wwPDB EM Validation Summary Report (i)

Sep 9, 2026 – 12:19 am BST

PDB ID	:	6ZM5 / pdb_00006zm5
EMDB ID	:	EMD-11278
Title	:	Human mitochondrial ribosome in complex with OXA1L, mRNA, A/A tRNA, P/P tRNA and nascent polypeptide
Authors	:	Itoh, Y.; Andrell, J.; Amunts, A.
Deposited on	:	2020-07-01
Resolution	:	2.89 Å(reported)
Based on initial models	:	5OOL, 6RW4, 3J9M

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 (i)) were used in the production of this report:

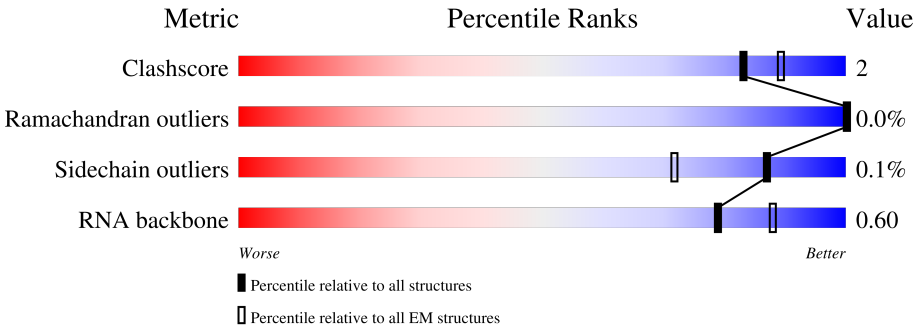
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

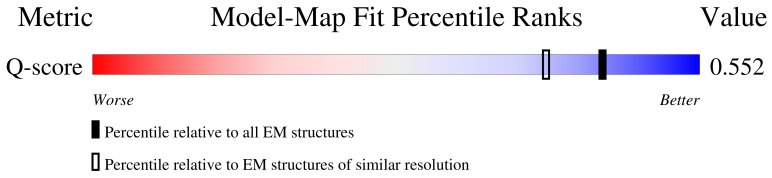
1 Overall quality at a glance

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

The reported resolution of this entry is 2.89 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	12148 (2.39 - 3.39)

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	A	1561	75% 21%
2	B	72	75% 25%
3	D	305	71% 7% 22%

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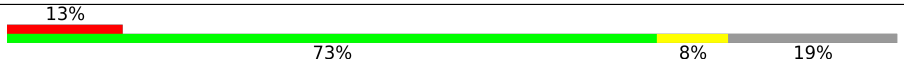
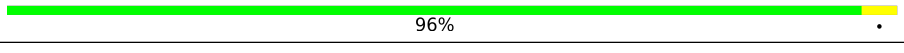
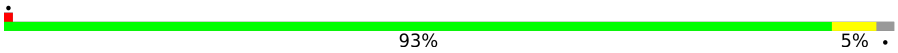
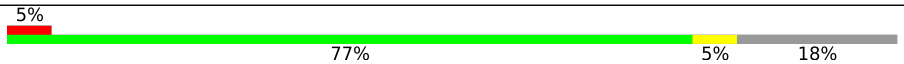
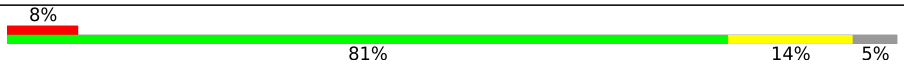
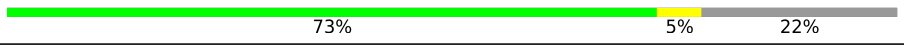
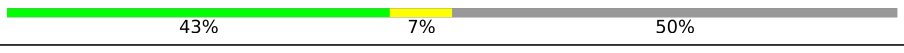
Mol	Chain	Length	Quality of chain
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	177	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	152	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	
28	3	188	

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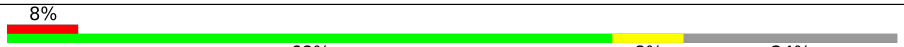
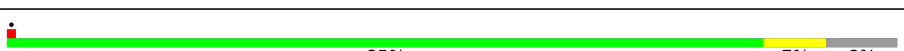
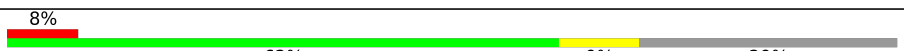
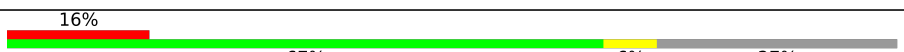
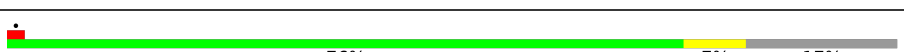
Mol	Chain	Length	Quality of chain
29	4	103	
30	5	423	
31	6	380	
32	7	338	
33	8	206	
34	9	137	
35	a	142	
36	b	214	
37	c	332	
38	d	306	
39	e	279	
40	f	212	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	111	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	t1	198	

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Mol	Chain	Length	Quality of chain
53	t2	198	5% 12% 5% 84%
53	t3	198	16% 16% 84%
53	t4	198	15% 15% 84%
53	t5	198	16% 15% 84%
53	t6	198	16% 16% 84%
54	AA	954	81% 17%
55	AB	296	73% 24%
56	AC	167	69% 10% 21%
57	AD	430	75% 5% 20%
58	AE	125	91% 6%
59	AF	242	80% 6% 14%
60	AG	396	74% 21%
61	AH	201	62% 7% 30%
62	AI	194	64% 6% 29%
63	AJ	138	75% 22%
64	AK	128	73% 5% 21%
65	AL	257	5% 65% 32%
66	AM	137	82% 5% 13%
67	AN	130	77% 8% 15%
68	AO	258	71% 25%
69	AP	142	63% 6% 32%
70	AQ	86	93% 7%
71	AR	360	76% 6% 18%
72	AS	190	68% 29%
73	AT	173	91% 6%

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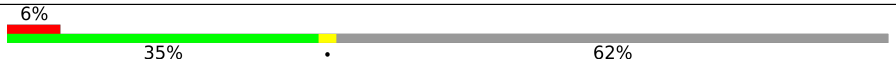
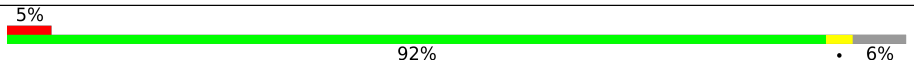
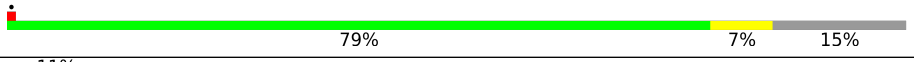
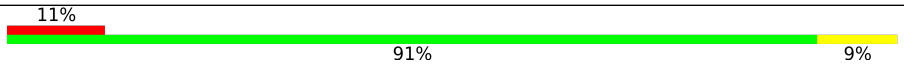
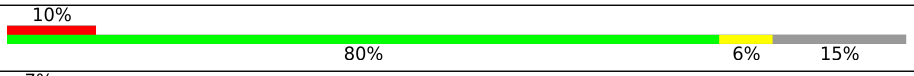
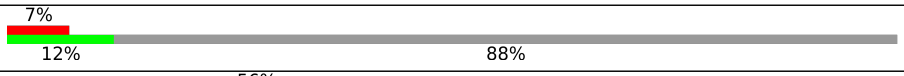
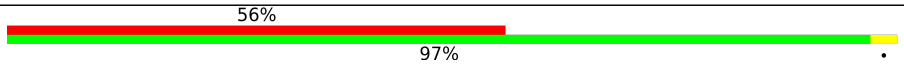
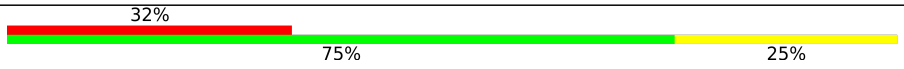
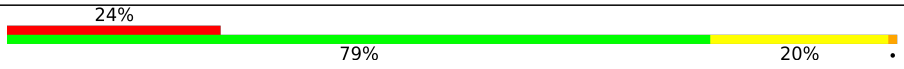
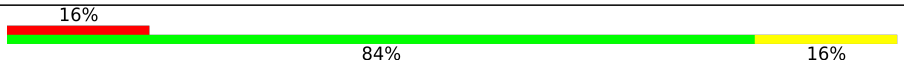
Mol	Chain	Length	Quality of chain
74	AU	205	
75	AV	414	
76	AW	187	
77	AX	398	
78	AY	395	
79	AZ	106	
80	A0	218	
81	A1	323	
82	A2	117	
83	A3	199	
84	A4	689	
85	u	435	
86	v	32	
87	w	68	
88	x	70	
89	y	19	

2 Entry composition (i)

There are 97 unique types of molecules in this entry. The entry contains 326964 atoms, of which 149830 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 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	1534	49092	14611	16532	5870	10545	1534	0	0

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	B	72	2298	683	776	269	498	72	0	0

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	238	3780	1157	1921	376	317	9	0	0

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	E	305	4823	1545	2417	418	432	11	0	0

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	252	4097	1305	2066	370	350	6	0	0

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
6	H	97	1649	508	847	155	139	0	0

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	212	Total	C	H	N	O	S	0	0
			3481	1088	1786	304	292	11		

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	177	Total	C	H	N	O	S	0	0
			2909	936	1454	259	253	7		

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	115	Total	C	H	N	O	S	0	0
			1832	559	942	171	155	5		

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	291	Total	C	H	N	O	S	0	0
			4723	1483	2396	430	408	6		

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	222	Total	C	H	N	O	S	0	0
			3605	1143	1819	326	307	10		

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	154	Total	C	H	N	O	S	0	0
			2554	792	1295	241	219	7		

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	144	Total	C	H	N	O	S	0	0
			2339	733	1166	224	211	5		

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	238	Total	C	H	N	O	S	0	0
			4002	1268	2023	352	350	9		

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	140	Total	C	H	N	O	S	0	0
			2369	732	1215	231	187	4		

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	161	Total	C	H	N	O	S	0	0
			2659	835	1366	227	227	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	166	Total	C	H	N	O	S	0	0
			2780	875	1411	254	233	7		

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	133	Total	C	H	N	O	S	0	0
			2215	702	1108	214	189	2		

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	205	Total	C	H	N	O	S	0	0
			3364	1068	1688	298	302	8		

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	W	116	Total	C	H	N	O	S	0	0
			1841	577	937	171	153	3		

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	X	244	Total	C	H	N	O	S	0	0
			4105	1322	2061	352	365	5		

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Y	181	Total	C	H	N	O	S	0	0
			3154	995	1598	298	259	4		

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	122	Total	C	H	N	O	S	0	0
			2041	636	1045	186	171	3		

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	0	110	Total	C	H	N	O	S	0	0
			1815	554	917	176	162	6		

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	55	Total	C	H	N	O	S	0	0
			954	290	499	87	76	2		

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	2	46	Total	C	H	N	O	S	0	0
			784	233	407	83	60	1		

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	3	95	Total	C	H	N	O	S	0	0
			1716	539	884	162	128	3		

- Molecule 29 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	38	Total	C	H	N	O	S	0	0
			704	217	362	72	49	4		

- Molecule 30 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	5	394	Total	C	H	N	O	S	0	0
			6418	2073	3208	560	566	11		

- Molecule 31 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	6	354	Total	C	H	N	O	S	0	0
			5792	1881	2844	525	533	9		

- Molecule 32 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	7	294	Total	C	H	N	O	S	0	0
			4789	1529	2399	405	438	18		

- Molecule 33 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	8	157	Total	C	H	N	O	S	0	0
			2696	844	1369	235	246	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
34	9	124	Total	C	H	N	O	S	0	0
			1985	644	988	170	181	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
35	a	100	Total	C	H	N	O	S	0	0
			1652	529	812	152	154	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
36	b	150	Total	C	H	N	O	S	0	0
			2392	744	1196	231	218	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
37	c	286	Total	C	H	N	O	S	0	0
			4621	1470	2322	397	423	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
38	d	242	Total	C	H	N	O	S	0	0
			3970	1275	1982	343	358	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
39	e	228	Total	C	H	N	O	S	0	0
			3699	1174	1851	326	342	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
40	f	157	Total	C	H	N	O	S	0	0
			2523	799	1271	207	242	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
41	g	134	Total	C	H	N	O	S	0	0
			2210	719	1097	193	199	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
42	h	110	Total	C	H	N	O	S	0	0
			1777	568	882	156	168	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
43	i	97	Total	C	H	N	O	S	0	0
			1687	532	859	165	127	4		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
45	k	101	Total	C	H	N	O	S	0	0
			1558	479	784	148	142	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
46	l	82	Total	C	H	N	O	S	0	0
			1363	437	675	120	128	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
47	m	87	Total	C	H	N	O	S	0	0
			1515	466	761	152	134	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
48	o	94	Total	C	H	N	O	S	0	0
			1605	501	807	165	129	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
49	p	147	Total	C	H	N	O	S	0	0
			2431	748	1226	228	225	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	q	161	Total	C	H	N	O	S	0	0
			2678	841	1328	260	244	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
51	r	162	Total	C	H	N	O	S	0	0
			2671	839	1349	252	223	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
52	s	386	Total	C	H	N	O	S	0	0
			6298	2023	3143	559	559	14		

- Molecule 53 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t1	46	Total	C	H	N	O	0	0
			732	228	378	56	70		
53	t2	32	Total	C	H	N	O	0	0
			541	168	284	40	49		
53	t3	32	Total	C	H	N	O	0	0
			541	168	284	40	49		
53	t4	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
53	t5	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
53	t6	31	Total	C	H	N	O	0	0
			520	159	275	39	47		

- Molecule 54 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	AA	954	Total	C	H	N	O	P	0	0
			30542	9081	10289	3647	6571	954		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
55	AB	225	Total	C	H	N	O	S	0	0
			3644	1164	1816	331	323	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
56	AC	132	Total	C	H	N	O	S	0	0
			2172	699	1089	195	185	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
57	AD	343	Total	C	H	N	O	S	0	0
			5536	1713	2805	518	487	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
58	AE	122	Total	C	H	N	O	S	0	0
			1973	614	1001	177	177	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
59	AF	208	Total	C	H	N	O	S	0	0
			3495	1104	1770	312	298	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
60	AG	312	Total	C	H	N	O	S	0	0
			5126	1632	2558	455	467	14		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
61	AH	140	Total	C	H	N	O	S	0	0
			2336	745	1184	194	210	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
62	AI	137	Total	C	H	N	O	S	0	0
			2076	641	1058	192	181	4		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
63	AJ	108	Total	C	H	N	O	S	0	0
			1727	521	888	169	143	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
64	AK	101	Total	C	H	N	O	S	0	0
			1748	537	886	179	141	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
65	AL	174	Total	C	H	N	O	S	0	0
			2994	925	1541	270	251	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
66	AM	119	Total	C	H	N	O	S	0	0
			1908	594	966	185	157	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
67	AN	110	Total	C	H	N	O	S	0	0
			1797	562	929	156	147	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
68	AO	193	Total	C	H	N	O	S	0	0
			3149	1014	1557	294	277	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
69	AP	97	Total	C	H	N	O	S	0	0
			1588	501	807	134	138	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
70	AQ	86	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
71	AR	295	Total	C	H	N	O	S	0	0
			4838	1533	2429	413	455	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
72	AS	135	Total	C	H	N	O	S	0	0
			2227	716	1116	198	196	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
73	AT	168	Total	C	H	N	O	S	0	0
			2765	877	1394	239	244	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
74	AU	176	Total	C	H	N	O	S	0	0
			2988	916	1500	301	267	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
75	AV	362	Total	C	H	N	O	S	0	0
			5933	1904	2964	495	558	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
76	AW	100	Total	C	H	N	O	S	0	0
			1592	498	803	141	146	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
77	AX	352	Total	C	H	N	O	S	0	0
			5694	1822	2845	499	517	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
78	AY	149	Total	C	H	N	O	S	0	0
			2444	801	1198	207	234	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
79	AZ	100	Total	C	H	N	O	S	0	0
			1699	534	860	153	148	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
80	A0	215	Total	C	H	N	O	S	0	0
			3584	1130	1797	339	313	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
81	A1	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
82	A2	117	Total	C	H	N	O	S	0	0
			1904	579	969	182	166	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
83	A3	70	Total	C	H	N	O	S	0	0
			1325	401	700	134	89	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
84	A4	588	Total	C	H	N	O	S	0	0
			9536	3053	4768	808	879	28		

- Molecule 85 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	u	51	Total	C	H	N	O	S	0	0
			863	265	432	87	77	2		

- Molecule 86 is a protein called Nascent polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	v	32	Total	C	H	N	O	0	0
			320	96	160	32	32		

- Molecule 87 is a RNA chain called A-site tRNA with aminoacylation.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	w	68	Total	C	H	N	O	P	0	0
			2163	647	725	251	472	68		

- Molecule 88 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	x	70	Total	C	H	N	O	P	0	0
			2234	665	751	261	487	70		

- Molecule 89 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	y	19	Total	C	H	N	O	P	0	0
			598	179	199	63	138	19		

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	A	128	Total	Mg	0
			128	128	
90	D	3	Total	Mg	0
			3	3	
90	E	1	Total	Mg	0
			1	1	
90	g	1	Total	Mg	0
			1	1	
90	AA	53	Total	Mg	0
			53	53	
90	AB	1	Total	Mg	0
			1	1	
90	AX	1	Total	Mg	0
			1	1	
90	A3	1	Total	Mg	0
			1	1	

- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
91	A	30	Total	K	0
			30	30	
91	M	1	Total	K	0
			1	1	
91	N	1	Total	K	0
			1	1	
91	P	1	Total	K	0
			1	1	
91	i	1	Total	K	0
			1	1	

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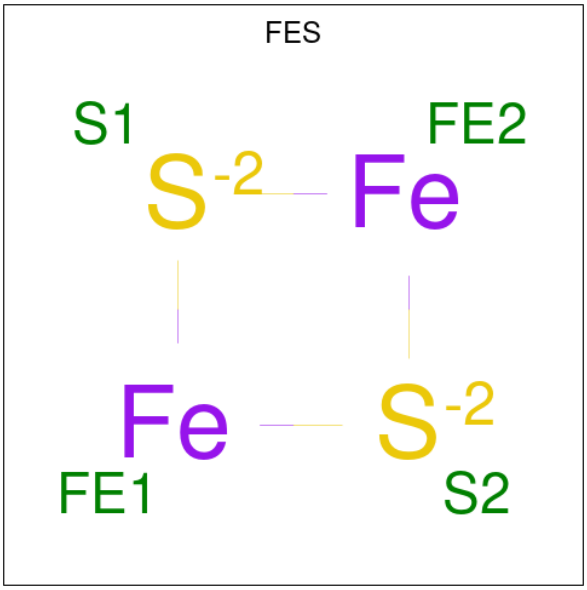
Mol	Chain	Residues	Atoms	AltConf
91	o	1	Total K 1 1	0
91	AA	9	Total K 9 9	0

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

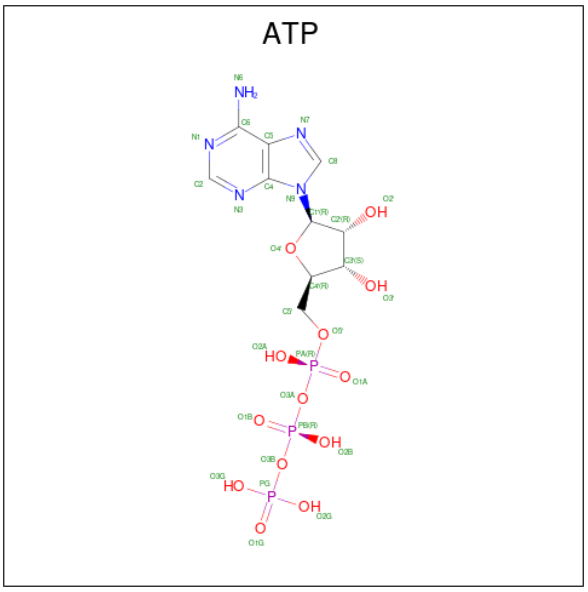
Mol	Chain	Residues	Atoms	AltConf
92	0	1	Total Zn 1 1	0
92	4	1	Total Zn 1 1	0
92	AO	1	Total Zn 1 1	0

- Molecule 93 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



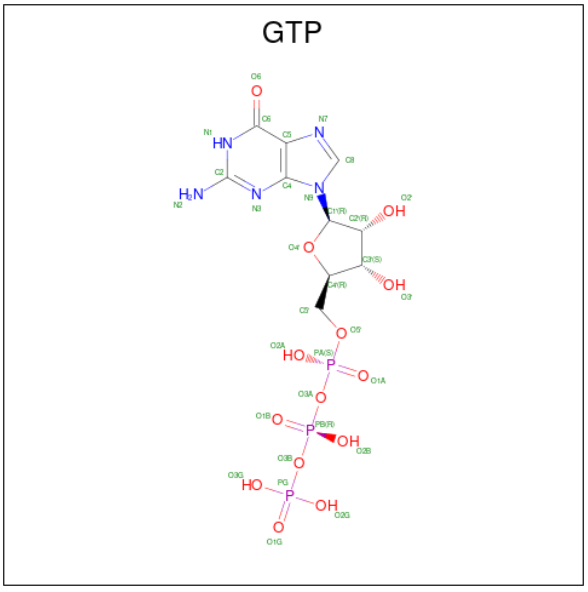
Mol	Chain	Residues	Atoms	AltConf
93	r	1	Total Fe S 4 2 2	0
93	AP	1	Total Fe S 4 2 2	0
93	AT	1	Total Fe S 4 2 2	0

- Molecule 94 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



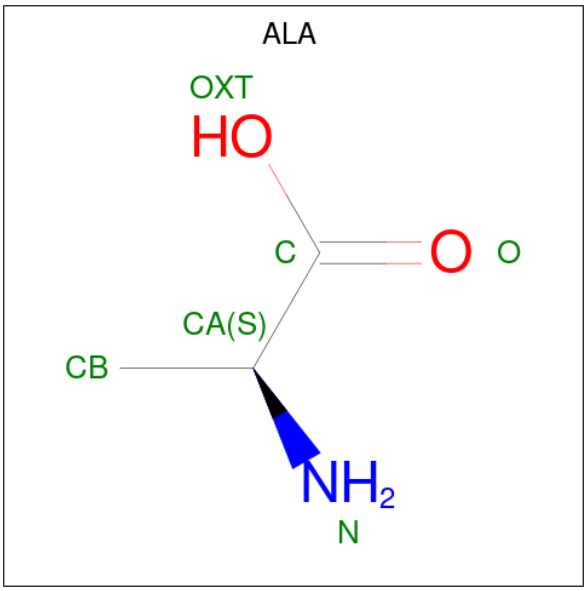
Mol	Chain	Residues	Atoms						AltConf
94	AX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 95 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						AltConf
95	AX	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

- Molecule 96 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms					AltConf
96	w	1	Total	C	H	N	O	0
			12	3	7	1	1	

- Molecule 97 is water.

