



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 07:21 pm BST

PDB ID : 7NSJ
EMDB ID : EMD-12569
Title : 55S mammalian mitochondrial ribosome with tRNA(P/P) and tRNA(E*)
Authors : Kummer, E.; Schubert, K.; Ban, N.
Deposited on : 2021-03-07
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

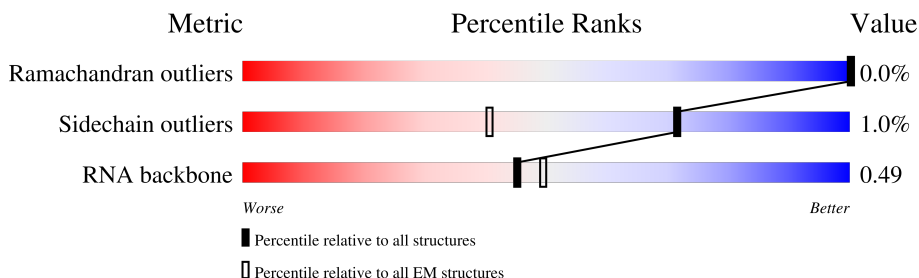
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B0	148	
2	B1	256	
3	B2	252	
4	B3	161	
5	B4	126	
6	B5	188	
7	B6	65	
8	BB	73	

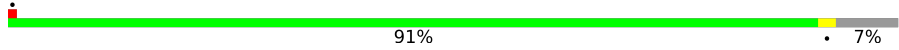

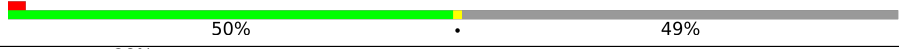



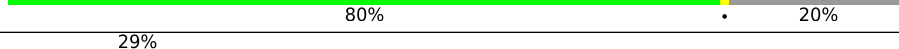
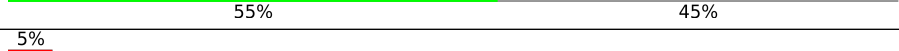
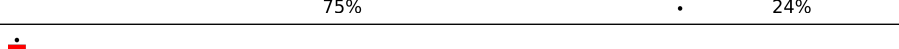

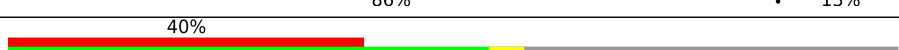

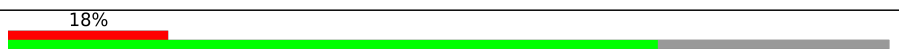

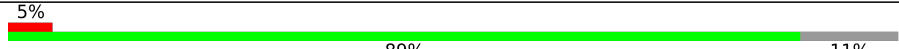





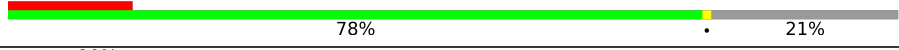
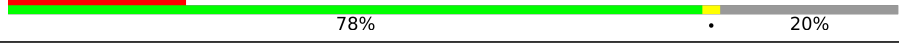



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Mol	Chain	Length	Quality of chain
9	B7	95	
10	BD	306	
11	BE	399	
12	BF	294	
13	BI	268	
14	BJ	262	
15	BK	192	
16	BN	178	
17	BO	145	
18	BP	296	
19	BQ	251	
20	BR	169	
21	BS	180	
22	BT	292	
23	BU	149	
24	BV	209	
25	BW	210	
26	BX	150	
27	BY	216	
28	Ba	423	
29	Bb	380	
30	Bc	334	
31	Bd	206	
32	Be	135	
33	Bf	142	

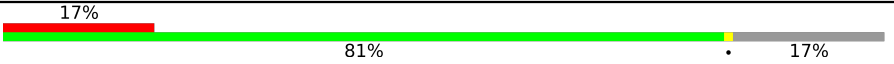

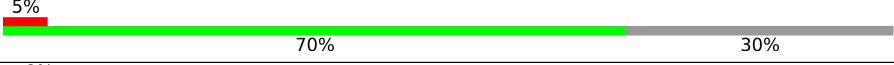

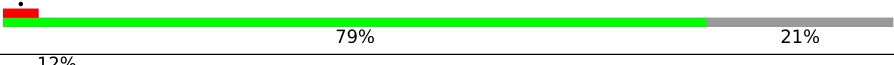
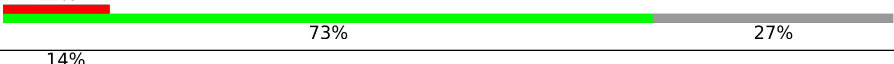
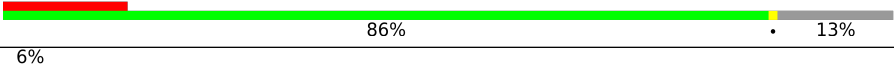

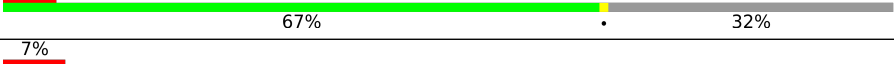
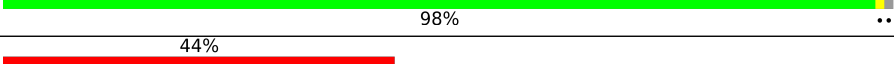
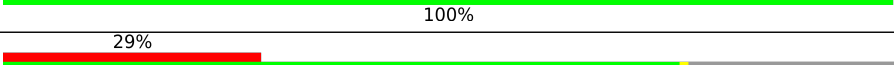
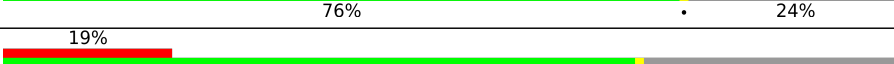
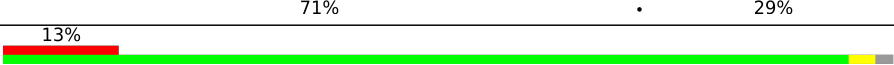
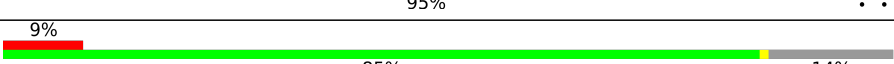

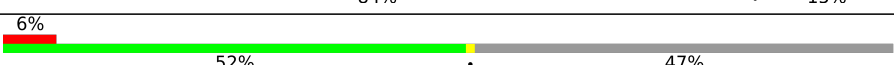
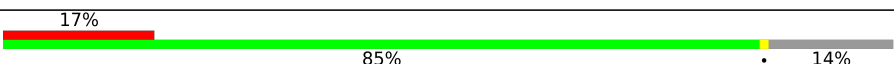
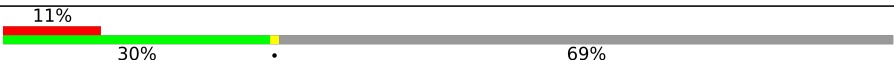
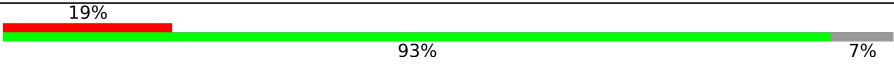
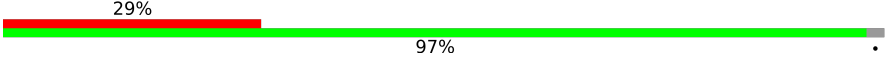

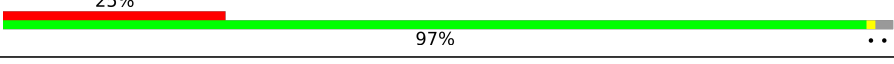



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Mol	Chain	Length	Quality of chain
34	Bg	159	
35	Bh	332	
36	B8	188	
37	Bi	306	
38	Bj	279	
39	Bk	269	
40	Bl	166	
41	Bm	198	
42	Bn	128	
43	Bo	124	
44	Bp	112	
45	Bq	138	
46	Bt	102	
47	Bu	205	
48	Bv	222	
49	Bw	433	
50	Bx	196	
51	AA	962	
52	B9	100	
53	BA	1571	
54	AB	289	
55	AC	167	
56	AE	430	
57	AF	276	
58	AG	242	

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Mol	Chain	Length	Quality of chain
59	AI	397	
60	AJ	200	
61	AK	196	
62	AL	139	
63	AN	128	
64	AO	239	
65	AP	135	
66	AQ	130	
67	AR	143	
68	AU	87	
69	AZ	18	
70	Aa	382	
71	Ab	190	
72	Ac	173	
73	Ad	205	
74	Ae	455	
75	Af	188	
76	Ag	410	
77	Ah	387	
78	Ai	106	
79	Aj	218	
80	Ak	325	
81	Am	118	
82	An	199	
83	Ao	690	

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Mol	Chain	Length	Quality of chain
84	Ap	258	
85	CL	198	
85	DL	198	
85	EL	198	
85	FL	198	
85	GL	198	
85	HL	198	
86	AV	71	
86	AY	71	
87	AX	6	

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 174837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Mitochondrial ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B0	110	Total	C	N	O	S	0	0
			857	553	156	145	3		

- Molecule 2 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 3 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B2	179	Total	C	N	O	S	0	0
			1548	992	290	260	6		

- Molecule 4 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 5 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B4	62	Total	C	N	O	S	0	0
			474	296	94	81	3		

- Molecule 6 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 7 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B6	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 8 is a RNA chain called CP tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BB	67	Total	C	N	O	P	0	0
			1427	640	261	459	67		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	71	C	-	insertion	GB 76262549

- Molecule 9 is a protein called Mitochondrial ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 10 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BD	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 11 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BE	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 12 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BF	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 13 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	BI	98	Total	C	N	O		
			805	509	155	141	0	0

- Molecule 14 is a protein called Mitochondrial ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	212	Total	C	N	O	S		
			1705	1100	306	290	9	0	0

- Molecule 15 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BK	176	Total	C	N	O	S		
			1303	830	236	235	2	0	0

- Molecule 16 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BN	177	Total	C	N	O	S		
			1444	926	258	253	7	0	0

- Molecule 17 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BO	115	Total	C	N	O	S		
			896	562	176	154	4	0	0

- Molecule 18 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BP	288	Total	C	N	O	S		
			2312	1473	430	403	6	0	0

- Molecule 19 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BQ	222	Total	C	N	O	S		
			1803	1156	331	306	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 20 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BR	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 21 is a protein called Mitochondrial ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BS	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 22 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BT	230	Total	C	N	O	S	0	0
			1890	1215	325	341	9		

- Molecule 23 is a protein called Mitochondrial ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BU	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 24 is a protein called Mitochondrial ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BV	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 25 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BW	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 26 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BX	149	Total	C	N	O	S	0	0
			1181	752	227	200	2		

- Molecule 27 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BY	206	Total	C	N	O	S	0	0
			1678	1056	308	309	5		

- Molecule 28 is a protein called Mitochondrial ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ba	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 29 is a protein called Mitochondrial ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bb	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 30 is a protein called Mitochondrial ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bc	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 31 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bd	141	Total	C	N	O	S	0	0
			1183	746	216	220	1		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Be	122	Total	C	N	O	S	0	0
			972	628	168	173	3		

- Molecule 33 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bf	108	Total	C	N	O	S	0	0
			827	519	154	150	4		

- Molecule 34 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 35 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bh	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 36 is a protein called Mitochondrial ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 37 is a protein called Mitochondrial ribosomal protein L45.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bi	260	Total	C	N	O	S	0	0
			2138	1370	379	379	10		

- Molecule 38 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bj	228	Total	C	N	O	S	0	0
			1872	1197	324	345	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bk	165	Total	C	N	O	S	0	0
			1327	848	229	245	5		

- Molecule 40 is a protein called Mrpl34.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bl	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bl	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 41 is a protein called Mitochondrial ribosomal protein L50.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bm	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 42 is a protein called Mitochondrial ribosomal protein L51.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bn	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 43 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bo	97	Total	C	N	O	S	0	0
			772	481	148	141	2		

- Molecule 44 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bp	12	ALA	SER	conflict	UNP A0A341D604
Bp	107	SER	GLY	conflict	UNP A0A341D604

- Molecule 45 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bq	80	Total	C	N	O	S	0	0
			672	431	123	116	2		

- Molecule 46 is a protein called Mitochondrial ribosomal protein L57.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 47 is a protein called mL62 (ICT1).

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bu	151	Total	C	N	O	S	0	0
			1198	738	233	222	5		

- Molecule 48 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bv	135	Total	C	N	O	S	0	0
			1131	692	223	211	5		

- Molecule 49 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bw	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 50 is a protein called Mitochondrial ribosomal protein S18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bx	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 51 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 52 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BA	1544	Total	C	N	O	P	0	0
			32844	14750	5972	10578	1544		

- Molecule 54 is a protein called Mitochondrial ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AB	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 55 is a protein called Mitochondrial ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 56 is a protein called 28S ribosomal protein S5, mitochondrial isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AE	343	Total	C	N	O	S	0	0
			2732	1707	527	487	11		

- Molecule 57 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AF	122	Total	C	N	O	S	0	0
			981	620	178	177	6		

- Molecule 58 is a protein called Mitochondrial ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AG	208	Total	C	N	O	S	0	0
			1721	1097	314	299	11		

- Molecule 59 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AI	328	Total	C	N	O	S	0	0
			2650	1678	478	481	13		

- Molecule 60 is a protein called Mitochondrial ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AJ	140	Total	C	N	O	S	0	0
			1155	746	197	208	4		

- Molecule 61 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AK	137	Total	C	N	O	S	0	0
			1007	631	193	180	3		

- Molecule 62 is a protein called Mitochondrial ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AL	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 63 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AN	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 64 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AO	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AP	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 66 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AQ	112	Total	C	N	O	S	0	0
			875	568	153	151	3		

- Molecule 67 is a protein called Mitochondrial ribosomal protein S18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 68 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 69 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	AZ	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 70 is a protein called Mitochondrial ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Aa	292	Total	C	N	O	S	0	0
			2378	1518	409	442	9		

- Molecule 71 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 72 is a protein called Mitochondrial ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 73 is a protein called Mitochondrial ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 74 is a protein called Mitochondrial ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ae	388	Total	C	N	O	S	0	0
			3109	1971	535	589	14		

- Molecule 75 is a protein called Mitoribosomal protein ms28, mrps28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Af	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 76 is a protein called Death associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ag	353	Total	C	N	O	S	0	0
			2875	1837	515	513	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ah	120	Total	C	N	O	S	0	0
			1015	659	168	185	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	133	THR	ALA	conflict	UNP A0A4X1SQW0
Ah	179	ARG	LYS	conflict	UNP A0A4X1SQW0
Ah	180	UNK	ALA	conflict	UNP A0A4X1SQW0

- Molecule 78 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ai	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 79 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Aj	213	Total	C	N	O	S	0	0
			1788	1131	338	311	8		

- Molecule 80 is a protein called Mitochondrial ribosomal protein S35.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 81 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 82 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 83 is a protein called Pentatricopeptide repeat domain 3,Pentatricopeptide repeat domain 3,Pentatricopeptide repeat domain 3,Pentatricopeptide repeat domain 3,mS39,Pentatricopeptide repeat domain 3,Pentatricopeptide repeat domain 3,Pentatricopeptide repeat domain 3,Pentatricopeptide repeat domain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ao	572	Total	C	N	O	S	0	0
			4527	2899	770	834	24		

- Molecule 84 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ap	190	Total	C	N	O	S	0	0
			1564	991	292	273	8		

- Molecule 85 is a protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
85	CL	45	Total	C	N	O	0	0
			317	203	52	62		

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Mol	Chain	Residues	Atoms				AltConf	Trace
85	DL	27	Total	C	N	O	0	0
			213	137	33	43		
85	EL	28	Total	C	N	O	0	0
			222	143	35	44		
85	FL	27	Total	C	N	O	0	0
			213	137	33	43		
85	GL	27	Total	C	N	O	0	0
			213	137	33	43		
85	HL	26	Total	C	N	O	0	0
			204	131	32	41		

- Molecule 86 is a RNA chain called tRNA(P/P) and tRNA(E*).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	AV	71	Total	C	N	O	P	0	0
			1419	640	147	562	70		
86	AY	71	Total	C	N	O	P	0	0
			1419	640	147	562	70		

- Molecule 87 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	AX	6	Total	C	N	O	P	0	0
			120	54	12	48	6		

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	B3	1	Total	Mg	0
			1	1	
88	BB	1	Total	Mg	0
			1	1	
88	BD	3	Total	Mg	0
			3	3	
88	BE	1	Total	Mg	0
			1	1	
88	BJ	1	Total	Mg	0
			1	1	
88	BP	2	Total	Mg	0
			2	2	
88	BQ	1	Total	Mg	0
			1	1	

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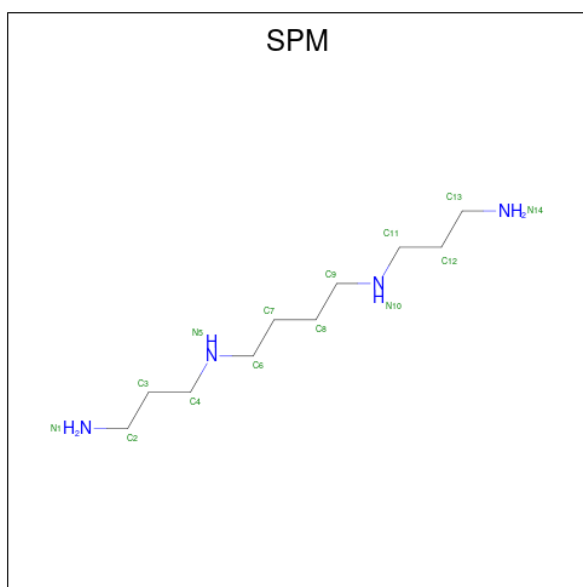
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Mol	Chain	Residues	Atoms		AltConf
88	Be	2	Total 2	Mg 2	0
88	Bl	1	Total 1	Mg 1	0
88	Bt	1	Total 1	Mg 1	0
88	AA	102	Total 102	Mg 102	0
88	BA	203	Total 203	Mg 203	0
88	AB	1	Total 1	Mg 1	0
88	AL	1	Total 1	Mg 1	0
88	Ag	1	Total 1	Mg 1	0
88	Am	1	Total 1	Mg 1	0
88	An	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

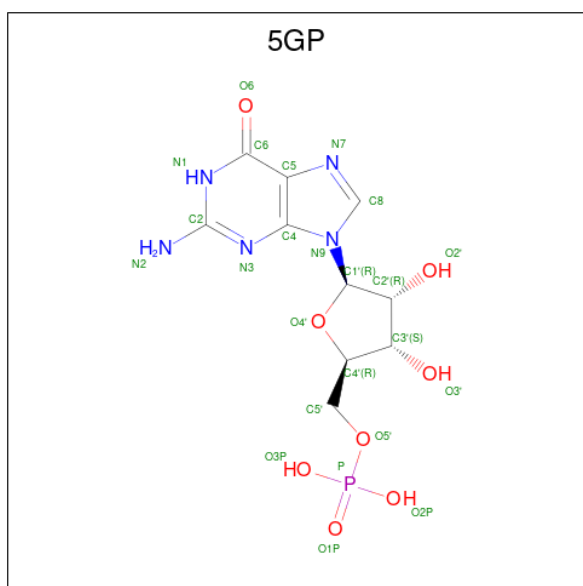
Mol	Chain	Residues	Atoms		AltConf
89	B5	1	Total 1	Zn 1	0
89	Bx	1	Total 1	Zn 1	0
89	B9	1	Total 1	Zn 1	0
89	AR	1	Total 1	Zn 1	0
89	Ac	1	Total 1	Zn 1	0
89	Ap	1	Total 1	Zn 1	0

- Molecule 90 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



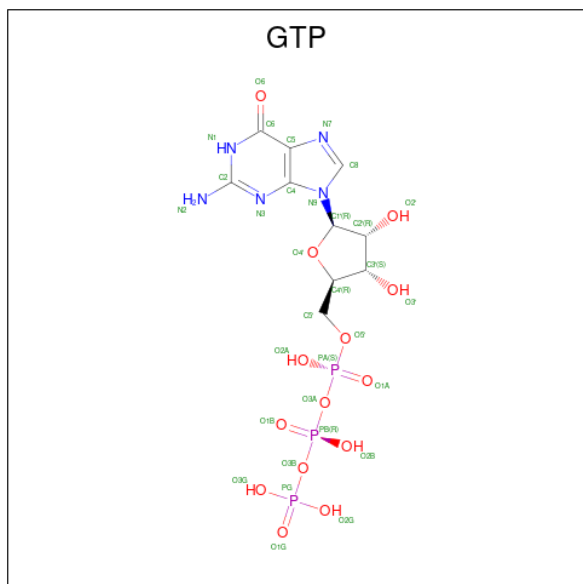
Mol	Chain	Residues	Atoms			AltConf
90	AA	1	Total	C	N	0
			14	10	4	
90	BA	1	Total	C	N	0
			14	10	4	
90	BA	1	Total	C	N	0
			14	10	4	

- Molecule 91 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					AltConf
91	BA	1	Total	C	N	O	P	0
			24	10	5	8	1	

- Molecule 92 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
92	Ag	1	Total	C	N	O	P	0
			32	10	5	14	3	

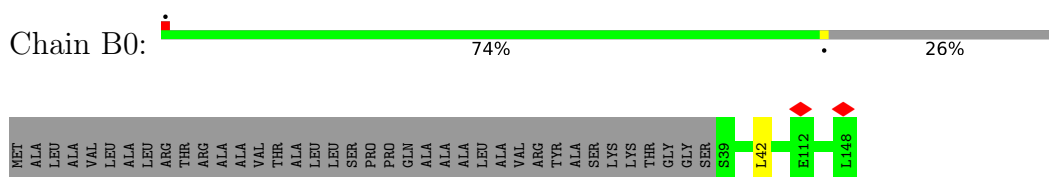
- Molecule 93 is water.

