wwPDB EM Validation Summary Report (i)

Sep 8, 2026 – 04:47 am BST

PDB ID	:	8ANY / pdb_00008any
EMDB ID	:	EMD-15544
Title	:	Human mitochondrial ribosome in complex with LRPPRC, SLIRP, A-site, P-site, E-site tRNAs and mRNA
Authors	:	Singh, V.; Itoh, Y.; Amunts, A.
Deposited on	:	2022-08-06
Resolution	:	2.85 Å(reported)

This is a wwPDB EM Validation Summary 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:

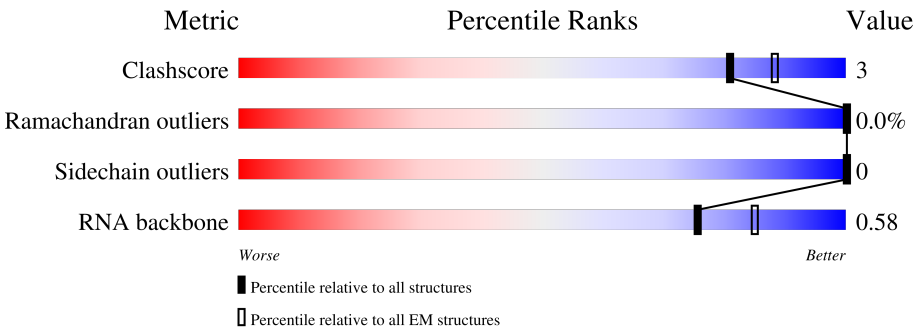
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

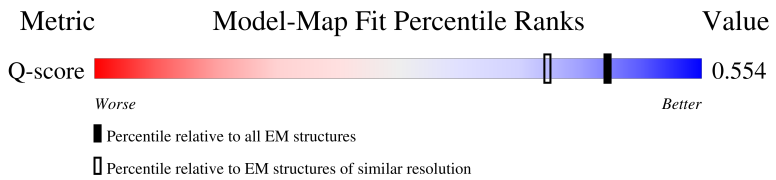
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	AA	954	74% 24% •
2	AB	296	• 73% • 24%
3	AC	167	73% 6% 21%

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Mol	Chain	Length	Quality of chain
4	AD	430	75% 20%
5	AE	125	93% 5%
6	AF	242	81% 5% 14%
7	AG	396	76% 6% 17%
8	AH	201	65% 5% 30%
9	AI	194	68% 29%
10	AJ	138	75% 22%
11	AK	128	76% 21%
12	AL	257	66% 32%
13	AM	137	83% 13%
14	AN	130	83% 15%
15	AO	258	73% 25%
16	AP	142	68% 32%
17	AQ	87	94% 5%
18	AR	360	80% 18%
19	AS	190	67% 29%
20	AT	173	92% 5%
21	AU	205	84% 14%
22	AV	414	84% 13%
23	AW	187	52% 47%
24	AX	398	82% 6% 12%
25	AZ	106	92% 6%
26	A0	217	94% 5%
27	A1	323	80% 5% 14%
28	A2	118	90% 9%

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Mol	Chain	Length	Quality of chain
29	A3	199	32% 65%
30	Aw	68	72% 28%
31	Ax	70	76% 19% 6%
32	Ay	70	39% 81% 16%
33	A	1561	71% 26%
34	B	72	67% 31%
35	D	305	75% 22%
36	E	348	84% 12%
37	F	311	76% 5% 19%
38	I	261	15% 79% 19%
39	J	192	88% 9%
40	K	178	97%
41	L	145	75% 21%
42	M	296	93% 5%
43	N	251	85% 12%
44	O	175	82% 6% 12%
45	P	180	77% 20%
46	Q	292	77% 5% 18%
47	R	149	94% 6%
48	S	205	74% 21%
49	T	206	78% 19%
50	U	153	93% 7%
51	V	216	88% 6% 5%
52	W	148	76% 22%
53	X	256	93% 5%

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Mol	Chain	Length	Quality of chain
54	Y	250	72% 28%
55	Z	161	73% 24%
56	0	188	57% 41%
57	1	65	82% 5% 14%
58	2	92	47% 50%
59	3	188	46% 5% 49%
60	4	103	33% 63%
61	5	423	91% 7%
62	6	380	88% 5% 7%
63	7	338	82% 5% 13%
64	8	206	74% 24%
65	9	137	88% 9%
66	a	142	68% 30%
67	b	215	66% 30%
68	c	332	83% 14%
69	d	306	75% 21%
70	e	279	80% 5% 15%
71	f	212	70% 26%
72	g	166	80% 19%
73	h	158	68% 30%
74	i	128	73% 24%
75	j	123	73% 24%
76	k	112	88% 10%
77	l	138	59% 41%
78	m	128	6% 70% 28%

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Mol	Chain	Length	Quality of chain
79	o	102	87% 5% 8%
80	p	206	68% 29%
81	q	222	15% 72% 26%
82	r	196	78% 5% 17%
83	s	439	86% 12%
84	t	198	11% 23% 77%
84	u	198	9% 16% 84%
84	v	198	16% 16% 84%
84	w	198	16% 16% 84%
84	x	198	16% 16% 84%
84	y	198	16% 16% 84%
85	H	267	25% 70% 6% 24%
86	z	325	60% 70% 8% 22%
87	AY	395	13% 49% 7% 44%
88	A5	1394	16% 37% 58%
89	A4	689	83% 14%
90	A6	109	50% 64% 32%
91	Az	42	10% 45% 40% 14%

2 Entry composition (i)

There are 103 unique types of molecules in this entry. The entry contains 355123 atoms, of which 160326 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	AA	954	30565	9088	10305	3647	6571	954	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	AB	225	3654	1164	1826	331	323	10	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	AC	132	2179	699	1096	195	185	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	AD	343	5545	1713	2814	518	487	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	AE	122	1976	614	1004	177	177	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	AF	208	3503	1104	1778	312	298	11	0	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	AG	327	5385	1710	2697	477	487	14	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	AH	140	2343	745	1191	194	210	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	AI	137	2086	642	1066	192	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	AJ	108	1731	521	892	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	AK	101	1751	537	889	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	AL	174	2998	925	1545	270	251	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	AM	119	1914	594	972	185	157	6	0	0

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	AN	110	1801	562	933	156	147	3	0	0

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	AO	193	3162	1014	1570	294	277	7	0	0

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	AP	97	1590	501	809	134	138	8	0	0

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	AQ	86	1504	460	760	150	126	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	variant	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	AR	295	4845	1533	2436	413	455	8	0	0

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	AS	135	2228	716	1117	198	196	1	0	0

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	AT	168	2767	877	1396	239	244	11	0	0

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	AU	176	2993	916	1505	301	267	4	0	0

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	AV	362	5941	1904	2972	495	558	12	0	0

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	AW	100	1595	498	806	141	146	4	0	0

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	AX	352	5708	1822	2859	499	517	11	0	0

- Molecule 25 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	AZ	100	1701	534	862	153	148	4	0	0

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	A0	215	3589	1130	1802	339	313	5	0	0

- Molecule 27 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	A1	277	4526	1424	2281	382	428	11	0	0

- Molecule 28 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	A2	117	1906	579	971	182	166	8	0	0

- Molecule 29 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	A3	70	1327	401	702	134	89	1	0	0

- Molecule 30 is a RNA chain called A/A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
30	Aw	68	2159	646	725	248	472	68	0	0

- Molecule 31 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
31	Ax	70	2232	665	750	260	487	70	0	0

- Molecule 32 is a RNA chain called E/E-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
32	Ay	70	2235	665	752	261	487	70	0	0

- Molecule 33 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
33	A	1558	49872	14843	16802	5963	10706	1558	0	0

- Molecule 34 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
34	B	72	2303	685	779	269	498	72	0	0

- Molecule 35 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	D	238	3787	1157	1928	376	317	9	0	0

- Molecule 36 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	E	305	4830	1545	2424	418	432	11	0	0

- Molecule 37 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	F	252	4106	1305	2075	370	350	6	0	0

- Molecule 38 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	I	212	3489	1088	1794	304	292	11	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	J	175	2739	847	1409	237	244	2	0	0

- Molecule 40 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	K	177	2915	936	1460	259	253	7	0	0

- Molecule 41 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	L	115	1835	559	945	171	155	5	0	0

- Molecule 42 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	M	289	4701	1476	2387	427	405	6	0	0

- Molecule 43 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	N	222	3610	1143	1824	326	307	10	0	0

- Molecule 44 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	O	154	2557	792	1298	241	219	7	0	0

- Molecule 45 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	P	144	2344	733	1171	224	211	5	0	0

- Molecule 46 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	Q	238	4004	1268	2025	352	350	9	0	0

- Molecule 47 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	R	140	2374	732	1220	231	187	4	0	0

- Molecule 48 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	S	161	2662	835	1369	227	227	4	0	0

- Molecule 49 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	T	166	2786	875	1417	254	233	7	0	0

- Molecule 50 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	U	152	2486	788	1235	234	226	3	0	0

- Molecule 51 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	V	205	3367	1068	1691	298	302	8	0	0

- Molecule 52 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
52	W	116	1847	577	943	171	153	3	0	0

- Molecule 53 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	X	244	4109	1322	2065	352	365	5	0	0

- Molecule 54 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	Y	181	3159	995	1603	298	259	4	0	0

- Molecule 55 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
55	Z	122	2048	636	1052	186	171	3	0	0

- Molecule 56 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	0	110	1817	554	919	176	162	6	0	0

- Molecule 57 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	1	56	977	296	513	89	77	2	0	0

- Molecule 58 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	2	46	786	233	409	83	60	1	0	0

- Molecule 59 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	3	95	1718	539	886	162	128	3	0	0

- Molecule 60 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	4	38	705	217	363	72	49	4	0	0

- Molecule 61 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
61	5	394	6432	2073	3222	560	566	11	0	0

- Molecule 62 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
62	6	354	5802	1881	2854	525	533	9	0	0

- Molecule 63 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
63	7	294	4796	1529	2406	405	438	18	0	0

- Molecule 64 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
64	8	157	2698	844	1371	235	246	2	0	0

- Molecule 65 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
65	9	124	1985	644	988	170	181	2	0	0

- Molecule 66 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
66	a	100	1659	529	819	152	154	5	0	0

- Molecule 67 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
67	b	151	2395	744	1199	231	218	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	2	ACE	-	acetylation	UNP Q8N983

- Molecule 68 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
68	c	286	4624	1470	2325	397	423	9	0	0

- Molecule 69 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
69	d	241	3971	1273	1986	340	359	13	0	0

- Molecule 70 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
70	e	238	3853	1222	1922	339	364	6	0	0

- Molecule 71 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
71	f	157	2529	799	1277	207	242	4	0	0

- Molecule 72 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
72	g	134	2214	719	1101	193	199	2	0	0

- Molecule 73 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
73	h	110	1780	568	885	156	168	3	0	0

- Molecule 74 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
74	i	97	1690	532	862	165	127	4	0	0

- Molecule 75 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
75	j	94	1492	463	747	144	136	2	0	0

- Molecule 76 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
76	k	101	1562	479	788	148	142	5	0	0

- Molecule 77 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
77	l	82	1364	437	676	120	128	3	0	0

- Molecule 78 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
78	m	92	1554	488	763	159	142	2	0	0

- Molecule 79 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
79	o	94	1608	501	810	165	129	3	0	0

- Molecule 80 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
80	p	147	2433	748	1228	228	225	4	0	0

- Molecule 81 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
81	q	165	2766	865	1377	270	249	5	0	0

- Molecule 82 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
82	r	162	2677	839	1355	252	223	8	0	0

- Molecule 83 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
83	s	386	6306	2023	3151	559	559	14	0	0

- Molecule 84 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
84	t	46	732	228	378	56	70	0	0
84	u	32	541	168	284	40	49	0	0
84	v	32	541	168	284	40	49	0	0
84	w	31	520	159	275	39	47	0	0
84	x	31	520	159	275	39	47	0	0
84	y	31	520	159	275	39	47	0	0

- Molecule 85 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
85	H	202	3398	1067	1737	304	286	4	0	0

- Molecule 86 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
86	z	252	4107	1304	2080	336	381	6	0	0

- Molecule 87 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
87	AY	221	3622	1159	1787	319	352	5	0	0

- Molecule 88 is a protein called Leucine-rich PPR motif-containing protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
88	A5	581	9336	2959	4690	790	871	26	0	0

- Molecule 89 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
89	A4	595	9643	3080	4828	815	892	28	0	0

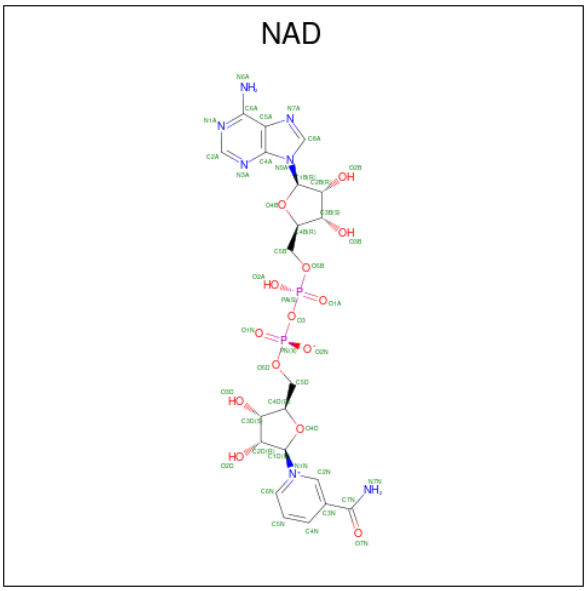
- Molecule 90 is a protein called SRA stem-loop-interacting RNA-binding protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
90	A6	74	1197	384	594	115	103	1	0	0

- Molecule 91 is a RNA chain called mRNA.

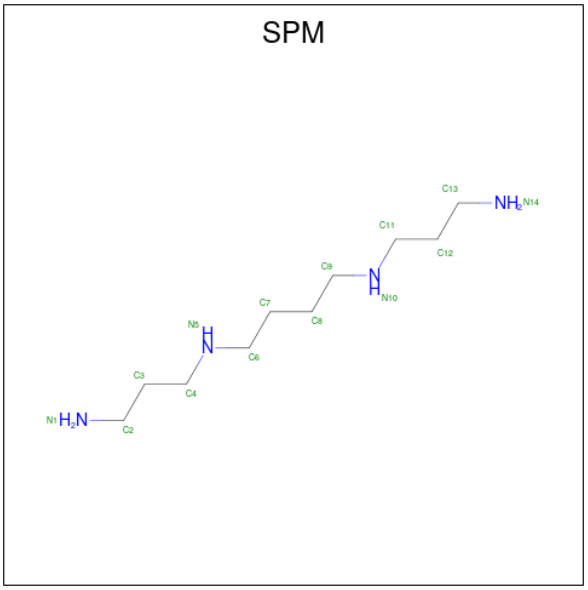
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
91	Az	42	1325	396	445	144	298	42	0	0

- Molecule 92 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



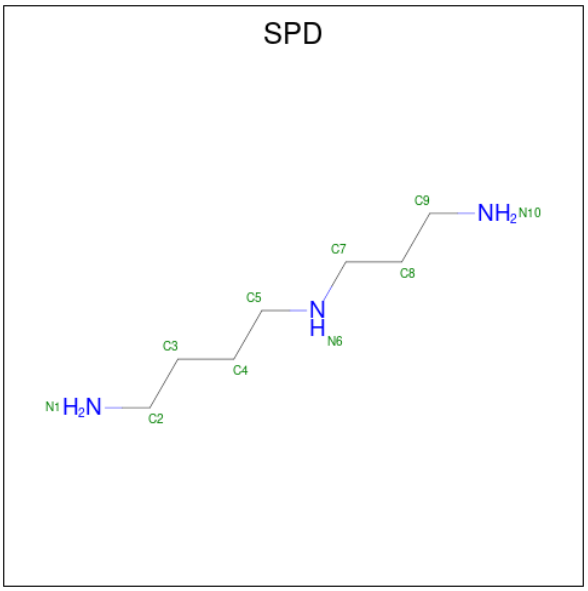
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
92	AA	1	70	21	26	7	14	2	0

- Molecule 93 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
93	AA	1	44	10	30	4	0

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
94	AA	1	32	7	22	3	0
94	A	1	32	7	22	3	0
94	A	1	32	7	22	3	0
94	A	1	32	7	22	3	0

- Molecule 95 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
95	AA	62	62	62	0
95	AB	1	1	1	0
95	AX	1	1	1	0
95	A3	1	1	1	0
95	Aw	1	1	1	0
95	A	136	136	136	0
95	D	2	2	2	0
95	E	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
95	g	1	1	1	0

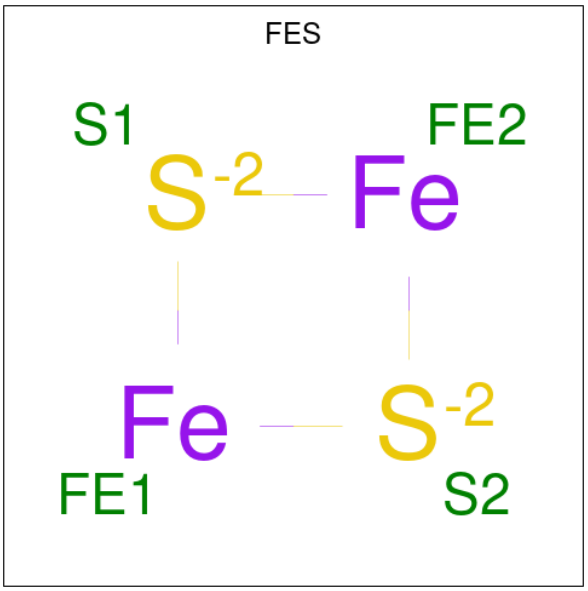
- Molecule 96 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
96	AA	16	16	16	0
			Total	K	
96	A	28	28	28	0
			Total	K	
96	D	1	1	1	0
			Total	K	
96	M	1	1	1	0
			Total	K	
96	P	1	1	1	0
			Total	K	
96	i	1	1	1	0
			Total	K	
96	o	1	1	1	0

- Molecule 97 is ZINC ION (CCD ID: ZN) (formula: Zn).