Mol	Chain	Residues	Atoms		AltConf
97	A	340	Total	O	0
			340	340	
97	B	1	Total	O	0
			1	1	
97	D	5	Total	O	0
			5	5	
97	E	4	Total	O	0
			4	4	
97	F	6	Total	O	0
			6	6	
97	K	3	Total	O	0
			3	3	
97	L	1	Total	O	0
			1	1	
97	M	7	Total	O	0
			7	7	
97	N	1	Total	O	0
			1	1	
97	O	2	Total	O	0
			2	2	
97	Q	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
97	R	3	Total O 3 3	0
97	S	1	Total O 1 1	0
97	T	1	Total O 1 1	0
97	U	1	Total O 1 1	0
97	W	2	Total O 2 2	0
97	6	1	Total O 1 1	0
97	c	1	Total O 1 1	0
97	f	1	Total O 1 1	0
97	i	1	Total O 1 1	0
97	o	2	Total O 2 2	0
97	r	1	Total O 1 1	0
97	s	2	Total O 2 2	0
97	AA	69	Total O 69 69	0
97	AC	1	Total O 1 1	0
97	AG	1	Total O 1 1	0
97	AH	3	Total O 3 3	0
97	AK	2	Total O 2 2	0
97	AX	2	Total O 2 2	0
97	A0	1	Total O 1 1	0
97	A3	3	Total O 3 3	0

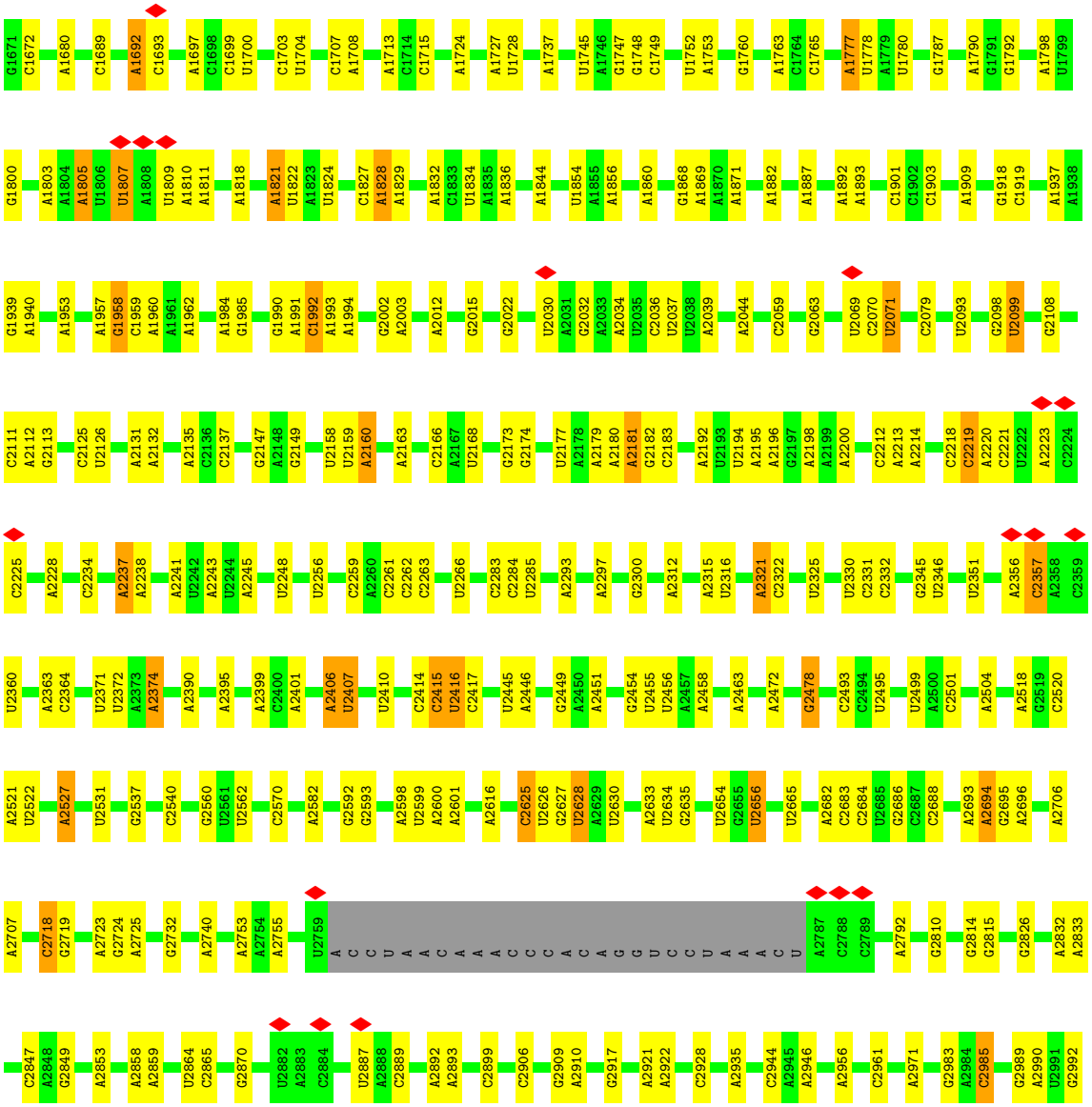
3 Residue-property plots (i)

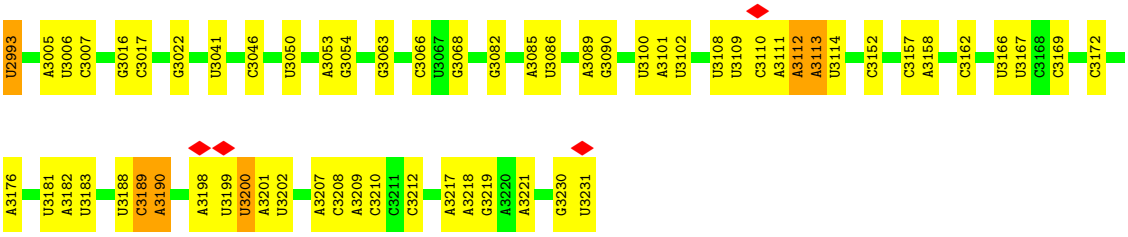
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S mitochondrial rRNA

Chain A:



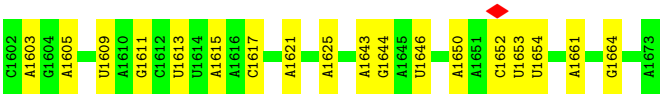




• Molecule 2: mitochondrial tRNAVal

Chain B:

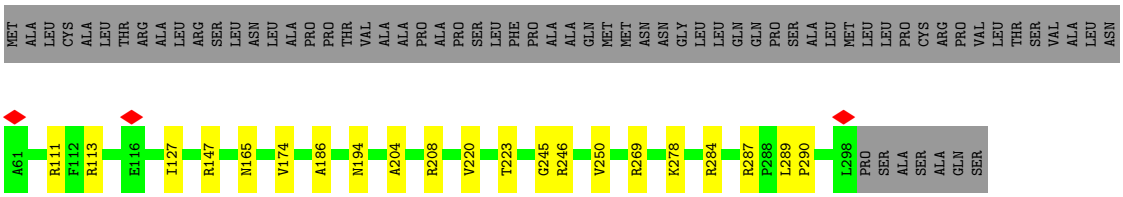




• Molecule 3: 39S ribosomal protein L2, mitochondrial

Chain D:

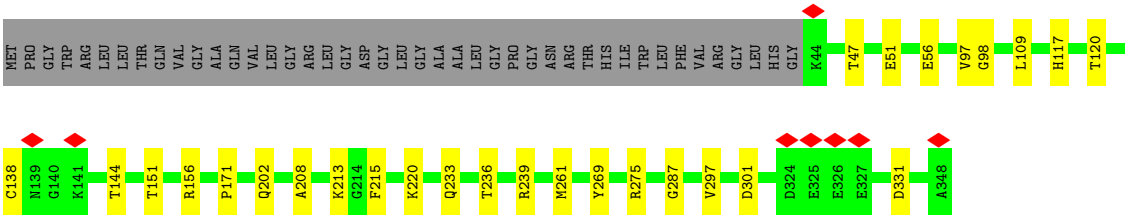




• Molecule 4: 39S ribosomal protein L3, mitochondrial

Chain E:

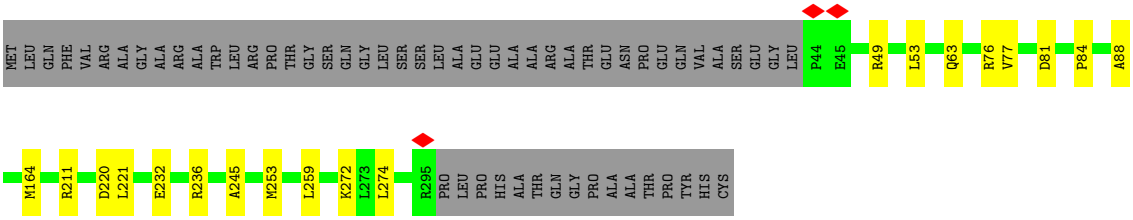




• Molecule 5: 39S ribosomal protein L4, mitochondrial

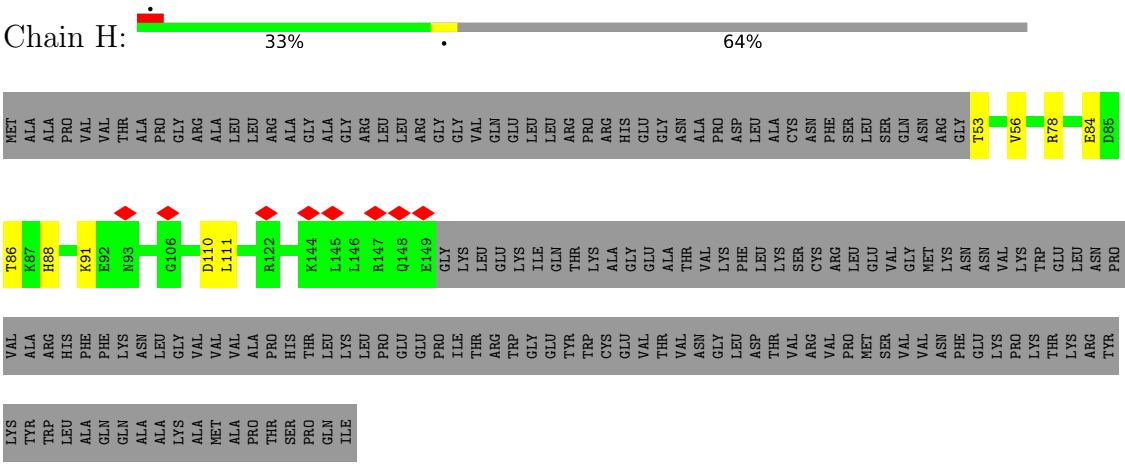
Chain F:





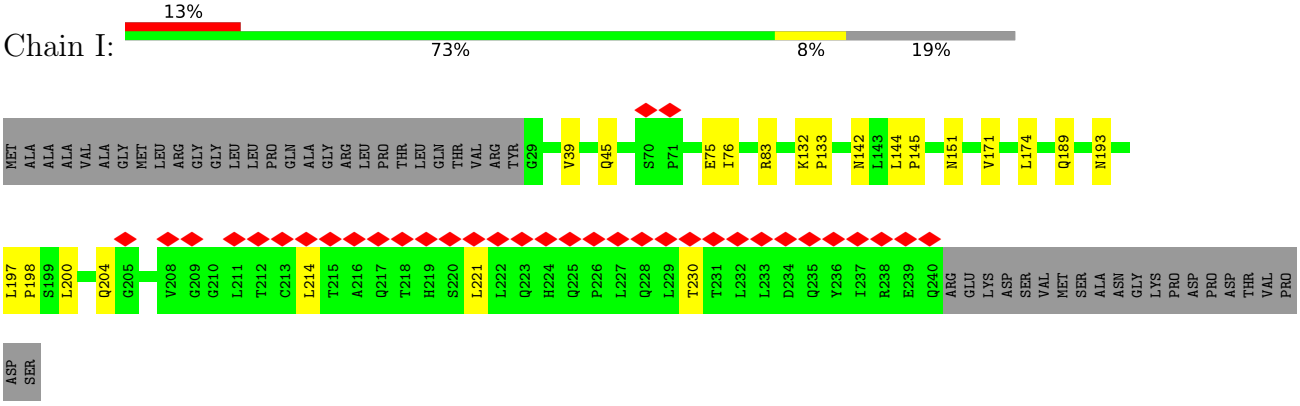
• Molecule 6: 39S ribosomal protein L9, mitochondrial

Chain H:



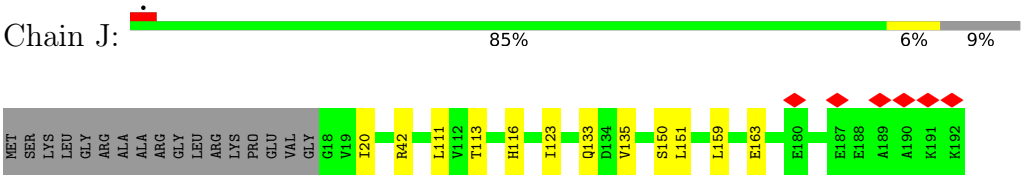
• Molecule 7: 39S ribosomal protein L10, mitochondrial

Chain I:



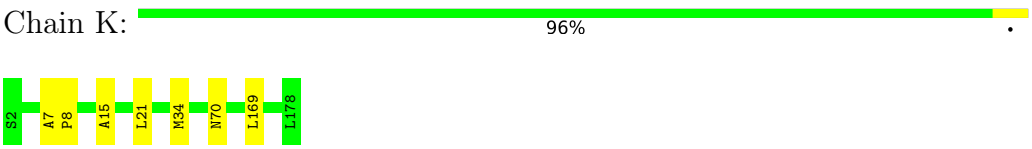
• Molecule 8: 39S ribosomal protein L11, mitochondrial

Chain J:



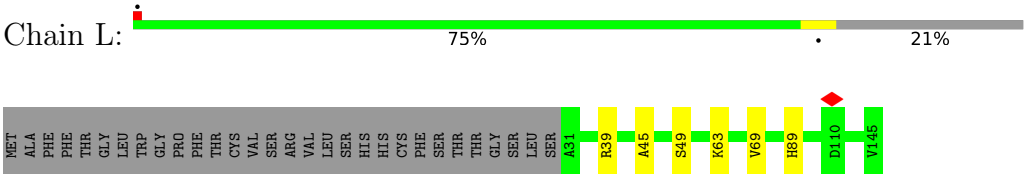
• Molecule 9: 39S ribosomal protein L13, mitochondrial

Chain K:



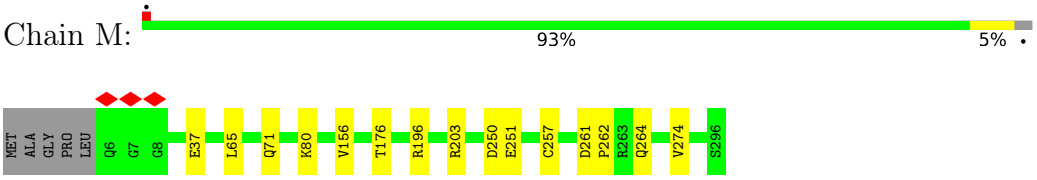
• Molecule 10: 39S ribosomal protein L14, mitochondrial

Chain L:



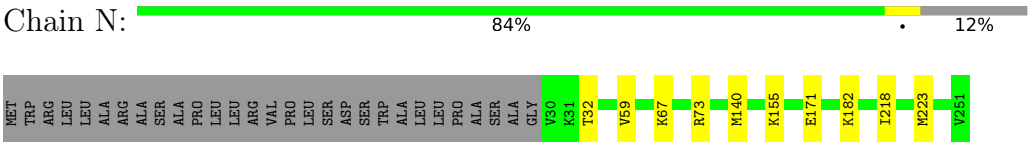
• Molecule 11: 39S ribosomal protein L15, mitochondrial

Chain M:



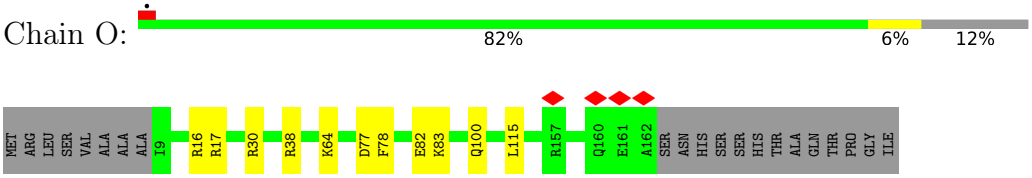
• Molecule 12: 39S ribosomal protein L16, mitochondrial

Chain N:



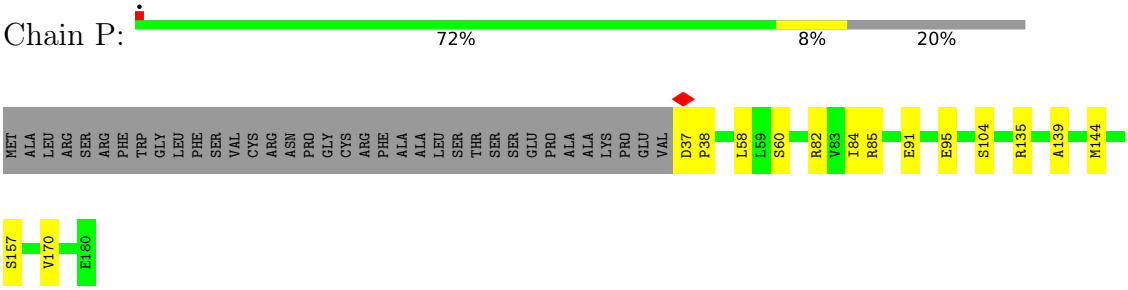
• Molecule 13: 39S ribosomal protein L17, mitochondrial

Chain O:



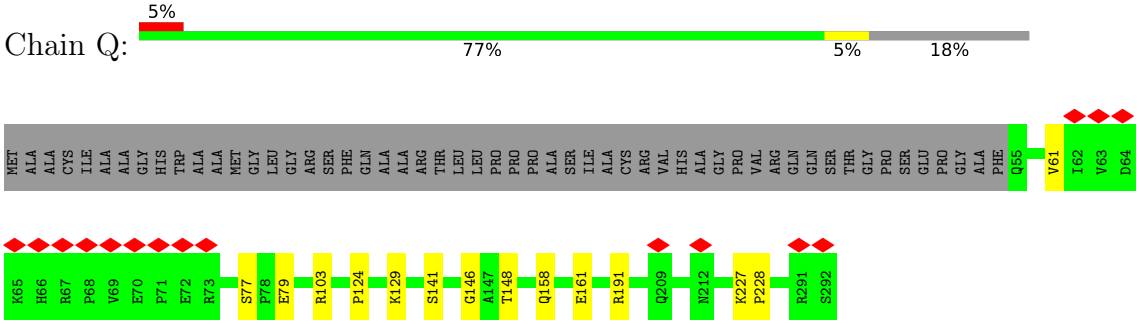
• Molecule 14: 39S ribosomal protein L18, mitochondrial

Chain P:



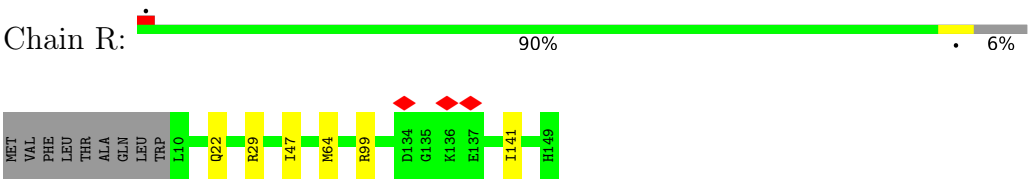
• Molecule 15: 39S ribosomal protein L19, mitochondrial

Chain Q:



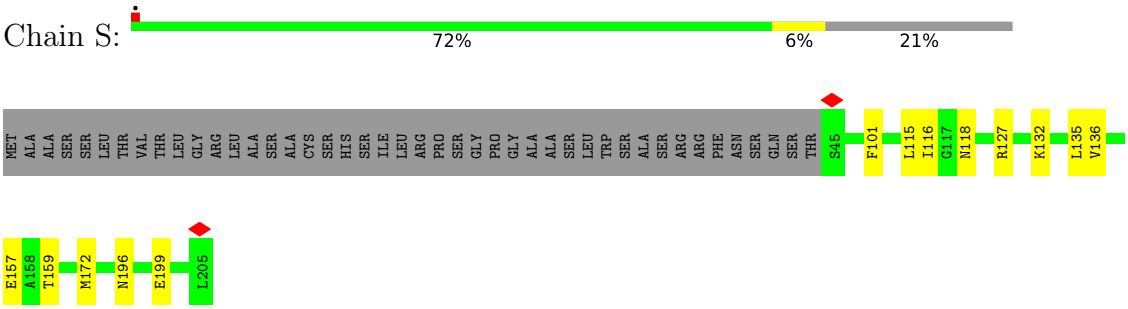
• Molecule 16: 39S ribosomal protein L20, mitochondrial

Chain R:



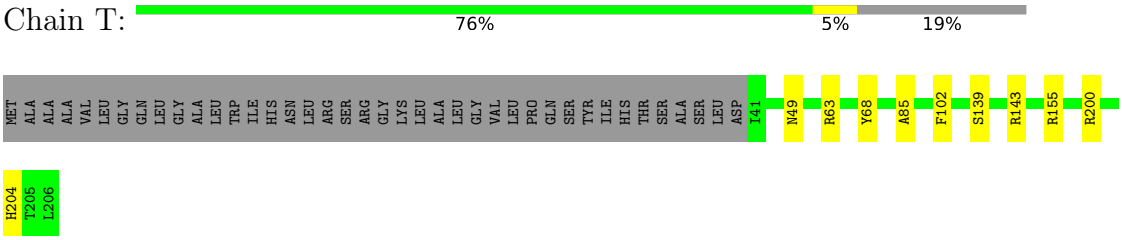
• Molecule 17: 39S ribosomal protein L21, mitochondrial

Chain S:



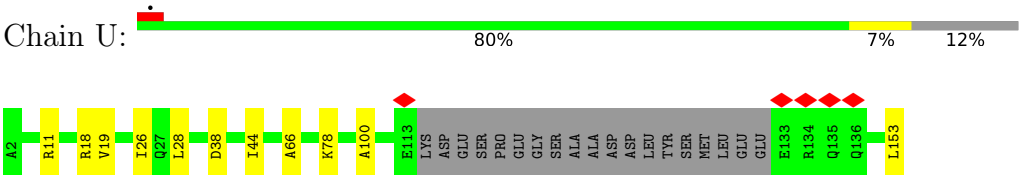
• Molecule 18: 39S ribosomal protein L22, mitochondrial

Chain T:



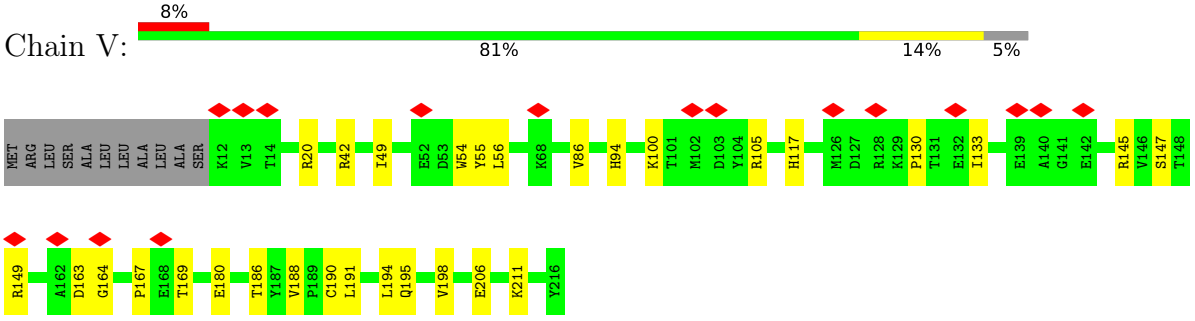
• Molecule 19: 39S ribosomal protein L23, mitochondrial

Chain U:



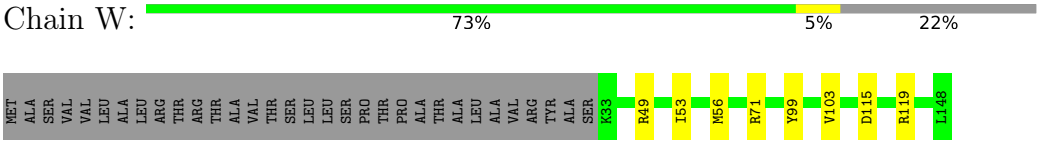
• Molecule 20: 39S ribosomal protein L24, mitochondrial

Chain V:



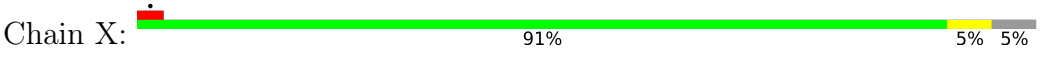
• Molecule 21: 39S ribosomal protein L27, mitochondrial

Chain W:



• Molecule 22: 39S ribosomal protein L28, mitochondrial

Chain X:





• Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y:



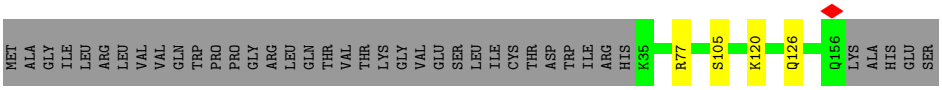




• Molecule 24: 39S ribosomal protein L30, mitochondrial

Chain Z:



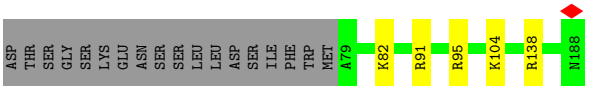


• Molecule 25: 39S ribosomal protein L32, mitochondrial

Chain 0:



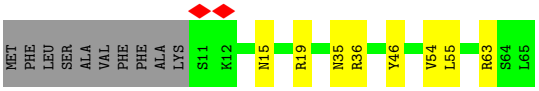




• Molecule 26: 39S ribosomal protein L33, mitochondrial

Chain 1:

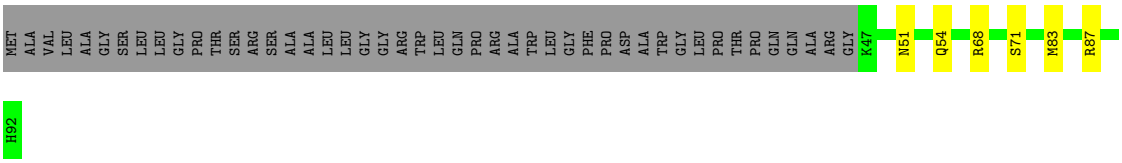




• Molecule 27: 39S ribosomal protein L34, mitochondrial

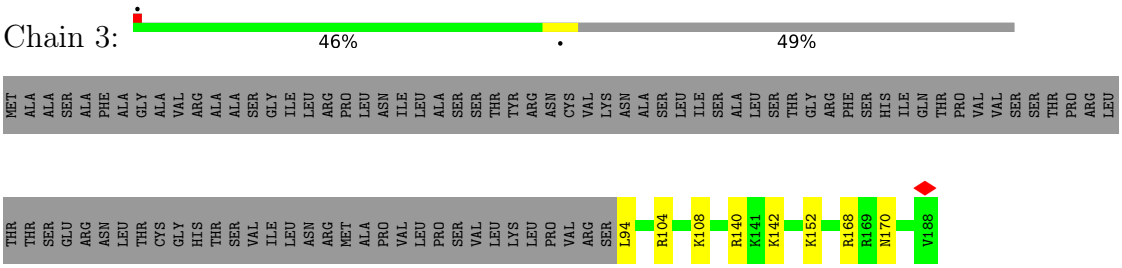
Chain 2:





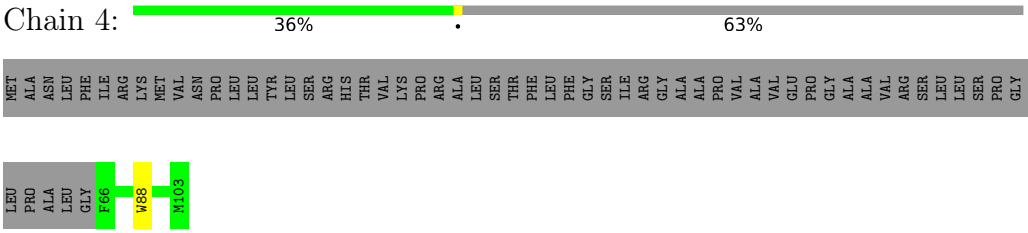
• Molecule 28: 39S ribosomal protein L35, mitochondrial

Chain 3:



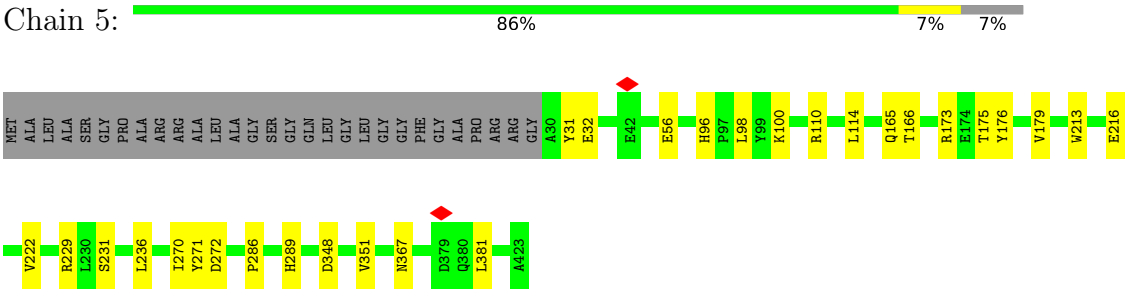
• Molecule 29: 39S ribosomal protein L36, mitochondrial

Chain 4:



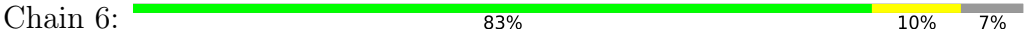
• Molecule 30: 39S ribosomal protein L37, mitochondrial

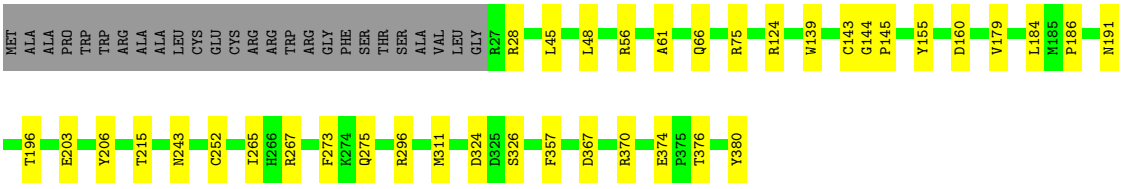
Chain 5:



• Molecule 31: 39S ribosomal protein L38, mitochondrial

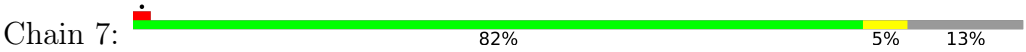
Chain 6:

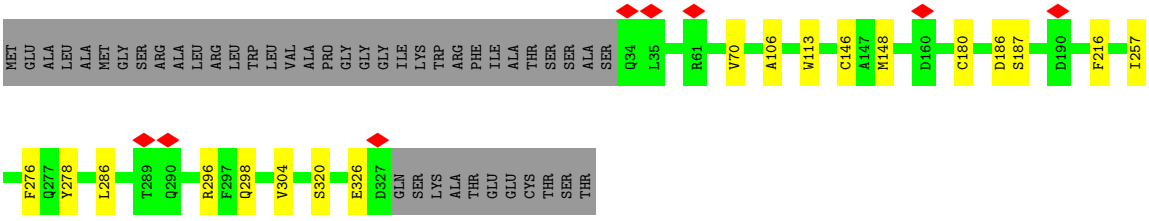




• Molecule 32: 39S ribosomal protein L39, mitochondrial

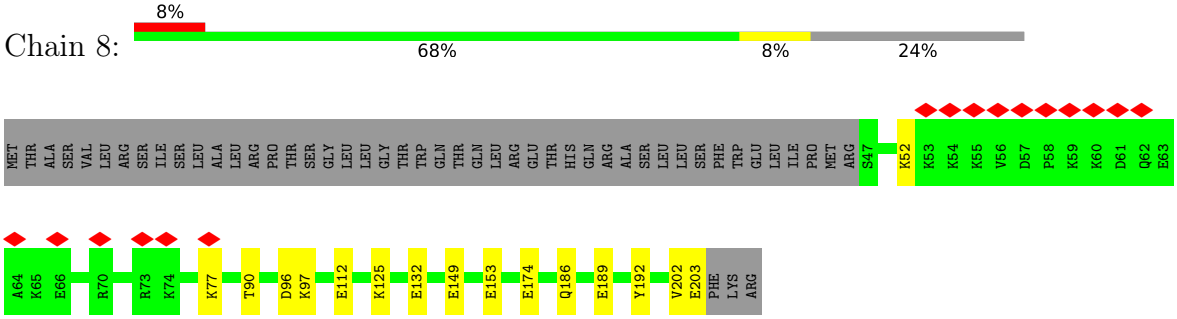
Chain 7:





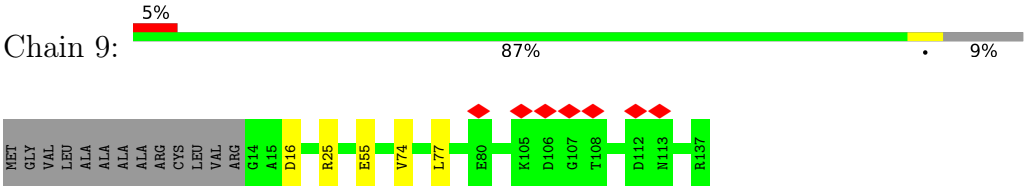
• Molecule 33: 39S ribosomal protein L40, mitochondrial

Chain 8:



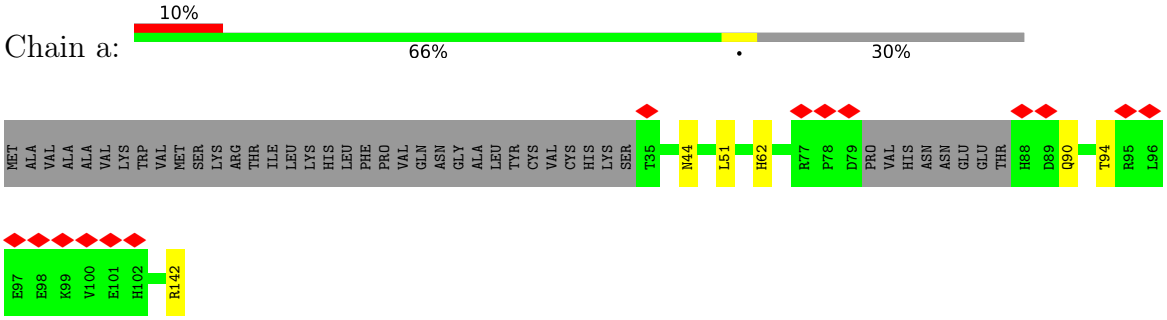
• Molecule 34: 39S ribosomal protein L41, mitochondrial

Chain 9:



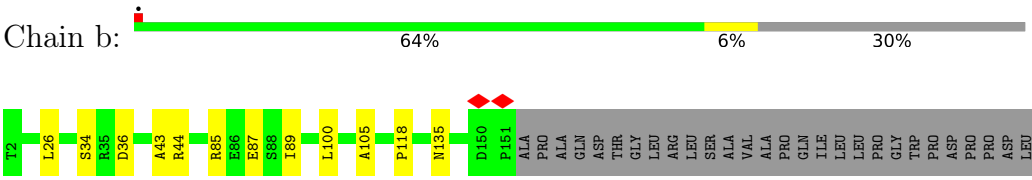
• Molecule 35: 39S ribosomal protein L42, mitochondrial

Chain a:



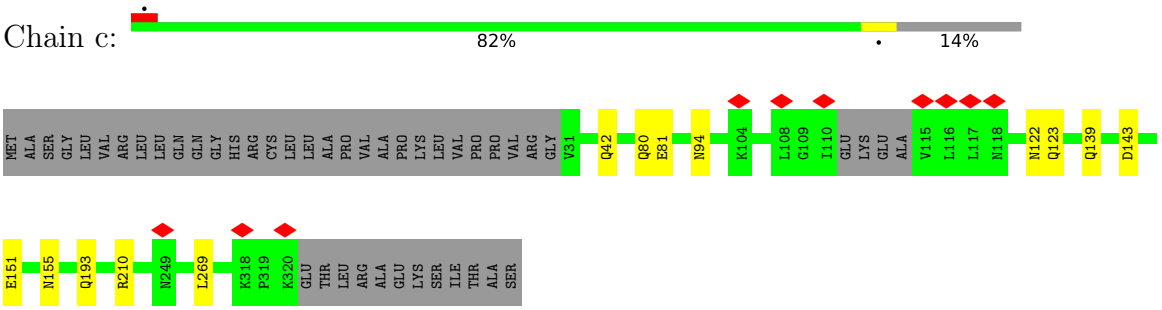
• Molecule 36: 39S ribosomal protein L43, mitochondrial

Chain b:



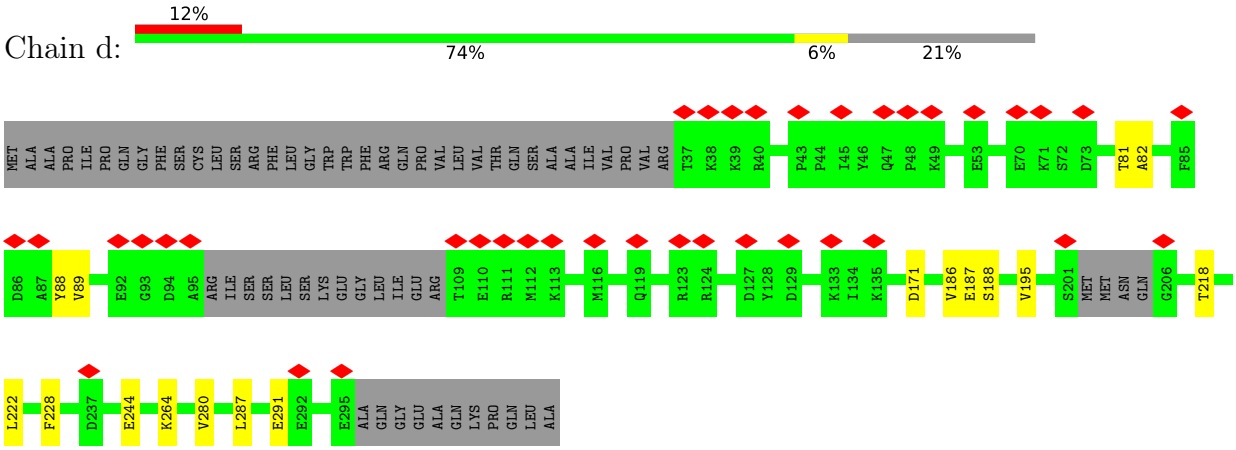
• Molecule 37: 39S ribosomal protein L44, mitochondrial

Chain c:



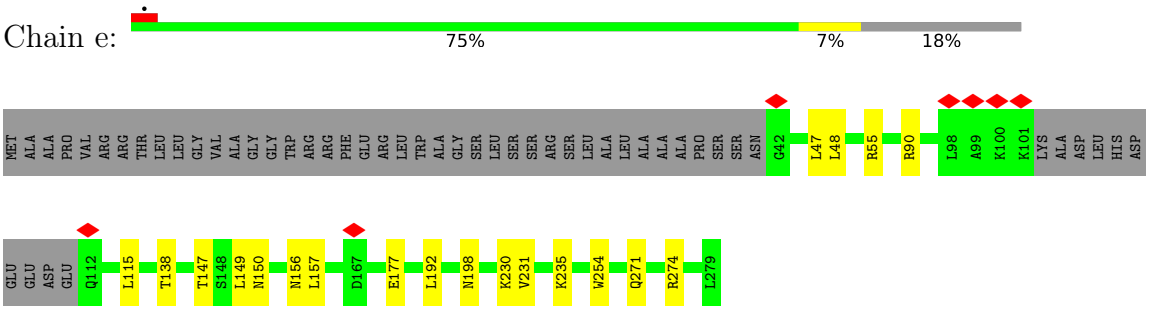
• Molecule 38: 39S ribosomal protein L45, mitochondrial

Chain d:



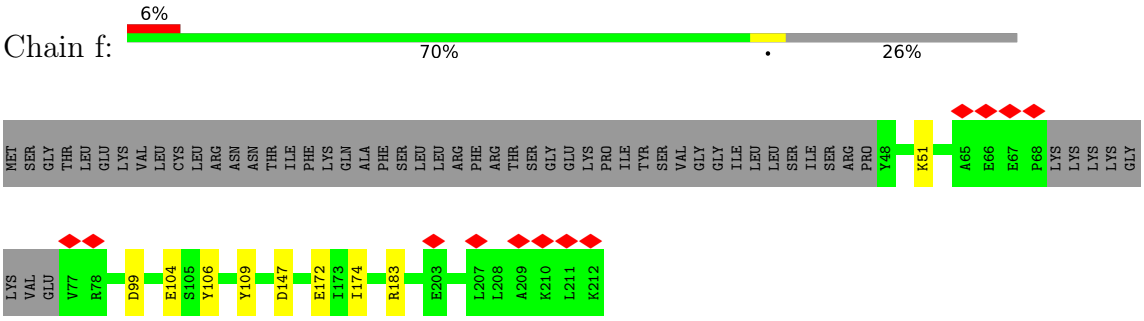
• Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e:



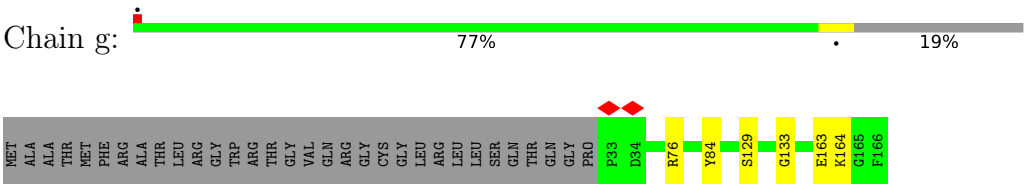
• Molecule 40: 39S ribosomal protein L48, mitochondrial

Chain f:



• Molecule 41: 39S ribosomal protein L49, mitochondrial

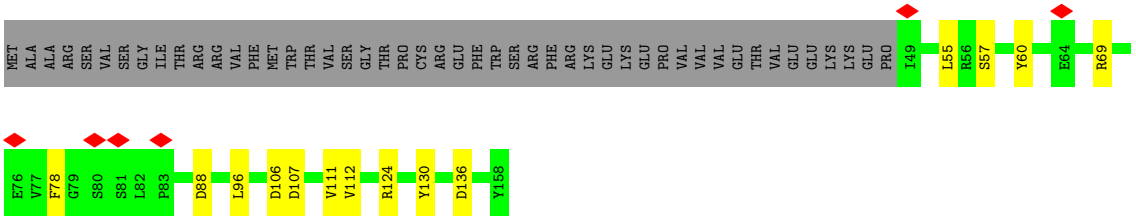
Chain g:



• Molecule 42: 39S ribosomal protein L50, mitochondrial

Chain h:





• Molecule 43: 39S ribosomal protein L51, mitochondrial

Chain i:

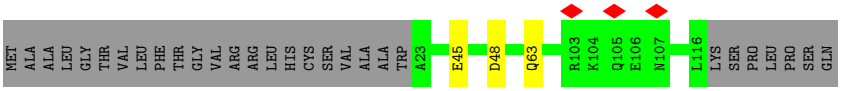




• Molecule 44: 39S ribosomal protein L52, mitochondrial

Chain j:

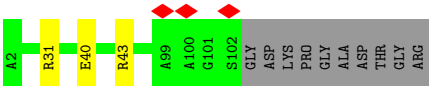




• Molecule 45: 39S ribosomal protein L53, mitochondrial

Chain k:

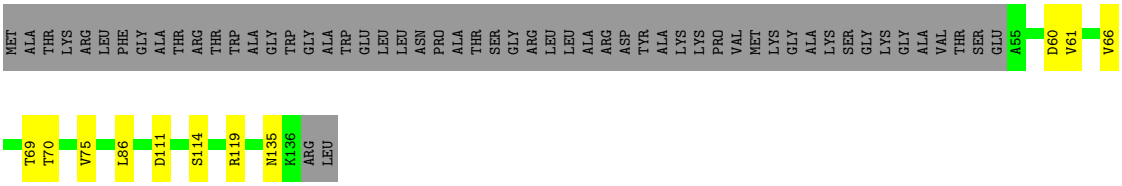




• Molecule 46: 39S ribosomal protein L54, mitochondrial

Chain l:

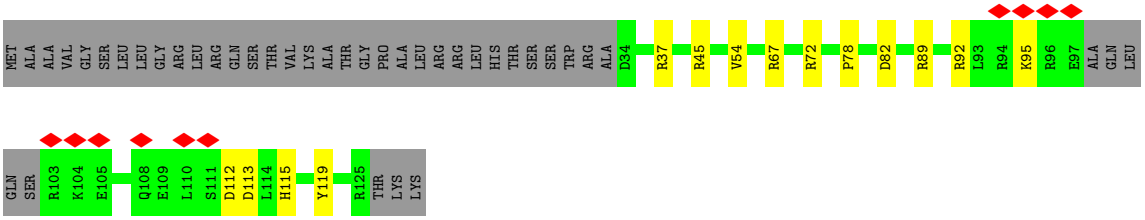




• Molecule 47: 39S ribosomal protein L55, mitochondrial

Chain m:

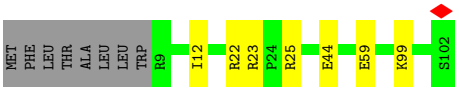




• Molecule 48: Ribosomal protein 63, mitochondrial

Chain o:

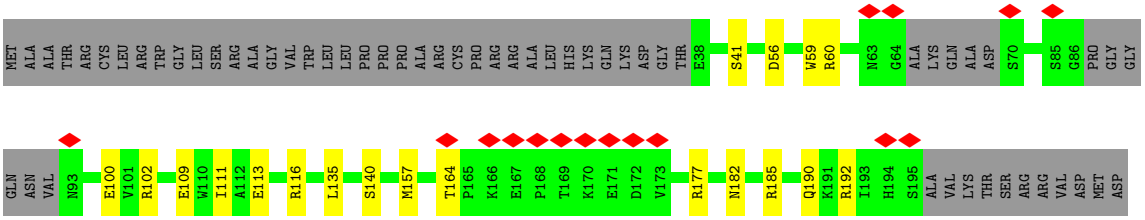




• Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:

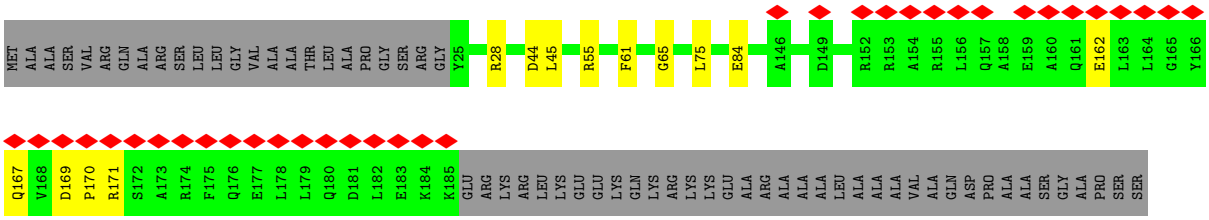




• Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:

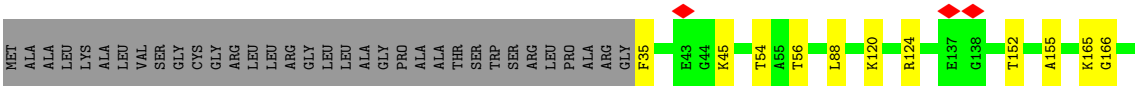


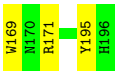


• Molecule 51: 39S ribosomal protein S18a, mitochondrial

Chain r:



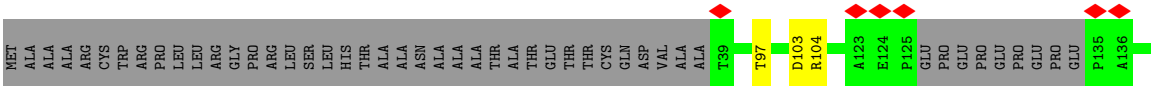


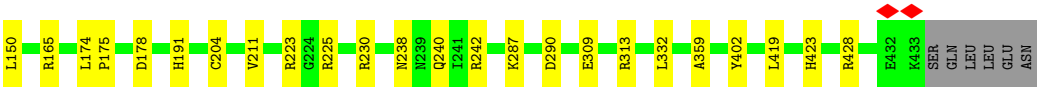


• Molecule 52: 39S ribosomal protein S30, mitochondrial

Chain s:



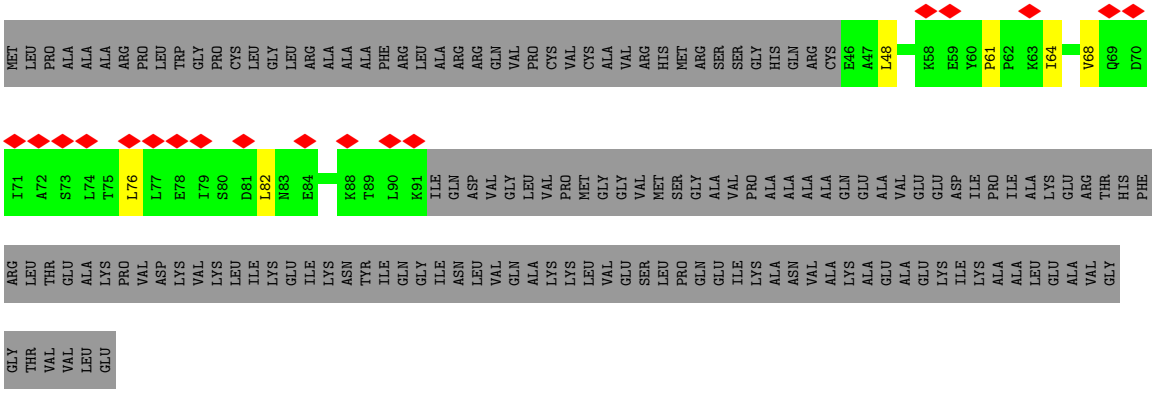




• Molecule 53: 39S ribosomal protein L12, mitochondrial

Chain t1:

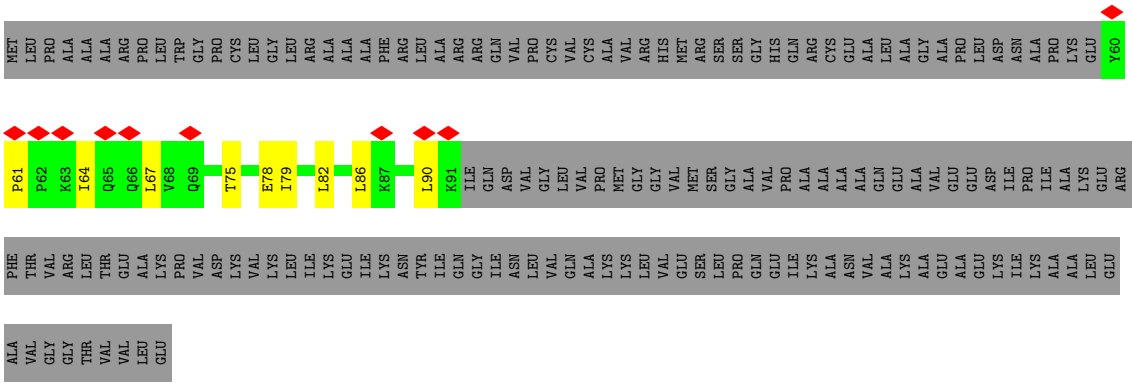




• Molecule 53: 39S ribosomal protein L12, mitochondrial

Chain t2:

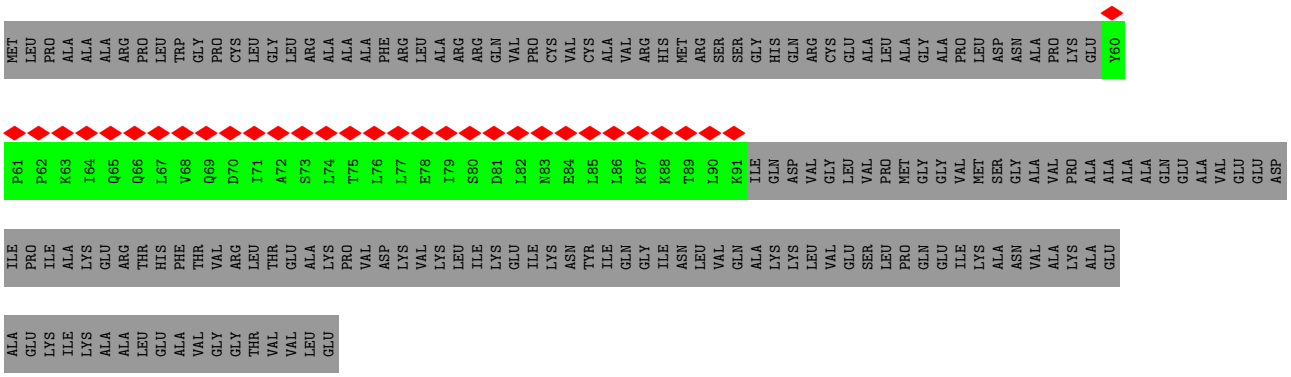




• Molecule 53: 39S ribosomal protein L12, mitochondrial

Chain t3:

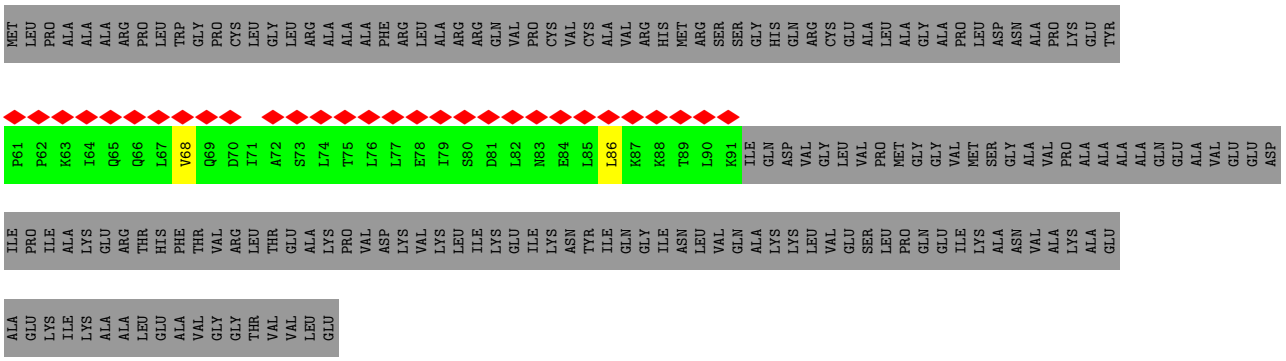




• Molecule 53: 39S ribosomal protein L12, mitochondrial

Chain t4:

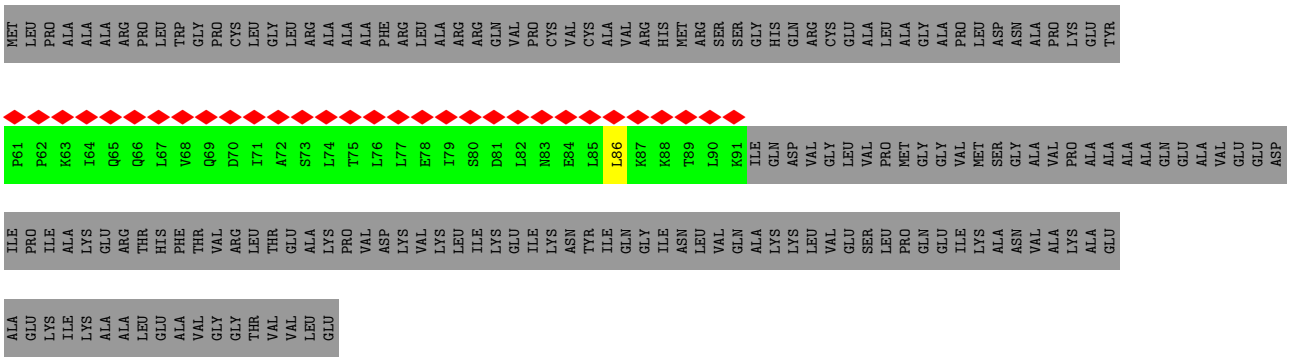




• Molecule 53: 39S ribosomal protein L12, mitochondrial

Chain t5:

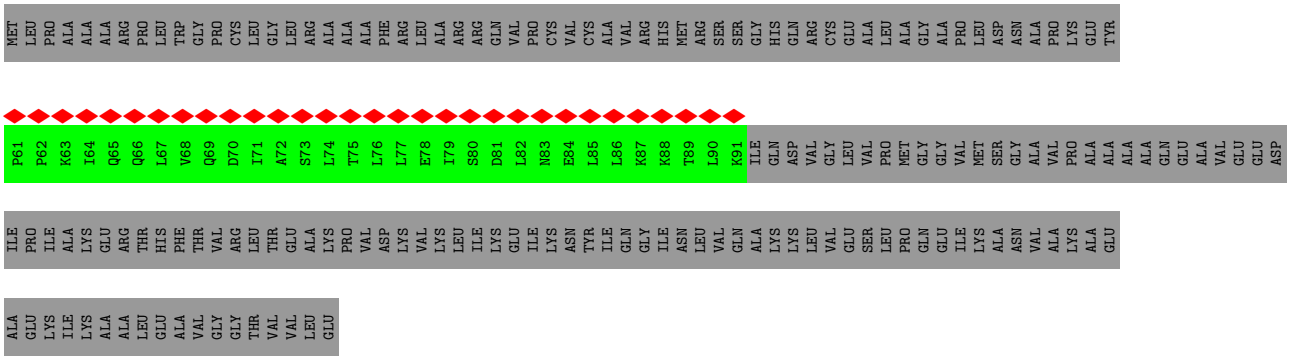




• Molecule 53: 39S ribosomal protein L12, mitochondrial

Chain t6:

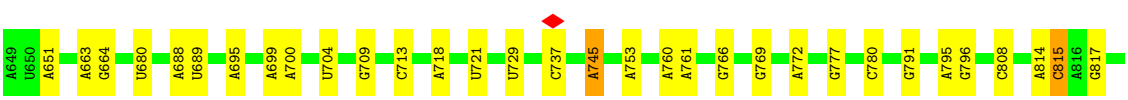


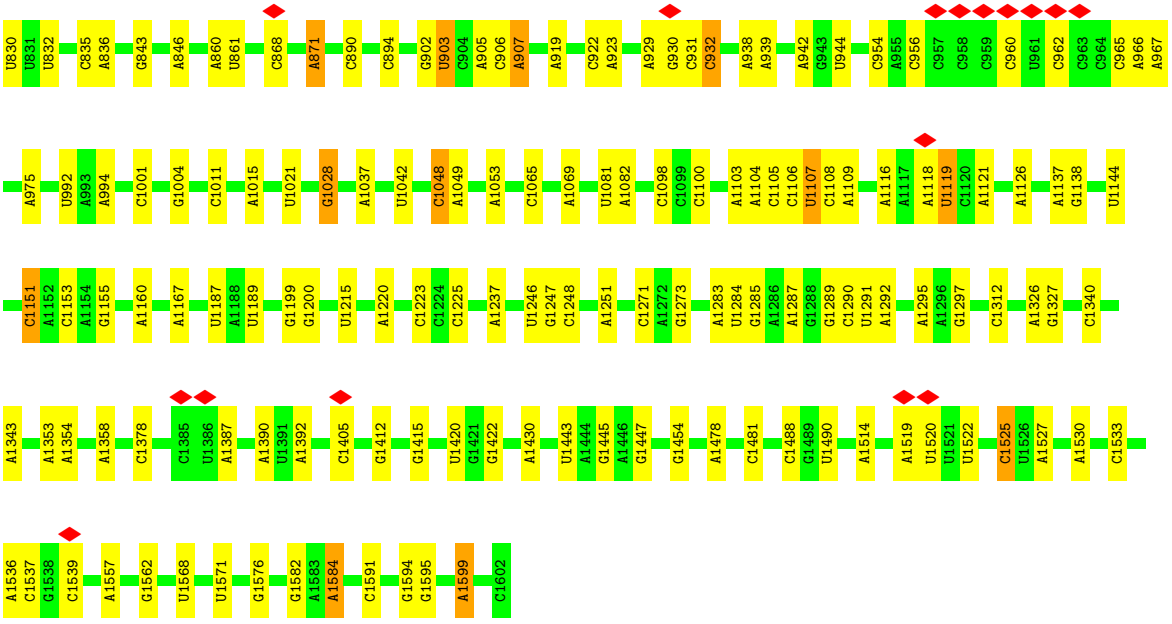


• Molecule 54: 12S mitochondrial rRNA

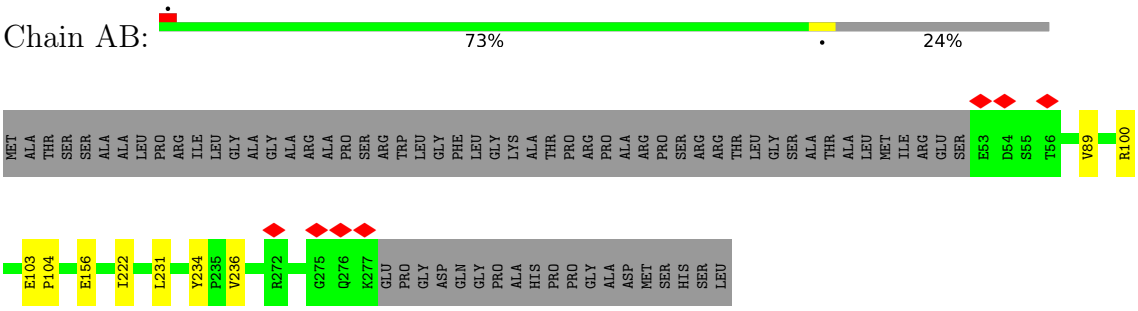
Chain AA:



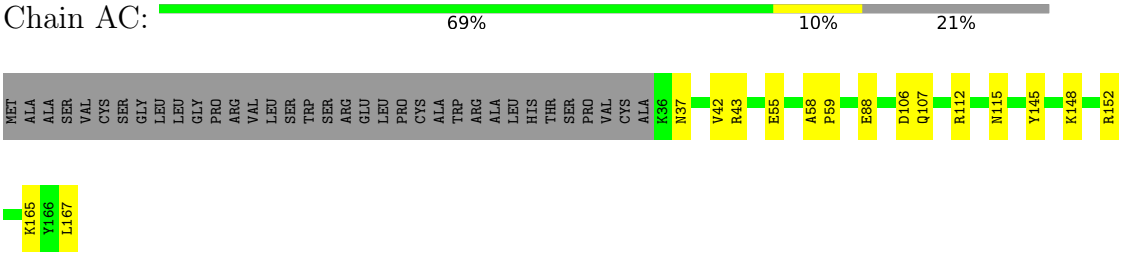




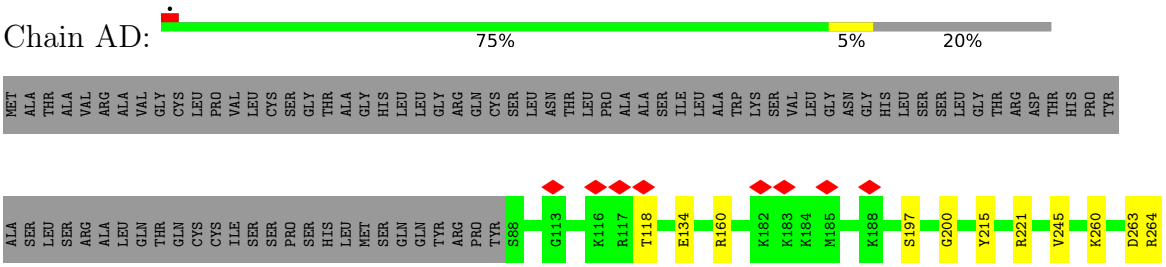
- Molecule 55: 28S ribosomal protein S2, mitochondrial

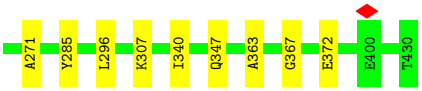


- Molecule 56: 28S ribosomal protein S24, mitochondrial



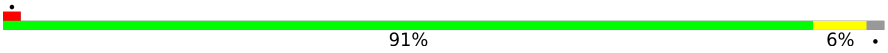
- Molecule 57: 28S ribosomal protein S5, mitochondrial

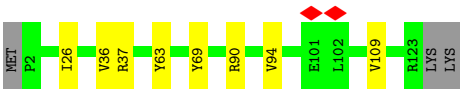




• Molecule 58: 28S ribosomal protein S6, mitochondrial

Chain AE:

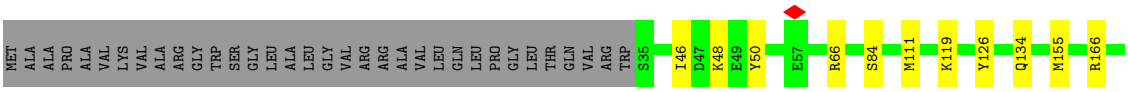


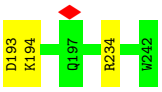


• Molecule 59: 28S ribosomal protein S7, mitochondrial

Chain AF:



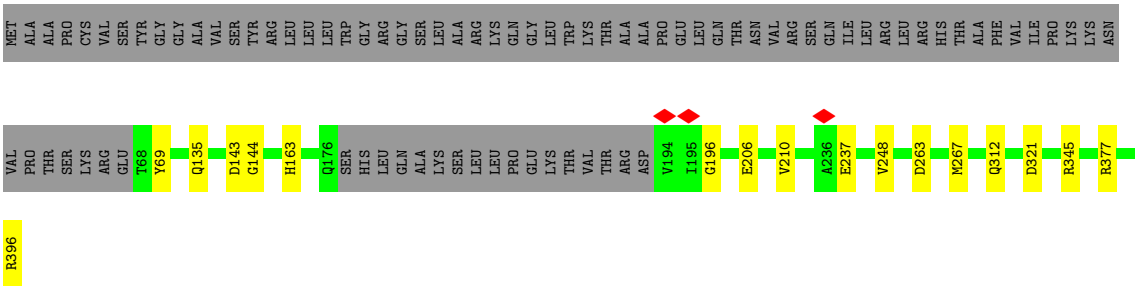




• Molecule 60: 28S ribosomal protein S9, mitochondrial

Chain AG:

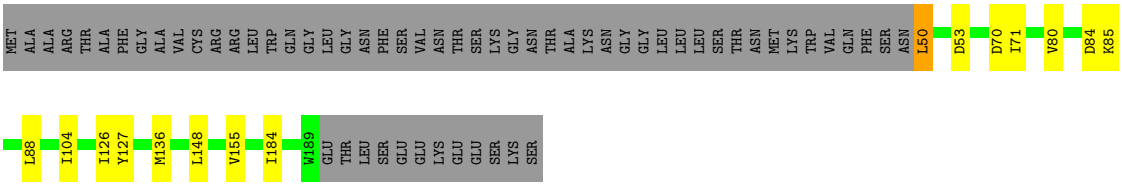




• Molecule 61: 28S ribosomal protein S10, mitochondrial

Chain AH:

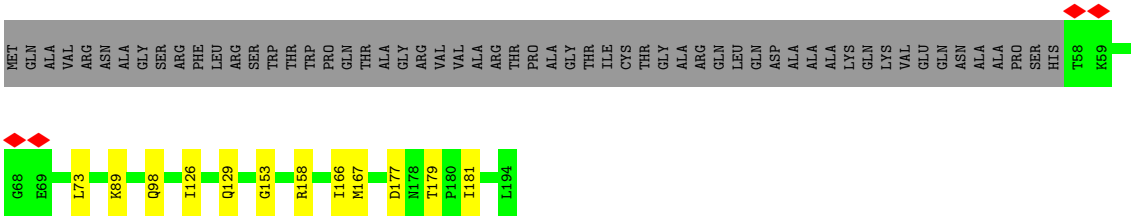




• Molecule 62: 28S ribosomal protein S11, mitochondrial

Chain AI:

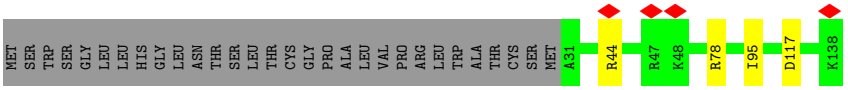




• Molecule 63: 28S ribosomal protein S12, mitochondrial

Chain AJ:





• Molecule 64: 28S ribosomal protein S14, mitochondrial

Chain AK:

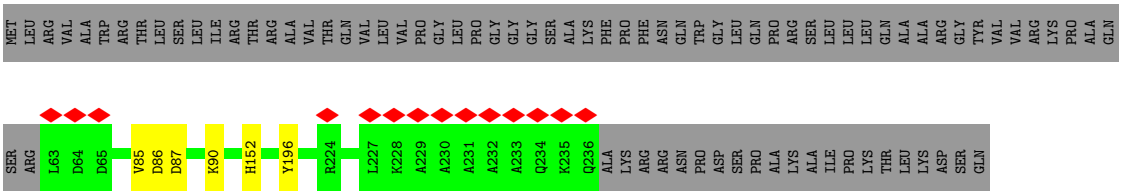




• Molecule 65: 28S ribosomal protein S15, mitochondrial

Chain AL:

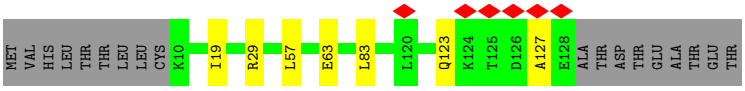




• Molecule 66: 28S ribosomal protein S16, mitochondrial

Chain AM:

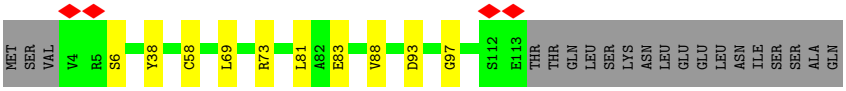




• Molecule 67: 28S ribosomal protein S17, mitochondrial

Chain AN:

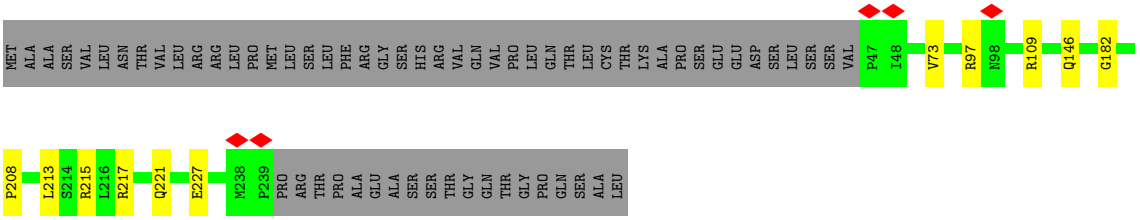




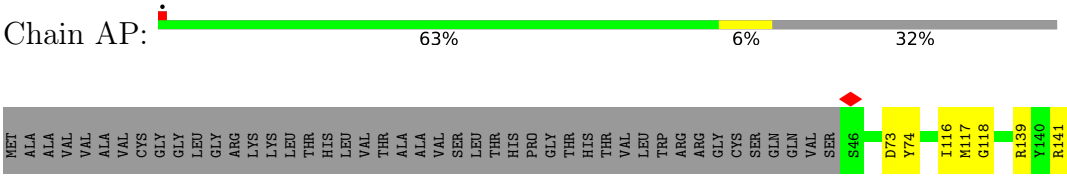
• Molecule 68: 28S ribosomal protein S18b, mitochondrial

Chain AO:

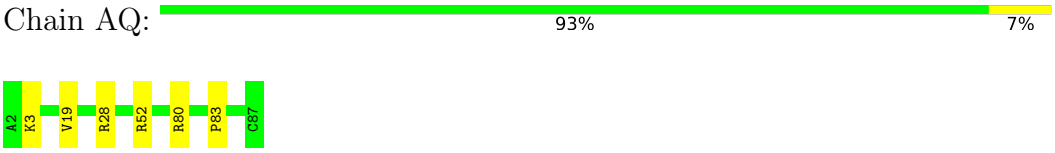




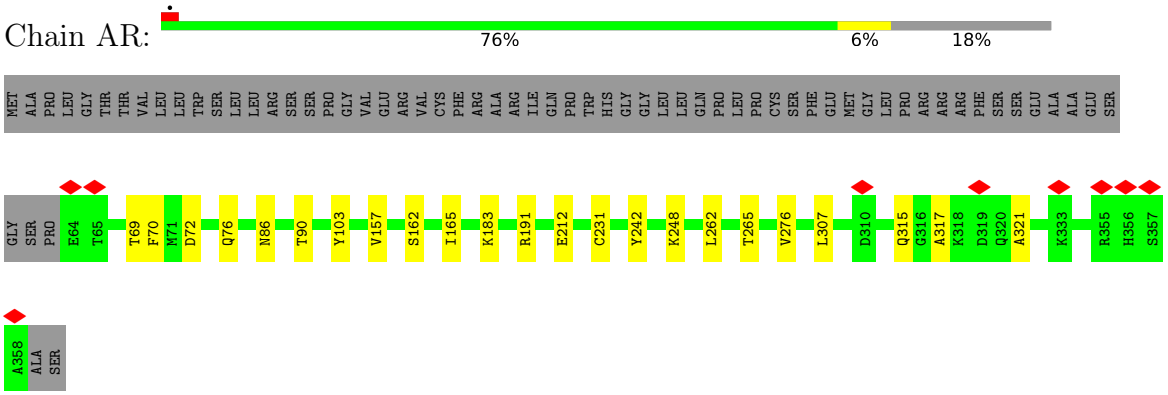
• Molecule 69: 28S ribosomal protein S18c, mitochondrial



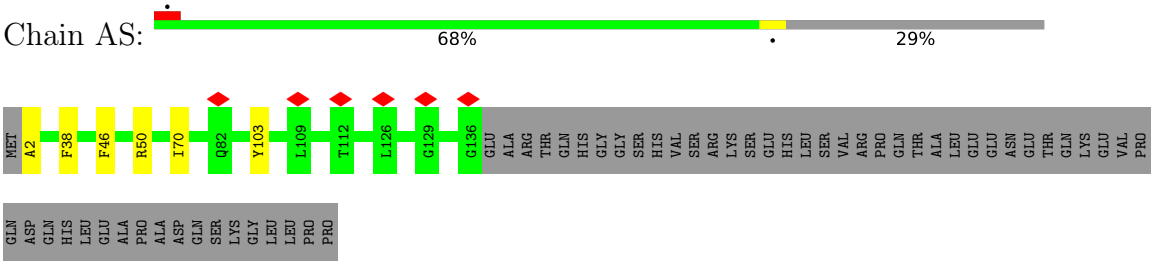
• Molecule 70: 28S ribosomal protein S21, mitochondrial



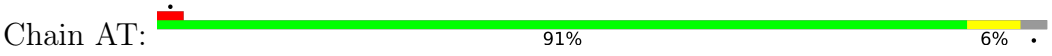
• Molecule 71: 28S ribosomal protein S22, mitochondrial

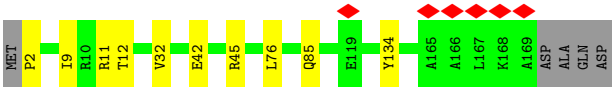


• Molecule 72: 28S ribosomal protein S23, mitochondrial

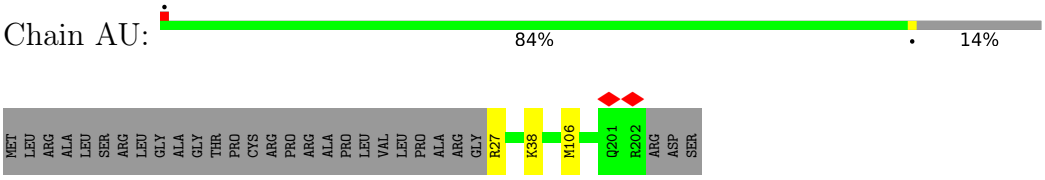


• Molecule 73: 28S ribosomal protein S25, mitochondrial

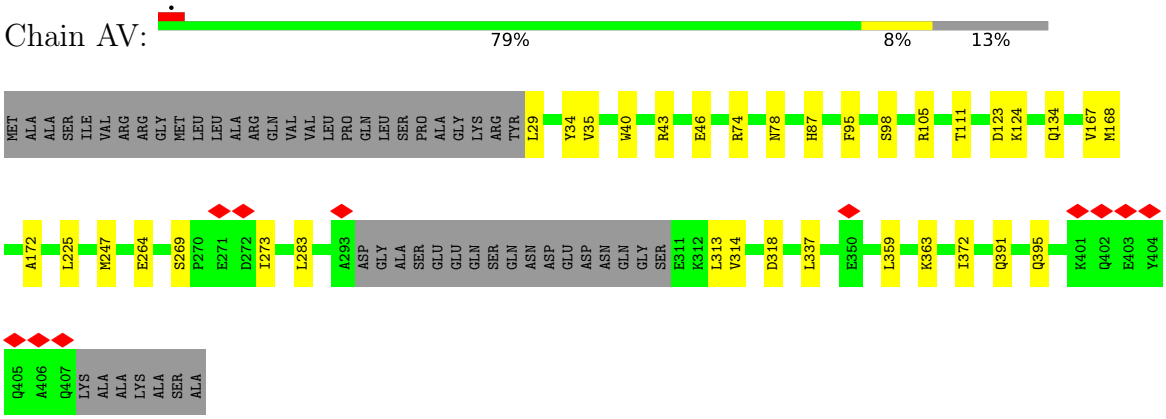




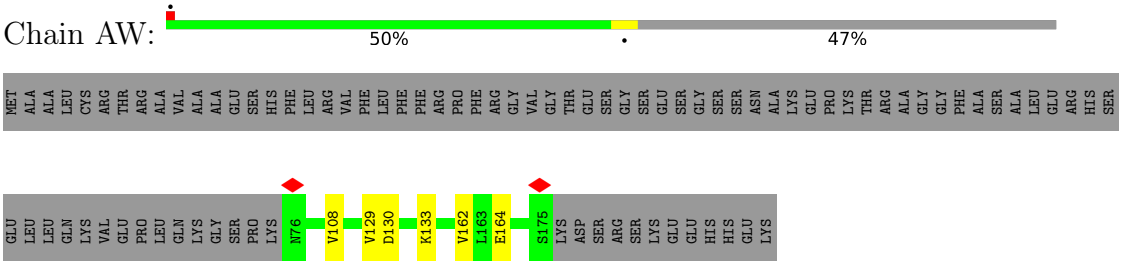
• Molecule 74: 28S ribosomal protein S26, mitochondrial



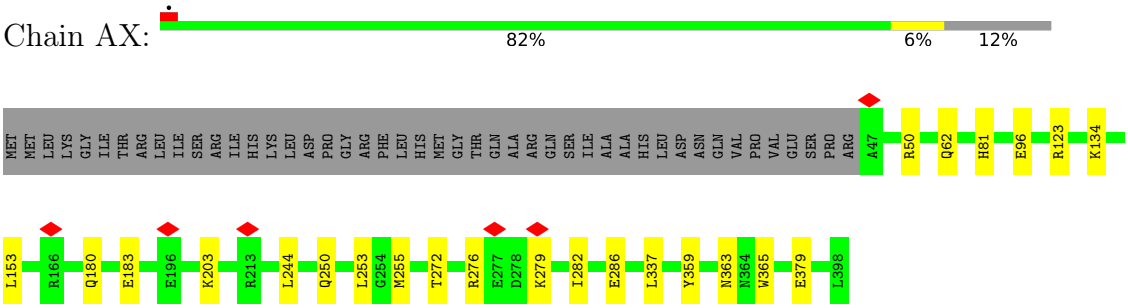
• Molecule 75: 28S ribosomal protein S27, mitochondrial



• Molecule 76: 28S ribosomal protein S28, mitochondrial

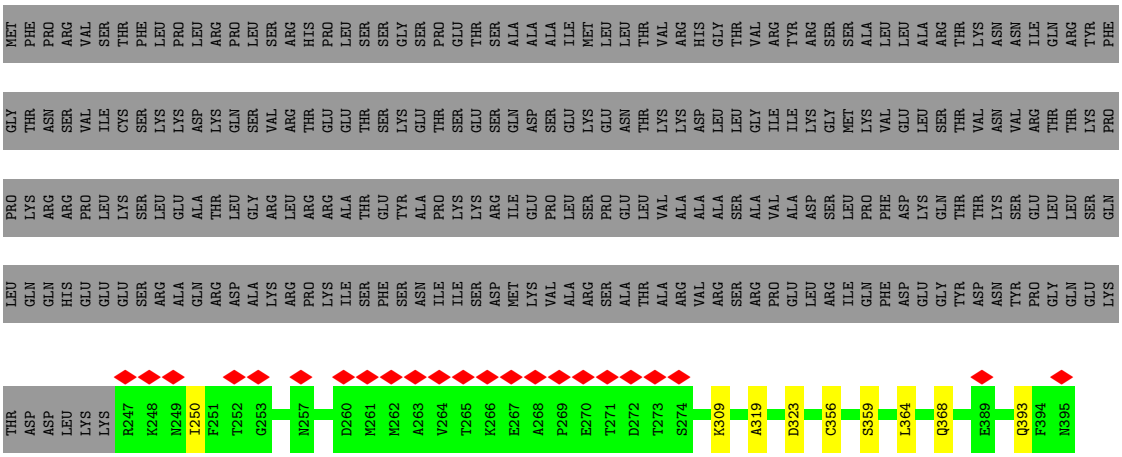


• Molecule 77: 28S ribosomal protein S29, mitochondrial



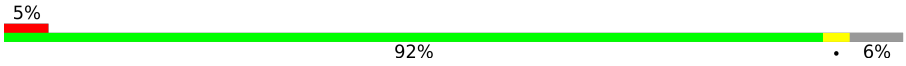
• Molecule 78: 28S ribosomal protein S31, mitochondrial

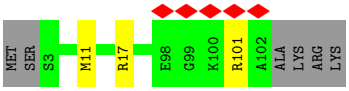




• Molecule 79: 28S ribosomal protein S33, mitochondrial

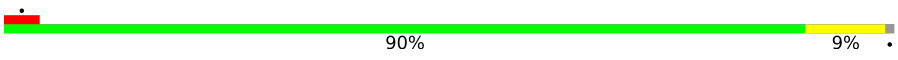
Chain AZ:

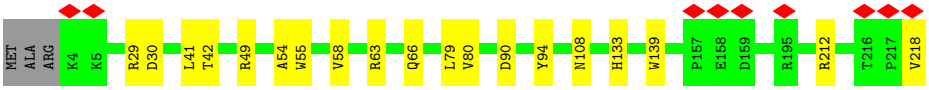




• Molecule 80: 28S ribosomal protein S34, mitochondrial

Chain A0:

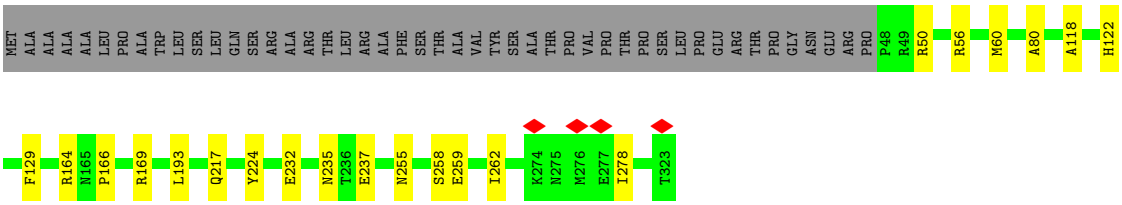




• Molecule 81: 28S ribosomal protein S35, mitochondrial

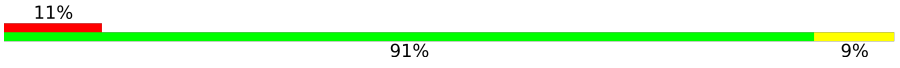
Chain A1:

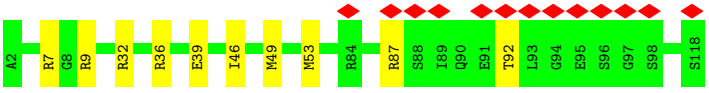




• Molecule 82: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2:

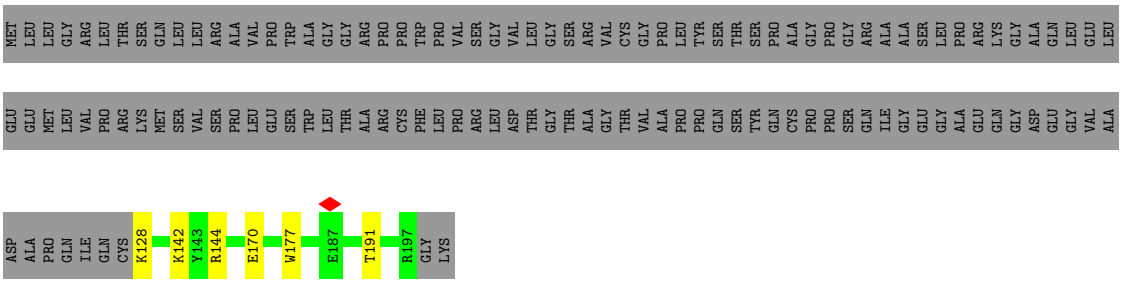




• Molecule 83: Aurora kinase A-interacting protein

Chain A3:

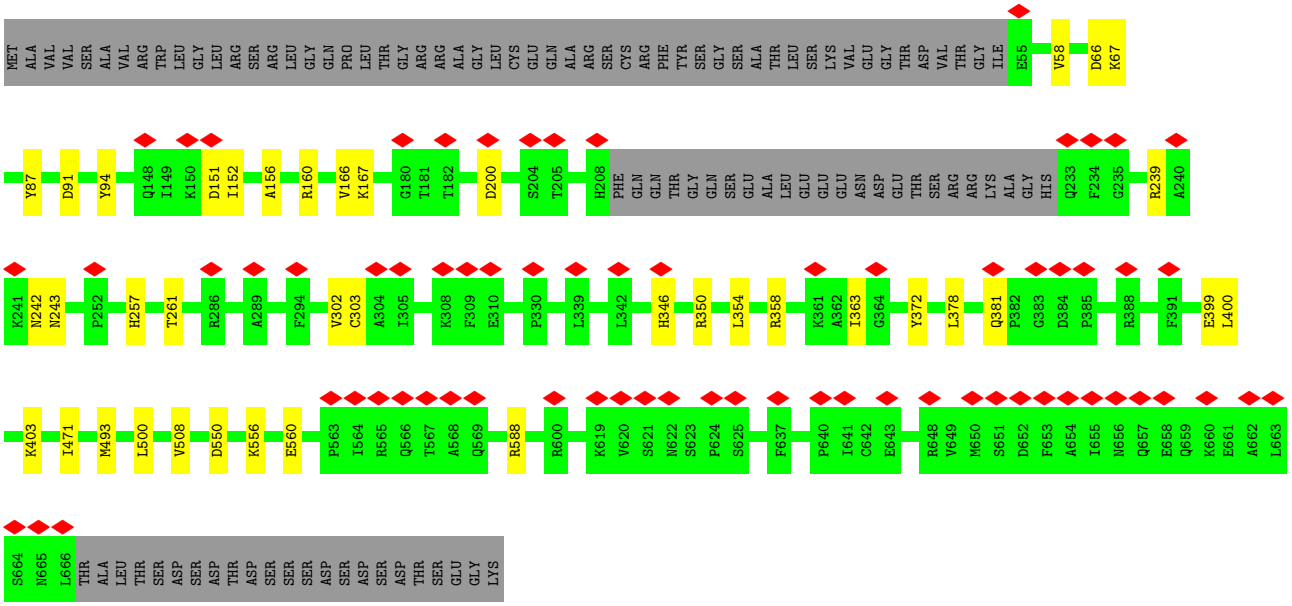




• Molecule 84: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4:

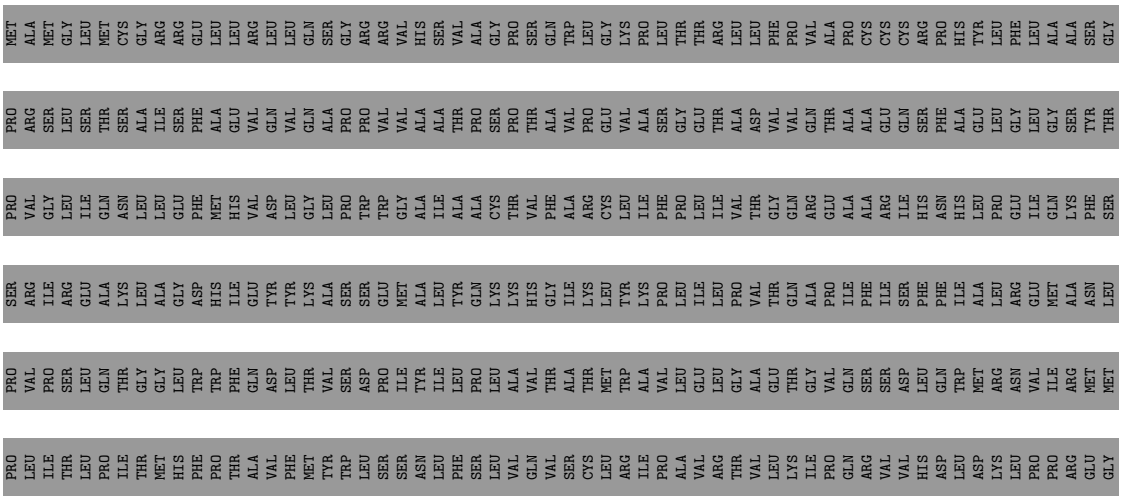


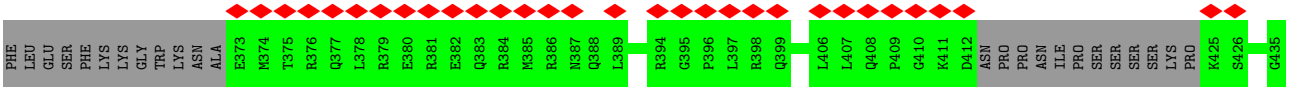


• Molecule 85: Mitochondrial inner membrane protein OXA1L

Chain u:

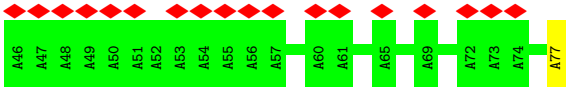






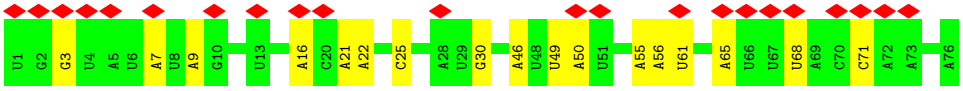
• Molecule 86: Nascent polypeptide



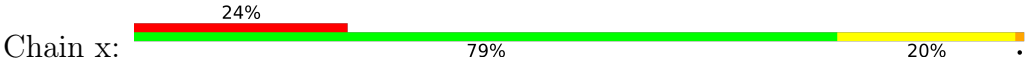


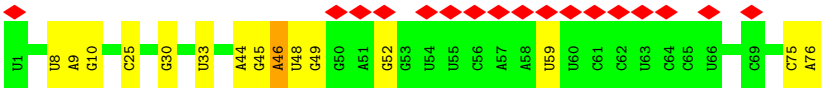
• Molecule 87: A-site tRNA with aminoacylation



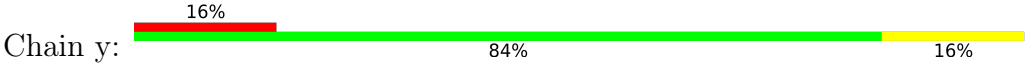


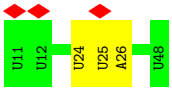
• Molecule 88: P-site tRNA





• Molecule 89: mRNA





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30744	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)	200	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	42.750	Depositor
Minimum map value	-22.327	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.092	Depositor
Recommended contour level	3	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: ATP, SAC, MG, ZN, FES, GTP, K, THC, IAS, 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	A	0.13	0/36431	0.20	0/56711
2	B	0.11	0/1700	0.19	0/2641
3	D	0.15	0/1896	0.29	0/2549
4	E	0.14	0/2475	0.25	0/3355
5	F	0.16	0/2090	0.29	0/2842
6	H	0.14	0/816	0.27	0/1097
7	I	0.18	0/1731	0.27	0/2345
8	J	0.16	0/1348	0.27	0/1813
9	K	0.19	0/1490	0.28	0/2021
10	L	0.15	0/905	0.28	0/1218
11	M	0.16	0/2381	0.29	0/3212
12	N	0.18	0/1833	0.28	0/2468
13	O	0.16	0/1283	0.27	0/1727
14	P	0.23	0/1199	0.30	0/1623
15	Q	0.13	0/2027	0.26	0/2734
16	R	0.18	0/1175	0.27	0/1572
17	S	0.16	0/1320	0.31	0/1789
18	T	0.16	0/1403	0.28	0/1886
19	U	0.16	0/1127	0.30	0/1523
20	V	0.12	0/1721	0.26	0/2333
21	W	0.23	0/926	0.31	0/1244
22	X	0.13	0/2099	0.25	0/2837
23	Y	0.15	0/1593	0.28	0/2136
24	Z	0.15	0/1021	0.27	0/1378
25	0	0.15	0/913	0.27	0/1224
26	1	0.15	0/460	0.27	0/610
27	2	0.19	0/383	0.33	0/507
28	3	0.19	0/853	0.31	0/1136
29	4	0.21	0/350	0.30	0/461
30	5	0.14	0/3305	0.26	0/4502
31	6	0.21	0/3043	0.31	0/4140
32	7	0.11	0/2447	0.24	0/3310

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	8	0.16	0/1354	0.26	0/1819
34	9	0.15	0/1025	0.25	0/1379
35	a	0.13	0/866	0.30	0/1174
36	b	0.16	0/1211	0.30	0/1639
37	c	0.14	0/2347	0.25	0/3171
38	d	0.10	0/2043	0.23	0/2764
39	e	0.15	0/1885	0.25	0/2542
40	f	0.20	0/1273	0.26	0/1716
41	g	0.15	0/1151	0.29	0/1569
42	h	0.11	0/918	0.23	0/1249
43	i	0.18	0/850	0.30	0/1135
44	j	0.15	0/760	0.27	0/1023
45	k	0.16	0/777	0.27	0/1048
46	l	0.15	0/707	0.27	0/960
47	m	0.17	0/767	0.30	0/1028
48	o	0.18	0/819	0.31	0/1097
49	p	0.13	0/1223	0.27	0/1641
50	q	0.12	0/1384	0.26	0/1869
51	r	0.20	0/1362	0.29	0/1846
52	s	0.15	0/3239	0.28	0/4400
53	t1	0.06	0/358	0.18	0/486
53	t2	0.07	0/259	0.19	0/350
53	t3	0.05	0/259	0.14	0/350
53	t4	0.06	0/246	0.16	0/331
53	t5	0.05	0/246	0.15	0/331
53	t6	0.06	0/246	0.15	0/331
54	AA	0.11	0/22655	0.17	0/35273
55	AB	0.15	0/1871	0.26	0/2531
56	AC	0.21	0/1113	0.28	0/1505
57	AD	0.16	0/2783	0.27	0/3724
58	AE	0.12	0/989	0.26	0/1335
59	AF	0.12	0/1767	0.25	0/2373
60	AG	0.14	0/2623	0.27	0/3515
61	AH	0.20	0/1178	0.28	0/1598
62	AI	0.13	0/1030	0.26	0/1386
63	AJ	0.15	0/855	0.27	0/1148
64	AK	0.20	0/880	0.31	0/1182
65	AL	0.12	0/1477	0.25	0/1974
66	AM	0.16	0/963	0.29	0/1295
67	AN	0.14	0/886	0.23	0/1199
68	AO	0.14	0/1648	0.27	0/2243
69	AP	0.13	0/798	0.26	0/1070
70	AQ	0.15	0/748	0.32	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
71	AR	0.13	0/2456	0.25	0/3317
72	AS	0.13	0/1138	0.25	0/1533
73	AT	0.13	0/1402	0.27	0/1883
74	AU	0.13	0/1510	0.28	0/2025
75	AV	0.09	0/3030	0.22	0/4093
76	AW	0.13	0/801	0.25	0/1079
77	AX	0.10	0/2921	0.23	0/3954
78	AY	0.14	0/1280	0.22	0/1725
79	AZ	0.16	0/857	0.27	0/1141
80	A0	0.13	0/1834	0.30	0/2484
81	A1	0.16	0/2285	0.25	0/3090
82	A2	0.13	0/941	0.30	0/1257
83	A3	0.17	0/636	0.37	0/839
84	A4	0.11	0/4877	0.24	0/6598
85	u	0.09	0/439	0.25	0/586
86	v	0.06	0/159	0.17	0/221
87	w	0.06	0/1608	0.14	0/2497
88	x	0.06	0/1656	0.15	0/2571
89	y	0.09	0/443	0.17	0/684
All	All	0.14	0/185856	0.24	0/264114