Mol	Chain	Residues	Atoms		AltConf
93	Ag	3	Total	O	0
			3	3	

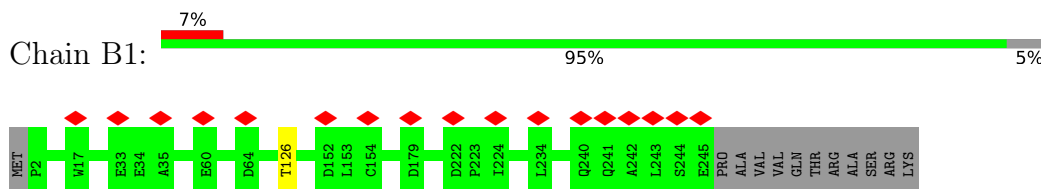
3 Residue-property plots [i](#)

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.

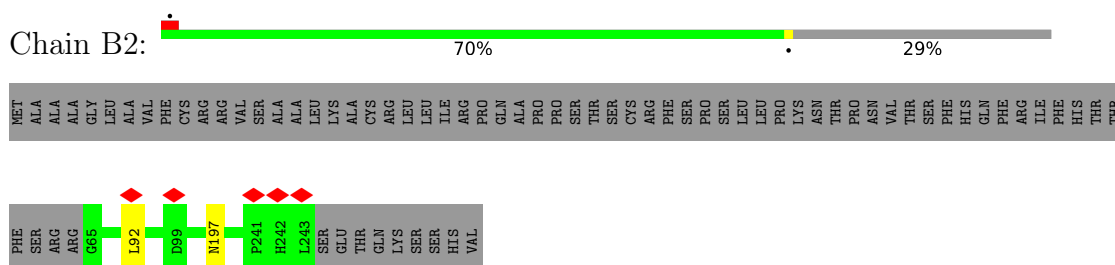
- Molecule 1: Mitochondrial ribosomal protein L27



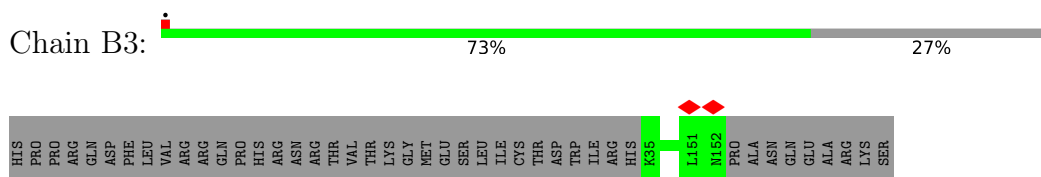
- Molecule 2: Mitochondrial ribosomal protein L28



- Molecule 3: Mitochondrial ribosomal protein L47

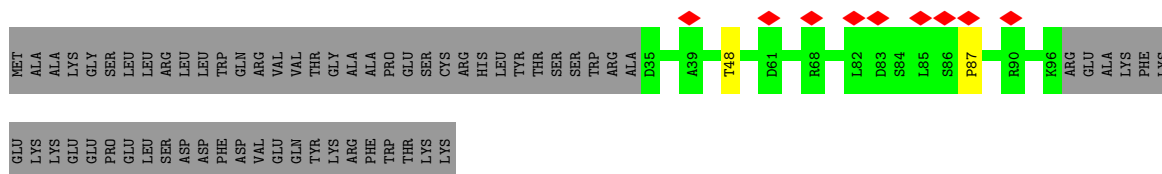


- Molecule 4: uL30m

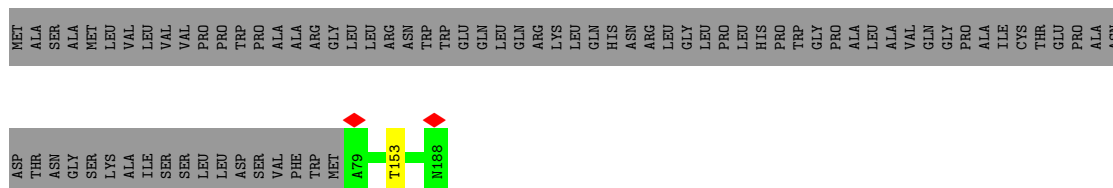


- Molecule 5: bL31m

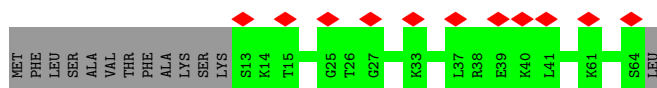
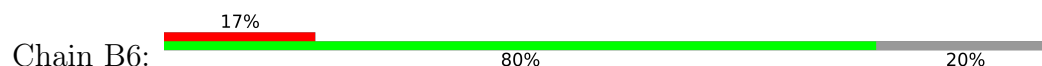




• Molecule 6: bL32m



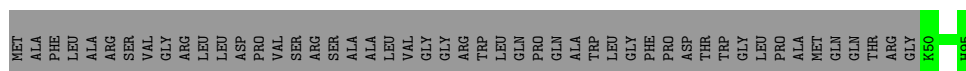
• Molecule 7: bL33m



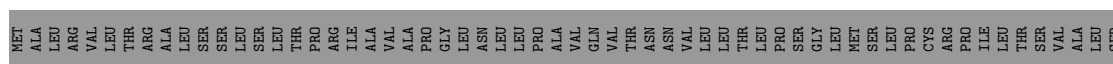
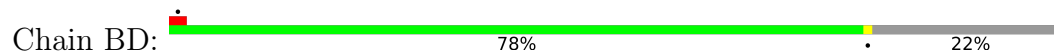
• Molecule 8: CP tRNAPhe



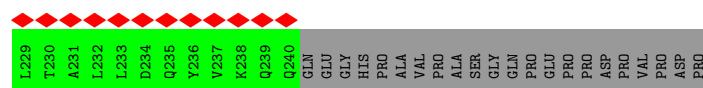
• Molecule 9: Mitochondrial ribosomal protein L34



• Molecule 10: uL2m

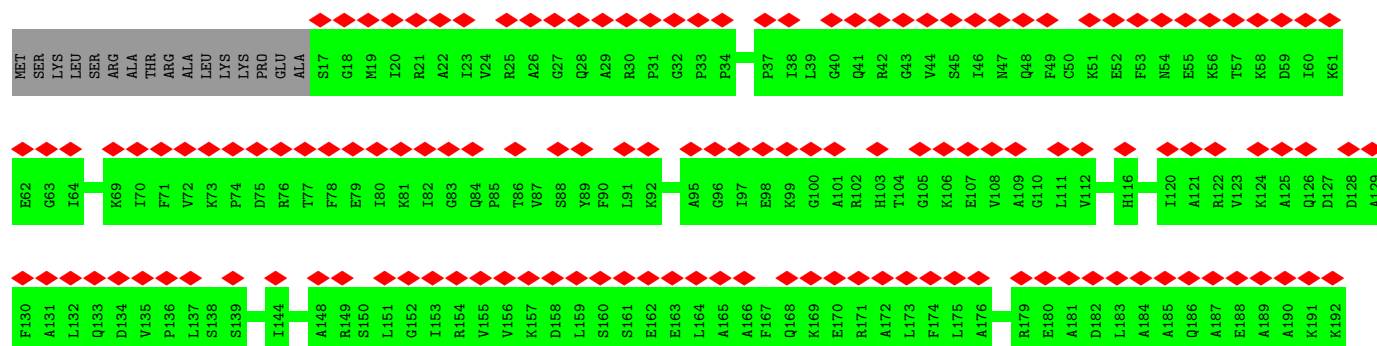


• Molecule 11: ICT1



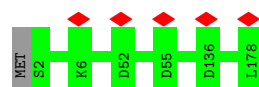
- Molecule 15: Mitochondrial ribosomal protein L11

Chain BK: 72% 92% 8%



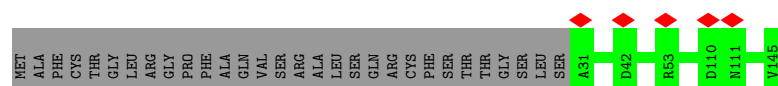
- Molecule 16: uL13m

Chain BN: 99%



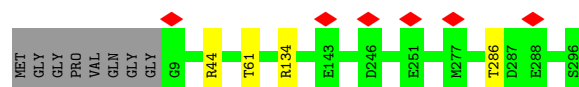
- Molecule 17: uL14m

Chain BO: 79% 21%



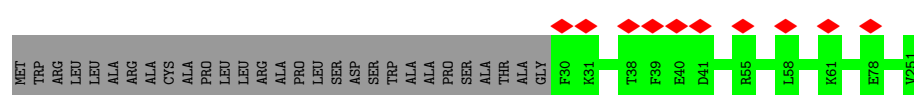
- Molecule 18: uL15m

Chain BP: 96%

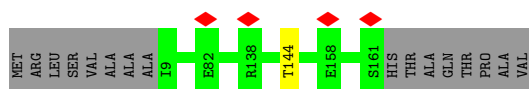


- Molecule 19: uL16m

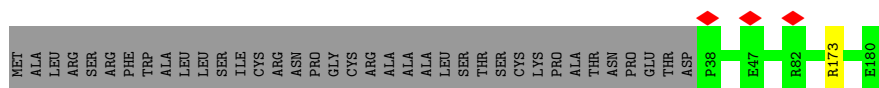
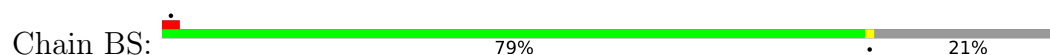
Chain BQ: 88% 12%



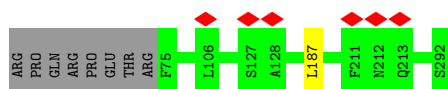
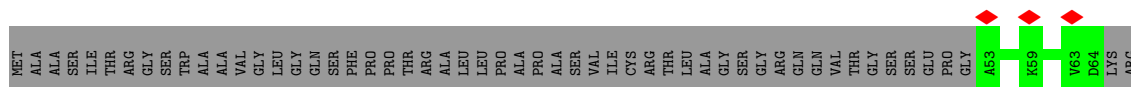
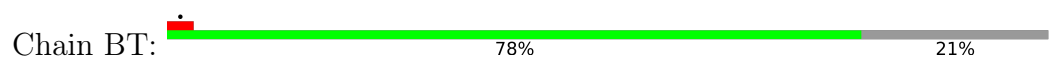
- Molecule 20: bL17m



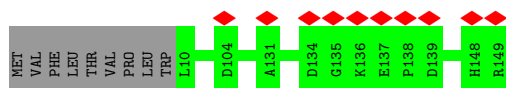
- Molecule 21: Mitochondrial ribosomal protein L18



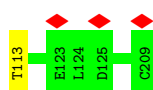
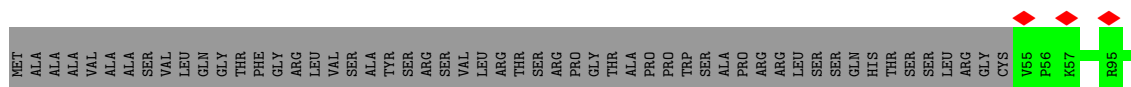
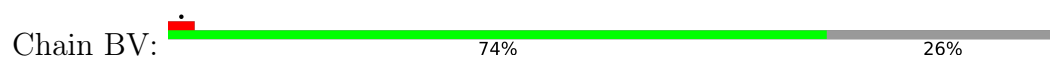
- Molecule 22: Mitochondrial ribosomal protein L19



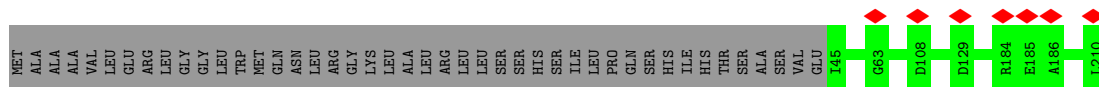
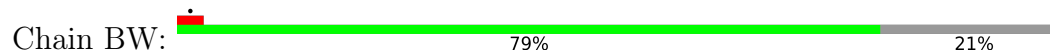
- Molecule 23: Mitochondrial ribosomal protein L20



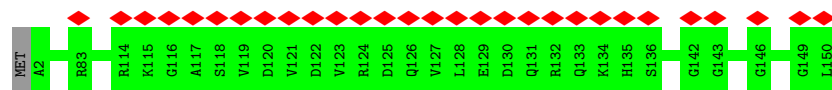
- Molecule 24: Mitochondrial ribosomal protein L21



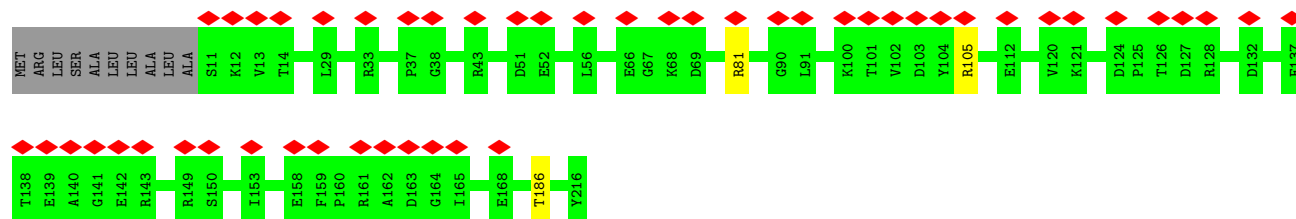
- Molecule 25: uL22m



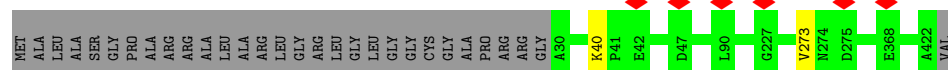
• Molecule 26: uL23m



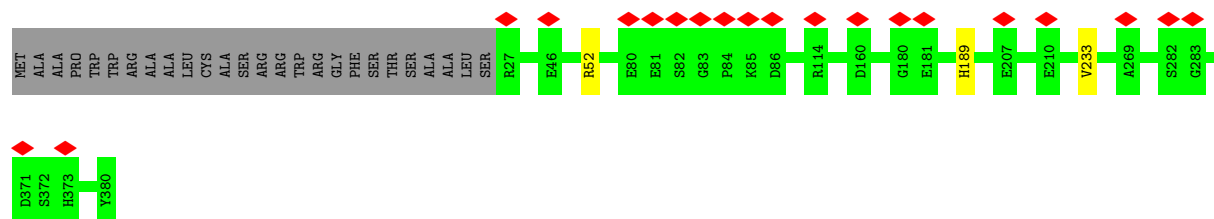
• Molecule 27: uL24m



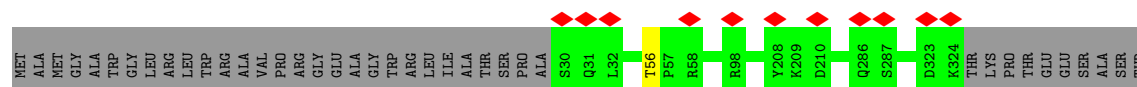
• Molecule 28: Mitochondrial ribosomal protein L37



• Molecule 29: Mitochondrial ribosomal protein L38

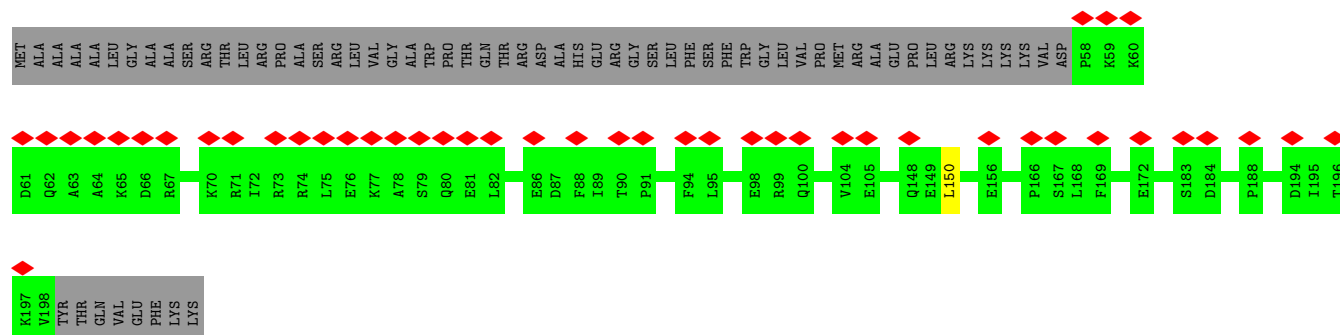


• Molecule 30: Mitochondrial ribosomal protein L39

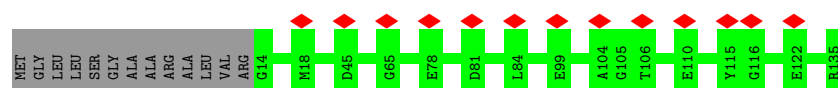


• Molecule 31: Mitochondrial ribosomal protein L40

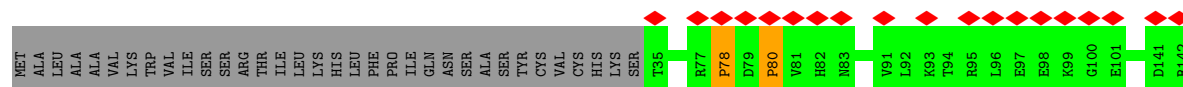
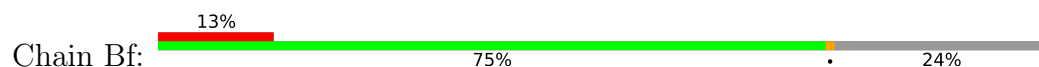




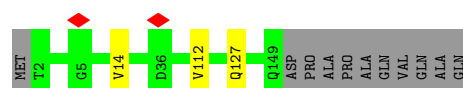
- Molecule 32: Mitochondrial ribosomal protein L41



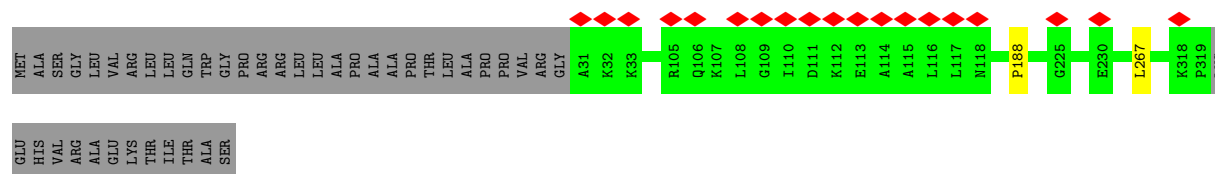
- Molecule 33: mL42



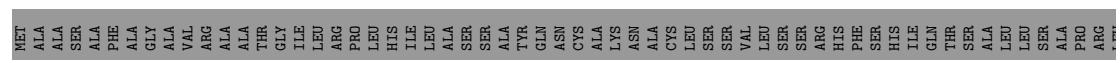
- Molecule 34: Mitochondrial ribosomal protein L43

