



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 11:08 AM UTC

PDB ID : 6VLZ / pdb_00006vlz
EMDB ID : EMD-21233
Title : Structure of the human mitochondrial ribosome-EF-G1 complex (ClassI)
Authors : Sharma, M.R.; Koripella, R.K.; Agrawal, R.K.
Deposited on : 2020-01-27
Resolution : 2.97 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:

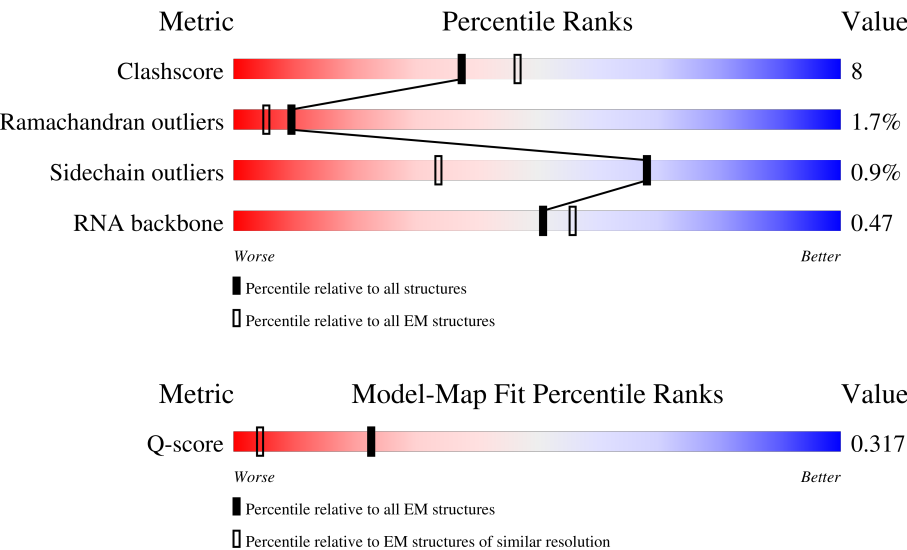
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.97 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13205 (2.47 - 3.47)

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	AA	954	
2	AB	296	
3	AC	167	

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Mol	Chain	Length	Quality of chain
4	AE	125	
5	AI	194	
6	AJ	138	
7	AK	128	
8	AM	137	
9	AN	130	
10	AO	258	
11	AP	142	
12	AQ	87	
13	AT	173	
14	AW	187	
15	AX	398	
16	A2	118	
17	AH	201	
18	AL	257	
19	AR	360	
20	AS	190	
21	AU	205	
22	AV	414	
23	AY	395	
24	AZ	106	
25	A1	323	
26	A0	218	
27	A3	199	
28	A4	689	

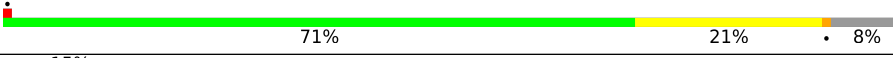
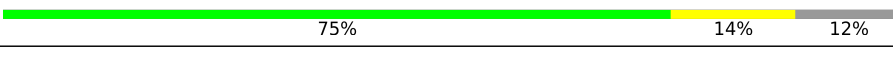
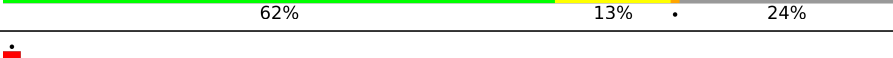
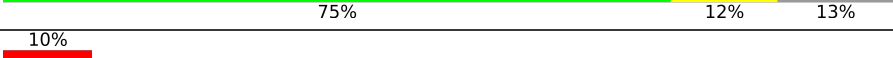
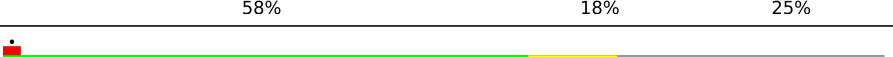
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Mol	Chain	Length	Quality of chain
29	AD	430	
30	AF	242	
31	AG	396	
32	A	1559	
33	B	73	
34	D	305	
35	F	311	
36	H	267	
37	K	178	
38	L	145	
39	M	296	
40	O	175	
41	R	149	
42	S	205	
43	T	212	
44	W	148	
45	X	256	
46	Y	250	
47	Z	161	
48	0	188	
49	1	65	
50	2	92	
51	3	188	
52	4	103	
53	8	206	

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Mol	Chain	Length	Quality of chain
54	b	155	
55	e	279	
56	g	166	
57	i	128	
58	j	123	
59	m	128	
60	o	102	
61	q	222	
62	r	196	
63	J	192	
64	I	261	
65	N	251	
66	P	179	
67	U	153	
68	V	216	
69	E	348	
70	5	423	
71	6	380	
72	7	338	
73	9	137	
74	a	142	
75	c	332	
76	d	306	
77	f	194	
78	h	158	

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Mol	Chain	Length	Quality of chain
79	k	112	
80	l	138	
81	p	206	
82	s	439	
83	Q	292	
84	TA	198	
84	TB	198	
84	TC	198	
85	u	65	
86	v	751	
87	A5	11	
88	A7	71	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	Y5P	A5	1	-	-	X	-
88	P5P	A7	1	-	-	X	-
92	GCP	v	802	-	-	X	-

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 174849 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 RNA chain called 12s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	944	Total	C	N	O	P	0	0
			20030	8980	3612	6494	944		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	220	Total	C	N	O	S	0	0
			1787	1141	324	312	10		

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

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

- Molecule 4 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 5 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 6 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 7 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 8 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 9 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 10 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AO	190	Total	C	N	O	S	0	0
			1570	998	291	274	7		

- Molecule 11 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 12 is a protein called 28S ribosomal protein S21, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 13 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 14 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 15 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AX	353	Total	C	N	O	S	0	0
			2860	1828	503	518	11		

- Molecule 16 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A2	116	Total	C	N	O	S	0	0
			925	574	181	162	8		

- Molecule 17 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AH	122	Total	C	N	O	S	0	0
			1014	656	172	183	3		

- Molecule 18 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AL	174	Total	C	N	O	S	0	0
			1451	924	271	249	7		

- Molecule 19 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AR	292	Total	C	N	O	S	0	0
			2388	1521	410	449	8		

- Molecule 20 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	177	Total	C	N	O	S	0	0
			1499	922	305	268	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	367	Total	C	N	O	S	0	0
			3009	1931	502	564	12		

- Molecule 23 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AY	120	Total	C	N	O	S	0	0
			1016	657	167	190	2		

- Molecule 24 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AZ	99	Total	C	N	O	S	0	0
			833	531	152	146	4		

- Molecule 25 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A1	275	Total	C	N	O	S	0	0
			2231	1414	380	426	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A0	214	Total	C	N	O	S	0	0
			1781	1125	341	310	5		

- Molecule 27 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A3	72	Total	C	N	O	S	0	0
			639	409	137	92	1		

- Molecule 28 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A4	549	Total	C	N	O	S	0	0
			3010	1841	573	593	3		

- Molecule 29 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AD	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 30 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AF	208	Total	C	N	O	S	0	0
			1724	1103	312	298	11		

- Molecule 31 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AG	315	Total	C	N	O	S	0	0
			2587	1640	462	471	14		

- Molecule 32 is a RNA chain called 16s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A	1527	Total	C	N	O	P	0	0
			32395	14536	5844	10488	1527		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	C	conflict	GB 1616239084

- Molecule 33 is a RNA chain called tRNA^{Val}.

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

- Molecule 34 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D	239	Total	C	N	O	S	0	0
			1866	1162	377	318	9		

- Molecule 35 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	H	98	Total	C	N	O		0	0
			806	510	156	140			

- Molecule 37 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L14, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L28, mitochondrial.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 46 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 48 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 49 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 50 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 51 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 52 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 53 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 54 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 55 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 56 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	g	132	Total	C	N	O	S	0	0
			1096	709	191	194	2		

- Molecule 57 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 58 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	j	93	Total	C	N	O	S	0	0
			740	460	143	135	2		

- Molecule 59 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 60 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 61 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	q	168	Total	C	N	O	S	0	0
			1294	801	255	233	5		

- Molecule 62 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 63 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	J	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 64 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	I	179	Total	C	N	O	S	0	0
			1435	925	258	242	10		

- Molecule 65 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 66 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	P	143	Total	C	N	O	S	0	0
			1165	729	223	208	5		

- Molecule 67 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	U	152	Total	C	N	O	S	0	0
			1224	774	233	214	3		

- Molecule 68 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	V	206	Total	C	N	O	S	0	0
			1682	1071	299	304	8		

- Molecule 69 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	E	306	Total	C	N	O	S	0	0
			2410	1547	419	433	11		

- Molecule 70 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 71 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 72 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	7	297	Total	C	N	O	S	0	0
			2410	1540	409	443	18		

- Molecule 73 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 74 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	a	108	Total	C	N	O	S	0	0
			896	560	162	169	5		

- Molecule 75 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	c	289	Total	C	N	O	S	0	0
			2322	1483	400	430	9		

- Molecule 76 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	d	257	Total	C	N	O	S	0	0
			2075	1326	363	372	14		

- Molecule 77 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	f	146	Total	C	N	O	S	0	0
			1126	714	186	222	4		

- Molecule 78 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	h	110	Total	C	N	O	S	0	0
			894	568	156	167	3		

- Molecule 79 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	k	96	Total	C	N	O	S	0	0
			743	462	143	133	5		

- Molecule 80 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	l	72	Total	C	N	O	S	0	0
			619	394	112	111	2		

- Molecule 81 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	p	152	Total	C	N	O	S	0	0
			1227	762	232	229	4		

- Molecule 82 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	s	393	Total	C	N	O	S	0	0
			3178	2036	565	563	14		

- Molecule 83 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Q	240	Total	C	N	O	S	0	0
			1995	1280	354	352	9		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
84	TA	45	Total	C	N	O	0	0
			345	222	54	69		
84	TB	27	Total	C	N	O	0	0
			213	137	33	43		
84	TC	71	Total	C	N	O	0	0
			352	210	71	71		

- Molecule 85 is a protein called P-site finger.