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	A	32560	16532	16529	146	0
2	B	1522	776	776	3	0
3	D	1859	1921	1920	15	0
4	E	2406	2417	2415	17	0
5	F	2031	2066	2065	13	0
6	H	802	847	846	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	1695	1786	1785	17	0
8	J	1330	1409	1407	9	0
9	K	1455	1454	1452	5	0
10	L	890	942	941	4	0
11	M	2327	2396	2395	13	0
12	N	1786	1819	1817	8	0
13	O	1259	1295	1294	8	0
14	P	1173	1166	1165	12	0
15	Q	1979	2023	2022	9	0
16	R	1154	1215	1214	5	0
17	S	1293	1366	1365	11	0
18	T	1369	1411	1410	8	0
19	U	1107	1108	1107	10	0
20	V	1676	1688	1687	24	0
21	W	904	937	935	6	0
22	X	2044	2061	2060	8	0
23	Y	1556	1598	1597	9	0
24	Z	996	1045	1044	4	0
25	0	898	917	916	5	0
26	1	455	499	498	6	0
27	2	377	407	406	4	0
28	3	832	884	883	7	0
29	4	342	362	361	1	0
30	5	3210	3208	3206	21	0
31	6	2948	2844	2841	26	0
32	7	2390	2399	2397	11	0
33	8	1327	1369	1368	15	0
34	9	997	988	987	4	0
35	a	840	812	810	5	0
36	b	1196	1196	1190	8	0
37	c	2299	2322	2320	8	0
38	d	1988	1982	1978	11	0
39	e	1848	1851	1849	13	0
40	f	1252	1271	1269	8	0
41	g	1113	1097	1097	3	0
42	h	895	882	881	8	0
43	i	828	859	857	8	0
44	j	745	747	746	2	0
45	k	774	784	784	2	0
46	l	688	675	674	8	0
47	m	754	761	758	13	0
48	o	798	807	804	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	p	1205	1226	1223	16	0
50	q	1350	1328	1327	9	0
51	r	1322	1349	1349	12	0
52	s	3155	3143	3139	17	0
53	t1	354	378	377	11	0
53	t2	257	284	283	10	0
53	t3	257	284	283	0	0
53	t4	245	275	275	4	0
53	t5	245	275	275	1	0
53	t6	245	275	275	0	0
54	AA	20253	10289	10287	62	0
55	AB	1828	1816	1815	7	0
56	AC	1083	1089	1088	10	0
57	AD	2731	2805	2804	13	0
58	AE	972	1001	1000	6	0
59	AF	1725	1770	1769	12	0
60	AG	2568	2558	2554	11	0
61	AH	1152	1184	1183	11	0
62	AI	1018	1058	1056	7	0
63	AJ	839	888	887	4	0
64	AK	862	886	885	5	0
65	AL	1453	1541	1540	5	0
66	AM	942	966	965	5	0
67	AN	868	929	928	7	0
68	AO	1592	1557	1557	10	0
69	AP	781	807	806	6	0
70	AQ	744	758	758	6	0
71	AR	2409	2429	2428	15	0
72	AS	1111	1116	1115	6	0
73	AT	1371	1394	1393	8	0
74	AU	1488	1500	1499	3	0
75	AV	2969	2964	2961	21	0
76	AW	789	803	802	5	0
77	AX	2849	2845	2843	15	0
78	AY	1246	1198	1197	8	0
79	AZ	839	860	858	3	0
80	A0	1787	1797	1796	13	0
81	A1	2238	2269	2269	15	0
82	A2	935	969	973	9	0
83	A3	625	700	699	5	0
84	A4	4768	4768	4766	24	0
85	u	431	432	429	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	v	160	160	159	2	0
87	w	1438	725	725	1	0
88	x	1483	751	752	6	0
89	y	399	199	201	1	0
90	A	128	0	0	0	0
90	A3	1	0	0	0	0
90	AA	53	0	0	0	0
90	AB	1	0	0	0	0
90	AX	1	0	0	0	0
90	D	3	0	0	0	0
90	E	1	0	0	0	0
90	g	1	0	0	0	0
91	A	30	0	0	0	0
91	AA	9	0	0	0	0
91	M	1	0	0	0	0
91	N	1	0	0	0	0
91	P	1	0	0	0	0
91	i	1	0	0	0	0
91	o	1	0	0	0	0
92	0	1	0	0	0	0
92	4	1	0	0	0	0
92	AO	1	0	0	0	0
93	AP	4	0	0	0	0
93	AT	4	0	0	0	0
93	r	4	0	0	0	0
94	AX	31	12	12	1	0
95	AX	32	12	12	0	0
96	w	5	7	4	2	0
97	6	1	0	0	0	0
97	A	340	0	0	11	0
97	A0	1	0	0	0	0
97	A3	3	0	0	0	0
97	AA	69	0	0	6	0
97	AC	1	0	0	0	0
97	AG	1	0	0	0	0
97	AH	3	0	0	1	0
97	AK	2	0	0	0	0
97	AX	2	0	0	0	0
97	B	1	0	0	0	0
97	D	5	0	0	0	0
97	E	4	0	0	0	0
97	F	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	K	3	0	0	1	0
97	L	1	0	0	0	0
97	M	7	0	0	0	0
97	N	1	0	0	0	0
97	O	2	0	0	0	0
97	Q	1	0	0	0	0
97	R	3	0	0	0	0
97	S	1	0	0	0	0
97	T	1	0	0	0	0
97	U	1	0	0	0	0
97	W	2	0	0	0	0
97	c	1	0	0	0	0
97	f	1	0	0	0	0
97	i	1	0	0	0	0
97	o	2	0	0	0	0
97	r	1	0	0	0	0
97	s	2	0	0	0	0
All	All	177134	149830	149709	755	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 2.

The worst 5 of 755 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)
1:A:1777:A:N6	1:A:1780:U:OP2	2.05	0.90
54:AA:992:U:O2'	54:AA:994:A:OP2	1.91	0.88
1:A:3152:C:OP1	15:Q:141:SER:OG	1.94	0.86
31:6:206:TYR:O	31:6:243:ASN:ND2	2.11	0.84
1:A:3063:G:O2'	1:A:3066:C:OP2	1.96	0.83

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	
3	D	236/305 (77%)	233 (99%)	3 (1%)	0	100	100
4	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100
5	F	250/311 (80%)	248 (99%)	2 (1%)	0	100	100
6	H	95/267 (36%)	94 (99%)	1 (1%)	0	100	100
7	I	210/261 (80%)	205 (98%)	5 (2%)	0	100	100
8	J	173/192 (90%)	173 (100%)	0	0	100	100
9	K	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
10	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
11	M	289/296 (98%)	287 (99%)	2 (1%)	0	100	100
12	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
13	O	152/175 (87%)	152 (100%)	0	0	100	100
14	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
15	Q	236/292 (81%)	234 (99%)	2 (1%)	0	100	100
16	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
17	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
18	T	164/206 (80%)	164 (100%)	0	0	100	100
19	U	129/152 (85%)	128 (99%)	1 (1%)	0	100	100
20	V	203/216 (94%)	203 (100%)	0	0	100	100
21	W	114/148 (77%)	114 (100%)	0	0	100	100
22	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
23	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
24	Z	120/161 (74%)	117 (98%)	3 (2%)	0	100	100
25	0	108/188 (57%)	108 (100%)	0	0	100	100
26	1	53/65 (82%)	53 (100%)	0	0	100	100
27	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
29	4	36/103 (35%)	36 (100%)	0	0	100	100
30	5	392/423 (93%)	388 (99%)	4 (1%)	0	100	100
31	6	352/380 (93%)	338 (96%)	14 (4%)	0	100	100
32	7	292/338 (86%)	287 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	8	155/206 (75%)	154 (99%)	1 (1%)	0	100	100
34	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
35	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
36	b	148/214 (69%)	143 (97%)	5 (3%)	0	100	100
37	c	282/332 (85%)	277 (98%)	5 (2%)	0	100	100
38	d	236/306 (77%)	232 (98%)	4 (2%)	0	100	100
39	e	224/279 (80%)	219 (98%)	5 (2%)	0	100	100
40	f	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
41	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
42	h	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
43	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
44	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
45	k	99/111 (89%)	99 (100%)	0	0	100	100
46	l	80/138 (58%)	80 (100%)	0	0	100	100
47	m	83/128 (65%)	81 (98%)	2 (2%)	0	100	100
48	o	92/102 (90%)	92 (100%)	0	0	100	100
49	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
50	q	159/222 (72%)	159 (100%)	0	0	100	100
51	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
52	s	382/439 (87%)	378 (99%)	4 (1%)	0	100	100
53	t1	44/198 (22%)	43 (98%)	1 (2%)	0	100	100
53	t2	30/198 (15%)	30 (100%)	0	0	100	100
53	t3	30/198 (15%)	30 (100%)	0	0	100	100
53	t4	29/198 (15%)	29 (100%)	0	0	100	100
53	t5	29/198 (15%)	29 (100%)	0	0	100	100
53	t6	29/198 (15%)	29 (100%)	0	0	100	100
55	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100	100
56	AC	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
57	AD	341/430 (79%)	335 (98%)	6 (2%)	0	100	100
58	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
59	AF	206/242 (85%)	206 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	AG	308/396 (78%)	305 (99%)	3 (1%)	0	100	100
61	AH	138/201 (69%)	134 (97%)	3 (2%)	1 (1%)	18	48
62	AI	133/194 (69%)	130 (98%)	3 (2%)	0	100	100
63	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
64	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
65	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
66	AM	117/137 (85%)	117 (100%)	0	0	100	100
67	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
68	AO	191/258 (74%)	187 (98%)	4 (2%)	0	100	100
69	AP	95/142 (67%)	95 (100%)	0	0	100	100
70	AQ	84/86 (98%)	84 (100%)	0	0	100	100
71	AR	293/360 (81%)	291 (99%)	2 (1%)	0	100	100
72	AS	133/190 (70%)	133 (100%)	0	0	100	100
73	AT	166/173 (96%)	166 (100%)	0	0	100	100
74	AU	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
75	AV	358/414 (86%)	357 (100%)	1 (0%)	0	100	100
76	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
77	AX	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
78	AY	147/395 (37%)	146 (99%)	1 (1%)	0	100	100
79	AZ	98/106 (92%)	98 (100%)	0	0	100	100
80	A0	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
81	A1	274/323 (85%)	269 (98%)	5 (2%)	0	100	100
82	A2	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
83	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
84	A4	584/689 (85%)	575 (98%)	9 (2%)	0	100	100
85	u	47/435 (11%)	47 (100%)	0	0	100	100
86	v	30/32 (94%)	30 (100%)	0	0	100	100
All	All	14361/19621 (73%)	14193 (99%)	167 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
61	AH	126	ILE

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	
3	D	192/245 (78%)	192 (100%)	0	100	100
4	E	260/290 (90%)	260 (100%)	0	100	100
5	F	219/262 (84%)	219 (100%)	0	100	100
6	H	88/228 (39%)	88 (100%)	0	100	100
7	I	194/232 (84%)	194 (100%)	0	100	100
8	J	138/150 (92%)	138 (100%)	0	100	100
9	K	154/154 (100%)	154 (100%)	0	100	100
10	L	98/124 (79%)	98 (100%)	0	100	100
11	M	246/249 (99%)	246 (100%)	0	100	100
12	N	189/211 (90%)	189 (100%)	0	100	100
13	O	134/150 (89%)	134 (100%)	0	100	100
14	P	126/155 (81%)	126 (100%)	0	100	100
15	Q	220/256 (86%)	220 (100%)	0	100	100
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	146/180 (81%)	146 (100%)	0	100	100
18	T	146/176 (83%)	146 (100%)	0	100	100
19	U	118/134 (88%)	118 (100%)	0	100	100
20	V	183/191 (96%)	183 (100%)	0	100	100
21	W	94/119 (79%)	94 (100%)	0	100	100
22	X	220/229 (96%)	220 (100%)	0	100	100
23	Y	163/223 (73%)	163 (100%)	0	100	100
24	Z	113/147 (77%)	113 (100%)	0	100	100
25	0	99/164 (60%)	99 (100%)	0	100	100
26	1	52/60 (87%)	52 (100%)	0	100	100
27	2	40/72 (56%)	40 (100%)	0	100	100
28	3	88/166 (53%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	4	37/89 (42%)	37 (100%)	0	100	100
30	5	353/368 (96%)	353 (100%)	0	100	100
31	6	313/332 (94%)	313 (100%)	0	100	100
32	7	270/303 (89%)	270 (100%)	0	100	100
33	8	146/190 (77%)	146 (100%)	0	100	100
34	9	104/112 (93%)	104 (100%)	0	100	100
35	a	96/133 (72%)	96 (100%)	0	100	100
36	b	131/184 (71%)	131 (100%)	0	100	100
37	c	251/288 (87%)	251 (100%)	0	100	100
38	d	221/274 (81%)	220 (100%)	1 (0%)	81	93
39	e	198/236 (84%)	198 (100%)	0	100	100
40	f	139/188 (74%)	139 (100%)	0	100	100
41	g	124/148 (84%)	124 (100%)	0	100	100
42	h	104/148 (70%)	104 (100%)	0	100	100
43	i	86/110 (78%)	86 (100%)	0	100	100
44	j	74/97 (76%)	74 (100%)	0	100	100
45	k	83/89 (93%)	83 (100%)	0	100	100
46	l	76/116 (66%)	76 (100%)	0	100	100
47	m	81/113 (72%)	81 (100%)	0	100	100
48	o	80/87 (92%)	80 (100%)	0	100	100
49	p	135/181 (75%)	135 (100%)	0	100	100
50	q	138/178 (78%)	138 (100%)	0	100	100
51	r	147/169 (87%)	147 (100%)	0	100	100
52	s	340/381 (89%)	340 (100%)	0	100	100
53	t1	40/158 (25%)	40 (100%)	0	100	100
53	t2	31/158 (20%)	31 (100%)	0	100	100
53	t3	31/158 (20%)	31 (100%)	0	100	100
53	t4	30/158 (19%)	30 (100%)	0	100	100
53	t5	30/158 (19%)	30 (100%)	0	100	100
53	t6	30/158 (19%)	30 (100%)	0	100	100
55	AB	198/249 (80%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	AC	115/143 (80%)	115 (100%)	0	100	100
57	AD	286/357 (80%)	285 (100%)	1 (0%)	86	96
58	AE	104/107 (97%)	104 (100%)	0	100	100
59	AF	185/209 (88%)	185 (100%)	0	100	100
60	AG	271/342 (79%)	271 (100%)	0	100	100
61	AH	130/180 (72%)	129 (99%)	1 (1%)	73	90
62	AI	104/146 (71%)	102 (98%)	2 (2%)	50	79
63	AJ	93/118 (79%)	93 (100%)	0	100	100
64	AK	91/113 (80%)	91 (100%)	0	100	100
65	AL	158/226 (70%)	158 (100%)	0	100	100
66	AM	97/113 (86%)	97 (100%)	0	100	100
67	AN	96/115 (84%)	96 (100%)	0	100	100
68	AO	174/230 (76%)	174 (100%)	0	100	100
69	AP	88/123 (72%)	88 (100%)	0	100	100
70	AQ	78/78 (100%)	78 (100%)	0	100	100
71	AR	264/318 (83%)	264 (100%)	0	100	100
72	AS	116/164 (71%)	116 (100%)	0	100	100
73	AT	153/157 (98%)	153 (100%)	0	100	100
74	AU	152/174 (87%)	152 (100%)	0	100	100
75	AV	325/364 (89%)	324 (100%)	1 (0%)	86	96
76	AW	87/158 (55%)	87 (100%)	0	100	100
77	AX	311/351 (89%)	310 (100%)	1 (0%)	86	96
78	AY	137/357 (38%)	137 (100%)	0	100	100
79	AZ	90/95 (95%)	90 (100%)	0	100	100
80	A0	188/190 (99%)	188 (100%)	0	100	100
81	A1	254/291 (87%)	254 (100%)	0	100	100
82	A2	100/100 (100%)	100 (100%)	0	100	100
83	A3	65/166 (39%)	65 (100%)	0	100	100
84	A4	526/609 (86%)	526 (100%)	0	100	100
85	u	46/373 (12%)	46 (100%)	0	100	100
All	All	12839/16871 (76%)	12832 (100%)	7 (0%)	87	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
62	AI	73	LEU
62	AI	181	ILE
77	AX	81	HIS
75	AV	29	LEU
61	AH	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
52	s	71	HIS
61	AH	183	HIS
84	A4	540	HIS
52	s	239	ASN
57	AD	288	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1532/1561 (98%)	217 (14%)	1 (0%)
2	B	71/72 (98%)	13 (18%)	0
54	AA	953/954 (99%)	125 (13%)	0
87	w	67/68 (98%)	16 (23%)	0
88	x	68/70 (97%)	8 (11%)	0
89	y	17/19 (89%)	2 (11%)	0
All	All	2708/2744 (98%)	381 (14%)	1 (0%)

5 of 381 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1689	C
1	A	1692	A
1	A	1700	U
1	A	1704	U
1	A	1707	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2112	A

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

7 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	$\#\|Z\| > 2$
82	AYA	A2	2	82	6,7,8	0.80	0	5,8,10	0.68	0
62	IAS	AI	184	62	5,6,8	0.79	0	3,6,10	1.21	0
9	SAC	K	2	9	7,8,9	0.88	0	8,9,11	0.52	0
70	AYA	AQ	2	70	6,7,8	0.78	0	5,8,10	0.57	0
36	THC	b	2	36	8,9,10	0.77	0	9,11,13	0.63	0
45	AYA	k	2	45	6,7,8	0.79	0	5,8,10	0.73	0
19	AYA	U	2	19	6,7,8	0.78	0	5,8,10	0.52	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
82	AYA	A2	2	82	-	0/4/6/8	-
62	IAS	AI	184	62	-	1/3/5/8	-
9	SAC	K	2	9	-	0/7/8/10	-
70	AYA	AQ	2	70	-	0/4/6/8	-
36	THC	b	2	36	-	0/8/10/12	-
45	AYA	k	2	45	-	0/4/6/8	-
19	AYA	U	2	19	-	1/4/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	AI	184	IAS	O-C-CA-CB
19	U	2	AYA	C-CA-N-CT

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 242 ligands modelled in this entry, 236 are monoatomic - leaving 6 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	FES	AP	201	58,69	0,4,4	-	-	-		
94	ATP	AX	501	90	29,33,33	1.02	3 (10%)	44,52,52	1.61	7 (15%)
93	FES	AT	201	66,73	0,4,4	-	-	-		
95	GTP	AX	503	-	30,34,34	0.97	2 (6%)	46,54,54	1.58	8 (17%)
96	ALA	w	101	87	3,4,5	0.69	0	2,4,6	0.88	0
93	FES	r	201	7,51	0,4,4	-	-	-		

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	FES	AP	201	58,69	-	-	0/1/1/1
94	ATP	AX	501	90	-	0/22/38/38	0/3/3/3
93	FES	AT	201	66,73	-	-	0/1/1/1
95	GTP	AX	503	-	-	0/22/38/38	0/3/3/3
96	ALA	w	101	87	-	0/0/2/4	-
93	FES	r	201	7,51	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
95	AX	503	GTP	C6-N1	-2.87	1.33	1.38
94	AX	501	ATP	C5-C6	2.81	1.48	1.41
95	AX	503	GTP	C2-N3	2.28	1.38	1.33
94	AX	501	ATP	C5-N7	-2.16	1.34	1.39
94	AX	501	ATP	C8-N7	2.16	1.35	1.31

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
94	AX	501	ATP	C5-C4-N3	-5.51	119.56	126.75
95	AX	503	GTP	C2-N1-C6	-4.89	116.19	125.10
95	AX	503	GTP	C5-C4-N3	-4.86	120.58	128.46
94	AX	501	ATP	N3-C4-N9	3.77	133.29	127.08
95	AX	503	GTP	C5-C6-N1	3.44	121.92	113.19

There are no chirality outliers.

There are no torsion outliers.

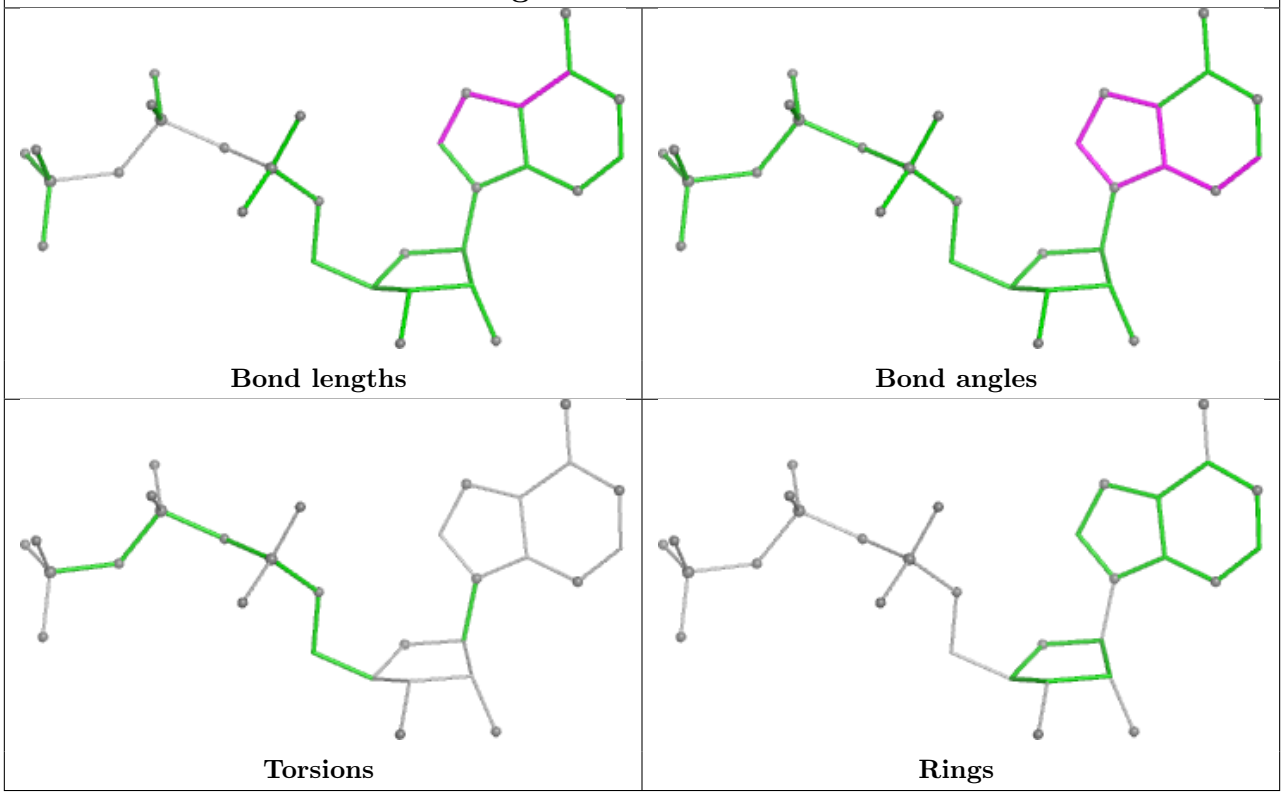
There are no ring outliers.