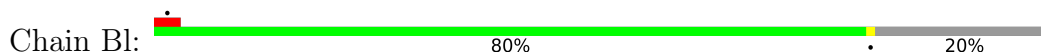


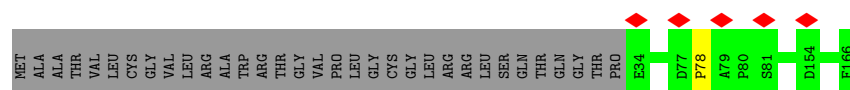
- Molecule 35: mL44



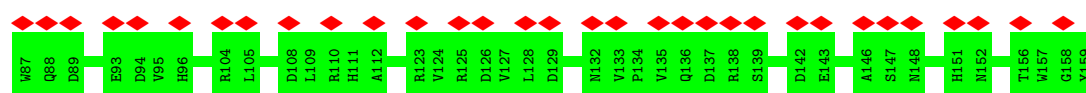
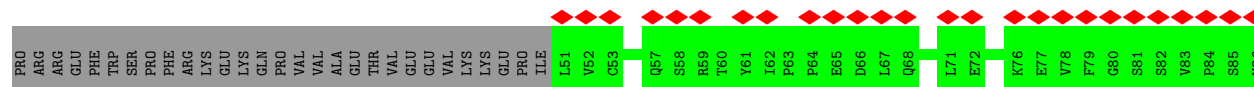
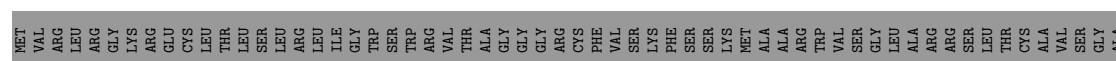
- Molecule 36: Mitochondrial ribosomal protein L35



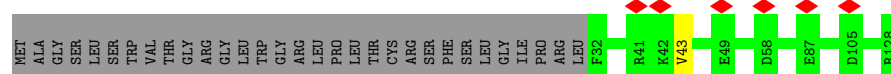
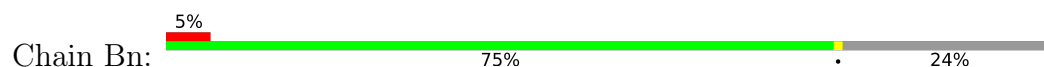




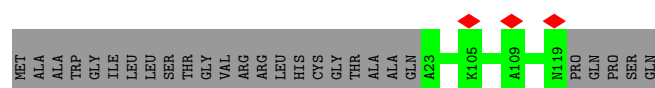
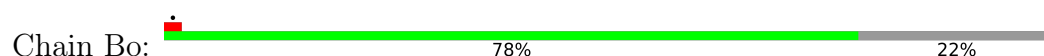
• Molecule 41: Mitochondrial ribosomal protein L50



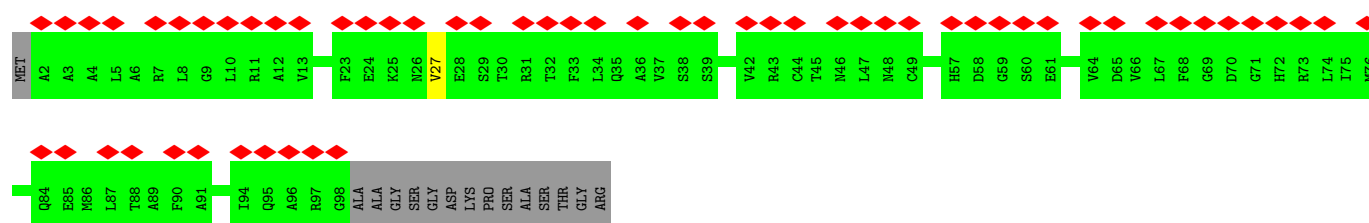
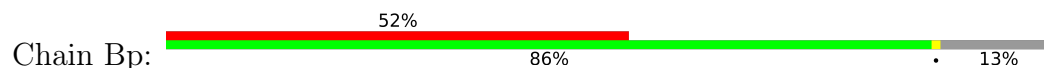
• Molecule 42: Mitochondrial ribosomal protein L51



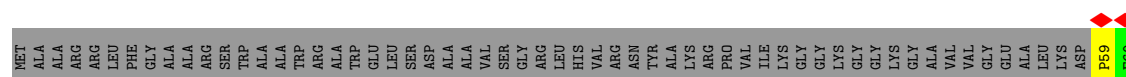
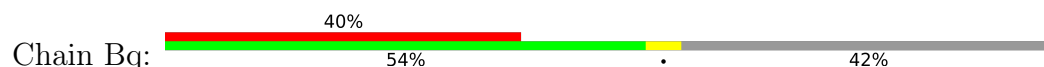
• Molecule 43: mL52

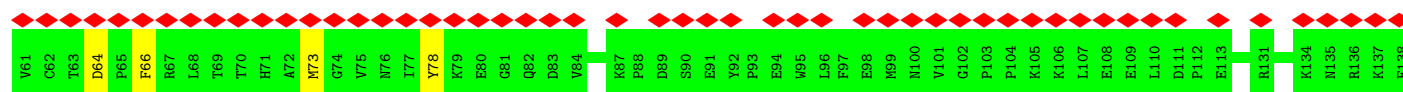


• Molecule 44: mL53

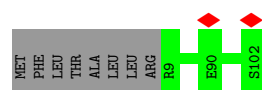


• Molecule 45: mL54

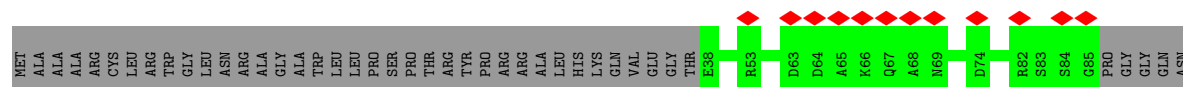
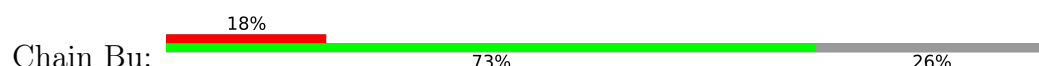




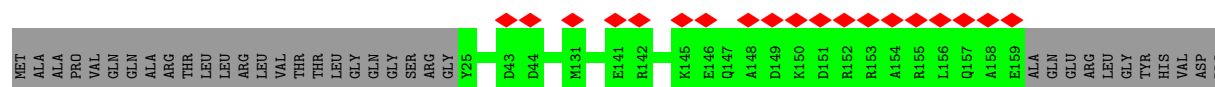
- Molecule 46: Mitochondrial ribosomal protein L57



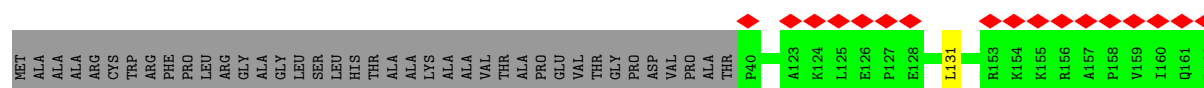
- Molecule 47: mL62 (ICT1)



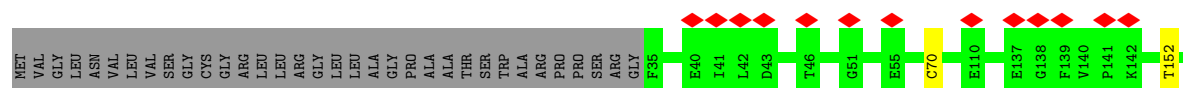
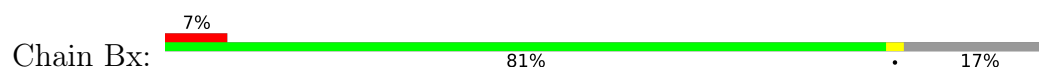
- Molecule 48: mL64



- Molecule 49: 39S ribosomal protein S30, mitochondrial



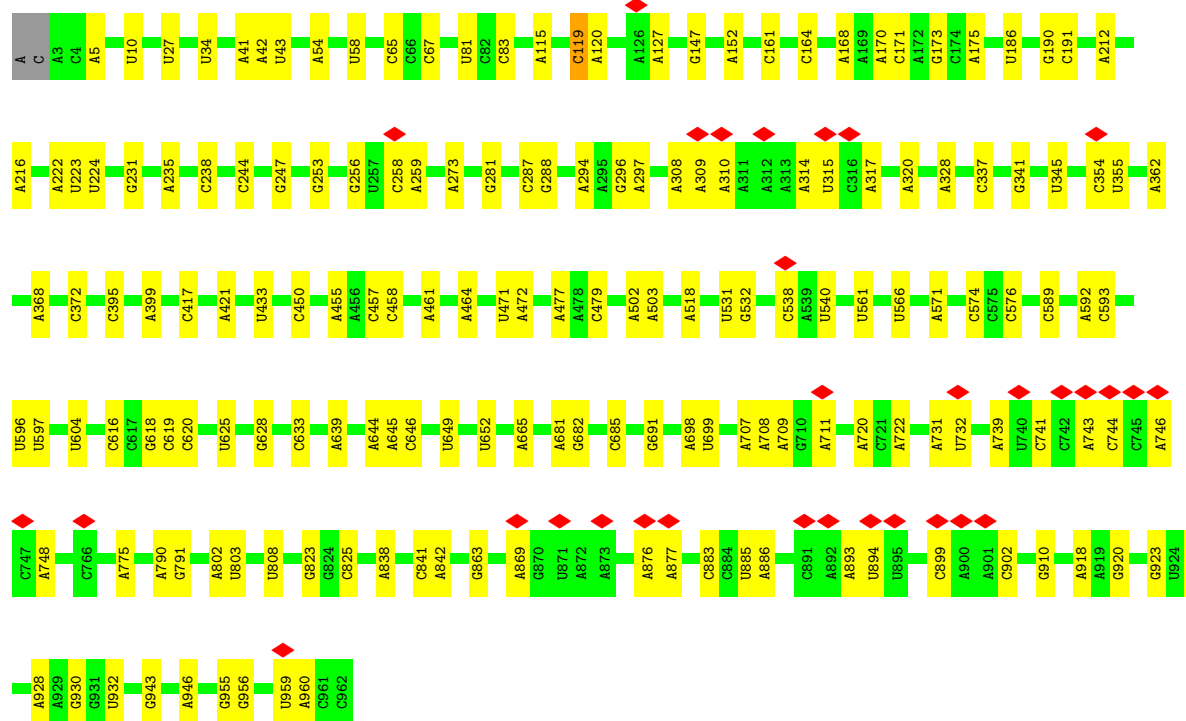
- Molecule 50: Mitochondrial ribosomal protein S18A





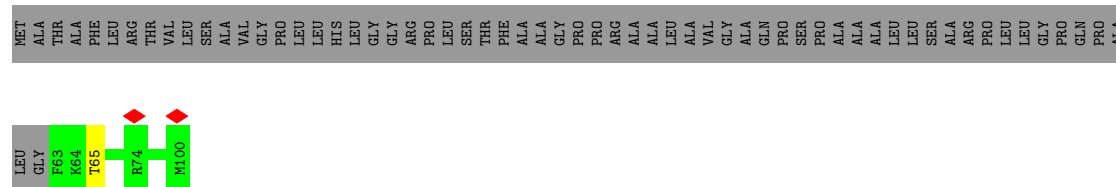
• Molecule 51: 12S rRNA

Chain AA: 82% 17%



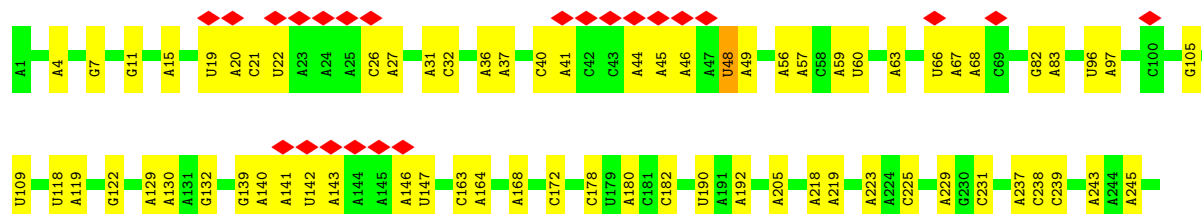
• Molecule 52: Ribosomal protein

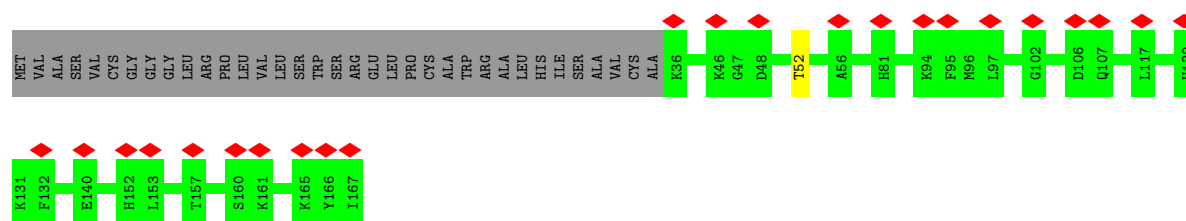
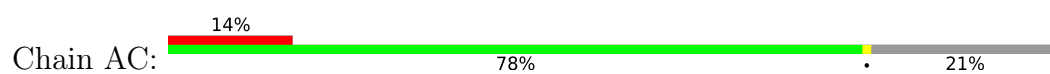
Chain B9: 37% 62%



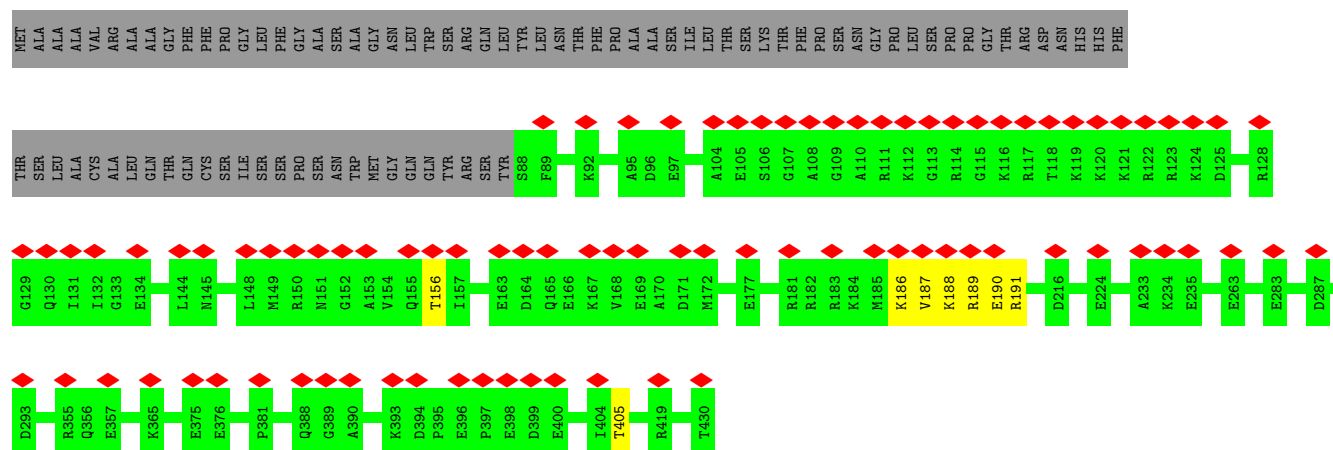
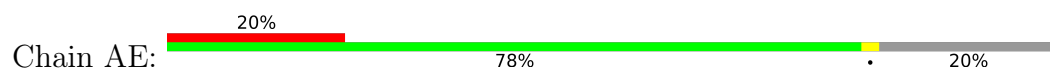
• Molecule 53: 16S rRNA

Chain BA: 72% 26%

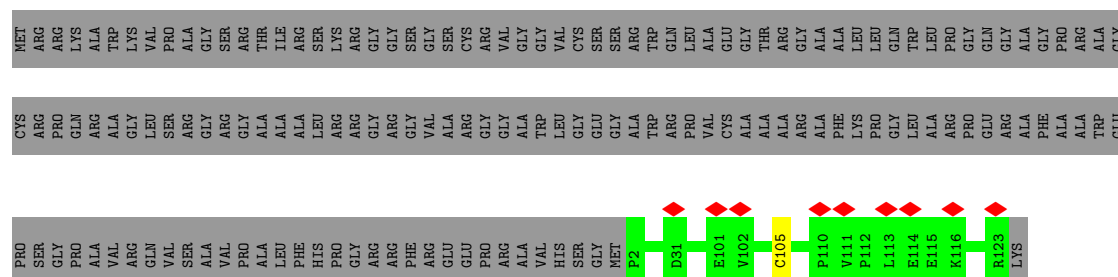




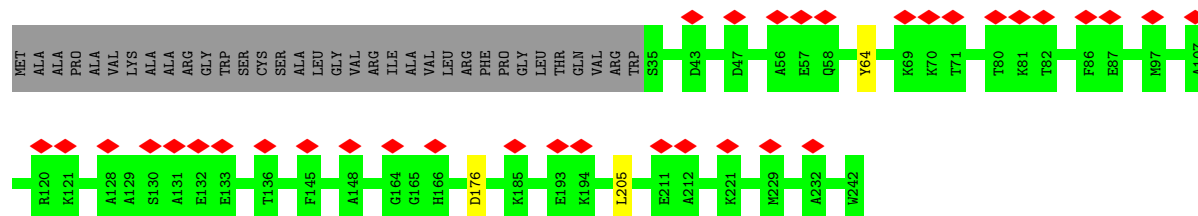
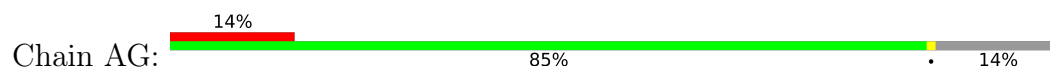
- Molecule 56: 28S ribosomal protein S5, mitochondrial isoform X2



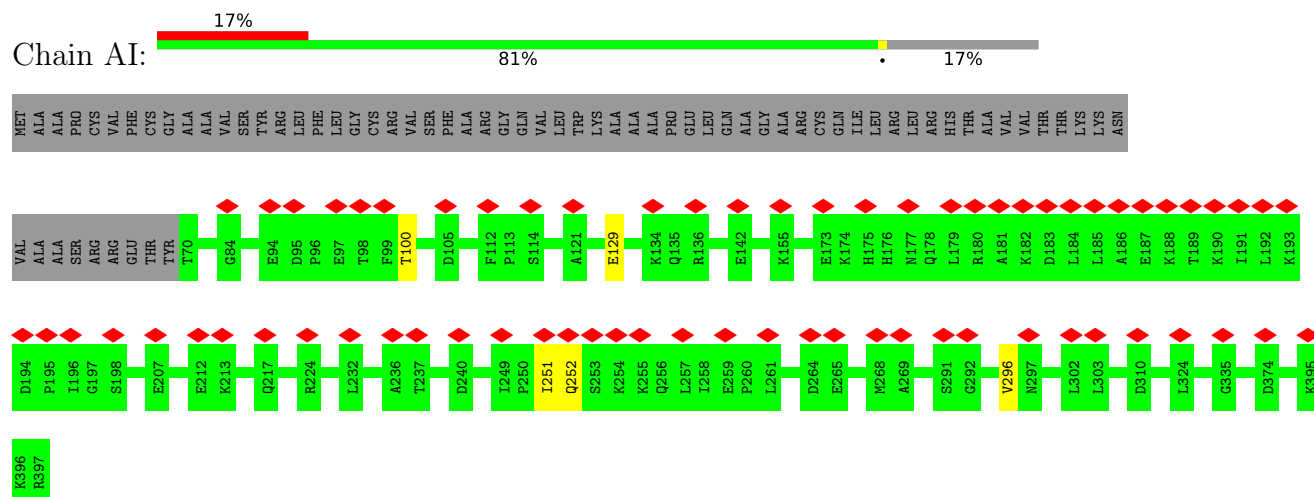
- Molecule 57: bS6m



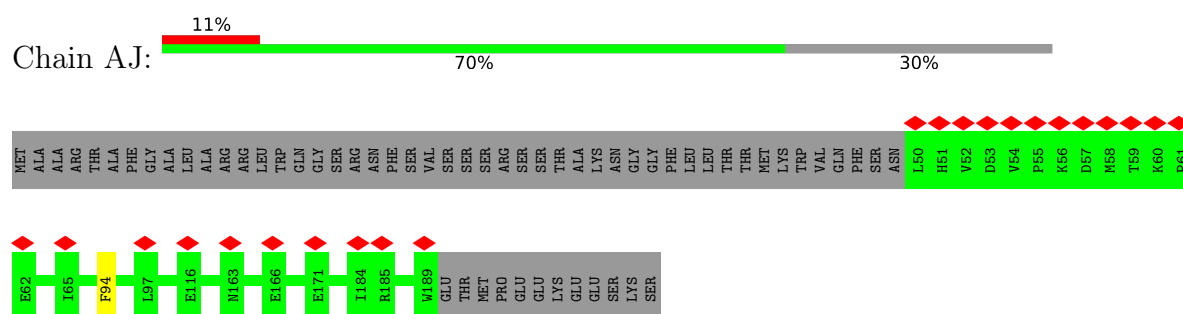
- Molecule 58: Mitochondrial ribosomal protein S7



