Full wwPDB EM Validation Report (i)

Dec 18, 2022 – 07:54 am GMT

PDB ID	:	7A5K
EMDB ID	:	EMD-11646
Title	:	Structure of the human mitoribosome in the post translocation state bound to mtEF-G1
Authors	:	Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on	:	2020-08-21
Resolution	:	3.70 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 (i) 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 (1)) were used in the production of this report:

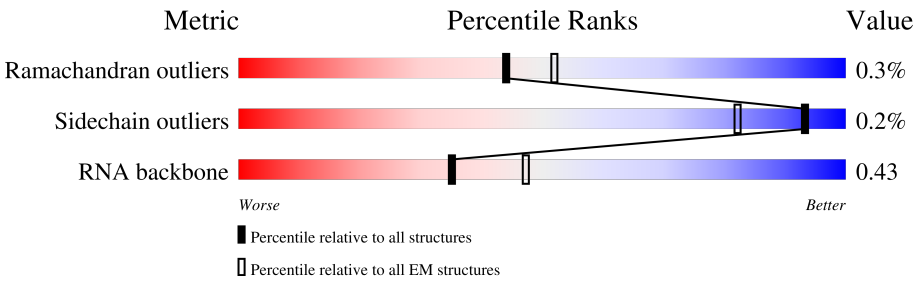
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	r1	751	38%, 87%, 5% • 7%
2	Y2	29	86%, 93%, 7%
3	8	1559	99%
3	A3	1559	•, 65%, 26%, 5% •
4	B3	73	16%, 52%, 23% • 23%
5	D3	305	9%, 76% • 23%
6	E3	348	5%, 84% • 14%
7	F3	311	•, 79% • 20%

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Mol	Chain	Length	Quality of chain
8	D	267	24% 28% 70%
8	H3	267	6% 35% 64%
9	I3	261	22% 60% 39%
10	J3	192	47% 71% 27%
11	K3	178	95%
12	L3	145	8% 79% 21%
13	M3	296	5% 93%
14	N3	251	6% 80% 18%
15	O3	175	5% 85% 13%
16	P3	179	72% 26%
17	Q3	292	10% 75% 25%
18	R3	149	6% 93% 6%
19	S3	205	74% 24%
20	T3	212	6% 77% 22%
21	U3	153	72% 27%
22	V3	216	19% 84% 12%
23	W3	148	74% 25%
24	X3	256	15% 93% 5%
25	Y3	250	8% 70% 30%
26	Z3	161	73% 25%
27	03	188	7% 56% 43%
28	13	65	8% 74% 6% 20%
29	23	92	50% 50%
30	33	188	50% 49%
31	43	103	35% 65%

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Mol	Chain	Length	Quality of chain
32	53	423	10% 87% 11%
33	63	380	11% 84% 14%
34	73	338	15% 78% 21%
35	93	137	9% 77% 20%
36	a3	142	58% 42%
37	b3	155	94% 5%
38	c3	332	7% 82% 17%
39	d3	306	13% 51% 47%
40	e3	279	67% 76% 22%
41	f3	194	38% 65% 32%
42	g3	166	77% 22%
43	h3	158	18% 60% 37%
44	i3	128	5% 74% 24%
45	j3	123	8% 67% 31%
46	k3	112	28% 75% 25%
47	l3	138	17% 83%
48	m3	128	22% 34% 65%
49	o3	102	91% 8%
50	p3	206	14% 61% 38%
51	q3	222	14% 56% 42%
52	r3	196	6% 74% 26%
53	s3	439	8% 83% 16%
54	u3	2	100%
55	A5	435	6% 6% 94%
56	B6	296	45% 72% 27%

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Mol	Chain	Length	Quality of chain
57	C6	167	78% / 79% / 21%
58	D6	430	43% / 73% / 25%
59	E6	125	78% / 97%
60	F6	242	83% / 81% / 17%
61	G6	396	70% / 76% / 23%
62	H6	201	59% / 60% / 39%
63	I6	194	50% / 69% / 30%
64	J6	138	14% / 77% / 22%
65	K6	128	77% / 78% / 21%
66	L6	257	37% / 63% / 36%
67	M6	137	53% / 82% / 15%
68	N6	130	38% / 79% / 18%
69	O6	258	51% / 68% / 28%
70	P6	142	48% / 65% / 32%
71	Q6	87	56% / 99%
72	R6	360	56% / 65% / 33%
73	S6	190	52% / 65% / 34%
74	T6	173	54% / 92% / 6%
75	U6	205	66% / 83% / 16%
76	V6	414	70% / 78% / 21%
77	W6	187	43% / 51% / 48%
78	X6	398	79% / 78% / 21%
79	Y6	395	27% / 27% / 73%
80	Z6	106	81% / 82% / 18%
81	a6	218	70% / 88% / 8%

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Mol	Chain	Length	Quality of chain
82	b6	323	78% 77% 21%
83	c6	118	73% 95%
84	d6	199	9% 35% 65%
85	e6	689	60% 59% 40%
86	A6	954	28% 65% 29%
87	24	73	95% 41% 53% 5%
87	FE	73	73% 41% 53% 5%
88	A	206	62% 74% 21%
89	n	286	73% 75% 24%
90	B	28	71% 100%

2 Entry composition (i)

There are 95 unique types of molecules in this entry. The entry contains 171122 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 Elongation factor G, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	r1	696	5452	3435	940	1044	33	0	0

- Molecule 2 is a protein called nascent chain.

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

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A3	1503	31913	14319	5761	10330	1503	0	0
3	8	8	Total	C	N	O	P	0	0
			175	79	37	51	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	3107	U	UNK	conflict	GB 1025814679
8	663	U	UNK	conflict	GB 1025814679

- Molecule 4 is a RNA chain called mt-tRNAVal.

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

- Molecule 5 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 16 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

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

- Molecule 17 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L28, mitochondrial.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 25 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	03	108	880	545	172	157	6	0	0

- Molecule 28 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	13	52	433	278	83	70	2	0	0

- Molecule 29 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	23	46	376	233	83	59	1	0	0

- Molecule 30 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	33	95	831	539	162	127	3	0	0

- Molecule 31 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	43	36	322	203	70	46	3	0	0

- Molecule 32 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	53	376	3064	1987	529	538	10	0	0

- Molecule 33 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	63	325	2636	1692	465	470	9	0	0

- Molecule 34 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	73	266	2158	1383	371	388	16	0	0

- Molecule 35 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	93	109	873	565	152	154	2	0	0

- Molecule 36 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L44, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 45 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

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

- Molecule 46 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	s3	370	3036	1946	542	534	14	0	0

- Molecule 54 is a RNA chain called RNA.

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

- Molecule 55 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	A5	28	136	80	28	28	0	0

- Molecule 56 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 68 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S21, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 73 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 74 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 75 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 76 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 77 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 78 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 79 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 80 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 81 is a protein called 28S ribosomal protein S34, mitochondrial.

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

- Molecule 82 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 83 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

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

- Molecule 84 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 85 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 86 is a RNA chain called 12S rRNA.

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

- Molecule 87 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
87	24	73	1547	696	280	499	72	0	0
			Total	C	N	O	P		
87	FE	73	1547	696	280	499	72	0	0

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

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

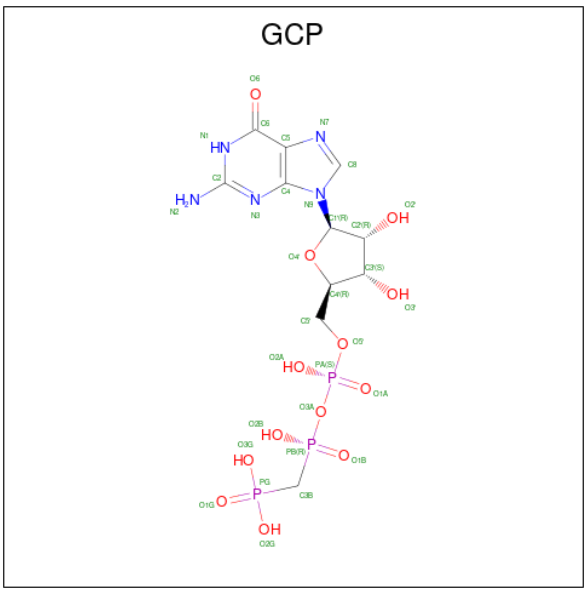
- Molecule 89 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
89	n	218	1744	1121	294	324	5	0	0

- Molecule 90 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
90	B	28	140	84	28	28	0	0

- Molecule 91 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

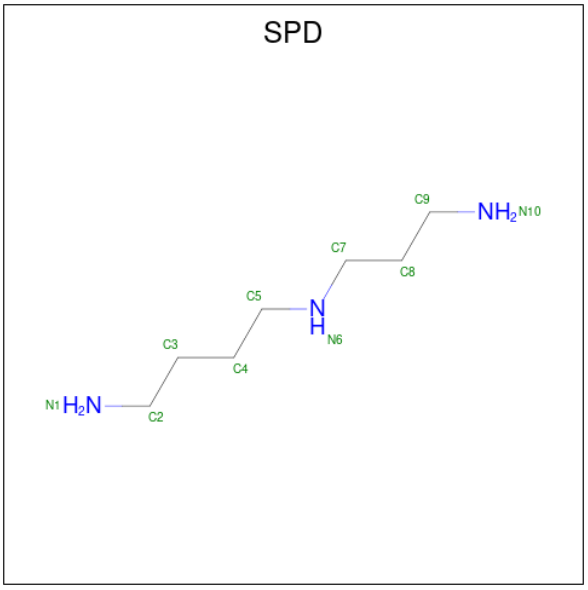


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
91	r1	1	32	11	5	13	3	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
92	r1	1	1	1	0
92	A3	95	95	95	0
92	D3	1	1	1	0
92	E3	1	1	1	0
92	M3	1	1	1	0
92	g3	1	1	1	0
92	A6	28	28	28	0

- Molecule 93 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

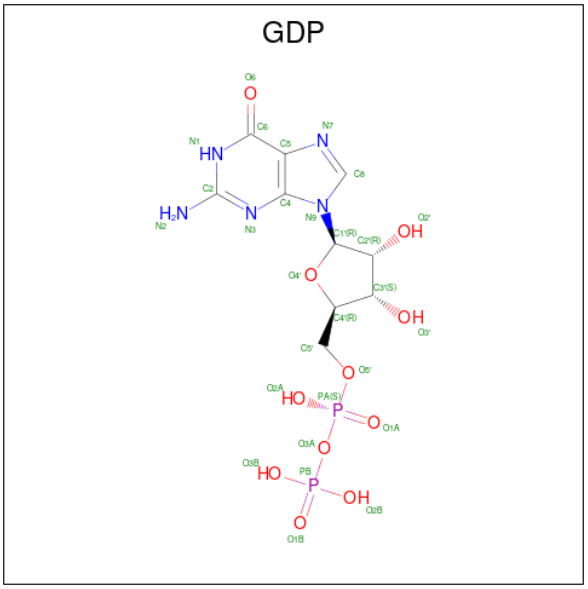


Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
93	A3	1	10	7	3	0

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

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

- Molecule 95 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



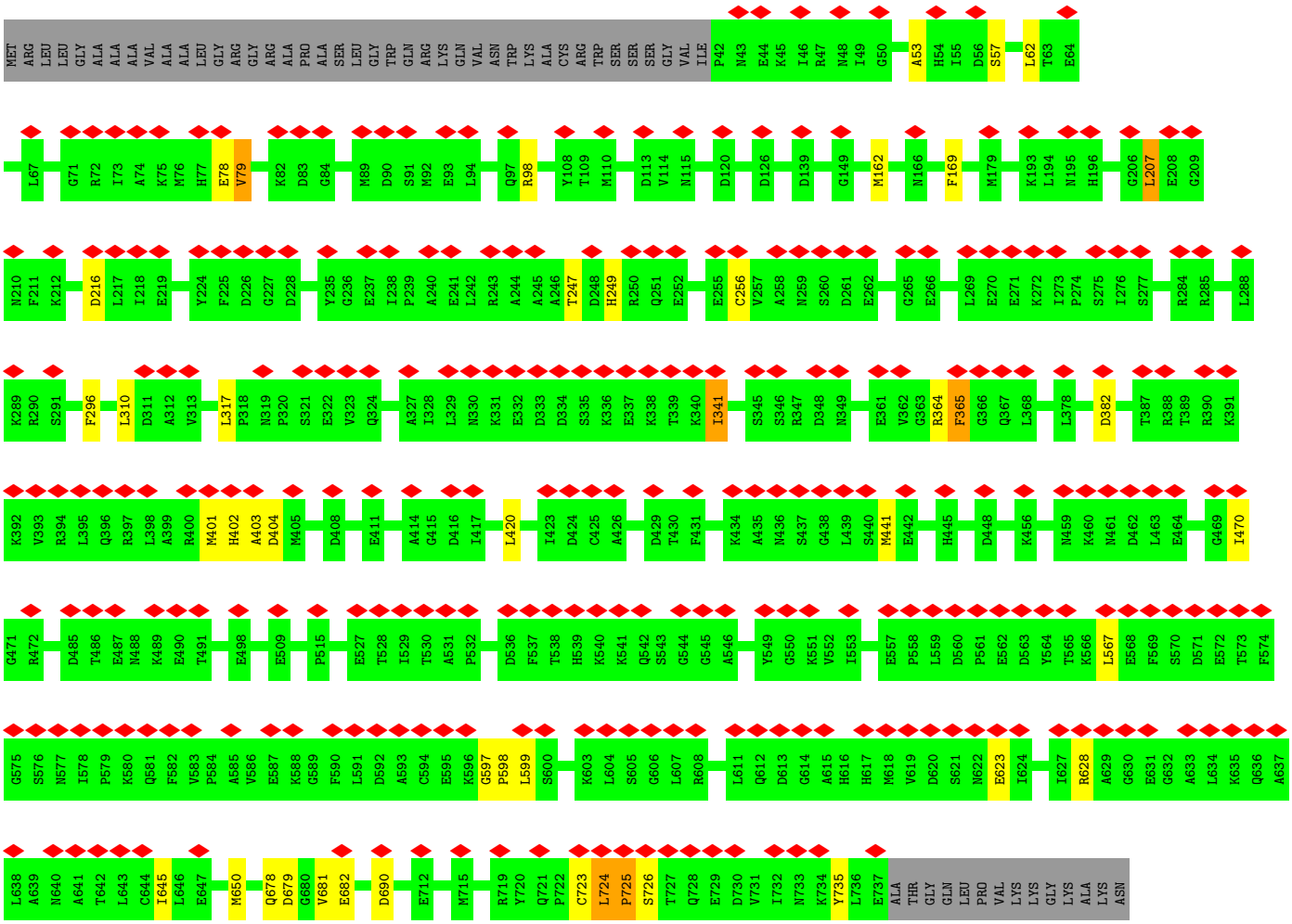
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
95	X6	1	28	10	5	11	2	0

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.

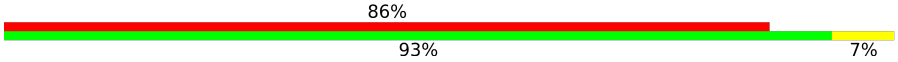
- Molecule 1: Elongation factor G, mitochondrial

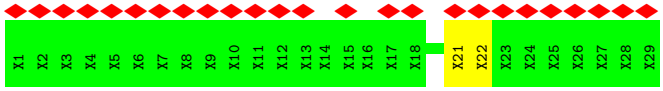
Chain r1:



- Molecule 2: nascent chain

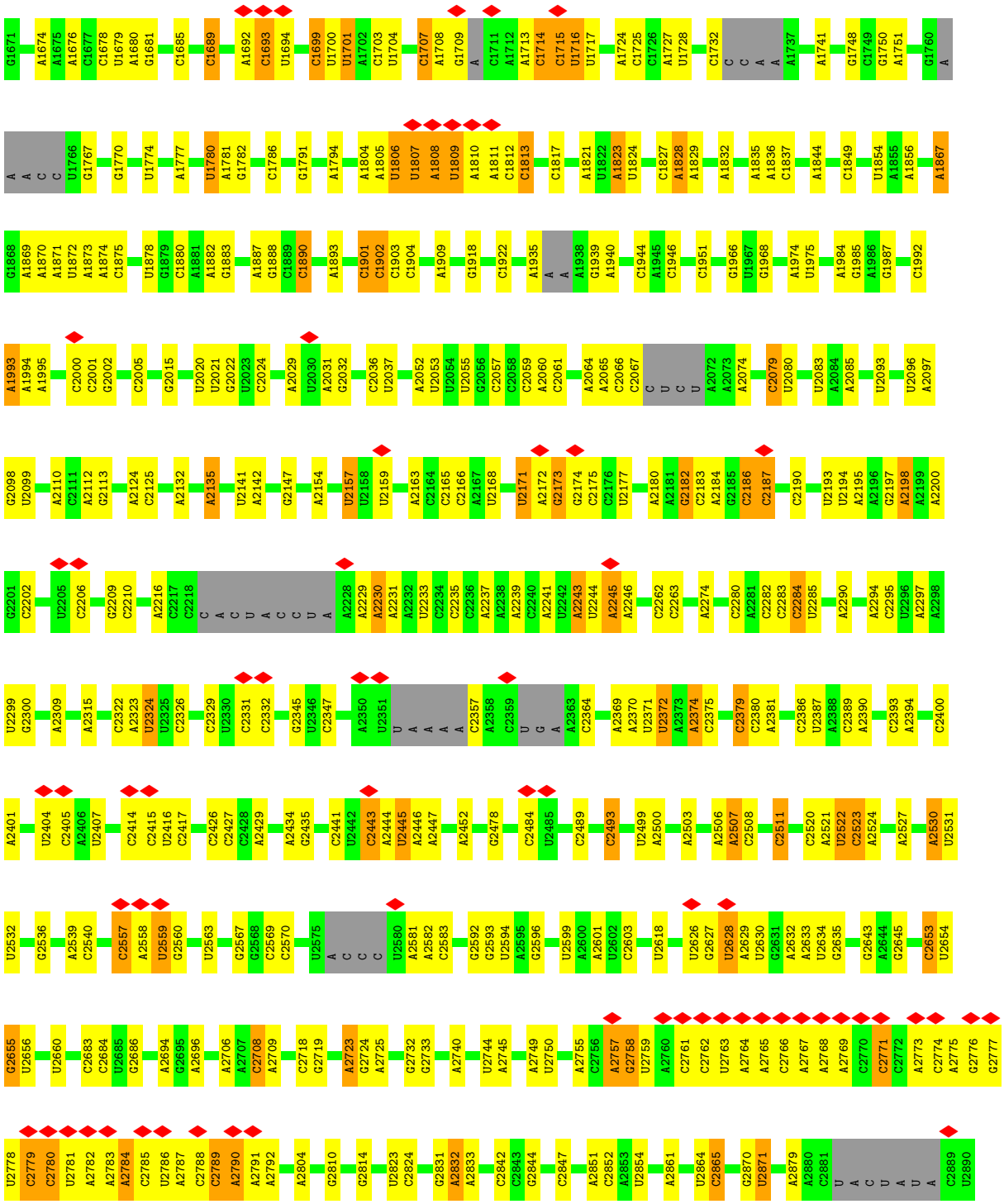
Chain Y2:

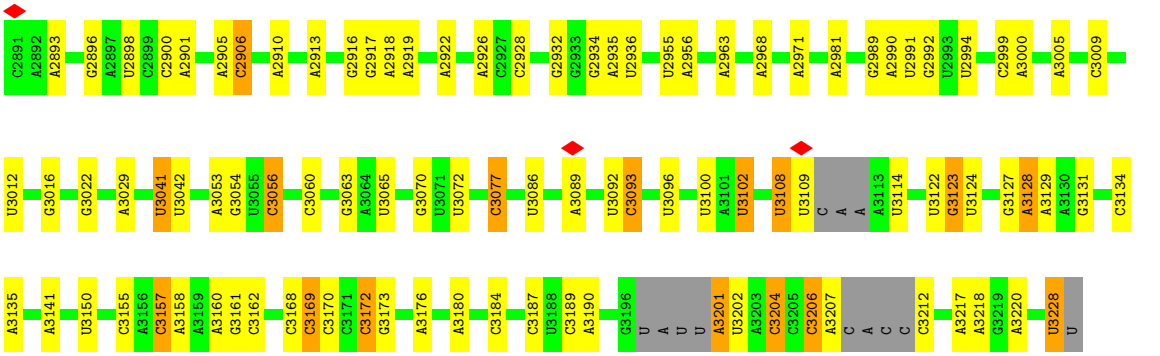




- Molecule 3: 16S rRNA

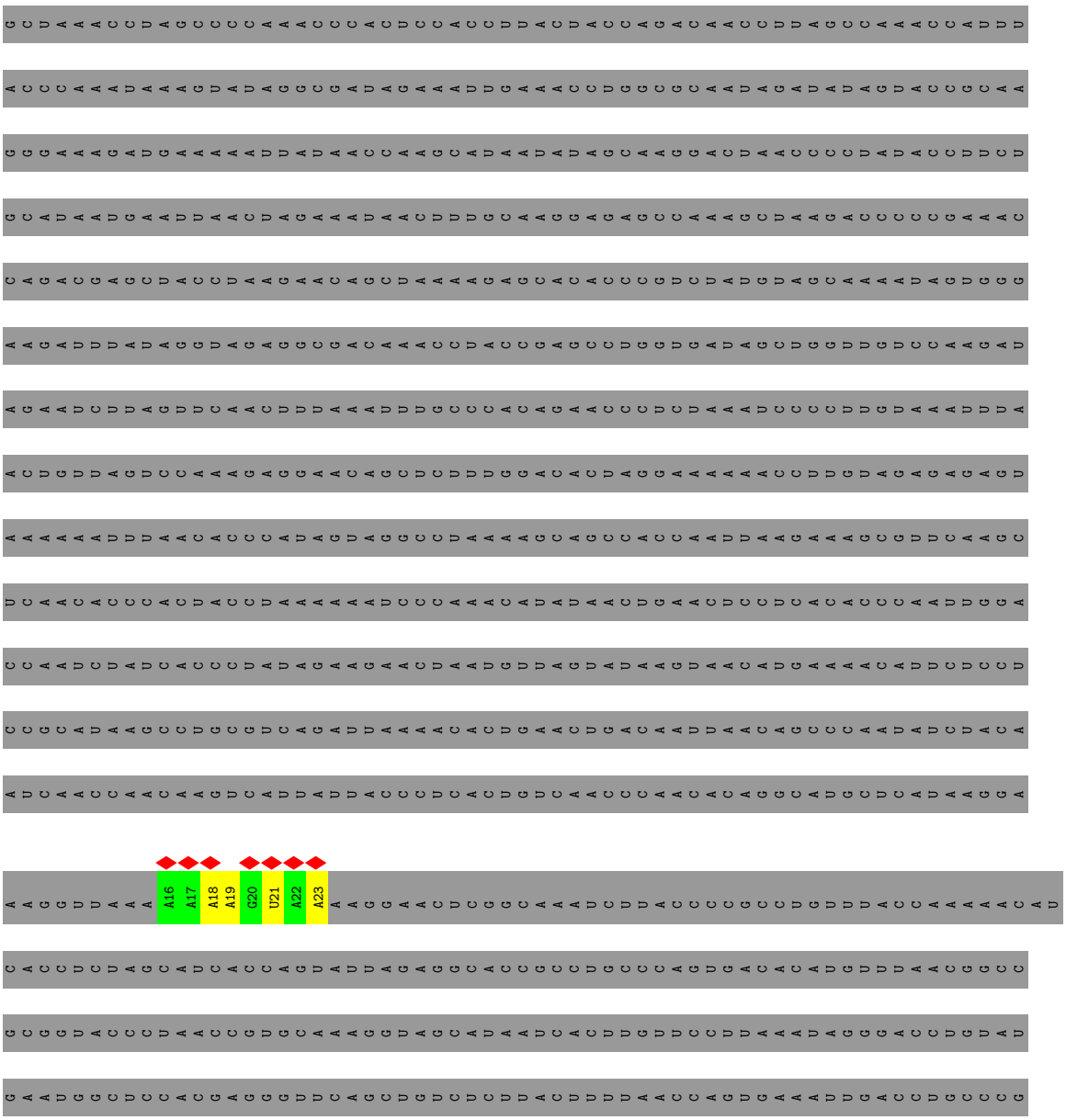
Chain A3:

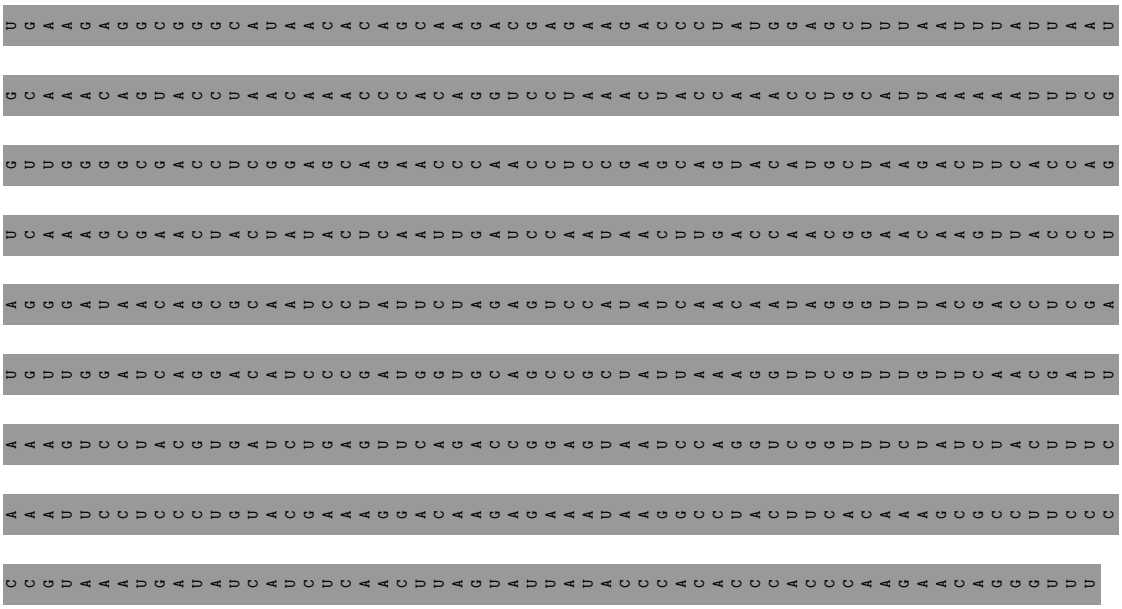




- Molecule 3: 16S rRNA

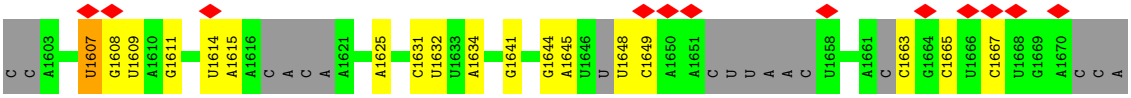
Chain 8: 99%





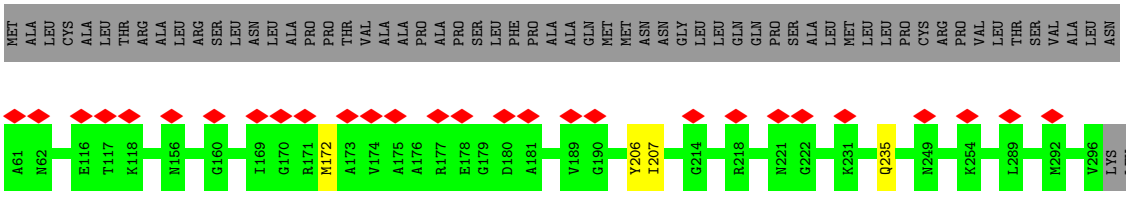
- Molecule 4: mt-tRNAVal

Chain B3:



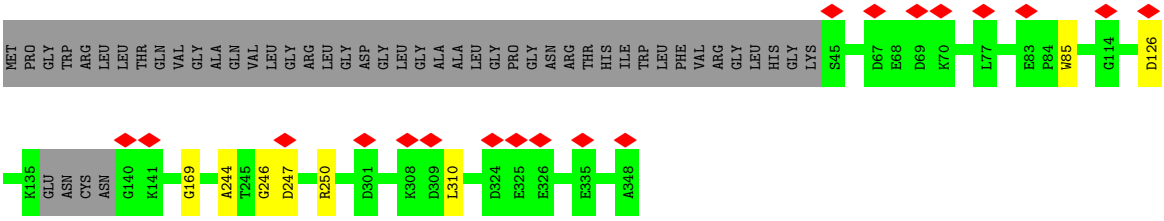
- Molecule 5: 39S ribosomal protein L2, mitochondrial

Chain D3:



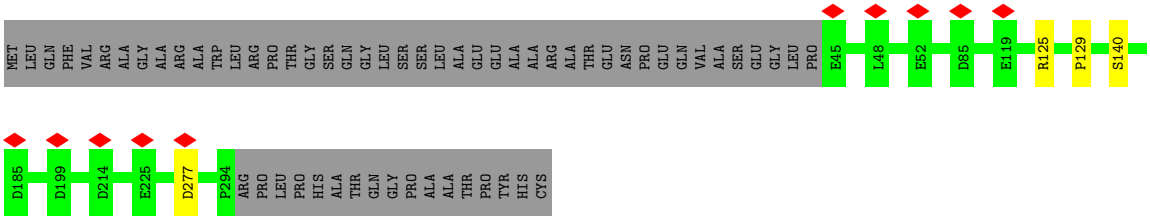
- Molecule 6: 39S ribosomal protein L3, mitochondrial

Chain E3:



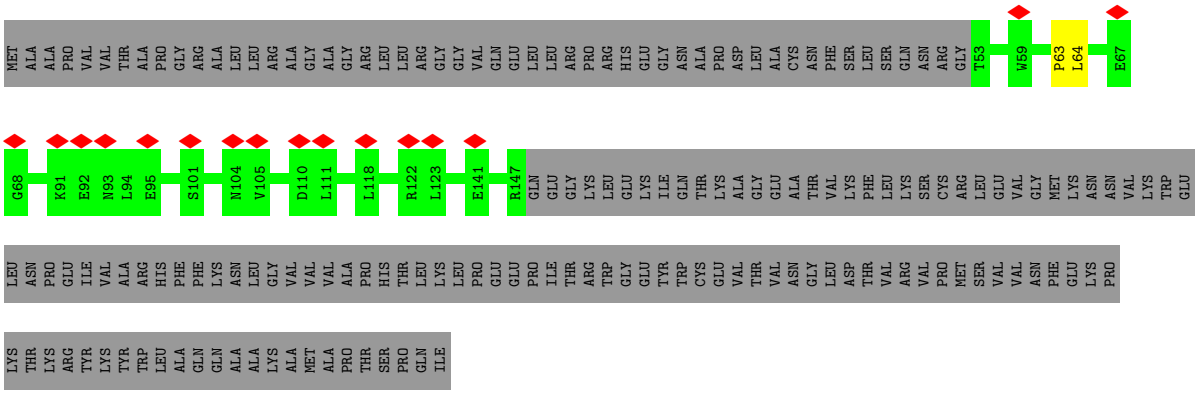
- Molecule 7: 39S ribosomal protein L4, mitochondrial

Chain F3:



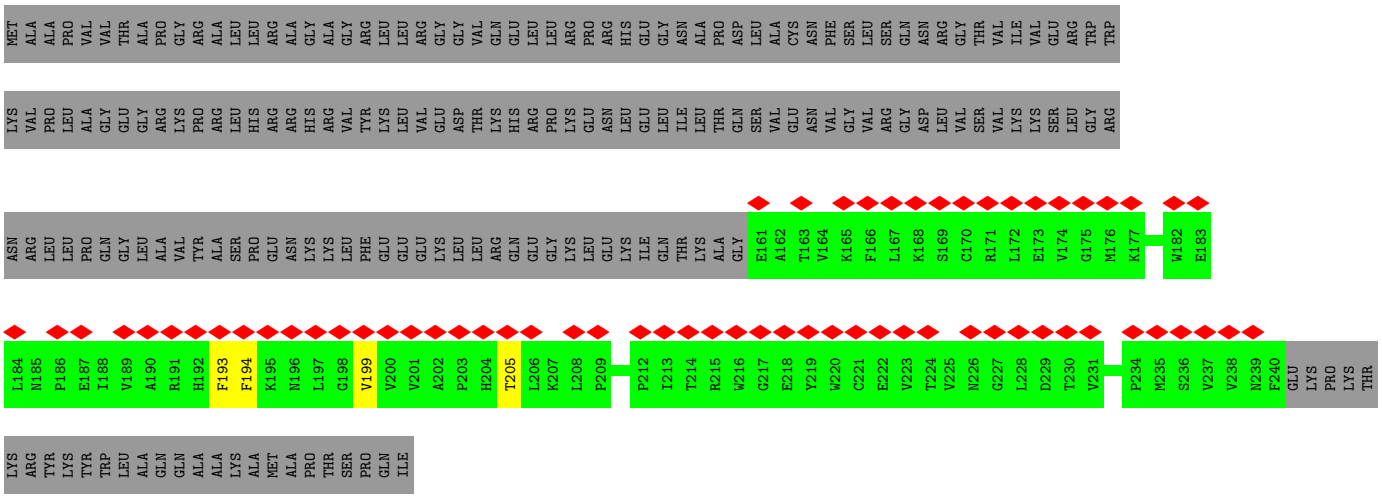
• Molecule 8: 39S ribosomal protein L9, mitochondrial

Chain H3:



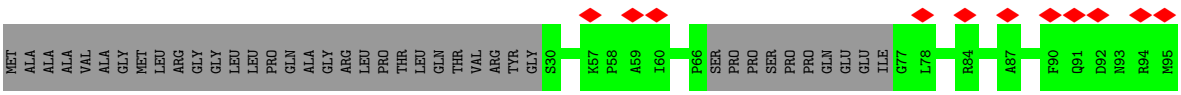
• Molecule 8: 39S ribosomal protein L9, mitochondrial

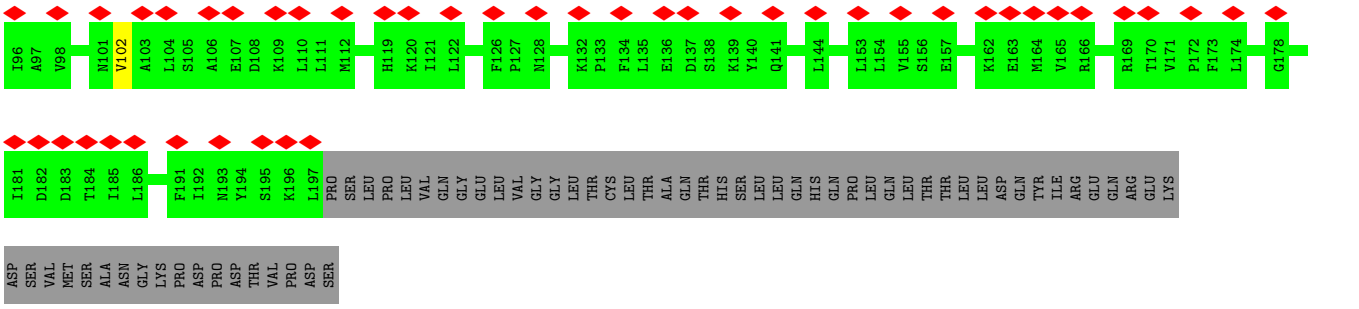
Chain D:



• Molecule 9: 39S ribosomal protein L10, mitochondrial

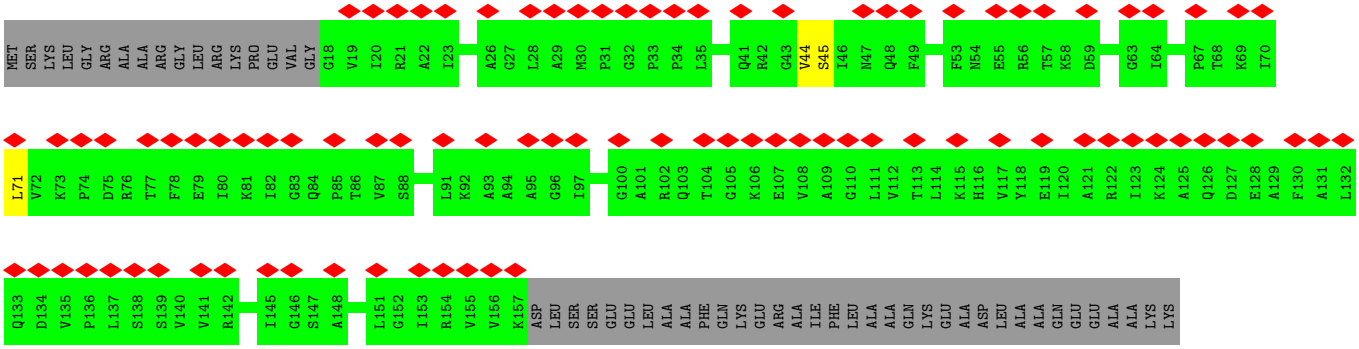
Chain I3:





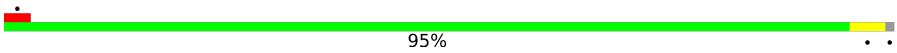
• Molecule 10: 39S ribosomal protein L11, mitochondrial

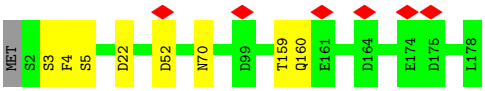
Chain J3:



• Molecule 11: 39S ribosomal protein L13, mitochondrial

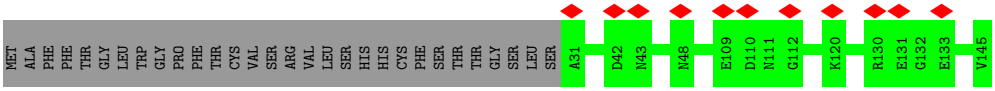
Chain K3:





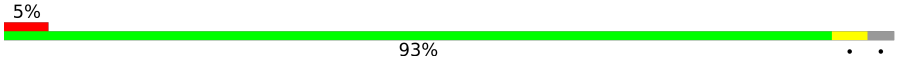
• Molecule 12: 39S ribosomal protein L14, mitochondrial

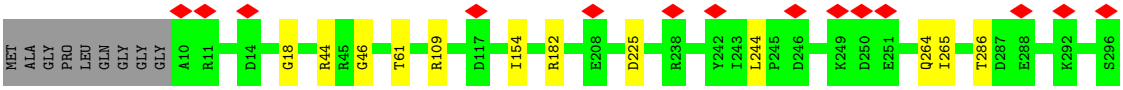
Chain L3:



• Molecule 13: 39S ribosomal protein L15, mitochondrial

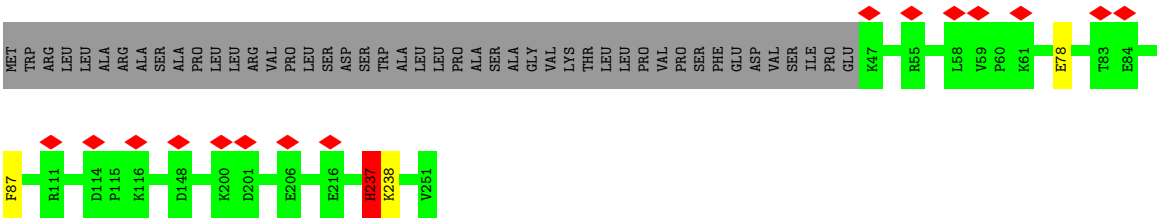
Chain M3:





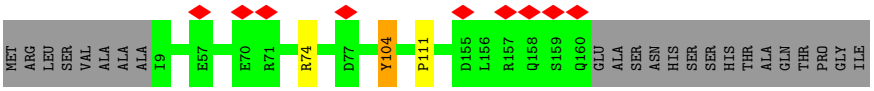
• Molecule 14: 39S ribosomal protein L16, mitochondrial

Chain N3:



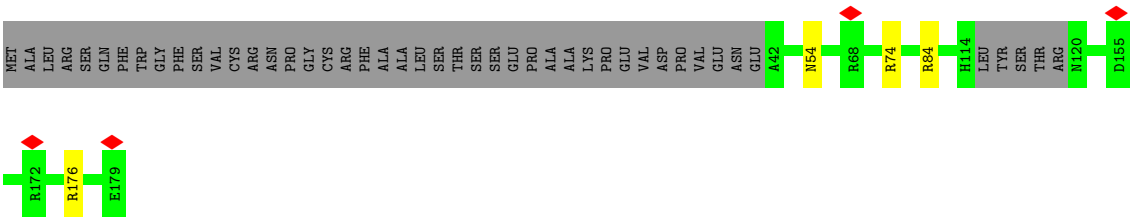
• Molecule 15: 39S ribosomal protein L17, mitochondrial

Chain O3:



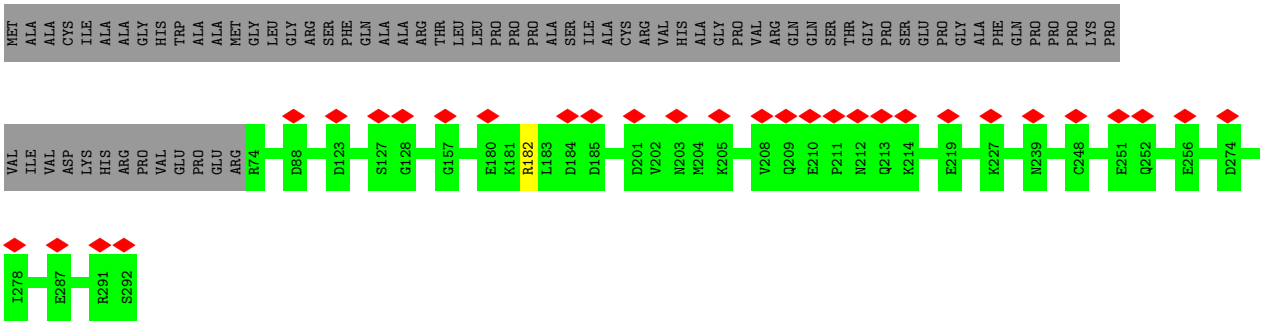
• Molecule 16: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain P3:



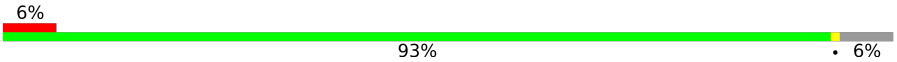
• Molecule 17: 39S ribosomal protein L19, mitochondrial

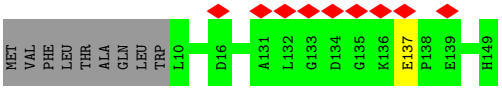
Chain Q3:



• Molecule 18: 39S ribosomal protein L20, mitochondrial

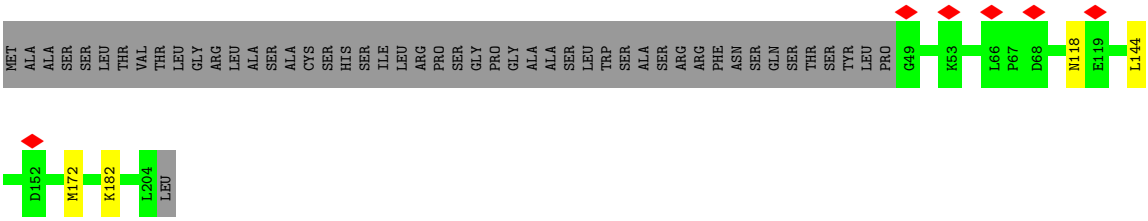
Chain R3:





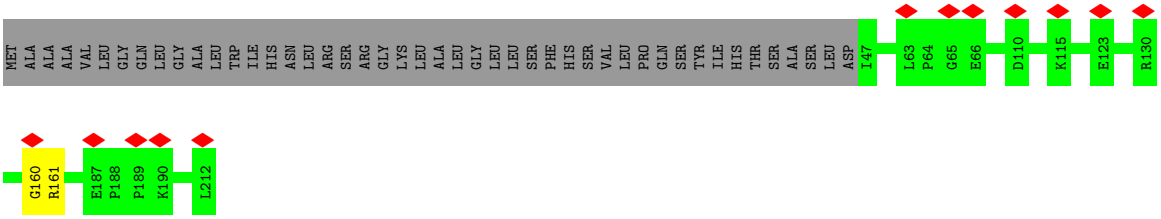
• Molecule 19: 39S ribosomal protein L21, mitochondrial

Chain S3:



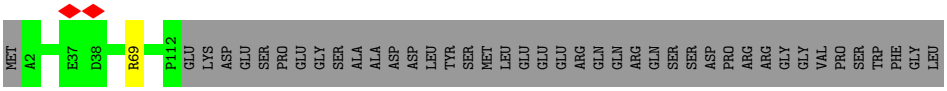
- Molecule 20: 39S ribosomal protein L22, mitochondrial

Chain T3:



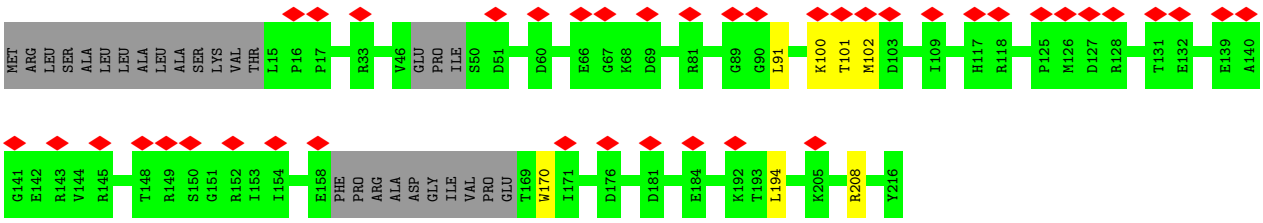
- Molecule 21: 39S ribosomal protein L23, mitochondrial

Chain U3:



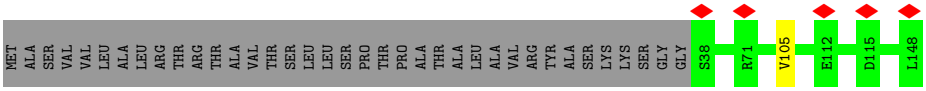
- Molecule 22: 39S ribosomal protein L24, mitochondrial

Chain V3:



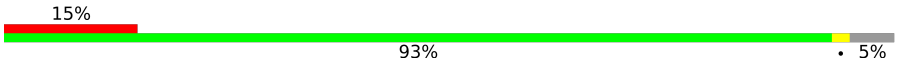
- Molecule 23: 39S ribosomal protein L27, mitochondrial

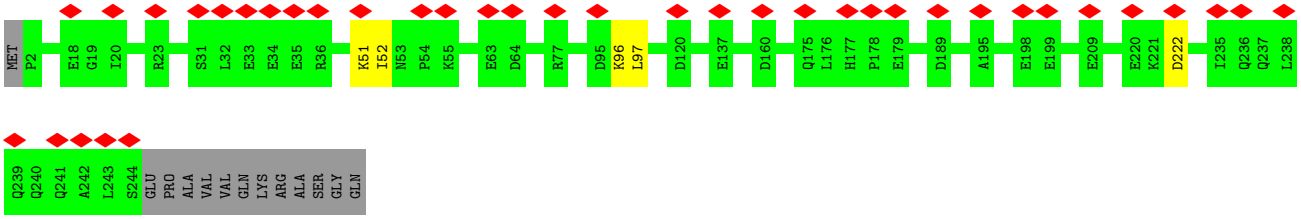
Chain W3:



- Molecule 24: 39S ribosomal protein L28, mitochondrial

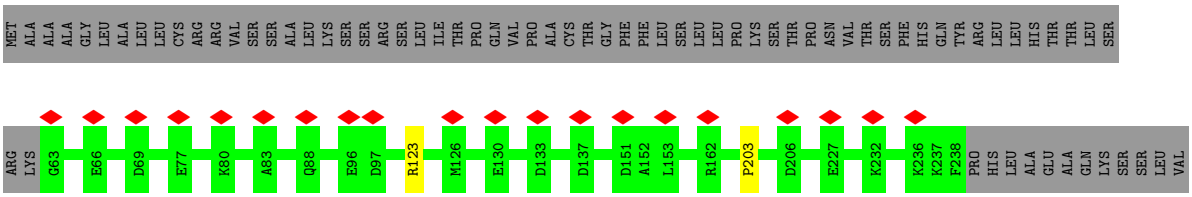
Chain X3:





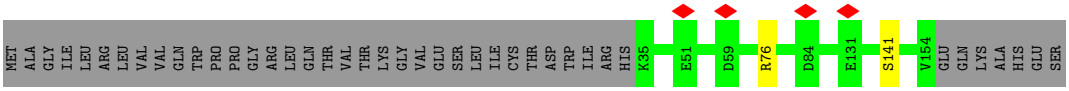
• Molecule 25: 39S ribosomal protein L47, mitochondrial

Chain Y3:



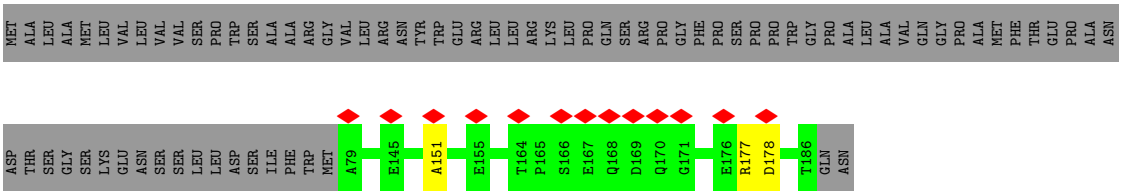
• Molecule 26: 39S ribosomal protein L30, mitochondrial

Chain Z3:



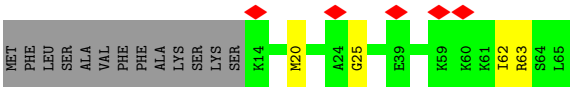
• Molecule 27: 39S ribosomal protein L32, mitochondrial

Chain 03:



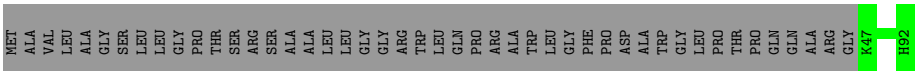
• Molecule 28: 39S ribosomal protein L33, mitochondrial

Chain 13:



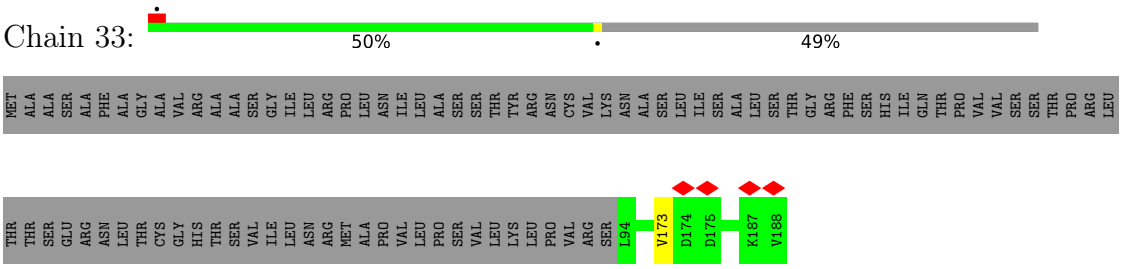
• Molecule 29: 39S ribosomal protein L34, mitochondrial

Chain 23:



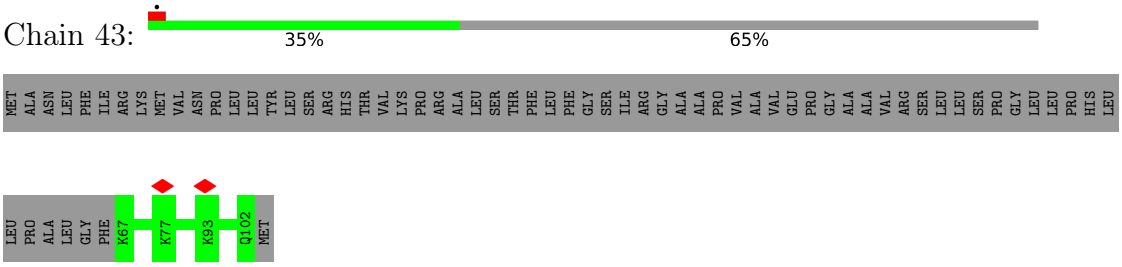
• Molecule 30: 39S ribosomal protein L35, mitochondrial

Chain 33:



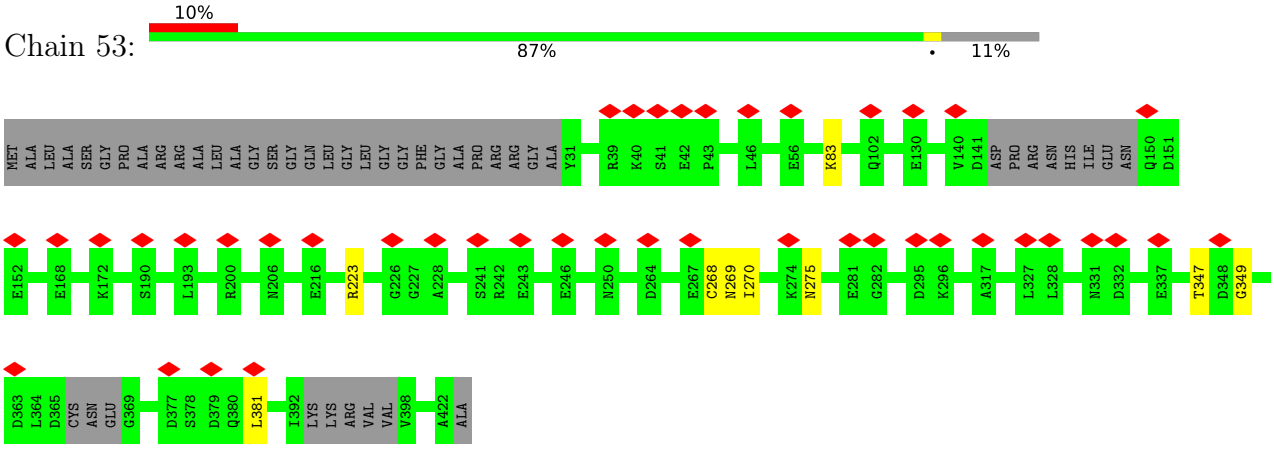
- Molecule 31: 39S ribosomal protein L36, mitochondrial

Chain 43:



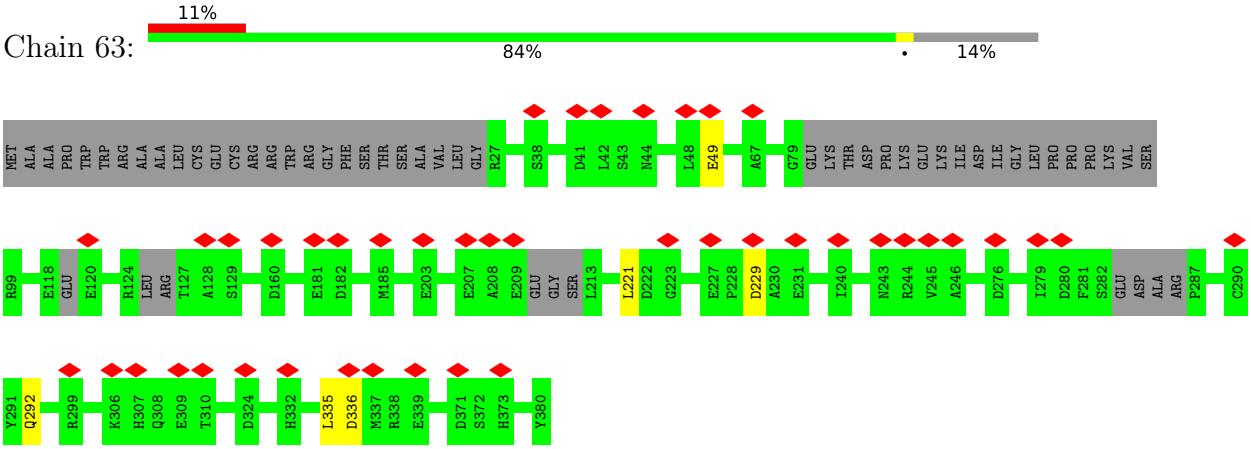
- Molecule 32: 39S ribosomal protein L37, mitochondrial

Chain 53:



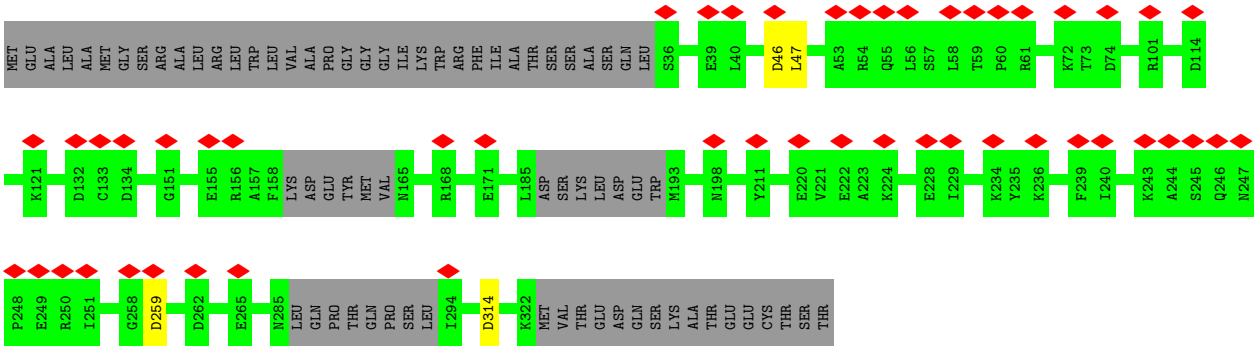
- Molecule 33: 39S ribosomal protein L38, mitochondrial

Chain 63:



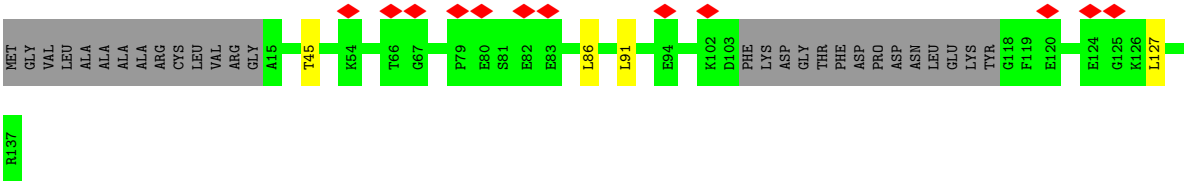
- Molecule 34: 39S ribosomal protein L39, mitochondrial

Chain 73:



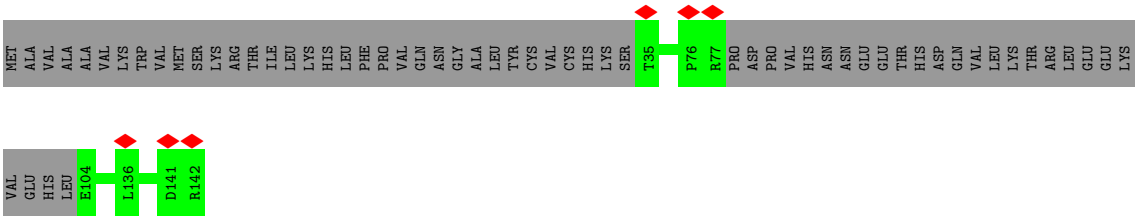
- Molecule 35: 39S ribosomal protein L41, mitochondrial

Chain 93:



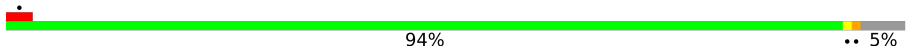
- Molecule 36: 39S ribosomal protein L42, mitochondrial

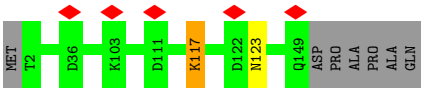
Chain a3:



- Molecule 37: 39S ribosomal protein L43, mitochondrial

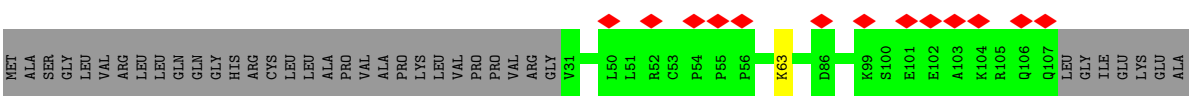
Chain b3:

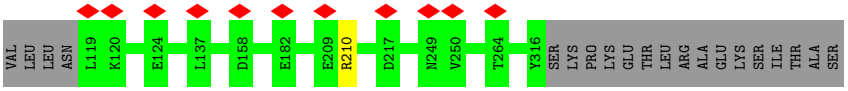




- Molecule 38: 39S ribosomal protein L44, mitochondrial

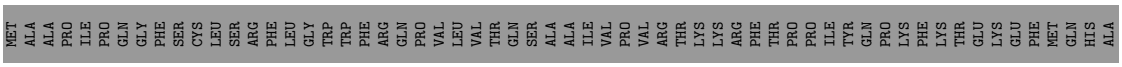
Chain c3:

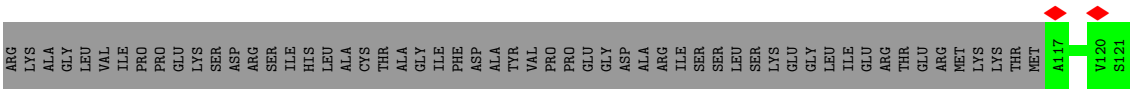


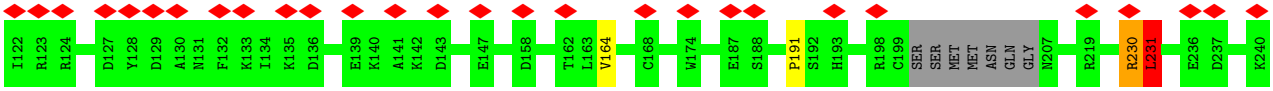


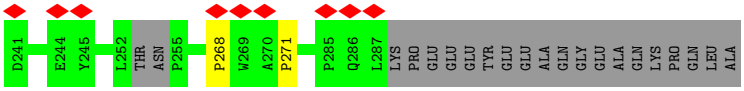
- Molecule 39: 39S ribosomal protein L45, mitochondrial

Chain d3:



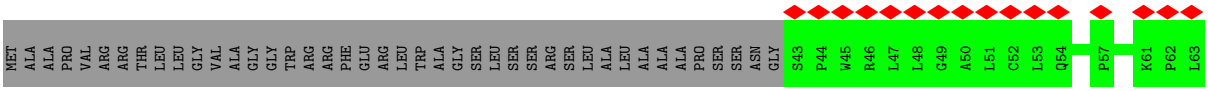


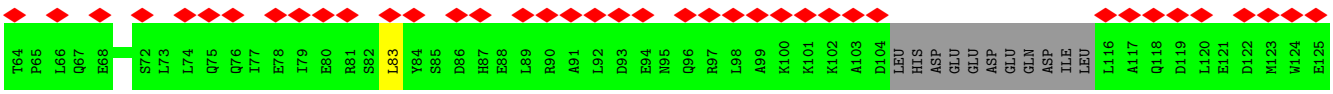


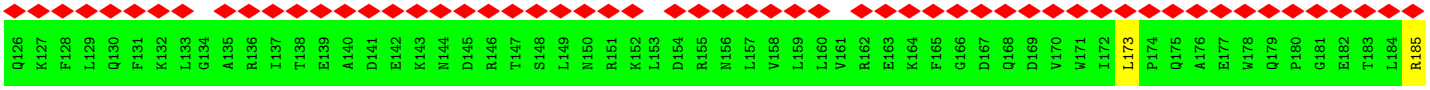


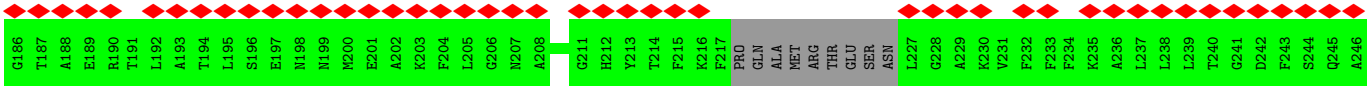
- Molecule 40: 39S ribosomal protein L46, mitochondrial

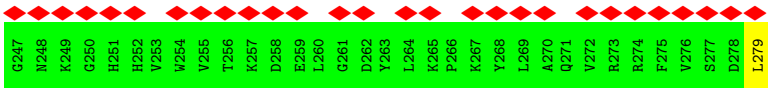
Chain e3:





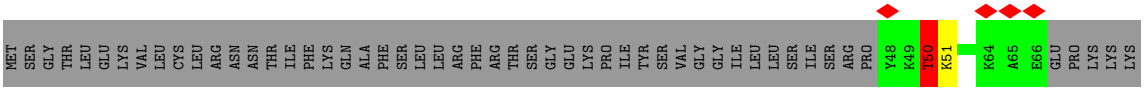


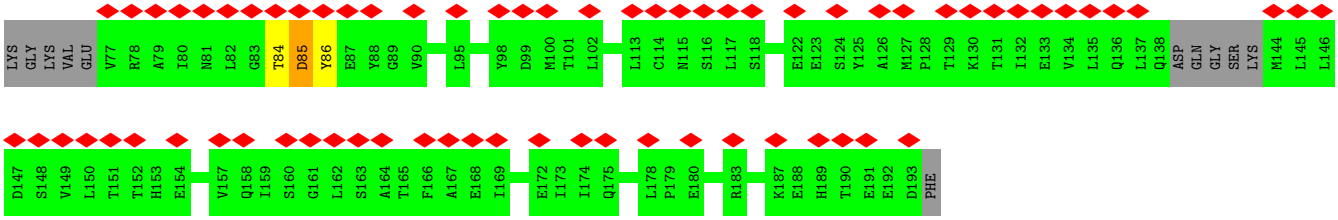




- Molecule 41: 39S ribosomal protein L48, mitochondrial

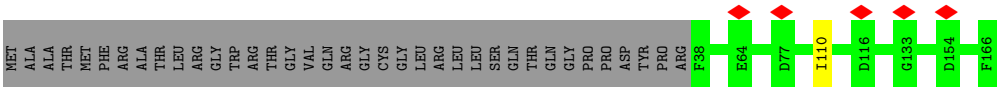
Chain f3:





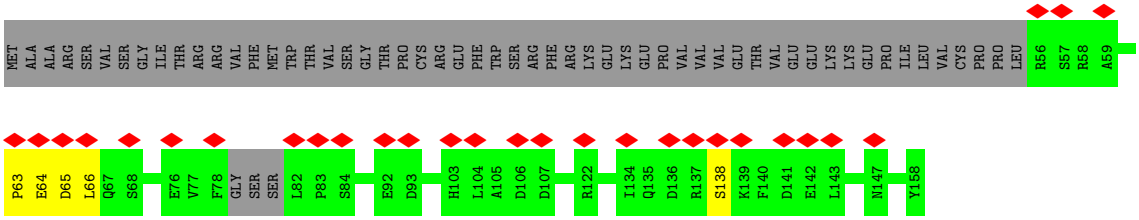
• Molecule 42: 39S ribosomal protein L49, mitochondrial

Chain g3:



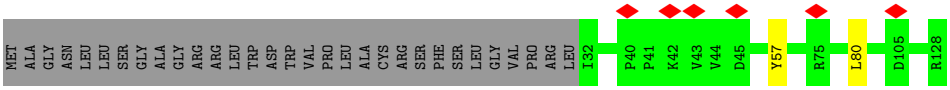
• Molecule 43: 39S ribosomal protein L50, mitochondrial

Chain h3:



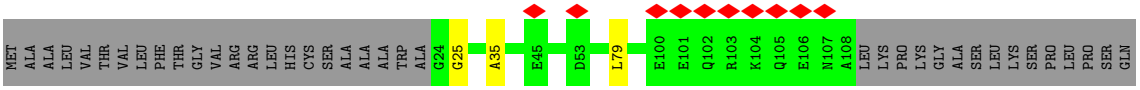
• Molecule 44: 39S ribosomal protein L51, mitochondrial

Chain i3:



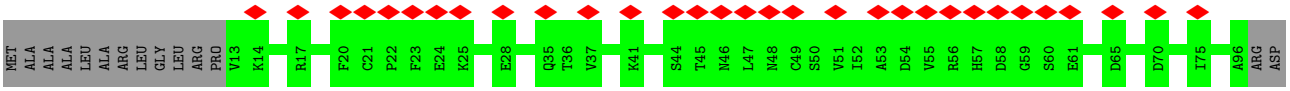
• Molecule 45: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA

Chain j3:



• Molecule 46: 39S ribosomal protein L53, mitochondrial

Chain k3:



ALA ALA GLY SER GLY ASP LYS PRO GLY ALA ASP THR GLY ARG

• Molecule 47: 39S ribosomal protein L54, mitochondrial

Chain l3:

MET ALA THR LYS ARG LEU PHE GLY ALA THR ARG THR TRP ALA GLY TRP GLY ALA TRP GLU LEU LEU ASN PRO ALA THR SER GLY ARG LEU LEU ALA ARG ASP TYR ALA LYS LYS PRO VAL MET LYS GLY ALA LYS SER GLY LYS GLY ALA VAL THR SER GLU ALA LEU LYS ASP PRO ASP

VAL CYS THR ASP PRO VAL GLN LEU THR THR TYR ALA MET GLY VAL ASN ILE TYR LYS GLU GLY GLN ASP VAL PRO LEU LYS PRO ASP ALA GLU TYR PRO GLU TRP LEU PHE GLU MET ASN LEU GLY PRO PRO LYS THR LEU GLU GLU LEU ASP PRO GLU S114 R115 K136 ARG LEU

• Molecule 48: 39S ribosomal protein L55, mitochondrial

Chain m3:

MET ALA ALA VAL GLY SER LEU LEU GLY ARG LEU ARG GLN SER THR VAL LYS ALA THR GLY PRO ALA LEU ARG ARG LEU HIS THR SER SER TRP ARG ALA D34 S35 S39 L40 H44 R45 Q46 A47 Y48 A49 R50 L51 L56 V57 K58 Q59 D60 G61 S62 T63 I64 H65 I66 R67

Y68 R69 E70 P71 R72 R73 M74 L75 A76 M77 P78 ILE ASP LEU ASP THR LEU SER PRO GLU GLU ARG ARG ALA ARG LEU ARG LYS ARG GLU ALA GLN LEU GLN SER ARG LYS GLU TYR GLU GLN GLU LEU SER ASP ASP LEU HIS VAL GLU ARG TYR ARG GLN PHE TRP THR ARG THR LYS

LYS

• Molecule 49: Ribosomal protein 63, mitochondrial

Chain o3:

MET PHE LEU THR ALA LEU LEU TRP R9 E42 D90 S102

• Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p3:

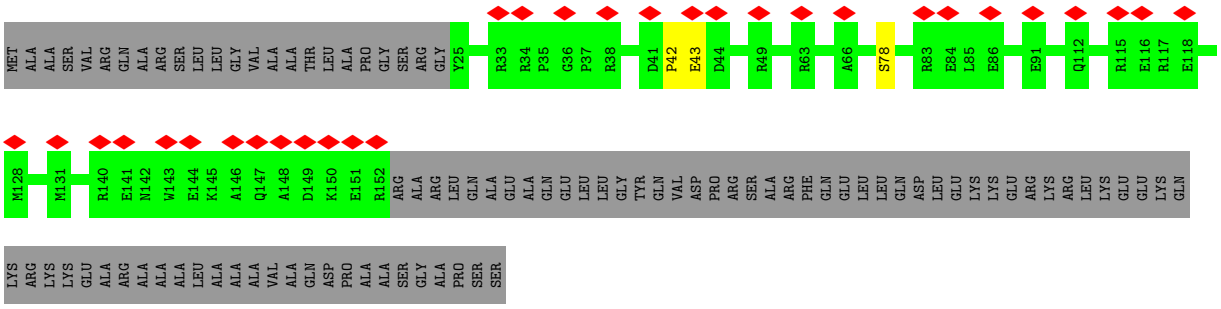
MET ALA ALA THR ARG CYS LEU ARG TRP GLY LEU SER ARG ALA GLY VAL TRP LEU LEU PRO PRO PRO ALA ARG CYS PRO ARG ARG ALA LEU HIS LYS GLN LYS ASP GLY THR E38 D46 Q53 G54 S55 D56 R60 V61 PRO ASN GLY ALA LYS GLN ALA ASP SER D70 R82

S83 SER GLY PRO GLY GLY GLN ASN VAL ASN LYS V95 N96 S97 T107 A108 E109 A112 I121 T122 H123 E138 E160 A161 S162 Q163 THR PRO LYS GLU PRO THR LYS GLU ASP VAL K174 L175 H176 I180 E186 Q190 K191 R192 I193 HIS SER ALA VAL LYS THR SER

ARG ARG VAL ASP MET ASP

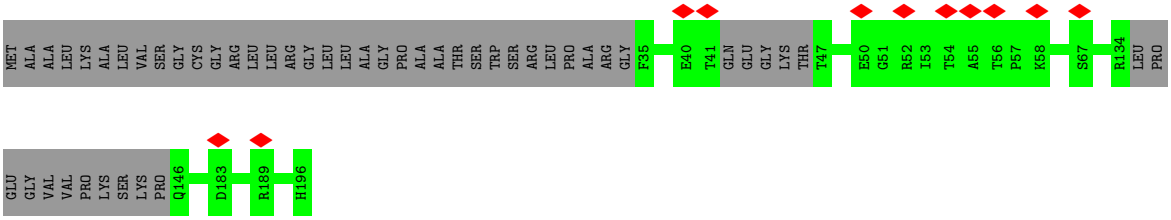
• Molecule 51: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q3:



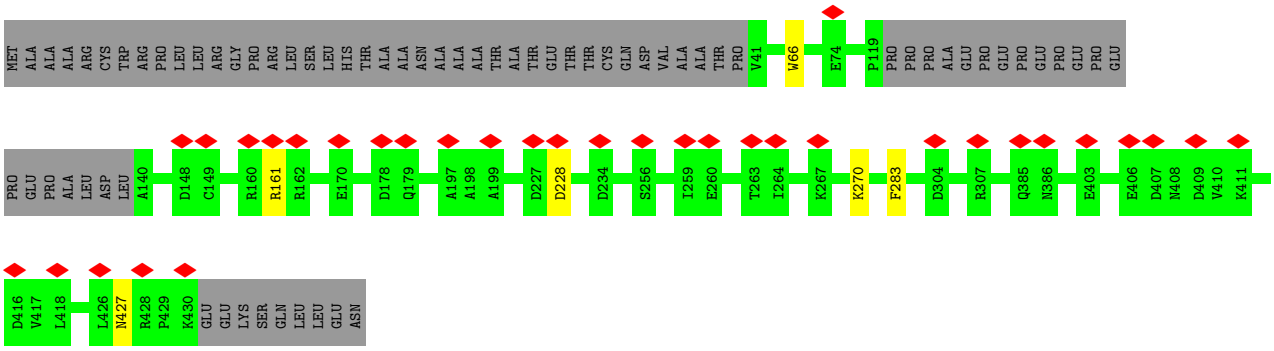
- Molecule 52: 39S ribosomal protein S18a, mitochondrial

Chain r3:



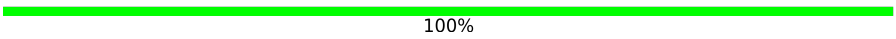
- Molecule 53: 39S ribosomal protein S30, mitochondrial

Chain s3:



- Molecule 54: RNA

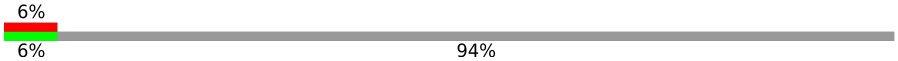
Chain u3:

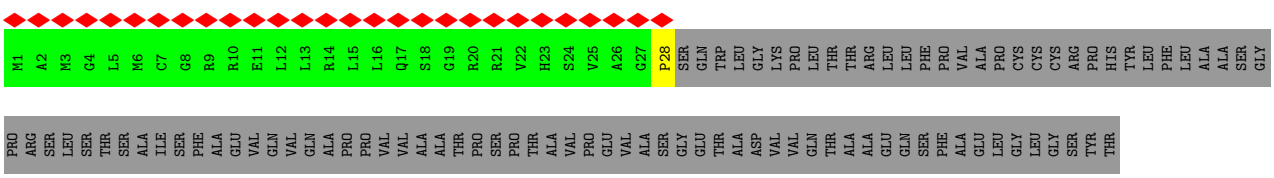


There are no outlier residues recorded for this chain.