2 monomers are involved in 3 short contacts:

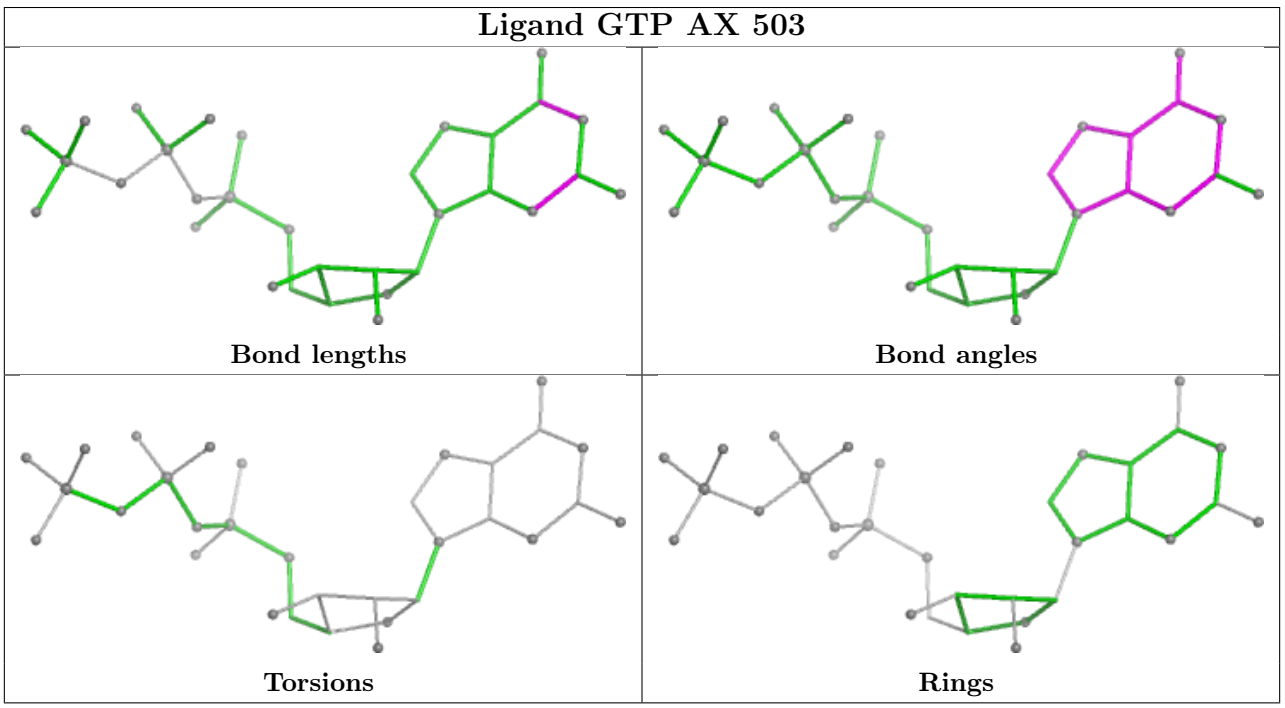
Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	AX	501	ATP	1	0
96	w	101	ALA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP AX 501



Ligand GTP AX 503



5.7 Other polymers

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
89	y	1
88	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	26:A	O3'	46:U	P	66.64
1	x	15:A	O3'	21:A	P	9.86

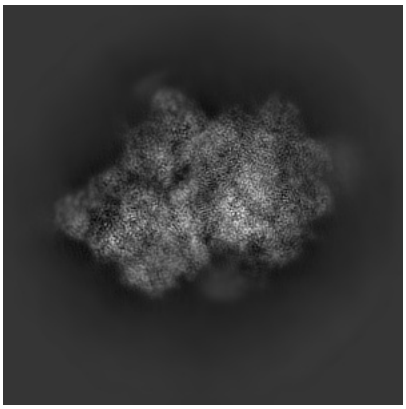
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11278. These allow visual inspection of the internal detail of the map and identification of artifacts.

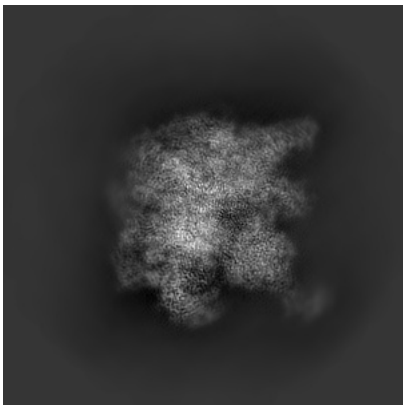
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

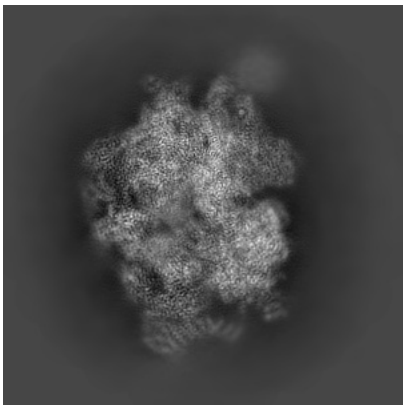
6.1.1 Primary map



X

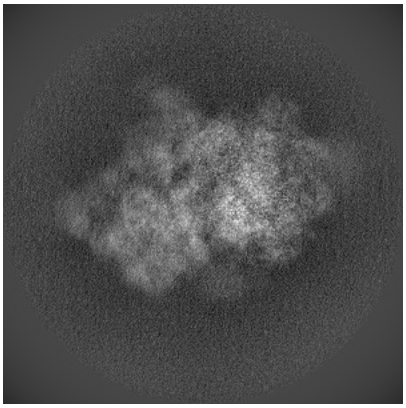


Y

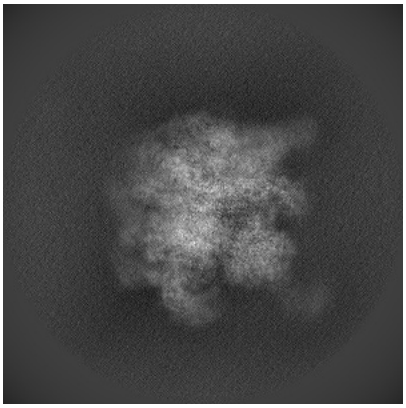


Z

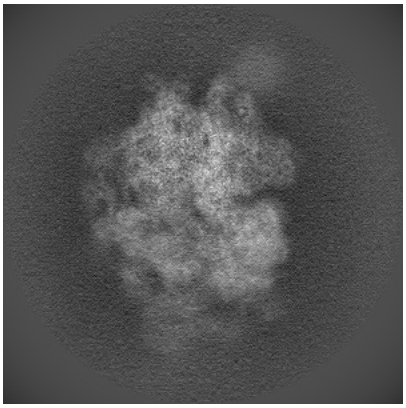
6.1.2 Raw map



X



Y

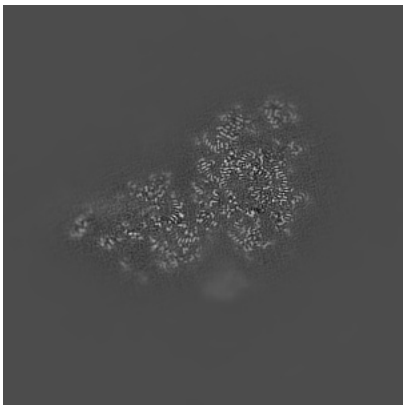


Z

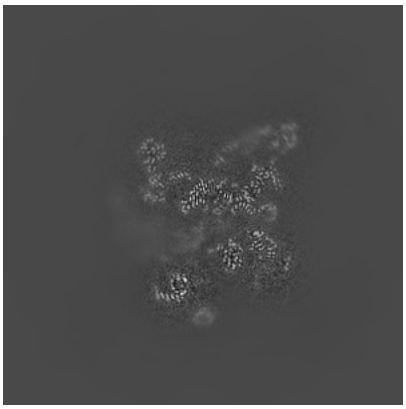
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

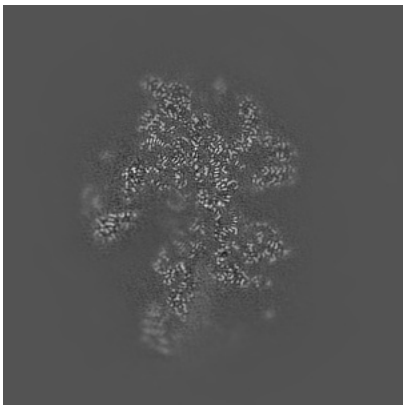
6.2.1 Primary map



X Index: 270

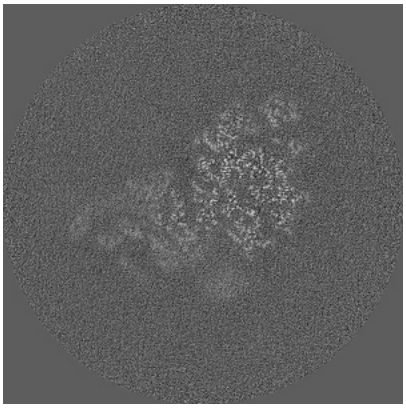


Y Index: 270

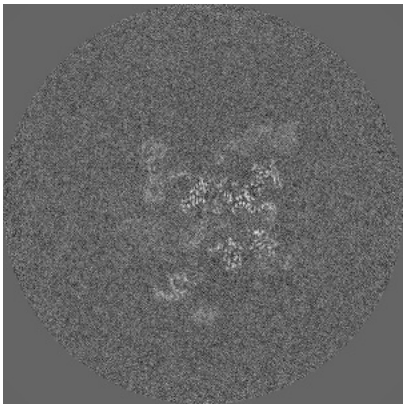


Z Index: 270

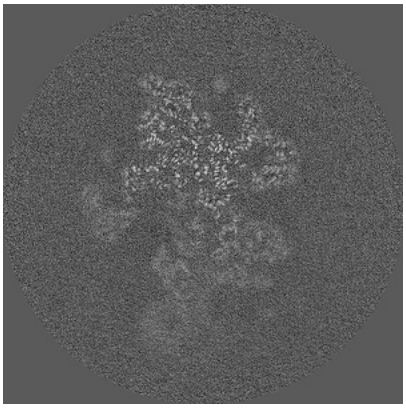
6.2.2 Raw map



X Index: 270



Y Index: 270

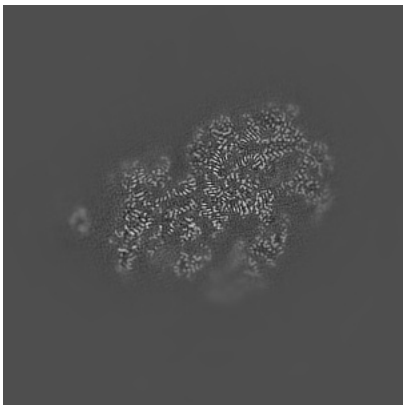


Z Index: 270

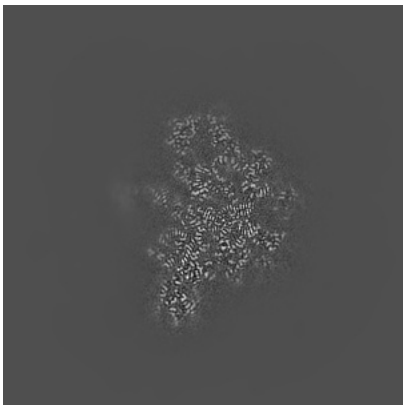
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

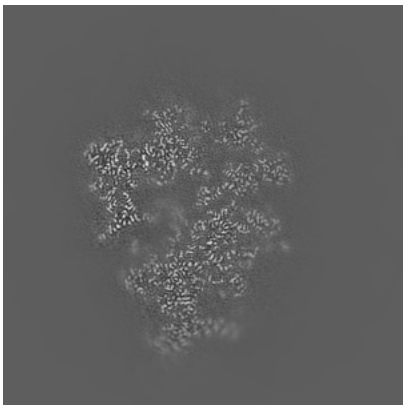
6.3.1 Primary map



X Index: 291

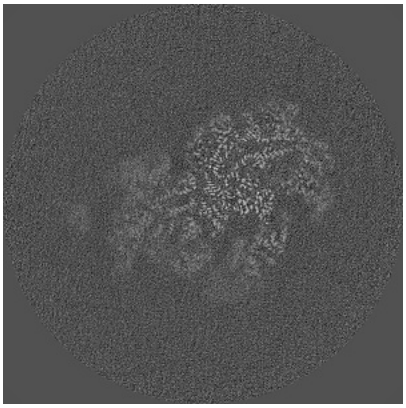


Y Index: 324

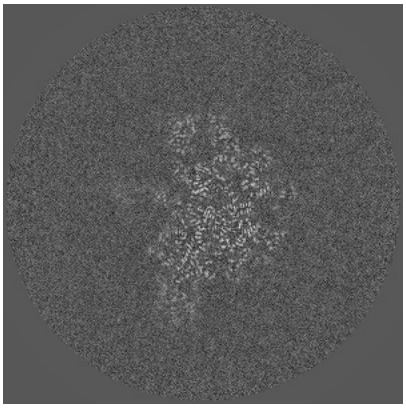


Z Index: 242

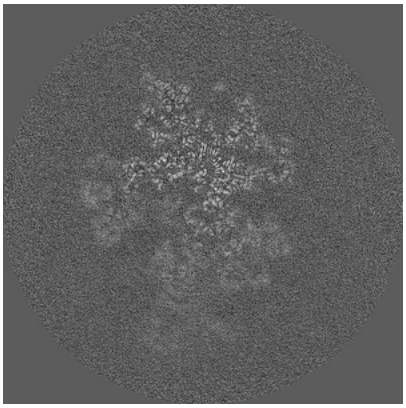
6.3.2 Raw map



X Index: 291



Y Index: 324

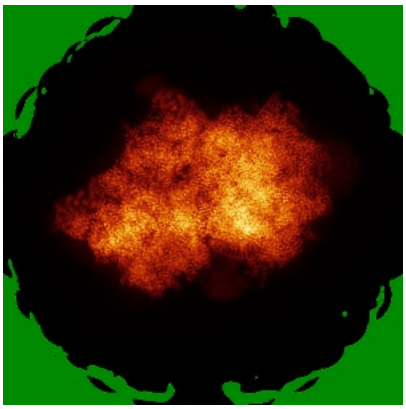


Z Index: 262

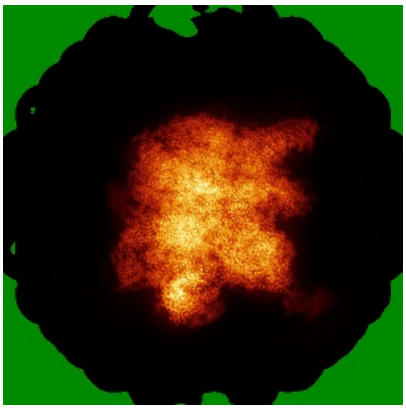
The images above show the largest variance slices of the map in three orthogonal directions.

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

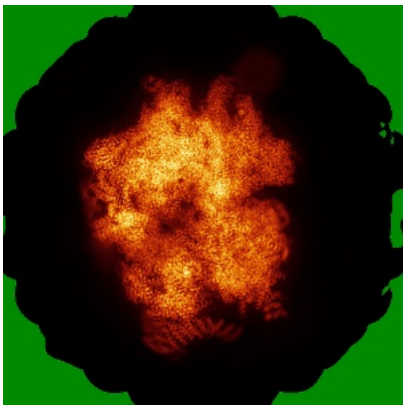
6.4.1 Primary map



X

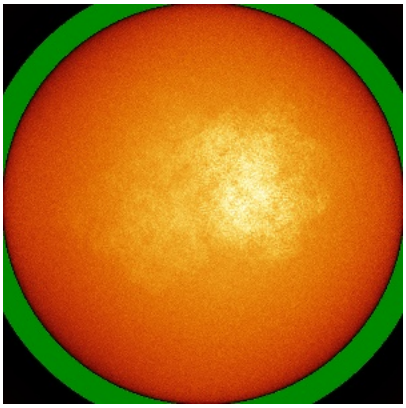


Y

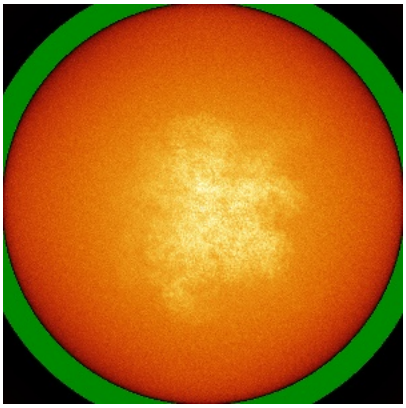


Z

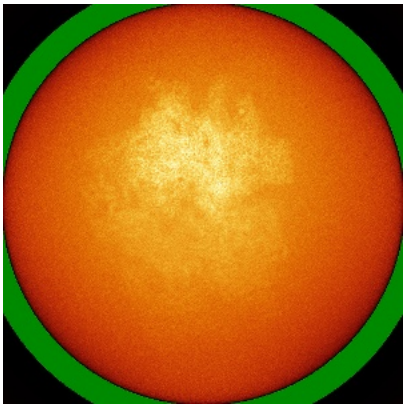
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

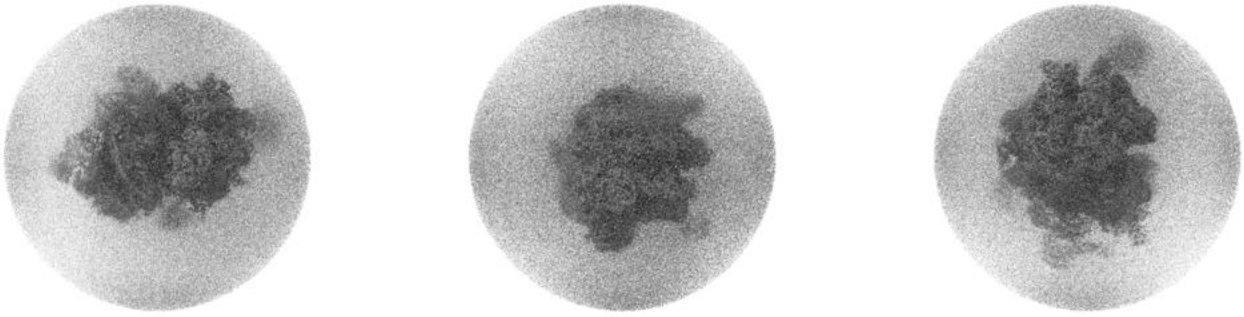
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

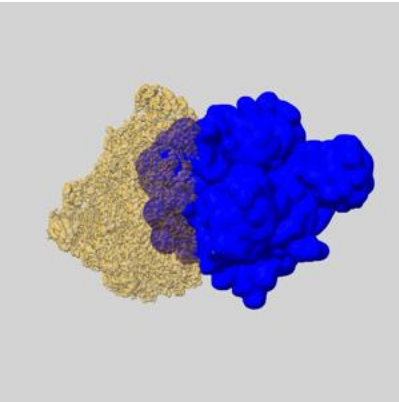
6.6 Mask visualisation (i)

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

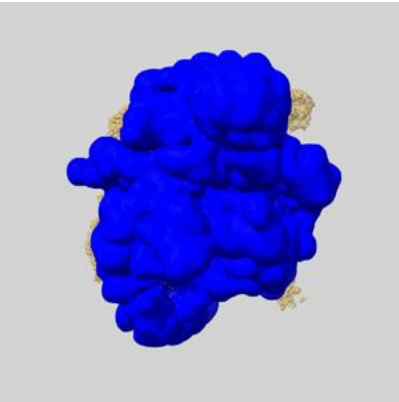
A mask typically either:

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

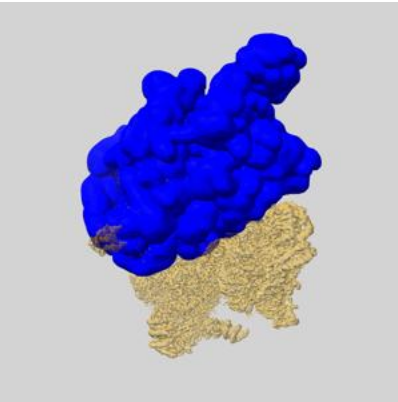
6.6.1 emd_11278_msk_1.map (i)