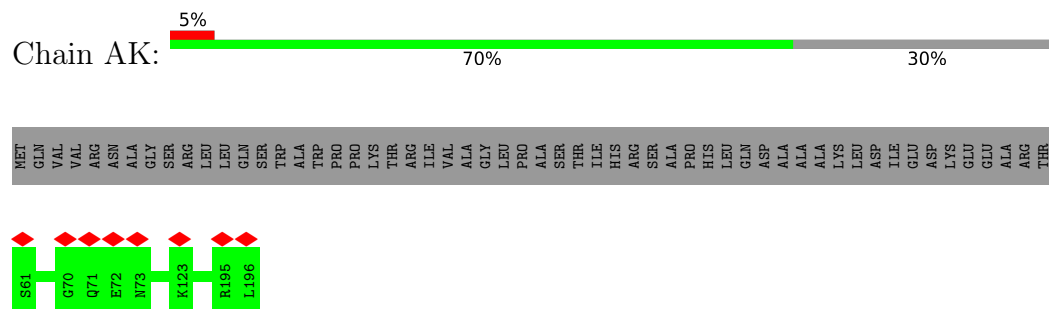
• Molecule 59: uS9m



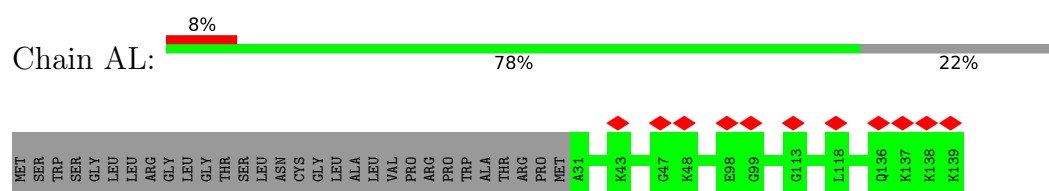
• Molecule 60: Mitochondrial ribosomal protein S10



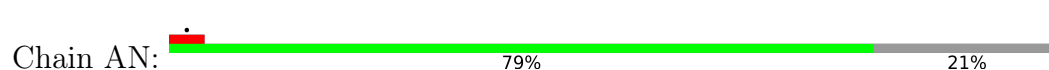
• Molecule 61: uS11m



• Molecule 62: Mitochondrial ribosomal protein S12

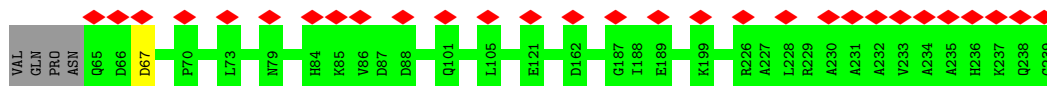
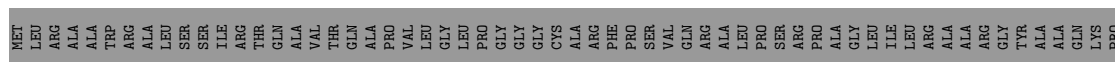
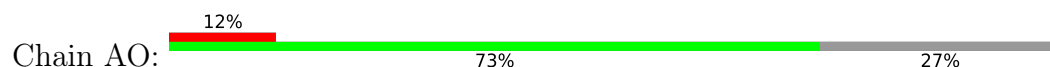


• Molecule 63: Mitochondrial ribosomal protein S14

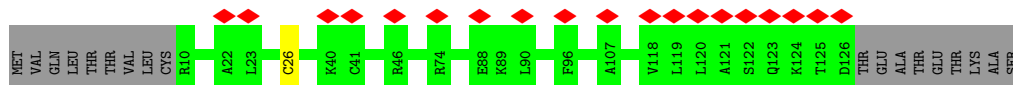
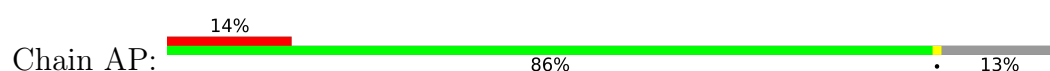




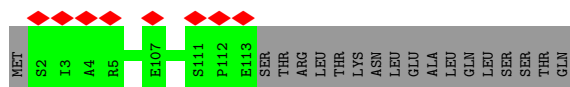
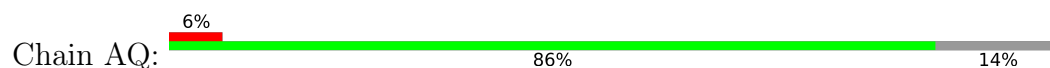
• Molecule 64: uS15m



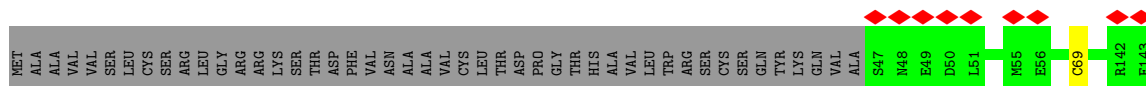
• Molecule 65: 28S ribosomal protein S16, mitochondrial



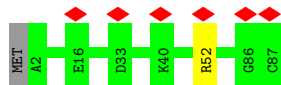
• Molecule 66: uS17m



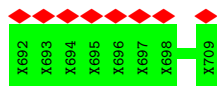
• Molecule 67: Mitochondrial ribosomal protein S18C



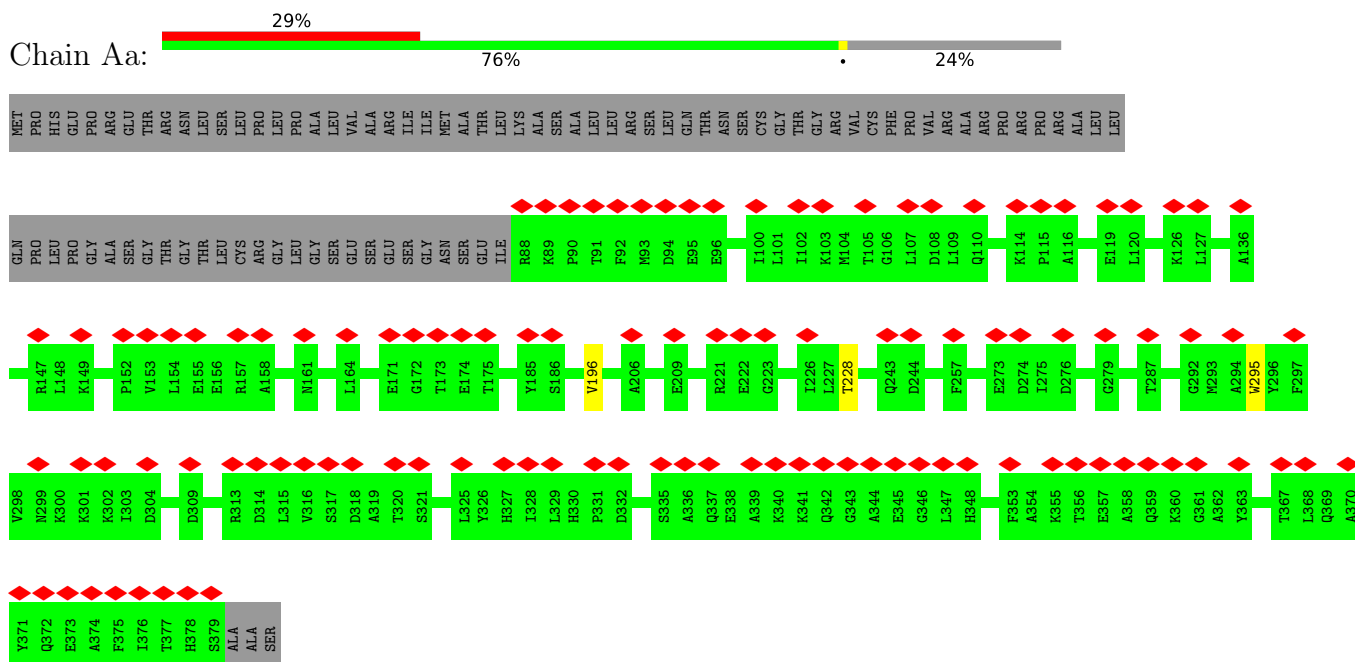
• Molecule 68: bS21m



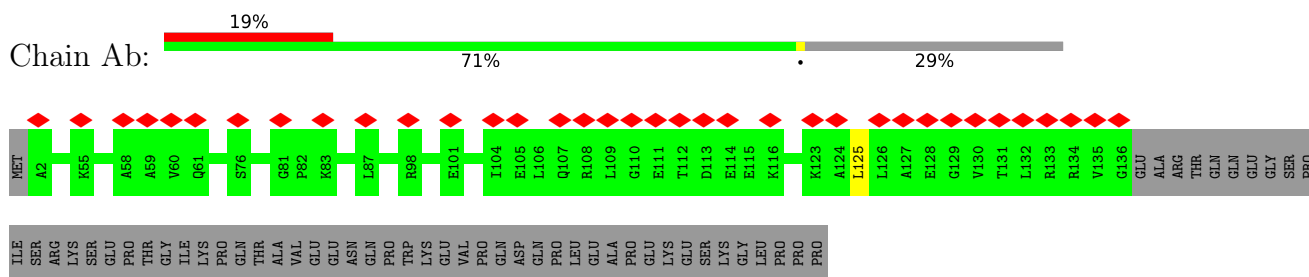
• Molecule 69: unknown



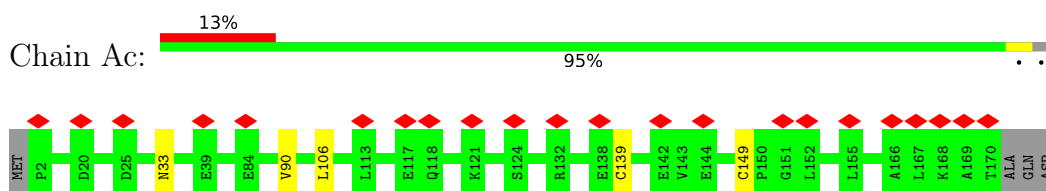
- Molecule 70: Mitochondrial ribosomal protein S22



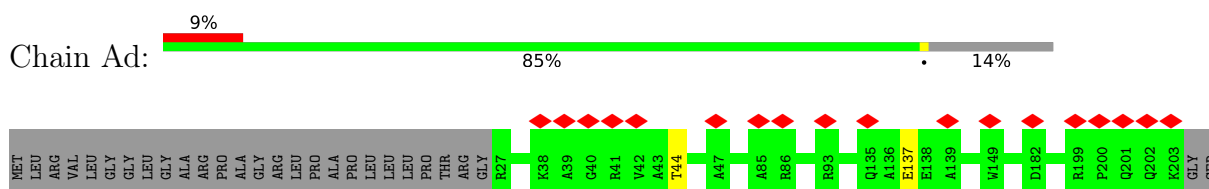
- Molecule 71: mS23



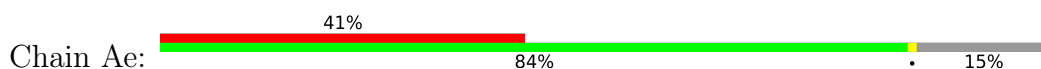
- Molecule 72: Mitochondrial ribosomal protein S25



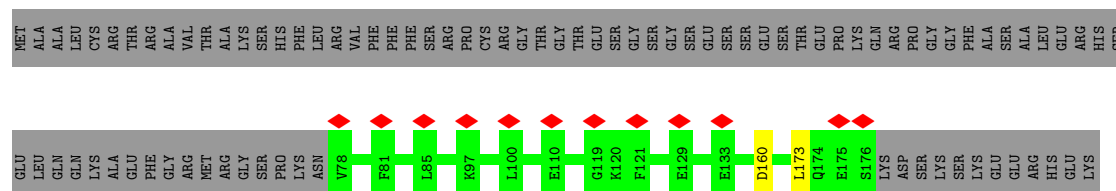
- Molecule 73: Mitochondrial ribosomal protein S26



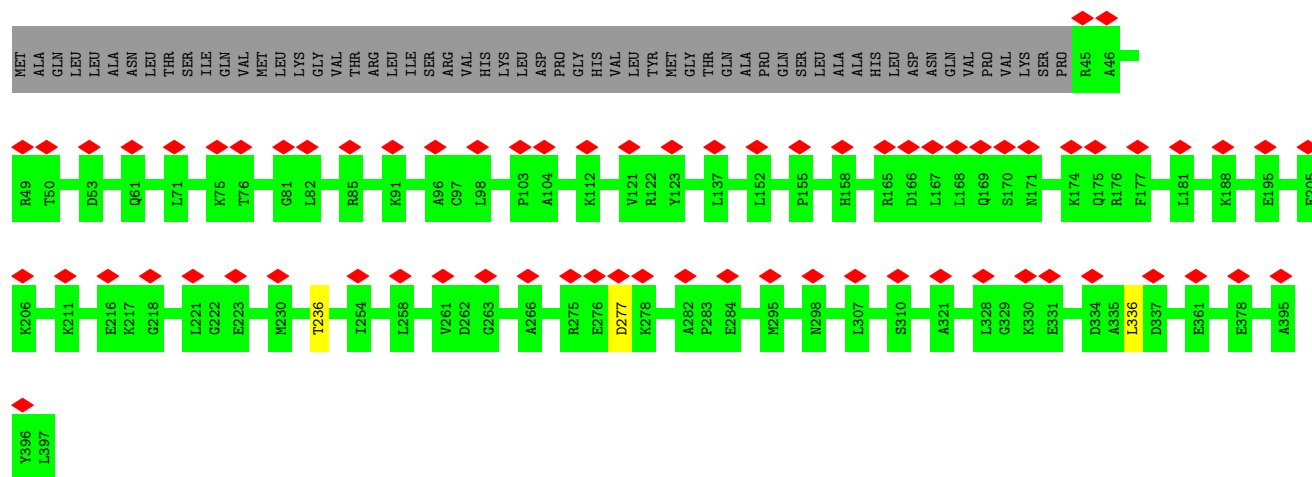
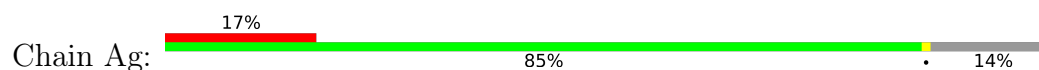
- Molecule 74: Mitochondrial ribosomal protein S27



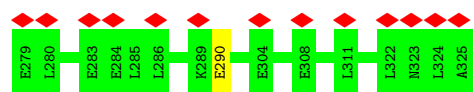
- Molecule 75: Mitoribosomal protein ms28, mrps28



- Molecule 76: Death associated protein 3



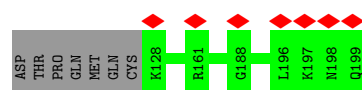
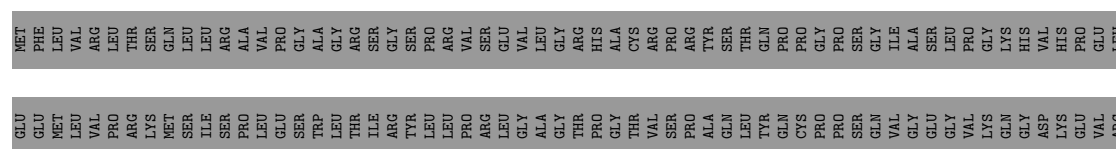
- Molecule 77: 28S ribosomal protein S31, mitochondrial



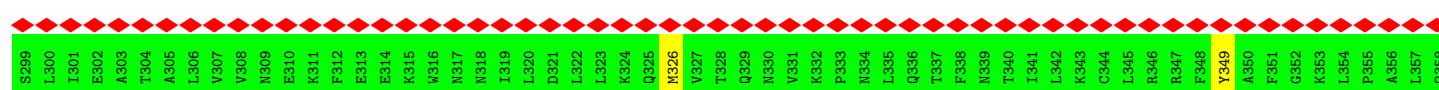
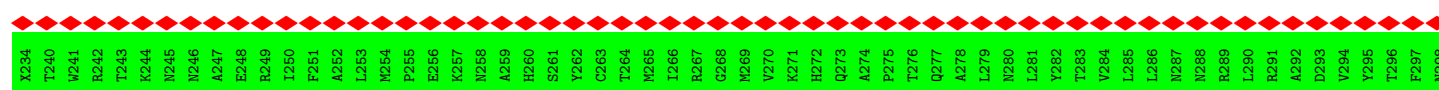
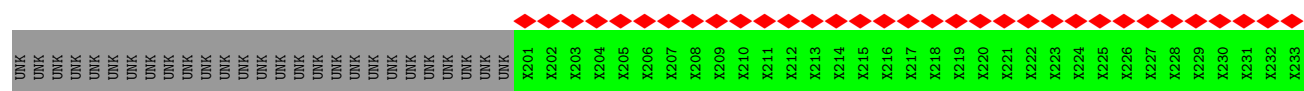
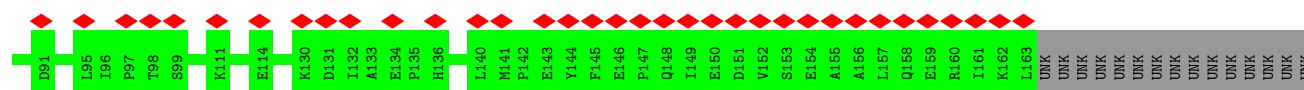
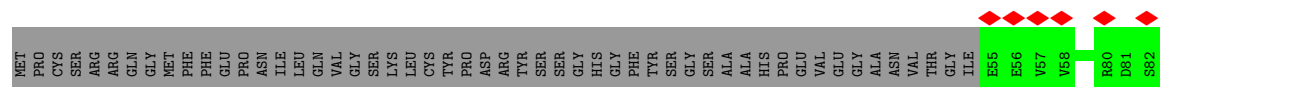
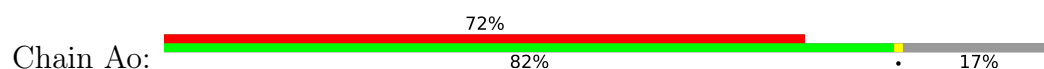
• Molecule 81: mS37



• Molecule 82: Aurora kinase A interacting protein 1

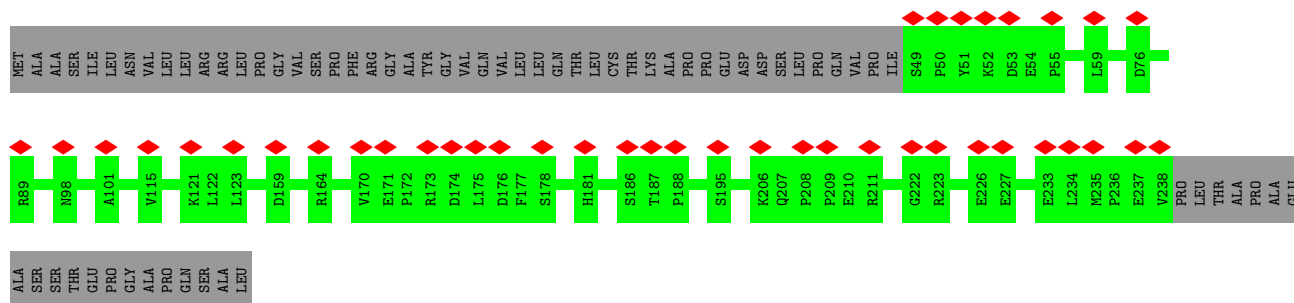
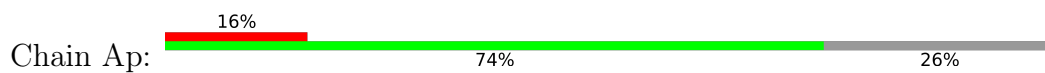


• Molecule 83: Pentatricopeptide repeat domain 3, Pentatricopeptide repeat domain 3, Pentatricopeptide repeat domain 3, mS39, Pentatricopeptide repeat domain 3, Pentatricopeptide repeat domain 3, Pentatricopeptide repeat domain 3, Pentatricopeptide repeat domain 3