- Molecule 55: Mitochondrial inner membrane protein OXA1L

Chain A5:





PRO VAL GLY LEU ILE GLN ASN LEU LEU GLU PHE MET HIS VAL ASP LEU GLY LEU PRO TRP TRP GLY ALA ILE ALA ALA CYS THR VAL PHE ALA ARG CYS LEU ILE PHE PRO LEU ILE VAL THR GLY GLN ARG GLU ALA ALA ARG ILE HIS ASN HIS LEU PRO GLU ILE GLN LYS PHE SER

SER ARG ILE ARG GLU ALA LYS LEU ALA GLY ASP HIS ILE GLU TYR TYR LYS ALA SER SER GLU MET ALA LEU TYR GLN LYS LYS HIS GLY ILE LYS LEU TYR LYS PRO LEU ILE LEU PRO VAL THR GLN ALA PRO ILE PHE ILE SER PHE PHE ILE ALA LEU ARG GLU MET ALA ASN LEU

PRO VAL PRO SER LEU GLN THR GLY GLY LEU TRP TRP PHE GLN ASP LEU THR VAL SER ASP PRO ILE TYR ILE LEU PRO LEU ALA VAL THR ALA THR MET TRP ALA VAL LEU GLU LEU GLY ALA GLU THR GLY VAL GLN SER SER ASP LEU GLN TRP MET ARG ASN VAL ILE ARG MET MET

PRO LEU ILE THR LEU PRO ILE THR MET HIS PHE PRO THR ALA VAL PHE MET TYR TRP LEU SER SER ASN LEU PHE SER LEU VAL GLN VAL SER CYS LEU ARG ILE PRO ALA VAL ARG THR VAL LEU LYS ILE PRO GLN ARG VAL VAL HIS ASP LEU ASP LYS LEU PRO PRO ARG GLU GLY

PHE LEU GLU SER PHE LYS LYS GLY TRP LYS ASN ALA GLU MET THR ARG GLN LEU ARG GLU ARG GLU GLN ARG MET ARG ASN GLN LEU GLU LEU ALA ALA ARG GLY PRO LEU ARG GLN THR PHE THR HIS ASN PRO LEU LEU GLN PRO GLY LYS ASP ASN PRO PRO ASN ILE PRO SER SER

SER SER LYS PRO LYS SER LYS LYS TYR PRO TRP HIS ASP THR LEU GLY

- Molecule 56: 28S ribosomal protein S2, mitochondrial

Chain B6:

MET ALA THR SER SER ALA ALA LEU PRO ARG ILE LEU GLY ALA GLY ALA ARG ALA PRO SER ARG TRP LEU GLY PHE LEU GLY LYS ALA THR PRO ARG PRO ALA ARG PRO SER ARG ARG THR LEU GLY SER ALA THR ALA LEU MET ILE ARG GLU SER GLU ASP SER THR ASP F58 N59 D60

K61 I62 L63 N64 E65 P66 L67 K68 H69 S70 D71 F72 F73 N74 V75 K76 E77 L78 F79 S80 V81 R82 S83 L84 F85 D86 A87 R88 V89 H90 L91 G92 H93 K94 A95 G96 C97 R98 M102 E103 I106 F107 G108 S109 R110 L111 D112 H113 D114 D117 L118 E119 Q120 T121 A122 T123 H124

L125 Q126 L127 A128 L129 N130 F131 T132 A133 H134 M135 A136 K139 G140 I141 I142 L143 F144 R147 N148 R149 Q150 Y153 L154 I155 E156 N157 R160 D161 C162 G163 E164 T168 R169 R172 M175 L176 A179 L182 F183 G184 R188 L192 I193 I194 F195 L196 H197

N201 I202 F203 E204 R210 D211 T219 I222 V223 D224 T225 N226 C227 N228 I232 P235 G238 N239 D240 D241 S242 P243 L244 A245 V246 H247 L248 Y249 C250 R251 Q254 T255 A256 I257 T258 R259 A260 K261 E262 Q265 Q266 V267 E268 A269 L270 Y271 R272 L273 Q274 GLY GLN LYS

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

- Molecule 57: 28S ribosomal protein S24, mitochondrial

Chain C6:

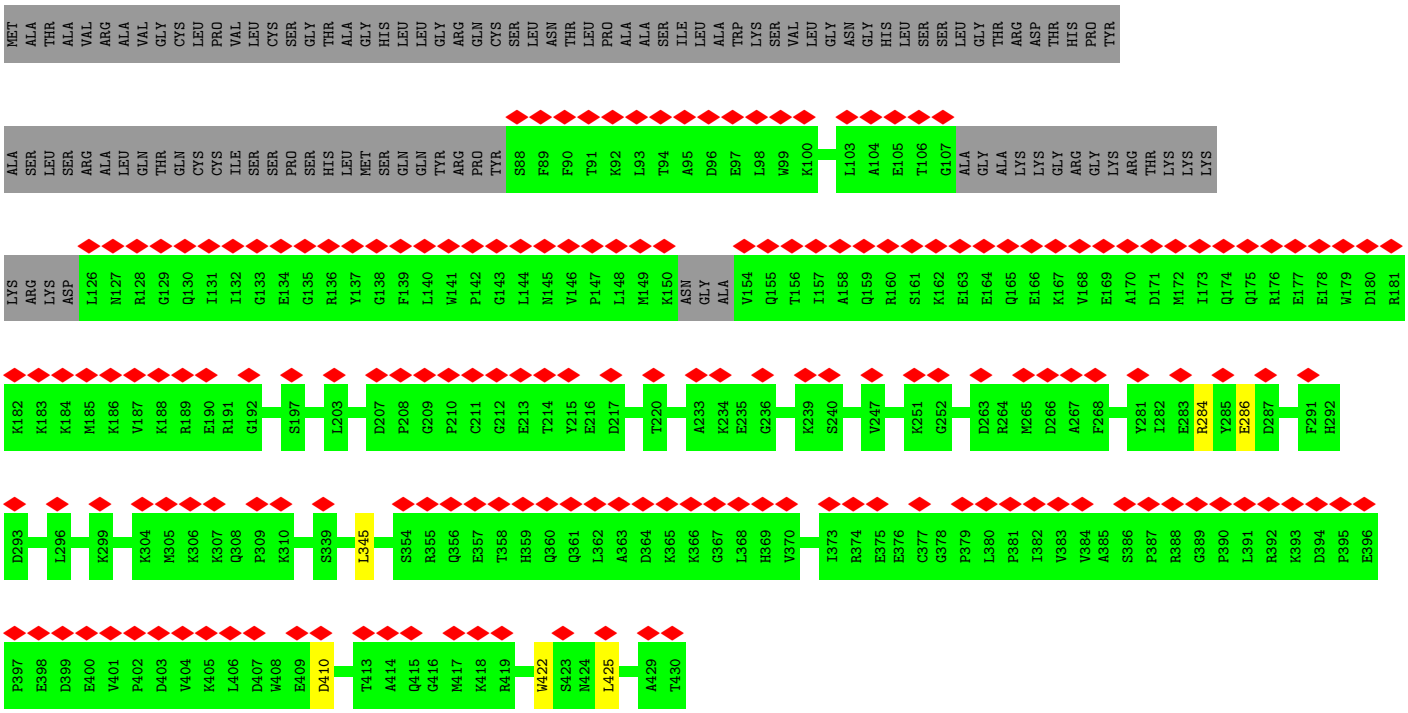
MET ALA ALA SER VAL CYS SER GLY LEU LEU GLY PRO ARG VAL LEU SER TRP SER ARG GLU LEU PRO CYS ALA TRP ARG ALA LEU HIS THR SER PRO VAL CYS ALA K36 N37 R38 A39 A40 R41 V42 R43 V44 S45 K46 G47 D48 K49 P50 V51 T52 Y53 E54 E55 A56 H57 A58 P59 H60

Y61 I62 A63 H64 R65 K66 G67 W68 L69 S70 L71 H72 T73 G74 N75 L76 D77 G78 E79 D80 H81 A82 A83 E84 R85 T86 V87 E88 D89 V90 F91 L92 R93 K94 F95 M96 W97 G98 T99 F100 P101 G102 C103 L104 A105 D106 Q107 L108 V109 L110 K111 R112 R113 G114 N115 Q116 L117 E118 I119 C120

A121 V122 V123 L124 R125 Q126 L127 S128 P129 H130 K131 Y132 Y133 F134 L135 V136 G137 Y138 S139 E140 T141 L142 L143 S144 Y145 F146 Y147 K148 C149 P150 V151 R152 L153 H154 L155 Q156 T157 V158 P159 S160 K161 V162 V163 Y164 K165 Y166 L167

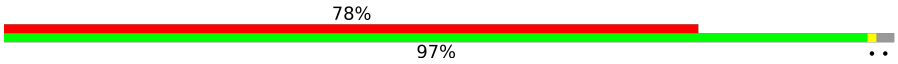
• Molecule 58: 28S ribosomal protein S5, mitochondrial

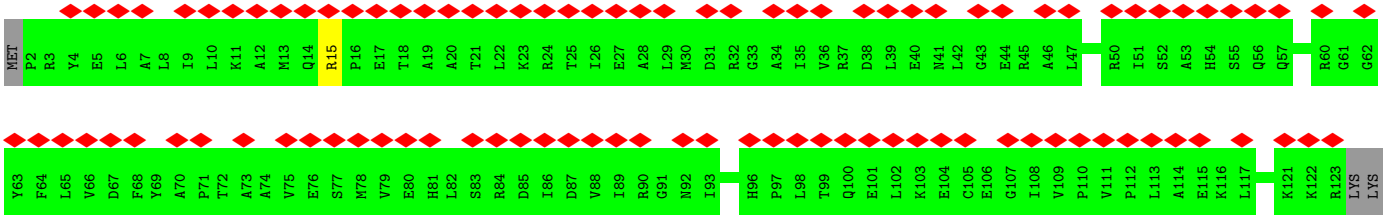
Chain D6:



• Molecule 59: 28S ribosomal protein S6, mitochondrial

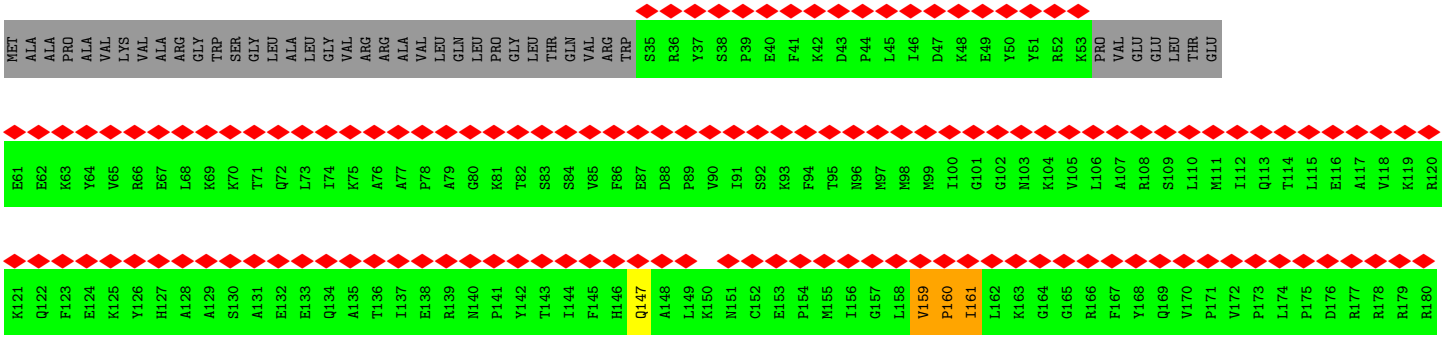
Chain E6:





• Molecule 60: 28S ribosomal protein S7, mitochondrial

Chain F6:



F181 L182 A183 M184 K185 W186 M187 I188 T189 E190 C191 R192 D193 K194 K195 H196 Q197 R198 T199 L200 M201 P202 E203 K204 L205 S206 H207 K208 L209 L210 E211 A212 F213 H214 N215 Q216 G217 P218 V219 I220 K221 R222 K223 H224 D225 L226 H227 K228 M229 A230 E231 A232 N233 R234 A235 L236 A237 H238 Y239 R240

W241 W242

• Molecule 61: 28S ribosomal protein S9, mitochondrial

Chain G6:

MET ALA ALA PRO CYS VAL SER TYR GLY GLY ALA VAL SER TYR ARG LEU LEU LEU TRP GLY ARG GLY SER LEU ALA ARG LYS GLN GLY LEU TRP LYS THR ALA ALA PRO GLU LEU GLN THR ASN VAL ARG SER GLN ILE LEU ARG LEU ARG HIS THR ALA PHE VAL ILE PRO LYS LYS ASN

VAL PRO THR SER LYS ARG GLU THR TYR THR E71 D72 F73 I74 K75 K76 Q77 I78 E79 E80 F81 N82 I83 G84 K85 R86 H87 L88 A89 N90 M91 M92 G93 E94 D95 P96 E97 T98 F99 T100 Q101 E102 D103 I104 D105 R106 A107 I108 A109 Y110 L111 F112 P113 S114 G115 L116 F117 E118 K119 R120

A121 R122 P123 V124 M125 K126 H127 P128 E129 Q130 I131 F132 P133 R134 Q135 R136 A137 I138 Q139 E142 D143 G144 R145 Y149 L150 T153 G154 K155 Y159 S160 L161 M162 H163 D164 V165 Y166 G167 M168 L169 L170 N171 L172 E173 K174 H175 Q176 SER HIS LEU GLN ALA LYS SER LEU LEU PRO

GLU LYS THR VAL THR ARG ASP VAL ILE GLY SER R198 I201 K202 E203 E204 L205 E206 E207 M208 L209 V210 E211 K212 D215 L216 D217 Y218 M219 Q220 F221 I222 R223 L224 L225 E226 K227 L228 L229 T230 S231 Q232 C233 G234 A235 A236 E237 E238 E239 F240 V241 Q242 R243 F244 R245 R246 S247 V248

T249 L250 E251 S252 K253 K254 Q255 L256 I257 E258 P259 V260 Q261 Y262 D263 E264 Q265 C266 M267 A268 F269 S270 K271 S272 E273 G274 K275 R276 K277 T278 A279 K280 A281 E282 A283 I284 V285 Y286 K287 H288 G289 S290 C291 R292 I293 K294 V295 N296 G297 I298 D299 Y300 Q301 L302 Y303 F304 P305 I306 T307 Q308

D309 R310 E311 Q312 L313 M314 F315 P316 F317 H318 F319 V320 D321 R322 L323 G324 K325 H326 D327 V328 T329 C330 T331 V332 S333 G334 G335 G336 R337 S338 A339 Q340 A341 G342 A343 I344 R345 L346 A347 M348 A349 K350 A351 L352 C353 S354 F355 V356 T357 E358 D359 E360 V361 E362 W363 M364 R365 Q366 A367 G368

L369 L370 T371 T372 D373 P374 R375 V376 R377 E378 R379 K380 K381 P382 G383 Q384 E385 G386 A387 R388 R389 K390 F391 T392 W393 K394 K395 R396

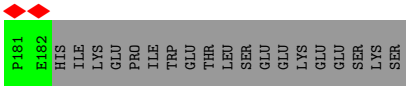
• Molecule 62: 28S ribosomal protein S10, mitochondrial

Chain H6:

MET ALA ALA ARG THR ALA PHE GLY ALA VAL CYS ARG ARG LEU TRP GLN GLY LEU GLY ASN PHE SER VAL ASN THR SER LYS GLY ASN THR ALA LYS ASN GLY GLY LEU LEU LEU SER THR ASN MET LYS TRP VAL GLN PHE SER ASN LEU HIS VAL ASP VAL PRO LYS ASP LEU THR LYS

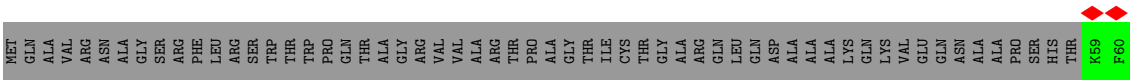
P61 V62 V63 T64 I65 S66 D67 E68 P69 D70 I71 L72 Y73 K74 R75 L76 S77 V78 L79 V80 K81 G82 H83 D84 K85 A86 V87 L88 D89 S90 Y91 E92 Y93 F94 A95 V96 L97 A98 A99 K100 E101 L102 G103 I104 S105 I106 K107 V108 H109 E110 P111 P112 R113 K114 I115 E116 R117 F118 T119 L120

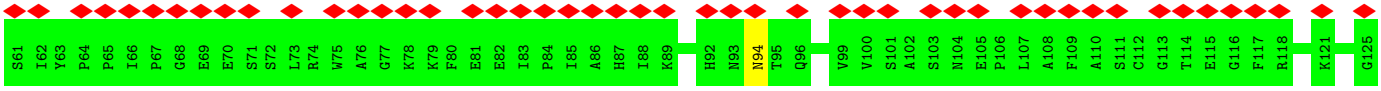
L121 Q122 S123 V124 H125 I126 Y127 K128 K129 H130 R131 V132 Q133 Y134 E135 M136 R137 T138 L139 Y140 R141 C142 L143 E144 L145 E146 H147 L148 T149 G150 S151 T152 A153 D154 V155 Y156 L157 E158 Y159 I160 Q161 R162 N163 L164 P165 E166 G167 V168 A169 M170 E171 V172 T173 K174 T175 Q176 L177 E178 Q179 L180

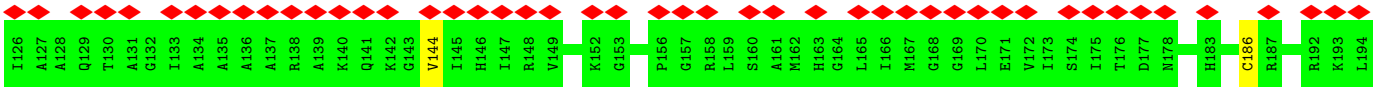


• Molecule 63: 28S ribosomal protein S11, mitochondrial

Chain I6:

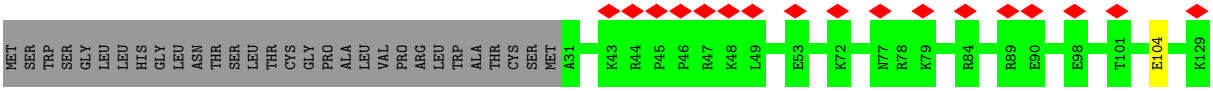


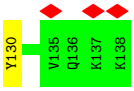




• Molecule 64: 28S ribosomal protein S12, mitochondrial

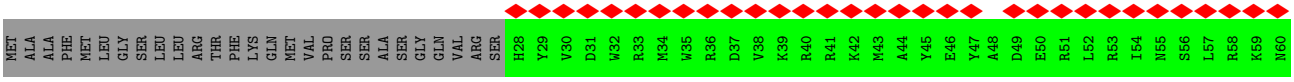
Chain J6:

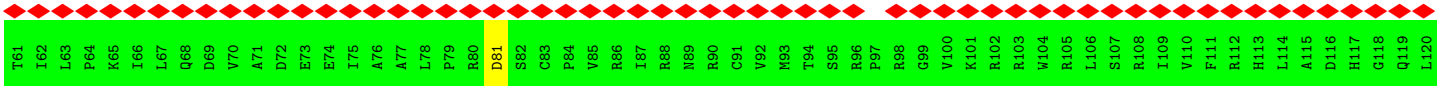


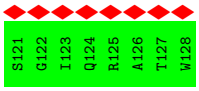


• Molecule 65: 28S ribosomal protein S14, mitochondrial

Chain K6:

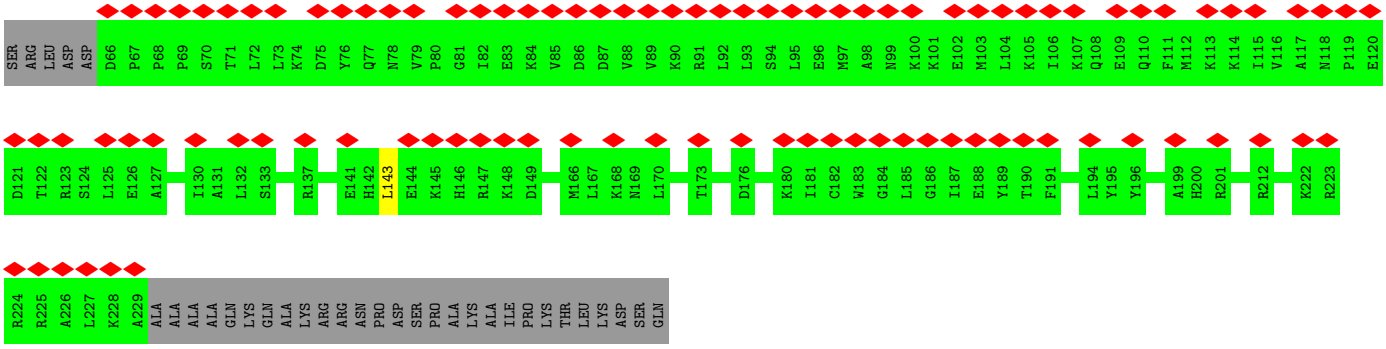






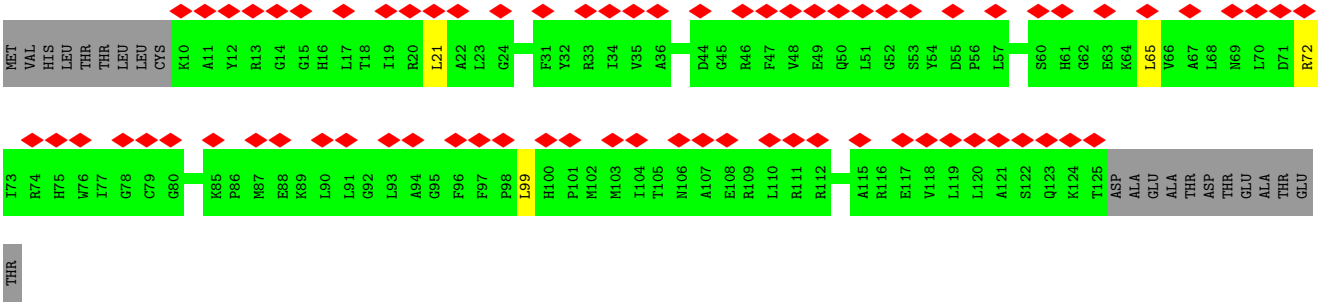
• Molecule 66: 28S ribosomal protein S15, mitochondrial

Chain L6:



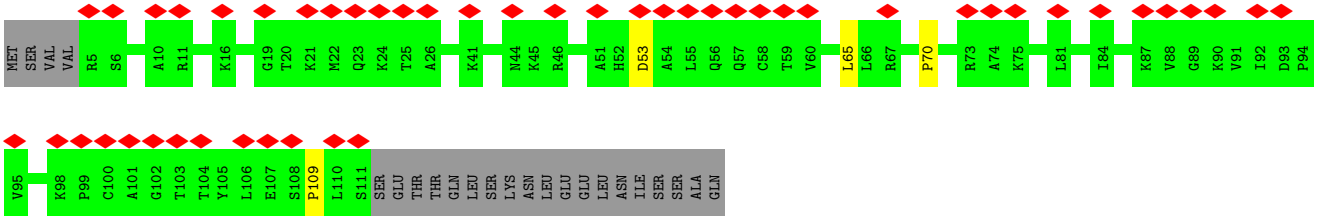
- Molecule 67: 28S ribosomal protein S16, mitochondrial

Chain M6:



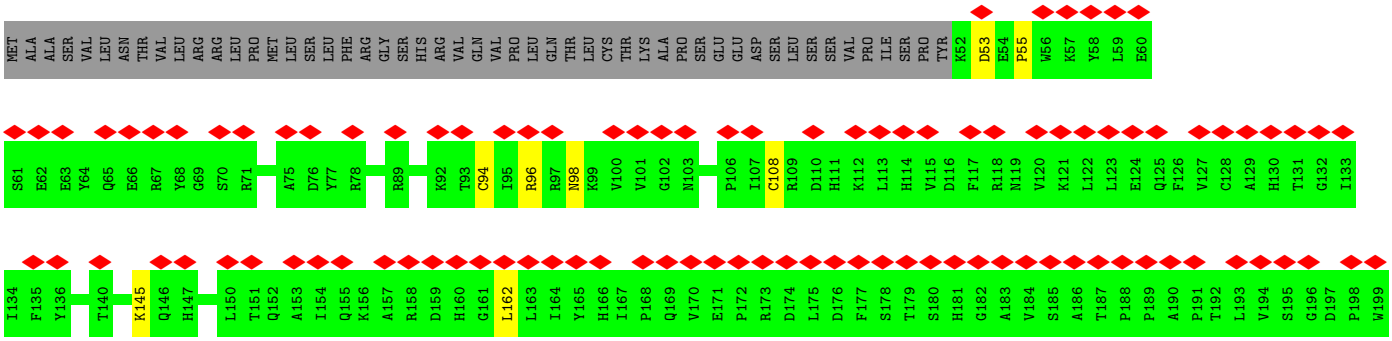
- Molecule 68: 28S ribosomal protein S17, mitochondrial

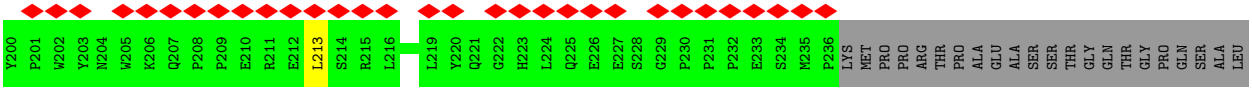
Chain N6:



- Molecule 69: 28S ribosomal protein S18b, mitochondrial

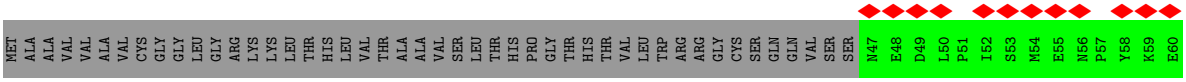
Chain O6:

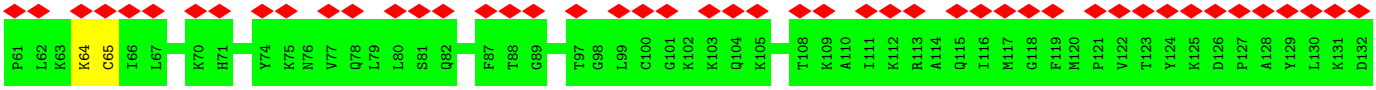


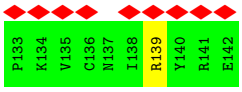


• Molecule 70: 28S ribosomal protein S18c, mitochondrial

Chain P6:

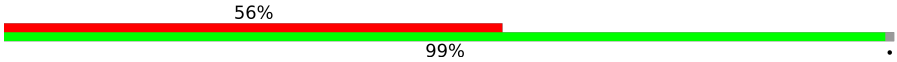


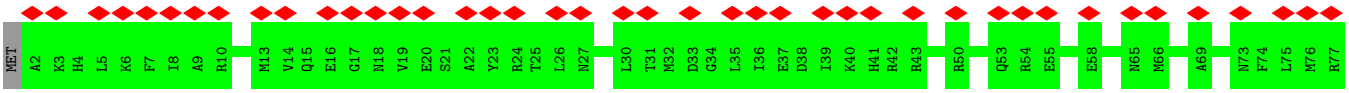


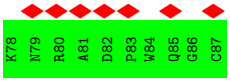


• Molecule 71: 28S ribosomal protein S21, mitochondrial

Chain Q6:

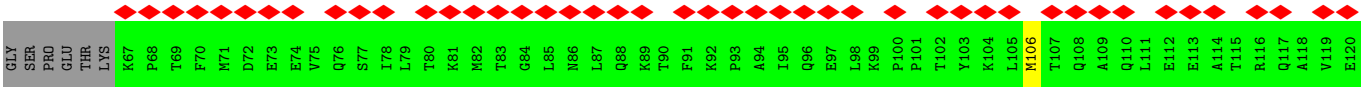


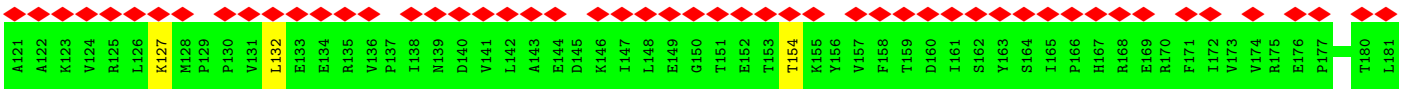


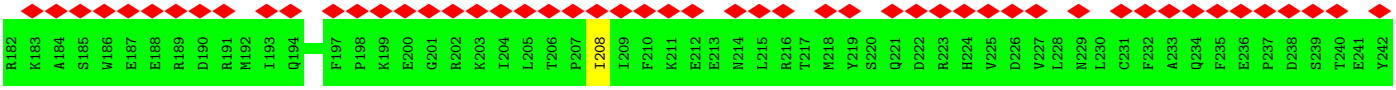


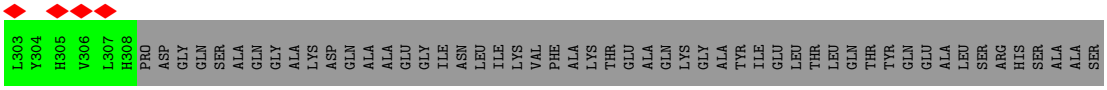
• Molecule 72: 28S ribosomal protein S22, mitochondrial

Chain R6:



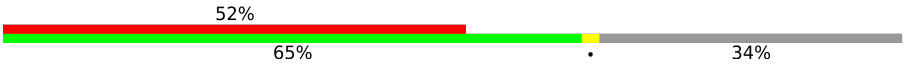


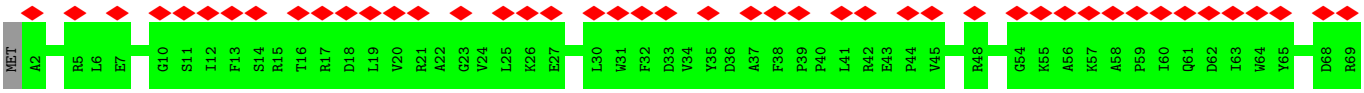


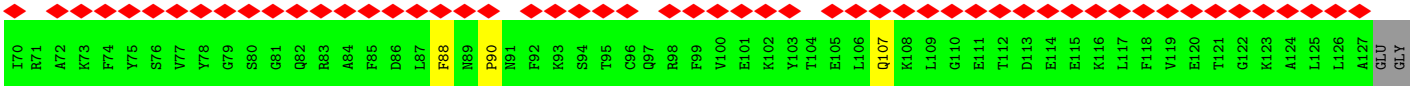


• Molecule 73: 28S ribosomal protein S23, mitochondrial

Chain S6:

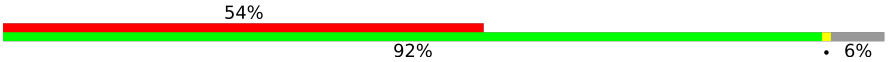


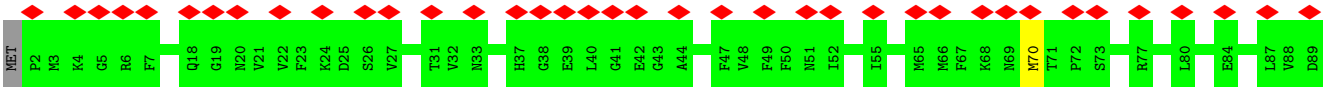


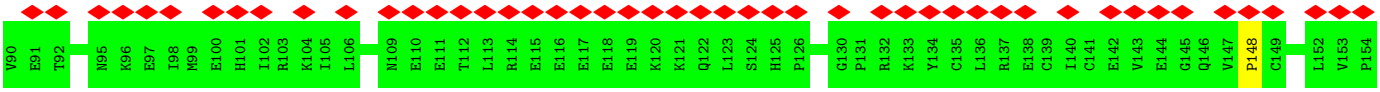


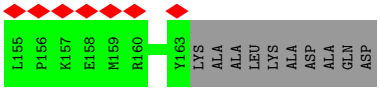
• Molecule 74: 28S ribosomal protein S25, mitochondrial

Chain T6:



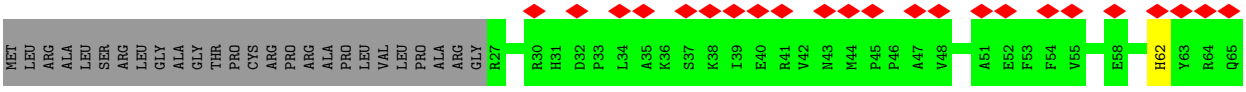


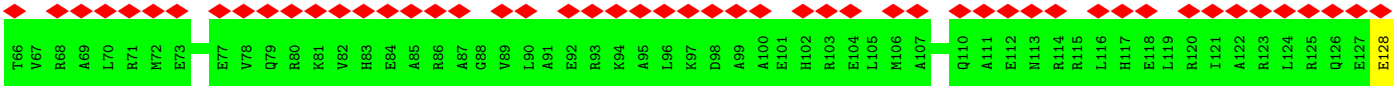


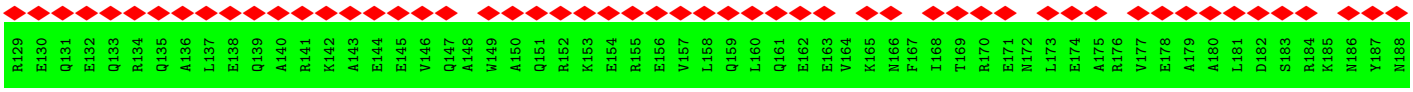


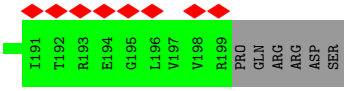
• Molecule 75: 28S ribosomal protein S26, mitochondrial

Chain U6:



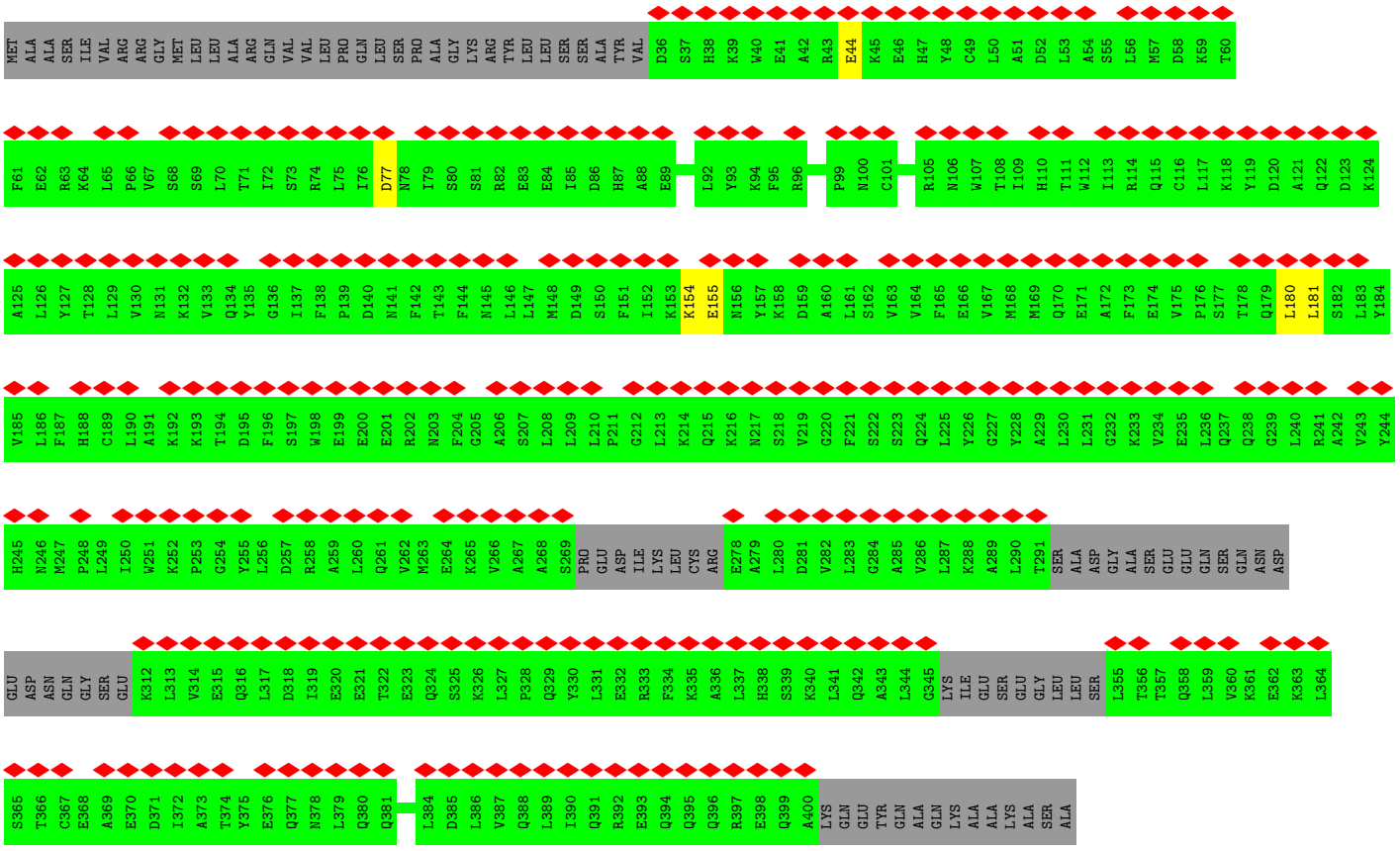






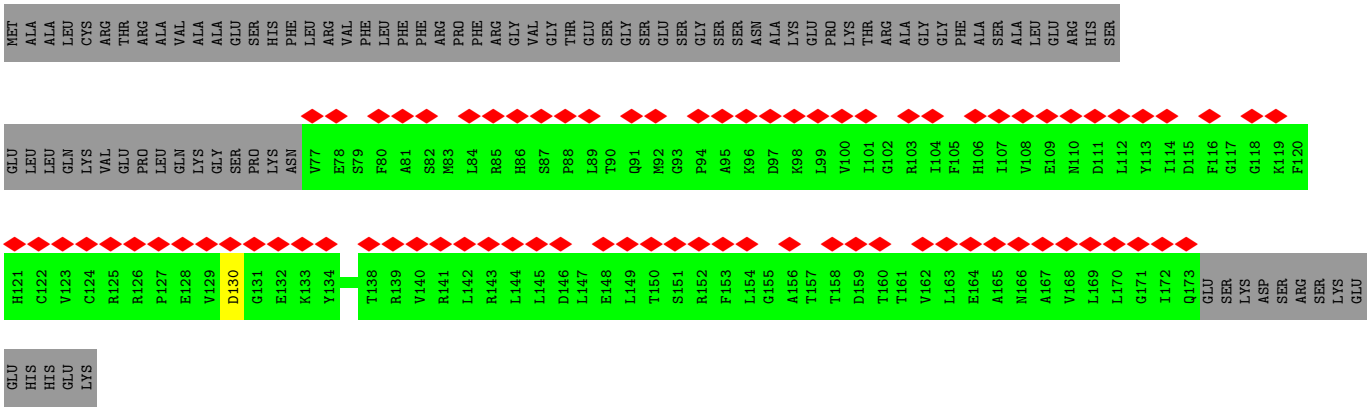
- Molecule 76: 28S ribosomal protein S27, mitochondrial

Chain V6:



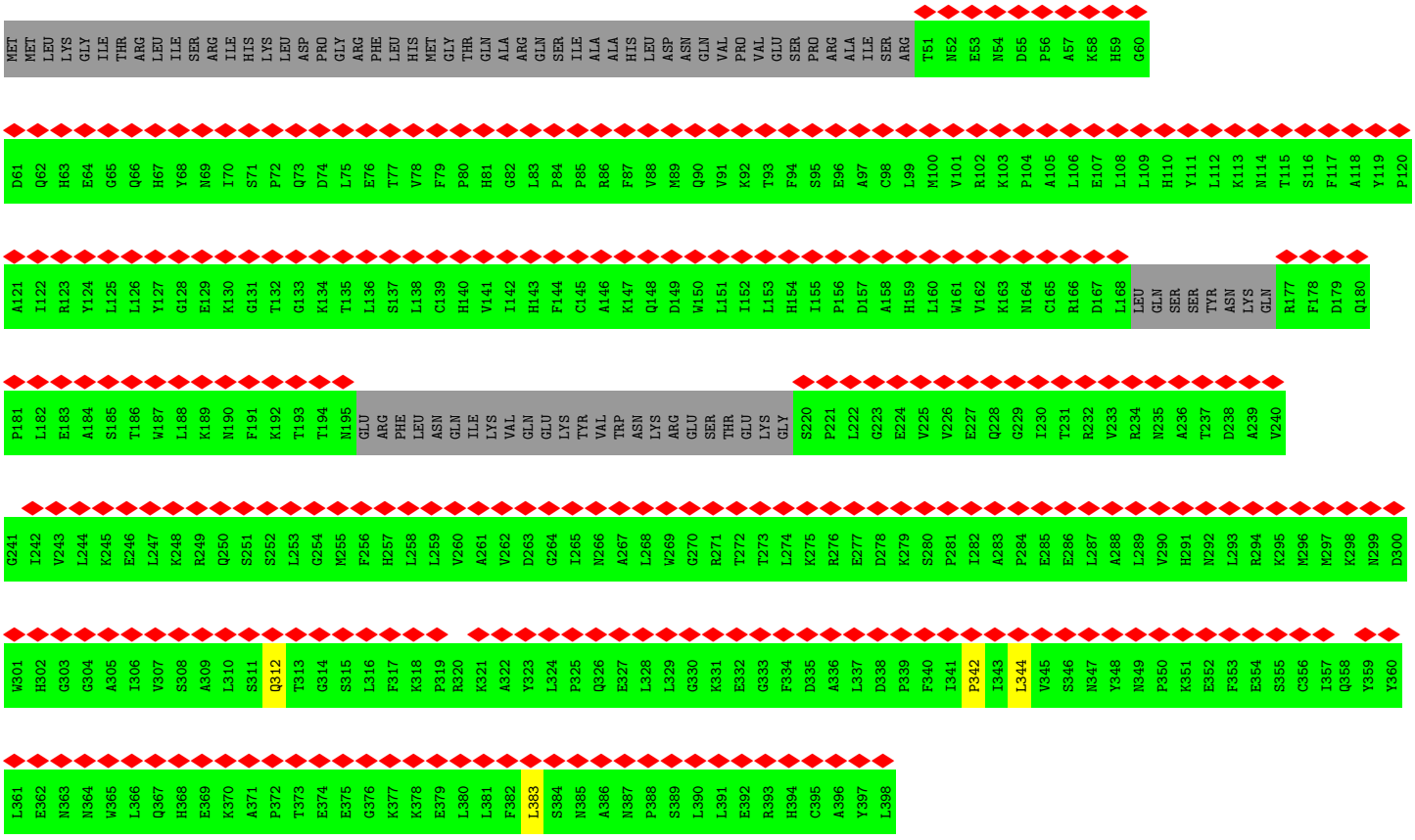
- Molecule 77: 28S ribosomal protein S28, mitochondrial

Chain W6:



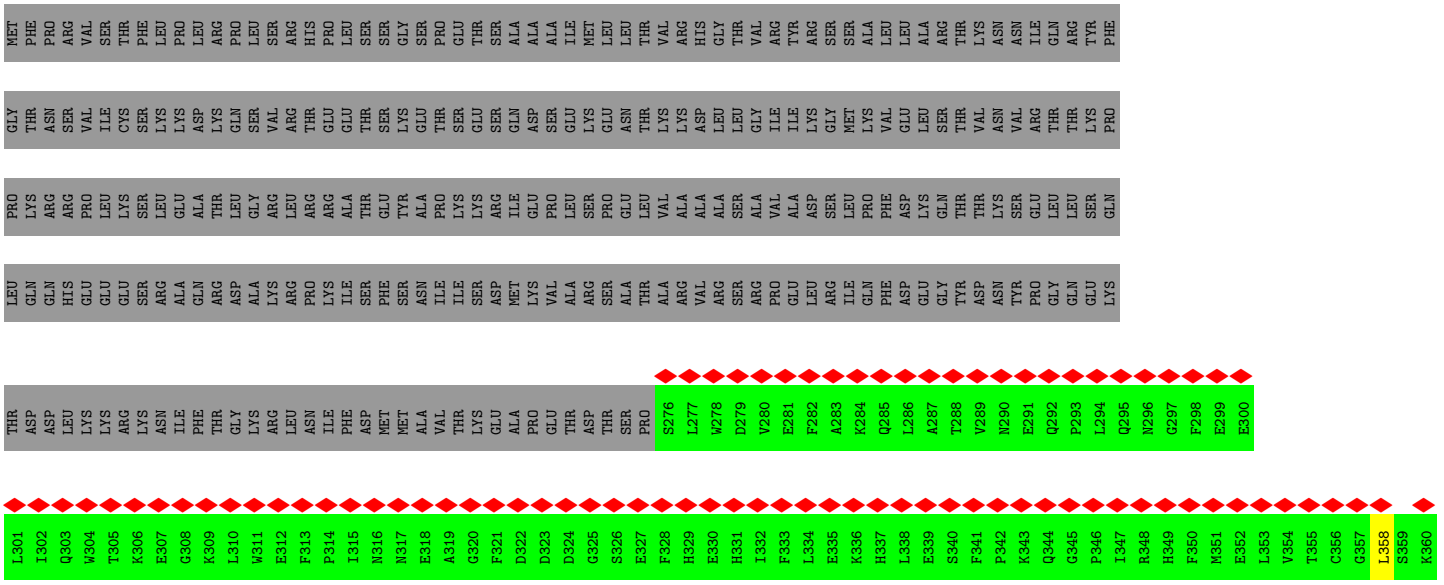
- Molecule 78: 28S ribosomal protein S29, mitochondrial

Chain X6:



- Molecule 79: 28S ribosomal protein S31, mitochondrial

Chain Y6:



N361 P362 Y363 L364 S365 V366 K367 Q368 K369 V370 E371 H372 I373 E374 W375 F376 R377 N378 Y379 F380 N381 E382 K383 LYS ASP ILE LEU LYS GLU SER ASN ILE GLN PHE ASN

- Molecule 80: 28S ribosomal protein S33, mitochondrial

Chain Z6: 81% 82% 18%

MET SER SER LEU S5 E6 Y7 A8 F9 R10 M11 S12 R13 L14 S15 A16 R17 L18 F19 G20 E21 V22 T23 R24 P25 T26 N27 S28 K29 S30 M31 K32 V33 V34 K35 L36 F37 S38 E39 L40 P41 L42 A43 K44 K45 K46 E47 T48 Y49 D50 W51 Y52 P53 N54 H55 H56 T57 Y58 A59 E60

L61 M62 Q63 T64 L65 R66 F67 L68 G69 L70 Y71 R72 D73 E74 H75 Q76 D77 F78 M79 D80 E81 Q82 K83 R84 L85 K86 K87 L88 R89 G90 K91 GLU LYS PRO LYS LYS GLY GLU GLY LYS ARG ALA ALA LYS ARG LYS

- Molecule 81: 28S ribosomal protein S34, mitochondrial

Chain a6: 70% 88% • 8%

MET ALA ARG LYS LYS V6 R7 P8 R9 L10 E13 L14 A15 R16 R17 V18 R19 A20 L21 R22 E23 Q24 L25 N26 R27 P28 R29 D30 S31 Q32 L33 D37 Y38 E39 T40 L41 T42 R43 P44 F45 S46 G47 R48 R49 L50 P51 V52 R53 A56 D57 V58 R59 R60 E61 S62 R63 L64

L65 Q66 L67 L68 G69 R70 L71 P72 L73 L76 G77 R78 L79 R82 K83 S84 W85 L86 W87 Q88 H89 D90 E91 P92 C93 Y94 W95 R96 L97 T98 R99 V100 R101 P102 D103 A106 Q107 N108 L109 D110 H111 G112 K113 A114 W115 G116 I117 L118 T119 F120 K121 G122 K123 T124 E125 S126 E127

A128 R129 E130 I131 E132 H133 V134 M135 Y136 H137 D138 W139 R140 L141 V142 P143 K144 H145 E146 E147 E148 A149 F150 T151 A152 F153 T154 PRO ALA PRO GLU ASP SER LEU A162 S163 V164 P165 Y166 P167 P168 L169 L170 M173 I174 I175 A176 E177 R178 Q179 K180 N181 G182 D183 T184 S185 T186 E187 E188

P189 M190 L191 N192 V193 Q194 R195 I196 R197 M198 E199 Y203 P204 A205 K206 Q207 E208 D209 K210 G211 R212 A213 LYS GLY THR PRO VAL

- Molecule 82: 28S ribosomal protein S35, mitochondrial

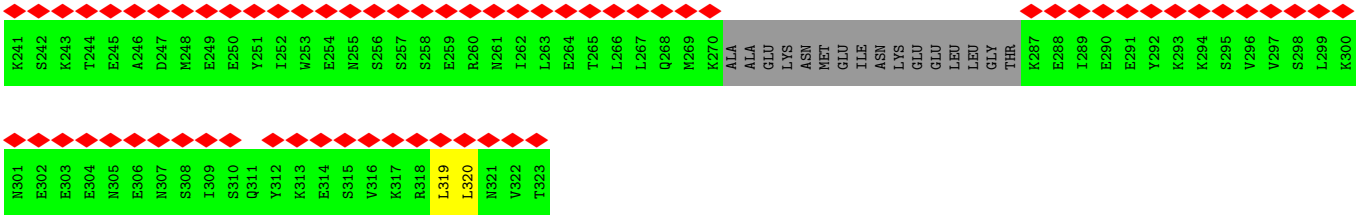
Chain b6: 78% 77% • 21%

MET ALA ALA ALA ALA LEU PRO ALA TRP LEU SER LEU GLN SER ARG ALA ARG THR LEU ARG ALA PHE SER THR ALA VAL TYR SER ALA THR PRO VAL PRO THR PRO SER LEU PRO GLU ARG THR PRO GLY ASN GLU ARG PRO PRO ARG ARG LYS A52 L53 P54 P55 R56 T57 E58 K59 M60

A61 V62 D63 Q64 D65 W66 P67 S68 V69 Y70 P71 V72 A73 A74 P75 F76 K77 P78 S79 A80 V81 P82 L83 P84 V85 R86 M87 G88 Y89 P90 V91 K92 K93 G94 V95 P96 M97 A98 K99 E100 G101 N102 L103 E104 L105 L106 K107 I108 P109 N110 F111 L112 H113 L114 T115 P116 V117 A118 I119 K120

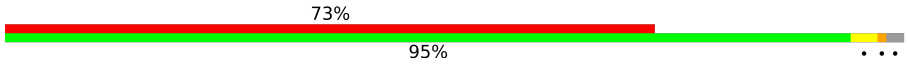
K121 H122 C123 E124 A125 L126 K127 D128 F129 C130 T131 E132 W133 P134 A135 A136 L137 D138 S139 D140 E141 K142 C143 E144 K145 H146 F147 P148 I149 E150 I151 D152 S153 T154 D155 Y156 V157 S158 S159 G160 P161 S162 V163 R164 N165 P166 R167 A168 R169 V170 V171 V172 L173 R174 V175 K176 L177 S178 S179 L180

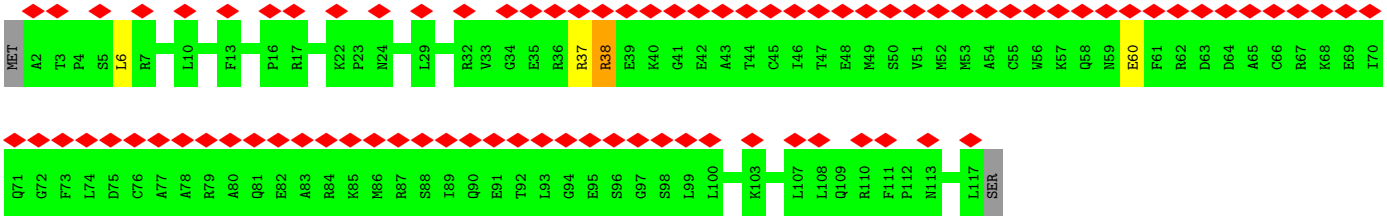
N181 L182 D183 D184 H185 A186 K187 K188 K189 L190 I191 K192 L193 V194 G195 E196 R197 Y198 C199 K200 T201 T202 D203 V204 L205 T206 I207 K208 T209 D210 R211 C212 P213 L214 R215 R216 Q217 N218 Y219 D220 Y221 A222 V223 Y224 L225 L226 T227 V228 L229 Y230 H231 E232 S233 W234 N235 T236 E237 E238 W239 E240



• Molecule 83: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

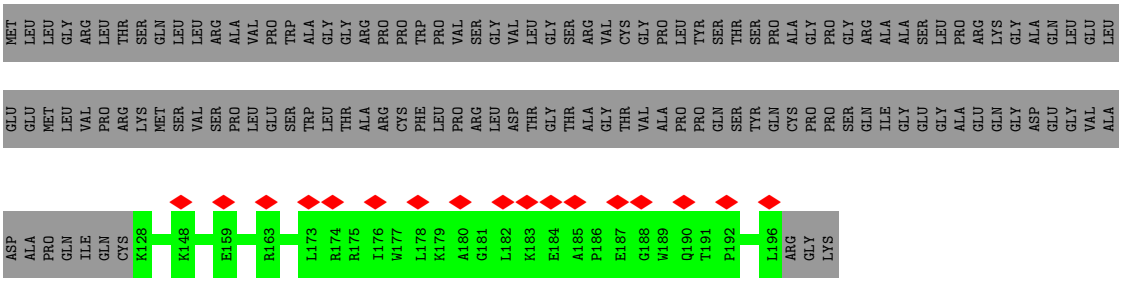
Chain c6:





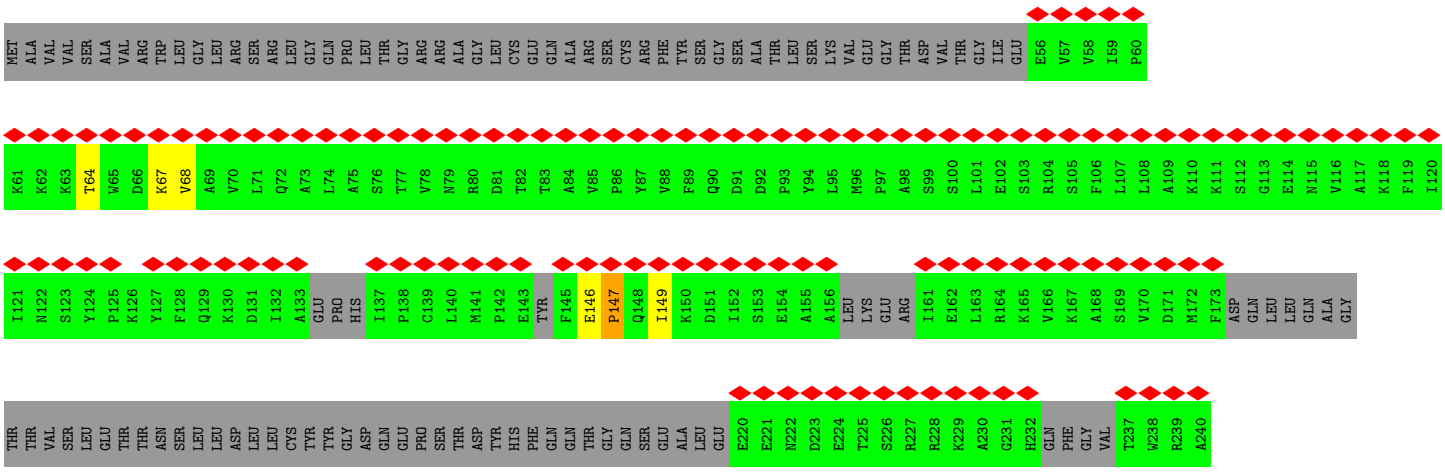
• Molecule 84: Aurora kinase A-interacting protein

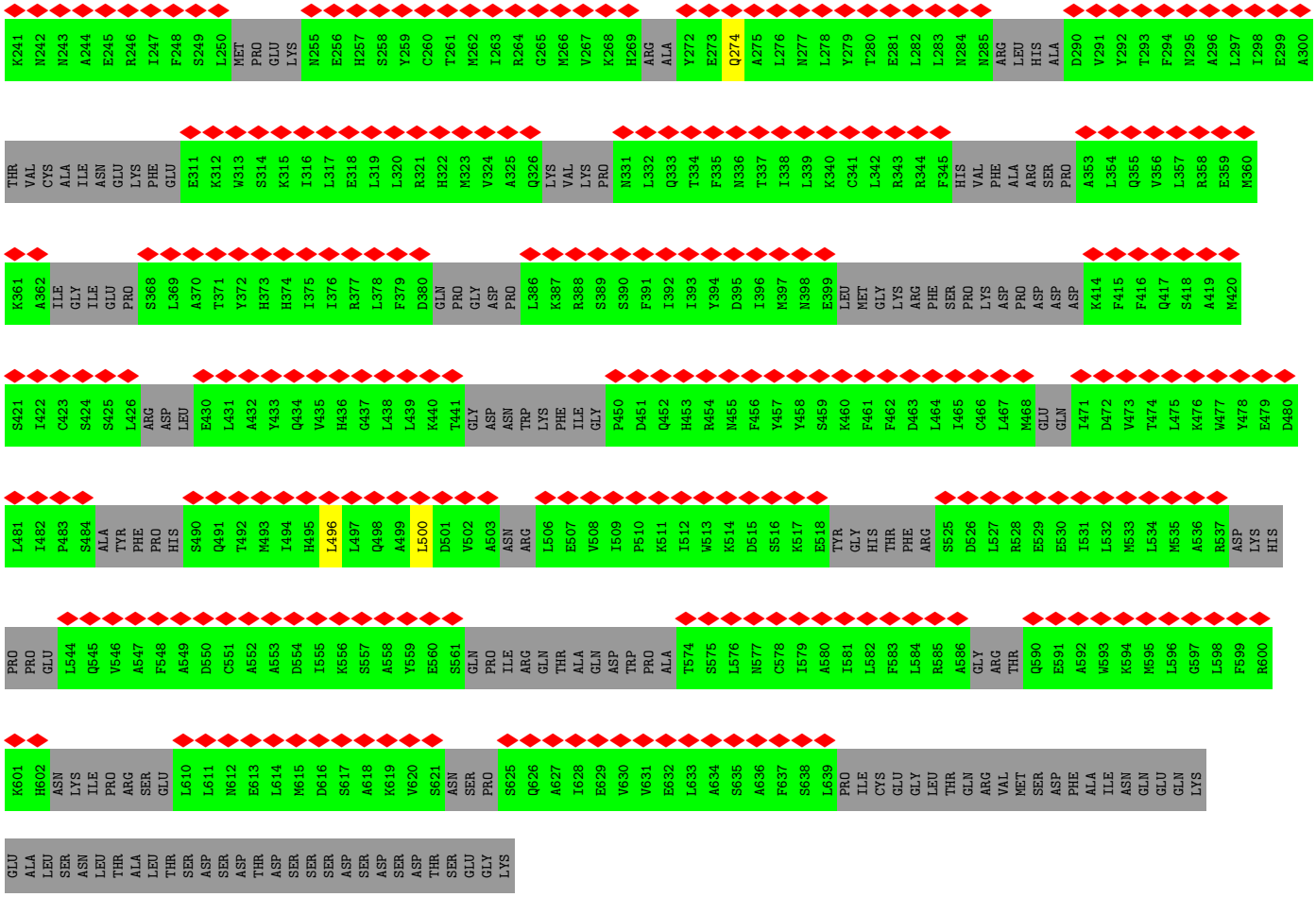
Chain d6:



• Molecule 85: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

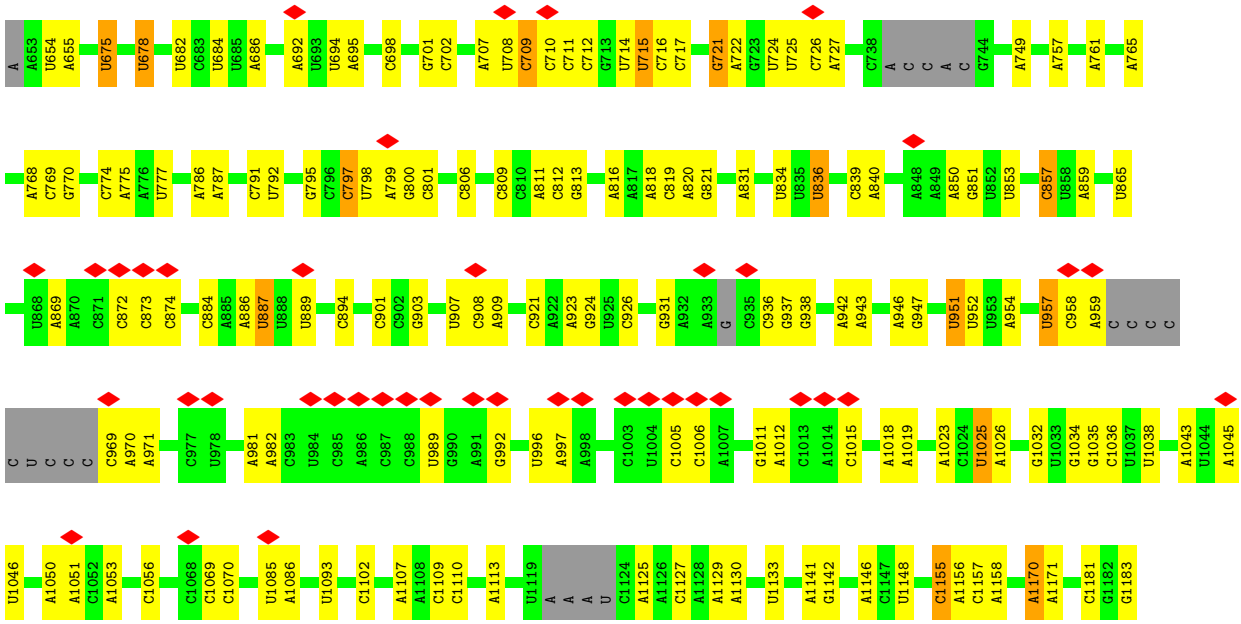
Chain e6:

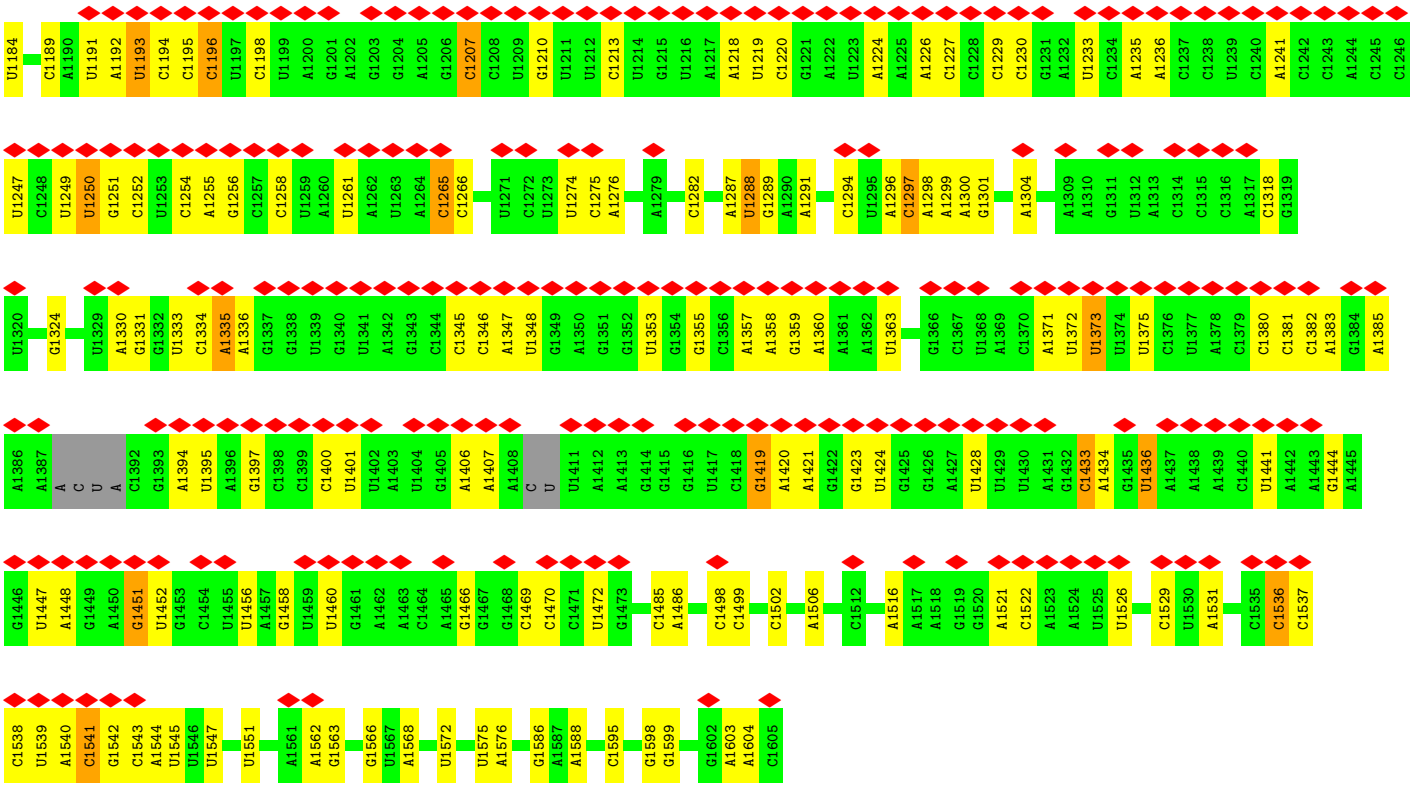




- Molecule 86: 12S rRNA

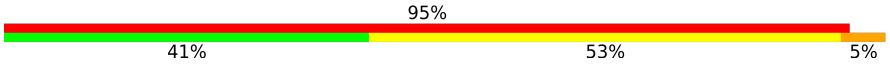
Chain A6:

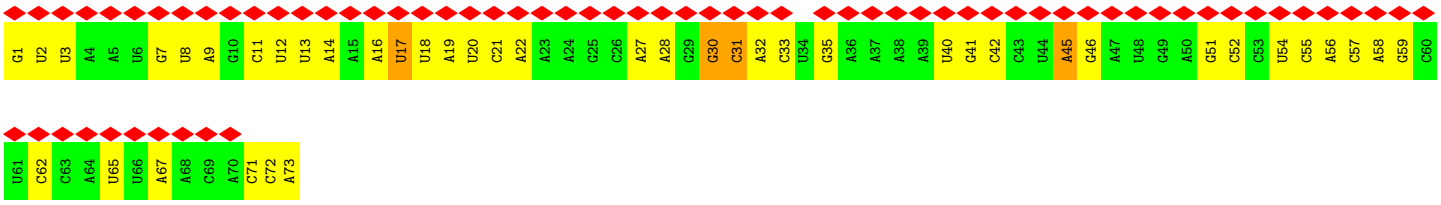




- Molecule 87: mt-tRNA

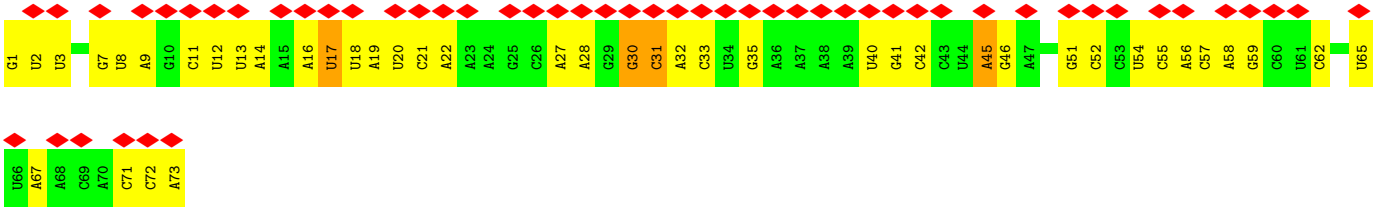
Chain 24:





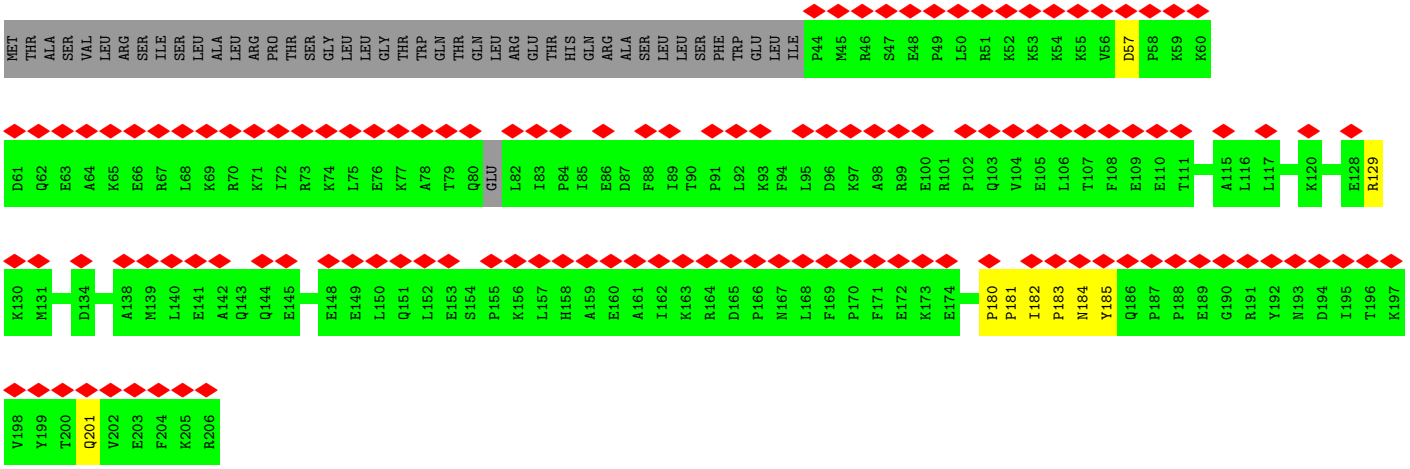
- Molecule 87: mt-tRNA

Chain FE:



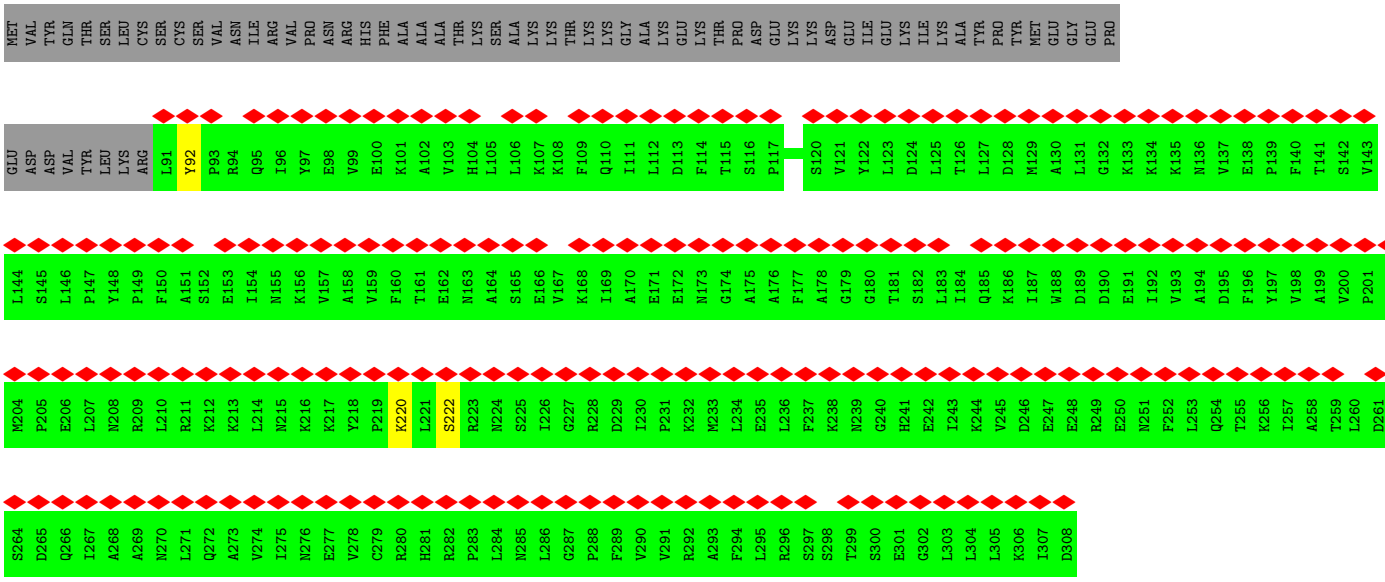
- Molecule 88: 39S ribosomal protein L40, mitochondrial

Chain A:



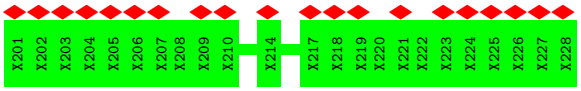
- Molecule 89: 39S ribosomal protein L1, mitochondrial

Chain n:



- Molecule 90: Unknown protein

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19767	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	0.294	Depositor
Minimum map value	-0.153	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, GCP, GDP, MG, SPD

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	r1	0.47	0/5552	0.93	15/7490 (0.2%)
3	8	0.52	0/197	1.06	0/305
3	A3	1.06	7/35697 (0.0%)	1.18	306/55544 (0.6%)
4	B3	0.57	0/1328	1.02	6/2056 (0.3%)
5	D3	0.46	0/1879	0.69	2/2527 (0.1%)
6	E3	0.54	0/2433	0.68	3/3299 (0.1%)
7	F3	0.55	0/2071	0.75	1/2817 (0.0%)
8	D	4.69	3/665 (0.5%)	1.19	7/905 (0.8%)
8	H3	0.44	0/798	0.73	1/1073 (0.1%)
9	I3	0.41	0/1308	0.71	0/1761
10	J3	0.39	0/1077	0.74	1/1452 (0.1%)
11	K3	0.55	0/1495	0.70	2/2029 (0.1%)
12	L3	0.47	0/904	0.71	0/1218
13	M3	0.55	1/2359 (0.0%)	0.73	4/3185 (0.1%)
14	N3	0.55	0/1697	0.73	2/2281 (0.1%)
15	O3	0.56	1/1269 (0.1%)	0.77	1/1708 (0.1%)
16	P3	0.54	0/1103	0.77	2/1491 (0.1%)
17	Q3	0.49	0/1863	0.70	0/2509
18	R3	0.60	0/1174	0.66	0/1572
19	S3	0.55	0/1276	0.72	3/1729 (0.2%)
20	T3	0.56	0/1402	0.64	1/1886 (0.1%)
21	U3	0.60	0/946	0.71	0/1283
22	V3	0.47	0/1590	0.75	2/2151 (0.1%)
23	W3	0.64	0/893	0.71	1/1204 (0.1%)
24	X3	0.46	0/2081	0.78	3/2812 (0.1%)
25	Y3	0.53	1/1552 (0.1%)	0.64	0/2079
26	Z3	0.51	0/1003	0.69	1/1354 (0.1%)
27	03	0.47	0/895	0.65	0/1201
28	13	0.47	0/438	0.87	1/583 (0.2%)
29	23	0.53	0/382	0.64	0/507
30	33	0.60	0/852	0.69	1/1136 (0.1%)
31	43	0.58	0/329	0.61	0/435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	53	0.46	0/3154	0.67	1/4295 (0.0%)
33	63	0.49	0/2722	0.72	3/3709 (0.1%)
34	73	0.45	0/2207	0.74	4/2978 (0.1%)
35	93	0.48	0/896	0.74	3/1205 (0.2%)
36	a3	0.51	0/709	0.65	0/963
37	b3	0.51	0/1202	0.67	1/1626 (0.1%)
38	c3	0.48	0/2264	0.68	1/3059 (0.0%)
39	d3	0.45	0/1385	0.81	2/1877 (0.1%)
40	e3	0.35	0/1797	0.76	3/2422 (0.1%)
41	f3	0.43	0/1055	0.83	1/1427 (0.1%)
42	g3	0.58	0/1102	0.69	0/1503
43	h3	0.41	0/847	0.71	2/1150 (0.2%)
44	i3	0.58	0/849	0.76	1/1135 (0.1%)
45	j3	0.48	0/698	0.62	1/940 (0.1%)
46	k3	0.35	0/665	0.74	0/897
47	l3	0.45	0/226	0.63	0/299
48	m3	0.36	0/379	0.73	0/510
49	o3	0.58	0/818	0.62	0/1097
50	p3	0.37	0/1071	0.59	0/1433
51	q3	0.42	0/1107	0.62	0/1498
52	r3	0.56	0/1238	0.70	0/1676
53	s3	0.51	1/3114 (0.0%)	0.74	3/4225 (0.1%)
54	u3	1.03	0/46	0.98	0/69
55	A5	0.28	0/135	0.72	1/185 (0.5%)
56	B6	0.39	0/1811	0.76	2/2451 (0.1%)
57	C6	0.36	0/1112	0.63	0/1505
58	D6	0.40	0/2607	0.74	2/3498 (0.1%)
59	E6	0.39	0/989	0.74	0/1335
60	F6	0.41	1/1708 (0.1%)	0.68	2/2291 (0.1%)
61	G6	0.38	0/2570	0.72	4/3443 (0.1%)
62	H6	0.34	0/1019	0.71	1/1379 (0.1%)
63	I6	0.35	0/1031	0.65	1/1390 (0.1%)
64	J6	0.56	1/854 (0.1%)	0.77	0/1148
65	K6	0.36	0/879	0.66	1/1182 (0.1%)
66	L6	0.35	0/1406	0.69	1/1878 (0.1%)
67	M6	0.41	0/941	1.00	5/1265 (0.4%)
68	N6	0.54	1/864 (0.1%)	0.85	5/1169 (0.4%)
69	O6	0.43	1/1580 (0.1%)	0.76	4/2150 (0.2%)
70	P6	0.39	0/791	0.76	0/1062
71	Q6	0.43	0/752	0.74	0/1001
72	R6	0.36	0/2050	0.75	2/2770 (0.1%)
73	S6	0.62	1/1069 (0.1%)	0.98	5/1441 (0.3%)
74	T6	0.42	0/1361	0.74	0/1829

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	U6	0.36	0/1482	0.62	0/1987
76	V6	0.36	0/2758	0.71	4/3724 (0.1%)
77	W6	0.35	0/778	0.78	1/1048 (0.1%)
78	X6	0.34	0/2596	0.70	2/3519 (0.1%)
79	Y6	0.34	0/943	0.65	1/1274 (0.1%)
80	Z6	0.31	0/757	0.63	0/1011
81	a6	0.40	0/1727	0.82	7/2338 (0.3%)
82	b6	0.33	0/2121	0.74	4/2873 (0.1%)
83	c6	0.34	0/939	0.69	1/1256 (0.1%)
84	d6	0.42	0/621	0.72	0/820
85	e6	0.29	0/2859	0.58	3/3864 (0.1%)
86	A6	0.67	0/22053	1.10	125/34324 (0.4%)
87	24	1.16	6/1731 (0.3%)	1.31	21/2693 (0.8%)
87	FE	1.16	6/1731 (0.3%)	1.31	20/2693 (0.7%)
88	A	0.35	0/1403	0.73	3/1880 (0.2%)
89	n	4.89	7/1776 (0.4%)	0.75	3/2397 (0.1%)
All	All	0.87	38/179863 (0.0%)	0.92	623/255648 (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	r1	0	23
2	Y2	0	2
5	D3	0	1
6	E3	0	5
7	F3	0	2
8	D	0	2
8	H3	0	1
9	I3	0	1
10	J3	0	2
11	K3	0	2
13	M3	0	4
14	N3	0	2
15	O3	0	1
17	Q3	0	1
18	R3	0	1
20	T3	0	1
22	V3	0	2
24	X3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	Z3	0	1
27	03	0	2
28	13	0	2
32	53	0	4
33	63	0	2
35	93	0	1
38	c3	0	1
39	d3	0	5
41	f3	0	4
42	g3	0	1
43	h3	0	2
44	i3	0	1
45	j3	0	1
49	o3	0	1
51	q3	0	1
53	s3	0	2
56	B6	0	1
58	D6	0	4
60	F6	0	4
61	G6	0	1
63	I6	0	2
64	J6	0	1
68	N6	0	1
69	O6	0	3
70	P6	0	3
72	R6	0	3
73	S6	0	1
75	U6	0	2
76	V6	0	2
81	a6	0	1
82	b6	0	1
83	c6	0	1
85	e6	0	2
88	A	0	6
89	n	0	1
All	All	0	125

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	n	220	LYS	CE-NZ	125.36	4.62	1.49
8	D	194	PHE	CB-CG	119.68	3.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	n	92	TYR	CD1-CE1	88.52	2.72	1.39
89	n	92	TYR	CD2-CE2	84.32	2.65	1.39
89	n	92	TYR	CE2-CZ	59.95	2.16	1.38
89	n	92	TYR	CE1-CZ	59.69	2.16	1.38
89	n	92	TYR	CG-CD2	47.04	2.00	1.39
89	n	92	TYR	CG-CD1	46.67	1.99	1.39
87	FE	17	U	C2-N3	24.50	1.54	1.37
87	24	17	U	C2-N3	24.48	1.54	1.37
87	FE	17	U	N3-C4	18.45	1.55	1.38
87	24	17	U	N3-C4	18.40	1.55	1.38
87	FE	17	U	N1-C2	17.73	1.54	1.38
87	24	17	U	N1-C2	17.65	1.54	1.38
87	24	17	U	N1-C6	16.81	1.53	1.38
87	FE	17	U	N1-C6	16.75	1.53	1.38
73	S6	90	PRO	CG-CD	-14.78	1.01	1.50
87	24	17	U	C4-C5	14.01	1.56	1.43
87	FE	17	U	C4-C5	14.00	1.56	1.43
87	24	17	U	C5-C6	12.54	1.45	1.34
87	FE	17	U	C5-C6	12.46	1.45	1.34
8	D	194	PHE	CG-CD2	11.07	1.55	1.38
8	D	194	PHE	CG-CD1	10.64	1.54	1.38
68	N6	70	PRO	CG-CD	-9.57	1.19	1.50
60	F6	159	VAL	C-N	9.02	1.51	1.34
3	A3	1828	A	N9-C4	-8.57	1.32	1.37
25	Y3	123	ARG	C-N	-6.42	1.19	1.34
13	M3	61	THR	C-N	-6.34	1.19	1.34
3	A3	1867	A	N9-C4	-6.33	1.34	1.37
53	s3	66	TRP	CB-CG	-5.96	1.39	1.50
3	A3	2755	A	N9-C4	-5.80	1.34	1.37
3	A3	2503	A	N9-C4	-5.51	1.34	1.37
64	J6	104	GLU	CA-C	5.32	1.66	1.52
3	A3	2052	A	N9-C4	-5.31	1.34	1.37
69	O6	94	CYS	CB-SG	-5.13	1.73	1.81
15	O3	104	TYR	CD1-CE1	-5.06	1.31	1.39
3	A3	2723	A	N9-C4	-5.05	1.34	1.37
3	A3	2198	A	N7-C5	-5.00	1.36	1.39

All (623) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	2790	A	OP1-P-OP2	-28.97	76.15	119.60
3	A3	2790	A	O5'-P-OP2	-28.55	76.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	S6	90	PRO	N-CD-CG	-18.72	75.12	103.20
3	A3	2790	A	O5'-P-OP1	15.95	129.84	110.70
87	24	30	G	C8-N9-C4	-15.63	100.15	106.40
87	FE	30	G	C8-N9-C4	-15.60	100.16	106.40
53	s3	427	ASN	C-N-CA	15.18	159.64	121.70
8	D	194	PHE	CD1-CG-CD2	-14.92	98.91	118.30
8	D	194	PHE	CB-CG-CD2	14.40	130.88	120.80
3	A3	2789	C	OP2-P-O3'	14.28	136.62	105.20
24	X3	97	LEU	CA-CB-CG	13.61	146.61	115.30
8	D	194	PHE	CB-CG-CD1	13.38	130.17	120.80
3	A3	1732	C	N1-C2-O2	12.90	126.64	118.90
87	24	30	G	N7-C8-N9	12.78	119.49	113.10
87	FE	30	G	N7-C8-N9	12.78	119.49	113.10
3	A3	2789	C	OP1-P-O3'	-12.53	77.63	105.20
1	r1	645	ILE	CG1-CB-CG2	-11.86	85.31	111.40
3	A3	1699	C	N1-C2-O2	11.83	126.00	118.90
86	A6	1373	U	N1-C2-O2	11.82	131.08	122.80
24	X3	97	LEU	CB-CG-CD2	11.57	130.67	111.00
3	A3	1732	C	C2-N1-C1'	11.44	131.38	118.80
86	A6	1373	U	C2-N1-C1'	11.29	131.24	117.70
86	A6	1373	U	N3-C2-O2	-11.24	114.33	122.20
73	S6	90	PRO	CA-CB-CG	-11.01	83.08	104.00
3	A3	1732	C	N3-C2-O2	-10.92	114.25	121.90
87	FE	31	C	O4'-C1'-N1	10.81	116.85	108.20
87	24	31	C	O4'-C1'-N1	10.77	116.82	108.20
3	A3	2780	C	N1-C2-O2	10.62	125.27	118.90
68	N6	70	PRO	N-CD-CG	-10.43	87.56	103.20
3	A3	3204	C	N1-C2-O2	10.26	125.06	118.90
3	A3	1699	C	N3-C2-O2	-10.01	114.89	121.90
67	M6	21	LEU	CB-CG-CD2	9.99	127.99	111.00
3	A3	2653	C	C6-N1-C2	-9.93	116.33	120.30
3	A3	1714	C	N1-C2-O2	9.54	124.62	118.90
3	A3	1902	C	C2-N1-C1'	9.54	129.29	118.80
3	A3	2079	C	N1-C2-O2	9.53	124.62	118.90
3	A3	1902	C	N1-C2-O2	9.44	124.56	118.90
3	A3	2079	C	N3-C2-O2	-9.39	115.33	121.90
3	A3	2066	C	N1-C2-O2	9.32	124.49	118.90
3	A3	3204	C	C2-N1-C1'	9.32	129.05	118.80
3	A3	2493	C	N1-C2-O2	9.26	124.46	118.90
3	A3	1699	C	C2-N1-C1'	9.26	128.98	118.80
3	A3	1837	C	C2-N1-C1'	9.25	128.97	118.80
3	A3	2522	U	C2-N1-C1'	9.22	128.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	3212	C	C2-N1-C1'	9.21	128.93	118.80
68	N6	70	PRO	CA-N-CD	-9.17	98.66	111.50
3	A3	3134	C	N1-C2-O2	9.12	124.37	118.90
67	M6	21	LEU	CA-CB-CG	9.08	136.18	115.30
3	A3	1837	C	N1-C2-O2	9.03	124.31	118.90
3	A3	1901	C	N1-C2-O2	8.98	124.29	118.90
3	A3	1732	C	C6-N1-C2	-8.93	116.73	120.30
3	A3	2080	U	N3-C2-O2	-8.91	115.96	122.20
3	A3	2779	C	P-O3'-C3'	8.90	130.39	119.70
3	A3	3212	C	N1-C2-O2	8.90	124.24	118.90
3	A3	2493	C	C2-N1-C1'	8.90	128.59	118.80
3	A3	2066	C	N3-C2-O2	-8.87	115.69	121.90
3	A3	2080	U	N1-C2-O2	8.82	128.97	122.80
3	A3	2066	C	C2-N1-C1'	8.81	128.50	118.80
3	A3	3134	C	N3-C2-O2	-8.74	115.78	121.90
3	A3	3204	C	N3-C2-O2	-8.67	115.83	121.90
3	A3	3157	C	N1-C2-O2	8.64	124.09	118.90
86	A6	809	C	C2-N1-C1'	8.59	128.25	118.80
3	A3	2780	C	C2-N1-C1'	8.58	128.24	118.80
86	A6	809	C	N1-C2-O2	8.47	123.98	118.90
3	A3	2079	C	C2-N1-C1'	8.40	128.04	118.80
87	FE	17	U	C6-N1-C2	8.37	126.02	121.00
34	73	314	ASP	CB-CG-OD1	8.35	125.81	118.30
87	24	17	U	C6-N1-C2	8.33	126.00	121.00
72	R6	293	LEU	CA-CB-CG	8.27	134.33	115.30
86	A6	769	C	C2-N1-C1'	8.26	127.89	118.80
3	A3	2235	C	C2-N1-C1'	8.23	127.86	118.80
86	A6	936	C	N3-C2-O2	-8.21	116.15	121.90
3	A3	1901	C	C2-N1-C1'	8.20	127.82	118.80
34	73	259	ASP	CB-CG-OD1	8.19	125.67	118.30
3	A3	1993	A	C2-N3-C4	8.16	114.68	110.60
3	A3	3157	C	C2-N1-C1'	8.14	127.76	118.80
3	A3	2493	C	N3-C2-O2	-8.14	116.20	121.90
3	A3	1902	C	N3-C2-O2	-8.07	116.25	121.90
34	73	47	LEU	CA-CB-CG	8.06	133.83	115.30
3	A3	2171	U	C2-N1-C1'	8.04	127.35	117.70
86	A6	715	U	C2-N1-C1'	7.99	127.28	117.70
86	A6	710	C	C2-N1-C1'	7.91	127.50	118.80
3	A3	2096	U	C2-N1-C1'	7.90	127.18	117.70
3	A3	2780	C	N3-C2-O2	-7.89	116.37	121.90
86	A6	1193	U	C2-N1-C1'	7.87	127.14	117.70
3	A3	2171	U	N3-C2-O2	-7.87	116.69	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	FE	17	U	N1-C2-N3	-7.86	110.19	114.90
87	24	17	U	N1-C2-N3	-7.83	110.20	114.90
86	A6	1070	C	C6-N1-C2	-7.81	117.18	120.30
81	a6	141	LEU	CA-CB-CG	7.79	133.22	115.30
3	A3	2080	U	C2-N1-C1'	7.78	127.03	117.70
61	G6	373	ASP	CB-CG-OD2	7.78	125.30	118.30
3	A3	2372	U	N3-C2-O2	-7.74	116.78	122.20
3	A3	2372	U	N1-C2-O2	7.72	128.20	122.80
86	A6	936	C	N1-C2-O2	7.72	123.53	118.90
3	A3	2898	U	C2-N1-C1'	7.71	126.95	117.70
3	A3	1714	C	N3-C2-O2	-7.71	116.50	121.90
3	A3	1699	C	C6-N1-C2	-7.69	117.22	120.30
86	A6	809	C	N3-C2-O2	-7.68	116.53	121.90
3	A3	2235	C	N1-C2-O2	7.67	123.50	118.90
53	s3	228	ASP	CB-CG-OD1	7.65	125.18	118.30
8	D	194	PHE	CG-CD2-CE2	7.62	129.18	120.80
3	A3	2061	C	N1-C2-O2	7.59	123.46	118.90
3	A3	1837	C	N3-C2-O2	-7.58	116.59	121.90
86	A6	769	C	N1-C2-O2	7.54	123.42	118.90
3	A3	1732	C	C6-N1-C1'	-7.52	111.78	120.80
3	A3	2157	U	C5-C6-N1	7.48	126.44	122.70
3	A3	2757	A	P-O3'-C3'	7.48	128.67	119.70
3	A3	2372	U	C2-N1-C1'	7.47	126.66	117.70
3	A3	3157	C	N3-C2-O2	-7.47	116.67	121.90
66	L6	143	LEU	CA-CB-CG	7.47	132.47	115.30
3	A3	3157	C	O4'-C1'-N1	7.46	114.17	108.20
11	K3	22	ASP	CB-CG-OD1	7.46	125.01	118.30
3	A3	2230	A	O5'-P-OP1	7.44	119.63	110.70
86	A6	1373	U	C6-N1-C1'	-7.44	110.78	121.20
3	A3	1813	C	N1-C2-O2	7.43	123.36	118.90
3	A3	1813	C	N3-C2-O2	-7.42	116.70	121.90
86	A6	1193	U	N1-C2-O2	7.40	127.98	122.80
3	A3	1813	C	C2-N1-C1'	7.39	126.92	118.80
86	A6	1541	C	N1-C2-O2	7.38	123.33	118.90
56	B6	251	ARG	NE-CZ-NH1	7.35	123.98	120.30
3	A3	2443	C	N1-C2-O2	7.29	123.28	118.90
89	n	92	TYR	CB-CG-CD2	-7.29	116.62	121.00
86	A6	1541	C	C6-N1-C2	-7.28	117.39	120.30
8	D	194	PHE	CG-CD1-CE1	7.28	128.81	120.80
3	A3	2484	C	N1-C2-O2	7.28	123.27	118.90
3	A3	3169	C	N1-C2-O2	7.27	123.26	118.90
86	A6	714	U	C2-N1-C1'	7.27	126.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K3	52	ASP	CB-CG-OD1	7.27	124.84	118.30
3	A3	2171	U	N1-C2-O2	7.26	127.88	122.80
73	S6	90	PRO	CB-CG-CD	7.25	134.80	106.50
3	A3	2522	U	N1-C2-O2	7.25	127.88	122.80
3	A3	2557	C	N1-C2-O2	7.17	123.20	118.90
3	A3	2235	C	N3-C2-O2	-7.17	116.88	121.90
3	A3	3134	C	C6-N1-C2	-7.17	117.43	120.30
73	S6	88	PHE	C-N-CA	7.14	139.56	121.70
3	A3	3009	C	C2-N1-C1'	7.11	126.62	118.80
87	24	30	G	N3-C4-C5	-7.10	125.05	128.60
86	A6	715	U	N1-C2-O2	7.09	127.76	122.80
86	A6	710	C	N1-C2-O2	7.09	123.15	118.90
87	FE	30	G	N3-C4-C5	-7.08	125.06	128.60
82	b6	182	LEU	CA-CB-CG	7.06	131.53	115.30
83	c6	6	LEU	CA-CB-CG	7.02	131.45	115.30
3	A3	2522	U	C6-N1-C1'	-7.02	111.38	121.20
3	A3	1707	C	N1-C2-O2	6.98	123.09	118.90
3	A3	3228	U	C2-N1-C1'	6.97	126.07	117.70
3	A3	2182	G	P-O3'-C3'	6.97	128.06	119.70
3	A3	1716	U	N3-C2-O2	-6.96	117.33	122.20
3	A3	3201	A	P-O3'-C3'	6.95	128.04	119.70
76	V6	77	ASP	CB-CG-OD1	6.94	124.54	118.30
86	A6	769	C	N3-C2-O2	-6.94	117.04	121.90
61	G6	150	LEU	CA-CB-CG	6.92	131.21	115.30
3	A3	3170	C	C2-N1-C1'	6.91	126.41	118.80
3	A3	3170	C	N1-C2-O2	6.91	123.05	118.90
3	A3	1701	U	C2-N1-C1'	6.90	125.97	117.70
3	A3	1806	U	P-O3'-C3'	6.89	127.97	119.70
3	A3	2061	C	C2-N1-C1'	6.88	126.36	118.80
22	V3	102	MET	CA-CB-CG	6.86	124.97	113.30
3	A3	2484	C	C2-N1-C1'	6.85	126.34	118.80
86	A6	710	C	C6-N1-C1'	-6.85	112.58	120.80
3	A3	3134	C	C2-N1-C1'	6.83	126.31	118.80
3	A3	1901	C	N3-C2-O2	-6.80	117.14	121.90
3	A3	1809	U	N1-C2-O2	6.77	127.54	122.80
81	a6	65	LEU	CA-CB-CG	6.75	130.82	115.30
69	O6	108	CYS	CA-CB-SG	6.74	126.13	114.00
3	A3	3009	C	N3-C2-O2	-6.73	117.19	121.90
3	A3	3204	C	C6-N1-C1'	-6.73	112.73	120.80
3	A3	1902	C	C6-N1-C1'	-6.71	112.75	120.80
33	63	229	ASP	CB-CG-OD1	6.70	124.33	118.30
3	A3	2771	C	N1-C2-O2	6.70	122.92	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	1837	C	C6-N1-C1'	-6.69	112.77	120.80
4	B3	1649	C	N1-C2-O2	6.68	122.91	118.90
3	A3	2324	U	N1-C2-O2	6.68	127.47	122.80
86	A6	1155	C	N1-C2-O2	6.67	122.90	118.90
3	A3	3212	C	N3-C2-O2	-6.66	117.24	121.90
3	A3	2061	C	N3-C2-O2	-6.64	117.25	121.90
86	A6	1499	C	C6-N1-C2	-6.64	117.64	120.30
86	A6	936	C	C2-N1-C1'	6.63	126.09	118.80
3	A3	2096	U	N1-C2-O2	6.62	127.43	122.80
3	A3	2493	C	C6-N1-C1'	-6.61	112.87	120.80
1	r1	382	ASP	CB-CG-OD1	6.60	124.24	118.30
3	A3	1828	A	C2-N3-C4	-6.60	107.30	110.60
89	n	92	TYR	CD1-CG-CD2	6.60	125.16	117.90
67	M6	99	LEU	CA-CB-CG	6.59	130.47	115.30
3	A3	2898	U	N3-C2-O2	-6.59	117.59	122.20
3	A3	1701	U	N1-C2-O2	6.59	127.41	122.80
86	A6	1193	U	OP1-P-O3'	6.58	119.67	105.20
86	A6	936	C	C6-N1-C2	-6.58	117.67	120.30
40	e3	279	LEU	CA-CB-CG	6.57	130.42	115.30
3	A3	1807	U	P-O3'-C3'	6.55	127.56	119.70
3	A3	2079	C	C6-N1-C2	-6.55	117.68	120.30
86	A6	857	C	C6-N1-C2	-6.55	117.68	120.30
3	A3	2780	C	C6-N1-C2	-6.54	117.68	120.30
86	A6	1025	U	P-O3'-C3'	6.54	127.55	119.70
3	A3	1693	C	C2-N1-C1'	6.51	125.97	118.80
38	c3	210	ARG	NE-CZ-NH1	6.51	123.55	120.30
87	24	33	C	N1-C2-O2	6.50	122.80	118.90
1	r1	650	MET	CA-CB-CG	6.49	124.34	113.30
3	A3	2871	U	C5-C6-N1	6.49	125.95	122.70
3	A3	3212	C	C6-N1-C1'	-6.49	113.02	120.80
86	A6	1335	A	P-O3'-C3'	6.47	127.47	119.70
87	FE	33	C	N1-C2-O2	6.46	122.78	118.90
3	A3	2295	C	N3-C2-O2	-6.45	117.39	121.90
86	A6	1541	C	N3-C2-O2	-6.44	117.39	121.90
3	A3	1693	C	N1-C2-O2	6.40	122.74	118.90
81	a6	173	MET	CB-CG-SD	6.39	131.57	112.40
86	A6	712	C	C6-N1-C2	-6.39	117.75	120.30
3	A3	3009	C	N1-C2-O2	6.38	122.73	118.90
3	A3	2530	A	P-O3'-C3'	6.38	127.35	119.70
7	F3	277	ASP	CB-CG-OD1	6.38	124.04	118.30
86	A6	1127	C	N1-C2-O2	6.37	122.72	118.90
86	A6	1250	U	OP2-P-O3'	6.37	119.22	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	1689	C	N1-C2-O2	6.36	122.71	118.90
3	A3	2759	U	N1-C2-O2	6.34	127.24	122.80
5	D3	172	MET	CG-SD-CE	6.33	110.33	100.20
3	A3	1875	C	O5'-P-OP1	-6.32	100.01	105.70
13	M3	225	ASP	CB-CG-OD2	6.32	123.99	118.30
3	A3	1835	A	O4'-C1'-N9	6.32	113.26	108.20
86	A6	857	C	C5-C6-N1	6.30	124.15	121.00
6	E3	310	LEU	CA-CB-CG	6.29	129.78	115.30
87	24	11	C	N1-C2-O2	6.29	122.67	118.90
3	A3	2064	A	N1-C6-N6	-6.29	114.83	118.60
32	53	381	LEU	CA-CB-CG	6.29	129.76	115.30
3	A3	1901	C	C6-N1-C1'	-6.28	113.27	120.80
67	M6	72	ARG	NE-CZ-NH1	6.26	123.43	120.30
8	D	199	VAL	CG1-CB-CG2	-6.26	100.88	110.90
3	A3	2206	C	C6-N1-C2	-6.25	117.80	120.30
88	A	129	ARG	NE-CZ-NH2	6.25	123.42	120.30
3	A3	1714	C	C2-N1-C1'	6.25	125.67	118.80
3	A3	2523	C	C2-N1-C1'	6.24	125.66	118.80
55	A5	28	PRO	N-CA-CB	6.24	110.78	103.30
3	A3	3228	U	N1-C2-O2	6.23	127.16	122.80
86	A6	715	U	N3-C2-O2	-6.23	117.84	122.20
3	A3	2417	C	N1-C2-O2	6.22	122.63	118.90
86	A6	1288	U	N3-C2-O2	-6.22	117.85	122.20
87	FE	11	C	N1-C2-O2	6.21	122.63	118.90
3	A3	3173	G	C2-N3-C4	-6.18	108.81	111.90
26	Z3	76	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	r1	420	LEU	CB-CG-CD1	-6.16	100.54	111.00
3	A3	3169	C	C2-N1-C1'	6.15	125.56	118.80
86	A6	1193	U	P-O3'-C3'	6.14	127.06	119.70
3	A3	2175	C	C6-N1-C2	-6.13	117.85	120.30
3	A3	3157	C	C6-N1-C1'	-6.13	113.44	120.80
3	A3	3128	A	C8-N9-C4	6.13	108.25	105.80
3	A3	2784	A	P-O3'-C3'	6.12	127.05	119.70
85	e6	496	LEU	CA-CB-CG	6.12	129.37	115.30
3	A3	3077	C	C6-N1-C2	-6.11	117.86	120.30
86	A6	1297	C	N1-C2-O2	6.11	122.56	118.90
15	O3	74	ARG	NE-CZ-NH1	6.10	123.35	120.30
3	A3	2324	U	N3-C2-O2	-6.10	117.93	122.20
3	A3	2066	C	C6-N1-C2	-6.10	117.86	120.30
3	A3	2758	G	O5'-P-OP1	-6.10	100.21	105.70
3	A3	2780	C	C5-C6-N1	6.09	124.04	121.00
3	A3	1984	A	C4-C5-N7	6.08	113.74	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	1701	U	N3-C2-O2	-6.08	117.94	122.20
3	A3	2759	U	N3-C2-O2	-6.08	117.95	122.20
86	A6	1353	U	C5-C6-N1	6.07	125.74	122.70
3	A3	2852	C	N1-C2-O2	6.06	122.54	118.90
86	A6	1070	C	C5-C6-N1	6.06	124.03	121.00
86	A6	1433	C	P-O3'-C3'	6.05	126.96	119.70
3	A3	2559	U	P-O3'-C3'	6.04	126.95	119.70
87	FE	42	C	C6-N1-C2	-6.04	117.89	120.30
19	S3	144	LEU	CA-CB-CG	6.04	129.19	115.30
39	d3	230	ARG	C-N-CA	6.04	136.79	121.70
87	FE	33	C	C2-N1-C1'	6.04	125.44	118.80
1	r1	216	ASP	CB-CG-OD1	6.03	123.73	118.30
87	24	33	C	C2-N1-C1'	6.03	125.43	118.80
3	A3	2569	C	N1-C2-O2	6.03	122.52	118.90
3	A3	1715	C	N1-C2-O2	6.02	122.51	118.90
3	A3	1732	C	C5-C6-N1	6.01	124.00	121.00
53	s3	161	ARG	NE-CZ-NH1	6.01	123.31	120.30
60	F6	209	LEU	CA-CB-CG	6.01	129.12	115.30
86	A6	721	G	P-O3'-C3'	6.01	126.91	119.70
3	A3	2386	C	N1-C2-O2	6.01	122.50	118.90
3	A3	1689	C	C2-N1-C1'	6.00	125.41	118.80
3	A3	2067	C	C6-N1-C2	-6.00	117.90	120.30
3	A3	2523	C	N1-C2-O2	6.00	122.50	118.90
3	A3	2999	C	C6-N1-C2	-6.00	117.90	120.30
86	A6	1181	C	C6-N1-C2	-5.99	117.90	120.30
87	24	42	C	C6-N1-C2	-5.99	117.90	120.30
86	A6	797	C	C2-N1-C1'	5.99	125.39	118.80
86	A6	1156	A	C4-N9-C1'	5.98	137.06	126.30
1	r1	310	LEU	CB-CG-CD2	-5.98	100.84	111.00
3	A3	2066	C	C6-N1-C1'	-5.96	113.64	120.80
86	A6	1170	A	P-O3'-C3'	5.96	126.86	119.70
58	D6	410	ASP	CB-CG-OD1	5.96	123.67	118.30
3	A3	1716	U	N1-C2-O2	5.95	126.96	122.80
23	W3	105	VAL	CG1-CB-CG2	-5.95	101.38	110.90
81	a6	43	ARG	NE-CZ-NH1	-5.93	117.33	120.30
86	A6	1541	C	P-O3'-C3'	5.93	126.82	119.70
3	A3	2243	A	P-O3'-C3'	5.93	126.81	119.70
3	A3	1993	A	C8-N9-C4	-5.93	103.43	105.80
3	A3	2898	U	N1-C2-O2	5.92	126.95	122.80
3	A3	1809	U	N3-C2-O2	-5.92	118.06	122.20
86	A6	1419	G	P-O3'-C3'	5.92	126.81	119.70
14	N3	237	HIS	C-N-CA	5.92	136.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	1806	U	OP2-P-O3'	5.92	118.22	105.20
1	r1	690	ASP	CB-CG-OD1	5.91	123.62	118.30
86	A6	809	C	C6-N1-C1'	-5.91	113.71	120.80
3	A3	2441	C	C6-N1-C2	-5.91	117.94	120.30
3	A3	1902	C	C6-N1-C2	-5.90	117.94	120.30
3	A3	2557	C	C2-N1-C1'	5.89	125.28	118.80
86	A6	1155	C	N3-C2-O2	-5.89	117.78	121.90
3	A3	2209	G	OP1-P-O3'	5.89	118.16	105.20
82	b6	319	LEU	CA-CB-CG	5.88	128.82	115.30
3	A3	1699	C	C6-N1-C1'	-5.87	113.75	120.80
86	A6	678	U	N3-C2-O2	-5.87	118.09	122.20
8	H3	64	LEU	CA-CB-CG	5.86	128.79	115.30
86	A6	1093	U	N3-C2-O2	-5.86	118.10	122.20
3	A3	2245	A	P-O3'-C3'	5.85	126.72	119.70
3	A3	2499	U	C2-N1-C1'	5.84	124.71	117.70
86	A6	951	U	N1-C2-O2	5.84	126.89	122.80
86	A6	769	C	C6-N1-C1'	-5.83	113.80	120.80
3	A3	3169	C	N3-C2-O2	-5.83	117.82	121.90
3	A3	2174	G	N3-C4-N9	5.83	129.50	126.00
4	B3	1649	C	N3-C2-O2	-5.83	117.82	121.90
68	N6	65	LEU	CA-CB-CG	5.82	128.69	115.30
13	M3	46	GLY	C-N-CA	5.82	136.25	121.70
3	A3	1809	U	P-O3'-C3'	5.82	126.68	119.70
3	A3	1725	C	N1-C2-O2	5.81	122.39	118.90
3	A3	2096	U	N3-C2-O2	-5.81	118.13	122.20
86	A6	711	C	N1-C2-O2	5.81	122.39	118.90
3	A3	1951	C	C6-N1-C2	-5.81	117.98	120.30
34	73	46	ASP	CB-CG-OD2	5.79	123.52	118.30
3	A3	1993	A	N3-C4-C5	-5.79	122.75	126.80
3	A3	3206	C	C2-N1-C1'	5.79	125.17	118.80
86	A6	926	C	C5-C6-N1	5.79	123.89	121.00
60	F6	160	PRO	N-CA-C	5.78	127.13	112.10
78	X6	383	LEU	CA-CB-CG	5.78	128.58	115.30
86	A6	1193	U	N3-C2-O2	-5.77	118.16	122.20
3	A3	2274	A	O4'-C1'-N9	5.77	112.81	108.20
3	A3	3056	C	C6-N1-C2	-5.77	117.99	120.30
3	A3	1823	A	P-O3'-C3'	5.76	126.61	119.70
3	A3	1993	A	C4-N9-C1'	5.76	136.66	126.30
33	63	335	LEU	CA-CB-CG	5.75	128.53	115.30
86	A6	702	C	C6-N1-C2	-5.75	118.00	120.30
3	A3	1707	C	N3-C2-O2	-5.75	117.87	121.90
87	FE	30	G	N9-C4-C5	5.75	107.70	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	2832	A	C4-N9-C1'	5.75	136.64	126.30
87	24	30	G	N9-C4-C5	5.75	107.70	105.40
86	A6	1499	C	C5-C6-N1	5.74	123.87	121.00
3	A3	3093	C	C6-N1-C2	-5.74	118.00	120.30
86	A6	714	U	N1-C2-O2	5.74	126.82	122.80
3	A3	1808	A	OP1-P-O3'	5.73	117.81	105.20
3	A3	1828	A	N3-C4-C5	5.73	130.81	126.80
3	A3	2280	C	N1-C2-O2	5.73	122.34	118.90
8	D	194	PHE	CA-CB-CG	5.73	127.64	113.90
3	A3	2445	U	N1-C2-O2	5.72	126.81	122.80
82	b6	320	LEU	CA-CB-CG	5.72	128.46	115.30
3	A3	2173	G	O5'-P-OP1	-5.72	100.56	105.70
3	A3	2379	C	N1-C2-O2	5.71	122.33	118.90
3	A3	3108	U	C5-C6-N1	5.71	125.56	122.70
3	A3	2599	U	C2-N1-C1'	5.70	124.54	117.70
3	A3	3212	C	C6-N1-C2	-5.70	118.02	120.30
30	33	173	VAL	CG1-CB-CG2	-5.69	101.79	110.90
87	FE	40	U	C2-N1-C1'	5.69	124.53	117.70
61	G6	373	ASP	CB-CG-OD1	-5.69	113.18	118.30
87	24	31	C	C6-N1-C1'	5.69	127.62	120.80
3	A3	3228	U	N3-C2-O2	-5.68	118.22	122.20
87	24	40	U	C2-N1-C1'	5.68	124.52	117.70
3	A3	3093	C	C5-C6-N1	5.68	123.84	121.00
86	A6	797	C	N1-C2-O2	5.68	122.31	118.90
86	A6	809	C	C6-N1-C2	-5.68	118.03	120.30
86	A6	1250	U	P-O3'-C3'	5.68	126.51	119.70
3	A3	2280	C	C6-N1-C2	-5.67	118.03	120.30
77	W6	130	ASP	CB-CG-OD1	5.67	123.40	118.30
3	A3	2347	C	C6-N1-C2	-5.67	118.03	120.30
86	A6	1193	U	C6-N1-C1'	-5.66	113.28	121.20
87	FE	31	C	C6-N1-C1'	5.66	127.59	120.80
3	A3	2235	C	C6-N1-C2	-5.65	118.04	120.30
86	A6	791	C	N1-C2-O2	5.65	122.29	118.90
86	A6	1282	C	N1-C2-O2	5.65	122.29	118.90
85	e6	147	PRO	N-CA-CB	5.65	110.08	103.30
3	A3	2557	C	N3-C2-O2	-5.65	117.95	121.90
86	A6	1536	C	N1-C2-O2	5.64	122.29	118.90
3	A3	1904	C	C6-N1-C2	-5.64	118.05	120.30
3	A3	2171	U	C6-N1-C1'	-5.64	113.31	121.20
86	A6	1266	C	N3-C2-O2	-5.64	117.95	121.90
86	A6	1541	C	C5-C6-N1	5.63	123.81	121.00
3	A3	2024	C	N1-C2-O2	5.62	122.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	2832	A	N7-C8-N9	5.61	116.60	113.80
3	A3	2780	C	C6-N1-C1'	-5.60	114.08	120.80
87	24	30	G	P-O3'-C3'	5.60	126.42	119.70
87	FE	30	G	P-O3'-C3'	5.59	126.41	119.70
3	A3	3077	C	C5-C6-N1	5.59	123.80	121.00
3	A3	2235	C	C6-N1-C1'	-5.59	114.09	120.80
68	N6	70	PRO	CA-CB-CG	-5.58	93.39	104.00
3	A3	2569	C	N3-C2-O2	-5.58	117.99	121.90
58	D6	345	LEU	CA-CB-CG	5.58	128.13	115.30
86	A6	1436	U	N1-C2-O2	5.58	126.70	122.80
3	A3	2096	U	C6-N1-C1'	-5.58	113.39	121.20
3	A3	2489	C	C6-N1-C2	-5.58	118.07	120.30
3	A3	3123	G	OP2-P-O3'	5.58	117.47	105.20
3	A3	2282	C	N1-C2-O2	5.57	122.24	118.90
3	A3	1707	C	C2-N1-C1'	5.57	124.92	118.80
3	A3	2757	A	OP1-P-O3'	5.57	117.45	105.20
86	A6	801	C	N1-C2-O2	5.56	122.24	118.90
86	A6	951	U	N3-C2-O2	-5.56	118.31	122.20
16	P3	74	ARG	NE-CZ-NH2	5.55	123.08	120.30
63	I6	186	CYS	C-N-CA	-5.55	107.83	121.70
3	A3	1984	A	C4-N9-C1'	5.55	136.28	126.30
3	A3	2653	C	C5-C6-N1	5.55	123.77	121.00
3	A3	2005	C	C6-N1-C2	-5.54	118.08	120.30
3	A3	3102	U	N3-C2-O2	-5.53	118.33	122.20
3	A3	2067	C	C5-C6-N1	5.53	123.76	121.00
3	A3	2374	A	P-O3'-C3'	5.52	126.33	119.70
13	M3	154	ILE	CG1-CB-CG2	-5.52	99.26	111.40
86	A6	836	U	N1-C2-O2	5.52	126.66	122.80
86	A6	1213	C	C6-N1-C2	-5.52	118.09	120.30
86	A6	1051	A	C2-N3-C4	5.51	113.36	110.60
86	A6	1288	U	N1-C2-O2	5.51	126.66	122.80
3	A3	2096	U	O4'-C1'-N1	5.51	112.61	108.20
3	A3	2530	A	OP2-P-O3'	5.51	117.32	105.20
3	A3	2484	C	N3-C2-O2	-5.50	118.05	121.90
3	A3	3170	C	N3-C2-O2	-5.50	118.05	121.90
86	A6	1451	G	N3-C4-N9	5.50	129.30	126.00
3	A3	2443	C	N3-C2-O2	-5.49	118.06	121.90
3	A3	2522	U	C5-C6-N1	5.49	125.44	122.70
56	B6	251	ARG	NE-CZ-NH2	-5.48	117.56	120.30
86	A6	1472	U	N3-C2-O2	-5.48	118.36	122.20
40	e3	173	LEU	CA-CB-CG	5.48	127.90	115.30
86	A6	1127	C	N3-C2-O2	-5.48	118.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	2379	C	C2-N1-C1'	5.47	124.82	118.80
4	B3	1648	U	N1-C2-O2	5.47	126.63	122.80
86	A6	801	C	N3-C2-O2	-5.47	118.07	121.90
3	A3	2445	U	N3-C2-O2	-5.47	118.37	122.20
1	r1	317	LEU	CA-CB-CG	5.46	127.87	115.30
3	A3	1823	A	N7-C8-N9	5.46	116.53	113.80
86	A6	801	C	C6-N1-C2	-5.46	118.11	120.30
85	e6	500	LEU	CA-CB-CG	5.45	127.83	115.30
3	A3	2079	C	C6-N1-C1'	-5.45	114.26	120.80
3	A3	2135	A	C2-N3-C4	5.45	113.32	110.60
44	i3	80	LEU	CB-CG-CD1	5.45	120.26	111.00
86	A6	1433	C	OP2-P-O3'	5.44	117.18	105.20
86	A6	921	C	C6-N1-C2	-5.44	118.12	120.30
86	A6	1196	C	N1-C2-O2	5.44	122.16	118.90
3	A3	2080	U	C6-N1-C1'	-5.43	113.59	121.20
76	V6	181	LEU	CA-CB-CG	-5.43	102.81	115.30
86	A6	1156	A	N3-C4-N9	5.43	131.74	127.40
86	A6	715	U	C5-C6-N1	5.43	125.42	122.70
3	A3	2684	C	C2-N1-C1'	5.42	124.77	118.80
3	A3	1780	U	C5-C4-O4	-5.42	122.65	125.90
87	24	31	C	C2-N1-C1'	-5.42	112.84	118.80
3	A3	2771	C	C5-C6-N1	5.42	123.71	121.00
3	A3	2771	C	C6-N1-C2	-5.42	118.13	120.30
3	A3	2523	C	C6-N1-C2	-5.41	118.14	120.30
3	A3	2434	A	O4'-C1'-N9	5.41	112.53	108.20
86	A6	1266	C	N1-C2-O2	5.40	122.14	118.90
3	A3	2569	C	C2-N1-C1'	5.40	124.74	118.80
3	A3	2112	A	C5-C6-N6	-5.40	119.38	123.70
86	A6	714	U	C6-N1-C1'	-5.39	113.65	121.20
87	FE	31	C	C2-N1-C1'	-5.39	112.87	118.80
86	A6	1156	A	C8-N9-C1'	-5.39	118.00	127.70
3	A3	2284	C	N1-C2-O2	5.39	122.13	118.90
45	j3	79	LEU	CA-CB-CG	5.38	127.69	115.30
86	A6	1447	U	N3-C2-O2	-5.38	118.43	122.20
3	A3	2789	C	N1-C2-O2	5.38	122.13	118.90
86	A6	1472	U	N1-C2-O2	5.38	126.56	122.80
43	h3	64	GLU	C-N-CA	5.38	135.14	121.70
86	A6	1472	U	C5-C6-N1	5.38	125.39	122.70
3	A3	2655	G	O4'-C1'-N9	-5.37	103.90	108.20
86	A6	1345	C	C6-N1-C2	-5.37	118.15	120.30
86	A6	926	C	C6-N1-C2	-5.37	118.15	120.30
3	A3	2784	A	OP1-P-O3'	5.37	117.01	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	f3	50	THR	C-N-CA	5.37	135.12	121.70
4	B3	1607	U	P-O3'-C3'	5.37	126.14	119.70
86	A6	1297	C	N3-C2-O2	-5.36	118.15	121.90
3	A3	2441	C	N1-C2-O2	5.36	122.12	118.90
3	A3	1813	C	C6-N1-C2	-5.36	118.16	120.30
3	A3	2186	C	P-O3'-C3'	5.36	126.13	119.70
3	A3	2282	C	C2-N1-C1'	5.35	124.68	118.80
3	A3	2865	C	C2-N1-C1'	5.35	124.68	118.80
3	A3	2112	A	C5-C6-N1	5.35	120.37	117.70
3	A3	2507	A	P-O3'-C3'	5.35	126.12	119.70
81	a6	118	LEU	CA-CB-CG	5.35	127.60	115.30
87	24	30	G	C5-N7-C8	-5.33	101.63	104.30
40	e3	83	LEU	CA-CB-CG	5.33	127.55	115.30
79	Y6	358	LEU	CA-CB-CG	5.33	127.55	115.30
43	h3	63	PRO	C-N-CA	5.33	135.02	121.70
3	A3	2628	U	P-O3'-C3'	5.33	126.09	119.70
73	S6	90	PRO	CA-N-CD	-5.32	104.05	111.50
10	J3	71	LEU	CA-CB-CG	5.32	127.54	115.30
87	FE	30	G	C5-N7-C8	-5.32	101.64	104.30
3	A3	3127	G	C8-N9-C4	-5.32	104.27	106.40
68	N6	53	ASP	CB-CG-OD1	5.32	123.08	118.30
3	A3	3102	U	N1-C2-O2	5.31	126.52	122.80
16	P3	84	ARG	NE-CZ-NH1	5.31	122.96	120.30
33	63	336	ASP	CB-CG-OD1	5.31	123.08	118.30
86	A6	1265	C	N1-C2-O2	5.31	122.09	118.90
3	A3	2900	C	C5-C6-N1	5.30	123.65	121.00
3	A3	2906	C	C5-C6-N1	5.30	123.65	121.00
3	A3	2523	C	N3-C2-O2	-5.29	118.19	121.90
6	E3	246	GLY	N-CA-C	5.29	126.33	113.10
65	K6	81	ASP	CB-CG-OD2	5.29	123.06	118.30
3	A3	3041	U	OP1-P-O3'	5.29	116.83	105.20
35	93	86	LEU	CA-CB-CG	5.29	127.46	115.30
89	n	92	TYR	CB-CG-CD1	-5.29	117.83	121.00
3	A3	2295	C	N1-C2-O2	5.28	122.07	118.90
3	A3	3201	A	C4-N9-C1'	5.28	135.81	126.30
3	A3	1699	C	C5-C6-N1	5.28	123.64	121.00
37	b3	117	LYS	CA-CB-CG	5.28	125.00	113.40
86	A6	1373	U	C5-C6-N1	5.27	125.34	122.70
14	N3	87	PHE	CB-CG-CD2	-5.27	117.11	120.80
3	A3	3204	C	C6-N1-C2	-5.27	118.19	120.30
78	X6	344	LEU	CA-CB-CG	5.27	127.42	115.30
3	A3	2445	U	C2-N1-C1'	5.26	124.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X3	222	ASP	CB-CG-OD1	5.26	123.04	118.30
88	A	183	PRO	C-N-CA	5.26	134.86	121.70
19	S3	172	MET	CG-SD-CE	-5.26	91.78	100.20
3	A3	1984	A	C6-C5-N7	-5.26	128.62	132.30
87	24	33	C	N3-C2-O2	-5.26	118.22	121.90
3	A3	1890	C	C6-N1-C2	-5.26	118.20	120.30
35	93	127	LEU	CA-CB-CG	5.26	127.39	115.30
86	A6	1318	C	C6-N1-C2	-5.25	118.20	120.30
3	A3	2280	C	N3-C2-O2	-5.25	118.23	121.90
86	A6	1207	C	N1-C2-O2	5.25	122.05	118.90
86	A6	1093	U	N1-C2-O2	5.25	126.47	122.80
86	A6	1025	U	OP2-P-O3'	5.25	116.74	105.20
69	O6	213	LEU	CA-CB-CG	5.24	127.36	115.30
86	A6	1127	C	C2-N1-C1'	5.24	124.56	118.80
19	S3	182	LYS	CD-CE-NZ	-5.24	99.66	111.70
4	B3	1648	U	C5-C6-N1	5.23	125.32	122.70
3	A3	1828	A	N3-C4-N9	-5.23	123.22	127.40
3	A3	2326	C	C6-N1-C2	-5.23	118.21	120.30
87	FE	33	C	N3-C2-O2	-5.22	118.25	121.90
69	O6	96	ARG	NE-CZ-NH2	-5.21	117.69	120.30
3	A3	2157	U	N1-C2-O2	5.21	126.45	122.80
3	A3	2171	U	O4'-C1'-N1	5.21	112.37	108.20
3	A3	2187	C	N1-C2-O2	5.21	122.03	118.90
87	FE	42	C	N1-C2-O2	5.21	122.03	118.90
3	A3	3228	U	C6-N1-C1'	-5.21	113.91	121.20
86	A6	901	C	C5-C6-N1	5.20	123.60	121.00
86	A6	809	C	O4'-C1'-N1	5.20	112.36	108.20
3	A3	1984	A	C5-N7-C8	-5.19	101.30	103.90
3	A3	2898	U	O4'-C1'-N1	5.19	112.35	108.20
1	r1	62	LEU	CA-CB-CG	5.19	127.23	115.30
86	A6	1318	C	C5-C6-N1	5.19	123.59	121.00
86	A6	1156	A	C2-N3-C4	5.18	113.19	110.60
3	A3	1946	C	C6-N1-C2	-5.18	118.23	120.30
3	A3	3172	C	N1-C2-O2	5.18	122.01	118.90
3	A3	2511	C	C2-N1-C1'	5.18	124.50	118.80
82	b6	138	ASP	C-N-CA	5.17	134.62	121.70
1	r1	207	LEU	CB-CA-C	5.17	120.01	110.20
87	24	42	C	N1-C2-O2	5.16	122.00	118.90
86	A6	1526	U	N1-C2-O2	5.16	126.41	122.80
5	D3	235	GLN	CA-CB-CG	5.15	124.72	113.40
86	A6	957	U	C2-N1-C1'	5.14	123.87	117.70
76	V6	154	LYS	C-N-CA	5.14	134.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A3	3201	A	C2-N3-C4	5.14	113.17	110.60
86	A6	969	C	N1-C2-O2	5.14	121.98	118.90
3	A3	1837	C	C6-N1-C2	-5.13	118.25	120.30
4	B3	1663	C	N1-C2-O2	5.13	121.98	118.90
87	FE	40	U	N1-C2-O2	5.13	126.39	122.80
3	A3	1880	C	C6-N1-C2	-5.13	118.25	120.30
3	A3	2186	C	N1-C2-O2	5.13	121.98	118.90
86	A6	709	C	N1-C2-O2	5.12	121.97	118.90
3	A3	2583	C	C5-C6-N1	5.12	123.56	121.00
3	A3	3041	U	P-O3'-C3'	5.12	125.84	119.70
86	A6	1373	U	C6-N1-C2	-5.11	117.93	121.00
3	A3	2282	C	N3-C2-O2	-5.11	118.32	121.90
62	H6	180	LEU	CA-CB-CG	5.11	127.06	115.30
3	A3	2708	C	N1-C2-O2	5.11	121.96	118.90
3	A3	2771	C	N3-C2-O2	-5.11	118.32	121.90
3	A3	1786	C	C6-N1-C2	-5.11	118.26	120.30
87	24	45	A	C2-N3-C4	5.11	113.15	110.60
3	A3	1725	C	N3-C2-O2	-5.10	118.33	121.90
72	R6	208	ILE	CG1-CB-CG2	-5.10	100.17	111.40
3	A3	2898	U	C6-N1-C1'	-5.10	114.06	121.20
69	O6	162	LEU	CA-CB-CG	5.10	127.03	115.30
3	A3	1689	C	N3-C2-O2	-5.10	118.33	121.90
3	A3	1823	A	C8-N9-C4	-5.10	103.76	105.80
86	A6	1541	C	C2-N1-C1'	5.09	124.40	118.80
1	r1	470	ILE	CG1-CB-CG2	-5.09	100.19	111.40
3	A3	2684	C	N1-C2-O2	5.09	121.95	118.90
86	A6	1472	U	C2-N1-C1'	5.09	123.81	117.70
3	A3	3122	U	N3-C2-O2	-5.09	118.64	122.20
86	A6	675	U	N1-C2-O2	5.08	126.36	122.80
20	T3	161	ARG	N-CA-C	-5.08	97.28	111.00
22	V3	91	LEU	CA-CB-CG	5.08	126.99	115.30
3	A3	2852	C	N3-C2-O2	-5.08	118.35	121.90
86	A6	678	U	N1-C2-O2	5.08	126.35	122.80
3	A3	2386	C	C2-N1-C1'	5.07	124.38	118.80
3	A3	3123	G	P-O3'-C3'	5.07	125.79	119.70
1	r1	365	PHE	CA-C-N	5.07	126.34	116.20
87	24	40	U	N1-C2-O2	5.07	126.35	122.80
3	A3	2583	C	C6-N1-C2	-5.07	118.27	120.30
39	d3	231	LEU	CA-CB-CG	5.07	126.96	115.30
86	A6	1447	U	C2-N1-C1'	5.07	123.78	117.70
3	A3	3170	C	C6-N1-C2	-5.07	118.27	120.30
3	A3	1984	A	N9-C4-C5	-5.06	103.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	A6	1451	G	C4-N9-C1'	5.06	133.08	126.50
86	A6	1127	C	C6-N1-C2	-5.06	118.28	120.30
1	r1	567	LEU	CA-CB-CG	5.05	126.93	115.30
87	FE	45	A	C2-N3-C4	5.05	113.12	110.60
86	A6	887	U	O5'-P-OP1	5.05	116.76	110.70
81	a6	135	MET	CB-CG-SD	-5.05	97.25	112.40
81	a6	78	ARG	NE-CZ-NH1	-5.04	117.78	120.30
86	A6	1324	G	O4'-C1'-N9	5.04	112.23	108.20
88	A	180	PRO	C-N-CD	-5.04	109.52	120.60
1	r1	79	VAL	CG1-CB-CG2	-5.03	102.85	110.90
3	A3	2489	C	C5-C6-N1	5.03	123.52	121.00
3	A3	2824	C	C6-N1-C2	-5.03	118.29	120.30
13	M3	244	LEU	CA-CB-CG	5.03	126.87	115.30
3	A3	2372	U	C6-N1-C1'	-5.03	114.16	121.20
3	A3	3187	C	C6-N1-C2	-5.03	118.29	120.30
3	A3	1693	C	C5-C6-N1	5.03	123.51	121.00
3	A3	2357	C	N3-C2-O2	-5.03	118.38	121.90
87	24	33	C	C6-N1-C2	-5.02	118.29	120.30
61	G6	302	LEU	CA-CB-CG	5.02	126.85	115.30
28	13	20	MET	CB-CG-SD	5.02	127.45	112.40
76	V6	180	LEU	CA-CB-CG	5.02	126.84	115.30
86	A6	1502	C	N1-C2-O2	5.01	121.91	118.90
86	A6	806	C	C6-N1-C2	-5.01	118.30	120.30
3	A3	1984	A	C8-N9-C1'	-5.01	118.68	127.70
3	A3	3206	C	N1-C2-O2	5.01	121.91	118.90
1	r1	725	PRO	C-N-CA	5.01	134.22	121.70
6	E3	247	ASP	CB-CG-OD1	5.01	122.81	118.30
3	A3	3206	C	P-O3'-C3'	5.00	125.71	119.70
35	93	91	LEU	CA-CB-CG	5.00	126.81	115.30
3	A3	1993	A	N3-C4-N9	5.00	131.40	127.40
3	A3	2135	A	C4-N9-C1'	5.00	135.30	126.30
67	M6	65	LEU	CA-CB-CG	5.00	126.80	115.30
86	A6	715	U	C6-N1-C1'	-5.00	114.20	121.20