X



Y

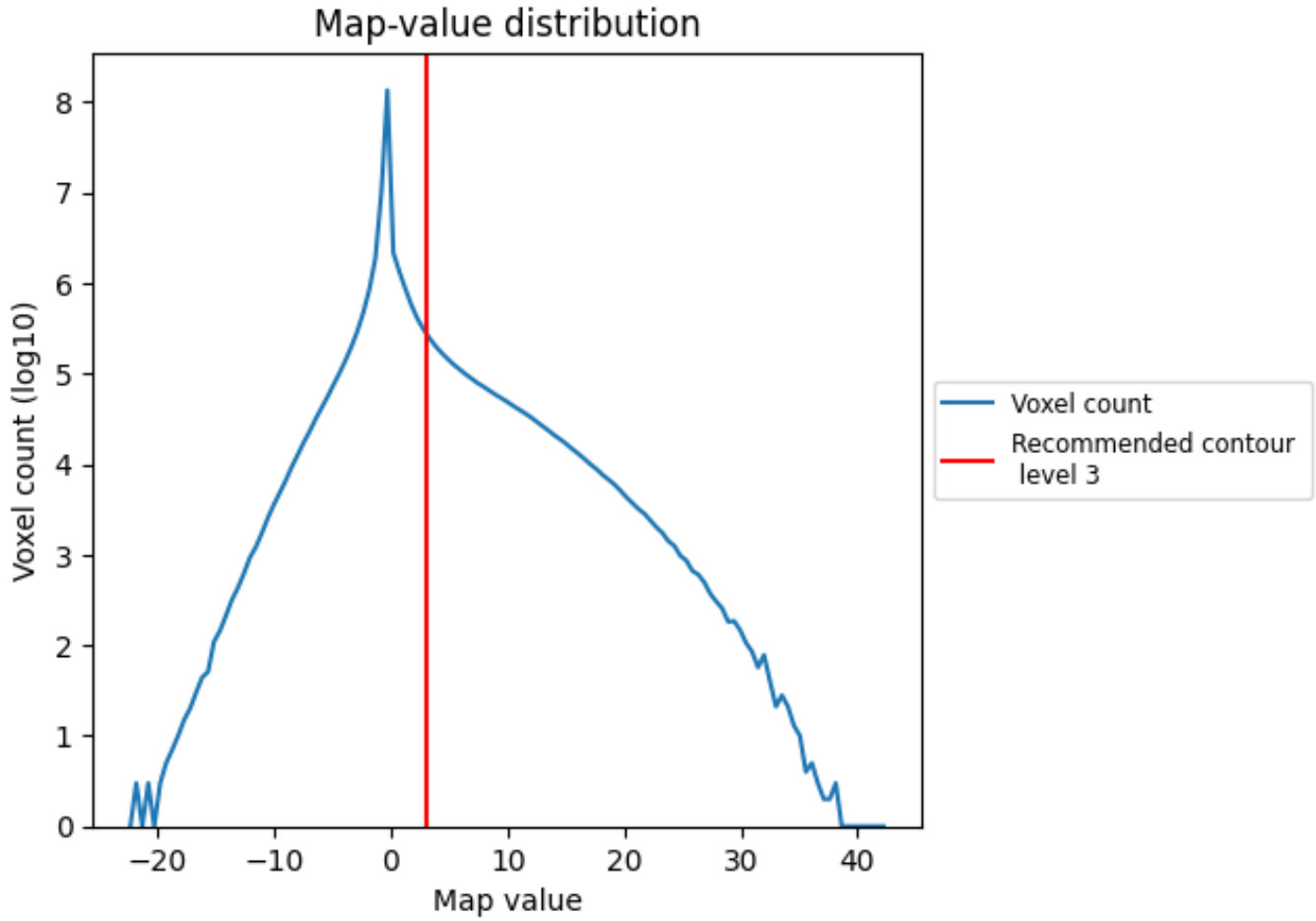


Z

7 Map analysis

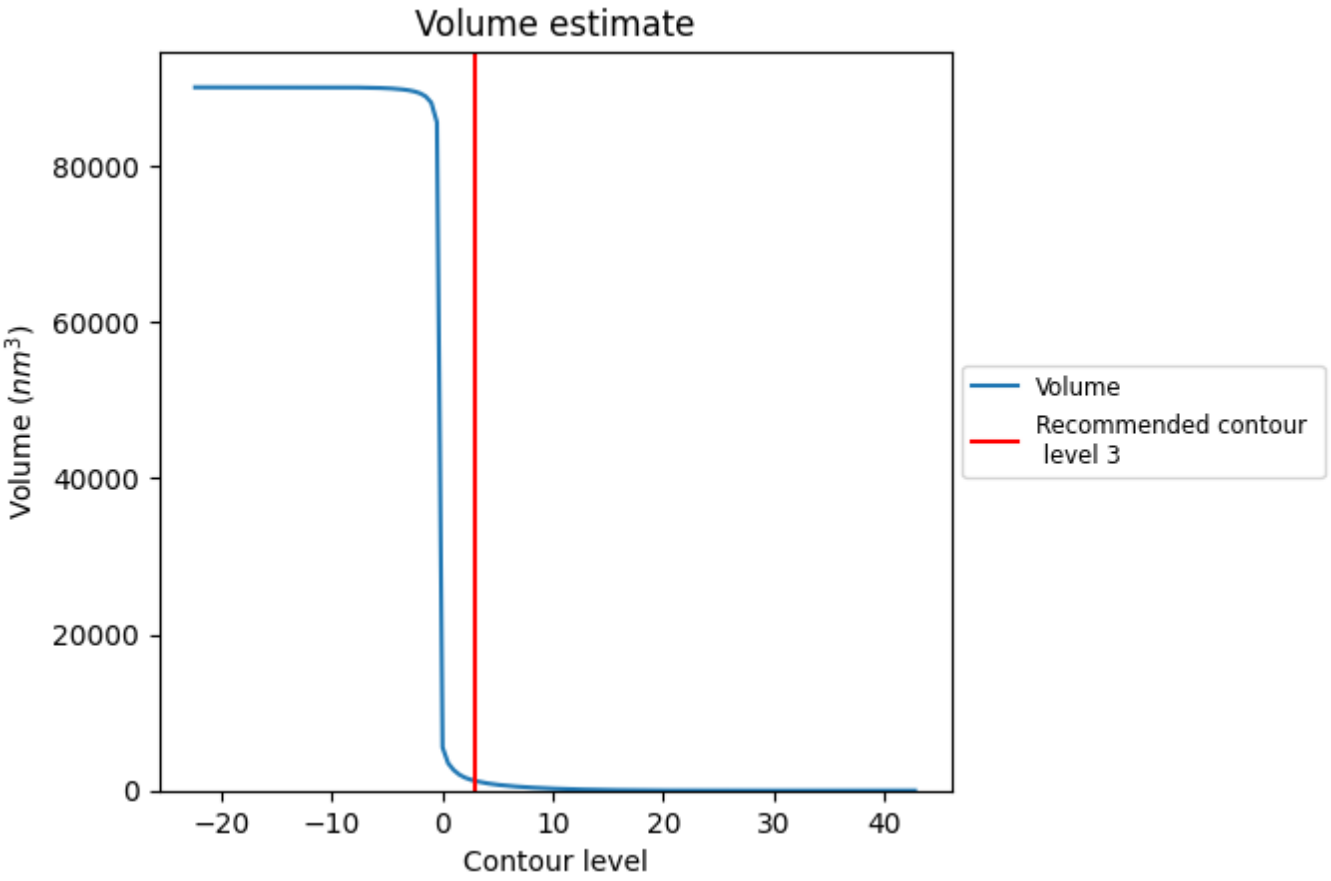
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

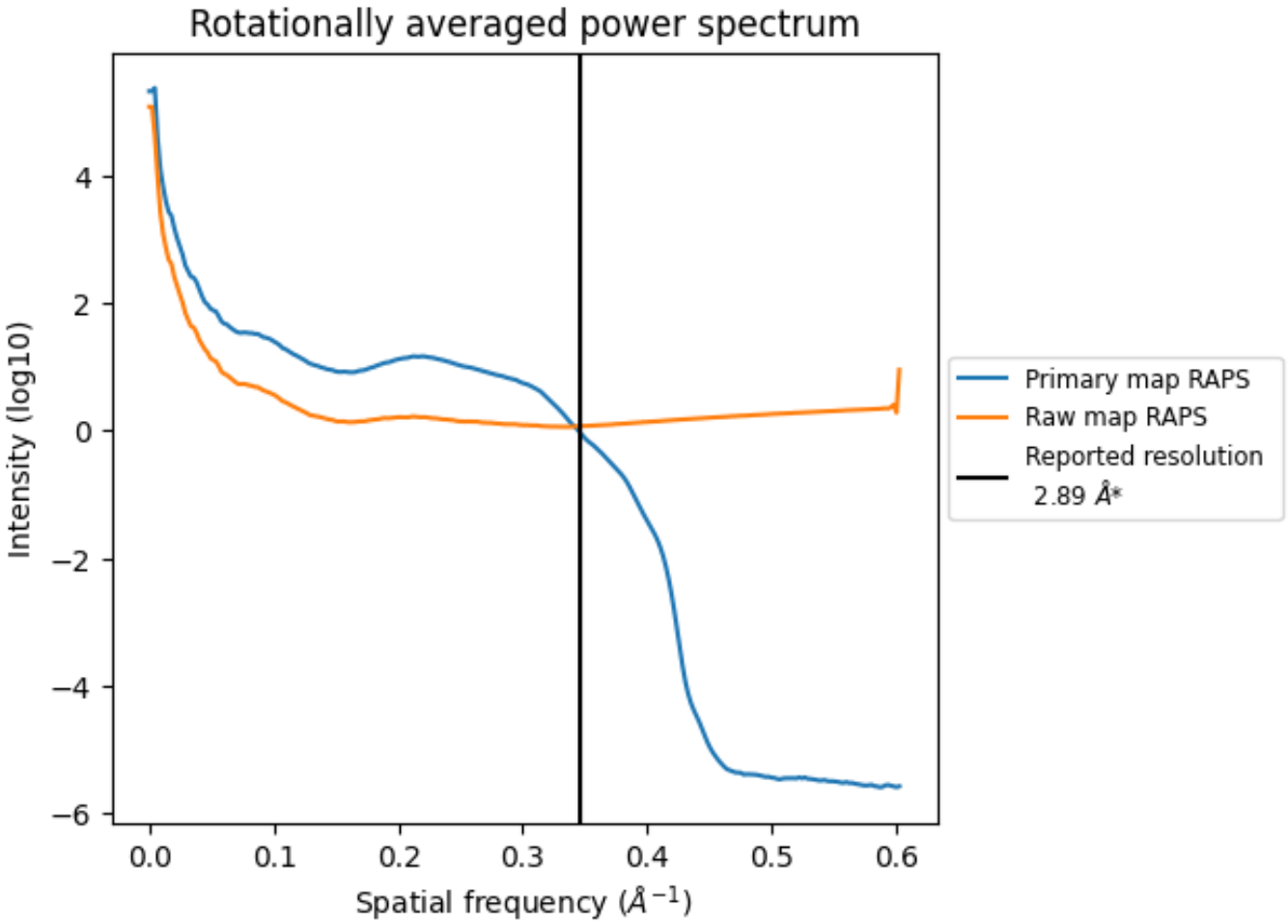
7.2 Volume estimate (i)



The volume at the recommended contour level is 1233 nm^3; this corresponds to an approximate mass of 1114 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)

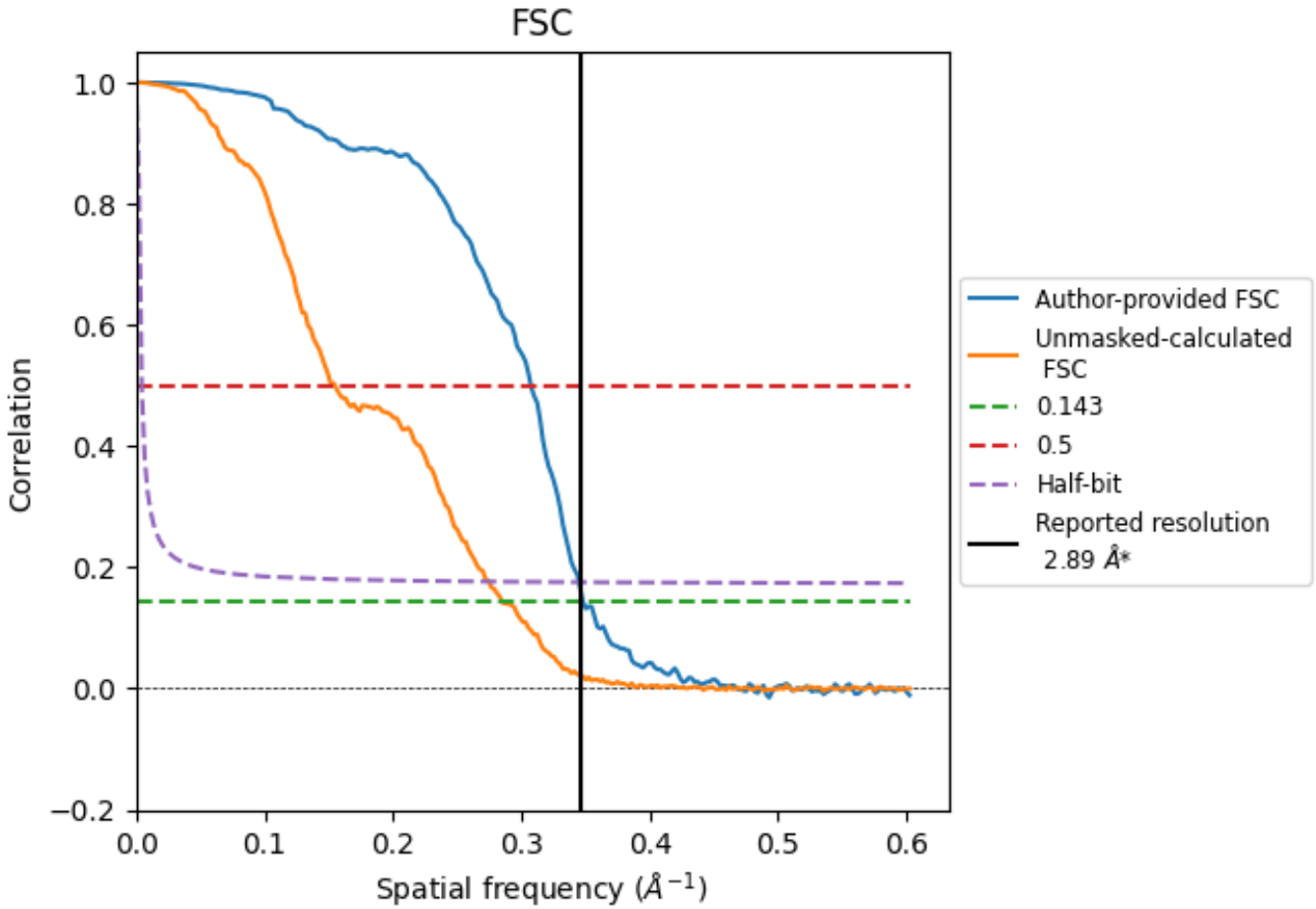


*Reported resolution corresponds to spatial frequency of 0.346 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.346 Å^{-1}

8.2 Resolution estimates (i)

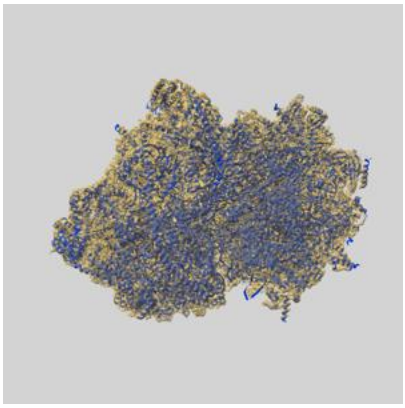
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.87	3.25	2.90
Unmasked-calculated*	3.51	6.46	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 2.89 by more than 10 %

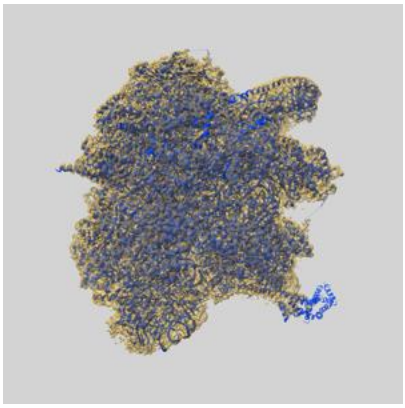
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11278 and PDB model 6ZM5. Per-residue inclusion information can be found in section 3 on page 25.

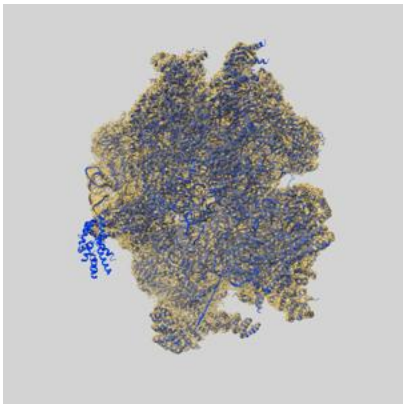
9.1 Map-model overlay



X



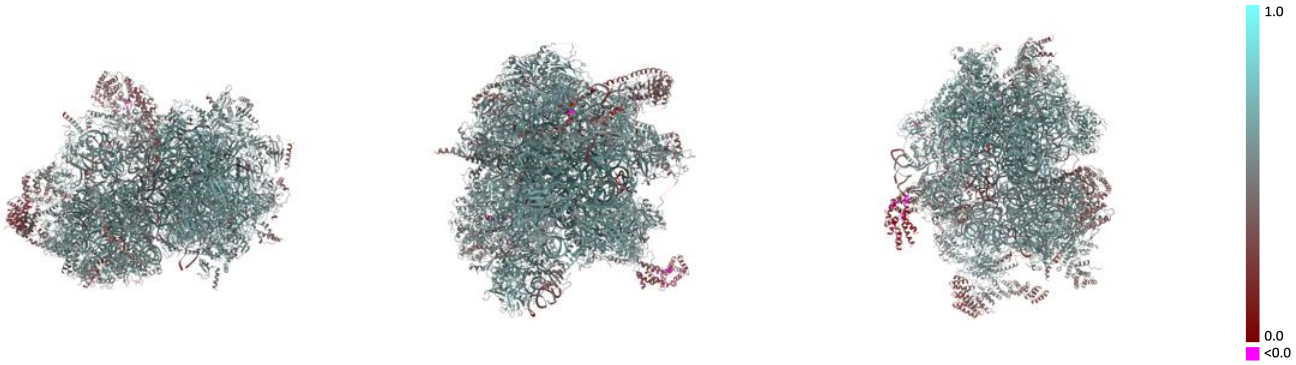
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

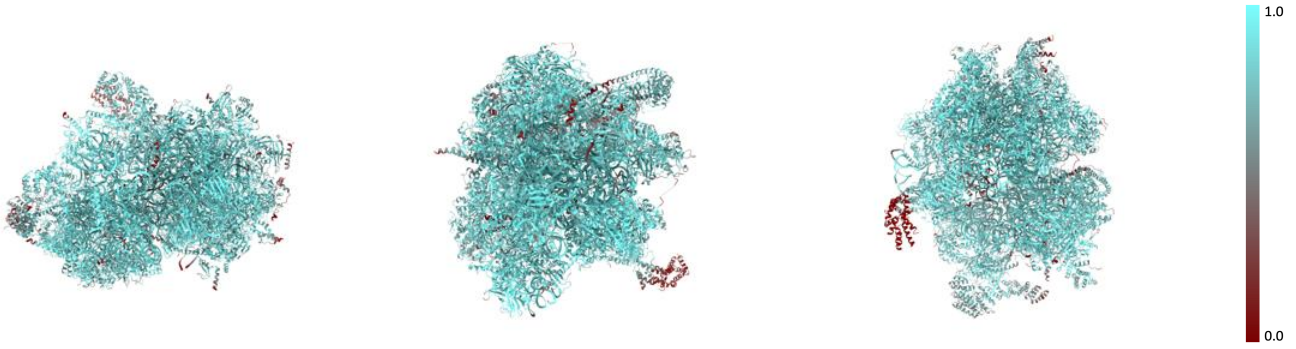
9.2 Q-score mapped to coordinate model



X Y Z

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

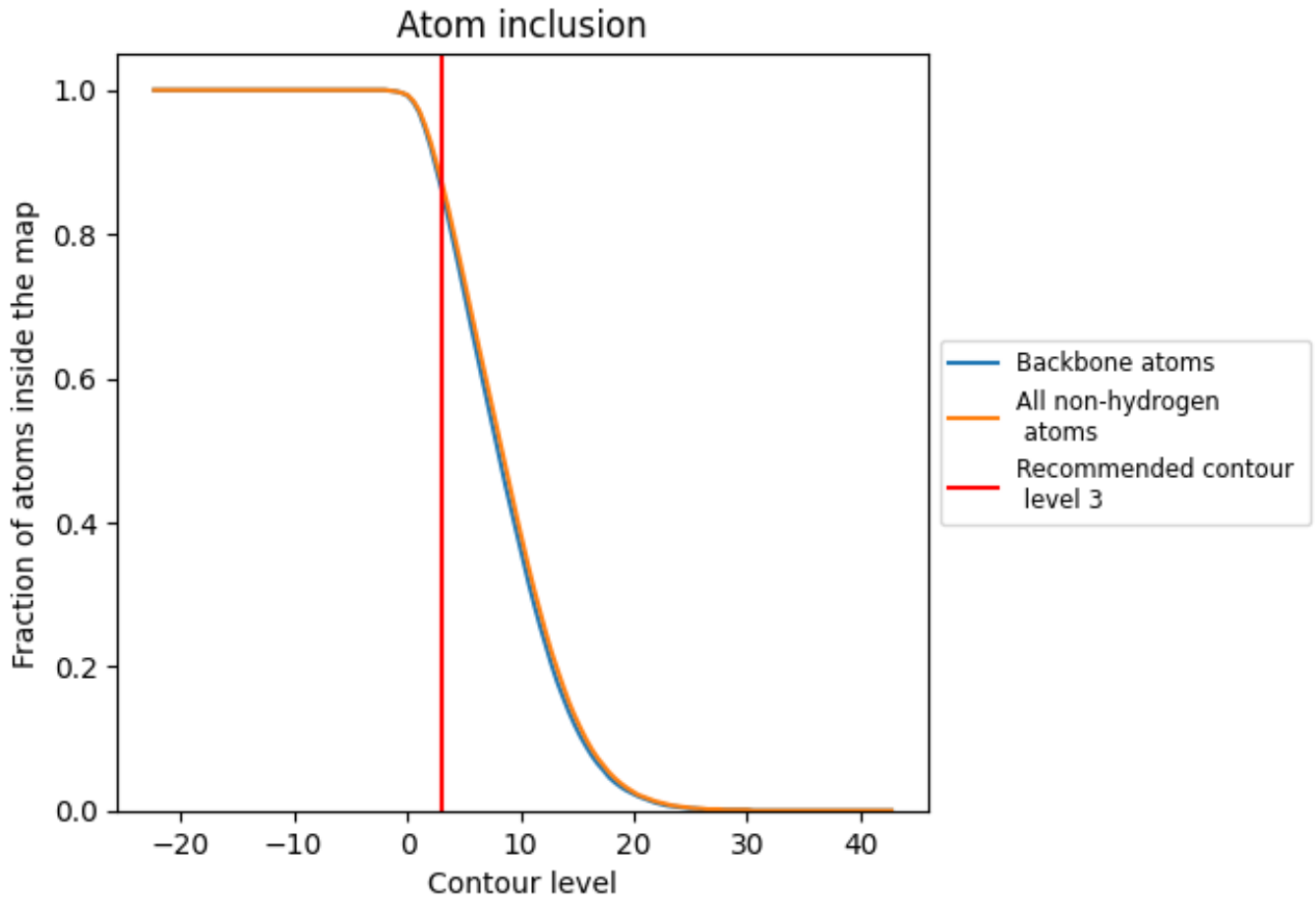
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8760	0.5520
0	0.8820	0.5890
1	0.8480	0.5640
2	0.9780	0.6720
3	0.9680	0.6480
4	0.9540	0.6260
5	0.8840	0.5710
6	0.9360	0.5750
7	0.7890	0.5120
8	0.7570	0.4450
9	0.8280	0.5520
A	0.9610	0.6190
A0	0.8280	0.5040
A1	0.8660	0.5250
A2	0.7960	0.4880
A3	0.8730	0.5660
A4	0.6960	0.3580
AA	0.9560	0.5930
AB	0.8990	0.5480
AC	0.9520	0.6120
AD	0.8670	0.5370
AE	0.8540	0.5520
AF	0.8410	0.5300
AG	0.8720	0.5320
AH	0.8960	0.5580
AI	0.8540	0.5320
AJ	0.8320	0.5470
AK	0.9520	0.6100
AL	0.7940	0.5040
AM	0.8870	0.5580
AN	0.9030	0.5700
AO	0.8830	0.5370
AP	0.8830	0.5580
AQ	0.8970	0.5780
AR	0.8350	0.4850



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Chain	Atom inclusion	Q-score
AS	0.8260	0.4760
AT	0.8730	0.5430
AU	0.8010	0.4630
AV	0.7220	0.3790
AW	0.8720	0.5280
AX	0.8310	0.5180
AY	0.7560	0.4600
AZ	0.8640	0.5430
B	0.9130	0.4760
D	0.9270	0.6060
E	0.9110	0.5990
F	0.9290	0.6170
H	0.7600	0.5200
I	0.7490	0.4570
J	0.8090	0.4410
K	0.9470	0.6230
L	0.9080	0.5970
M	0.9140	0.5970
N	0.9200	0.5930
O	0.9040	0.6030
P	0.9480	0.6050
Q	0.8320	0.5490
R	0.9530	0.6360
S	0.9170	0.6100
T	0.9220	0.6210
U	0.8940	0.6030
V	0.7760	0.5310
W	0.9400	0.6220
X	0.8470	0.5650
Y	0.8880	0.5950
Z	0.9230	0.6050
a	0.7820	0.5210
b	0.9370	0.6190
c	0.8440	0.5550
d	0.6850	0.4900
e	0.8640	0.4610
f	0.8200	0.5060
g	0.9070	0.5900
h	0.7800	0.5210
i	0.9510	0.6490
j	0.8730	0.5490
k	0.8500	0.5150

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Chain	Atom inclusion	Q-score
l	0.8390	0.4680
m	0.7720	0.4420
o	0.9530	0.6310
p	0.7670	0.4840
q	0.6420	0.4280
r	0.9260	0.5890
s	0.8960	0.5900
t1	0.5070	0.2850
t2	0.4650	0.2780
t3	0.0000	0.1520
t4	0.0290	0.0720
t5	0.0000	0.1240
t6	0.0000	0.0560
u	0.3830	0.3490
v	0.4060	0.3310
w	0.5160	0.3440
x	0.6590	0.4180
y	0.7970	0.4540