Mol	Chain	Residues	Atoms				AltConf	Trace
85	u	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 86 is a protein called Elongation factor G, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	v	712	Total	C	N	O	S	0	0
			5546	3494	957	1062	33		

- Molecule 87 is a DNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	A5	11	Total	C	N	O	P	0	0
			213	104	32	66	11		

- Molecule 88 is a DNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	A7	62	Total	C	N	O	P	0	0
			1197	586	180	370	61		

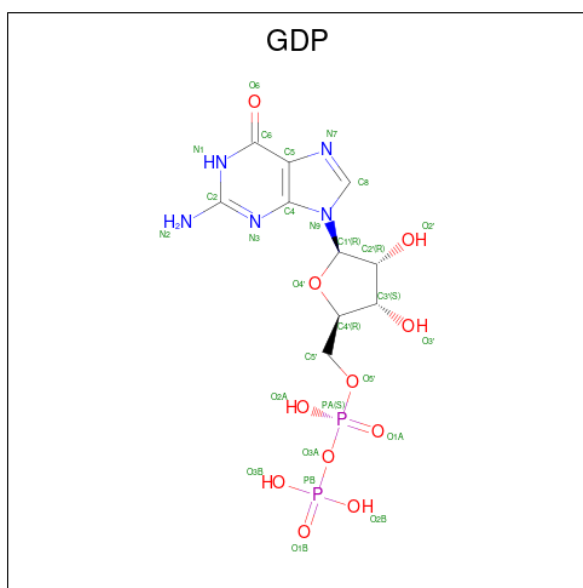
- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	AA	26	Total	Mg	0
			26	26	
89	A2	1	Total	Mg	0
			1	1	
89	AH	1	Total	Mg	0
			1	1	
89	A	97	Total	Mg	0
			97	97	
89	D	1	Total	Mg	0
			1	1	
89	W	1	Total	Mg	0
			1	1	
89	g	1	Total	Mg	0
			1	1	
89	E	1	Total	Mg	0
			1	1	
89	v	1	Total	Mg	0
			1	1	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

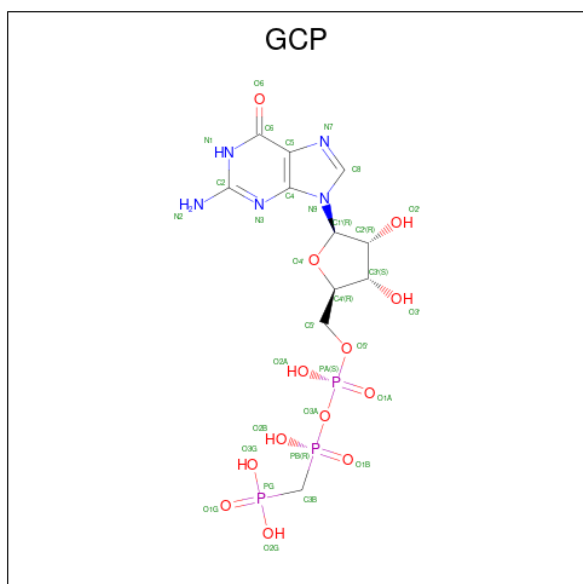
Mol	Chain	Residues	Atoms		AltConf
90	AB	1	Total	Zn	0
			1	1	
90	AO	1	Total	Zn	0
			1	1	
90	AP	1	Total	Zn	0
			1	1	
90	AT	1	Total	Zn	0
			1	1	
90	0	1	Total	Zn	0
			1	1	
90	4	1	Total	Zn	0
			1	1	
90	r	1	Total	Zn	0
			1	1	