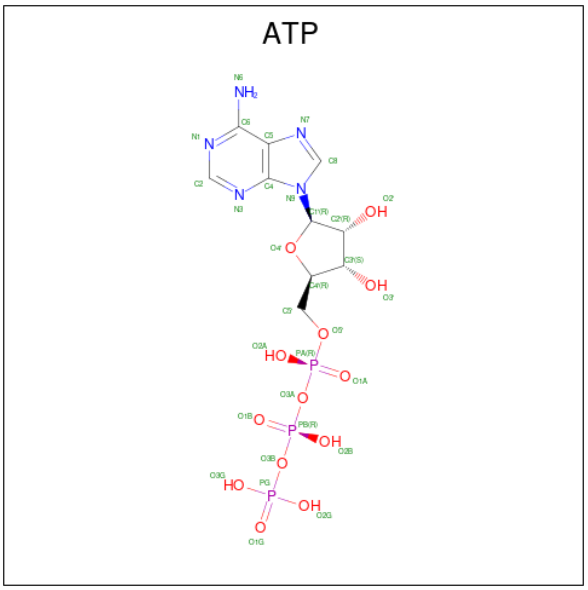
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
97	AO	1	1	1	0
			Total	Zn	
97	0	1	1	1	0
			Total	Zn	
97	4	1	1	1	0

- Molecule 98 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



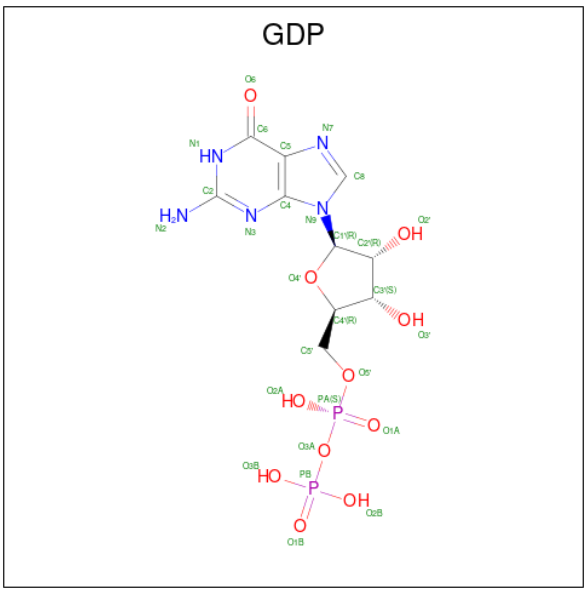
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
98	AP	1	4	2	2	0
98	AT	1	4	2	2	0
98	r	1	4	2	2	0

- Molecule 99 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



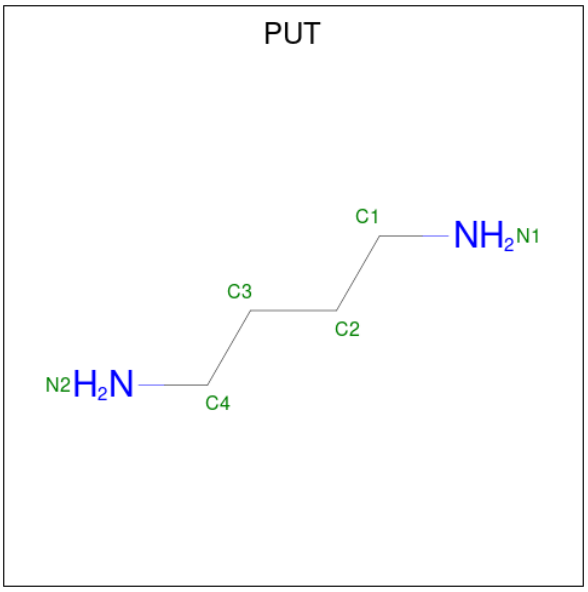
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
99	AX	1	43	10	12	5	13	3	0

- Molecule 100 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



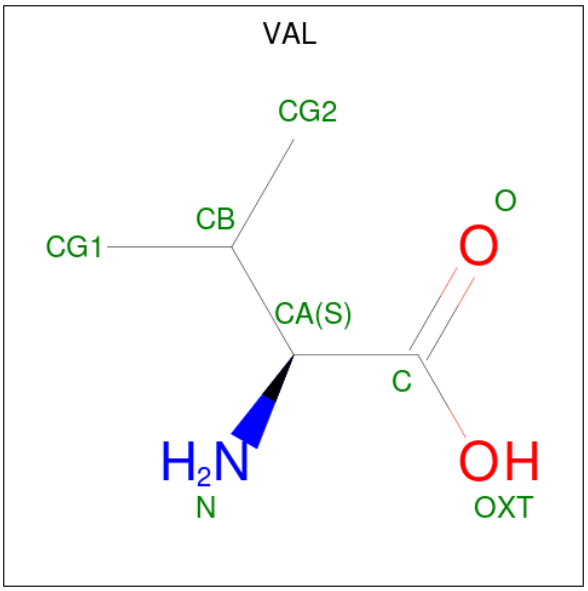
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
100	AX	1	40	10	12	5	11	2	0

- Molecule 101 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
101	A	1	20	4	14	2	0

- Molecule 102 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
102	B	1	18	5	11	1	1	0

- Molecule 103 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
103	AA	1747	1747	1747	0
103	AB	60	60	60	0
103	AC	48	48	48	0
103	AD	66	66	66	0
103	AE	20	20	20	0
103	AF	29	29	29	0
103	AG	53	53	53	0
103	AH	46	46	46	0
103	AI	30	30	30	0
103	AJ	14	14	14	0
103	AK	49	49	49	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
103	AL	42	42	42	0
			Total	O	
103	AM	13	13	13	0
			Total	O	
103	AN	29	29	29	0
			Total	O	
103	AO	33	33	33	0
			Total	O	
103	AP	23	23	23	0
			Total	O	
103	AQ	52	52	52	0
			Total	O	
103	AR	9	9	9	0
			Total	O	
103	AS	18	18	18	0
			Total	O	
103	AT	26	26	26	0
			Total	O	
103	AU	4	4	4	0
			Total	O	
103	AW	9	9	9	0
			Total	O	
103	AX	44	44	44	0
			Total	O	
103	AZ	24	24	24	0
			Total	O	
103	A0	2	2	2	0
			Total	O	
103	A1	36	36	36	0
			Total	O	
103	A2	26	26	26	0
			Total	O	
103	A3	43	43	43	0
			Total	O	
103	Aw	4	4	4	0
			Total	O	
103	Ax	8	8	8	0
			Total	O	
103	Ay	1	1	1	0
			Total	O	
103	A	2847	2847	2847	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
103	B	55	55	55	0
			Total	O	
103	D	68	68	68	0
			Total	O	
103	E	57	57	57	0
			Total	O	
103	F	74	74	74	0
			Total	O	
103	I	21	21	21	0
			Total	O	
103	K	68	68	68	0
			Total	O	
103	L	27	27	27	0
			Total	O	
103	M	46	46	46	0
			Total	O	
103	N	50	50	50	0
			Total	O	
103	O	34	34	34	0
			Total	O	
103	P	69	69	69	0
			Total	O	
103	Q	26	26	26	0
			Total	O	
103	R	59	59	59	0
			Total	O	
103	S	43	43	43	0
			Total	O	
103	T	47	47	47	0
			Total	O	
103	U	25	25	25	0
			Total	O	
103	V	6	6	6	0
			Total	O	
103	W	49	49	49	0
			Total	O	
103	X	11	11	11	0
			Total	O	
103	Y	23	23	23	0
			Total	O	
103	Z	35	35	35	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
103	0	27	27	27	0
			Total	O	
103	1	2	2	2	0
			Total	O	
103	2	33	33	33	0
			Total	O	
103	3	43	43	43	0
			Total	O	
103	4	11	11	11	0
			Total	O	
103	5	15	15	15	0
			Total	O	
103	6	69	69	69	0
			Total	O	
103	7	11	11	11	0
			Total	O	
103	8	14	14	14	0
			Total	O	
103	9	16	16	16	0
			Total	O	
103	a	9	9	9	0
			Total	O	
103	b	32	32	32	0
			Total	O	
103	c	16	16	16	0
			Total	O	
103	d	6	6	6	0
			Total	O	
103	e	8	8	8	0
			Total	O	
103	f	18	18	18	0
			Total	O	
103	g	10	10	10	0
			Total	O	
103	i	50	50	50	0
			Total	O	
103	j	21	21	21	0
			Total	O	
103	l	1	1	1	0
			Total	O	
103	m	8	8	8	0

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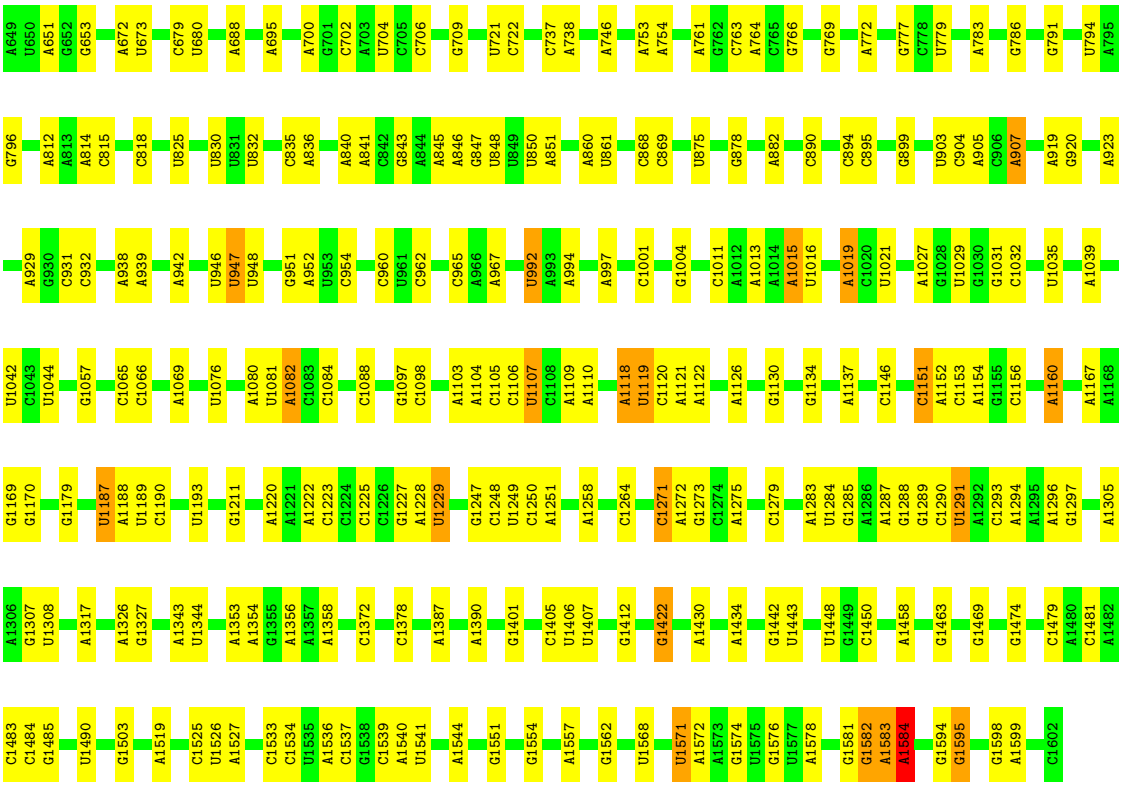
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
103	o	33	33	33	0
			Total	O	
103	p	4	4	4	0
			Total	O	
103	r	35	35	35	0
			Total	O	
103	s	40	40	40	0
			Total	O	
103	H	7	7	7	0
			Total	O	
103	AY	20	20	20	0
			Total	O	
103	A4	7	7	7	0
			Total	O	
103	Az	12	12	12	0

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.

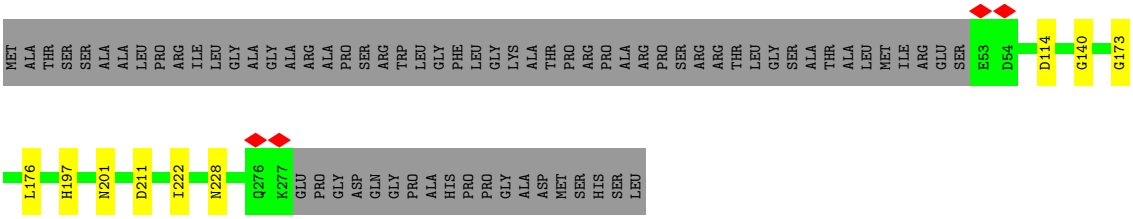
- Molecule 1: 12S mitochondrial rRNA

Chain AA: 74% 24%



- Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain AB: 73% 24%

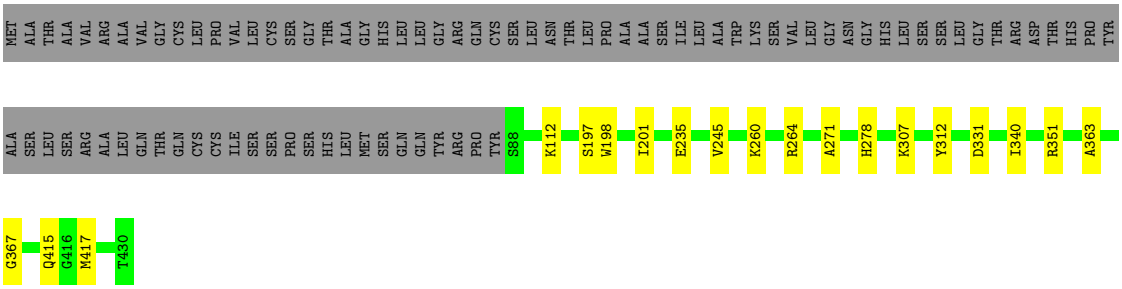


• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC:

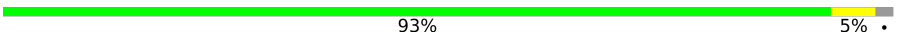
• Molecule 4: 28S ribosomal protein S5, mitochondrial

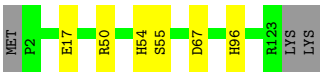
Chain AD:



• Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain AE:



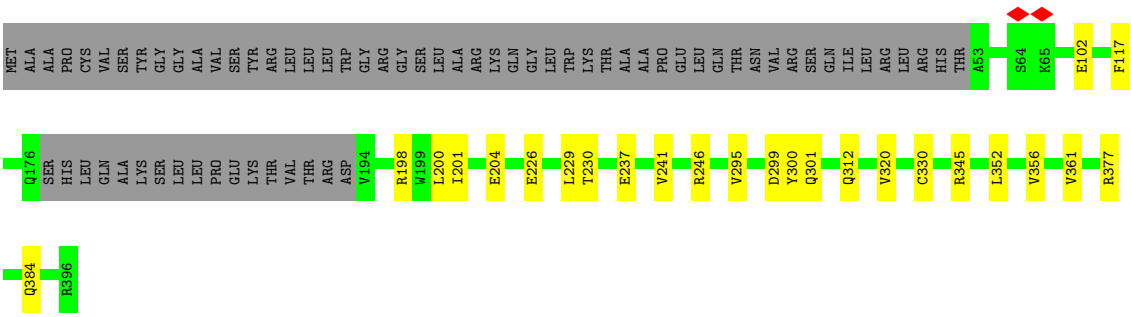


• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain AF:

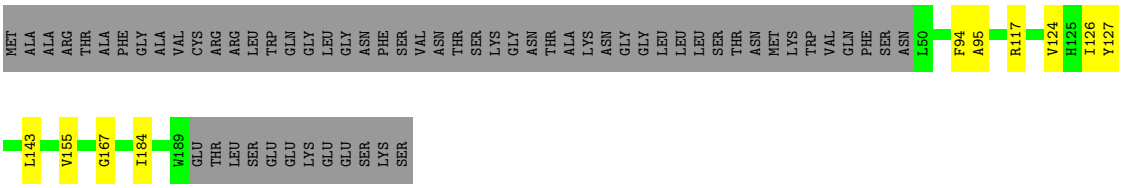
• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain AG:



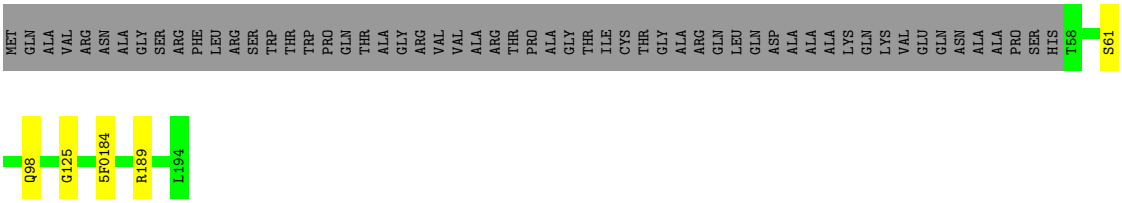
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain AH: 65% 5% 30%



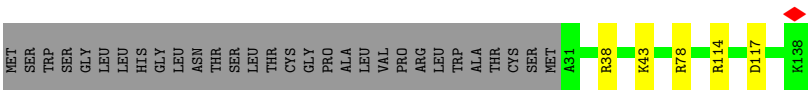
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain AI: 68% 29%



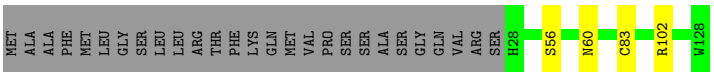
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain AJ: 75% 22%



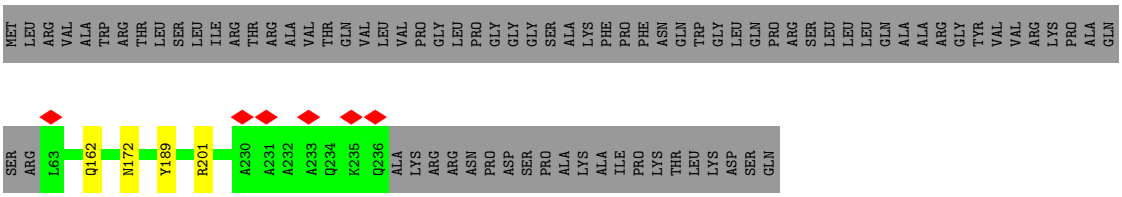
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain AK: 76% 21%



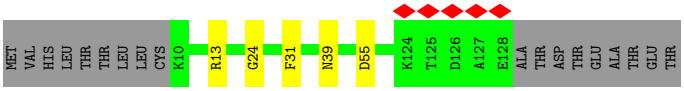
• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain AL: 66% 32%



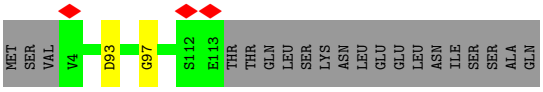
• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain AM: 83% 13%



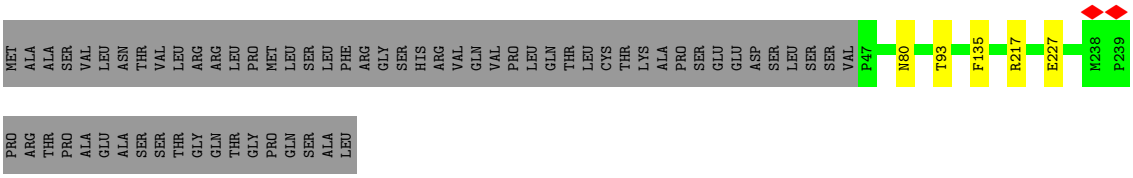
- Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain AN:



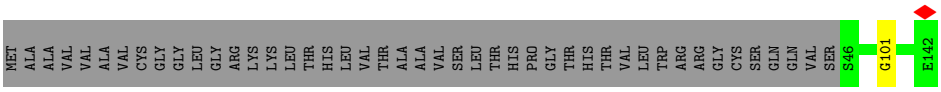
- Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain AO:



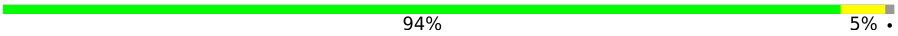
- Molecule 16: 28S ribosomal protein S18c, mitochondrial

Chain AP:



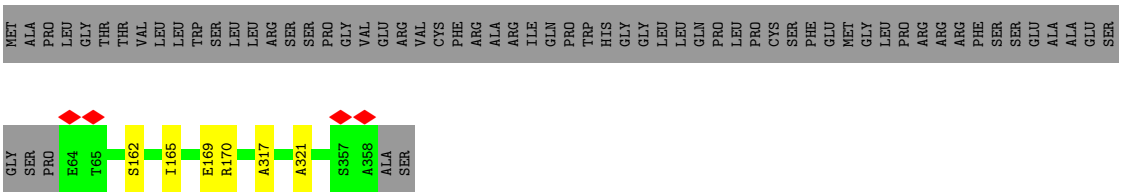
- Molecule 17: 28S ribosomal protein S21, mitochondrial

Chain AQ:



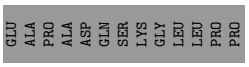
- Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain AR:



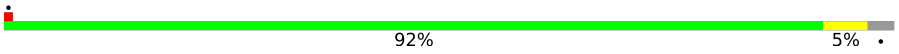
- Molecule 19: 28S ribosomal protein S23, mitochondrial

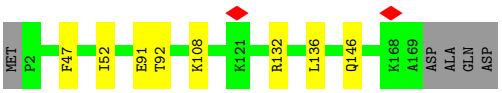
Chain AS:



• Molecule 20: 28S ribosomal protein S25, mitochondrial

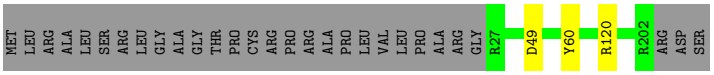
Chain AT:





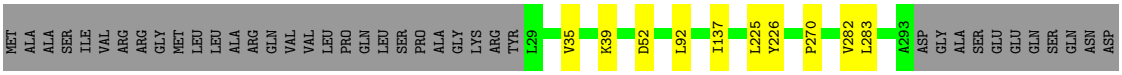
• Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain AU:



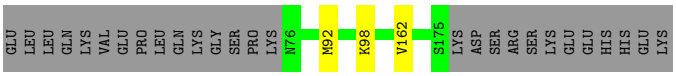
• Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain AV:



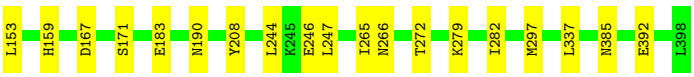
• Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain AW:



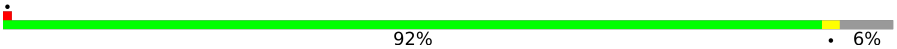
• Molecule 24: 28S ribosomal protein S29, mitochondrial

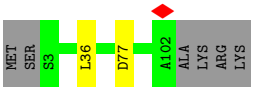
Chain AX:



• Molecule 25: 28S ribosomal protein S33, mitochondrial

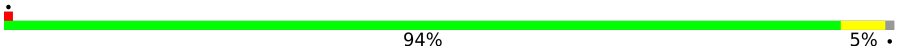
Chain AZ:

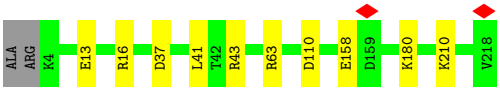




• Molecule 26: 28S ribosomal protein S34, mitochondrial

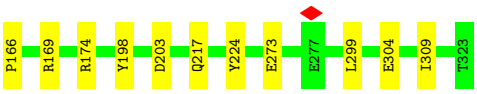
Chain A0:





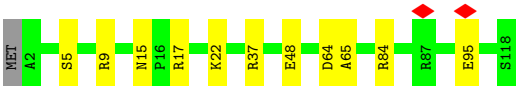
• Molecule 27: 28S ribosomal protein S35, mitochondrial

Chain A1:



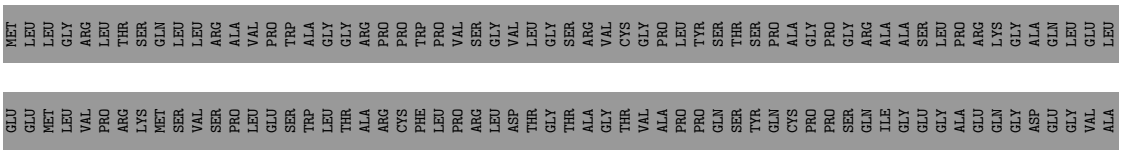
• Molecule 28: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

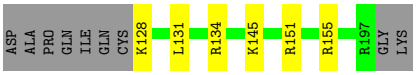
Chain A2:



• Molecule 29: Aurora kinase A-interacting protein

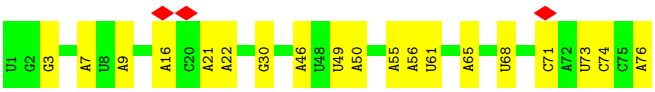
Chain A3:





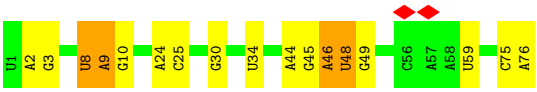
• Molecule 30: A/A-tRNA

Chain Aw:



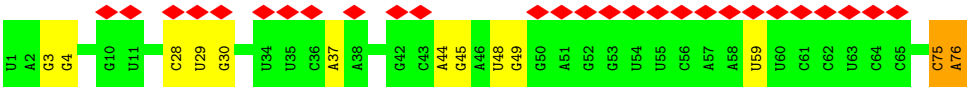
• Molecule 31: P/P-tRNA

Chain Ax:



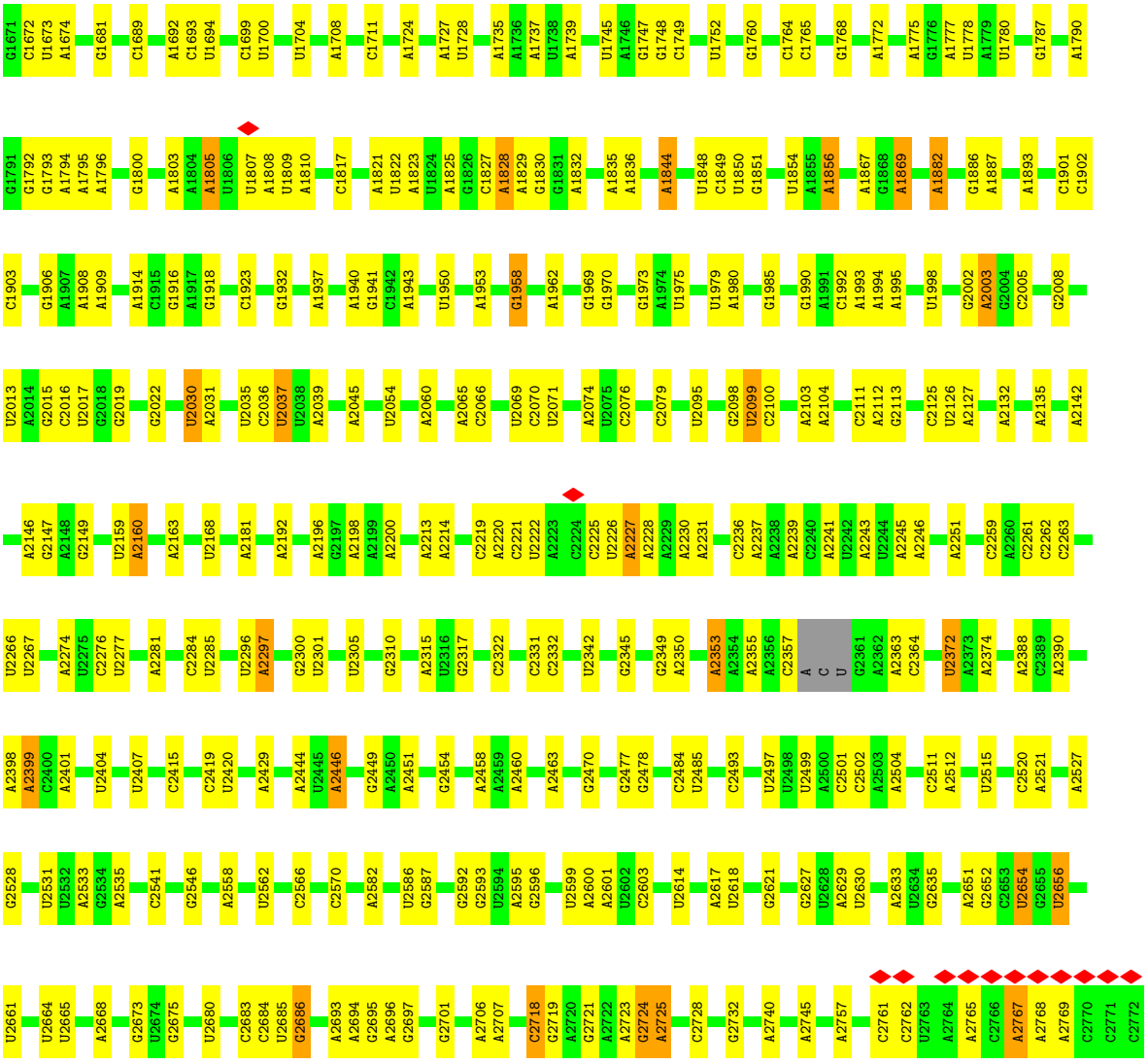
• Molecule 32: E/E-tRNA

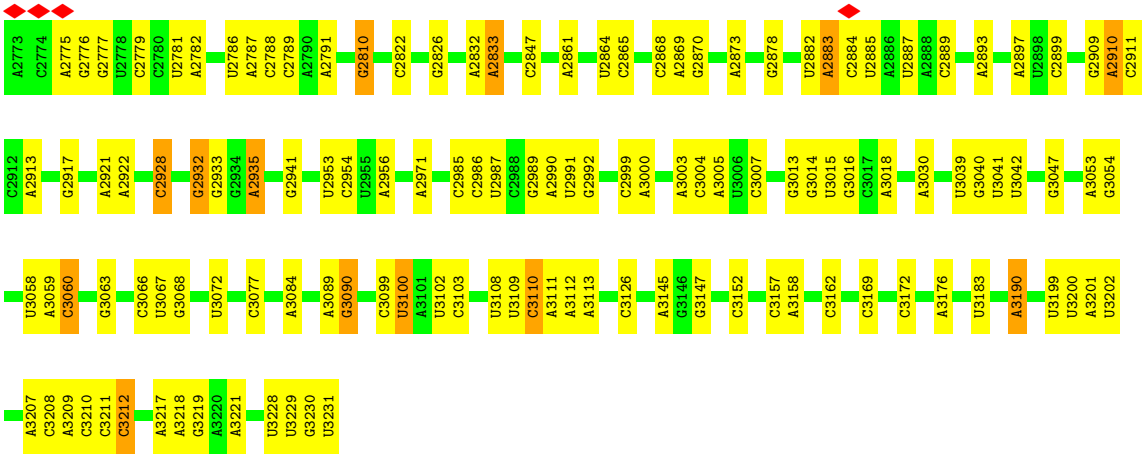
Chain Ay:



• Molecule 33: 16S mitochondrial rRNA

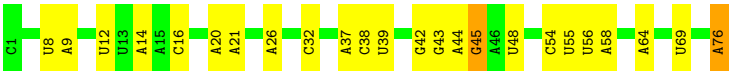
Chain A:





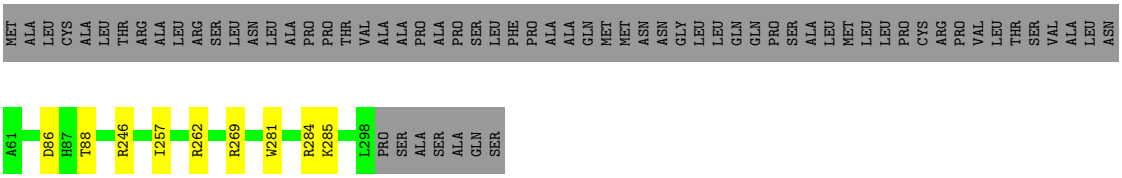
- Molecule 34: mitochondrial tRNAVal

Chain B: 67% 31% •



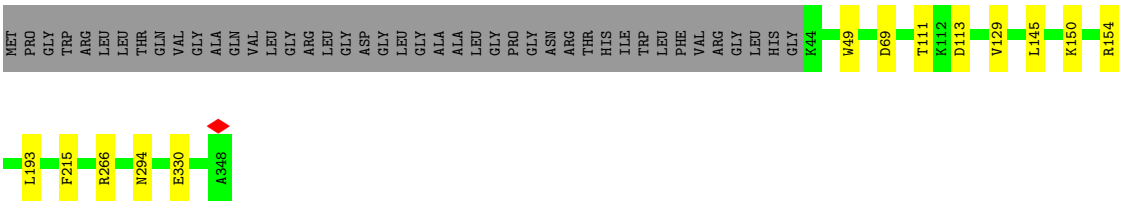
- Molecule 35: 39S ribosomal protein L2, mitochondrial

Chain D: 75% • 22%



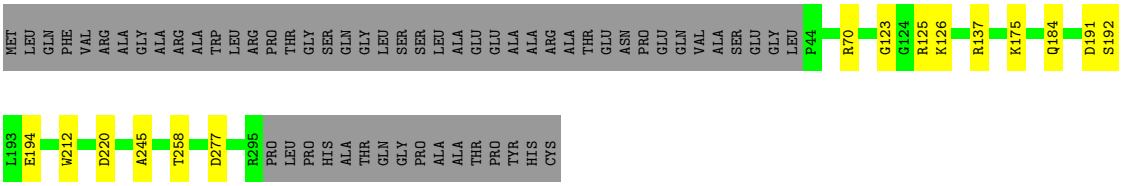
- Molecule 36: 39S ribosomal protein L3, mitochondrial

Chain E: 84% • 12%



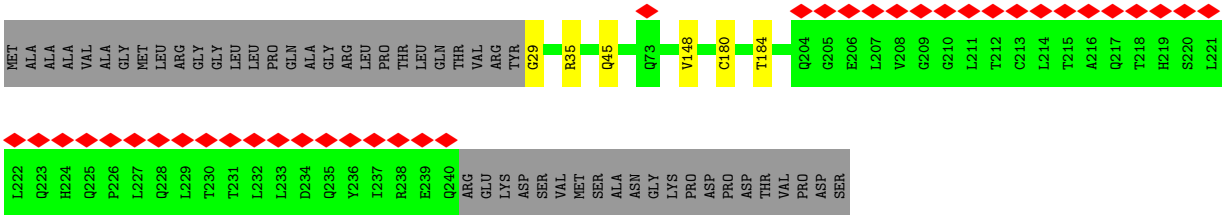
- Molecule 37: 39S ribosomal protein L4, mitochondrial

Chain F: 76% 5% 19%



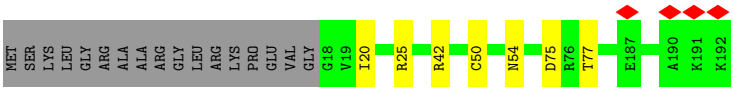
• Molecule 38: 39S ribosomal protein L10, mitochondrial

Chain I: 15% 79% • 19%



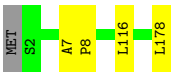
• Molecule 39: 39S ribosomal protein L11, mitochondrial

Chain J: • 88% • 9%



• Molecule 40: 39S ribosomal protein L13, mitochondrial

Chain K: 97% • •



• Molecule 41: 39S ribosomal protein L14, mitochondrial

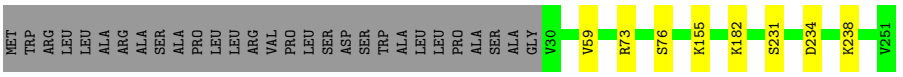
Chain L: 75% • 21%

• Molecule 42: 39S ribosomal protein L15, mitochondrial

Chain M: 93% 5% •

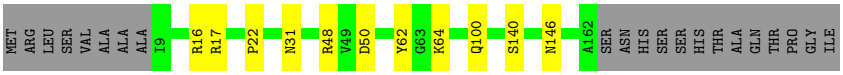
• Molecule 43: 39S ribosomal protein L16, mitochondrial

Chain N: 85% • 12%



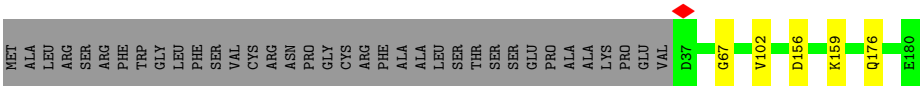
• Molecule 44: 39S ribosomal protein L17, mitochondrial

Chain O: 82% 6% 12%



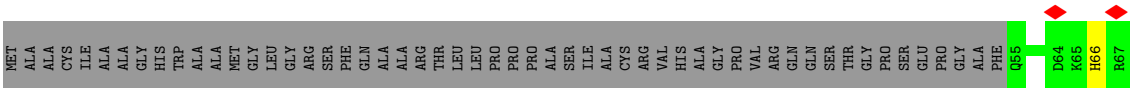
• Molecule 45: 39S ribosomal protein L18, mitochondrial

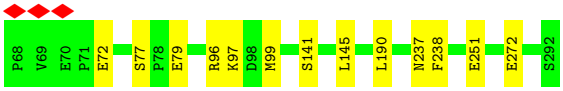
Chain P: 77% 20%



• Molecule 46: 39S ribosomal protein L19, mitochondrial

Chain Q: 77% 5% 18%



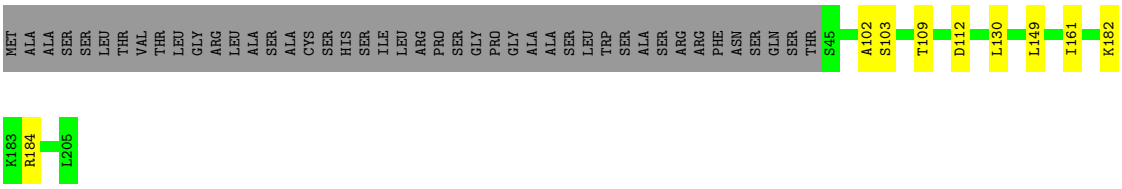


• Molecule 47: 39S ribosomal protein L20, mitochondrial

Chain R: 94% 6%

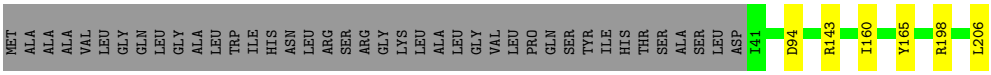
• Molecule 48: 39S ribosomal protein L21, mitochondrial

Chain S: 74% 21%



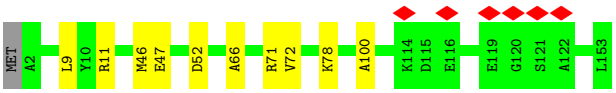
• Molecule 49: 39S ribosomal protein L22, mitochondrial

Chain T: 78% 19%



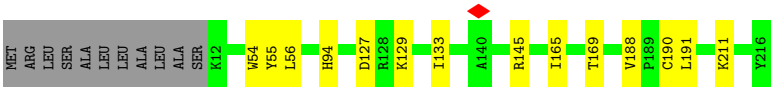
• Molecule 50: 39S ribosomal protein L23, mitochondrial

Chain U: 93% 7%



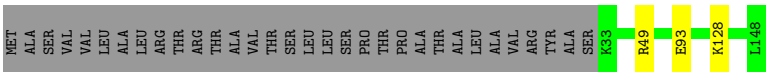
• Molecule 51: 39S ribosomal protein L24, mitochondrial

Chain V: 88% 6% 5%



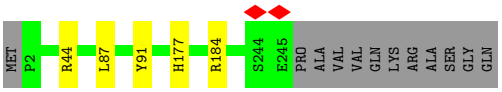
• Molecule 52: 39S ribosomal protein L27, mitochondrial

Chain W: 76% 22%



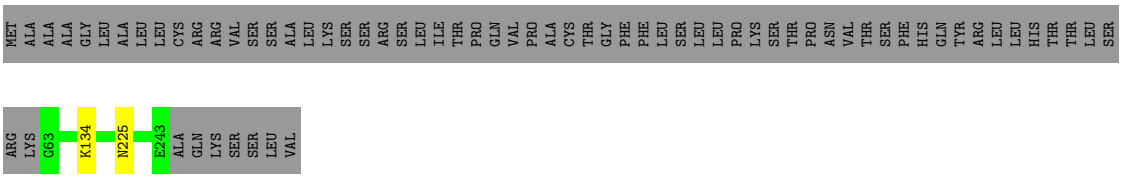
• Molecule 53: 39S ribosomal protein L28, mitochondrial

Chain X: 93% 5%



• Molecule 54: 39S ribosomal protein L47, mitochondrial

Chain Y: 72% 28%



• Molecule 55: 39S ribosomal protein L30, mitochondrial

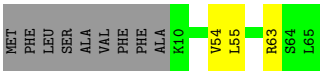
Chain Z: 73% 24%

• Molecule 56: 39S ribosomal protein L32, mitochondrial

Chain 0: 57% 41%

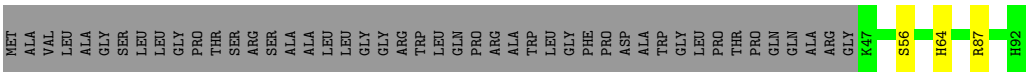
- Molecule 57: 39S ribosomal protein L33, mitochondrial

Chain 1:



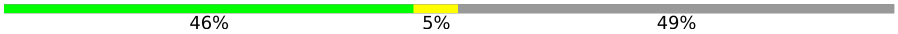
- Molecule 58: 39S ribosomal protein L34, mitochondrial