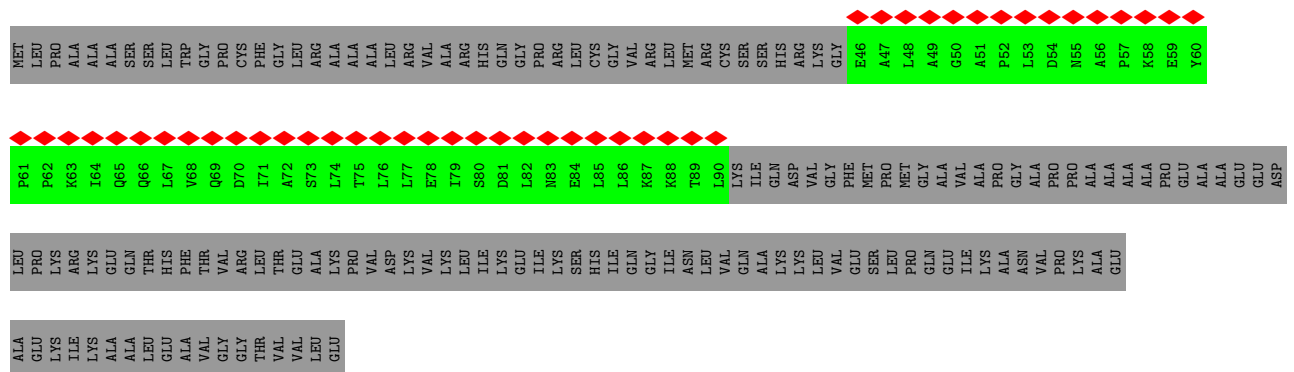




• Molecule 84: 28S ribosomal protein S18b, mitochondrial

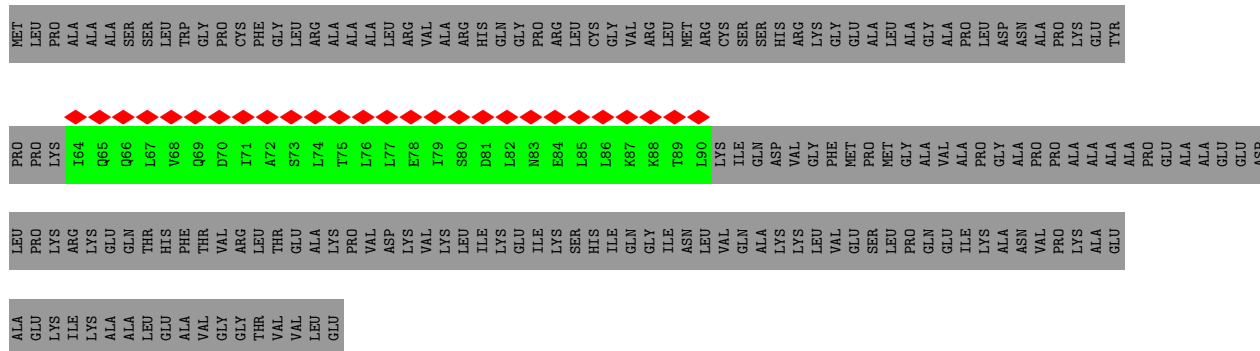


• Molecule 85: Mitochondrial ribosomal protein L12



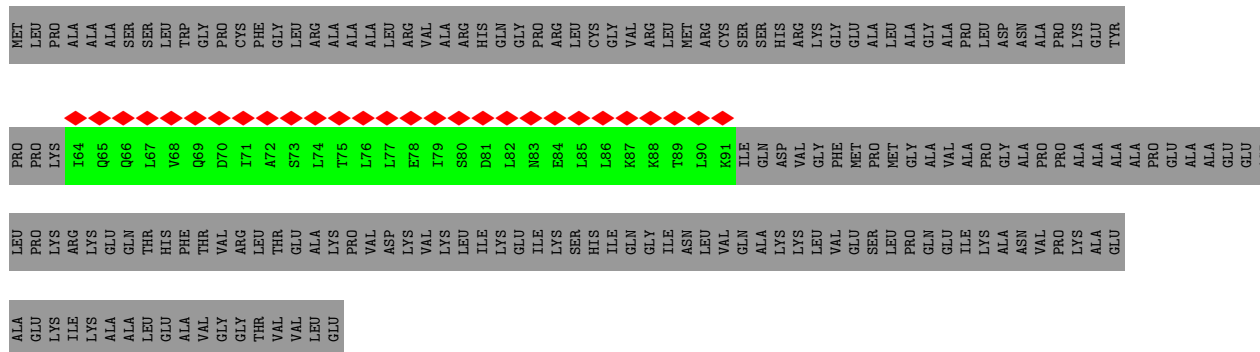
• Molecule 85: Mitochondrial ribosomal protein L12

Chain DL:  14% 86%



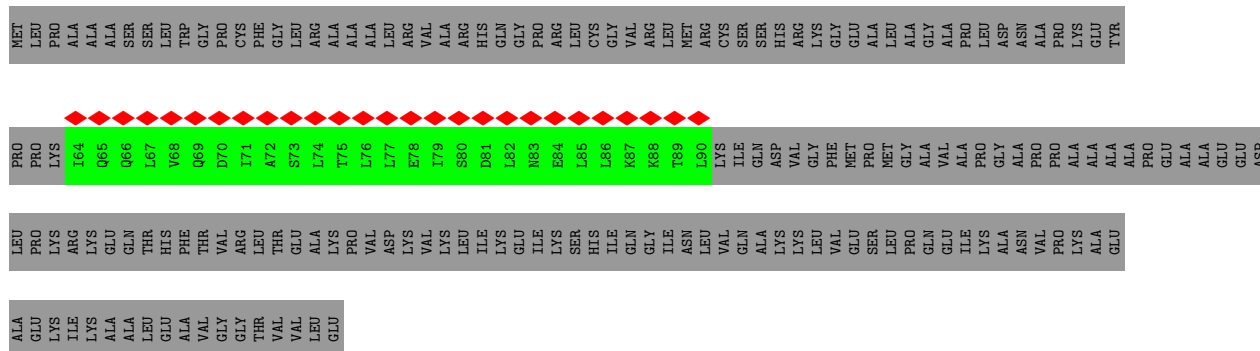
• Molecule 85: Mitochondrial ribosomal protein L12

Chain EL:  14% 86%



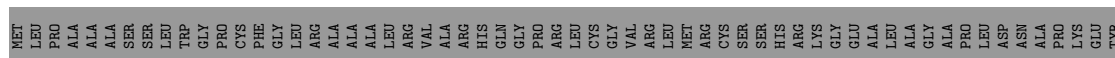
• Molecule 85: Mitochondrial ribosomal protein L12

Chain FL:  14% 86%



• Molecule 85: Mitochondrial ribosomal protein L12

Chain GL:  14% 86%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26001	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	521.76, 521.76, 521.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.087, 1.087, 1.087	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5GP, GTP, MG, SPM

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	B0	0.25	0/880	0.45	0/1189
2	B1	0.24	0/2093	0.46	0/2835
3	B2	0.24	0/1586	0.47	0/2123
4	B3	0.24	0/993	0.46	0/1341
5	B4	0.23	0/481	0.59	1/653 (0.2%)
6	B5	0.24	0/917	0.51	0/1227
7	B6	0.24	0/430	0.49	0/570
8	BB	0.31	1/1595 (0.1%)	0.75	0/2475
9	B7	0.23	0/395	0.54	0/524
10	BD	0.24	0/1898	0.52	0/2555
11	BE	0.25	0/2493	0.45	0/3387
12	BF	0.23	0/2069	0.48	0/2816
13	BI	0.23	0/819	0.53	0/1101
14	BJ	0.24	0/1742	0.47	0/2358
15	BK	0.25	0/1323	0.47	0/1785
16	BN	0.24	0/1487	0.43	0/2017
17	BO	0.23	0/912	0.52	0/1231
18	BP	0.25	0/2368	0.50	0/3198
19	BQ	0.24	0/1850	0.50	0/2491
20	BR	0.23	0/1262	0.50	0/1700
21	BS	0.23	0/1197	0.53	0/1624
22	BT	0.25	0/1936	0.47	0/2615
23	BU	0.23	0/1179	0.52	0/1578
24	BV	0.24	0/1256	0.48	0/1706
25	BW	0.25	0/1407	0.48	0/1891
26	BX	0.25	0/1211	0.52	0/1646
27	BY	0.24	0/1719	0.50	0/2329
28	Ba	0.24	0/3267	0.46	0/4455
29	Bb	0.25	0/3047	0.49	0/4139
30	Bc	0.24	0/2464	0.45	0/3330
31	Bd	0.24	0/1209	0.49	0/1627
32	Be	0.26	0/1000	0.46	0/1345

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Bf	0.24	0/851	0.57	2/1159 (0.2%)
34	Bg	0.24	0/1191	0.53	0/1614
35	Bh	0.24	0/2372	0.46	0/3211
36	B8	0.23	0/853	0.51	0/1136
37	Bi	0.25	0/2199	0.47	0/2980
38	Bj	0.23	0/1910	0.46	0/2572
39	Bk	0.24	0/1353	0.46	0/1823
40	Bl	0.25	0/1135	0.48	0/1549
41	Bm	0.23	0/917	0.44	0/1248
42	Bn	0.23	0/860	0.48	0/1150
43	Bo	0.24	0/787	0.46	0/1056
44	Bp	0.24	0/752	0.51	0/1013
45	Bq	0.24	0/692	0.51	1/936 (0.1%)
46	Bt	0.23	0/798	0.54	0/1073
47	Bu	0.23	0/1214	0.53	1/1630 (0.1%)
48	Bv	0.23	0/1157	0.49	0/1560
49	Bw	0.24	0/3206	0.46	0/4354
50	Bx	0.24	0/1364	0.48	0/1849
51	AA	0.17	0/22852	0.75	3/35580 (0.0%)
52	B9	0.24	0/342	0.52	0/450
53	BA	0.20	0/36784	0.77	12/57270 (0.0%)
54	AB	0.24	0/1804	0.48	0/2445
55	AC	0.24	0/1105	0.48	0/1496
56	AE	0.25	0/2785	0.50	0/3735
57	AF	0.24	0/999	0.50	0/1347
58	AG	0.24	0/1763	0.45	0/2368
59	AI	0.26	0/2707	0.48	0/3636
60	AJ	0.24	0/1181	0.48	0/1597
61	AK	0.25	0/1027	0.49	0/1389
62	AL	0.24	0/858	0.51	0/1152
63	AN	0.22	0/874	0.54	0/1171
64	AO	0.24	0/1473	0.45	0/1970
65	AP	0.24	0/954	0.53	0/1284
66	AQ	0.24	0/894	0.47	0/1213
67	AR	0.24	0/802	0.44	0/1079
68	AU	0.23	0/745	0.53	0/993
70	Aa	0.23	0/2428	0.43	0/3279
71	Ab	0.25	0/1126	0.49	0/1514
72	Ac	0.25	0/1399	0.46	0/1881
73	Ad	0.24	0/1490	0.49	0/2005
74	Ae	0.24	0/3171	0.47	1/4292 (0.0%)
75	Af	0.25	0/790	0.48	0/1064
76	Ag	0.24	0/2945	0.46	0/3984

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	Ah	0.25	0/1045	0.40	0/1409
78	Ai	0.24	0/841	0.50	0/1121
79	Aj	0.23	0/1835	0.52	0/2484
80	Ak	0.23	0/2268	0.44	0/3069
81	Am	0.24	0/947	0.51	0/1268
82	An	0.23	0/650	0.53	0/858
83	Ao	0.24	0/4458	0.44	0/6036
84	Ap	0.24	0/1616	0.48	0/2195
85	CL	0.23	0/319	0.40	0/435
85	DL	0.22	0/212	0.43	0/286
85	EL	0.22	0/221	0.42	0/297
85	FL	0.22	0/212	0.41	0/286
85	GL	0.22	0/212	0.40	0/286
85	HL	0.22	0/203	0.41	0/273
86	AV	0.98	32/1561 (2.0%)	1.23	2/2411 (0.1%)
86	AY	0.98	32/1561 (2.0%)	1.23	2/2411 (0.1%)
87	AX	1.17	1/131 (0.8%)	1.33	0/200
All	All	0.26	66/183686 (0.0%)	0.62	25/261293 (0.0%)

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BB	1	G	OP3-P	-10.58	1.48	1.61
86	AV	14	U	C1'-N1	6.38	1.58	1.48
86	AY	14	U	C1'-N1	6.29	1.58	1.48
86	AY	40	U	C1'-N1	6.28	1.58	1.48
86	AV	41	U	C1'-N1	6.25	1.58	1.48

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	AA	119	C	C2-N1-C1'	7.95	127.54	118.80
86	AY	69	C	C2-N1-C1'	-6.75	111.38	118.80
86	AV	69	C	C2-N1-C1'	-6.73	111.40	118.80
33	Bf	80	PRO	N-CA-CB	6.60	111.22	103.30
47	Bu	167	PRO	N-CA-CB	6.47	111.06	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B0	108/148 (73%)	108 (100%)	0	0	100	100
2	B1	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
3	B2	177/252 (70%)	176 (99%)	1 (1%)	0	100	100
4	B3	116/161 (72%)	113 (97%)	3 (3%)	0	100	100
5	B4	60/126 (48%)	54 (90%)	6 (10%)	0	100	100
6	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
7	B6	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
9	B7	44/95 (46%)	44 (100%)	0	0	100	100
10	BD	238/306 (78%)	231 (97%)	7 (3%)	0	100	100
11	BE	305/399 (76%)	293 (96%)	12 (4%)	0	100	100
12	BF	248/294 (84%)	245 (99%)	3 (1%)	0	100	100
13	BI	96/268 (36%)	96 (100%)	0	0	100	100
14	BJ	210/262 (80%)	200 (95%)	10 (5%)	0	100	100
15	BK	174/192 (91%)	171 (98%)	3 (2%)	0	100	100
16	BN	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
17	BO	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
18	BP	286/296 (97%)	276 (96%)	10 (4%)	0	100	100
19	BQ	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
20	BR	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
21	BS	141/180 (78%)	132 (94%)	9 (6%)	0	100	100
22	BT	226/292 (77%)	221 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	BU	138/149 (93%)	138 (100%)	0	0	100	100
24	BV	153/209 (73%)	150 (98%)	3 (2%)	0	100	100
25	BW	164/210 (78%)	160 (98%)	4 (2%)	0	100	100
26	BX	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
27	BY	204/216 (94%)	199 (98%)	5 (2%)	0	100	100
28	Ba	391/423 (92%)	375 (96%)	16 (4%)	0	100	100
29	Bb	352/380 (93%)	339 (96%)	13 (4%)	0	100	100
30	Bc	293/334 (88%)	279 (95%)	14 (5%)	0	100	100
31	Bd	139/206 (68%)	134 (96%)	5 (4%)	0	100	100
32	Be	120/135 (89%)	114 (95%)	6 (5%)	0	100	100
33	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	6	34
34	Bg	146/159 (92%)	137 (94%)	9 (6%)	0	100	100
35	Bh	287/332 (86%)	276 (96%)	11 (4%)	0	100	100
36	B8	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
37	Bi	258/306 (84%)	253 (98%)	5 (2%)	0	100	100
38	Bj	224/279 (80%)	213 (95%)	11 (5%)	0	100	100
39	Bk	163/269 (61%)	156 (96%)	7 (4%)	0	100	100
40	Bl	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
41	Bm	107/198 (54%)	105 (98%)	2 (2%)	0	100	100
42	Bn	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
43	Bo	95/124 (77%)	94 (99%)	1 (1%)	0	100	100
44	Bp	95/112 (85%)	91 (96%)	4 (4%)	0	100	100
45	Bq	78/138 (56%)	72 (92%)	5 (6%)	1 (1%)	10	41
46	Bt	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
47	Bu	147/205 (72%)	142 (97%)	3 (2%)	2 (1%)	9	39
48	Bv	133/222 (60%)	133 (100%)	0	0	100	100
49	Bw	385/433 (89%)	367 (95%)	18 (5%)	0	100	100
50	Bx	160/196 (82%)	154 (96%)	6 (4%)	0	100	100
52	B9	36/100 (36%)	36 (100%)	0	0	100	100
54	AB	218/289 (75%)	211 (97%)	7 (3%)	0	100	100
55	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	AE	341/430 (79%)	329 (96%)	12 (4%)	0	100	100
57	AF	120/276 (44%)	117 (98%)	3 (2%)	0	100	100
58	AG	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
59	AI	326/397 (82%)	315 (97%)	11 (3%)	0	100	100
60	AJ	138/200 (69%)	130 (94%)	8 (6%)	0	100	100
61	AK	135/196 (69%)	128 (95%)	7 (5%)	0	100	100
62	AL	107/139 (77%)	102 (95%)	5 (5%)	0	100	100
63	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
64	AO	173/239 (72%)	168 (97%)	5 (3%)	0	100	100
65	AP	115/135 (85%)	112 (97%)	3 (3%)	0	100	100
66	AQ	110/130 (85%)	109 (99%)	1 (1%)	0	100	100
67	AR	95/143 (66%)	93 (98%)	2 (2%)	0	100	100
68	AU	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
70	Aa	290/382 (76%)	283 (98%)	7 (2%)	0	100	100
71	Ab	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
72	Ac	167/173 (96%)	167 (100%)	0	0	100	100
73	Ad	175/205 (85%)	174 (99%)	1 (1%)	0	100	100
74	Ae	386/455 (85%)	364 (94%)	20 (5%)	2 (0%)	25	60
75	Af	97/188 (52%)	94 (97%)	3 (3%)	0	100	100
76	Ag	351/410 (86%)	336 (96%)	15 (4%)	0	100	100
77	Ah	118/387 (30%)	117 (99%)	1 (1%)	0	100	100
78	Ai	97/106 (92%)	95 (98%)	2 (2%)	0	100	100
79	Aj	211/218 (97%)	207 (98%)	4 (2%)	0	100	100
80	Ak	273/325 (84%)	269 (98%)	4 (2%)	0	100	100
81	Am	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
82	An	70/199 (35%)	69 (99%)	1 (1%)	0	100	100
83	Ao	532/690 (77%)	518 (97%)	14 (3%)	0	100	100
84	Ap	188/258 (73%)	183 (97%)	5 (3%)	0	100	100
85	CL	43/198 (22%)	42 (98%)	1 (2%)	0	100	100
85	DL	25/198 (13%)	25 (100%)	0	0	100	100
85	EL	26/198 (13%)	26 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
85	FL	25/198 (13%)	25 (100%)	0	0	100	100
85	GL	25/198 (13%)	25 (100%)	0	0	100	100
85	HL	24/198 (12%)	24 (100%)	0	0	100	100
All	All	14187/19424 (73%)	13772 (97%)	408 (3%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	Bf	78	PRO
33	Bf	80	PRO
47	Bu	167	PRO
45	Bq	64	ASP
74	Ae	342	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B0	90/115 (78%)	89 (99%)	1 (1%)	70	79
2	B1	219/229 (96%)	218 (100%)	1 (0%)	86	90
3	B2	164/228 (72%)	162 (99%)	2 (1%)	67	78
4	B3	110/150 (73%)	110 (100%)	0	100	100
5	B4	45/114 (40%)	44 (98%)	1 (2%)	47	65
6	B5	99/163 (61%)	98 (99%)	1 (1%)	73	81
7	B6	49/60 (82%)	49 (100%)	0	100	100
9	B7	41/78 (53%)	41 (100%)	0	100	100
10	BD	193/248 (78%)	191 (99%)	2 (1%)	73	81
11	BE	263/320 (82%)	260 (99%)	3 (1%)	70	79
12	BF	217/251 (86%)	215 (99%)	2 (1%)	75	83
13	BI	88/228 (39%)	87 (99%)	1 (1%)	70	79
14	BJ	192/230 (84%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	BK	129/151 (85%)	129 (100%)	0	100	100
16	BN	156/157 (99%)	156 (100%)	0	100	100
17	BO	99/123 (80%)	99 (100%)	0	100	100
18	BP	245/249 (98%)	241 (98%)	4 (2%)	58	73
19	BQ	190/210 (90%)	190 (100%)	0	100	100
20	BR	132/143 (92%)	131 (99%)	1 (1%)	79	84
21	BS	123/153 (80%)	122 (99%)	1 (1%)	79	84
22	BT	208/258 (81%)	207 (100%)	1 (0%)	86	90
23	BU	118/127 (93%)	118 (100%)	0	100	100
24	BV	136/178 (76%)	135 (99%)	1 (1%)	81	86
25	BW	144/180 (80%)	144 (100%)	0	100	100
26	BX	116/134 (87%)	116 (100%)	0	100	100
27	BY	185/192 (96%)	182 (98%)	3 (2%)	58	73
28	Ba	348/365 (95%)	346 (99%)	2 (1%)	84	88
29	Bb	310/328 (94%)	307 (99%)	3 (1%)	73	81
30	Bc	271/299 (91%)	270 (100%)	1 (0%)	89	91
31	Bd	130/181 (72%)	129 (99%)	1 (1%)	79	84
32	Be	100/108 (93%)	100 (100%)	0	100	100
33	Bf	80/133 (60%)	80 (100%)	0	100	100
34	Bg	128/136 (94%)	125 (98%)	3 (2%)	45	64
35	Bh	251/284 (88%)	249 (99%)	2 (1%)	79	84
36	B8	87/162 (54%)	86 (99%)	1 (1%)	70	79
37	Bi	236/275 (86%)	233 (99%)	3 (1%)	65	76
38	Bj	201/242 (83%)	192 (96%)	9 (4%)	23	48
39	Bk	144/226 (64%)	140 (97%)	4 (3%)	38	59
40	Bl	122/147 (83%)	121 (99%)	1 (1%)	79	84
41	Bm	103/178 (58%)	103 (100%)	0	100	100
42	Bn	88/113 (78%)	87 (99%)	1 (1%)	70	79
43	Bo	77/97 (79%)	77 (100%)	0	100	100
44	Bp	79/88 (90%)	78 (99%)	1 (1%)	65	76
45	Bq	70/114 (61%)	67 (96%)	3 (4%)	25	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Bt	75/82 (92%)	75 (100%)	0	100	100
47	Bu	126/177 (71%)	126 (100%)	0	100	100
48	Bv	115/183 (63%)	115 (100%)	0	100	100
49	Bw	340/373 (91%)	338 (99%)	2 (1%)	84	88
50	Bx	149/173 (86%)	146 (98%)	3 (2%)	50	68
52	B9	36/77 (47%)	35 (97%)	1 (3%)	38	59
54	AB	187/233 (80%)	186 (100%)	1 (0%)	86	90
55	AC	115/142 (81%)	114 (99%)	1 (1%)	75	83
56	AE	282/351 (80%)	274 (97%)	8 (3%)	38	59
57	AF	107/210 (51%)	106 (99%)	1 (1%)	75	83
58	AG	181/205 (88%)	178 (98%)	3 (2%)	56	72
59	AI	273/333 (82%)	268 (98%)	5 (2%)	54	71
60	AJ	130/180 (72%)	129 (99%)	1 (1%)	79	84
61	AK	103/151 (68%)	103 (100%)	0	100	100
62	AL	92/116 (79%)	92 (100%)	0	100	100
63	AN	92/114 (81%)	92 (100%)	0	100	100
64	AO	159/205 (78%)	158 (99%)	1 (1%)	84	88
65	AP	97/113 (86%)	96 (99%)	1 (1%)	73	81
66	AQ	97/114 (85%)	97 (100%)	0	100	100
67	AR	89/127 (70%)	88 (99%)	1 (1%)	70	79
68	AU	77/78 (99%)	76 (99%)	1 (1%)	65	76
70	Aa	258/330 (78%)	255 (99%)	3 (1%)	67	78
71	Ab	113/162 (70%)	112 (99%)	1 (1%)	75	83
72	Ac	152/155 (98%)	147 (97%)	5 (3%)	33	56
73	Ad	149/168 (89%)	147 (99%)	2 (1%)	65	76
74	Ae	325/393 (83%)	322 (99%)	3 (1%)	75	83
75	Af	86/160 (54%)	84 (98%)	2 (2%)	45	64
76	Ag	312/361 (86%)	309 (99%)	3 (1%)	73	81
77	Ah	109/346 (32%)	105 (96%)	4 (4%)	29	53
78	Ai	86/93 (92%)	86 (100%)	0	100	100
79	Aj	188/190 (99%)	187 (100%)	1 (0%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	Ak	249/289 (86%)	248 (100%)	1 (0%)	89	91
81	Am	100/102 (98%)	99 (99%)	1 (1%)	73	81
82	An	66/174 (38%)	66 (100%)	0	100	100
83	Ao	478/541 (88%)	472 (99%)	6 (1%)	65	76
84	Ap	170/225 (76%)	170 (100%)	0	100	100
85	CL	30/157 (19%)	30 (100%)	0	100	100
85	DL	26/157 (17%)	26 (100%)	0	100	100
85	EL	27/157 (17%)	27 (100%)	0	100	100
85	FL	26/157 (17%)	26 (100%)	0	100	100
85	GL	26/157 (17%)	26 (100%)	0	100	100
85	HL	24/157 (15%)	24 (100%)	0	100	100
All	All	12498/16513 (76%)	12376 (99%)	122 (1%)	71	81