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



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

- Molecule 92 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

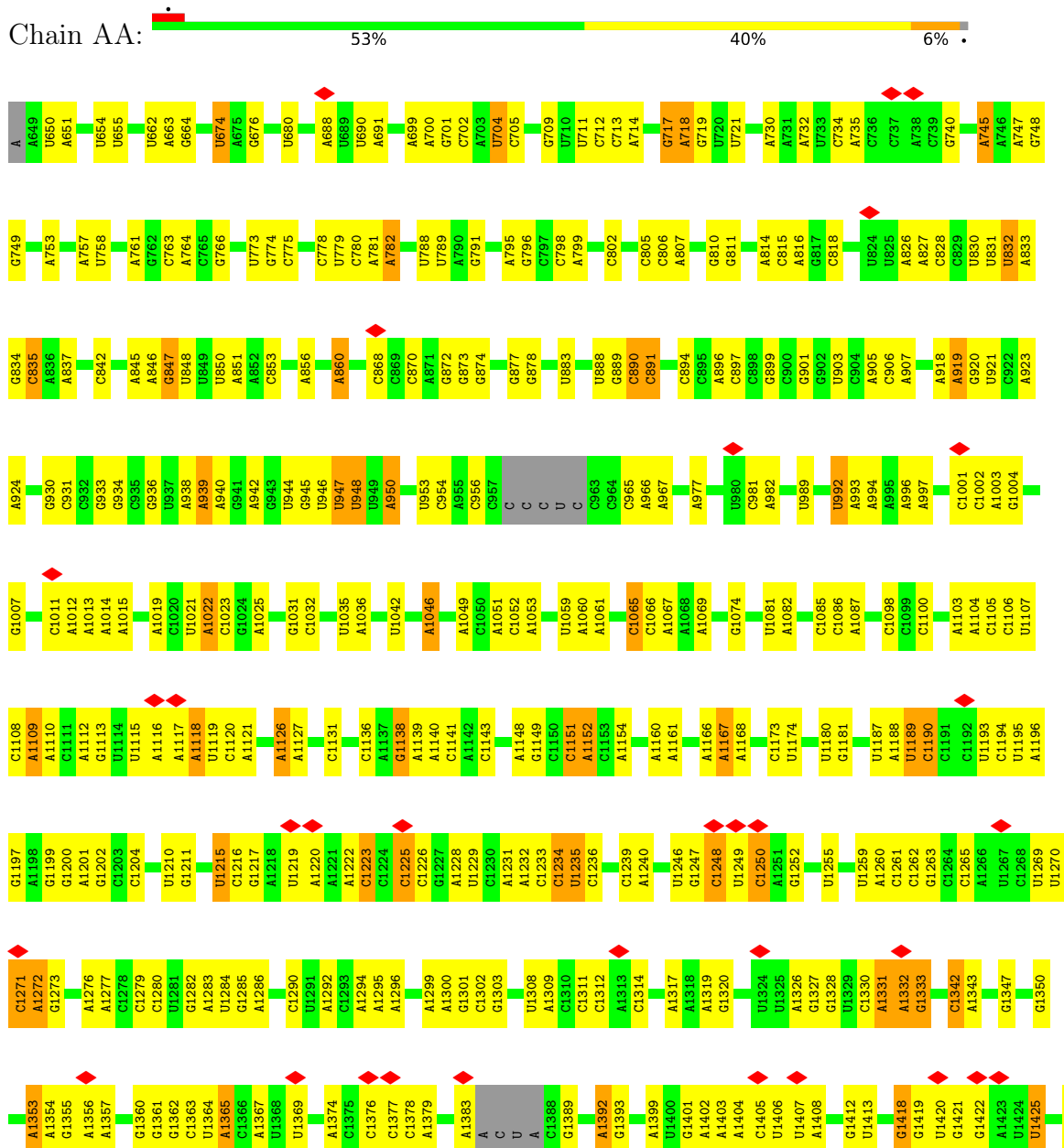


Mol	Chain	Residues	Atoms					AltConf
92	v	1	Total	C	N	O	P	0
			32	11	5	13	3	

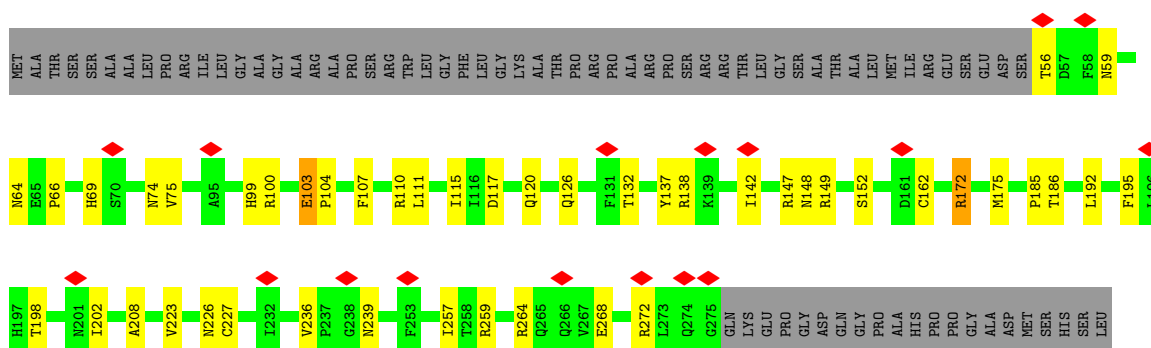
3 Residue-property plots

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

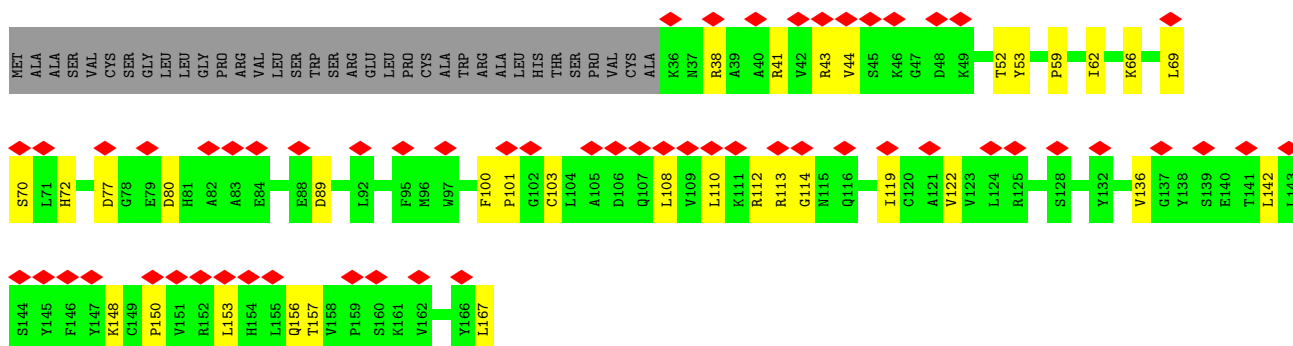
• Molecule 1: 12s rRNA



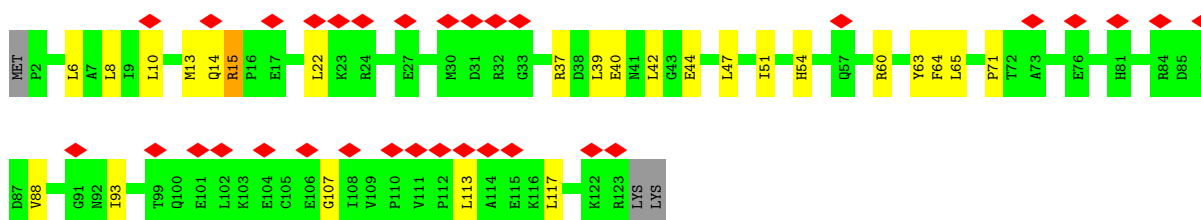
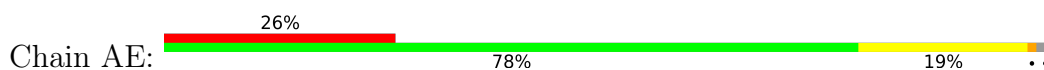
- Molecule 2: 28S ribosomal protein S2, mitochondrial



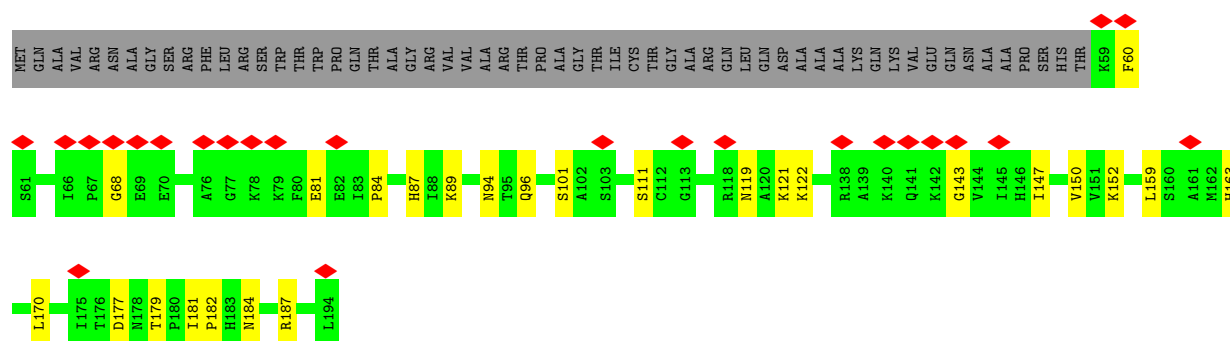
- Molecule 3: 28S ribosomal protein S24, mitochondrial



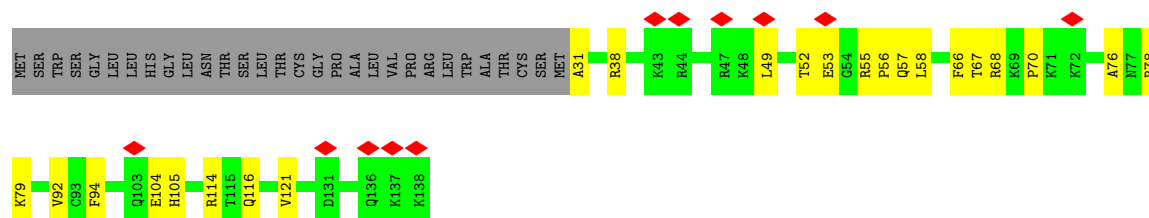
- Molecule 4: 28S ribosomal protein S6, mitochondrial



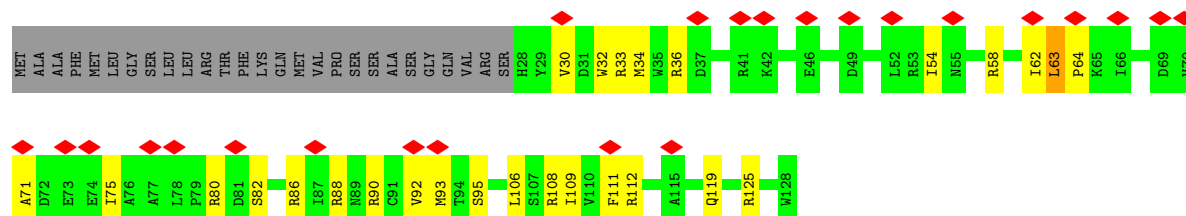
- Molecule 5: 28S ribosomal protein S11, mitochondrial



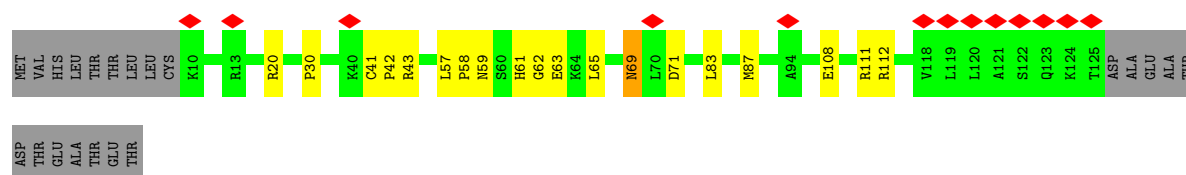
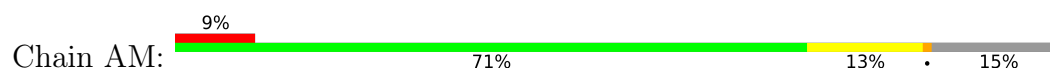
- Molecule 6: 28S ribosomal protein S12, mitochondrial