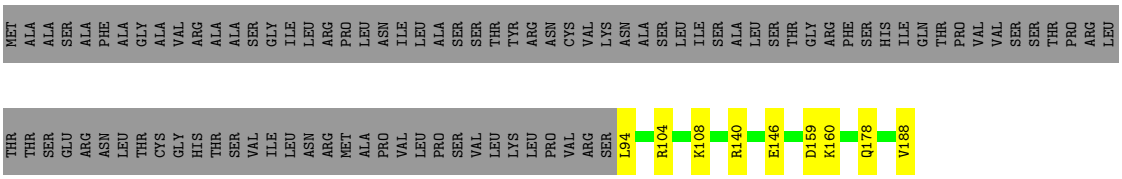
Chain 2:



- Molecule 59: 39S ribosomal protein L35, mitochondrial

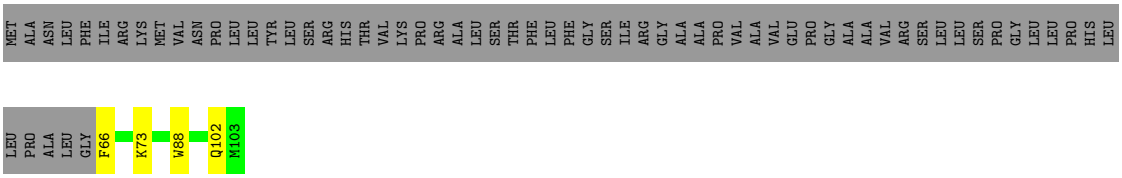
Chain 3:





- Molecule 60: 39S ribosomal protein L36, mitochondrial

Chain 4:

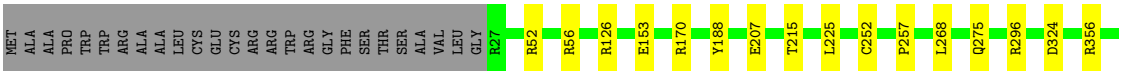


- Molecule 61: 39S ribosomal protein L37, mitochondrial

Chain 5:

- Molecule 62: 39S ribosomal protein L38, mitochondrial

Chain 6:

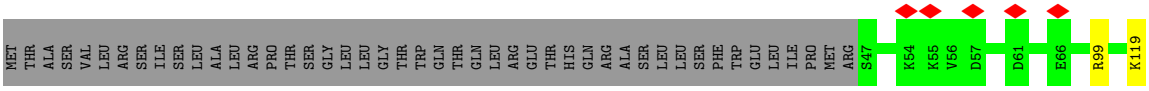


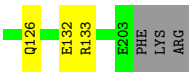
• Molecule 63: 39S ribosomal protein L39, mitochondrial

Chain 7:

• Molecule 64: 39S ribosomal protein L40, mitochondrial

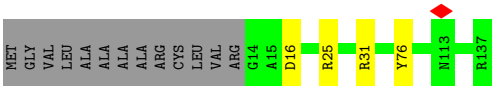
Chain 8:





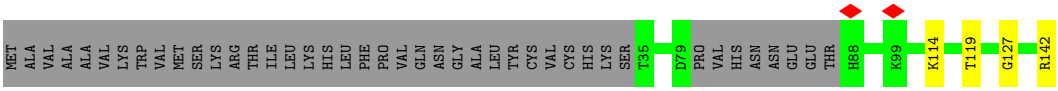
• Molecule 65: 39S ribosomal protein L41, mitochondrial

Chain 9:



• Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a:

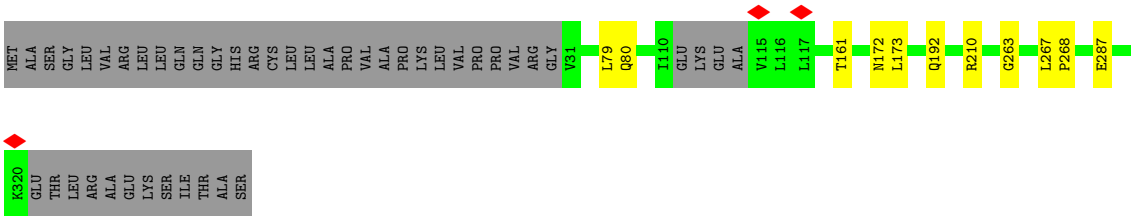


• Molecule 67: Large ribosomal subunit protein mL43

Chain b:

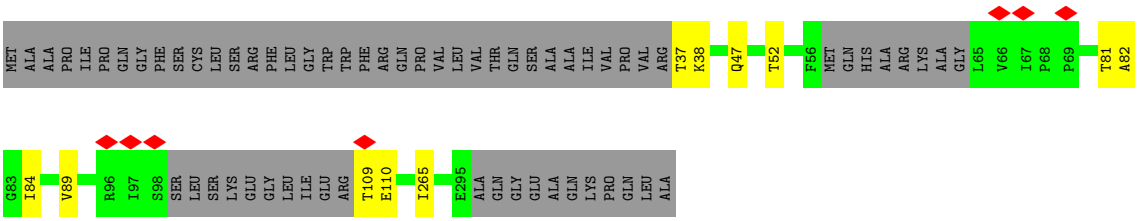
• Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c:



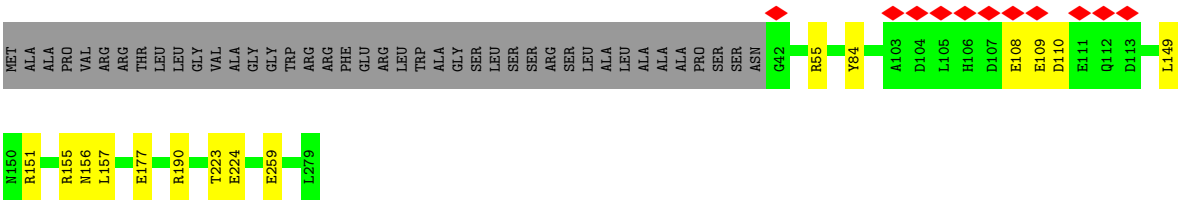
- Molecule 69: 39S ribosomal protein L45, mitochondrial

Chain d:



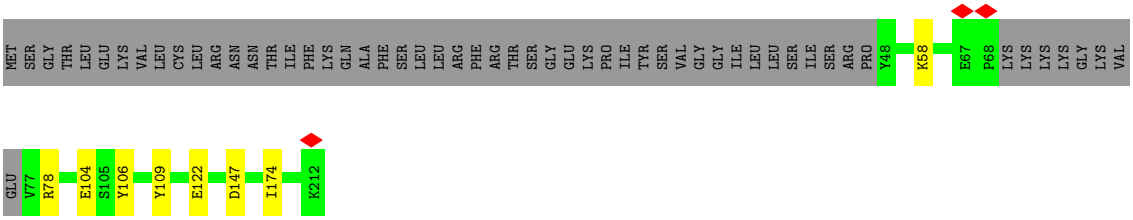
- Molecule 70: 39S ribosomal protein L46, mitochondrial

Chain e:



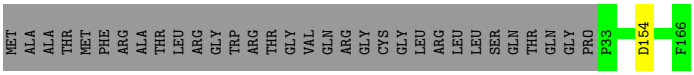
- Molecule 71: 39S ribosomal protein L48, mitochondrial

Chain f:



- Molecule 72: 39S ribosomal protein L49, mitochondrial

Chain g:



• Molecule 73: 39S ribosomal protein L50, mitochondrial

Chain h: 68% • 30%

MET ALA ALA ARG SER VAL SER GLY ILE THR ARG ARG VAL PHE MET TRP THR VAL SER GLY THR PRO CYS ARG GLU PHE TRP SER ARG PHE ARG LYS GLU LYS GLU PRO VAL VAL VAL GLU THR VAL GLU GLU LYS LYS GLU PRO I49 R69 D107 Y158

• Molecule 74: 39S ribosomal protein L51, mitochondrial

Chain i: 73% • 24%

MET ALA GLY ASN LEU LEU SER GLY ALA GLY ARG ARG LEU TRP ASP TRP VAL PRO LEU ALA CYS ARG SER PHE SER LEU GLY VAL PRO ARG LEU I32 G33 I34 K42 K50 Y57 R128

• Molecule 75: 39S ribosomal protein L52, mitochondrial

Chain j: 73% • 24%

MET ALA ALA LEU GLY THR VAL LEU PHE THR GLY VAL ARG ARG LEU HIS CYS SER VAL ALA ALA TRP A23 E45 D53 G54 R70 L116 LYS SER PRO LEU PRO SER GLN

• Molecule 76: 39S ribosomal protein L53, mitochondrial

Chain k: 88% • 10%

MET A2 L10 N46 S102 GLY ASP LYS PRO GLY ALA ASP THR GLY ARG

• Molecule 77: 39S ribosomal protein L54, mitochondrial

Chain l: 59% • 41%

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 A55 D58 K136 ARG

LEU

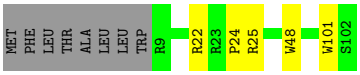
• Molecule 78: 39S ribosomal protein L55, mitochondrial

Chain m: 6% 70% • 28%

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 R72 R94 E97 A98 Q99 L100 Q101 S102 R103 K104 E105 H115 R125 THR LYS LYS

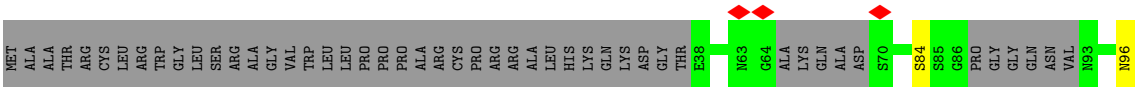
• Molecule 79: Ribosomal protein 63, mitochondrial

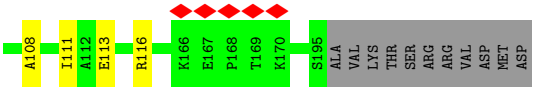
Chain o: 87% 5% 8%



• Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

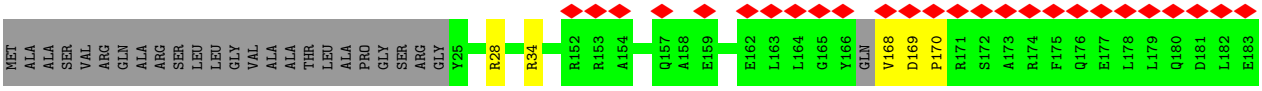
Chain p:

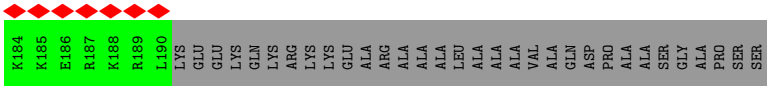




• Molecule 81: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



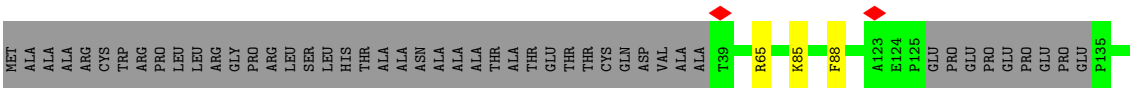


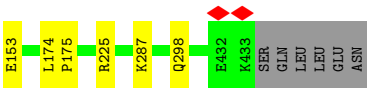
• Molecule 82: 39S ribosomal protein S18a, mitochondrial

Chain r:

• Molecule 83: 39S ribosomal protein S30, mitochondrial

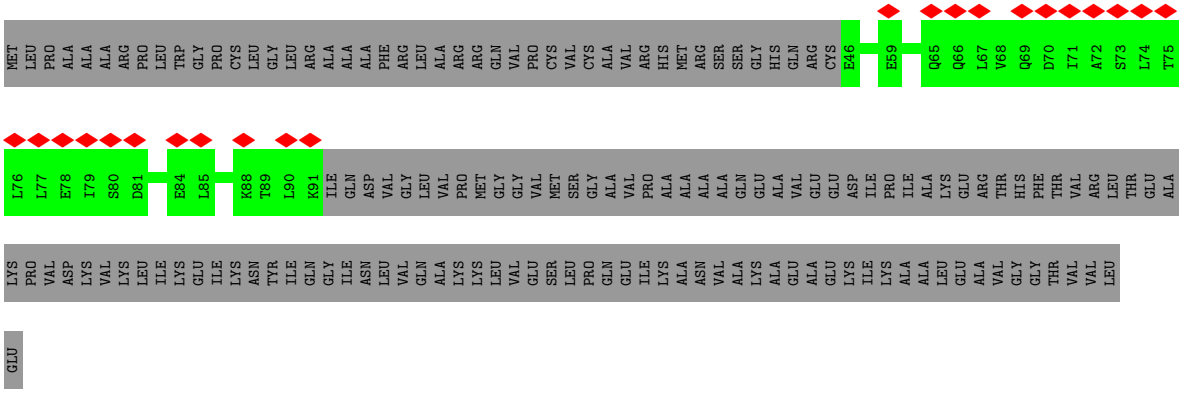
Chain s:





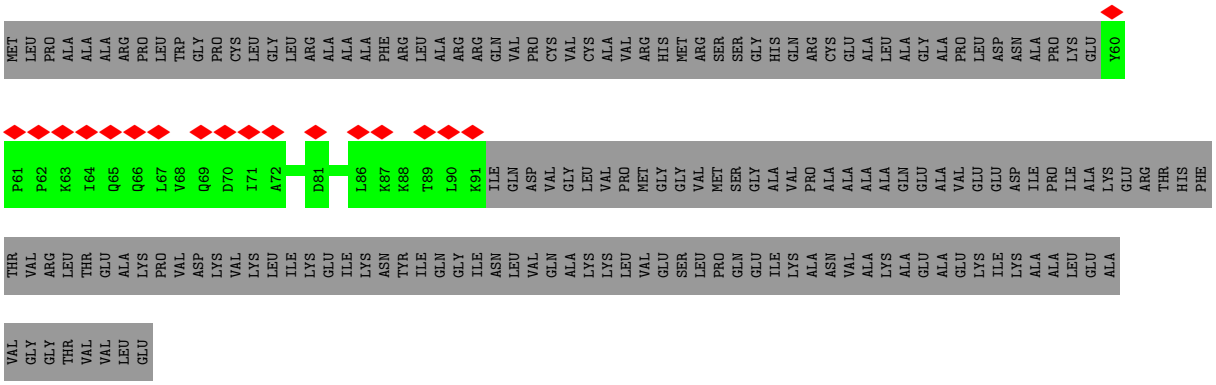
• Molecule 84: 39S ribosomal protein L12, mitochondrial

Chain t:



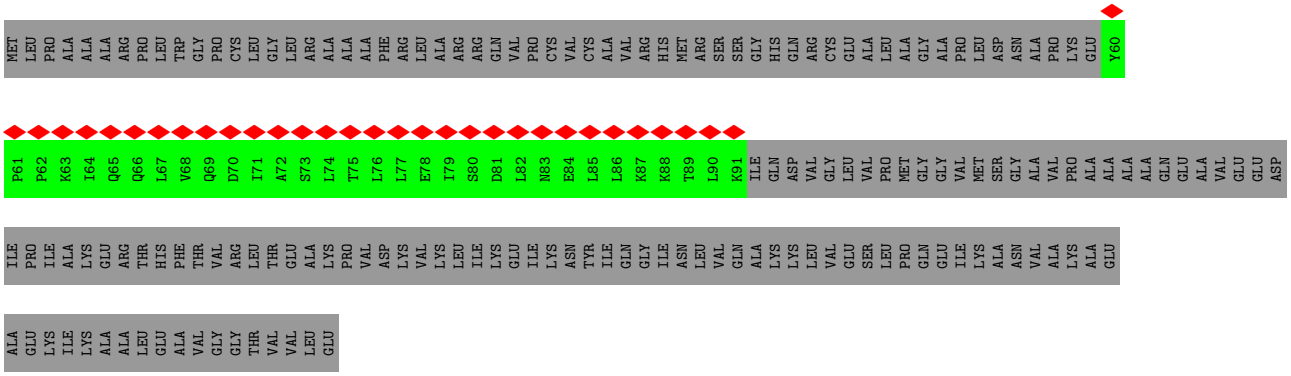
• Molecule 84: 39S ribosomal protein L12, mitochondrial

Chain u:



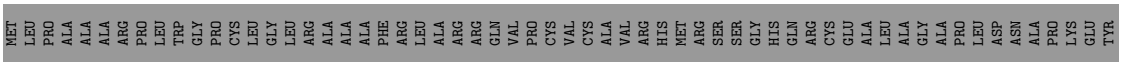
• Molecule 84: 39S ribosomal protein L12, mitochondrial

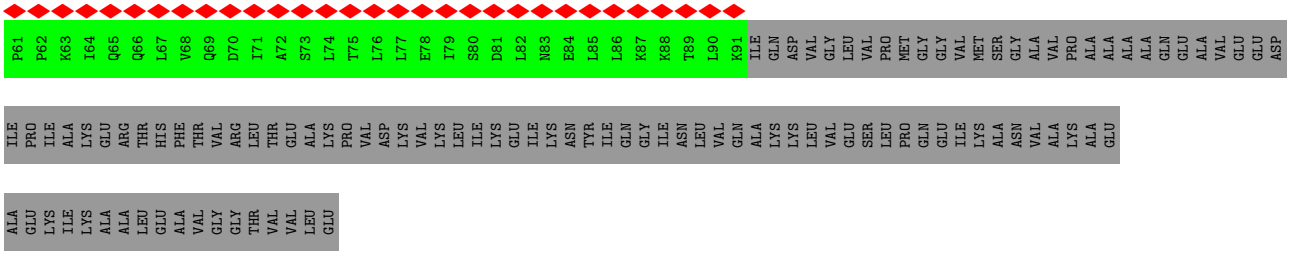
Chain v:



• Molecule 84: 39S ribosomal protein L12, mitochondrial

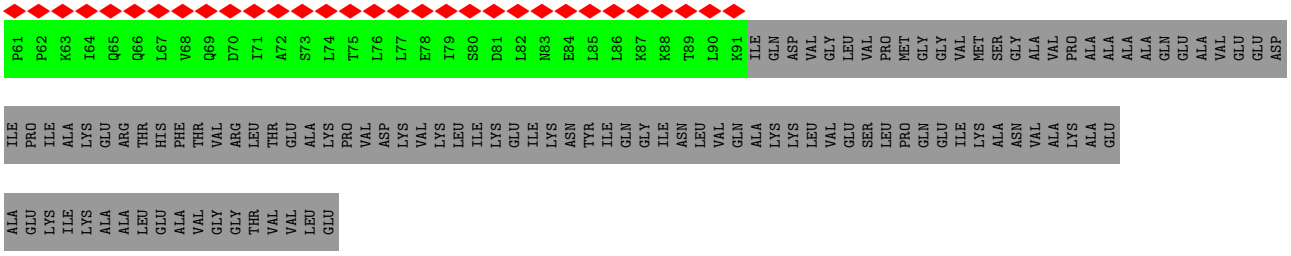
Chain w:





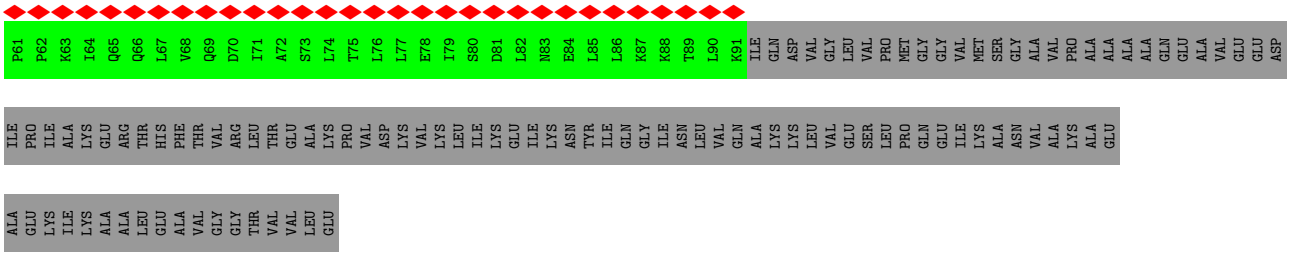
- Molecule 84: 39S ribosomal protein L12, mitochondrial