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	Bq	66	PHE
77	Ah	284	ARG
56	AE	188	LYS
77	Ah	276	LYS
83	Ao	407	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
49	Bw	352	GLN
59	AI	156	GLN
59	AI	139	GLN
59	AI	327	HIS
14	BJ	151	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	AA	959/962 (99%)	169 (17%)	0
53	BA	1542/1571 (98%)	411 (26%)	2 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	BB	64/73 (87%)	17 (26%)	0
86	AV	70/71 (98%)	24 (34%)	3 (4%)
86	AY	70/71 (98%)	24 (34%)	3 (4%)
87	AX	5/6 (83%)	5 (100%)	0
All	All	2710/2754 (98%)	650 (23%)	8 (0%)

5 of 650 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	BB	3	U
8	BB	5	A
8	BB	7	G
8	BB	8	U
8	BB	9	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
86	AY	70	C
86	AY	69	C
86	AV	70	C
86	AV	69	C
86	AY	43	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 335 ligands modelled in this entry, 330 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
90	SPM	BA	1792	-	13,13,13	0.33	0	12,12,12	0.79	0
90	SPM	AA	3001	-	13,13,13	0.34	0	12,12,12	0.79	0
90	SPM	BA	1793	-	13,13,13	0.34	0	12,12,12	0.79	0
92	GTP	Ag	500	88	26,34,34	1.12	2 (7%)	32,54,54	1.65	7 (21%)
91	5GP	BA	1791	88	22,26,26	1.24	2 (9%)	26,40,40	1.24	4 (15%)

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
90	SPM	BA	1792	-	-	3/11/11/11	-
90	SPM	AA	3001	-	-	2/11/11/11	-
90	SPM	BA	1793	-	-	4/11/11/11	-
92	GTP	Ag	500	88	-	0/18/38/38	0/3/3/3
91	5GP	BA	1791	88	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	BA	1791	5GP	C5-C6	-4.10	1.39	1.47
92	Ag	500	GTP	C5-C6	-3.99	1.39	1.47
91	BA	1791	5GP	C6-N1	-2.49	1.34	1.37
92	Ag	500	GTP	C2-N3	2.20	1.38	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	Ag	500	GTP	PA-O3A-PB	-4.07	118.85	132.83
92	Ag	500	GTP	PB-O3B-PG	-3.78	119.85	132.83
92	Ag	500	GTP	C5-C6-N1	3.28	119.74	113.95
92	Ag	500	GTP	C3'-C2'-C1'	3.26	105.89	100.98
91	BA	1791	5GP	C5-C6-N1	3.07	119.38	113.95

There are no chirality outliers.

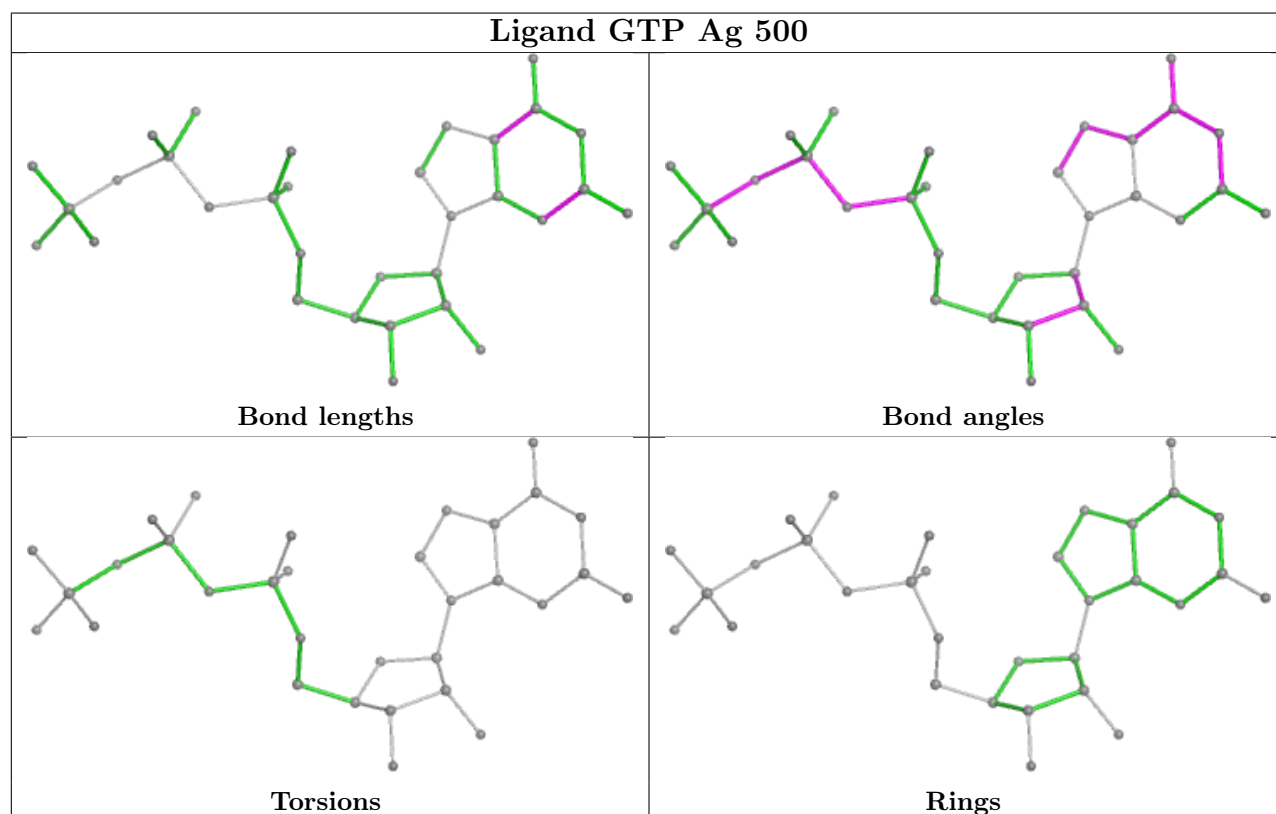
5 of 9 torsion outliers are listed below:

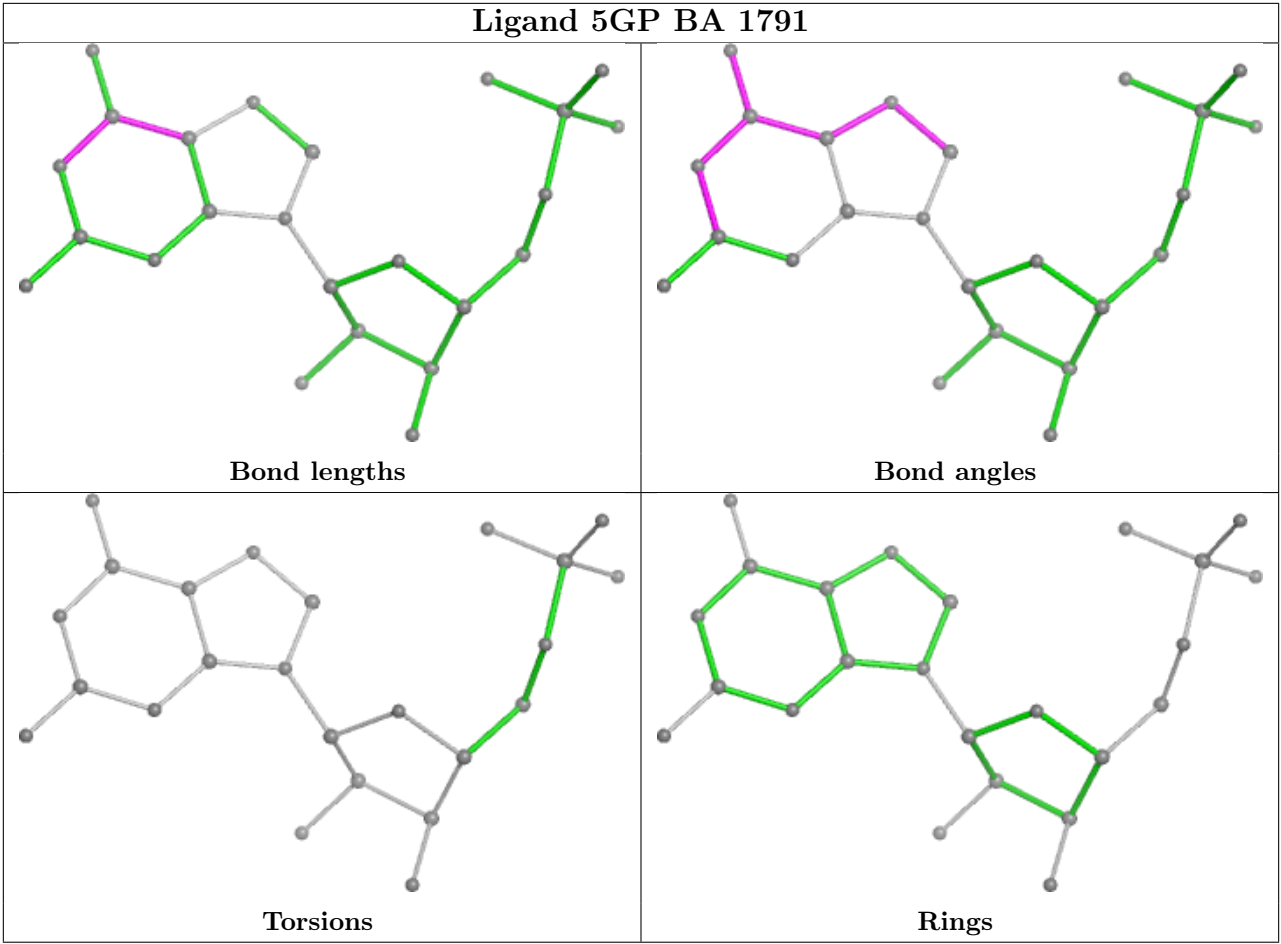
Mol	Chain	Res	Type	Atoms
90	BA	1793	SPM	N5-C6-C7-C8
90	AA	3001	SPM	C8-C9-N10-C11
90	BA	1792	SPM	C7-C8-C9-N10
90	BA	1793	SPM	C8-C9-N10-C11
90	BA	1793	SPM	C7-C8-C9-N10

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
83	Ao	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ao	234:UNK	C	240:THR	N	8.00

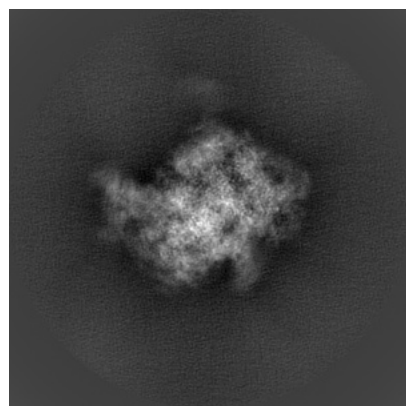
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12569. These allow visual inspection of the internal detail of the map and identification of artifacts.

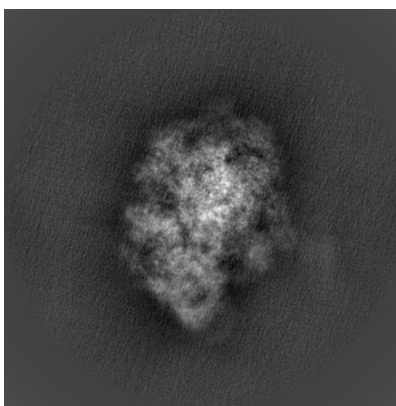
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

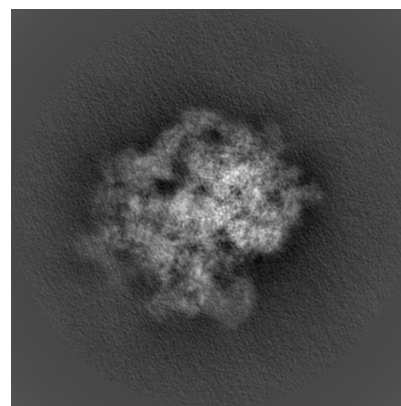
6.1.1 Primary map



X

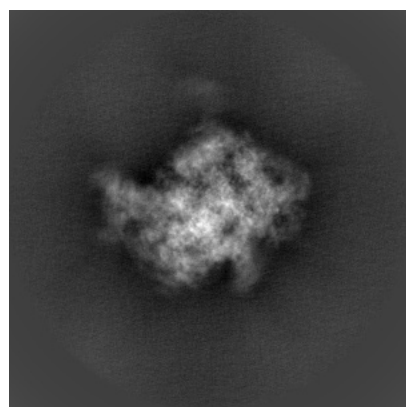


Y

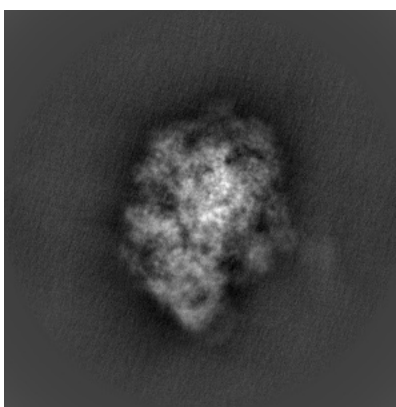


Z

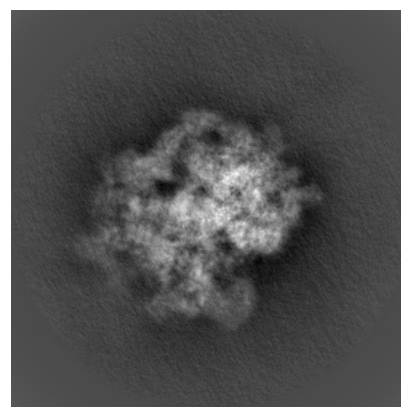
6.1.2 Raw map



X



Y

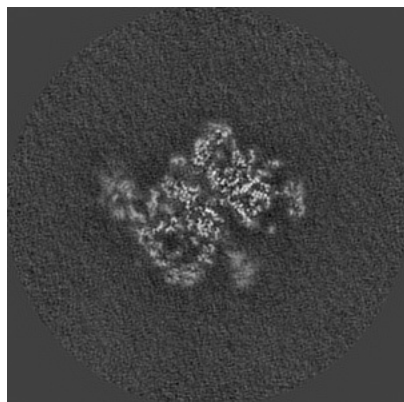


Z

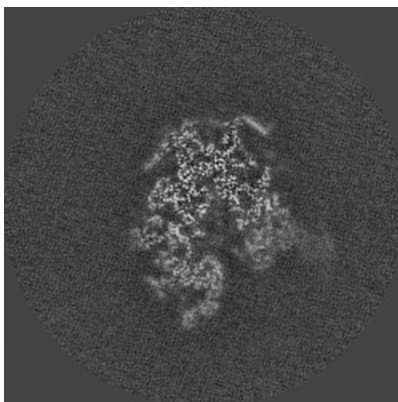
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