There are no chirality outliers.

All (125) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	03	151	ALA	Peptide
27	03	177	ARG	Peptide
28	13	25	GLY	Peptide
28	13	62	ILE	Peptide

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Mol	Chain	Res	Type	Group
32	53	223	ARG	Peptide
32	53	268	CYS	Peptide
32	53	269	ASN	Peptide
32	53	347	THR	Peptide
33	63	221	LEU	Peptide
33	63	49	GLU	Peptide
35	93	45	THR	Peptide
88	A	181	PRO	Peptide
88	A	182	ILE	Peptide
88	A	184	ASN	Peptide
88	A	185	TYR	Peptide
88	A	201	GLN	Peptide
88	A	57	ASP	Peptide
56	B6	164	GLU	Peptide
8	D	193	PHE	Peptide
8	D	205	THR	Peptide
5	D3	206	TYR	Peptide
58	D6	284	ARG	Peptide
58	D6	286	GLU	Peptide
58	D6	422	TRP	Peptide
58	D6	425	LEU	Peptide
6	E3	126	ASP	Peptide
6	E3	169	GLY	Peptide
6	E3	244	ALA	Peptide
6	E3	250	ARG	Peptide
6	E3	85	TRP	Peptide
7	F3	129	PRO	Peptide
7	F3	140	SER	Peptide
60	F6	147	GLN	Peptide
60	F6	159	VAL	Peptide
60	F6	160	PRO	Mainchain
60	F6	161	ILE	Peptide
61	G6	103	ASP	Peptide
8	H3	63	PRO	Peptide
9	I3	102	VAL	Peptide
63	I6	144	VAL	Peptide
63	I6	94	ASN	Peptide
10	J3	44	VAL	Peptide
10	J3	45	SER	Peptide
64	J6	130	TYR	Peptide
11	K3	3	SER	Peptide
11	K3	5	SER	Peptide

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Mol	Chain	Res	Type	Group
13	M3	109	ARG	Peptide
13	M3	18	GLY	Peptide
13	M3	264	GLN	Peptide
13	M3	286	THR	Peptide
14	N3	237	HIS	Peptide
14	N3	78	GLU	Peptide
68	N6	109	PRO	Peptide
15	O3	104	TYR	Peptide
69	O6	53	ASP	Peptide
69	O6	55	PRO	Peptide
69	O6	98	ASN	Peptide
70	P6	139	ARG	Peptide
70	P6	64	LYS	Peptide
70	P6	65	CYS	Peptide
17	Q3	182	ARG	Peptide
18	R3	137	GLU	Peptide
72	R6	132	LEU	Peptide
72	R6	154	THR	Peptide
72	R6	291	ARG	Peptide
73	S6	107	GLN	Peptide
20	T3	160	GLY	Peptide
75	U6	128	GLU	Peptide
75	U6	62	HIS	Peptide
22	V3	100	LYS	Peptide
22	V3	170	TRP	Peptide
76	V6	155	GLU	Peptide
76	V6	44	GLU	Peptide
24	X3	51	LYS	Peptide
2	Y2	21	UNK	Peptide
2	Y2	22	UNK	Peptide
26	Z3	141	SER	Peptide
81	a6	21	LEU	Peptide
82	b6	228	VAL	Peptide
38	c3	63	LYS	Peptide
83	c6	38	ARG	Peptide
39	d3	191	PRO	Peptide
39	d3	230	ARG	Peptide
39	d3	231	LEU	Peptide
39	d3	268	PRO	Peptide
39	d3	271	PRO	Peptide
85	e6	64	THR	Peptide
85	e6	67	LYS	Peptide

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Mol	Chain	Res	Type	Group
41	f3	50	THR	Peptide
41	f3	84	THR	Peptide
41	f3	85	ASP	Peptide
41	f3	86	TYR	Peptide
42	g3	110	ILE	Peptide
43	h3	138	SER	Peptide
43	h3	65	ASP	Peptide
44	i3	57	TYR	Peptide
45	j3	25	GLY	Peptide
89	n	222	SER	Peptide
49	o3	42	GLU	Peptide
51	q3	78	SER	Peptide
1	r1	162	MET	Peptide
1	r1	169	PHE	Peptide
1	r1	207	LEU	Peptide
1	r1	247	THR	Peptide
1	r1	249	HIS	Peptide
1	r1	256	CYS	Peptide
1	r1	296	PHE	Peptide
1	r1	341	ILE	Peptide
1	r1	364	ARG	Peptide
1	r1	401	MET	Peptide
1	r1	402	HIS	Peptide
1	r1	441	MET	Peptide
1	r1	53	ALA	Peptide
1	r1	57	SER	Peptide
1	r1	597	GLY	Peptide
1	r1	678	GLN	Peptide
1	r1	681	VAL	Peptide
1	r1	723	CYS	Peptide
1	r1	724	LEU	Peptide
1	r1	726	SER	Peptide
1	r1	735	TYR	Peptide
1	r1	78	GLU	Peptide
1	r1	98	ARG	Peptide
53	s3	270	LYS	Peptide
53	s3	283	PHE	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	r1	694/751 (92%)	523 (75%)	159 (23%)	12 (2%)	9 42
5	D3	234/305 (77%)	216 (92%)	17 (7%)	1 (0%)	34 69
6	E3	296/348 (85%)	258 (87%)	38 (13%)	0	100 100
7	F3	248/311 (80%)	224 (90%)	24 (10%)	0	100 100
8	D	78/267 (29%)	60 (77%)	18 (23%)	0	100 100
8	H3	93/267 (35%)	84 (90%)	9 (10%)	0	100 100
9	I3	154/261 (59%)	145 (94%)	9 (6%)	0	100 100
10	J3	138/192 (72%)	124 (90%)	14 (10%)	0	100 100
11	K3	175/178 (98%)	153 (87%)	19 (11%)	3 (2%)	9 42
12	L3	113/145 (78%)	104 (92%)	9 (8%)	0	100 100
13	M3	285/296 (96%)	254 (89%)	30 (10%)	1 (0%)	34 69
14	N3	203/251 (81%)	189 (93%)	12 (6%)	2 (1%)	15 51
15	O3	150/175 (86%)	130 (87%)	19 (13%)	1 (1%)	22 59
16	P3	129/179 (72%)	118 (92%)	11 (8%)	0	100 100
17	Q3	217/292 (74%)	192 (88%)	25 (12%)	0	100 100
18	R3	138/149 (93%)	128 (93%)	10 (7%)	0	100 100
19	S3	154/205 (75%)	139 (90%)	15 (10%)	0	100 100
20	T3	164/212 (77%)	152 (93%)	12 (7%)	0	100 100
21	U3	109/153 (71%)	96 (88%)	13 (12%)	0	100 100
22	V3	183/216 (85%)	155 (85%)	26 (14%)	2 (1%)	14 50
23	W3	109/148 (74%)	103 (94%)	6 (6%)	0	100 100
24	X3	241/256 (94%)	220 (91%)	20 (8%)	1 (0%)	34 69
25	Y3	174/250 (70%)	161 (92%)	12 (7%)	1 (1%)	25 62
26	Z3	118/161 (73%)	108 (92%)	10 (8%)	0	100 100
27	03	106/188 (56%)	94 (89%)	11 (10%)	1 (1%)	17 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	13	50/65 (77%)	46 (92%)	3 (6%)	1 (2%)	7	39
29	23	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
30	33	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
31	43	34/103 (33%)	34 (100%)	0	0	100	100
32	53	368/423 (87%)	326 (89%)	40 (11%)	2 (0%)	29	66
33	63	313/380 (82%)	283 (90%)	30 (10%)	0	100	100
34	73	258/338 (76%)	233 (90%)	25 (10%)	0	100	100
35	93	105/137 (77%)	88 (84%)	17 (16%)	0	100	100
36	a3	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
37	b3	146/155 (94%)	132 (90%)	13 (9%)	1 (1%)	22	59
38	c3	271/332 (82%)	251 (93%)	20 (7%)	0	100	100
39	d3	156/306 (51%)	139 (89%)	15 (10%)	2 (1%)	12	47
40	e3	211/279 (76%)	193 (92%)	18 (8%)	0	100	100
41	f3	125/194 (64%)	103 (82%)	19 (15%)	3 (2%)	6	35
42	g3	127/166 (76%)	119 (94%)	8 (6%)	0	100	100
43	h3	96/158 (61%)	84 (88%)	11 (12%)	1 (1%)	15	51
44	i3	95/128 (74%)	87 (92%)	8 (8%)	0	100	100
45	j3	83/123 (68%)	78 (94%)	4 (5%)	1 (1%)	13	48
46	k3	82/112 (73%)	66 (80%)	16 (20%)	0	100	100
47	l3	21/138 (15%)	21 (100%)	0	0	100	100
48	m3	43/128 (34%)	36 (84%)	7 (16%)	0	100	100
49	o3	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
50	p3	119/206 (58%)	113 (95%)	6 (5%)	0	100	100
51	q3	126/222 (57%)	119 (94%)	5 (4%)	2 (2%)	9	43
52	r3	140/196 (71%)	125 (89%)	15 (11%)	0	100	100
53	s3	366/439 (83%)	340 (93%)	26 (7%)	0	100	100
55	A5	26/435 (6%)	17 (65%)	9 (35%)	0	100	100
56	B6	215/296 (73%)	200 (93%)	15 (7%)	0	100	100
57	C6	130/167 (78%)	122 (94%)	8 (6%)	0	100	100
58	D6	316/430 (74%)	272 (86%)	44 (14%)	0	100	100
59	E6	120/125 (96%)	113 (94%)	6 (5%)	1 (1%)	19	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	F6	197/242 (81%)	182 (92%)	14 (7%)	1 (0%)	29	66
61	G6	301/396 (76%)	276 (92%)	25 (8%)	0	100	100
62	H6	120/201 (60%)	103 (86%)	17 (14%)	0	100	100
63	I6	134/194 (69%)	122 (91%)	12 (9%)	0	100	100
64	J6	106/138 (77%)	93 (88%)	13 (12%)	0	100	100
65	K6	99/128 (77%)	88 (89%)	11 (11%)	0	100	100
66	L6	162/257 (63%)	151 (93%)	11 (7%)	0	100	100
67	M6	114/137 (83%)	100 (88%)	14 (12%)	0	100	100
68	N6	105/130 (81%)	93 (89%)	12 (11%)	0	100	100
69	O6	183/258 (71%)	159 (87%)	24 (13%)	0	100	100
70	P6	94/142 (66%)	82 (87%)	12 (13%)	0	100	100
71	Q6	84/87 (97%)	75 (89%)	9 (11%)	0	100	100
72	R6	240/360 (67%)	210 (88%)	30 (12%)	0	100	100
73	S6	124/190 (65%)	110 (89%)	14 (11%)	0	100	100
74	T6	160/173 (92%)	140 (88%)	19 (12%)	1 (1%)	25	62
75	U6	171/205 (83%)	159 (93%)	12 (7%)	0	100	100
76	V6	320/414 (77%)	287 (90%)	33 (10%)	0	100	100
77	W6	95/187 (51%)	81 (85%)	14 (15%)	0	100	100
78	X6	310/398 (78%)	264 (85%)	45 (14%)	1 (0%)	41	74
79	Y6	106/395 (27%)	96 (91%)	10 (9%)	0	100	100
80	Z6	85/106 (80%)	79 (93%)	6 (7%)	0	100	100
81	a6	197/218 (90%)	174 (88%)	23 (12%)	0	100	100
82	b6	252/323 (78%)	223 (88%)	29 (12%)	0	100	100
83	c6	114/118 (97%)	98 (86%)	15 (13%)	1 (1%)	17	54
84	d6	67/199 (34%)	62 (92%)	5 (8%)	0	100	100
85	e6	362/689 (52%)	328 (91%)	29 (8%)	5 (1%)	11	45
88	A	158/206 (77%)	139 (88%)	19 (12%)	0	100	100
89	n	216/286 (76%)	166 (77%)	50 (23%)	0	100	100
All	All	13828/19638 (70%)	12301 (89%)	1479 (11%)	48 (0%)	44	74

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	r1	365	PHE
1	r1	598	PRO
1	r1	623	GLU
1	r1	724	LEU
1	r1	725	PRO
22	V3	101	THR
39	d3	231	LEU
41	f3	51	LYS
85	e6	68	VAL
85	e6	147	PRO
1	r1	599	LEU
1	r1	682	GLU
11	K3	160	GLN
13	M3	265	ILE
22	V3	194	LEU
24	X3	52	ILE
32	53	270	ILE
51	q3	43	GLU
60	F6	161	ILE
1	r1	404	ASP
14	N3	238	LYS
27	03	178	ASP
28	13	63	ARG
41	f3	50	THR
41	f3	85	ASP
51	q3	42	PRO
78	X6	342	PRO
1	r1	679	ASP
5	D3	207	ILE
83	c6	60	GLU
1	r1	403	ALA
11	K3	4	PHE
45	j3	35	ALA
85	e6	146	GLU
85	e6	274	GLN
11	K3	159	THR
14	N3	237	HIS
43	h3	66	LEU
1	r1	79	VAL
32	53	349	GLY
85	e6	149	ILE
39	d3	164	VAL
74	T6	148	PRO