Chain x:



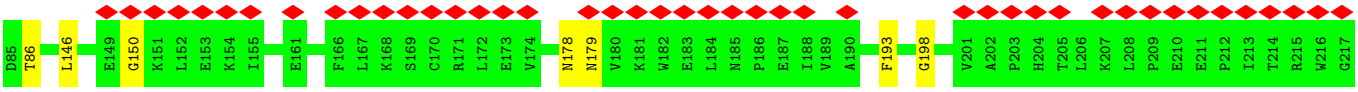
- Molecule 84: 39S ribosomal protein L12, mitochondrial

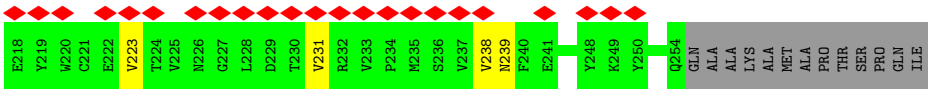
Chain y:



- Molecule 85: 39S ribosomal protein L9, mitochondrial

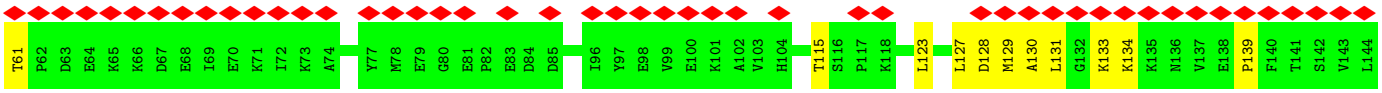
Chain H:

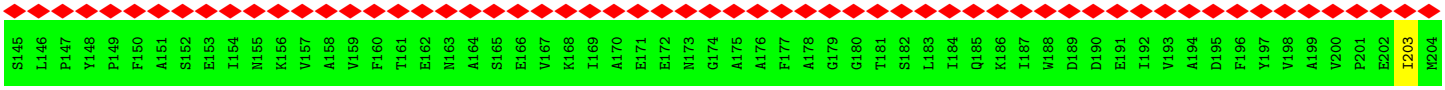


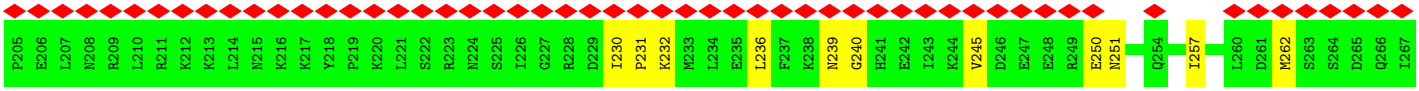


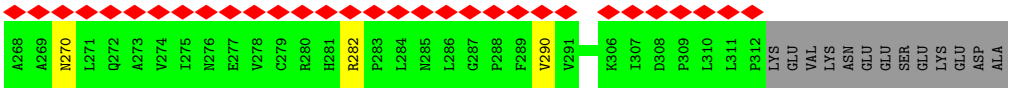
• Molecule 86: 39S ribosomal protein L1, mitochondrial

Chain z:



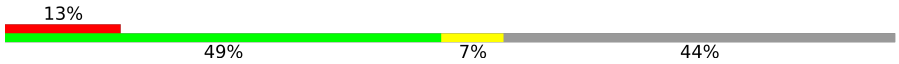


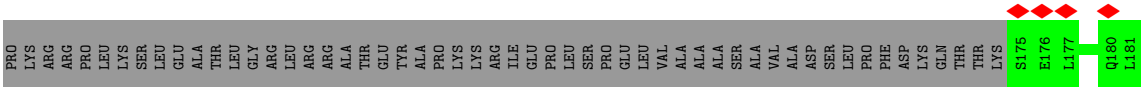


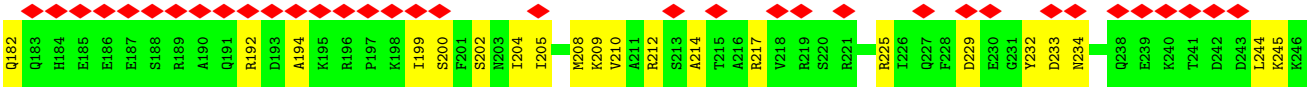


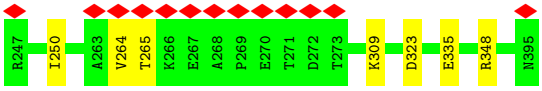
• Molecule 87: 28S ribosomal protein S31, mitochondrial

Chain AY:



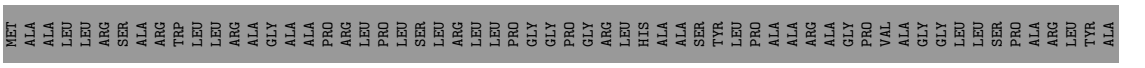


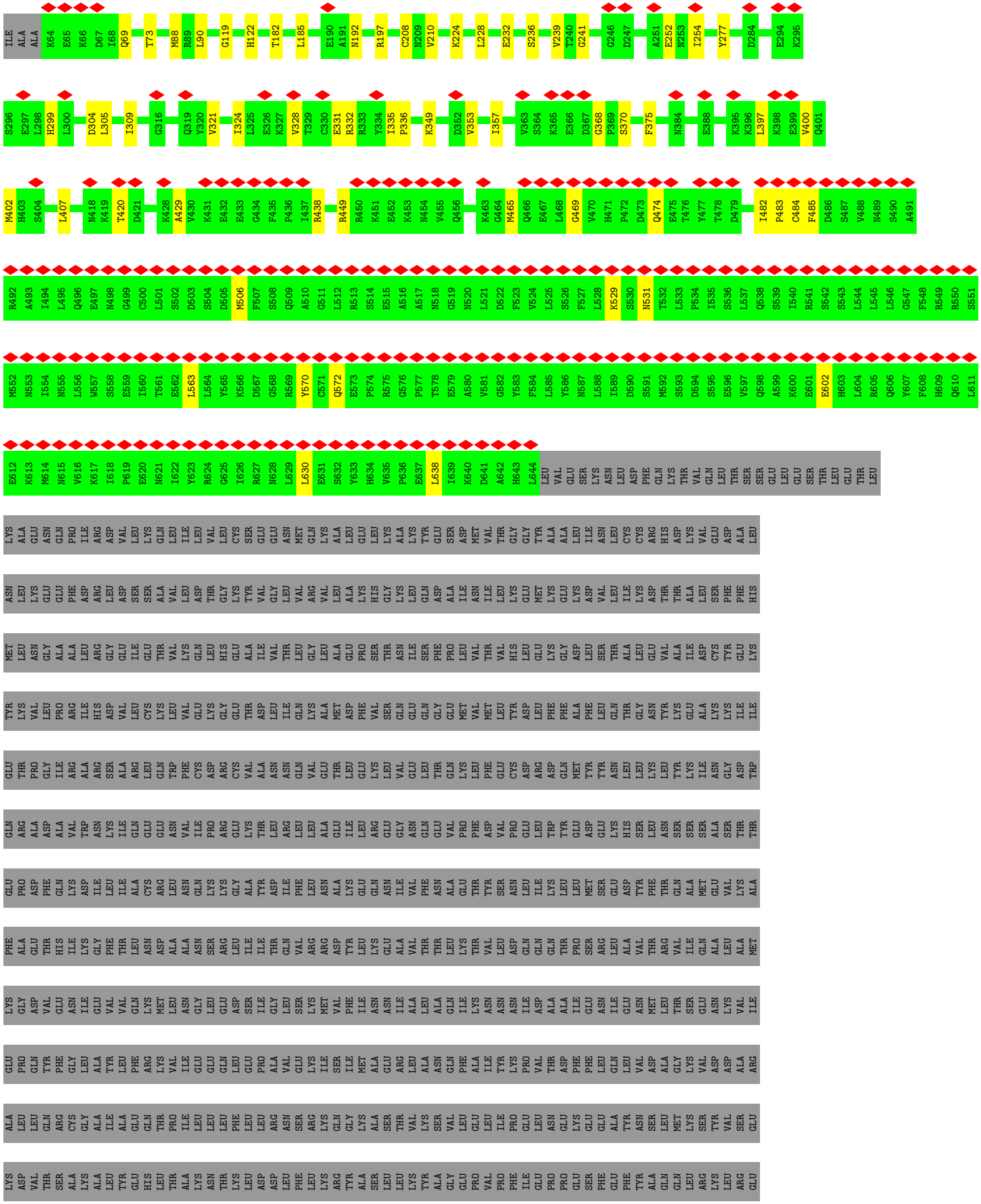




• Molecule 88: Leucine-rich PPR motif-containing protein, mitochondrial

Chain A5:




ILE ALA ALA K64 E65 K66 D67 I68 Q69 T73 M88 R89 L90 G119 H122 T182 L185 E190 A191 N192 R197 C208 N209 V210 K224 L228 E232 S236 V239 T240 G241 G246 D247 A251 E252 N253 I254 Y277 D284 E294 K295
S296 E297 L298 H299 L300 D304 L305 I309 G316 Q319 Y320 V321 I324 L325 E326 K327 V328 T329 G330 E331 R332 R333 Y334 I335 P336 K349 D352 V353 I357 V363 S364 K365 E366 D367 G368 P369 S370 F375 N384 E388 K395 K396 L397 K398 E399 V400 Q401
M402 H403 S404 L407 N418 K419 T420 D421 K428 A429 V430 K431 E432 E433 G434 F435 P436 I437 R438 R449 R450 K451 E452 K453 N454 V455 Q456 K463 G464 M465 Q466 E467 L468 G469 V470 H471 P472 D473 Q474 E475 T476 Y477 T478 D479 I482 P483 C484 F485 D486 S487 V488 N489 S490 A491
R492 A493 I494 L495 Q496 E497 N498 G499 C500 L501 S502 D503 S504 D505 M506 F507 S508 Q509 A510 G511 L512 R513 S514 E515 A516 A517 N518 G519 N520 L521 D522 F523 V524 L525 S526 F527 L528 K529 S530 N531 T532 L533 P534 I535 S536 L537 Q538 S539 I540 R541 S542 S543 L544 L545 L546 G547 F548 R549 R550 S551
M552 N553 I554 N555 L556 W557 S558 E559 I560 T561 E562 L563 L564 Y565 K566 D567 G568 R569 Y570 C571 Q572 E573 P574 R575 G576 P577 T578 E579 A580 V581 G582 Y583 F584 L585 Y586 N587 L588 I589 D590 S591 M592 S593 D594 S595 E596 V597 Q598 A599 K600 E601 E602 H603 L604 R605 Q606 Y607 F608 H609 Q610 L611
E612 K613 M614 N615 V616 K617 I618 P619 E620 N621 I622 Y623 R624 G625 I626 R627 N628 L629 L630 E631 S632 Y633 H634 V635 P636 E637 L638 I639 K640 D641 A642 H643 L644 LEU VAL GLU SER LYS ASN LEU ASP PHE GLN LYS THR VAL GLN LEU THR SER SER GLU LEU GLU SER THR LEU GLU THR LEU
LYS ALA GLU ASN GLN PRO ILE ARG ASP VAL LEU LYS GLN LEU ILE LEU VAL LEU CYS SER GLU GLU ASN MET GLN LYS ALA LEU GLU LEU LYS ALA LYS TYR GLU SER ASP MET VAL THR GLY GLY TYR ALA ALA LEU ILE ASN LEU CYS CYS ARG HIS ASP LYS VAL GLU ASP ALA LEU
ASN LEU LYS GLU GLU PHE ASP ARG LEU ASP SER SER ALA VAL LEU ASP THR GLY LYS TYR VAL GLY LEU VAL ARG VAL LEU ALA LYS HIS GLY LYS LEU GLN ASP ALA ILE ASN ILE LEU LYS GLU MET LYS GLU LYS ASP VAL LEU ILE LYS ASP THR THR ALA LEU SER PHE PHE HIS
MET LEU ASN GLY ALA ALA LEU ARG GLY GLU ILE GLU THR VAL LYS GLN LEU HIS GLU ALA ILE VAL THR LEU GLY LEU ALA GLU PRO SER THR ASN ILE SER PHE PRO LEU VAL THR VAL HIS LEU GLU LYS GLY ASP LEU SER THR ALA LEU GLU VAL ALA ILE ASP CYS TYR GLU LYS
TYR LYS VAL LEU PRO ARG ILE HIS ASP VAL LEU CYS LYS LEU VAL GLU LYS GLY GLU THR ASP LEU ILE GLN LYS ALA MET ASP PHE VAL SER GLN GLU GLN GLY GLU MET VAL MET LEU TYR ASP LEU PHE PHE PHE ALA ALA PHE LEU GLN THR THR GLY ASN TYR LYS ASP LEU ILE LYS LYS ILE ILE
GLU THR PRO GLY ILE ARG ALA ARG SER ALA ARG LEU GLN TRP PHE CYS ASP ARG CYS VAL ALA ASN ASN GLN VAL GLU THR LEU GLU LYS LEU VAL GLU LEU THR GLN LYS LEU PHE GLU CYS ASP ARG ASP GLN MET TYR TYR ASN LEU LEU LYS LYS TYR ILE ASN GLY ASP TRP
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GLU PRO ASP PHE GLN LYS ASP ILE LEU ILE ALA CYS ARG LEU ASN ALA GLN ILE LYS GLY ALA TYR ASP ILE PHE LEU ASN ALA LYS GLU GLN ASN ILE VAL PHE ASN ALA GLU THR TYR SER ASN LEU ILE LYS LEU LEU MET SER GLU ASP TYR PHE THR ASN SER GLN ALA MET GLU VAL LYS ALA
PHE ALA GLU THR HIS ILE LYS GLY PHE THR LEU ASN ASP ALA ALA ASN SER ARG LEU ILE ILE THR GLN VAL ARG ARG ASP TYR LEU LYS ASN GLU ALA VAL THR THR LEU ASP GLN GLN GLN THR PRO SER ARG LEU ALA VAL THR ARG VAL ILE GLN ALA LEU ALA MET
LYS GLY ASP VAL GLU ASN ILE GLU VAL VAL GLN LYS MET LEU ASN GLY LEU GLU SER LYS MET VAL PHE ILE ASN ASN ILE ALA LEU ALA LYS ASN ASN ILE ASP ALA ALA ILE GLU GLU ASN ILE ILE MET SER GLU ASP TYR ILE GLU ALA VAL THR ARG VAL LYS ILE
GLU PRO GLN TYR PHE GLY LEU ALA TYR LEU PHE ARG LYS VAL LEU ALA GLU GLU GLN GLU PRO ALA VAL GLU LYS ILE SER ILE ILE MET ALA GLU ARG LEU ALA ASN GLN PHE ALA ILE TYR LYS PRO VAL THR ASP PHE PHE LEU GLN LEU ASN ASN ILE ILE ALA LEU ALA ARG
ALA LEU LEU GLN ARG CYS GLY ALA ILE ALA LEU THR PRO ILE LEU LEU LEU PHE LEU ARG ASN SER ARG LYS GLN GLY LYS GLU ALA SER THR ASP VAL LEU GLU LYS ILE ILE ILE GLU LEU ILE ILE LYS LEU LEU MET SER GLU ASP ILE ILE ILE LYS ILE ILE ILE LEU ILE ILE
LYS ASP VAL THR SER ALA LYS ALA LEU TYR GLU HIS LEU THR ALA LYS ASN THR LYS LEU ASP LEU PHE LEU LYS ARG TYR ALA SER LEU LEU LYS TYR ALA GLY GLU PRO VAL PRO PHE ILE GLU PRO PRO GLU SER PHE GLU PHE TYR ALA LEU ARG LEU LYS GLU ALA ARG GLU ARG

ASN SER SER

• Molecule 89: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4:

MET ALA VAL VAL SER ALA VAL ARG TRP LEU GLY LEU ARG SER ARG LEU GLY GLN PRO LEU THR GLY ARG ARG ALA GLY LEU CYS GLU GLN ALA ARG SER CYS ARG PHE TYR SER GLY SER ALA THR LEU SER LYS VAL GLU GLY THR ASP VAL THR GLY ILE E55 V58 K67

Y87 E134 D200 H208 PHE GLN GLN THR GLY GLN SER GLU ALA LEU GLU GLU GLU ASN ASP GLU THR SER ARG ARG LYS ALA GLY HIS Q233 F234 N243 C303 N306 R344 L354 R358 Y372 Q381 P382 G383 D384 P385 L386 K387 R388 F391 L400

D501 R537 I564 R565 Q566 T567 A568 Q569 I605 M622 E632 S635 Q647 R648 S651 N656 N665 L666 T667 A668 L669 T670 S671 D672 S673 ASP THR ASP SER SER SER ASP SER ASP SER ASP THR SER GLU GLY LYS

• Molecule 90: SRA stem-loop-interacting RNA-binding protein, mitochondrial

Chain A6:

MET ALA ALA SER ALA ALA ARG GLY ALA ALA ALA LEU ARG ARG SER ILE ASN GLN PRO V20 V23 R24 R25 A30 A31 S32 S33 Q34 L35 K36 E37 H38 F39 A40 Q41 F42 G43 H44 V45 R46 R47 C48 I49 L50 P51 F52 D53 K54 E55 R60 G61 L62 G63 W64 V65 Q66 F67

S68 S69 E70 E71 G72 L73 R74 N75 A76 L77 Q78 Q79 E80 N81 H82 I83 I84 D85 G86 V87 K88 V91 H92 T93 ARG ARG PRO LYS LEU PRO GLN THR SER ASP ASP GLU LYS LYS ASP PHE

• Molecule 91: mRNA

Chain Az:

U-1 U0 U1 G6 G7 U8 U11 U12 U13 A14 U15 A18 A22 U25 A26 C27 G31 A32 U33 C34 A35 C36 C37 U38 U39 C40

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82522	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.335	Depositor
Minimum map value	-0.152	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	531.2, 531.2, 531.2	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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: GDP, SPM, ATP, PSU, NAD, SPD, OMG, 1MA, SAC, OMU, ZN, 5F0, 5MU, 5MC, MA6, K, MG, B8T, PUT, 2MG, ACE, FES, AYA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	AA	0.12	0/22537	0.19	0/35085
2	AB	0.09	0/1871	0.24	0/2531
3	AC	0.10	0/1113	0.24	0/1505
4	AD	0.09	0/2783	0.21	0/3724
5	AE	0.08	0/989	0.21	0/1335
6	AF	0.08	0/1767	0.21	0/2373
7	AG	0.09	0/2746	0.21	0/3681
8	AH	0.11	0/1178	0.25	0/1598
9	AI	0.08	0/1030	0.21	0/1386
10	AJ	0.10	0/855	0.25	0/1148
11	AK	0.09	0/880	0.21	0/1182
12	AL	0.08	0/1477	0.20	0/1974
13	AM	0.09	0/963	0.24	0/1295
14	AN	0.09	0/886	0.23	0/1199
15	AO	0.09	0/1648	0.22	0/2243
16	AP	0.10	0/798	0.24	0/1070
17	AQ	0.10	0/748	0.22	0/994
18	AR	0.08	0/2456	0.19	0/3317
19	AS	0.08	0/1138	0.19	0/1533
20	AT	0.09	0/1402	0.24	0/1883
21	AU	0.07	0/1510	0.17	0/2025
22	AV	0.09	0/3030	0.20	0/4093
23	AW	0.09	0/801	0.22	0/1079
24	AX	0.09	0/2921	0.23	0/3954
25	AZ	0.09	0/857	0.22	0/1141
26	A0	0.10	0/1834	0.24	0/2484
27	A1	0.09	0/2293	0.22	0/3102
28	A2	0.08	0/941	0.23	0/1257
29	A3	0.10	0/636	0.25	0/839
30	Aw	0.05	0/1603	0.13	0/2488
31	Ax	0.08	0/1655	0.16	0/2569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Ay	0.06	0/1656	0.15	0/2571
33	A	0.12	0/36876	0.21	0/57402
34	B	0.10	0/1627	0.17	0/2527
35	D	0.09	0/1896	0.25	0/2549
36	E	0.10	0/2475	0.25	0/3355
37	F	0.11	0/2090	0.27	0/2842
38	I	0.10	0/1731	0.25	0/2345
39	J	0.08	0/1348	0.21	0/1813
40	K	0.10	0/1490	0.24	0/2021
41	L	0.09	0/905	0.25	0/1218
42	M	0.10	0/2368	0.27	0/3195
43	N	0.10	0/1833	0.24	0/2468
44	O	0.09	0/1283	0.23	0/1727
45	P	0.12	0/1199	0.24	0/1623
46	Q	0.09	0/2027	0.23	0/2734
47	R	0.10	0/1175	0.22	0/1572
48	S	0.11	0/1320	0.28	0/1789
49	T	0.11	0/1403	0.27	0/1886
50	U	0.10	0/1274	0.24	0/1723
51	V	0.09	0/1721	0.24	0/2333
52	W	0.11	0/926	0.24	0/1244
53	X	0.10	0/2099	0.22	0/2837
54	Y	0.09	0/1593	0.22	0/2136
55	Z	0.10	0/1021	0.27	0/1378
56	0	0.10	0/913	0.23	0/1224
57	1	0.09	0/469	0.24	0/621
58	2	0.11	0/383	0.27	0/507
59	3	0.11	0/853	0.26	0/1136
60	4	0.10	0/350	0.22	0/461
61	5	0.10	0/3305	0.24	0/4502
62	6	0.12	0/3043	0.24	0/4140
63	7	0.09	0/2447	0.25	0/3310
64	8	0.09	0/1354	0.23	0/1819
65	9	0.10	0/1025	0.24	0/1379
66	a	0.11	0/866	0.27	0/1174
67	b	0.12	0/1219	0.25	0/1651
68	c	0.09	0/2347	0.22	0/3171
69	d	0.09	0/2039	0.22	0/2759
70	e	0.08	0/1970	0.22	0/2658
71	f	0.10	0/1273	0.21	0/1716
72	g	0.11	0/1151	0.24	0/1569
73	h	0.08	0/918	0.19	0/1249
74	i	0.11	0/850	0.24	0/1135

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	j	0.11	0/760	0.25	0/1023
76	k	0.08	0/777	0.19	0/1048
77	l	0.08	0/707	0.24	0/960
78	m	0.08	0/805	0.20	0/1081
79	o	0.11	0/819	0.26	0/1097
80	p	0.08	0/1223	0.21	0/1641
81	q	0.08	0/1422	0.19	0/1916
82	r	0.10	0/1362	0.26	0/1846
83	s	0.10	0/3239	0.24	0/4400
84	t	0.06	0/358	0.18	0/486
84	u	0.07	0/259	0.18	0/350
84	v	0.06	0/259	0.15	0/350
84	w	0.08	0/246	0.17	0/331
84	x	0.07	0/246	0.16	0/331
84	y	0.07	0/246	0.16	0/331
85	H	0.09	0/1698	0.22	0/2292
86	z	0.10	0/2067	0.27	0/2793
87	AY	0.11	0/1877	0.26	0/2524
88	A5	0.10	0/4737	0.27	0/6398
89	A4	0.09	0/4924	0.23	0/6663
90	A6	0.08	0/619	0.22	0/835
91	Az	0.10	0/981	0.24	0/1522
All	All	0.10	0/197088	0.22	0/279774

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	20260	10305	10285	129	0
2	AB	1828	1826	1815	9	0
3	AC	1083	1096	1088	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	2731	2814	2804	13	0
5	AE	972	1004	1000	4	0
6	AF	1725	1778	1769	9	0
7	AG	2688	2697	2687	17	0
8	AH	1152	1191	1183	10	0
9	AI	1020	1066	1053	5	0
10	AJ	839	892	887	6	0
11	AK	862	889	885	4	0
12	AL	1453	1545	1540	4	0
13	AM	942	972	965	4	0
14	AN	868	933	928	1	0
15	AO	1592	1570	1557	4	0
16	AP	781	809	806	1	0
17	AQ	744	760	758	5	0
18	AR	2409	2436	2428	4	0
19	AS	1111	1117	1115	6	0
20	AT	1371	1396	1393	6	0
21	AU	1488	1505	1499	3	0
22	AV	2969	2972	2961	9	0
23	AW	789	806	802	2	0
24	AX	2849	2859	2843	18	0
25	AZ	839	862	858	2	0
26	A0	1787	1802	1796	7	0
27	A1	2245	2281	2276	14	0
28	A2	935	971	971	10	0
29	A3	625	702	699	6	0
30	Aw	1434	725	725	2	0
31	Ax	1482	750	752	8	0
32	Ay	1483	752	753	4	0
33	A	33070	16802	16798	244	0
34	B	1524	779	779	13	0
35	D	1859	1928	1920	6	0
36	E	2406	2424	2415	10	0
37	F	2031	2075	2065	10	0
38	I	1695	1794	1785	5	0
39	J	1330	1409	1407	4	0
40	K	1455	1460	1452	3	0
41	L	890	945	941	5	0
42	M	2314	2387	2384	10	0
43	N	1786	1824	1817	7	0
44	O	1259	1298	1294	8	0
45	P	1173	1171	1165	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Q	1979	2025	2022	11	0
47	R	1154	1220	1214	0	0
48	S	1293	1369	1365	9	0
49	T	1369	1417	1410	6	0
50	U	1251	1235	1232	8	0
51	V	1676	1691	1687	11	0
52	W	904	943	935	4	0
53	X	2044	2065	2060	4	0
54	Y	1556	1603	1597	2	0
55	Z	996	1052	1044	4	0
56	0	898	919	916	2	0
57	1	464	513	511	2	0
58	2	377	409	406	3	0
59	3	832	886	883	8	0
60	4	342	363	361	4	0
61	5	3210	3222	3206	6	0
62	6	2948	2854	2841	15	0
63	7	2390	2406	2397	11	0
64	8	1327	1371	1368	5	0
65	9	997	988	987	4	0
66	a	840	819	810	4	0
67	b	1196	1199	1195	9	0
68	c	2299	2325	2320	8	0
69	d	1985	1986	1976	9	0
70	e	1931	1922	1916	9	0
71	f	1252	1277	1269	6	0
72	g	1113	1101	1097	1	0
73	h	895	885	881	1	0
74	i	828	862	857	4	0
75	j	745	747	746	3	0
76	k	774	788	784	1	0
77	l	688	676	674	1	0
78	m	791	763	796	2	0
79	o	798	810	804	6	0
80	p	1205	1228	1223	4	0
81	q	1389	1377	1374	4	0
82	r	1322	1355	1348	10	0
83	s	3155	3151	3139	8	0
84	t	354	378	377	0	0
84	u	257	284	283	0	0
84	v	257	284	283	0	0
84	w	245	275	275	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	x	245	275	275	0	0
84	y	245	275	275	0	0
85	H	1661	1737	1734	12	0
86	z	2027	2080	2076	20	0
87	AY	1835	1787	1780	23	0
88	A5	4646	4690	4674	44	0
89	A4	4815	4828	4810	17	0
90	A6	603	594	588	3	0
91	Az	880	445	445	7	0
92	AA	44	26	26	0	0
93	AA	14	30	26	0	0
94	A	30	66	57	0	0
94	AA	10	22	19	0	0
95	A	136	0	0	0	0
95	A3	1	0	0	0	0
95	AA	62	0	0	0	0
95	AB	1	0	0	0	0
95	AX	1	0	0	0	0
95	Aw	1	0	0	0	0
95	D	2	0	0	0	0
95	E	1	0	0	0	0
95	g	1	0	0	0	0
96	A	28	0	0	0	0
96	AA	16	0	0	1	0
96	D	1	0	0	0	0
96	M	1	0	0	0	0
96	P	1	0	0	1	0
96	i	1	0	0	0	0
96	o	1	0	0	0	0
97	0	1	0	0	0	0
97	4	1	0	0	0	0
97	AO	1	0	0	0	0
98	AP	4	0	0	0	0
98	AT	4	0	0	0	0
98	r	4	0	0	0	0
99	AX	31	12	12	0	0
100	AX	28	12	12	0	0
101	A	6	14	12	0	0
102	B	7	11	8	1	0
103	0	27	0	0	0	0
103	1	2	0	0	0	0
103	2	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
103	3	43	0	0	2	0
103	4	11	0	0	1	0
103	5	15	0	0	1	0
103	6	69	0	0	6	0
103	7	11	0	0	2	0
103	8	14	0	0	3	0
103	9	16	0	0	0	0
103	A	2847	0	0	153	0
103	A0	2	0	0	0	0
103	A1	36	0	0	0	0
103	A2	26	0	0	3	0
103	A3	43	0	0	2	0
103	A4	7	0	0	2	0
103	AA	1747	0	0	87	0
103	AB	60	0	0	8	0
103	AC	48	0	0	4	0
103	AD	66	0	0	3	0
103	AE	20	0	0	1	0
103	AF	29	0	0	1	0
103	AG	53	0	0	2	0
103	AH	46	0	0	4	0
103	AI	30	0	0	4	0
103	AJ	14	0	0	3	0
103	AK	49	0	0	3	0
103	AL	42	0	0	2	0
103	AM	13	0	0	0	0
103	AN	29	0	0	0	0
103	AO	33	0	0	3	0
103	AP	23	0	0	1	0
103	AQ	52	0	0	4	0
103	AR	9	0	0	0	0
103	AS	18	0	0	2	0
103	AT	26	0	0	1	0
103	AU	4	0	0	0	0
103	AW	9	0	0	0	0
103	AX	44	0	0	3	0
103	AY	20	0	0	0	0
103	AZ	24	0	0	2	0
103	Aw	4	0	0	1	0
103	Ax	8	0	0	1	0
103	Ay	1	0	0	1	0
103	Az	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
103	B	55	0	0	8	0
103	D	68	0	0	0	0
103	E	57	0	0	3	0
103	F	74	0	0	5	0
103	H	7	0	0	1	0
103	I	21	0	0	2	0
103	K	68	0	0	1	0
103	L	27	0	0	3	0
103	M	46	0	0	4	0
103	N	50	0	0	3	0
103	O	34	0	0	2	0
103	P	69	0	0	5	0
103	Q	26	0	0	2	0
103	R	59	0	0	0	0
103	S	43	0	0	4	0
103	T	47	0	0	3	0
103	U	25	0	0	2	0
103	V	6	0	0	0	0
103	W	49	0	0	3	0
103	X	11	0	0	0	0
103	Y	23	0	0	1	0
103	Z	35	0	0	1	0
103	a	9	0	0	2	0
103	b	32	0	0	4	0
103	c	16	0	0	2	0
103	d	6	0	0	2	0
103	e	8	0	0	0	0
103	f	18	0	0	2	0
103	g	10	0	0	0	0
103	i	50	0	0	1	0
103	j	21	0	0	0	0
103	l	1	0	0	0	0
103	m	8	0	0	0	0
103	o	33	0	0	4	0
103	p	4	0	0	0	0
103	r	35	0	0	6	0
103	s	40	0	0	4	0
All	All	194797	160326	159801	879	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 879 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:2317:G:OP2	103:A:3501:HOH:O	1.82	0.96
1:AA:1485:G:OP2	103:AA:1801:HOH:O	1.90	0.90
96:P:201:K:K	103:P:327:HOH:O	1.83	0.88
33:A:3047:G:N7	103:A:3564:HOH:O	2.08	0.86
30:Aw:76:A:O3'	33:A:3072:U:O4	1.93	0.86

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
3	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
4	AD	341/430 (79%)	329 (96%)	12 (4%)	0	100	100
5	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
6	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
7	AG	323/396 (82%)	315 (98%)	8 (2%)	0	100	100
8	AH	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	35
9	AI	134/194 (69%)	131 (98%)	3 (2%)	0	100	100
10	AJ	106/138 (77%)	106 (100%)	0	0	100	100
11	AK	99/128 (77%)	99 (100%)	0	0	100	100
12	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
13	AM	117/137 (85%)	117 (100%)	0	0	100	100
14	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
15	AO	191/258 (74%)	187 (98%)	4 (2%)	0	100	100
16	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
17	AQ	84/87 (97%)	81 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	293/360 (81%)	283 (97%)	10 (3%)	0	100	100
19	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
20	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	AU	174/205 (85%)	174 (100%)	0	0	100	100
22	AV	358/414 (86%)	351 (98%)	7 (2%)	0	100	100
23	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
24	AX	350/398 (88%)	343 (98%)	7 (2%)	0	100	100
25	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
26	A0	213/217 (98%)	209 (98%)	4 (2%)	0	100	100
27	A1	275/323 (85%)	271 (98%)	4 (2%)	0	100	100
28	A2	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
29	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
35	D	236/305 (77%)	232 (98%)	4 (2%)	0	100	100
36	E	303/348 (87%)	298 (98%)	4 (1%)	1 (0%)	36	54
37	F	250/311 (80%)	244 (98%)	6 (2%)	0	100	100
38	I	210/261 (80%)	201 (96%)	9 (4%)	0	100	100
39	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
40	K	175/178 (98%)	173 (99%)	2 (1%)	0	100	100
41	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
42	M	287/296 (97%)	284 (99%)	3 (1%)	0	100	100
43	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
44	O	152/175 (87%)	148 (97%)	4 (3%)	0	100	100
45	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
46	Q	236/292 (81%)	234 (99%)	2 (1%)	0	100	100
47	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
48	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
49	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
50	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
51	V	203/216 (94%)	198 (98%)	5 (2%)	0	100	100
52	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
53	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Y	179/250 (72%)	176 (98%)	3 (2%)	0	100	100
55	Z	120/161 (74%)	120 (100%)	0	0	100	100
56	0	108/188 (57%)	108 (100%)	0	0	100	100
57	1	54/65 (83%)	54 (100%)	0	0	100	100
58	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
59	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
60	4	36/103 (35%)	36 (100%)	0	0	100	100
61	5	392/423 (93%)	383 (98%)	9 (2%)	0	100	100
62	6	352/380 (93%)	344 (98%)	8 (2%)	0	100	100
63	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
64	8	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
65	9	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
66	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
67	b	149/215 (69%)	146 (98%)	3 (2%)	0	100	100
68	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
69	d	235/306 (77%)	231 (98%)	4 (2%)	0	100	100
70	e	236/279 (85%)	222 (94%)	13 (6%)	1 (0%)	30	48
71	f	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
72	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
73	h	108/158 (68%)	108 (100%)	0	0	100	100
74	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
75	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
76	k	99/112 (88%)	99 (100%)	0	0	100	100
77	l	80/138 (58%)	79 (99%)	1 (1%)	0	100	100
78	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
79	o	92/102 (90%)	92 (100%)	0	0	100	100
80	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
81	q	161/222 (72%)	160 (99%)	1 (1%)	0	100	100
82	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
83	s	382/439 (87%)	372 (97%)	10 (3%)	0	100	100
84	t	44/198 (22%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	u	30/198 (15%)	30 (100%)	0	0	100	100
84	v	30/198 (15%)	30 (100%)	0	0	100	100
84	w	29/198 (15%)	29 (100%)	0	0	100	100
84	x	29/198 (15%)	29 (100%)	0	0	100	100
84	y	29/198 (15%)	29 (100%)	0	0	100	100
85	H	200/267 (75%)	194 (97%)	6 (3%)	0	100	100
86	z	250/325 (77%)	240 (96%)	9 (4%)	1 (0%)	30	48
87	AY	219/395 (55%)	207 (94%)	11 (5%)	1 (0%)	24	42
88	A5	579/1394 (42%)	561 (97%)	17 (3%)	1 (0%)	43	62
89	A4	591/689 (86%)	577 (98%)	13 (2%)	1 (0%)	43	62
90	A6	72/109 (66%)	69 (96%)	3 (4%)	0	100	100
All	All	15427/20987 (74%)	15135 (98%)	285 (2%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AH	126	ILE
86	z	128	ASP
87	AY	233	ASP
36	E	150	LYS
70	e	109	GLU

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	
2	AB	198/249 (80%)	198 (100%)	0	100	100
3	AC	115/143 (80%)	115 (100%)	0	100	100
4	AD	286/357 (80%)	286 (100%)	0	100	100
5	AE	104/107 (97%)	104 (100%)	0	100	100
6	AF	185/209 (88%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	285/342 (83%)	285 (100%)	0	100	100
8	AH	130/180 (72%)	130 (100%)	0	100	100
9	AI	104/146 (71%)	104 (100%)	0	100	100
10	AJ	93/118 (79%)	93 (100%)	0	100	100
11	AK	91/113 (80%)	91 (100%)	0	100	100
12	AL	158/226 (70%)	158 (100%)	0	100	100
13	AM	97/113 (86%)	97 (100%)	0	100	100
14	AN	96/115 (84%)	96 (100%)	0	100	100
15	AO	174/230 (76%)	174 (100%)	0	100	100
16	AP	88/123 (72%)	88 (100%)	0	100	100
17	AQ	78/79 (99%)	78 (100%)	0	100	100
18	AR	264/318 (83%)	264 (100%)	0	100	100
19	AS	116/164 (71%)	116 (100%)	0	100	100
20	AT	153/157 (98%)	153 (100%)	0	100	100
21	AU	152/174 (87%)	152 (100%)	0	100	100
22	AV	325/364 (89%)	325 (100%)	0	100	100
23	AW	87/158 (55%)	87 (100%)	0	100	100
24	AX	311/351 (89%)	311 (100%)	0	100	100
25	AZ	90/95 (95%)	90 (100%)	0	100	100
26	A0	188/189 (100%)	188 (100%)	0	100	100
27	A1	255/291 (88%)	255 (100%)	0	100	100
28	A2	100/101 (99%)	100 (100%)	0	100	100
29	A3	65/166 (39%)	65 (100%)	0	100	100
35	D	192/245 (78%)	192 (100%)	0	100	100
36	E	260/290 (90%)	260 (100%)	0	100	100
37	F	219/262 (84%)	219 (100%)	0	100	100
38	I	194/232 (84%)	194 (100%)	0	100	100
39	J	138/150 (92%)	138 (100%)	0	100	100
40	K	154/155 (99%)	154 (100%)	0	100	100
41	L	98/124 (79%)	98 (100%)	0	100	100
42	M	245/249 (98%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	N	189/211 (90%)	189 (100%)	0	100	100
44	O	134/150 (89%)	134 (100%)	0	100	100
45	P	126/155 (81%)	126 (100%)	0	100	100
46	Q	220/256 (86%)	220 (100%)	0	100	100
47	R	118/126 (94%)	118 (100%)	0	100	100
48	S	146/180 (81%)	146 (100%)	0	100	100
49	T	146/176 (83%)	146 (100%)	0	100	100
50	U	134/135 (99%)	134 (100%)	0	100	100
51	V	183/191 (96%)	183 (100%)	0	100	100
52	W	94/119 (79%)	94 (100%)	0	100	100
53	X	220/229 (96%)	220 (100%)	0	100	100
54	Y	163/223 (73%)	163 (100%)	0	100	100
55	Z	113/147 (77%)	113 (100%)	0	100	100
56	0	99/164 (60%)	99 (100%)	0	100	100
57	1	53/60 (88%)	53 (100%)	0	100	100
58	2	40/72 (56%)	40 (100%)	0	100	100
59	3	88/166 (53%)	88 (100%)	0	100	100
60	4	37/89 (42%)	37 (100%)	0	100	100
61	5	353/368 (96%)	353 (100%)	0	100	100
62	6	313/332 (94%)	313 (100%)	0	100	100
63	7	270/303 (89%)	270 (100%)	0	100	100
64	8	146/190 (77%)	146 (100%)	0	100	100
65	9	104/112 (93%)	104 (100%)	0	100	100
66	a	96/133 (72%)	96 (100%)	0	100	100
67	b	132/185 (71%)	132 (100%)	0	100	100
68	c	251/288 (87%)	251 (100%)	0	100	100
69	d	223/274 (81%)	223 (100%)	0	100	100
70	e	207/236 (88%)	207 (100%)	0	100	100
71	f	139/188 (74%)	139 (100%)	0	100	100
72	g	124/148 (84%)	124 (100%)	0	100	100
73	h	104/148 (70%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	i	86/110 (78%)	86 (100%)	0	100	100
75	j	74/97 (76%)	74 (100%)	0	100	100
76	k	83/90 (92%)	83 (100%)	0	100	100
77	l	76/116 (66%)	76 (100%)	0	100	100
78	m	85/113 (75%)	85 (100%)	0	100	100
79	o	80/87 (92%)	80 (100%)	0	100	100
80	p	135/181 (75%)	135 (100%)	0	100	100
81	q	142/178 (80%)	142 (100%)	0	100	100
82	r	147/169 (87%)	147 (100%)	0	100	100
83	s	340/381 (89%)	340 (100%)	0	100	100
84	t	40/158 (25%)	40 (100%)	0	100	100
84	u	31/158 (20%)	31 (100%)	0	100	100
84	v	31/158 (20%)	31 (100%)	0	100	100
84	w	30/158 (19%)	30 (100%)	0	100	100
84	x	30/158 (19%)	30 (100%)	0	100	100
84	y	30/158 (19%)	30 (100%)	0	100	100
85	H	182/228 (80%)	182 (100%)	0	100	100
86	z	226/287 (79%)	226 (100%)	0	100	100
87	AY	202/357 (57%)	202 (100%)	0	100	100
88	A5	515/1219 (42%)	515 (100%)	0	100	100
89	A4	532/609 (87%)	532 (100%)	0	100	100
90	A6	63/90 (70%)	63 (100%)	0	100	100
All	All	13813/18099 (76%)	13813 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
86	z	266	GLN
87	AY	234	ASN
89	A4	495	HIS
35	D	276	HIS
35	D	221	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	953/954 (99%)	136 (14%)	1 (0%)
30	Aw	67/68 (98%)	18 (26%)	0
31	Ax	68/70 (97%)	12 (17%)	0
32	Ay	68/70 (97%)	13 (19%)	0
33	A	1556/1561 (99%)	224 (14%)	3 (0%)
34	B	71/72 (98%)	12 (16%)	0
91	Az	41/42 (97%)	21 (51%)	0
All	All	2824/2837 (99%)	436 (15%)	4 (0%)