- Molecule 7: 28S ribosomal protein S14, mitochondrial

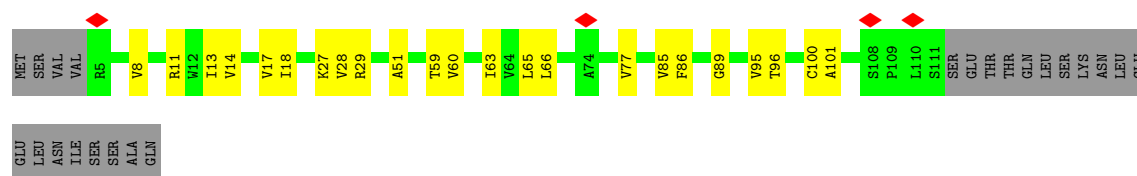


- Molecule 8: 28S ribosomal protein S16, mitochondrial

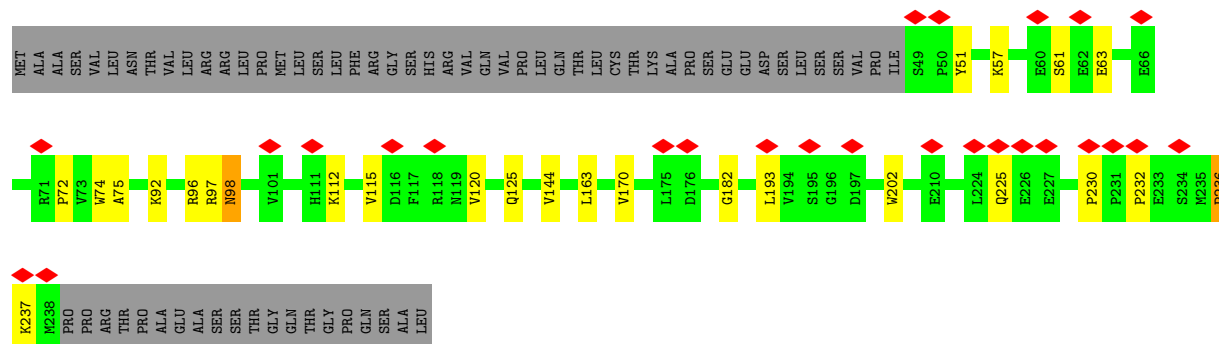


- Molecule 9: 28S ribosomal protein S17, mitochondrial

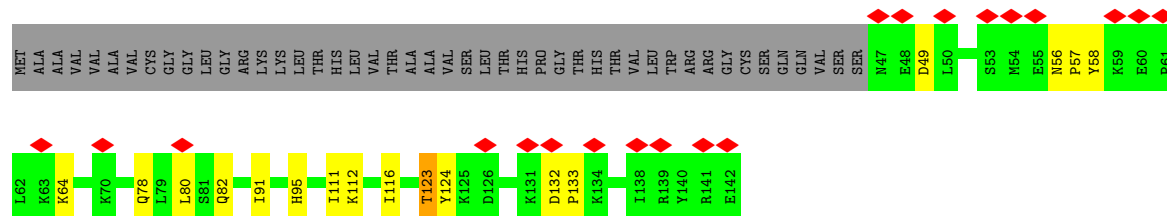




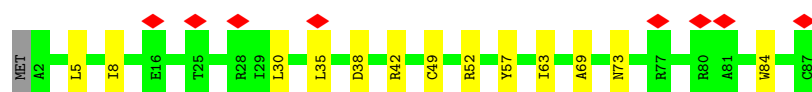
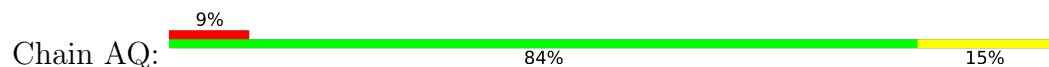
- Molecule 10: 28S ribosomal protein S18b, mitochondrial



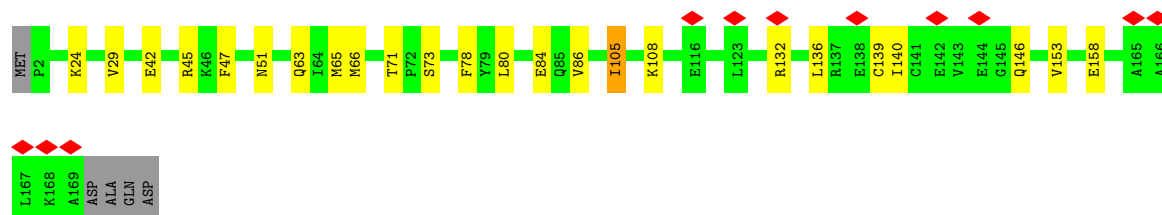
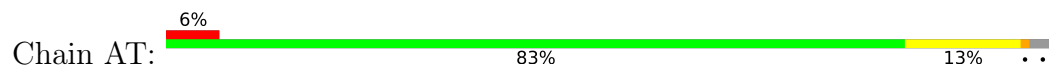
- Molecule 11: 28S ribosomal protein S18c, mitochondrial



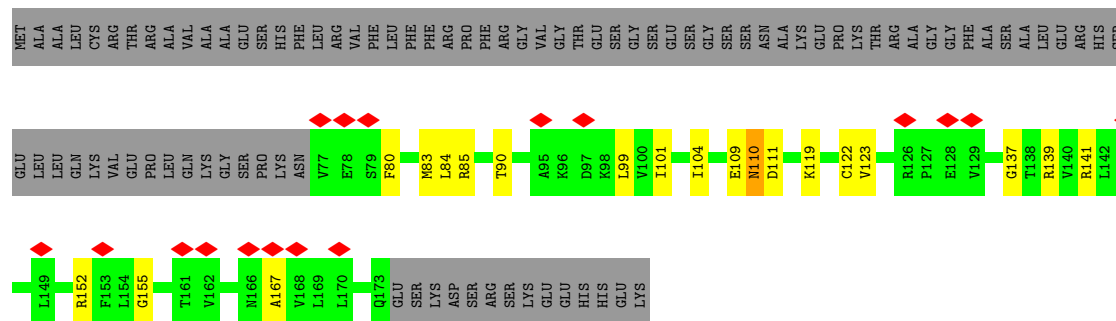
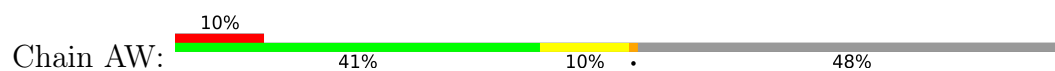
- Molecule 12: 28S ribosomal protein S21, mitochondrial



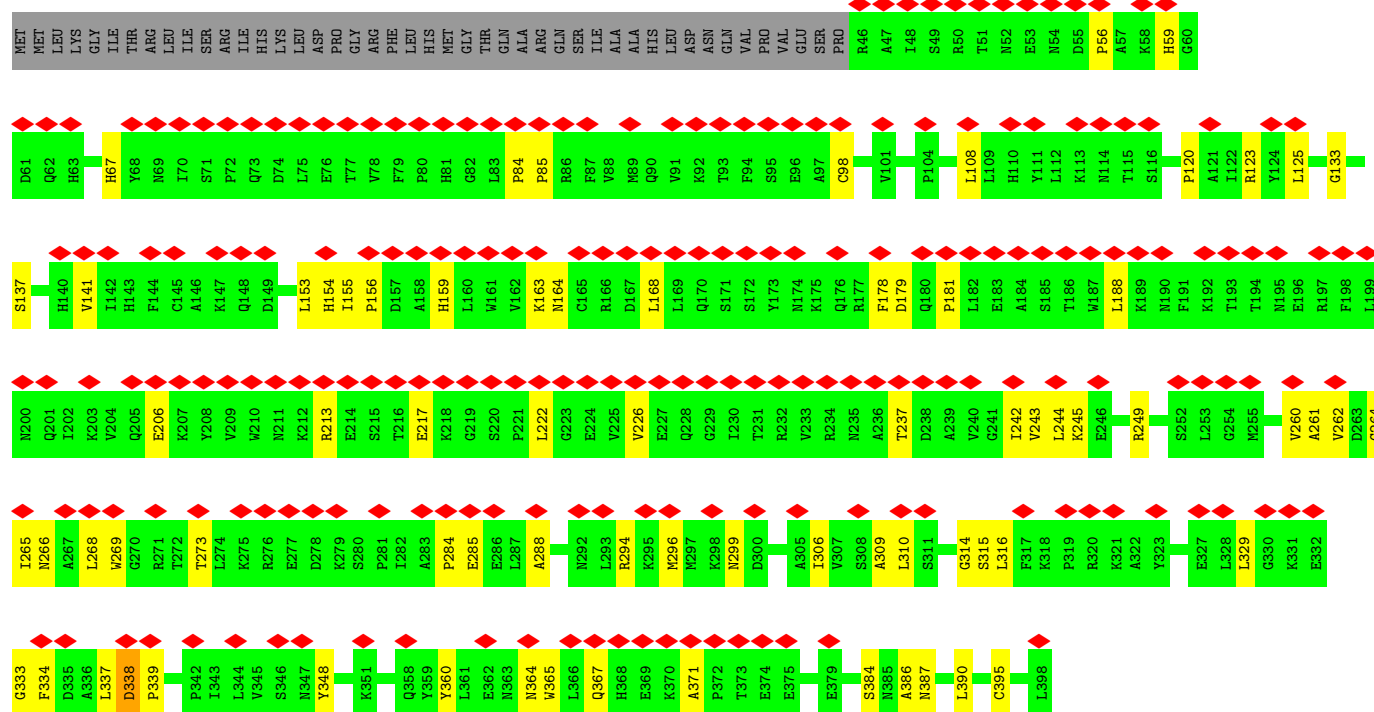
- Molecule 13: 28S ribosomal protein S25, mitochondrial



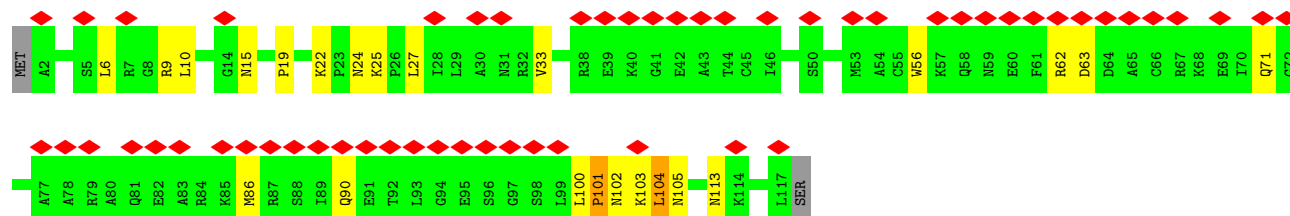
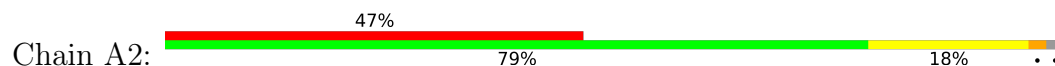
• Molecule 14: 28S ribosomal protein S28, mitochondrial