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Mol	Chain	Res	Type
1	r1	341	ILE
25	Y3	203	PRO
59	E6	15	ARG
15	O3	111	PRO
37	b3	117	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r1	592/630 (94%)	591 (100%)	1 (0%)	93	97
5	D3	190/245 (78%)	190 (100%)	0	100	100
6	E3	255/290 (88%)	255 (100%)	0	100	100
7	F3	217/262 (83%)	216 (100%)	1 (0%)	88	94
8	D	73/228 (32%)	73 (100%)	0	100	100
8	H3	86/228 (38%)	86 (100%)	0	100	100
9	I3	145/232 (62%)	145 (100%)	0	100	100
10	J3	113/150 (75%)	113 (100%)	0	100	100
11	K3	155/156 (99%)	154 (99%)	1 (1%)	86	93
12	L3	98/124 (79%)	98 (100%)	0	100	100
13	M3	245/249 (98%)	243 (99%)	2 (1%)	81	89
14	N3	172/211 (82%)	172 (100%)	0	100	100
15	O3	133/150 (89%)	133 (100%)	0	100	100
16	P3	115/154 (75%)	113 (98%)	2 (2%)	60	79
17	Q3	201/256 (78%)	201 (100%)	0	100	100
18	R3	118/126 (94%)	118 (100%)	0	100	100
19	S3	141/180 (78%)	140 (99%)	1 (1%)	84	91
20	T3	146/182 (80%)	146 (100%)	0	100	100
21	U3	99/135 (73%)	98 (99%)	1 (1%)	76	86
22	V3	169/191 (88%)	168 (99%)	1 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W3	91/119 (76%)	91 (100%)	0	100	100
24	X3	217/227 (96%)	216 (100%)	1 (0%)	88	94
25	Y3	159/223 (71%)	159 (100%)	0	100	100
26	Z3	111/147 (76%)	111 (100%)	0	100	100
27	03	97/164 (59%)	97 (100%)	0	100	100
28	13	49/60 (82%)	49 (100%)	0	100	100
29	23	40/72 (56%)	40 (100%)	0	100	100
30	33	88/166 (53%)	88 (100%)	0	100	100
31	43	35/89 (39%)	35 (100%)	0	100	100
32	53	337/368 (92%)	335 (99%)	2 (1%)	86	93
33	63	266/332 (80%)	265 (100%)	1 (0%)	91	95
34	73	242/303 (80%)	242 (100%)	0	100	100
35	93	91/112 (81%)	91 (100%)	0	100	100
36	a3	78/133 (59%)	78 (100%)	0	100	100
37	b3	130/135 (96%)	129 (99%)	1 (1%)	81	89
38	c3	241/288 (84%)	241 (100%)	0	100	100
39	d3	151/274 (55%)	151 (100%)	0	100	100
40	e3	188/236 (80%)	187 (100%)	1 (0%)	88	94
41	f3	117/173 (68%)	117 (100%)	0	100	100
42	g3	119/148 (80%)	119 (100%)	0	100	100
43	h3	95/148 (64%)	95 (100%)	0	100	100
44	i3	86/110 (78%)	86 (100%)	0	100	100
45	j3	68/97 (70%)	68 (100%)	0	100	100
46	k3	74/90 (82%)	74 (100%)	0	100	100
47	l3	23/116 (20%)	23 (100%)	0	100	100
48	m3	40/113 (35%)	39 (98%)	1 (2%)	47	70
49	o3	80/87 (92%)	80 (100%)	0	100	100
50	p3	117/181 (65%)	116 (99%)	1 (1%)	78	88
51	q3	110/178 (62%)	110 (100%)	0	100	100
52	r3	133/169 (79%)	133 (100%)	0	100	100
53	s3	326/381 (86%)	326 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	B6	191/249 (77%)	190 (100%)	1 (0%)	88	94
57	C6	115/143 (80%)	115 (100%)	0	100	100
58	D6	269/357 (75%)	269 (100%)	0	100	100
59	E6	104/107 (97%)	104 (100%)	0	100	100
60	F6	178/209 (85%)	178 (100%)	0	100	100
61	G6	265/342 (78%)	264 (100%)	1 (0%)	91	95
62	H6	112/180 (62%)	112 (100%)	0	100	100
63	I6	104/147 (71%)	104 (100%)	0	100	100
64	J6	93/118 (79%)	93 (100%)	0	100	100
65	K6	91/113 (80%)	91 (100%)	0	100	100
66	L6	152/226 (67%)	152 (100%)	0	100	100
67	M6	95/113 (84%)	95 (100%)	0	100	100
68	N6	93/115 (81%)	93 (100%)	0	100	100
69	O6	166/230 (72%)	165 (99%)	1 (1%)	86	93
70	P6	87/123 (71%)	87 (100%)	0	100	100
71	Q6	78/79 (99%)	78 (100%)	0	100	100
72	R6	224/318 (70%)	222 (99%)	2 (1%)	78	88
73	S6	109/164 (66%)	109 (100%)	0	100	100
74	T6	150/157 (96%)	149 (99%)	1 (1%)	84	91
75	U6	149/174 (86%)	149 (100%)	0	100	100
76	V6	295/364 (81%)	295 (100%)	0	100	100
77	W6	84/158 (53%)	84 (100%)	0	100	100
78	X6	275/351 (78%)	274 (100%)	1 (0%)	91	95
79	Y6	99/357 (28%)	99 (100%)	0	100	100
80	Z6	80/95 (84%)	80 (100%)	0	100	100
81	a6	176/190 (93%)	175 (99%)	1 (1%)	86	93
82	b6	237/291 (81%)	236 (100%)	1 (0%)	91	95
83	c6	99/101 (98%)	97 (98%)	2 (2%)	55	74
84	d6	63/166 (38%)	63 (100%)	0	100	100
85	e6	226/609 (37%)	226 (100%)	0	100	100
88	A	151/190 (80%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
89	n	194/254 (76%)	194 (100%)	0	100	100
All	All	12266/16608 (74%)	12237 (100%)	29 (0%)	93	97

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	r1	628	ARG
7	F3	125	ARG
11	K3	70	ASN
13	M3	44	ARG
13	M3	182	ARG
16	P3	54	ASN
16	P3	176	ARG
19	S3	118	ASN
21	U3	69	ARG
22	V3	208	ARG
24	X3	96	LYS
32	53	83	LYS
32	53	275	ASN
33	63	292	GLN
37	b3	123	ASN
40	e3	185	ARG
48	m3	72	ARG
50	p3	82	ARG
56	B6	113	HIS
61	G6	276	ARG
69	O6	145	LYS
72	R6	106	MET
72	R6	127	LYS
74	T6	70	MET
78	X6	312	GLN
81	a6	27	ARG
82	b6	211	ARG
83	c6	37	ARG
83	c6	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	r1	77	HIS
1	r1	152	GLN

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Mol	Chain	Res	Type
1	r1	196	HIS
1	r1	542	GLN
1	r1	548	GLN
6	E3	72	GLN
10	J3	103	GLN
16	P3	54	ASN
17	Q3	158	GLN
19	S3	179	ASN
22	V3	73	GLN
32	53	275	ASN
35	93	134	ASN
46	k3	35	GLN
63	I6	98	GLN
66	L6	172	ASN
70	P6	71	HIS
70	P6	115	GLN
74	T6	59	ASN
74	T6	128	ASN
76	V6	245	HIS
78	X6	190	ASN
79	Y6	295	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	8	7/1559 (0%)	4 (57%)	0
3	A3	1490/1559 (95%)	415 (27%)	38 (2%)
4	B3	51/73 (69%)	15 (29%)	1 (1%)
54	u3	1/2 (50%)	0	0
86	A6	921/954 (96%)	267 (28%)	14 (1%)
87	24	73/73 (100%)	38 (52%)	1 (1%)
87	FE	73/73 (100%)	38 (52%)	1 (1%)
All	All	2616/4293 (60%)	777 (29%)	55 (2%)

All (777) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A3	1674	A
3	A3	1676	A
3	A3	1678	C
3	A3	1679	U

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Mol	Chain	Res	Type
3	A3	1680	A
3	A3	1681	G
3	A3	1685	C
3	A3	1689	C
3	A3	1692	A
3	A3	1693	C
3	A3	1694	U
3	A3	1699	C
3	A3	1700	U
3	A3	1701	U
3	A3	1704	U
3	A3	1707	C
3	A3	1708	A
3	A3	1709	G
3	A3	1713	A
3	A3	1714	C
3	A3	1715	C
3	A3	1716	U
3	A3	1717	U
3	A3	1724	A
3	A3	1727	A
3	A3	1728	U
3	A3	1741	A
3	A3	1748	G
3	A3	1750	G
3	A3	1751	A
3	A3	1767	G
3	A3	1770	G
3	A3	1774	U
3	A3	1777	A
3	A3	1780	U
3	A3	1781	A
3	A3	1782	G
3	A3	1791	G
3	A3	1794	A
3	A3	1804	A
3	A3	1805	A
3	A3	1806	U
3	A3	1807	U
3	A3	1808	A
3	A3	1809	U
3	A3	1810	A

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Mol	Chain	Res	Type
3	A3	1811	A
3	A3	1812	C
3	A3	1813	C
3	A3	1817	C
3	A3	1821	A
3	A3	1824	U
3	A3	1827	C
3	A3	1828	A
3	A3	1829	A
3	A3	1832	A
3	A3	1836	A
3	A3	1844	A
3	A3	1849	C
3	A3	1854	U
3	A3	1856	A
3	A3	1867	A
3	A3	1869	A
3	A3	1870	A
3	A3	1872	U
3	A3	1873	A
3	A3	1874	A
3	A3	1878	U
3	A3	1882	A
3	A3	1883	G
3	A3	1887	A
3	A3	1888	G
3	A3	1890	C
3	A3	1893	A
3	A3	1902	C
3	A3	1903	C
3	A3	1909	A
3	A3	1918	G
3	A3	1922	C
3	A3	1935	A
3	A3	1939	G
3	A3	1940	A
3	A3	1944	C
3	A3	1966	G
3	A3	1968	G
3	A3	1974	A
3	A3	1975	U
3	A3	1985	G

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Mol	Chain	Res	Type
3	A3	1987	G
3	A3	1992	C
3	A3	1993	A
3	A3	1994	A
3	A3	1995	A
3	A3	2000	C
3	A3	2001	C
3	A3	2002	G
3	A3	2015	G
3	A3	2020	U
3	A3	2021	U
3	A3	2022	G
3	A3	2029	A
3	A3	2031	A
3	A3	2032	G
3	A3	2036	C
3	A3	2037	U
3	A3	2053	U
3	A3	2055	U
3	A3	2057	C
3	A3	2059	C
3	A3	2060	A
3	A3	2065	A
3	A3	2074	A
3	A3	2079	C
3	A3	2083	U
3	A3	2085	A
3	A3	2093	U
3	A3	2097	A
3	A3	2098	G
3	A3	2099	U
3	A3	2110	A
3	A3	2113	G
3	A3	2124	A
3	A3	2125	C
3	A3	2132	A
3	A3	2135	A
3	A3	2141	U
3	A3	2142	A
3	A3	2147	G
3	A3	2154	A
3	A3	2157	U

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Mol	Chain	Res	Type
3	A3	2159	U
3	A3	2163	A
3	A3	2165	C
3	A3	2166	C
3	A3	2168	U
3	A3	2171	U
3	A3	2172	A
3	A3	2173	G
3	A3	2177	U
3	A3	2180	A
3	A3	2182	G
3	A3	2183	C
3	A3	2184	A
3	A3	2187	C
3	A3	2190	C
3	A3	2193	U
3	A3	2194	U
3	A3	2195	A
3	A3	2197	G
3	A3	2198	A
3	A3	2200	A
3	A3	2202	C
3	A3	2210	C
3	A3	2216	A
3	A3	2229	A
3	A3	2230	A
3	A3	2231	A
3	A3	2233	U
3	A3	2237	A
3	A3	2239	A
3	A3	2241	A
3	A3	2243	A
3	A3	2244	U
3	A3	2245	A
3	A3	2246	A
3	A3	2262	C
3	A3	2263	C
3	A3	2283	C
3	A3	2284	C
3	A3	2285	U
3	A3	2290	A
3	A3	2294	A

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Mol	Chain	Res	Type
3	A3	2297	A
3	A3	2299	U
3	A3	2300	G
3	A3	2309	A
3	A3	2322	C
3	A3	2323	A
3	A3	2324	U
3	A3	2329	C
3	A3	2331	C
3	A3	2332	C
3	A3	2345	G
3	A3	2364	C
3	A3	2369	A
3	A3	2370	A
3	A3	2371	U
3	A3	2372	U
3	A3	2374	A
3	A3	2375	C
3	A3	2379	C
3	A3	2380	C
3	A3	2381	A
3	A3	2387	U
3	A3	2389	C
3	A3	2390	A
3	A3	2393	C
3	A3	2394	A
3	A3	2400	C
3	A3	2401	A
3	A3	2404	U
3	A3	2405	C
3	A3	2407	U
3	A3	2414	C
3	A3	2415	C
3	A3	2416	U
3	A3	2426	C
3	A3	2427	C
3	A3	2429	A
3	A3	2435	G
3	A3	2443	C
3	A3	2444	A
3	A3	2445	U
3	A3	2446	A

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Mol	Chain	Res	Type
3	A3	2447	A
3	A3	2452	A
3	A3	2478	G
3	A3	2493	C
3	A3	2500	A
3	A3	2506	A
3	A3	2508	C
3	A3	2511	C
3	A3	2520	C
3	A3	2521	A
3	A3	2522	U
3	A3	2523	C
3	A3	2524	A
3	A3	2527	A
3	A3	2530	A
3	A3	2531	U
3	A3	2532	U
3	A3	2536	G
3	A3	2539	A
3	A3	2540	C
3	A3	2557	C
3	A3	2558	A
3	A3	2559	U
3	A3	2560	G
3	A3	2563	U
3	A3	2567	G
3	A3	2570	C
3	A3	2581	A
3	A3	2582	A
3	A3	2592	G
3	A3	2593	G
3	A3	2594	U
3	A3	2596	G
3	A3	2601	A
3	A3	2603	C
3	A3	2618	U
3	A3	2626	U
3	A3	2627	G
3	A3	2629	A
3	A3	2630	U
3	A3	2632	A
3	A3	2633	A

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Mol	Chain	Res	Type
3	A3	2634	U
3	A3	2635	G
3	A3	2643	G
3	A3	2645	G
3	A3	2654	U
3	A3	2655	G
3	A3	2656	U
3	A3	2660	U
3	A3	2683	C
3	A3	2686	G
3	A3	2694	A
3	A3	2696	A
3	A3	2706	A
3	A3	2708	C
3	A3	2709	A
3	A3	2718	C
3	A3	2719	G
3	A3	2723	A
3	A3	2724	G
3	A3	2725	A
3	A3	2732	G
3	A3	2733	G
3	A3	2740	A
3	A3	2745	A
3	A3	2749	A
3	A3	2750	U
3	A3	2757	A
3	A3	2758	G
3	A3	2761	C
3	A3	2762	C
3	A3	2763	U
3	A3	2764	A
3	A3	2765	A
3	A3	2766	C
3	A3	2767	A
3	A3	2768	A
3	A3	2769	A
3	A3	2771	C
3	A3	2773	A
3	A3	2774	C
3	A3	2775	A
3	A3	2776	G

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Mol	Chain	Res	Type
3	A3	2777	G
3	A3	2778	U
3	A3	2779	C
3	A3	2780	C
3	A3	2781	U
3	A3	2782	A
3	A3	2783	A
3	A3	2784	A
3	A3	2785	C
3	A3	2786	U
3	A3	2787	A
3	A3	2788	C
3	A3	2789	C
3	A3	2790	A
3	A3	2791	A
3	A3	2792	A
3	A3	2804	A
3	A3	2810	G
3	A3	2814	G
3	A3	2823	U
3	A3	2831	G
3	A3	2832	A
3	A3	2833	A
3	A3	2842	C
3	A3	2844	G
3	A3	2847	C
3	A3	2851	A
3	A3	2854	U
3	A3	2861	A
3	A3	2864	U
3	A3	2865	C
3	A3	2870	G
3	A3	2871	U
3	A3	2879	A
3	A3	2893	A
3	A3	2896	G
3	A3	2901	A
3	A3	2906	C
3	A3	2910	A
3	A3	2913	A
3	A3	2916	G
3	A3	2917	G

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Mol	Chain	Res	Type
3	A3	2918	A
3	A3	2919	A
3	A3	2922	A
3	A3	2926	A
3	A3	2928	C
3	A3	2932	G
3	A3	2934	G
3	A3	2935	A
3	A3	2936	U
3	A3	2955	U
3	A3	2956	A
3	A3	2963	A
3	A3	2968	A
3	A3	2971	A
3	A3	2981	A
3	A3	2989	G
3	A3	2990	A
3	A3	2991	U
3	A3	2992	G
3	A3	2994	U
3	A3	3000	A
3	A3	3005	A
3	A3	3012	U
3	A3	3016	G
3	A3	3022	G
3	A3	3029	A
3	A3	3041	U
3	A3	3042	U
3	A3	3053	A
3	A3	3054	G
3	A3	3056	C
3	A3	3060	C
3	A3	3063	G
3	A3	3065	U
3	A3	3070	G
3	A3	3072	U
3	A3	3077	C
3	A3	3086	U
3	A3	3089	A
3	A3	3093	C
3	A3	3096	U
3	A3	3100	U

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Mol	Chain	Res	Type
3	A3	3102	U
3	A3	3108	U
3	A3	3109	U
3	A3	3114	U
3	A3	3123	G
3	A3	3124	U
3	A3	3128	A
3	A3	3129	A
3	A3	3131	G
3	A3	3135	A
3	A3	3141	A
3	A3	3150	U
3	A3	3155	C
3	A3	3157	C
3	A3	3158	A
3	A3	3160	A
3	A3	3161	G
3	A3	3162	C
3	A3	3168	C
3	A3	3169	C
3	A3	3172	C
3	A3	3176	A
3	A3	3180	A
3	A3	3184	C
3	A3	3189	C
3	A3	3190	A
3	A3	3202	U
3	A3	3204	C
3	A3	3207	A
3	A3	3217	A
3	A3	3218	A
3	A3	3220	A
3	A3	3228	U
4	B3	1607	U
4	B3	1608	G
4	B3	1609	U
4	B3	1611	G
4	B3	1614	U
4	B3	1615	A
4	B3	1625	A
4	B3	1631	C
4	B3	1632	U

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Mol	Chain	Res	Type
4	B3	1634	A
4	B3	1641	G
4	B3	1644	G
4	B3	1645	A
4	B3	1665	C
4	B3	1667	C
86	A6	654	U
86	A6	655	A
86	A6	675	U
86	A6	678	U
86	A6	682	U
86	A6	684	U
86	A6	686	A
86	A6	692	A
86	A6	694	U
86	A6	695	A
86	A6	698	C
86	A6	701	G
86	A6	707	A
86	A6	708	U
86	A6	709	C
86	A6	715	U
86	A6	716	C
86	A6	717	C
86	A6	722	A
86	A6	724	U
86	A6	725	U
86	A6	726	C
86	A6	727	A
86	A6	749	A
86	A6	757	A
86	A6	761	A
86	A6	765	A
86	A6	768	A
86	A6	770	G
86	A6	774	C
86	A6	775	A
86	A6	777	U
86	A6	786	A
86	A6	787	A
86	A6	792	U
86	A6	795	G

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Mol	Chain	Res	Type
86	A6	797	C
86	A6	798	U
86	A6	799	A
86	A6	800	G
86	A6	811	A
86	A6	812	C
86	A6	813	G
86	A6	816	A
86	A6	818	A
86	A6	819	C
86	A6	820	A
86	A6	821	G
86	A6	831	A
86	A6	834	U
86	A6	836	U
86	A6	839	C
86	A6	840	A
86	A6	850	A
86	A6	851	G
86	A6	853	U
86	A6	857	C
86	A6	859	A
86	A6	865	U
86	A6	869	A
86	A6	872	C
86	A6	873	C
86	A6	874	C
86	A6	884	C
86	A6	886	A
86	A6	887	U
86	A6	889	U
86	A6	894	C
86	A6	903	G
86	A6	907	U
86	A6	908	C
86	A6	909	A
86	A6	923	A
86	A6	924	G
86	A6	931	G
86	A6	937	G
86	A6	938	G
86	A6	942	A

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Mol	Chain	Res	Type
86	A6	943	A
86	A6	946	A
86	A6	947	G
86	A6	951	U
86	A6	952	U
86	A6	954	A
86	A6	957	U
86	A6	958	C
86	A6	959	A
86	A6	970	A
86	A6	971	A
86	A6	981	A
86	A6	982	A
86	A6	989	U
86	A6	992	G
86	A6	996	U
86	A6	997	A
86	A6	1005	C
86	A6	1006	C
86	A6	1011	G
86	A6	1012	A
86	A6	1015	C
86	A6	1018	A
86	A6	1019	A
86	A6	1023	A
86	A6	1026	A
86	A6	1032	G
86	A6	1035	G
86	A6	1036	C
86	A6	1038	U
86	A6	1043	A
86	A6	1046	U
86	A6	1050	A
86	A6	1053	A
86	A6	1056	C
86	A6	1069	C
86	A6	1085	U
86	A6	1086	A
86	A6	1102	C
86	A6	1107	A
86	A6	1109	C
86	A6	1110	C

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Mol	Chain	Res	Type
86	A6	1113	A
86	A6	1125	A
86	A6	1129	A
86	A6	1130	A
86	A6	1133	U
86	A6	1141	A
86	A6	1142	G
86	A6	1146	A
86	A6	1148	U
86	A6	1155	C
86	A6	1157	C
86	A6	1158	A
86	A6	1170	A
86	A6	1171	A
86	A6	1183	G
86	A6	1184	U
86	A6	1189	C
86	A6	1191	U
86	A6	1192	A
86	A6	1193	U
86	A6	1194	C
86	A6	1195	C
86	A6	1196	C
86	A6	1198	C
86	A6	1207	C
86	A6	1210	G
86	A6	1218	A
86	A6	1219	U
86	A6	1220	C
86	A6	1224	A
86	A6	1226	A
86	A6	1227	C
86	A6	1229	C
86	A6	1230	C
86	A6	1233	U
86	A6	1235	A
86	A6	1236	A
86	A6	1241	A
86	A6	1247	U
86	A6	1249	U
86	A6	1250	U
86	A6	1251	G

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Mol	Chain	Res	Type
86	A6	1252	C
86	A6	1254	C
86	A6	1255	A
86	A6	1256	G
86	A6	1258	C
86	A6	1261	U
86	A6	1265	C
86	A6	1274	U
86	A6	1275	C
86	A6	1276	A
86	A6	1287	A
86	A6	1288	U
86	A6	1289	G
86	A6	1291	A
86	A6	1294	C
86	A6	1296	A
86	A6	1297	C
86	A6	1298	A
86	A6	1299	A
86	A6	1300	A
86	A6	1301	G
86	A6	1304	A
86	A6	1330	A
86	A6	1331	G
86	A6	1333	U
86	A6	1334	C
86	A6	1336	A
86	A6	1346	C
86	A6	1347	A
86	A6	1348	U
86	A6	1355	G
86	A6	1357	A
86	A6	1358	A
86	A6	1359	G
86	A6	1360	A
86	A6	1363	U
86	A6	1371	A
86	A6	1372	U
86	A6	1373	U
86	A6	1375	U
86	A6	1380	C
86	A6	1381	C

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Mol	Chain	Res	Type
86	A6	1382	C
86	A6	1383	A
86	A6	1385	A
86	A6	1394	A
86	A6	1395	U
86	A6	1397	G
86	A6	1400	C
86	A6	1401	U
86	A6	1406	A
86	A6	1407	A
86	A6	1420	A
86	A6	1421	A
86	A6	1423	G
86	A6	1424	U
86	A6	1428	U
86	A6	1434	A
86	A6	1436	U
86	A6	1441	U
86	A6	1444	G
86	A6	1448	A
86	A6	1451	G
86	A6	1452	U
86	A6	1456	U
86	A6	1458	G
86	A6	1460	U
86	A6	1466	G
86	A6	1469	C
86	A6	1470	C
86	A6	1485	C
86	A6	1486	A
86	A6	1498	C
86	A6	1506	A
86	A6	1516	A
86	A6	1521	A
86	A6	1522	C
86	A6	1529	C
86	A6	1531	A
86	A6	1536	C
86	A6	1537	C
86	A6	1538	C
86	A6	1539	U
86	A6	1540	A

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Mol	Chain	Res	Type
86	A6	1541	C
86	A6	1542	G
86	A6	1543	C
86	A6	1544	A
86	A6	1545	U
86	A6	1547	U
86	A6	1551	U
86	A6	1562	A
86	A6	1563	G
86	A6	1566	G
86	A6	1568	A
86	A6	1572	U
86	A6	1575	U
86	A6	1576	A
86	A6	1586	G
86	A6	1588	A
86	A6	1595	C
86	A6	1598	G
86	A6	1599	G
86	A6	1603	A
86	A6	1604	A
87	24	2	U
87	24	3	U
87	24	7	G
87	24	8	U
87	24	9	A
87	24	12	U
87	24	13	U
87	24	14	A
87	24	16	A
87	24	17	U
87	24	18	U
87	24	19	A
87	24	20	U
87	24	21	C
87	24	22	A
87	24	27	A
87	24	28	A
87	24	30	G
87	24	31	C
87	24	32	A
87	24	35	G

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Mol	Chain	Res	Type
87	24	41	G
87	24	45	A
87	24	46	G
87	24	51	G
87	24	52	C
87	24	54	U
87	24	55	C
87	24	56	A
87	24	57	C
87	24	58	A
87	24	59	G
87	24	62	C
87	24	65	U
87	24	67	A
87	24	71	C
87	24	72	C
87	24	73	A
3	8	18	A
3	8	19	A
3	8	21	U
3	8	23	A
87	FE	2	U
87	FE	3	U
87	FE	7	G
87	FE	8	U
87	FE	9	A
87	FE	12	U
87	FE	13	U
87	FE	14	A
87	FE	16	A
87	FE	17	U
87	FE	18	U
87	FE	19	A
87	FE	20	U
87	FE	21	C
87	FE	22	A
87	FE	27	A
87	FE	28	A
87	FE	30	G
87	FE	31	C
87	FE	32	A
87	FE	35	G

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Mol	Chain	Res	Type
87	FE	41	G
87	FE	45	A
87	FE	46	G
87	FE	51	G
87	FE	52	C
87	FE	54	U
87	FE	55	C
87	FE	56	A
87	FE	57	C
87	FE	58	A
87	FE	59	G
87	FE	62	C
87	FE	65	U
87	FE	67	A
87	FE	71	C
87	FE	72	C
87	FE	73	A

All (55) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A3	1703	C
3	A3	1805	A
3	A3	1806	U
3	A3	1807	U
3	A3	1809	U
3	A3	1823	A
3	A3	1871	A
3	A3	1901	C
3	A3	1994	A
3	A3	2165	C
3	A3	2172	A
3	A3	2182	G
3	A3	2186	C
3	A3	2243	A
3	A3	2245	A
3	A3	2315	A
3	A3	2374	A
3	A3	2507	A
3	A3	2523	C
3	A3	2530	A
3	A3	2558	A

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Mol	Chain	Res	Type
3	A3	2559	U
3	A3	2628	U
3	A3	2653	C
3	A3	2744	U
3	A3	2757	A
3	A3	2779	C
3	A3	2784	A
3	A3	2788	C
3	A3	2789	C
3	A3	2905	A
3	A3	2989	G
3	A3	3041	U
3	A3	3092	U
3	A3	3123	G
3	A3	3157	C
3	A3	3201	A
3	A3	3206	C
4	B3	1607	U
86	A6	721	G
86	A6	797	C
86	A6	886	A
86	A6	1025	U
86	A6	1034	G
86	A6	1045	A
86	A6	1170	A
86	A6	1193	U
86	A6	1250	U
86	A6	1335	A
86	A6	1419	G
86	A6	1433	C
86	A6	1538	C
86	A6	1541	C
87	24	1	G
87	FE	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 138 ligands modelled in this entry, 135 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
95	GDP	X6	500	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
93	SPD	A3	3396	-	9,9,9	0.35	0	8,8,8	0.50	0
91	GCP	r1	801	1,92	27,34,34	3.59	11 (40%)	34,54,54	5.22	13 (38%)

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
95	GDP	X6	500	-	-	4/12/32/32	0/3/3/3
93	SPD	A3	3396	-	-	6/7/7/7	-
91	GCP	r1	801	1,92	-	8/15/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	r1	801	GCP	O4'-C1'	-8.41	1.29	1.41
91	r1	801	GCP	C2'-C3'	-8.15	1.31	1.53
91	r1	801	GCP	PB-O3A	6.28	1.65	1.58
91	r1	801	GCP	C2-N2	6.23	1.46	1.33
91	r1	801	GCP	O6-C6	6.18	1.40	1.24
91	r1	801	GCP	C2'-C1'	5.48	1.62	1.53
91	r1	801	GCP	O4'-C4'	4.14	1.54	1.45
91	r1	801	GCP	O3'-C3'	3.13	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	r1	801	GCP	C5'-C4'	-3.02	1.42	1.51
95	X6	500	GDP	C6-N1	-2.55	1.34	1.37
91	r1	801	GCP	PB-O2B	-2.29	1.51	1.56
91	r1	801	GCP	PG-O3G	-2.20	1.49	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	r1	801	GCP	O3G-PG-C3B	-16.88	65.45	106.40
91	r1	801	GCP	O3G-PG-O1G	-14.36	74.41	112.39
91	r1	801	GCP	O1G-PG-C3B	13.11	139.50	111.24
91	r1	801	GCP	O3G-PG-O2G	12.05	143.27	108.08
91	r1	801	GCP	PB-O3A-PA	-4.10	119.55	132.56
91	r1	801	GCP	C2-N3-C4	3.84	119.74	115.36
91	r1	801	GCP	C3'-C2'-C1'	3.72	106.58	100.98
91	r1	801	GCP	C4-C5-C6	-3.69	117.27	120.80
95	X6	500	GDP	C3'-C2'-C1'	3.68	106.51	100.98
91	r1	801	GCP	N3-C2-N1	-3.55	122.49	127.22
95	X6	500	GDP	PA-O3A-PB	-3.11	122.17	132.83
91	r1	801	GCP	C4-C5-N7	-2.93	106.34	109.40
91	r1	801	GCP	C2-N1-C6	2.49	119.88	115.93
91	r1	801	GCP	C5-C6-N1	-2.43	120.11	123.43
95	X6	500	GDP	C5-C6-N1	2.33	118.06	113.95
91	r1	801	GCP	O2G-PG-O1G	-2.28	106.37	112.39
95	X6	500	GDP	C8-N7-C5	2.22	107.22	102.99

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	r1	801	GCP	PG-C3B-PB-O1B
91	r1	801	GCP	PG-C3B-PB-O2B
91	r1	801	GCP	PG-C3B-PB-O3A
91	r1	801	GCP	C5'-O5'-PA-O1A
95	X6	500	GDP	C5'-O5'-PA-O1A
95	X6	500	GDP	C3'-C4'-C5'-O5'
93	A3	3396	SPD	N6-C7-C8-C9
93	A3	3396	SPD	C3-C4-C5-N6
95	X6	500	GDP	O4'-C4'-C5'-O5'
93	A3	3396	SPD	C8-C7-N6-C5
93	A3	3396	SPD	C7-C8-C9-N10
91	r1	801	GCP	O4'-C4'-C5'-O5'

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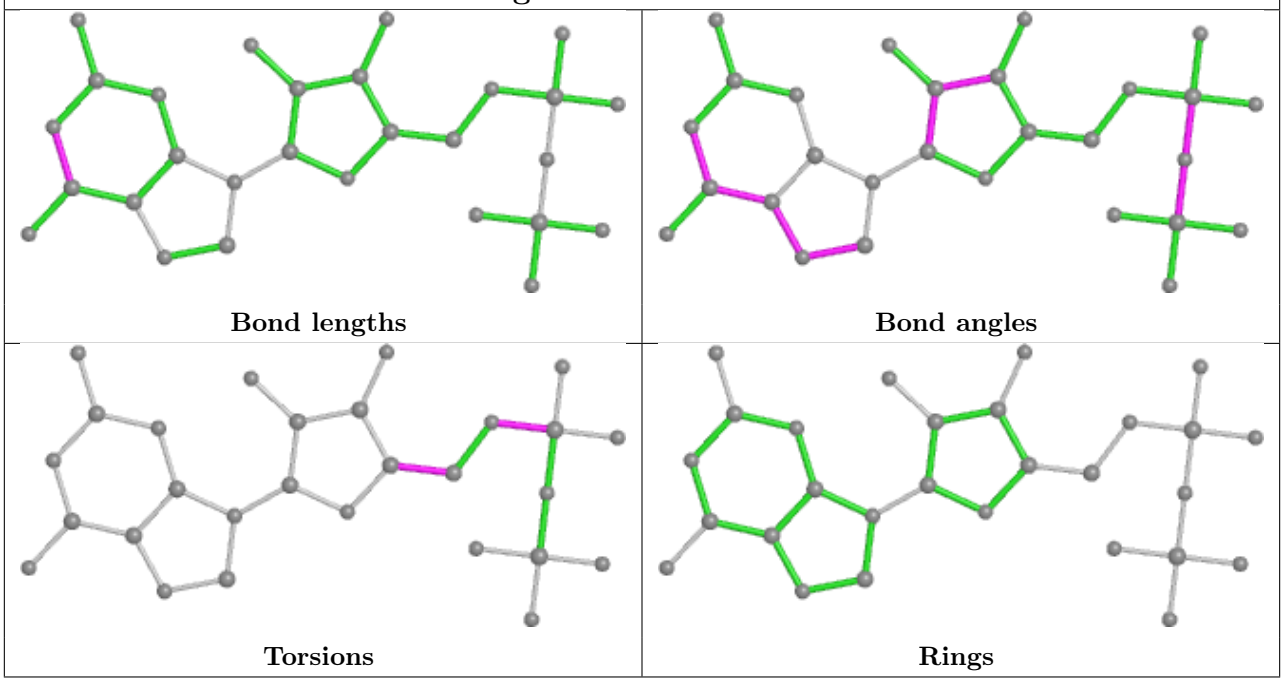
Mol	Chain	Res	Type	Atoms
91	r1	801	GCP	C3'-C4'-C5'-O5'
93	A3	3396	SPD	N1-C2-C3-C4
91	r1	801	GCP	C4'-C5'-O5'-PA
95	X6	500	GDP	C5'-O5'-PA-O3A
93	A3	3396	SPD	C2-C3-C4-C5
91	r1	801	GCP	C5'-O5'-PA-O3A

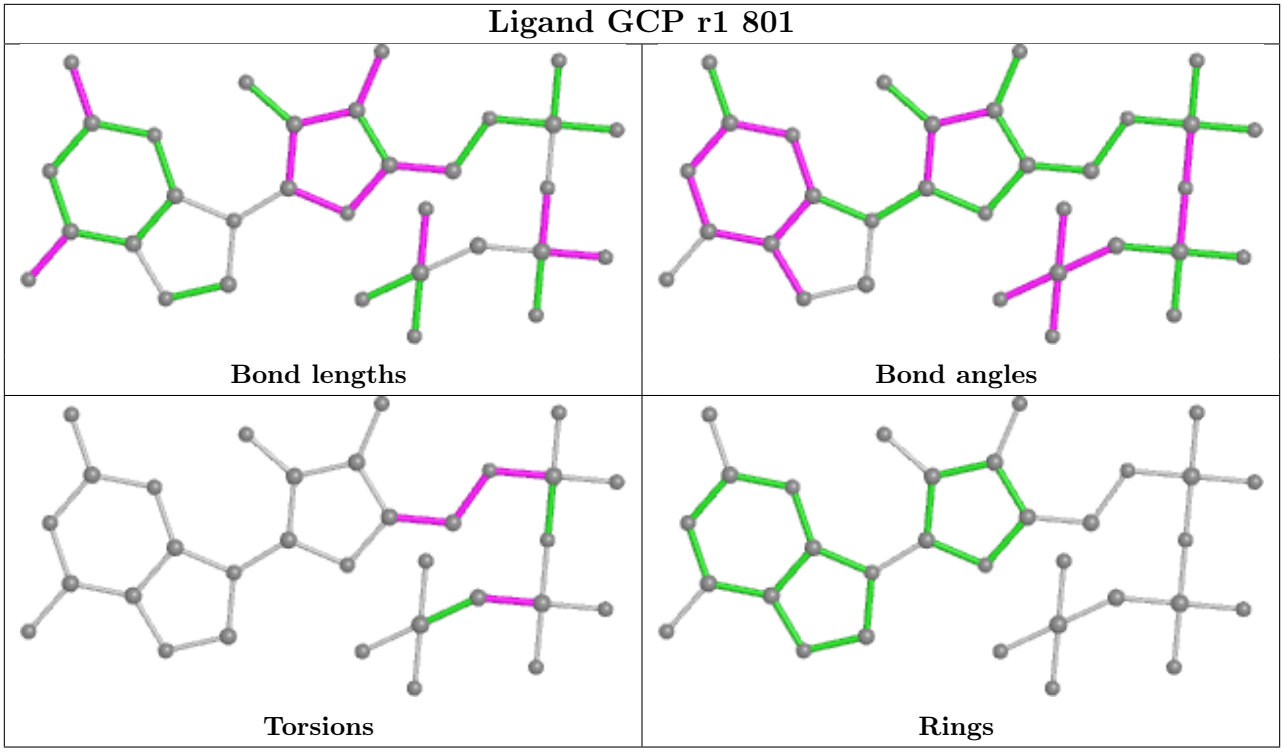
There are no ring outliers.