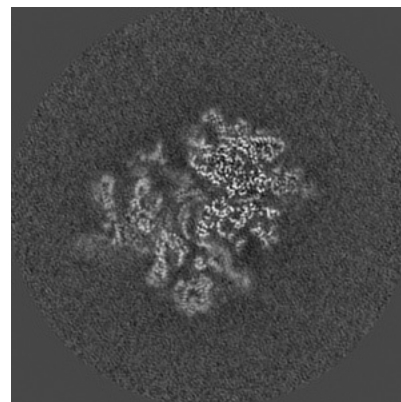
6.2.1 Primary map



X Index: 240

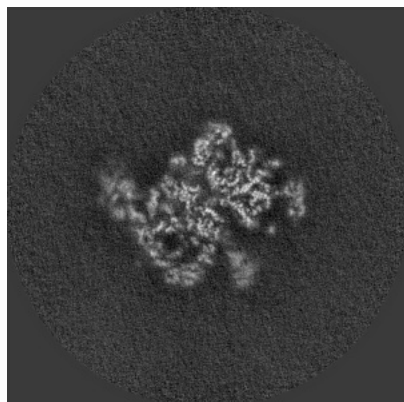


Y Index: 240

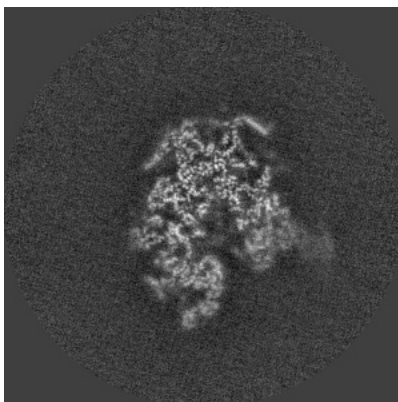


Z Index: 240

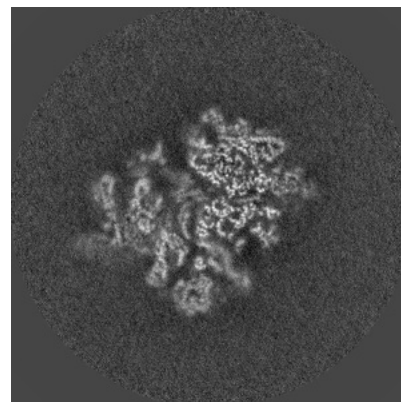
6.2.2 Raw map



X Index: 240



Y Index: 240

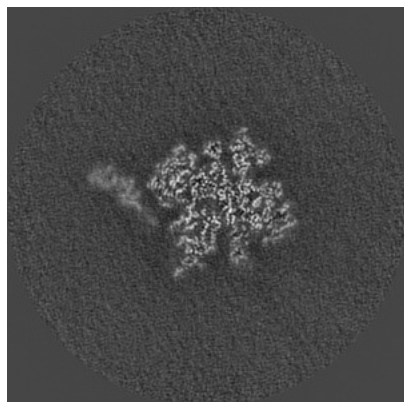


Z Index: 240

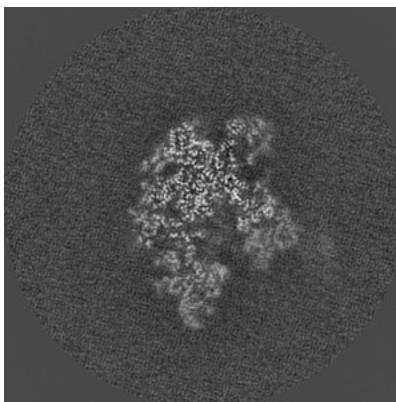
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

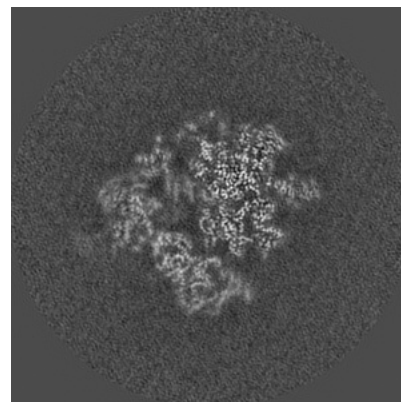
6.3.1 Primary map



X Index: 270

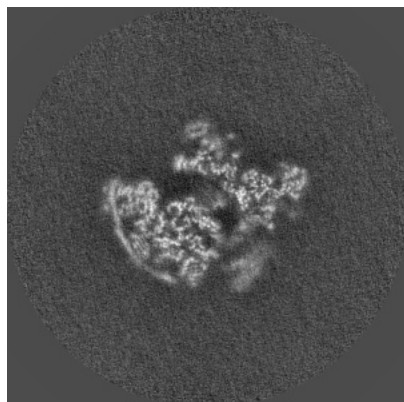


Y Index: 235

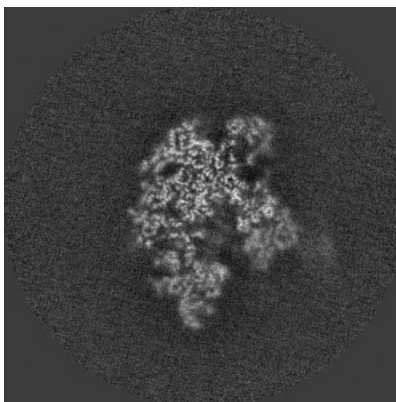


Z Index: 249

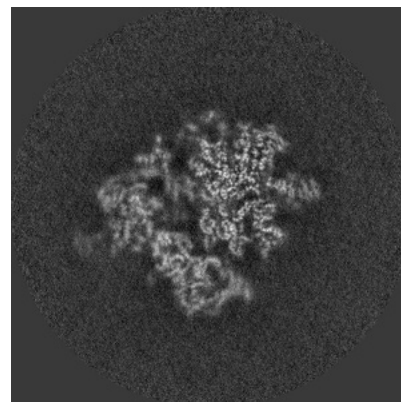
6.3.2 Raw map



X Index: 227



Y Index: 235

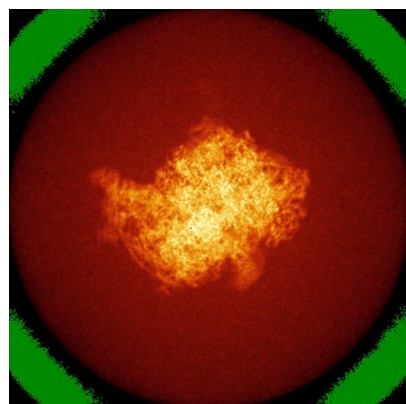


Z Index: 248

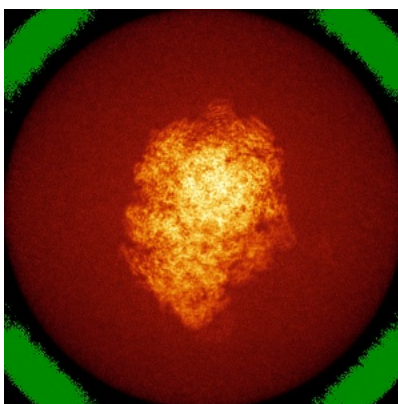
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

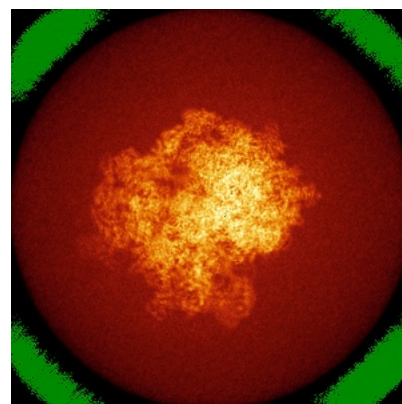
6.4.1 Primary map



X

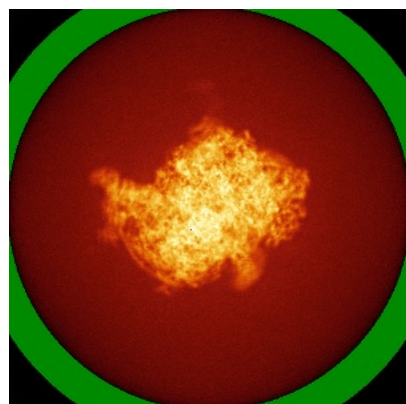


Y

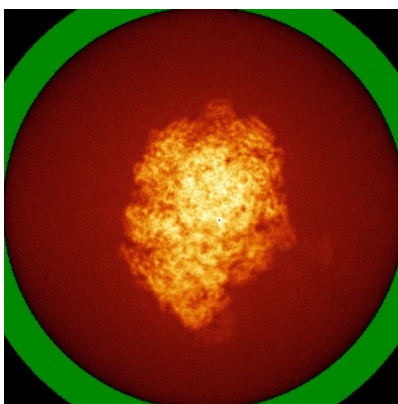


Z

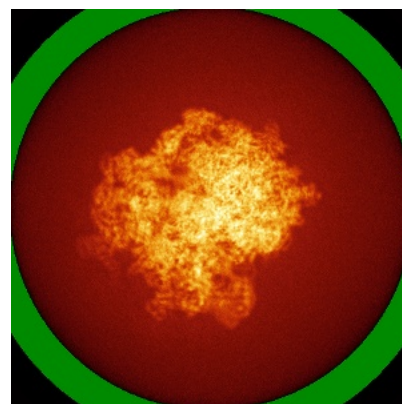
6.4.2 Raw map



X



Y

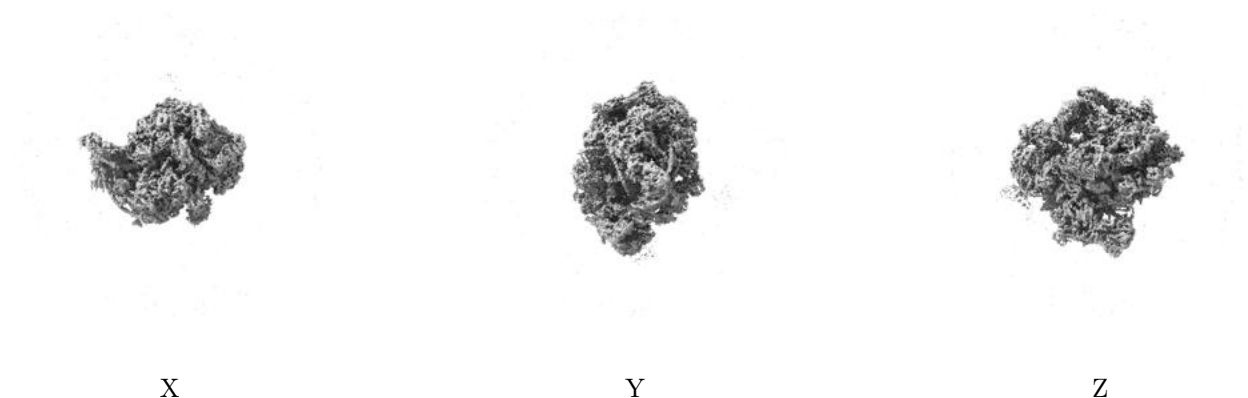


Z

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.

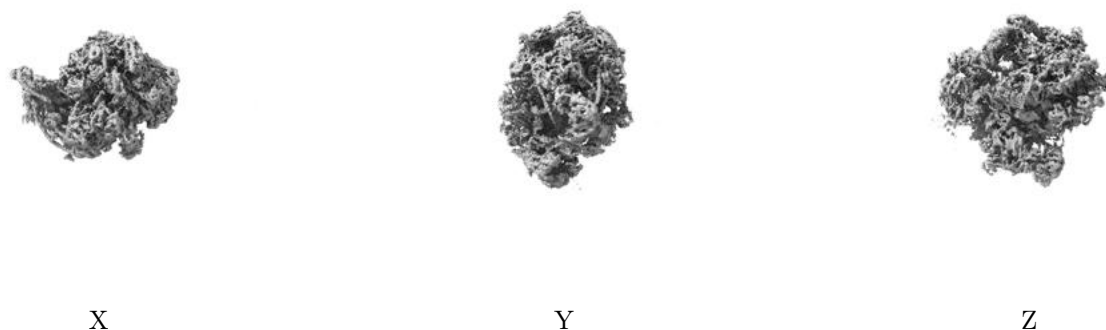
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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



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.

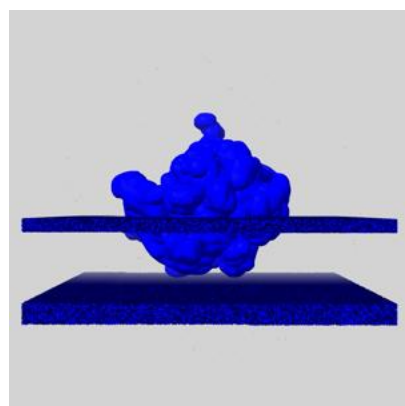
6.6 Mask visualisation [i](#)

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

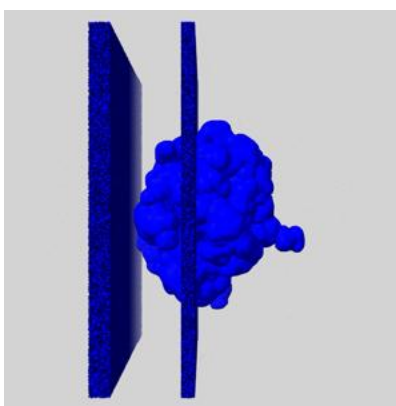
A mask typically either:

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

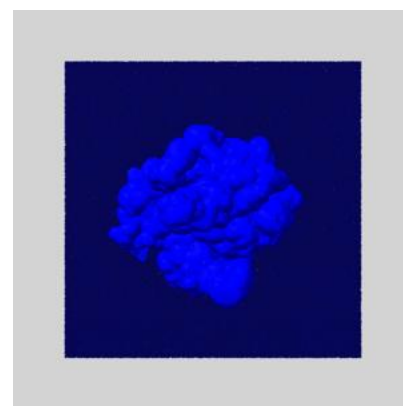
6.6.1 emd_12569_msk_1.map [i](#)



X



Y

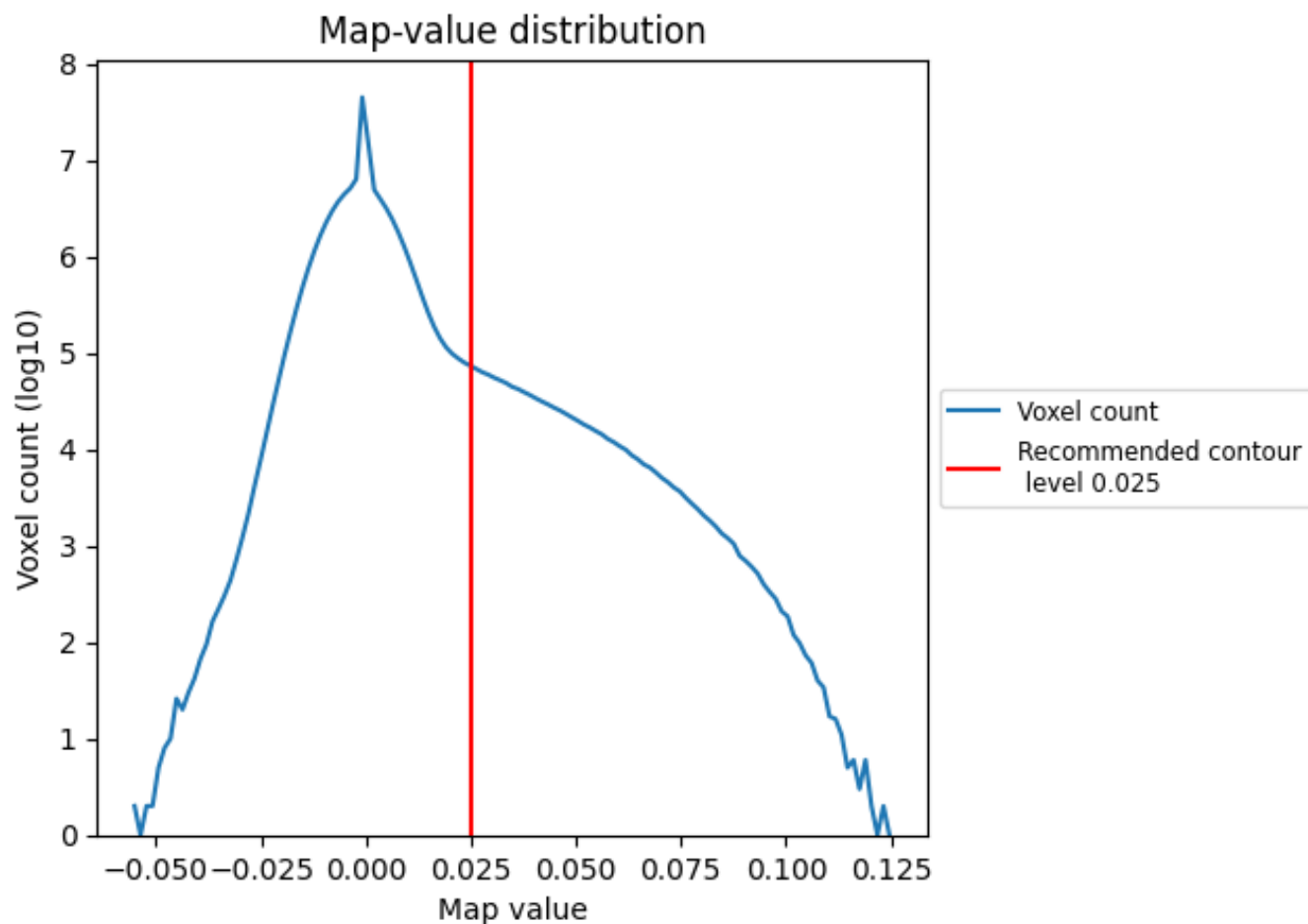


Z

7 Map analysis [i](#)

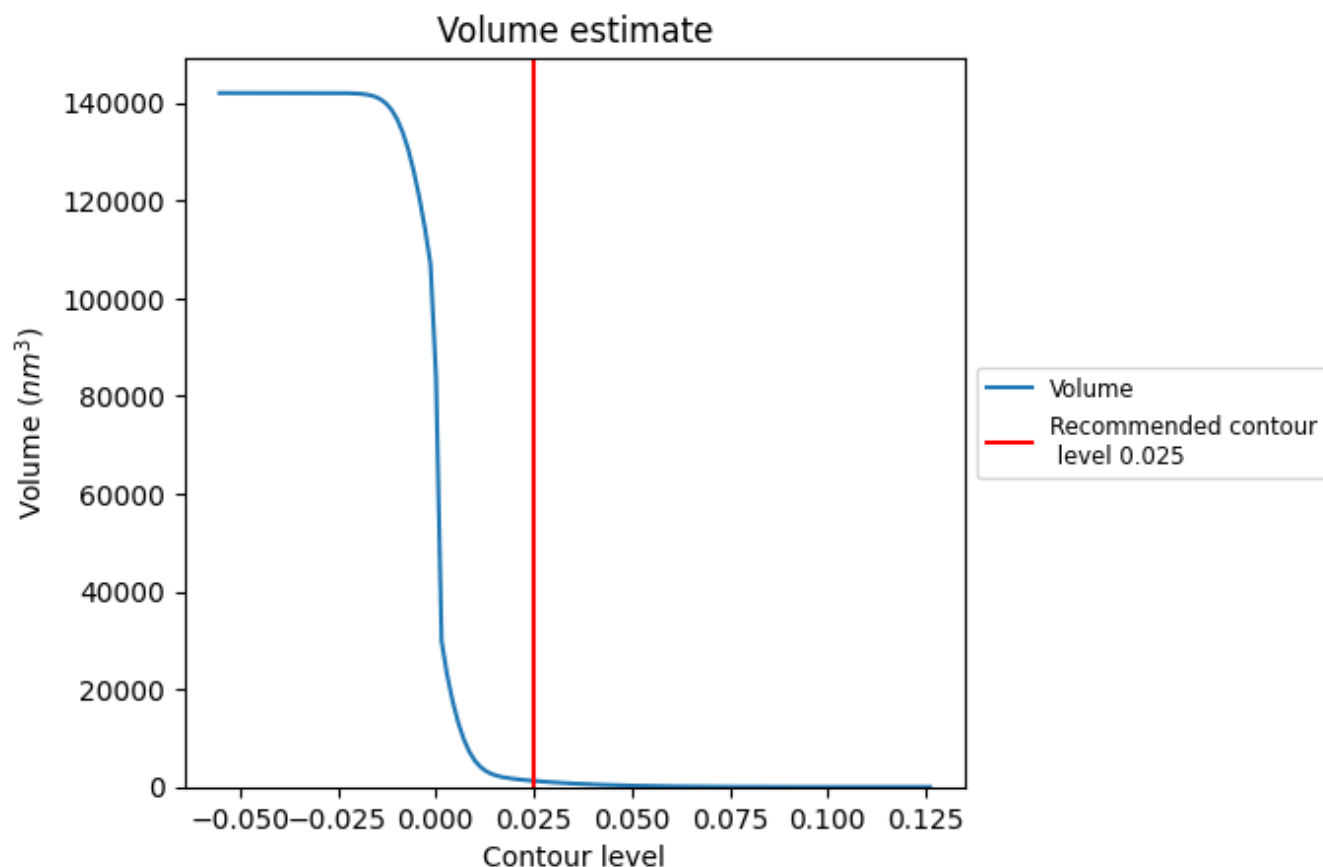
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