5 of 436 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	651	A
1	AA	673	U
1	AA	680	U
1	AA	688	A
1	AA	695	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1539	C
33	A	2030	U
33	A	2112	A
33	A	2245	A

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

19 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
33	OMU	A	3039	33,96	19,22,23	0.29	0	26,31,34	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MU	AA	1076	1	19,22,23	0.63	0	28,32,35	1.21	3 (10%)
33	PSU	A	3067	33	18,21,22	0.79	0	22,30,33	2.55	5 (22%)
76	AYA	k	2	76	6,7,8	0.82	0	5,8,10	0.50	0
1	5MC	AA	1488	1	18,22,23	0.32	0	26,32,35	0.42	0
40	SAC	K	2	40	7,8,9	0.21	0	8,9,11	0.55	0
28	AYA	A2	2	28	6,7,8	0.80	0	5,8,10	0.58	0
1	MA6	AA	1583	1	23,26,27	0.30	0	34,38,41	0.59	1 (2%)
33	OMG	A	2815	33,96,31	23,26,27	0.30	0	33,38,41	0.38	0
1	MA6	AA	1584	1	23,26,27	0.33	0	34,38,41	0.61	1 (2%)
34	2MG	B	10	34	23,26,27	0.48	0	32,38,41	0.54	0
9	5F0	AI	184	9	8,8,9	0.59	0	7,9,11	1.17	1 (14%)
1	B8T	AA	1486	95,1	19,22,23	0.30	0	26,31,34	0.35	0
34	1MA	B	9	34	21,25,26	0.75	1 (4%)	31,37,40	0.64	1 (3%)
50	AYA	U	2	50	6,7,8	0.77	0	5,8,10	0.58	0
33	1MA	A	2617	33	21,25,26	0.76	1 (4%)	31,37,40	0.65	1 (3%)
17	AYA	AQ	2	17	6,7,8	0.78	0	5,8,10	0.43	0
34	PSU	B	39	34	18,21,22	0.77	0	22,30,33	2.55	4 (18%)
33	OMG	A	3040	33,30	23,26,27	0.29	0	33,38,41	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	OMU	A	3039	33,96	-	0/9/27/28	0/2/2/2
1	5MU	AA	1076	1	-	0/7/25/26	0/2/2/2
33	PSU	A	3067	33	-	0/7/25/26	0/2/2/2
76	AYA	k	2	76	-	1/4/6/8	-
1	5MC	AA	1488	1	-	0/7/25/26	0/2/2/2
40	SAC	K	2	40	-	0/7/8/10	-
28	AYA	A2	2	28	-	0/4/6/8	-
1	MA6	AA	1583	1	-	0/11/29/30	0/3/3/3
33	OMG	A	2815	33,96,31	-	0/9/27/28	0/3/3/3
1	MA6	AA	1584	1	-	2/11/29/30	0/3/3/3
34	2MG	B	10	34	-	0/9/27/28	0/3/3/3
9	5F0	AI	184	9	-	0/9/9/10	-
1	B8T	AA	1486	95,1	-	1/7/27/28	0/2/2/2
34	1MA	B	9	34	-	0/7/25/26	0/3/3/3
50	AYA	U	2	50	-	1/4/6/8	-
33	1MA	A	2617	33	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	AYA	AQ	2	17	-	0/4/6/8	-
34	PSU	B	39	34	-	0/7/25/26	0/2/2/2
33	OMG	A	3040	33,30	-	0/9/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	2617	1MA	C6-N6	3.02	1.35	1.28
34	B	9	1MA	C6-N6	2.98	1.35	1.28

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	39	PSU	N1-C2-N3	8.07	124.27	115.13
33	A	3067	PSU	N1-C2-N3	8.04	124.24	115.13
34	B	39	PSU	C4-N3-C2	-6.57	116.87	126.34
33	A	3067	PSU	C4-N3-C2	-6.53	116.93	126.34
1	AA	1076	5MU	C4-N3-C2	-4.83	121.11	127.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1584	MA6	C5-C6-N6-C9
76	k	2	AYA	C-CA-N-CT
1	AA	1584	MA6	C4'-C5'-O5'-P
1	AA	1486	B8T	O4'-C4'-C5'-O5'
50	U	2	AYA	C-CA-N-CT

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	3039	OMU	2	0
1	AA	1583	MA6	2	0
1	AA	1584	MA6	1	0
33	A	3040	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 271 ligands modelled in this entry, 258 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
93	SPM	AA	1702	-	13,13,13	0.25	0	12,12,12	0.99	0
98	FES	r	201	38,82	0,4,4	-	-	-		
94	SPD	A	3301	-	9,9,9	0.22	0	8,8,8	1.24	0
94	SPD	AA	1703	-	9,9,9	0.24	0	8,8,8	1.34	2 (25%)
98	FES	AT	201	13,20	0,4,4	-	-	-		
99	ATP	AX	501	95	29,33,33	0.49	0	44,52,52	0.49	0
102	VAL	B	101	34	4,6,7	0.53	0	6,7,9	0.78	0
94	SPD	A	3303	-	9,9,9	0.26	0	8,8,8	1.18	0
101	PUT	A	3304	-	5,5,5	0.24	0	4,4,4	0.51	0
94	SPD	A	3302	-	9,9,9	0.25	0	8,8,8	1.15	0
98	FES	AP	201	16,5	0,4,4	-	-	-		
100	GDP	AX	503	-	28,30,30	0.42	0	44,47,47	0.40	0
92	NAD	AA	1701	95	45,48,48	0.38	0	63,73,73	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPM	AA	1702	-	-	0/11/11/11	-
98	FES	r	201	38,82	-	-	0/1/1/1
94	SPD	A	3301	-	-	1/7/7/7	-
98	FES	AP	201	16,5	-	-	0/1/1/1
94	SPD	AA	1703	-	-	0/7/7/7	-
98	FES	AT	201	13,20	-	-	0/1/1/1
99	ATP	AX	501	95	-	0/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
102	VAL	B	101	34	-	0/5/6/8	-
94	SPD	A	3303	-	-	2/7/7/7	-
101	PUT	A	3304	-	-	0/3/3/3	-
94	SPD	A	3302	-	-	0/7/7/7	-
100	GDP	AX	503	-	-	0/16/32/32	0/3/3/3
92	NAD	AA	1701	95	-	0/30/62/62	0/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
94	AA	1703	SPD	C4-C5-N6	-2.33	105.86	112.14
94	AA	1703	SPD	C8-C7-N6	-2.10	106.46	112.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
94	A	3303	SPD	C4-C5-N6-C7
94	A	3303	SPD	C8-C7-N6-C5
94	A	3301	SPD	N6-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
102	B	101	VAL	1	0

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
32	Ay	1
31	Ax	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ay	15:A	O3'	21:A	P	9.63
1	Ax	15:A	O3'	21:A	P	8.88

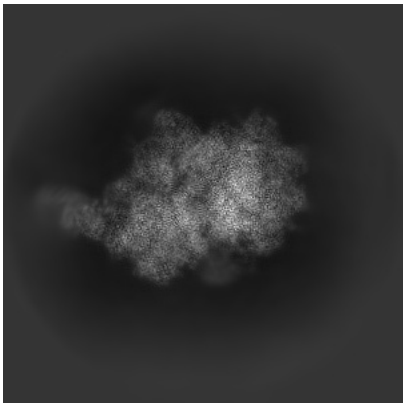
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15544. These allow visual inspection of the internal detail of the map and identification of artifacts.

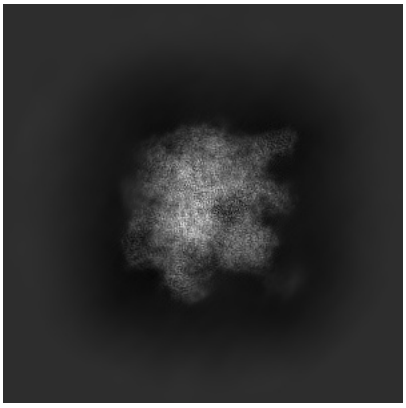
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

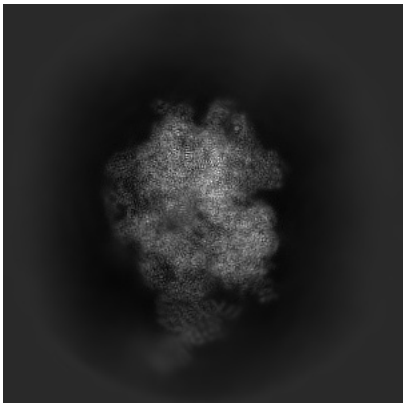
6.1.1 Primary map



X



Y



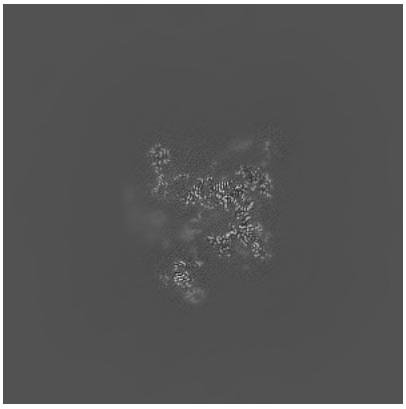
Z

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

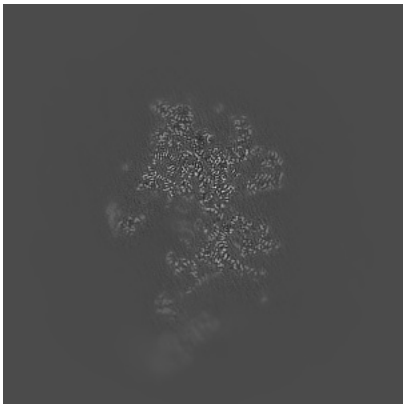
6.2 Central slices (i)

6.2.1 Primary map

X Index: 320



Y Index: 320

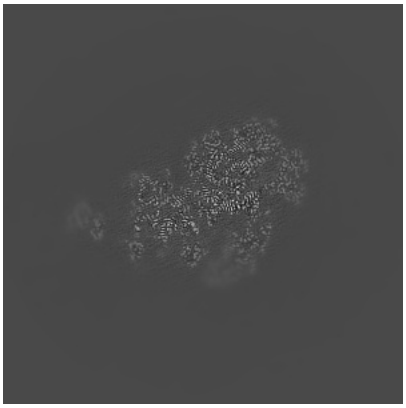


Z Index: 320

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

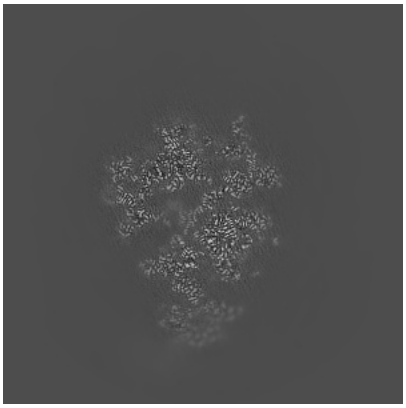
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 342

Y Index: 369

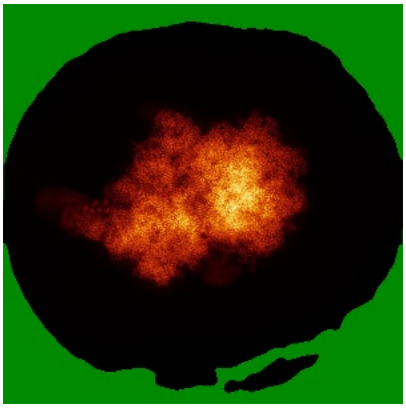


Z Index: 292

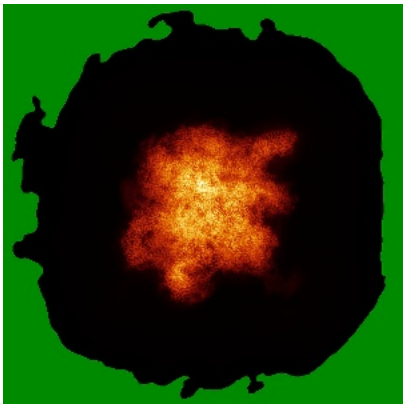
The images above show the largest variance slices of the map in three orthogonal directions.

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

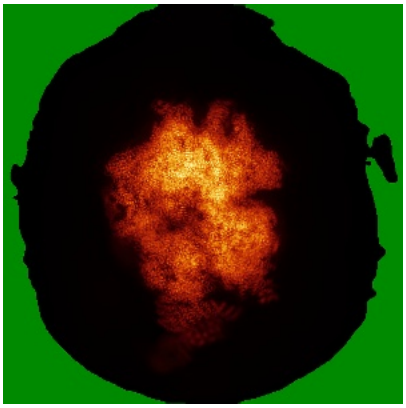
6.4.1 Primary map



X



Y

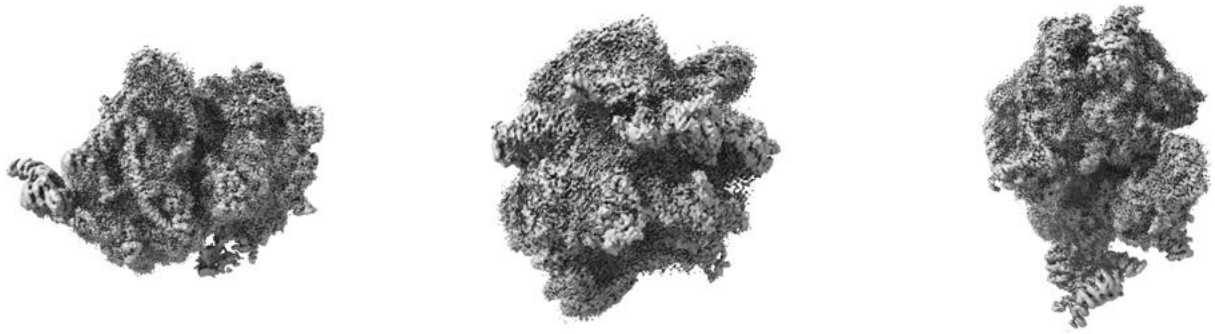


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

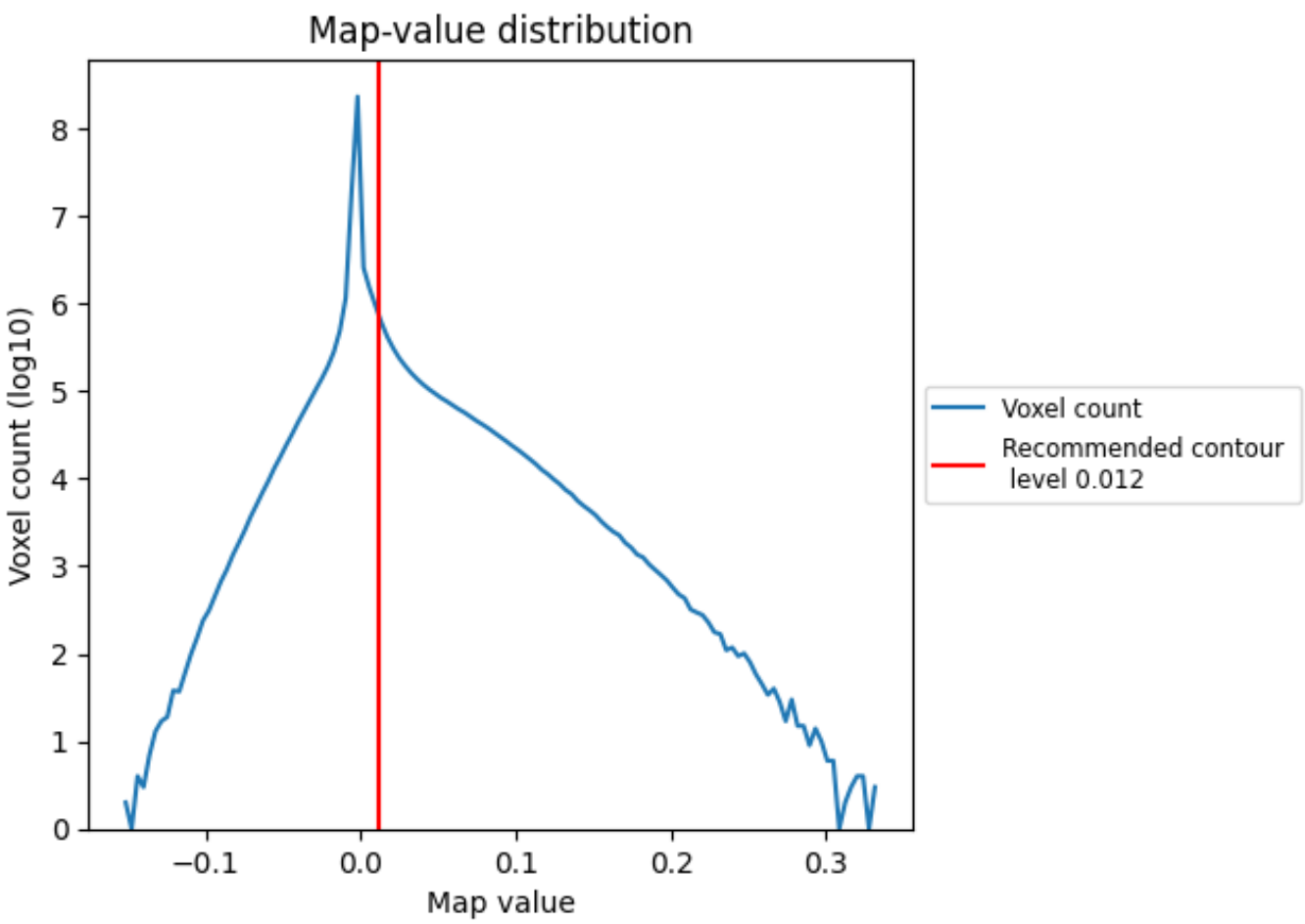
6.6 Mask visualisation (i)