• Molecule 15: 28S ribosomal protein S29, mitochondrial

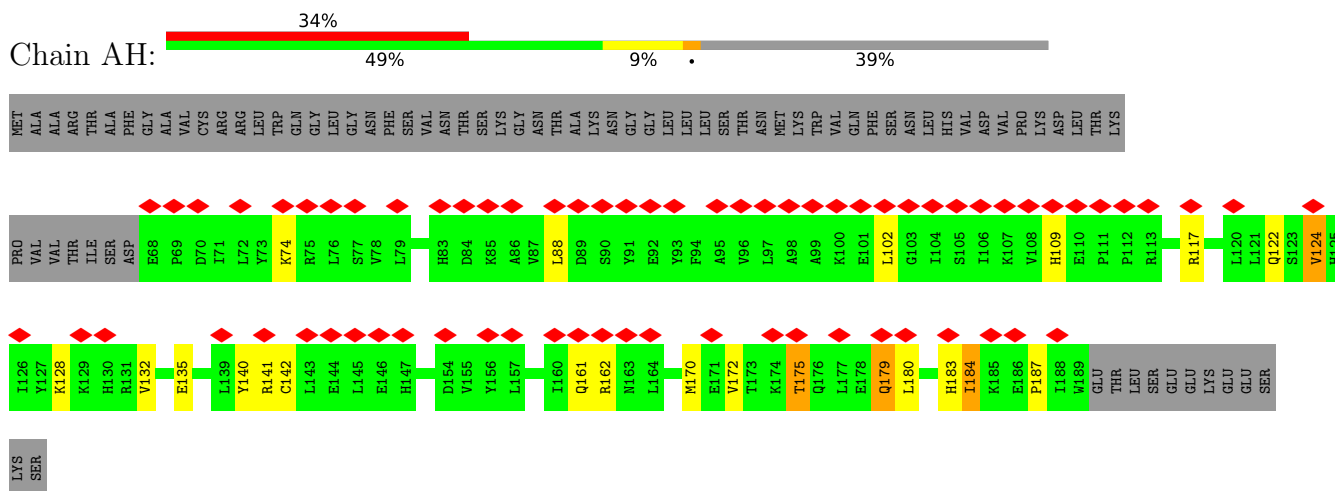


• Molecule 16: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1



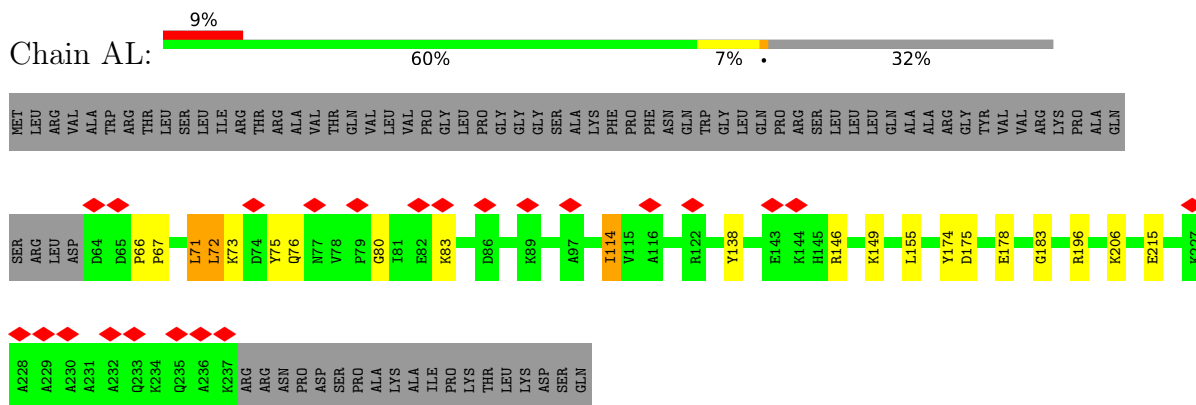
- Molecule 17: 28S ribosomal protein S10, mitochondrial

Chain AH:



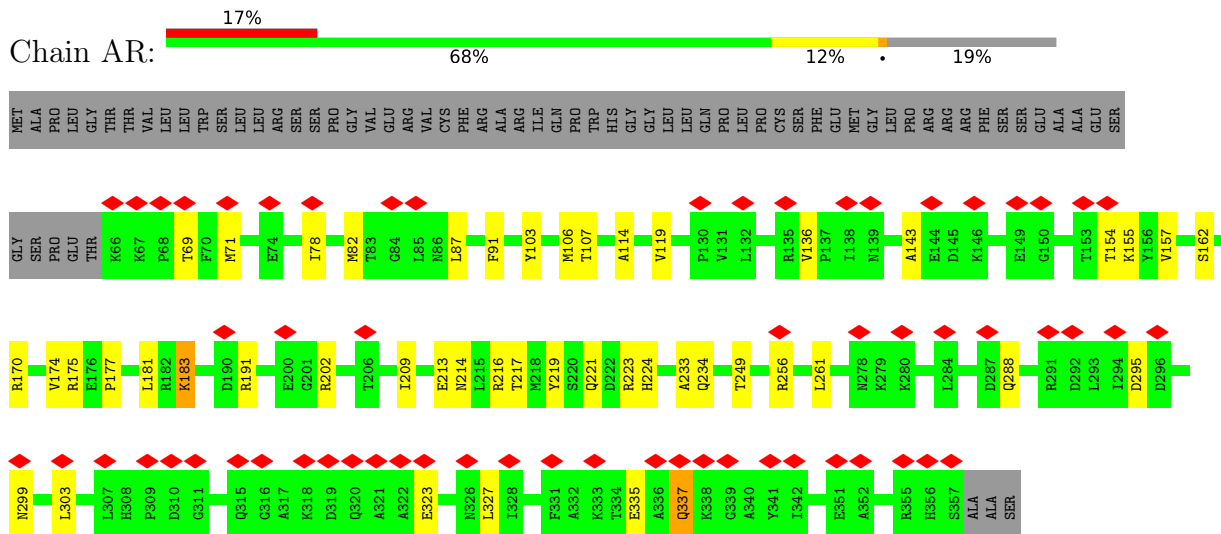
- Molecule 18: 28S ribosomal protein S15, mitochondrial

Chain AL:



- Molecule 19: 28S ribosomal protein S22, mitochondrial

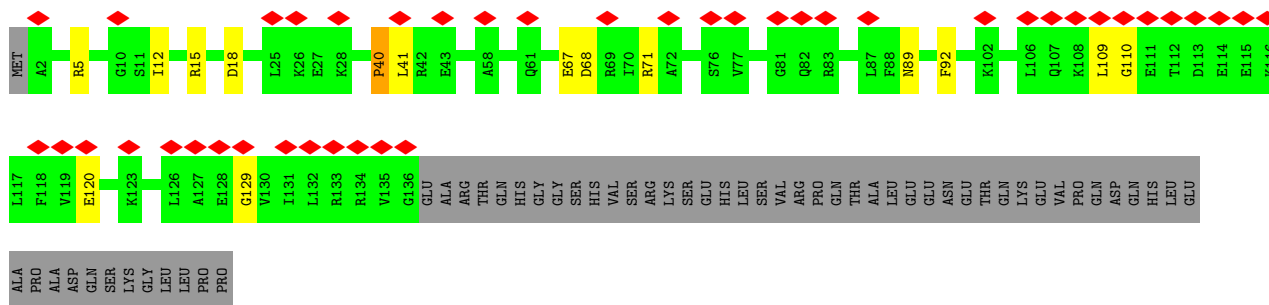
Chain AR:



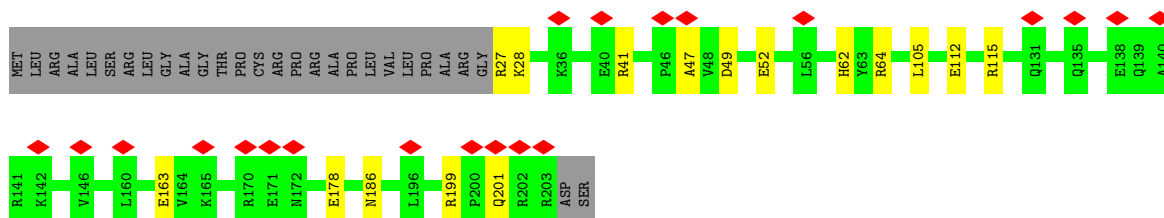
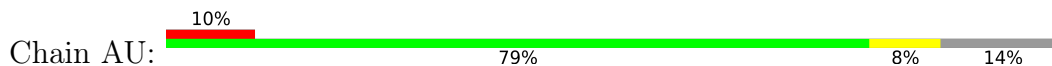
- Molecule 20: 28S ribosomal protein S23, mitochondrial

Chain AS:

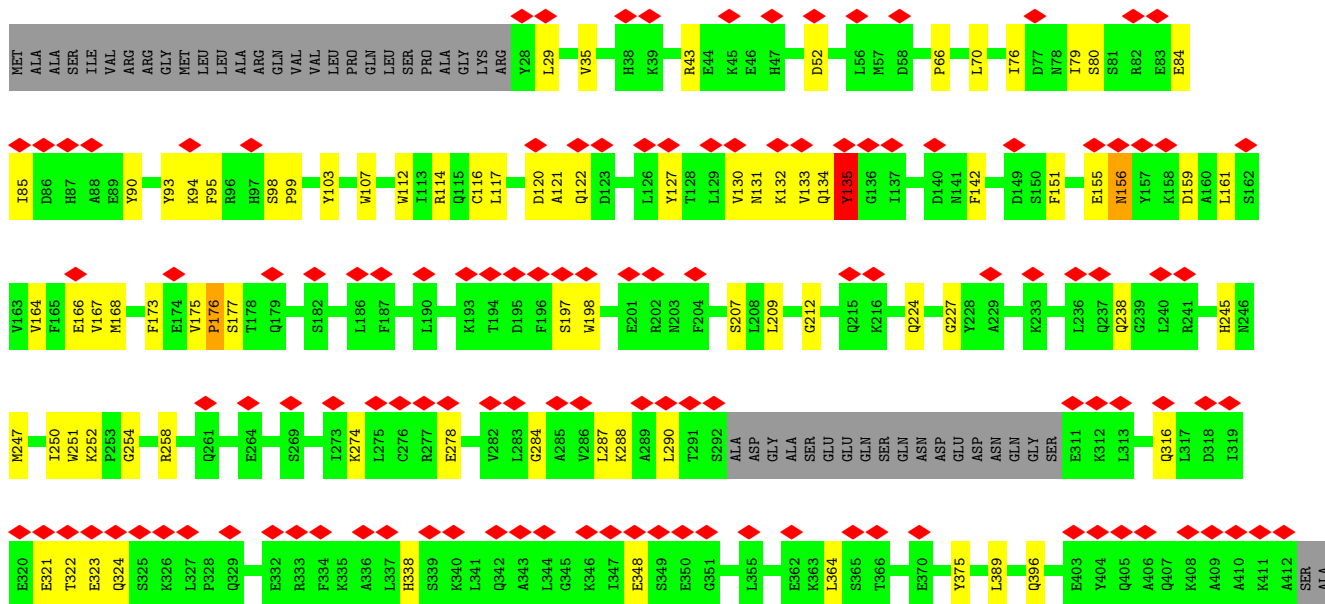
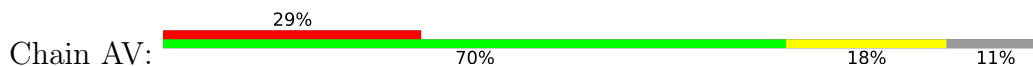




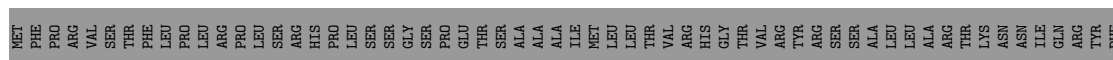
- Molecule 21: 28S ribosomal protein S26, mitochondrial

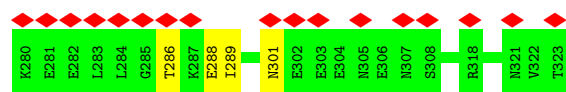


- Molecule 22: 28S ribosomal protein S27, mitochondrial

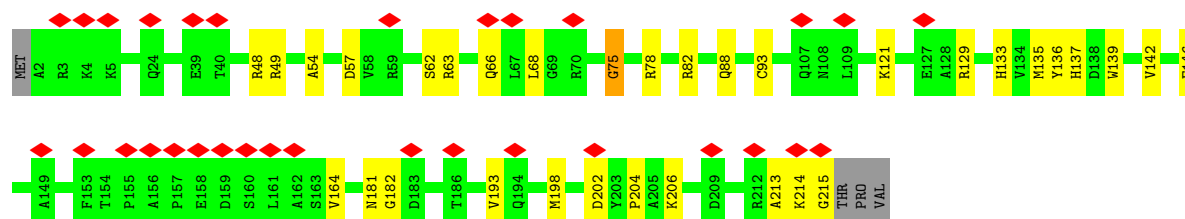
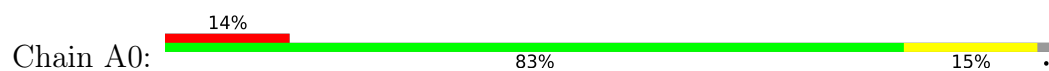


- Molecule 23: 28S ribosomal protein S31, mitochondrial

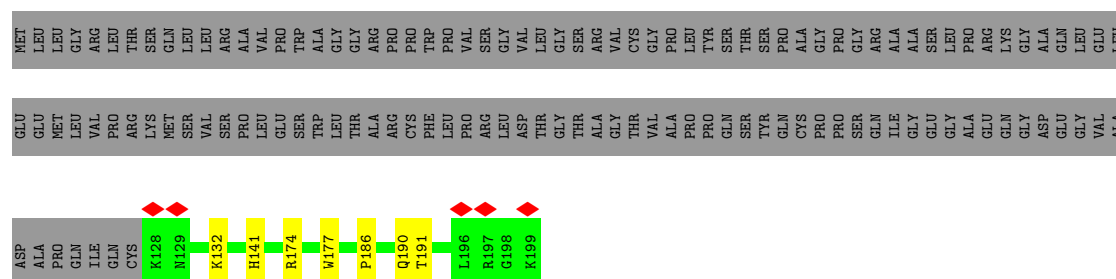




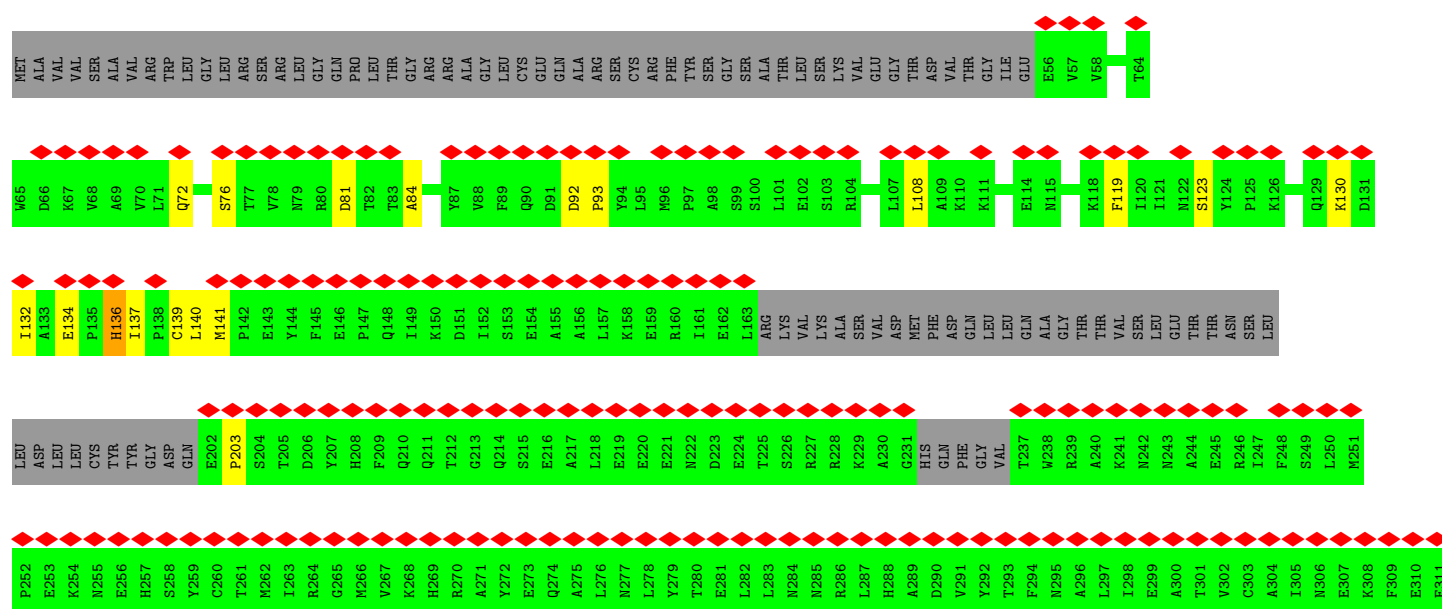
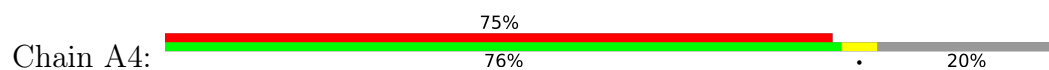
- Molecule 26: 28S ribosomal protein S34, mitochondrial