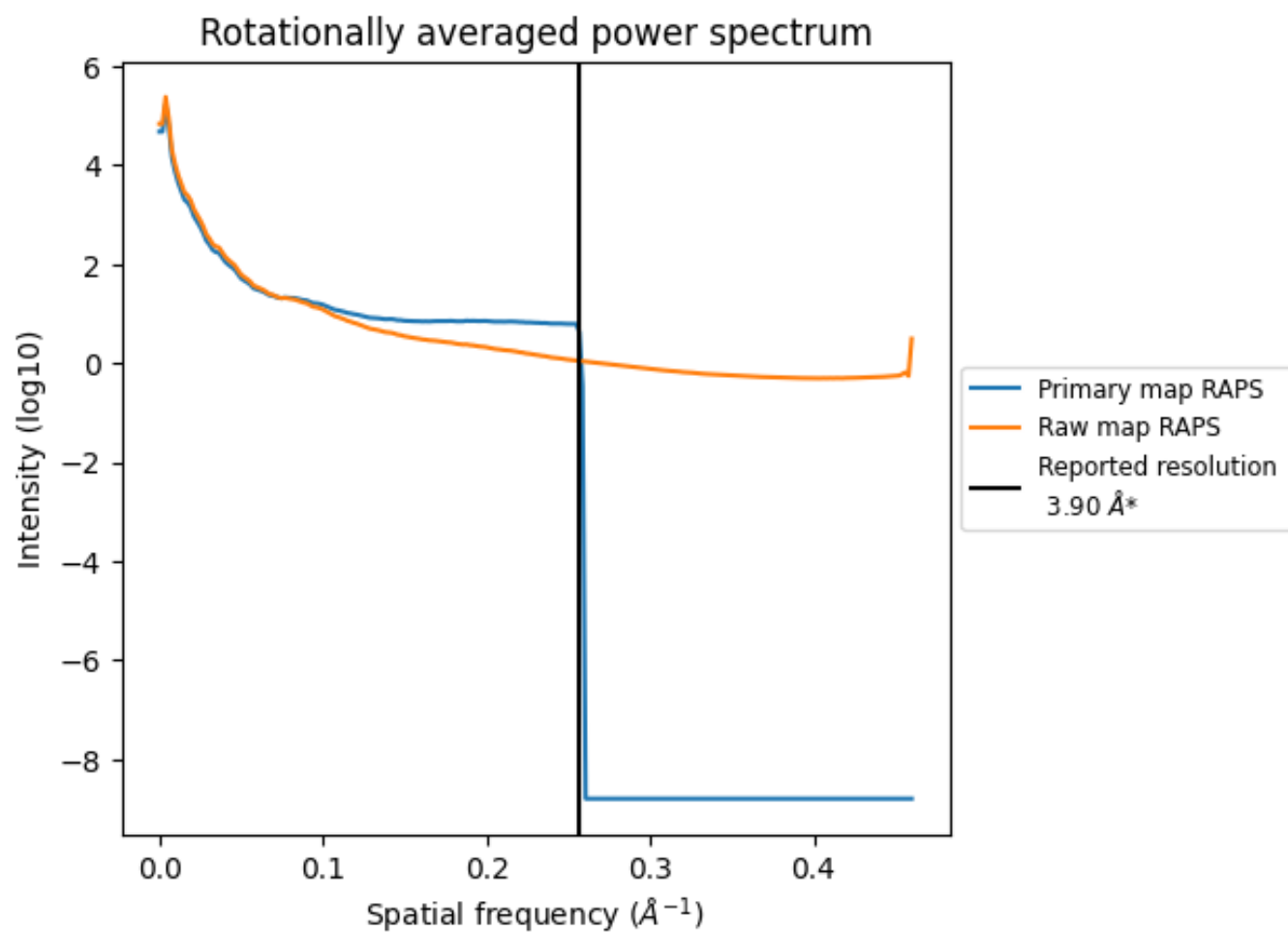
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1243 nm^3 ; this corresponds to an approximate mass of 1123 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 ⓘ

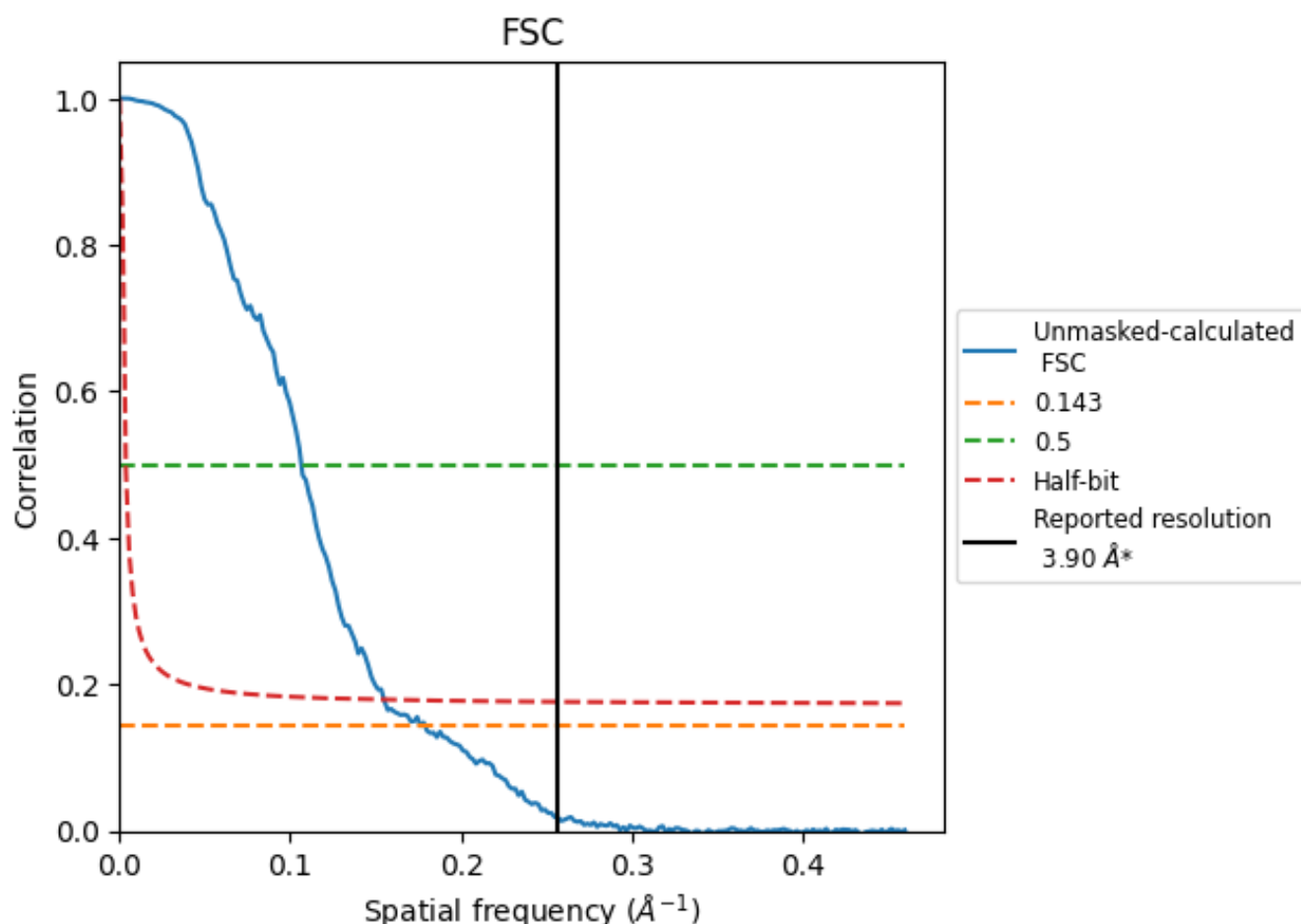


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

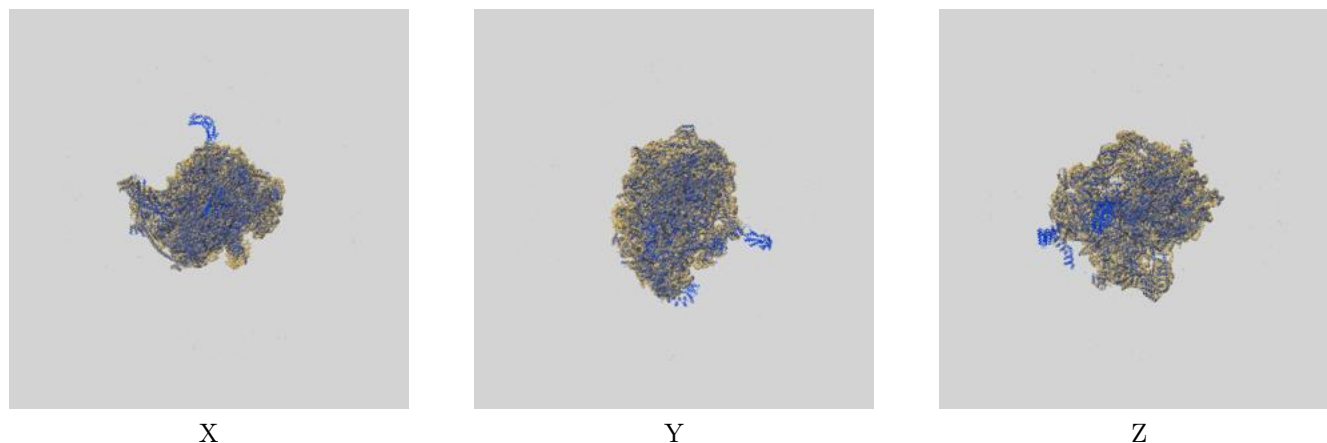
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.59	9.38	6.45

*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 5.59 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

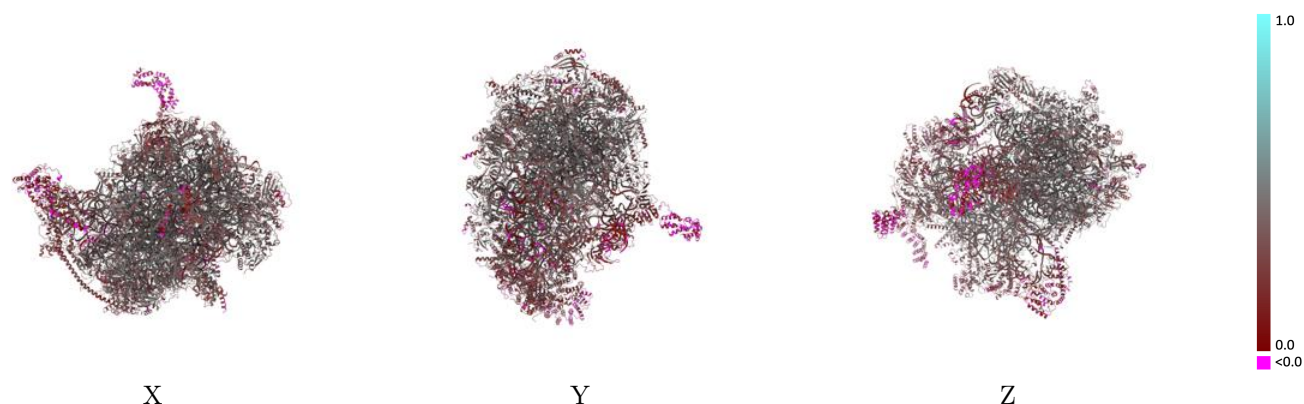
This section contains information regarding the fit between EMDB map EMD-12569 and PDB model 7NSJ. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



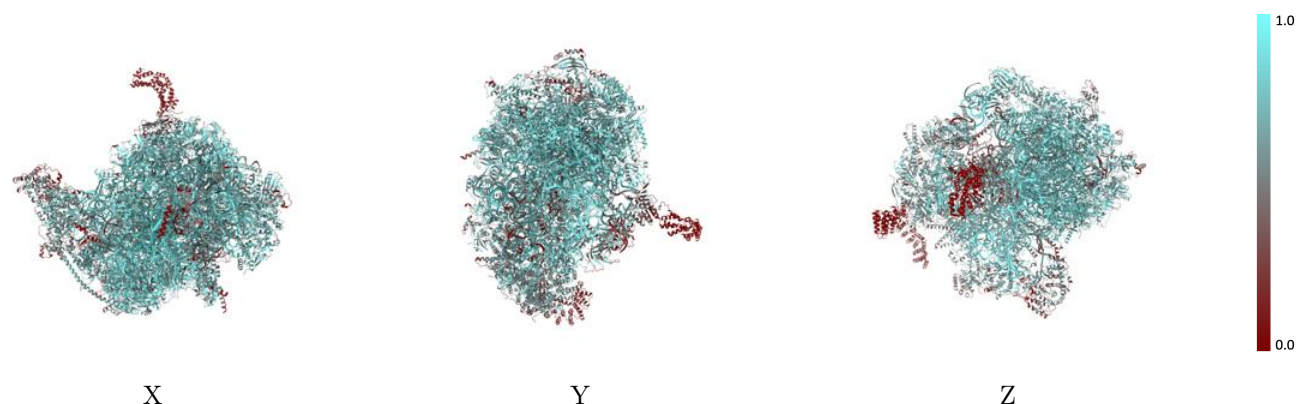
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



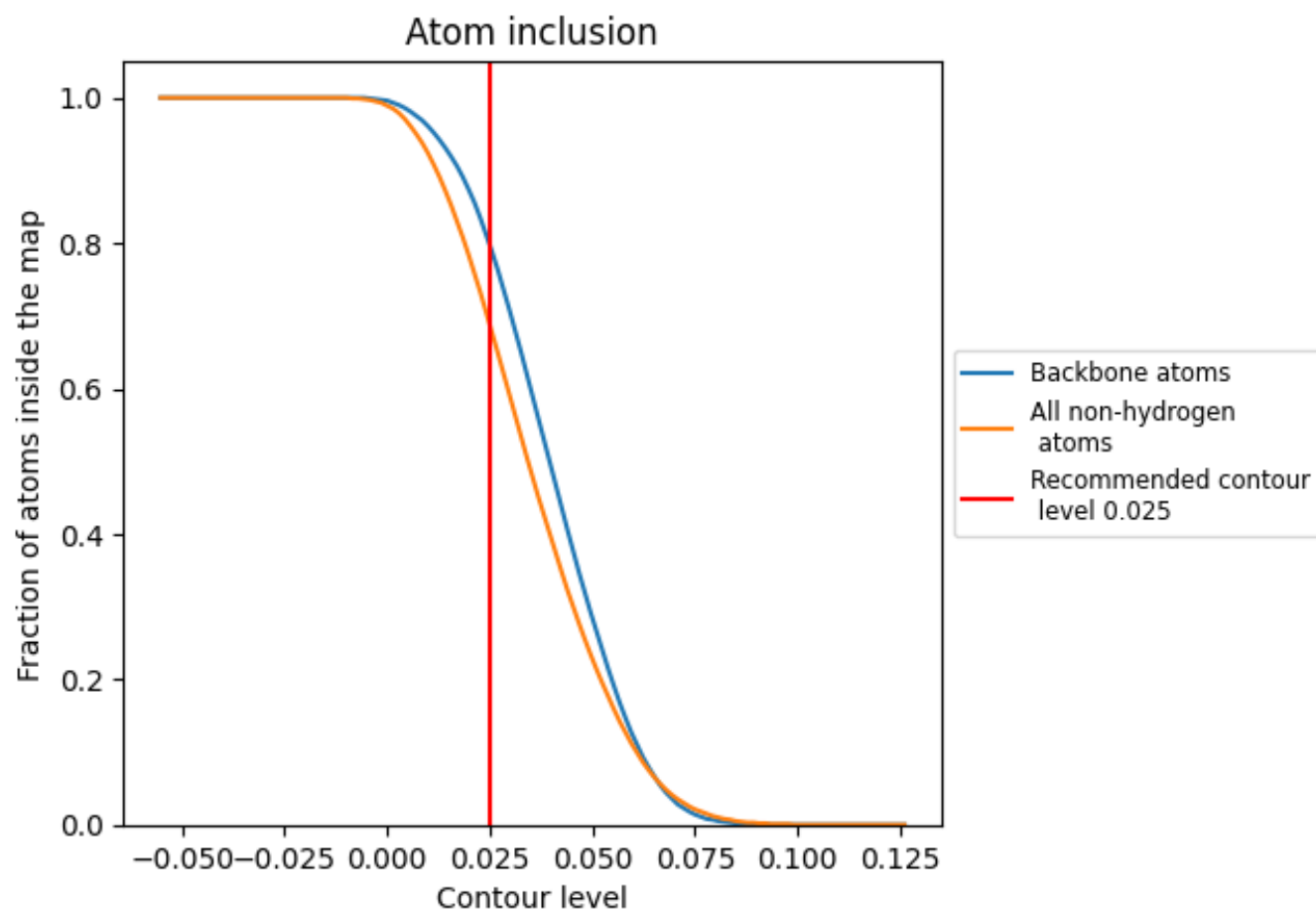
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6890	 0.3450
AA	 0.8720	 0.3700
AB	 0.6740	 0.3490
AC	 0.5700	 0.3490
AE	 0.5580	 0.3480
AF	 0.6910	 0.3910
AG	 0.5900	 0.3050
AI	 0.5980	 0.3020
AJ	 0.5890	 0.3180
AK	 0.6920	 0.3760
AL	 0.6560	 0.3840
AN	 0.6670	 0.3370
AO	 0.6170	 0.3420
AP	 0.5960	 0.2780
AQ	 0.6780	 0.3780
AR	 0.6750	 0.3800
AU	 0.6920	 0.3870
AV	 0.5960	 0.2780
AX	 0.6920	 0.3360
AY	 0.3010	 0.0800
AZ	 0.6330	 0.2350
Aa	 0.4910	 0.2570
Ab	 0.5430	 0.2920
Ac	 0.6630	 0.3500
Ad	 0.6400	 0.2650
Ae	 0.4210	 0.1380
Af	 0.6030	 0.3480
Ag	 0.5990	 0.2610
Ah	 0.4850	 0.2420
Ai	 0.5760	 0.3020
Aj	 0.5250	 0.2310
Ak	 0.5650	 0.2670
Am	 0.5710	 0.3140
An	 0.6590	 0.3810
Ao	 0.1080	 0.1160





































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Chain	Atom inclusion	Q-score
Ap	 0.5980	 0.2810
B0	 0.8010	 0.4490
B1	 0.6800	 0.3780
B2	 0.7470	 0.3850
B3	 0.7580	 0.4190
B4	 0.6790	 0.3270
B5	 0.7430	 0.4090
B6	 0.6030	 0.3360
B7	 0.7940	 0.4530
B8	 0.7570	 0.4400
B9	 0.8070	 0.4330
BA	 0.8720	 0.4050
BB	 0.7130	 0.2380
BD	 0.7530	 0.4320
BE	 0.7400	 0.4130
BF	 0.7290	 0.4150
BI	 0.6210	 0.3400
BJ	 0.3270	 0.2160
BK	 0.2280	 0.1670
BN	 0.7520	 0.4200
BO	 0.7150	 0.4180
BP	 0.7570	 0.4140
BQ	 0.7290	 0.4130
BR	 0.7520	 0.4250
BS	 0.7430	 0.3870
BT	 0.7060	 0.3910
BU	 0.7200	 0.4140
BV	 0.7190	 0.4110
BW	 0.7250	 0.4400
BX	 0.6990	 0.3970
BY	 0.5530	 0.3520
Ba	 0.7680	 0.3960
Bb	 0.7550	 0.3640
Bc	 0.6910	 0.3480
Bd	 0.5480	 0.2540
Be	 0.6650	 0.3550
Bf	 0.6670	 0.3660
Bg	 0.7490	 0.4200
Bh	 0.6990	 0.3630
Bi	 0.4960	 0.2980
Bj	 0.5420	 0.1900
Bk	 0.5420	 0.2950

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Chain	Atom inclusion	Q-score
Bl	 0.7830	 0.4140
Bm	 0.3810	 0.3000
Bn	 0.7520	 0.4350
Bo	 0.7320	 0.3810
Bp	 0.3740	 0.2330
Bq	 0.3100	 0.2450
Bt	 0.7880	 0.4190
Bu	 0.5900	 0.3200
Bv	 0.6160	 0.3020
Bw	 0.7520	 0.3930
Bx	 0.7190	 0.3730
CL	 0.0000	 0.0240
DL	 0.0000	 0.0300
EL	 0.0000	 0.0390
FL	 0.0050	 0.0480
GL	 0.0000	 0.0060
HL	 0.0000	 0.0140