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

7 Map analysis (i)

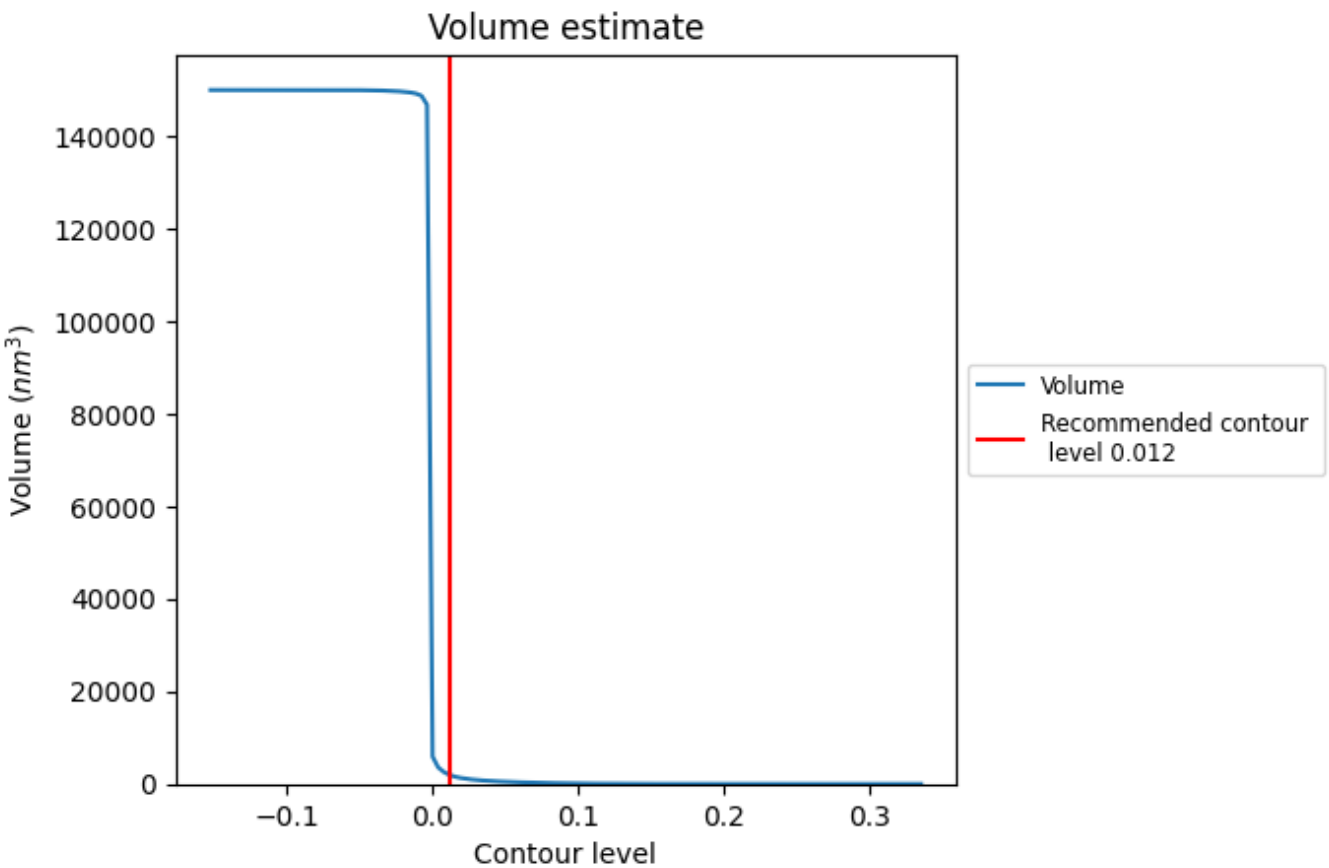
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

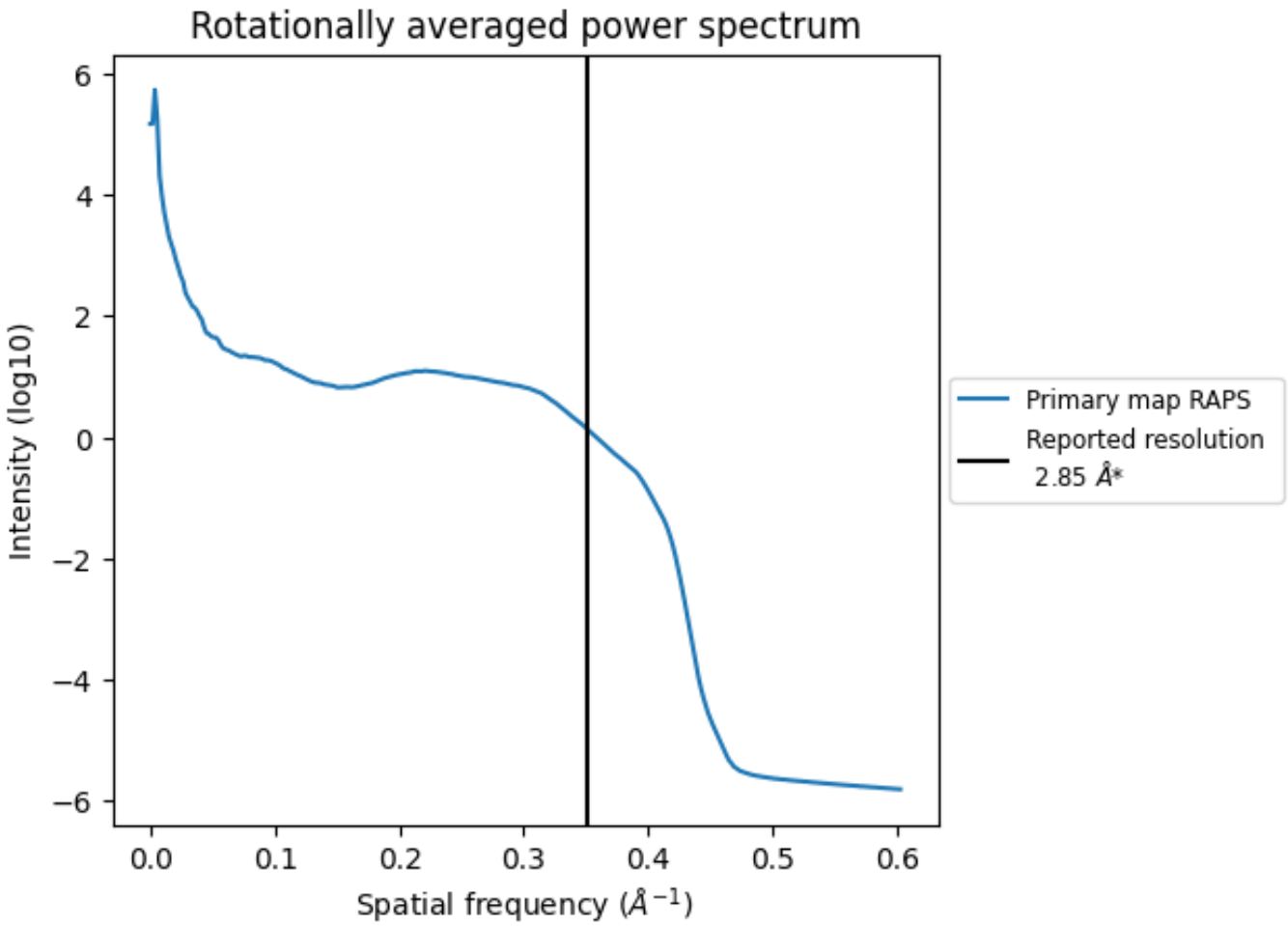
7.2 Volume estimate (i)



The volume at the recommended contour level is 1967 nm^3; this corresponds to an approximate mass of 1777 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 0.351 Å^{-1}

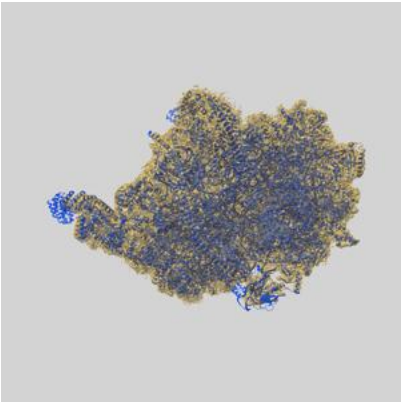
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

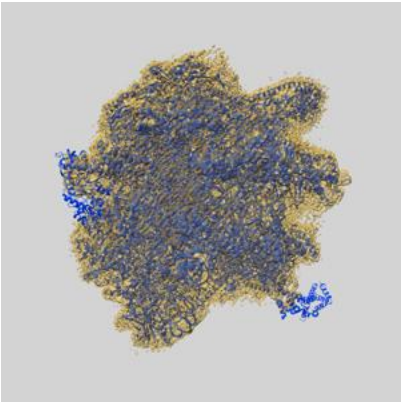
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15544 and PDB model 8ANY. Per-residue inclusion information can be found in section 3 on page 31.

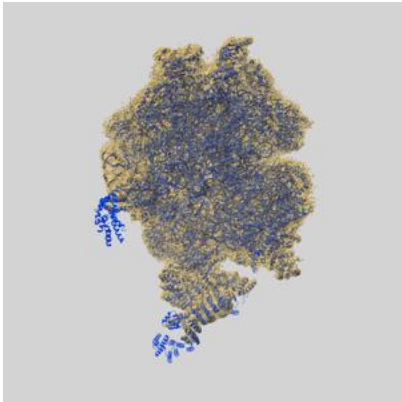
9.1 Map-model overlay (i)



X



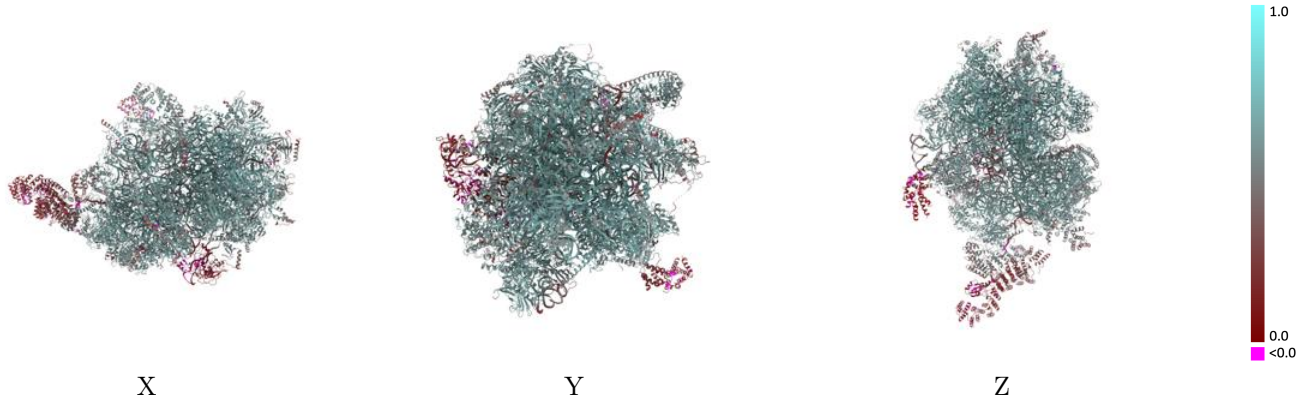
Y



Z

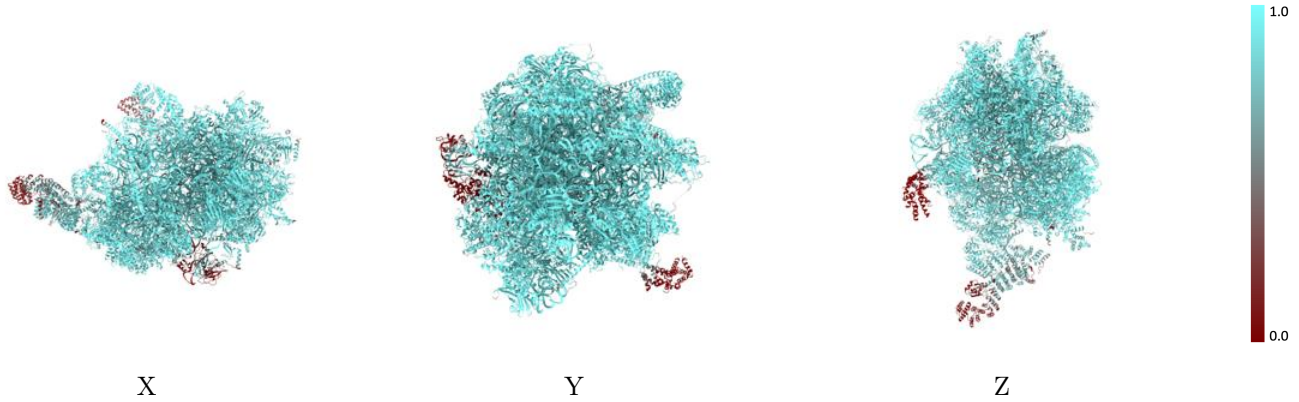
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



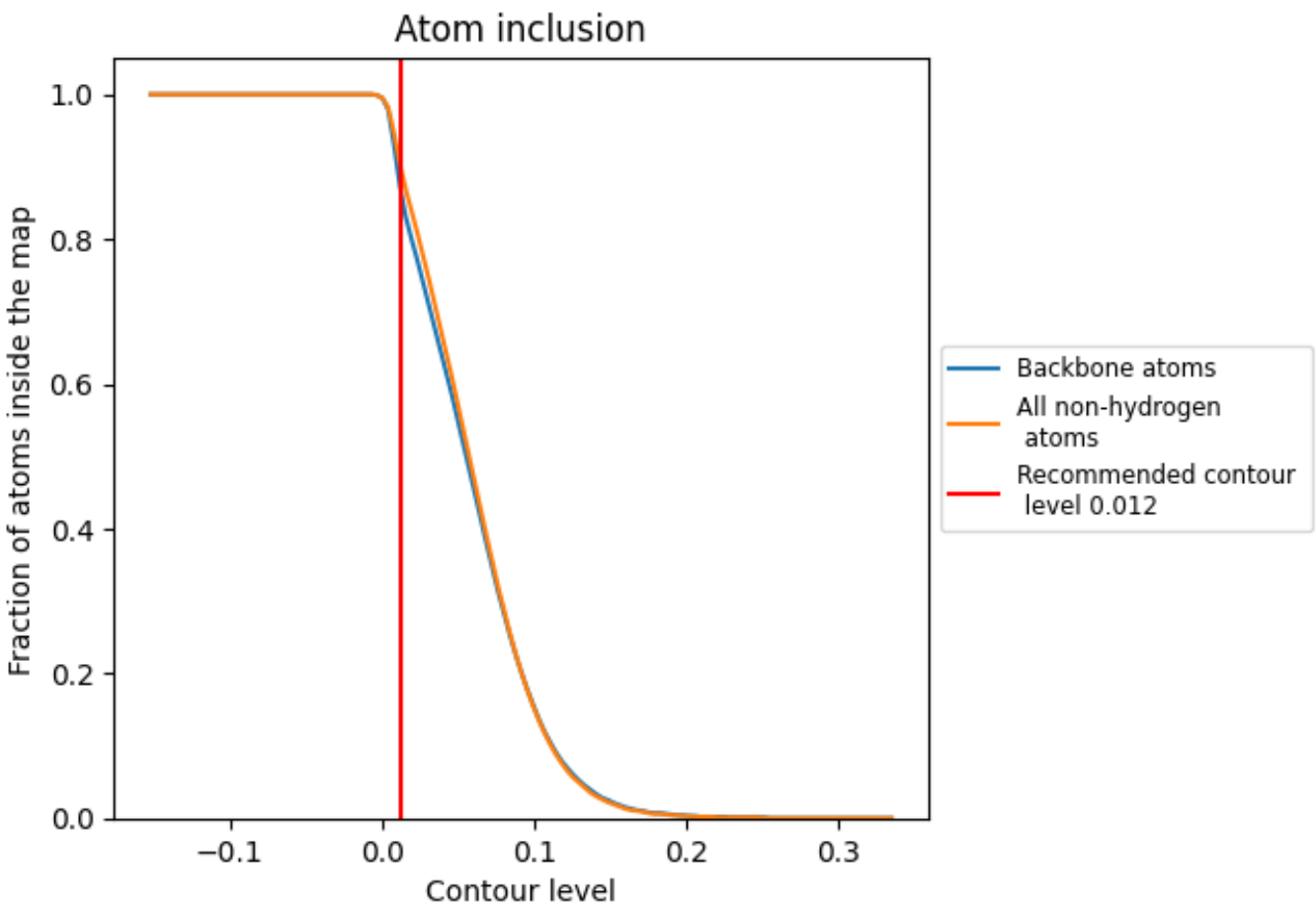
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 90% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9040	0.5540
0	0.9620	0.6050
1	0.9450	0.5770
2	0.9950	0.6820
3	0.9910	0.6710
4	0.9880	0.6420
5	0.9640	0.5810
6	0.9650	0.5940
7	0.9410	0.5410
8	0.8720	0.4880
9	0.9310	0.5690
A	0.9810	0.6290
A0	0.9360	0.5540
A1	0.9340	0.5680
A2	0.9070	0.5040
A3	0.9610	0.6000
A4	0.8590	0.4320
A5	0.4750	0.1750
A6	0.2210	0.1260
AA	0.9930	0.6240
AB	0.9610	0.5980
AC	0.9860	0.6490
AD	0.9500	0.5700
AE	0.9520	0.5800
AF	0.9550	0.5730
AG	0.9270	0.5530
AH	0.9570	0.5990
AI	0.9700	0.5910
AJ	0.9570	0.5740
AK	0.9890	0.6560
AL	0.9240	0.5440
AM	0.9290	0.5770
AN	0.9590	0.5930
AO	0.9510	0.5610
AP	0.9620	0.5930

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Chain	Atom inclusion	Q-score
AQ	0.9790	0.6240
AR	0.9040	0.4830
AS	0.9170	0.5270
AT	0.9440	0.5720
AU	0.9060	0.5090
AV	0.9290	0.5300
AW	0.9490	0.5580
AX	0.9680	0.5870
AY	0.7040	0.4040
AZ	0.9400	0.5880
Aw	0.7730	0.3380
Ax	0.9390	0.4600
Ay	0.5110	0.2100
Az	0.7640	0.2910
B	0.9740	0.5180
D	0.9830	0.6350
E	0.9720	0.6260
F	0.9820	0.6360
H	0.5850	0.3310
I	0.7680	0.4640
J	0.8970	0.4790
K	0.9760	0.6420
L	0.9830	0.6300
M	0.9780	0.6270
N	0.9660	0.6120
O	0.9770	0.6180
P	0.9820	0.6270
Q	0.9350	0.5810
R	0.9810	0.6560
S	0.9720	0.6220
T	0.9800	0.6390
U	0.9160	0.5650
V	0.9320	0.5310
W	0.9810	0.6490
X	0.9460	0.5770
Y	0.9710	0.6130
Z	0.9630	0.6260
a	0.9150	0.5520
b	0.9840	0.6320
c	0.9440	0.5700
d	0.8920	0.4830
e	0.8790	0.4870

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Chain	Atom inclusion	Q-score
f	0.9100	0.5390
g	0.9610	0.6090
h	0.9450	0.5290
i	0.9890	0.6640
j	0.9330	0.5710
k	0.9420	0.5240
l	0.9220	0.5190
m	0.8500	0.4660
o	0.9870	0.6520
p	0.8840	0.5060
q	0.7490	0.4140
r	0.9590	0.5940
s	0.9620	0.5980
t	0.3910	0.2650
u	0.3360	0.2270
v	0.0000	0.1330
w	0.0000	0.0430
x	0.0000	0.0870
y	0.0000	0.0560
z	0.1860	0.1010