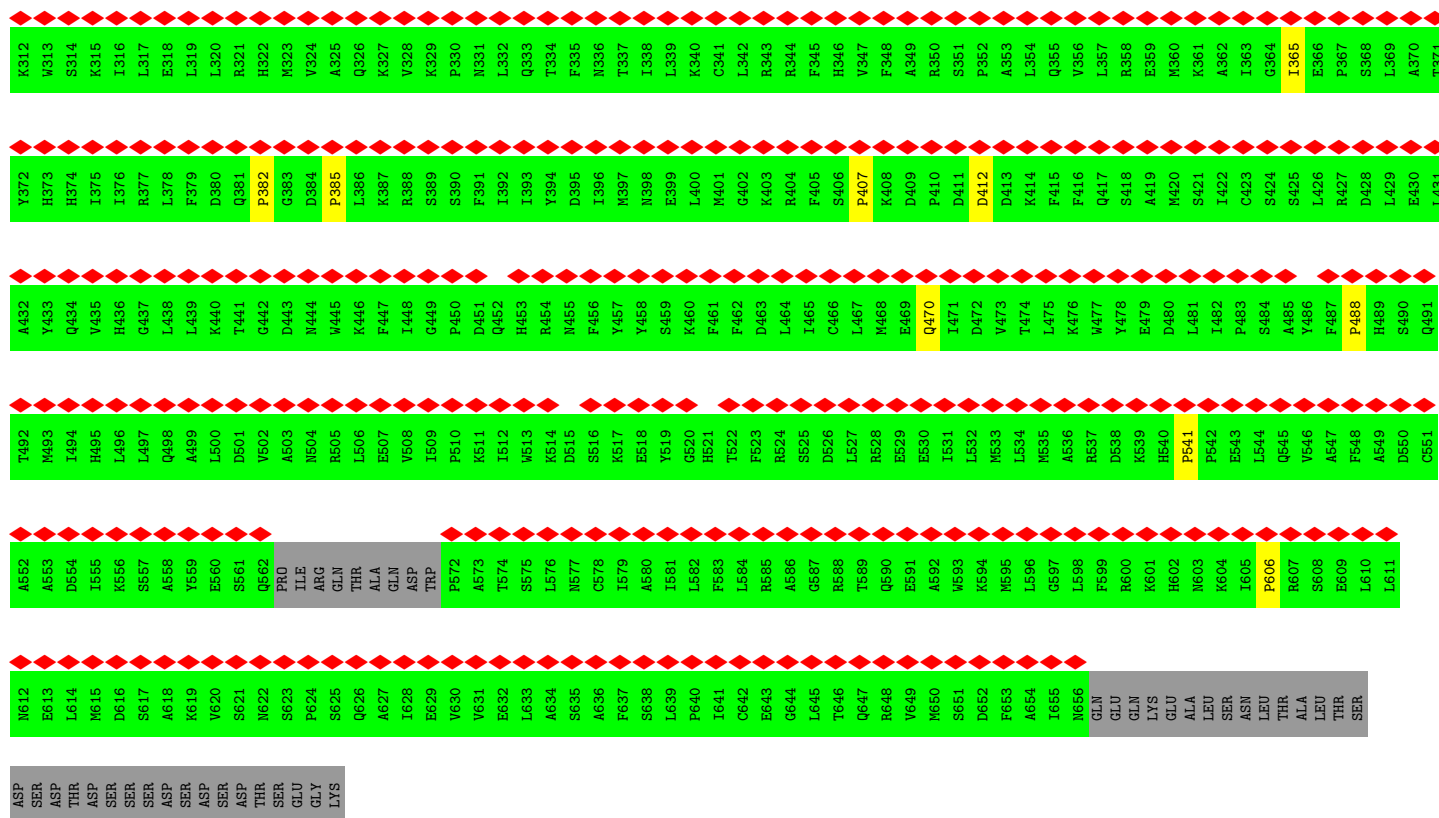


- Molecule 27: Aurora kinase A-interacting protein

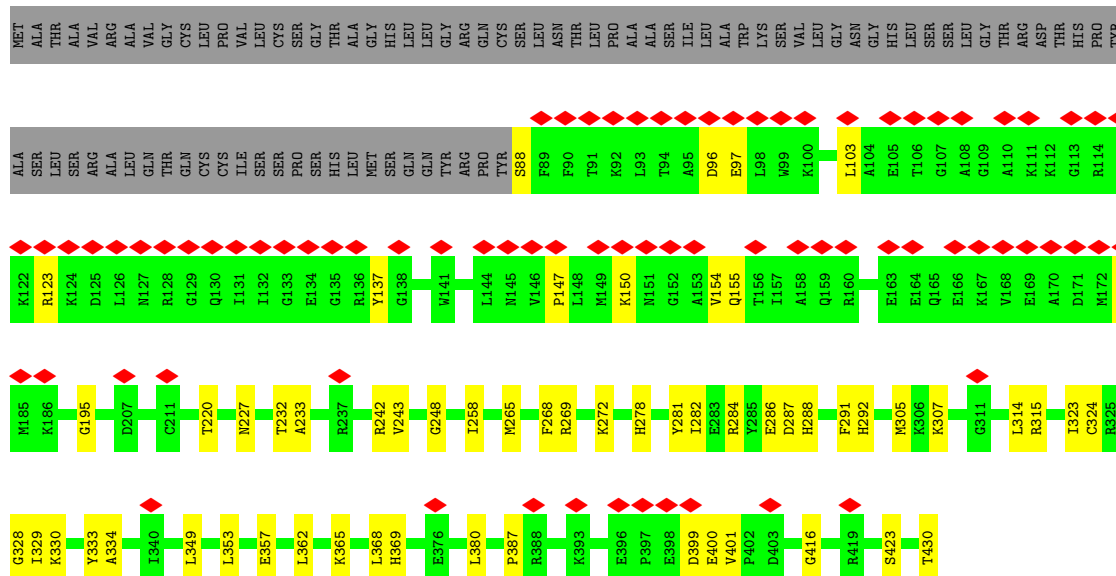


- Molecule 28: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

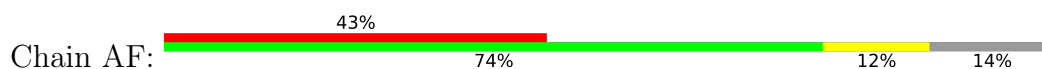




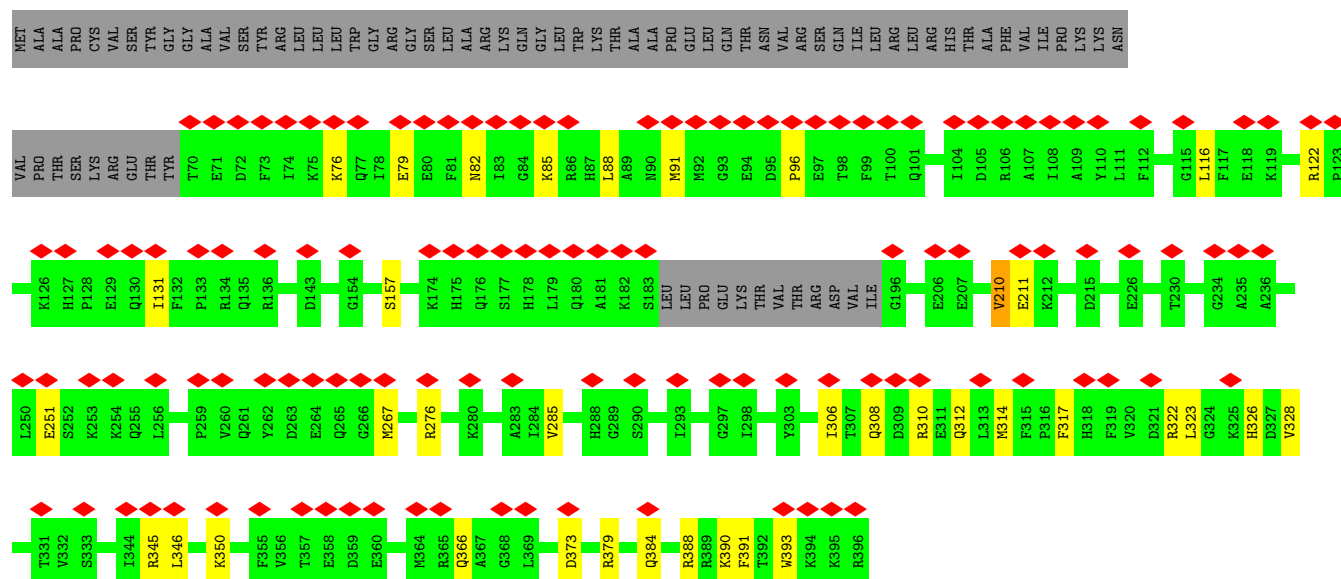
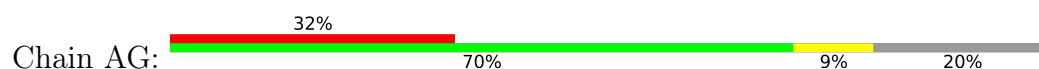
- Molecule 29: 28S ribosomal protein S5, mitochondrial



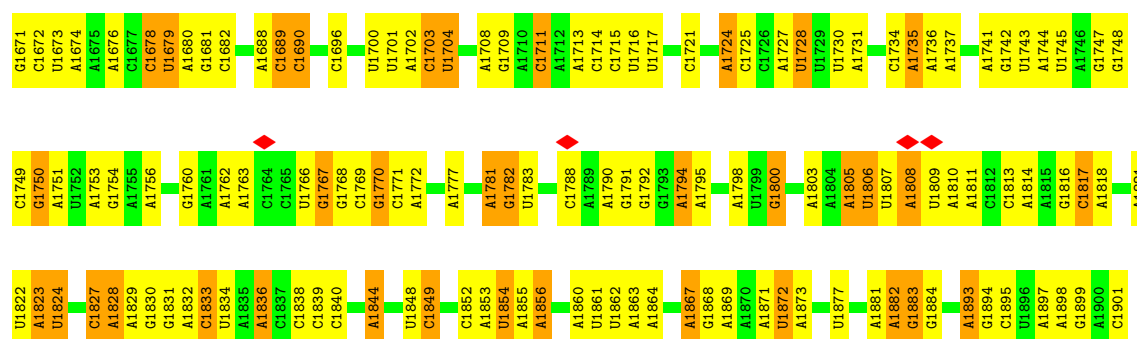
- Molecule 30: 28S ribosomal protein S7, mitochondrial