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M3	1
25	Y3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M3	61:THR	C	62:ARG	N	1.19
1	Y3	123:ARG	C	124:LEU	N	1.19

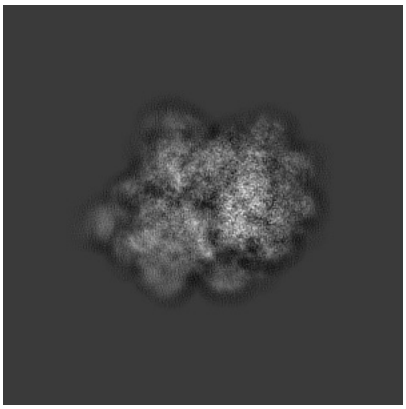
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11646. These allow visual inspection of the internal detail of the map and identification of artifacts.

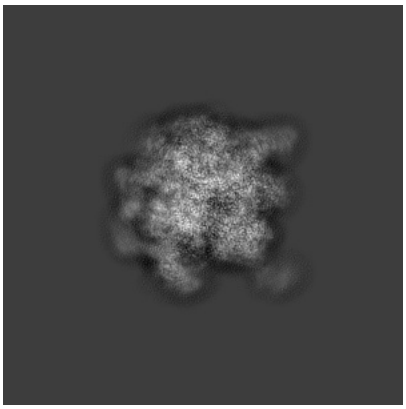
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

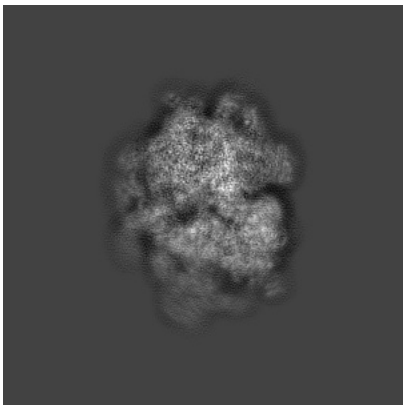
6.1.1 Primary map



X

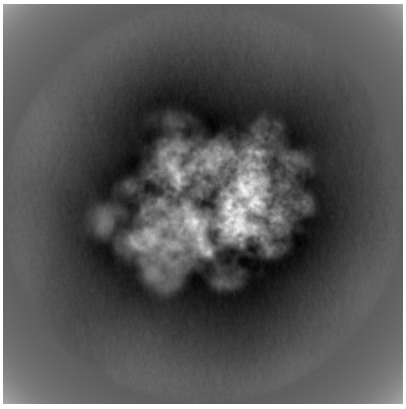


Y

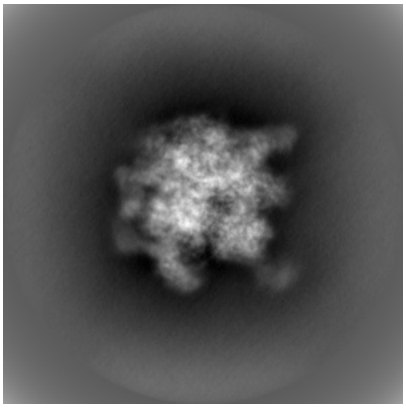


Z

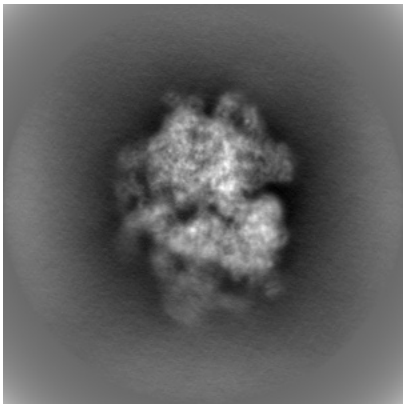
6.1.2 Raw map



X



Y

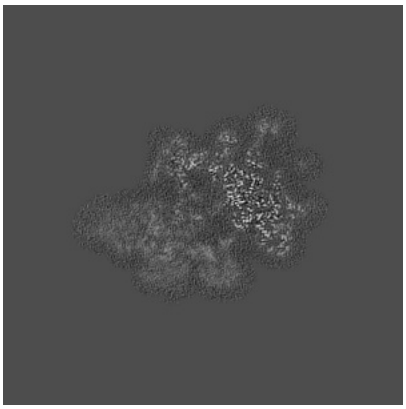


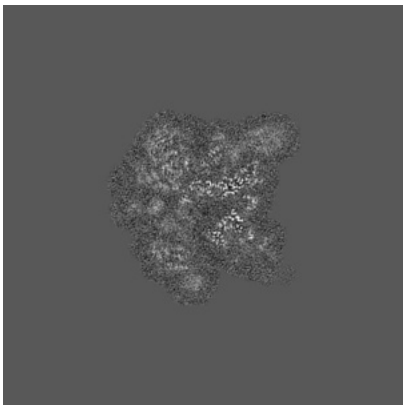
Z

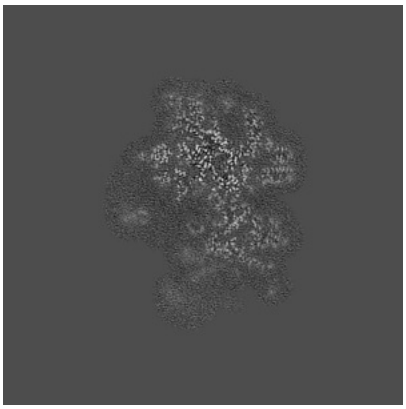
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

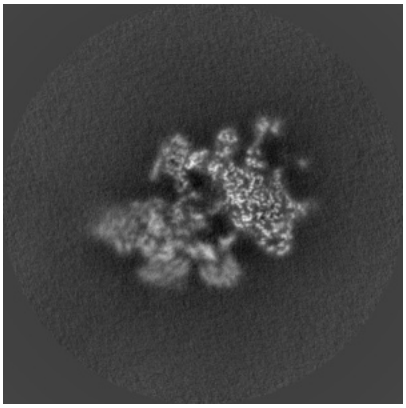
6.2.1 Primary map

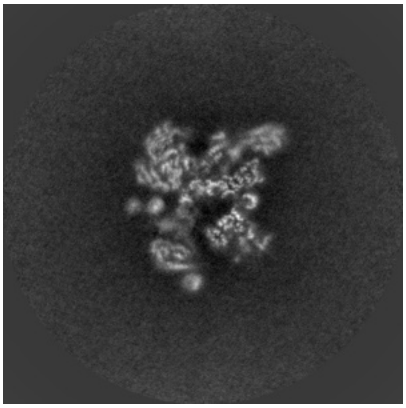

X Index: 256

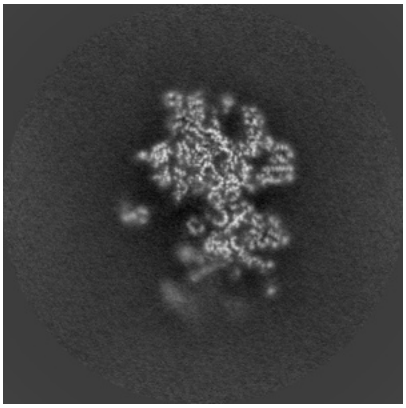

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

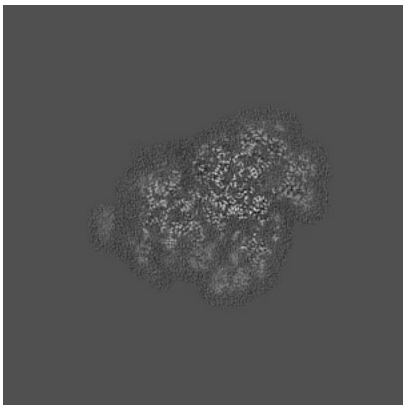

Y Index: 256


Z Index: 256

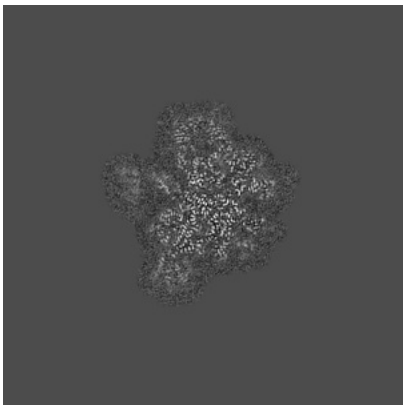
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

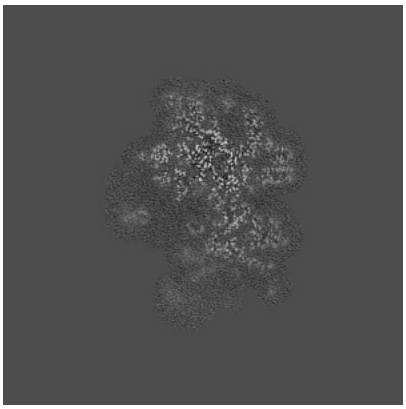
6.3.1 Primary map



X Index: 286

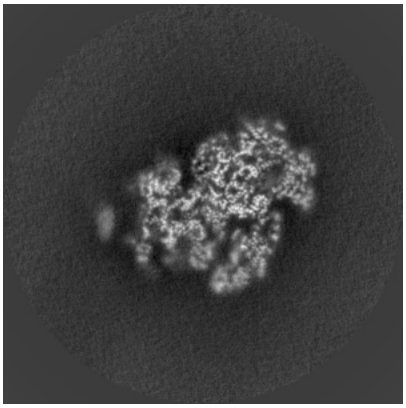


Y Index: 305

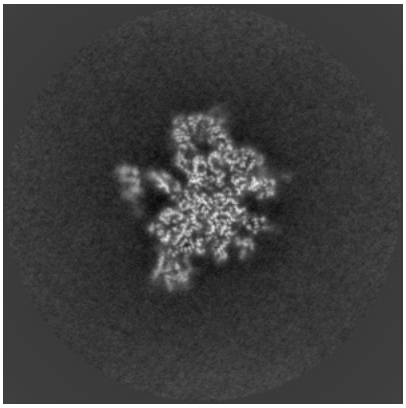


Z Index: 256

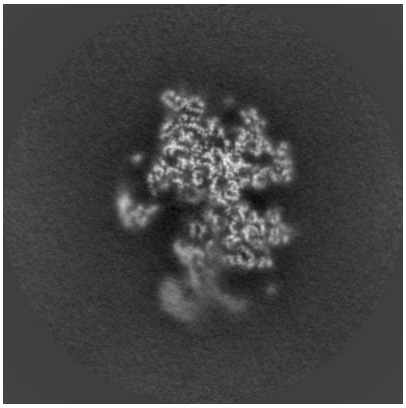
6.3.2 Raw map



X Index: 286



Y Index: 305



Z Index: 247

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

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

6.4.2 Raw map

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.

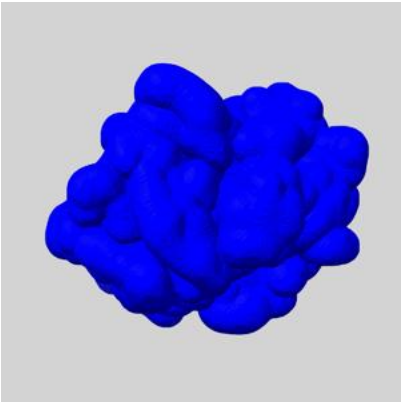
6.5 Mask visualisation (i)

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

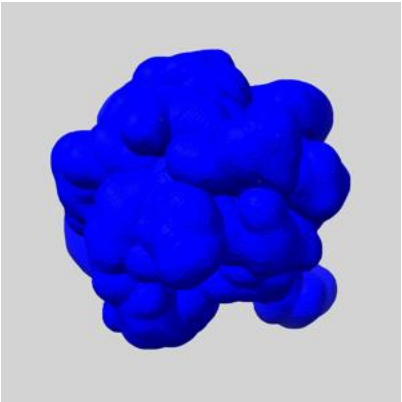
A mask typically either:

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

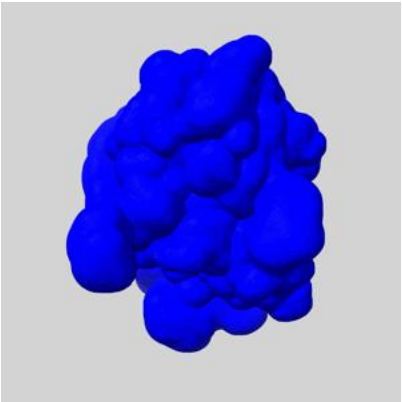
6.5.1 emd_11646_msk_1.map (i)



X



Y

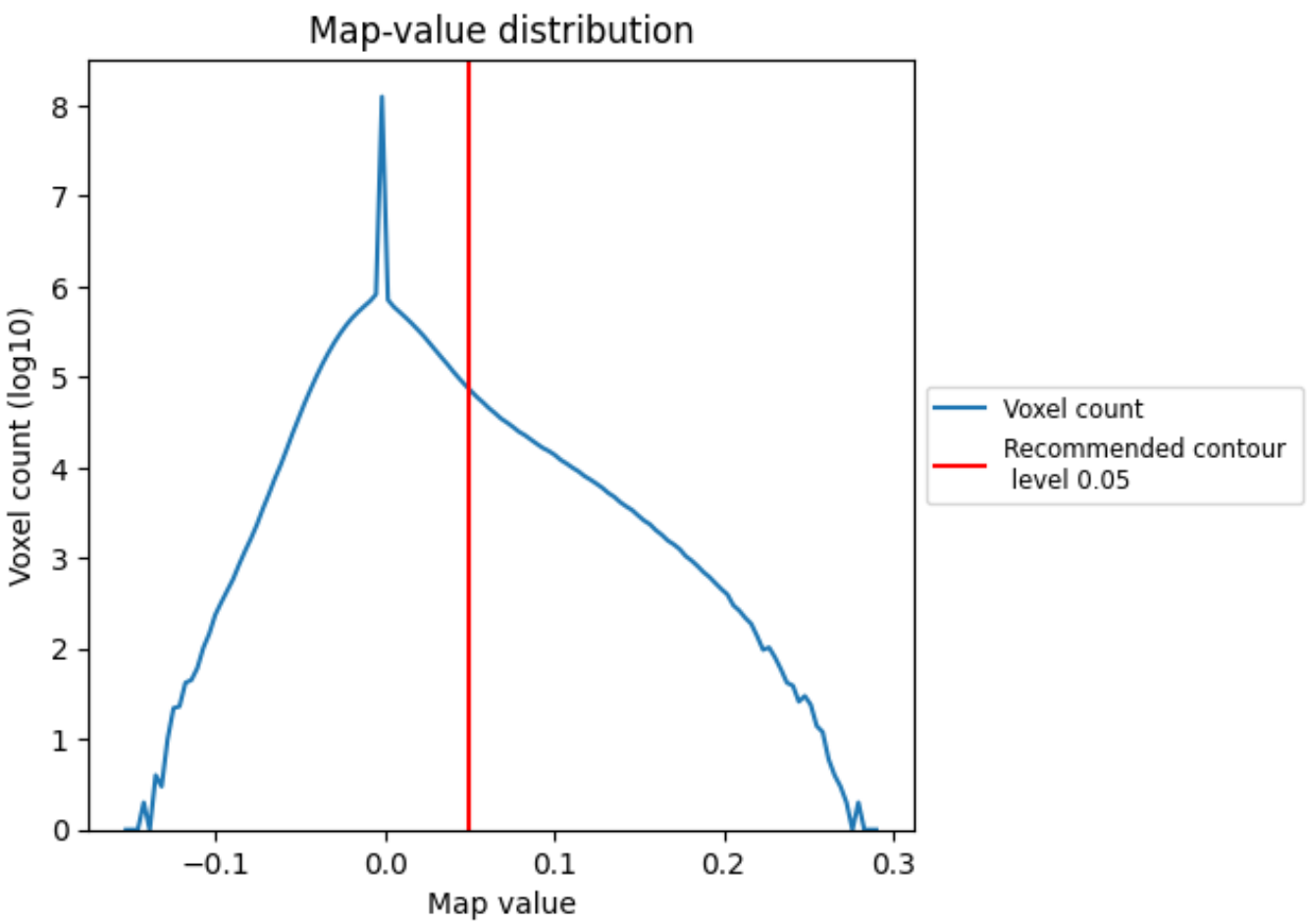


Z

7 Map analysis (i)

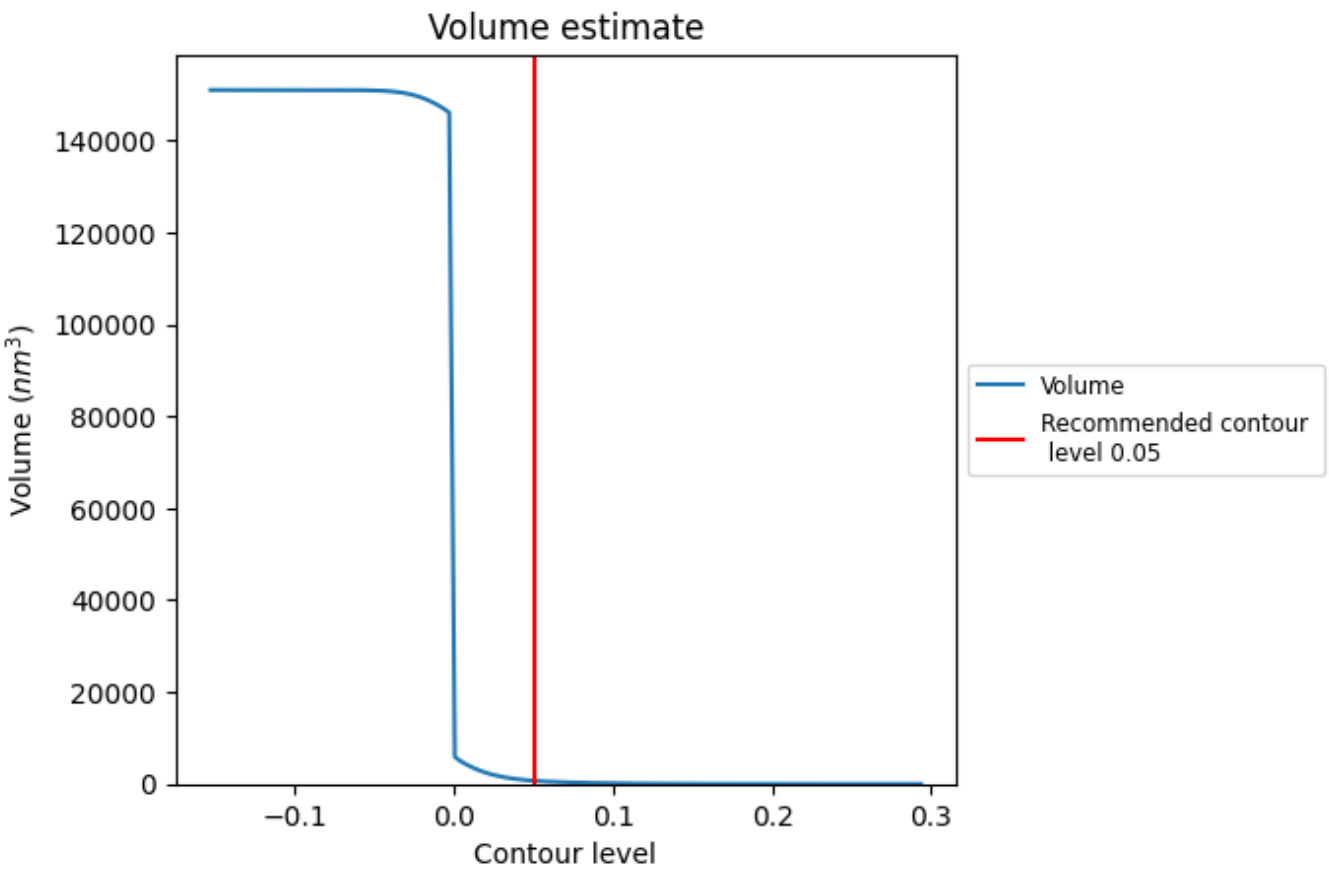
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

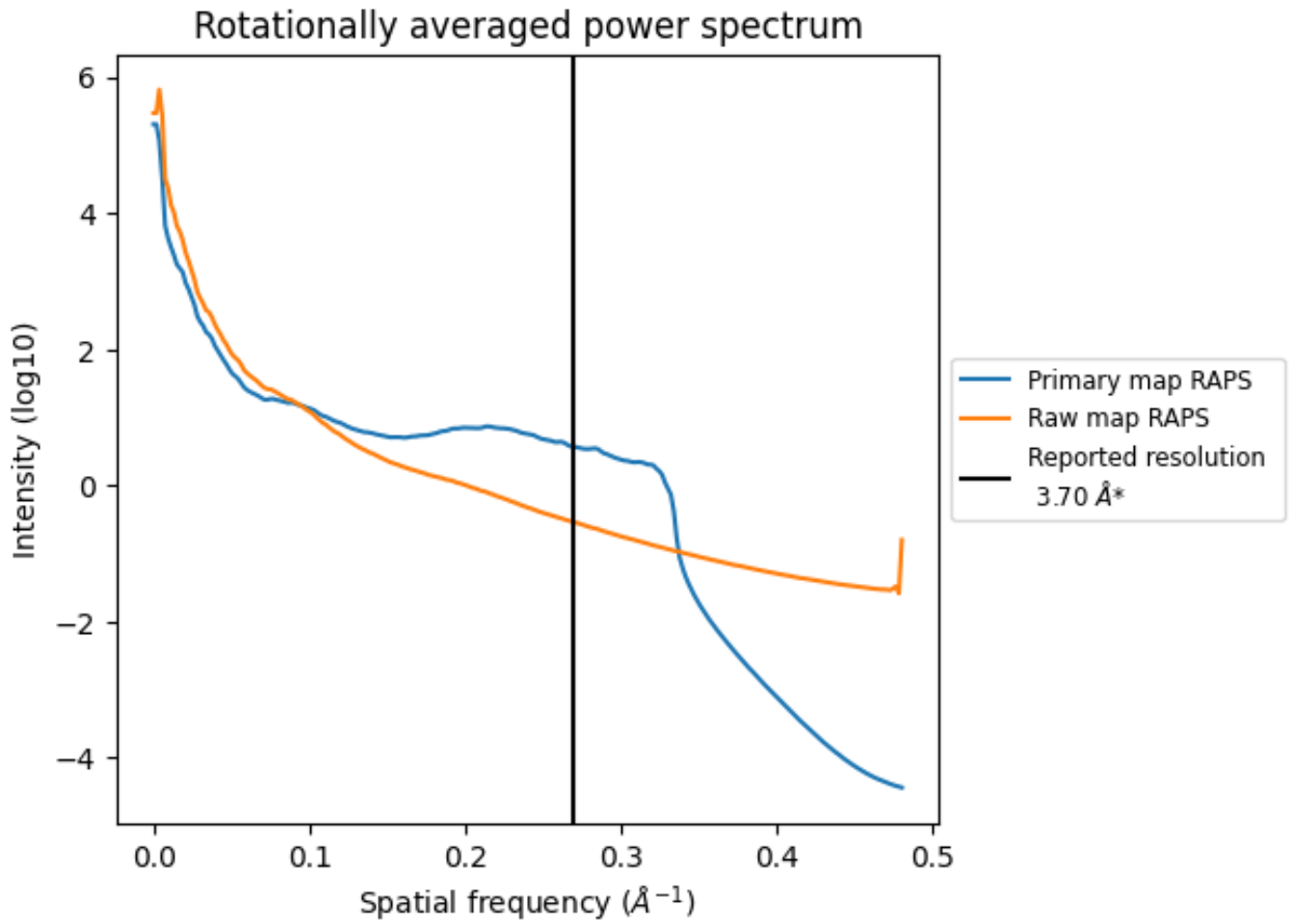
7.2 Volume estimate (i)



The volume at the recommended contour level is 706 nm^3; this corresponds to an approximate mass of 638 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)

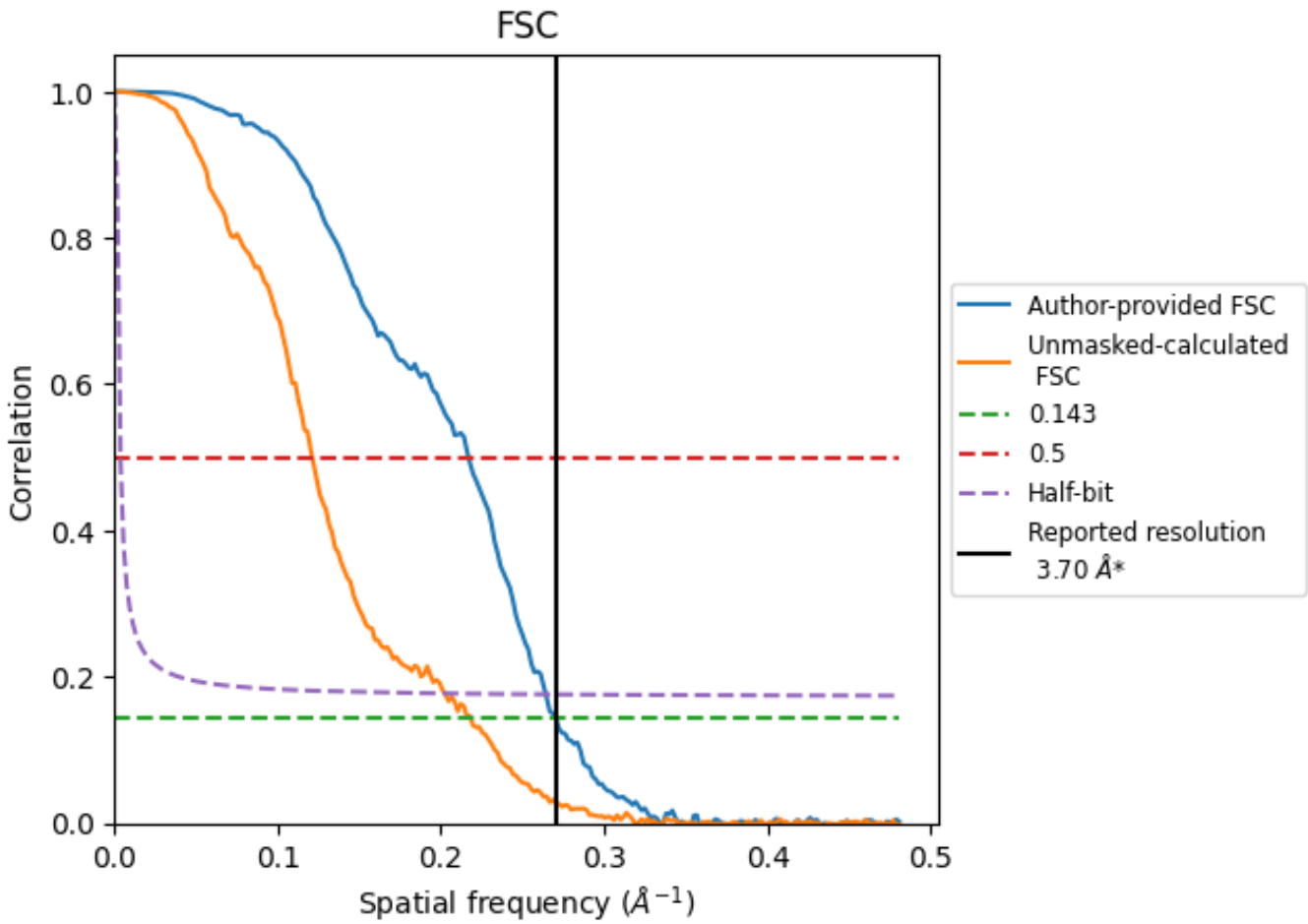


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

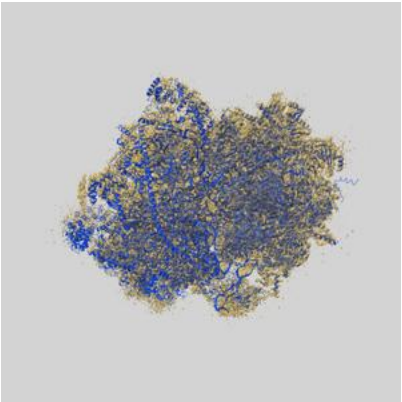
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.61	3.78
Unmasked-calculated*	4.58	8.26	4.94

*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 4.58 differs from the reported value 3.7 by more than 10 %

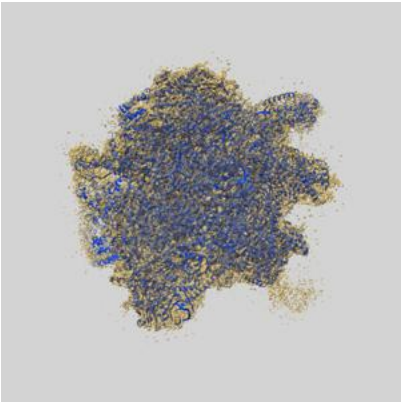
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11646 and PDB model 7A5K. Per-residue inclusion information can be found in section 3 on page 23.

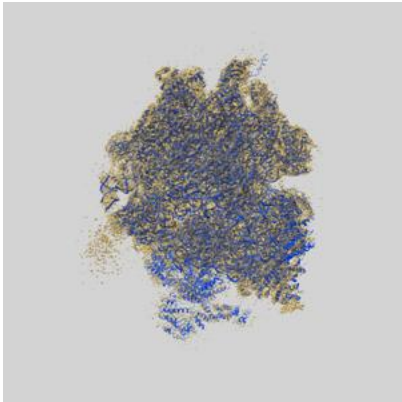
9.1 Map-model overlay (i)



X



Y



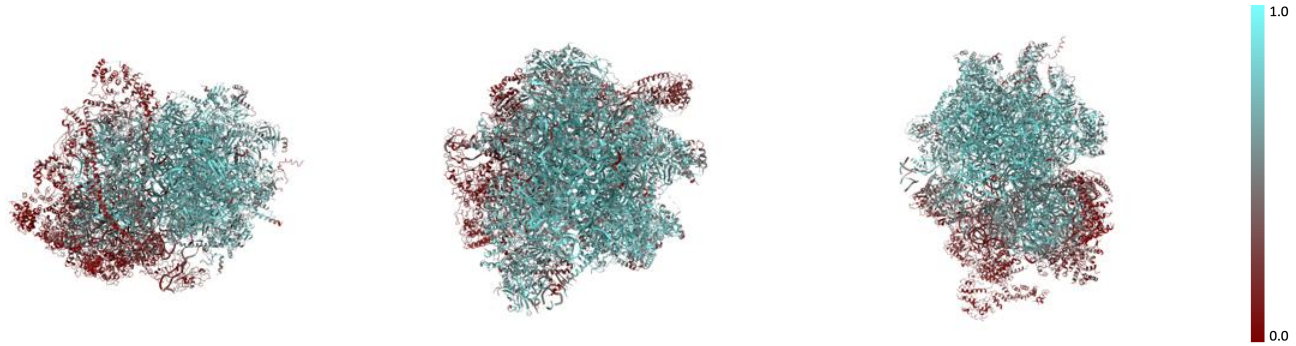
Z

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)

This section was not generated.

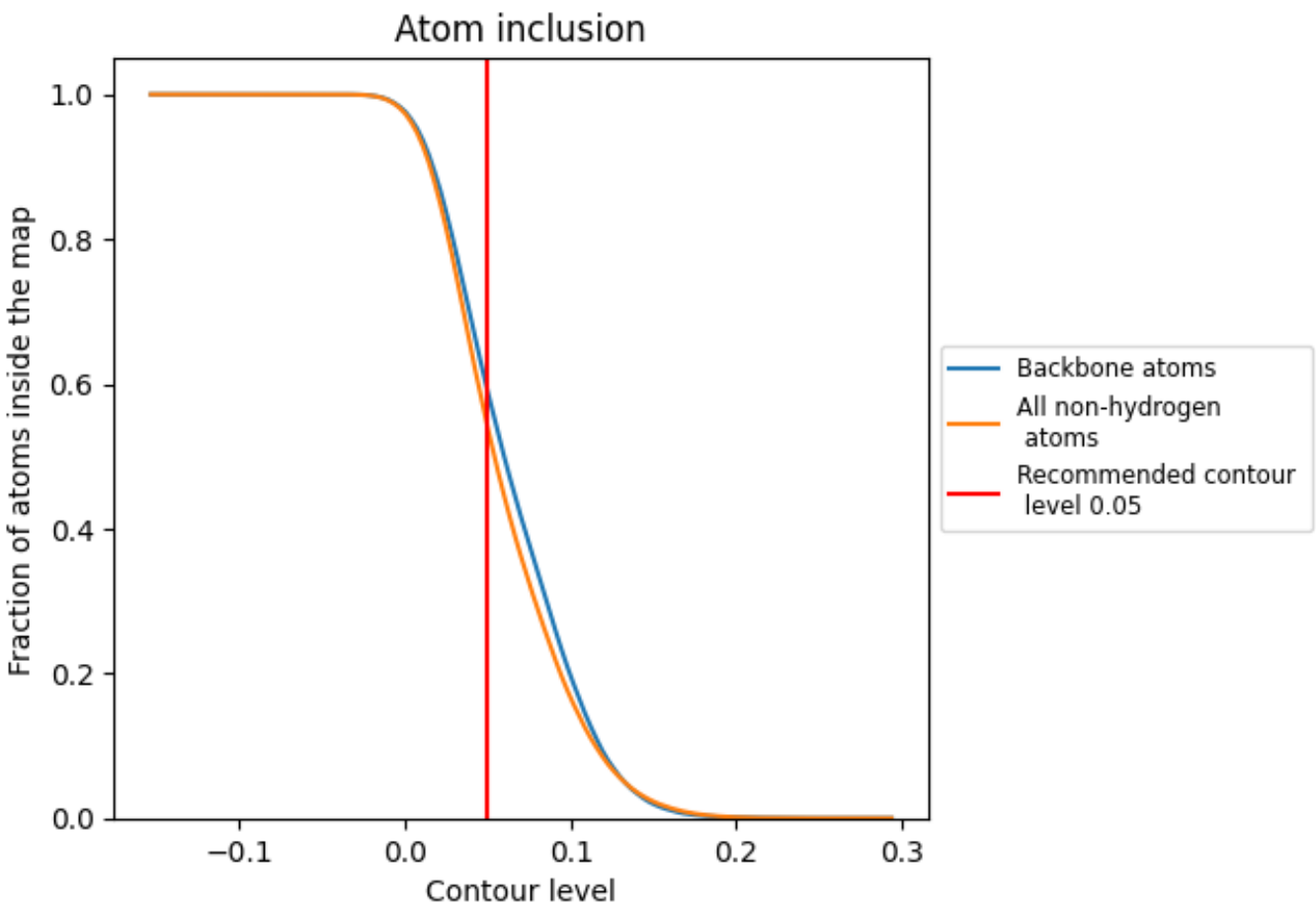
9.3 Atom inclusion mapped to coordinate model (i)



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, 59% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.5403
03	0.6659
13	0.6714
23	0.7889
24	0.1138
33	0.7807
43	0.7850
53	0.6443
63	0.6389
73	0.6060
8	0.1486
93	0.6365
A	0.2203
A3	0.8367
A5	0.0000
A6	0.5826
B	0.3000
B3	0.6331
B6	0.3386
C6	0.0752
D	0.1997
D3	0.6719
D6	0.3431
E3	0.7274
E6	0.2540
F3	0.7219
F6	0.0375
FE	0.2864
G6	0.1465
H3	0.5831
H6	0.0962
I3	0.4944
I6	0.2779
J3	0.3244
J6	0.5644

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Chain	Atom inclusion
K3	0.7544
K6	0.1152
L3	0.6371
L6	0.3696
M3	0.7177
M6	0.3202
N3	0.7013
N6	0.4547
O3	0.7108
O6	0.2784
P3	0.6715
P6	0.2852
Q3	0.6368
Q6	0.4077
R3	0.7292
R6	0.1849
S3	0.7250
S6	0.2376
T3	0.7151
T6	0.3367
U3	0.7556
U6	0.2359
V3	0.5650
V6	0.1583
W3	0.7368
W6	0.1952
X3	0.6322
X6	0.0481
Y2	0.1655
Y3	0.6990
Y6	0.0631
Z3	0.7312
Z6	0.0766
a3	0.7128
a6	0.2410
b3	0.7144
b6	0.0747
c3	0.6528
c6	0.2302
d3	0.5691
d6	0.5447
e3	0.2203

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Continued from previous page...

Chain	Atom inclusion
e6	0.0488
f3	0.3717
g3	0.6987
h3	0.5665
i3	0.7472
j3	0.6657
k3	0.4540
l3	0.7136
m3	0.3598
n	0.0909
o3	0.7546
p3	0.5773
q3	0.5620
r1	0.4441
r3	0.7461
s3	0.6872
u3	0.8571