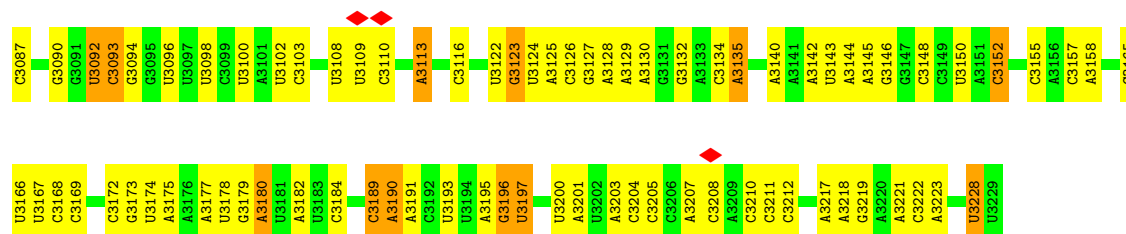
- Molecule 31: 28S ribosomal protein S9, mitochondrial



- Molecule 32: 16s rRNA



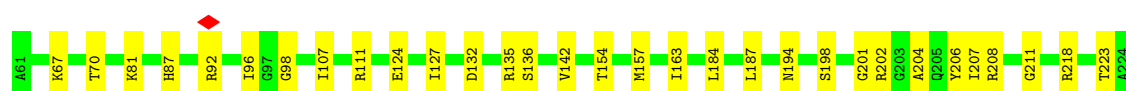
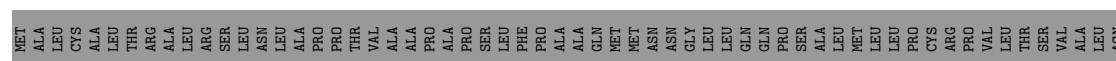
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G3001	C1903	A2084	G2170	C2335	U2312	A2390	U2483	A2581	C2653	A2745	A2833	A2921	G3002
A3003	A1907	A2085	A2171	A2236	A2313	C2393	C2484	C2584	U2654	U2749	C2836	A2926	A3004
G3005	C2001	A2086	A2172	A2237	A2314	A2394	C2489	G2585	U2655	U2750	U2841	C2927	G3006
U3006	A1909	U2087	G2173	A2241	A2315	A2395	C2493	U2586	U2656	A2753	C2842	C2928	G3007
G3007	C1910	U2088	G2174	A2244	U2316	U2404	C2496	C2587	C2657	A2754	C2843	U2930	G3010
G3010	C1911	C2092	A2178	U2245	A2317	A2405	A2503	A2588	U2658	A2755	G2844	A2931	A3011
A3011	A1912	U2093	A2179	A2246	G2318	C2406	A2507	A2590	U2659	C2756	C2847	C2932	G3012
U3012	C1915	G2094	A2180	A2246	A2319	A2407	C2508	A2591	U2660	A2757	A2848	U2933	U3013
G3013	G1916	C2095	A2181	A2246	A2320	U2407	U2510	G2592	U2661	G2758	G2849	A2935	G3016
G3016	A1917	G2096	C2183	A2250	C2322	C2414	C2511	U2593	U2662	U2759	A2853	U2936	G3022
G3022	G1918	G2011	A2184	A2251	U2325	C2415	C2519	C2597	A2672	A2760	U2854	A2937	G3023
G3023	U1924	G2015	C2187	A2252	C2331	U2421	G2520	A2598	G2673	C	U2855	A2938	U3024
U3024	A1925	C2016	A2188	U2253	C2332	G2421	A2521	C2602	U2674	U	G2860	U2939	G3027
G3031	A1926	G2017	C2189	U2254	C2339	A2425	U2522	U2603	U2675	A	U2861	C2942	U3032
G3032	U1930	U2021	C2190	U2255	G2343	C2426	C2523	C2606	C2676	C	C2862	G2943	U3033
U3033	G1935	G2022	A2196	U2256	G2344	C2427	A2524	U2607	C2683	A	U2863	C2944	U3034
U3034	A1936	U2023	A2197	U2257	G2345	A2432	U2528	U2610	C2686	C	C2864	C2945	G3031
U3041	A1937	U2024	G2197	U2258	G2346	C2433	U2529	C2611	U2687	C	A2865	A2946	G3032
U3042	A1938	C2025	A2199	U2259	G2347	U2439	U2530	C2612	G2688	A	A2866	U2947	U3033
C3043	A1939	A2026	A2200	U2260	U2350	U2441	A2531	U2613	C2689	C	C2867	C2948	U3034
U3049	A1940	A2027	G2201	U2261	A2350	C2442	A2532	U2618	U2690	C	U2868	U2949	U3041
A3052	A1941	G2028	G2202	U2262	U2351	U2443	U2533	G2620	G2691	C	C2869	A2950	U3042
G3053	A1942	A2031	G2203	U2263	U2352	A2444	U2534	G2621	G2692	C	U2870	A2951	U3043
G3054	A1943	A2032	U2204	U2264	U2353	U2445	U2535	G2622	G2693	C	A2706	U2952	U3044
C3060	C1944	A2033	U2205	U2265	U2354	U2446	U2536	G2623	G2694	C	A2707	U2953	U3045
G3063	C1951	C2036	A2206	U2266	U2355	U2447	U2537	A2624	G2695	A	C2710	C2954	C3066
U3067	U1952	U2037	U2043	U2267	U2356	G2448	U2538	C2625	U2696	C	A2711	A2955	G3068
G3068	A1953	A2038	U2047	U2268	U2357	U2449	A2539	U2626	G2697	C	C2712	C2956	G3070
A3069	A1954	G2040	U2048	U2269	U2358	G2453	A2540	U2627	U2698	C	C2713	U2907	U3071
U3070	G1955	A2060	A2060	U2270	U2359	A2457	A2541	U2628	G2699	C	A2714	A2908	U3072
U3072	G1956	A2065	A2065	U2271	U2360	A2458	A2542	U2629	U2700	C	U2715	U2909	C3073
C3073	U1957	C2066	C2066	U2272	A2361	A2461	C2557	U2630	G2706	C	U2716	C2910	A3074
A3074	G1958	A2065	A2065	U2273	A2362	A2462	A2558	U2631	G2707	C	C2717	A2911	U3077
C3077	U1979	C2067	C2067	U2274	A2363	A2463	U2559	U2632	A2708	C	G2718	C2912	C3078
G3079	A1980	C2068	U2069	U2275	A2364	A2464	G2560	U2633	G2709	C	G2719	A2913	G3079
A3081	G1981	U2070	C2070	U2276	A2365	A2465	A2561	U2634	U2724	C	A2720	C2914	G3080
G3082	G1982	C2071	C2071	U2277	A2366	A2466	A2562	U2635	G2725	C	U2721	G2915	A3081
A3085	G1985	U2076	C2076	U2278	A2367	A2467	A2563	U2636	U2726	C	C2722	U2916	G3082
U3086	U1986	C2077	C2077	U2279	A2368	A2468	A2564	U2637	U2727	C	G2723	C2917	U3085
	G1987	C2078	C2078	U2280	A2369	A2469	A2565	U2638	G2728	C	G2724	U2918	
	C1989	C2079	C2079	U2281	A2370	G2470	A2566	U2639	U2729	C	U2725	A2919	
	A1993	U2080	U2080	U2282	A2371	A2471	A2567	U2640	G2730	C	A2726	C2920	
	A1994	A2081	A2081	U2283	A2372	A2472	A2568	U2641	G2731	C	U2727	U2921	
	A1995	G2082	G2082	U2284	A2373	A2473	A2569	U2642	G2732	C	U2728	A2922	
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				U2287	A2376	A2476	A2572	U2645	G2735	C	U2731	U2925	
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				U2294	A2383	A2483	A2579	U2652		C	U2738	U2932	
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				U2300	A2389	A2489	A2585	U2658		C	U2744	U2938	
				U2301	A2390	A2490	A2586	U2659		C	U2745	U2939	
				U2302	A2391	A2491	A2587	U2660		C	U2746	U2940	
				U2303	A2392	A2492	A2588	U2661		C	U2747	U2941	
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				U2305	A2394	A2494	A2590	U2663		C	U2749	U2943	
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				U2308	A2397	A2497	A2593	U2666		C	U2752	U2946	
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				U2317	A2406	A2506	A2602	U2675		C	U2761	U2955	
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				U2331	A2420	A2520	A2616	U2689		C	U2775	U2969	
				U2332	A2421	A2521	A2617	U2690		C	U2776	U2970	
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				U2342	A2431	A2531	A2627	U2700		C	U2786	U2980	
				U2343	A2432	A2532	A2628	U2701		C	U2787	U2981	
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				U2345	A2434	A2534	A2630	U2703		C	U2789	U2983	
				U2346	A2435	A2535	A2631	U2704		C	U2790	U2984	
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				U2348	A2437								



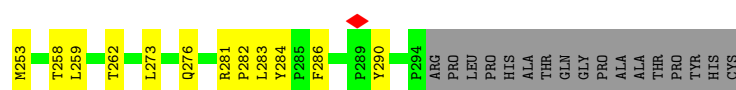
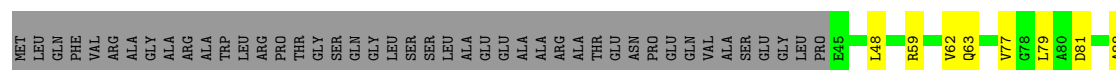
• Molecule 33: tRNAval



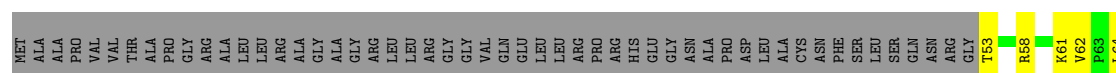
• Molecule 34: 39S ribosomal protein L2, mitochondrial

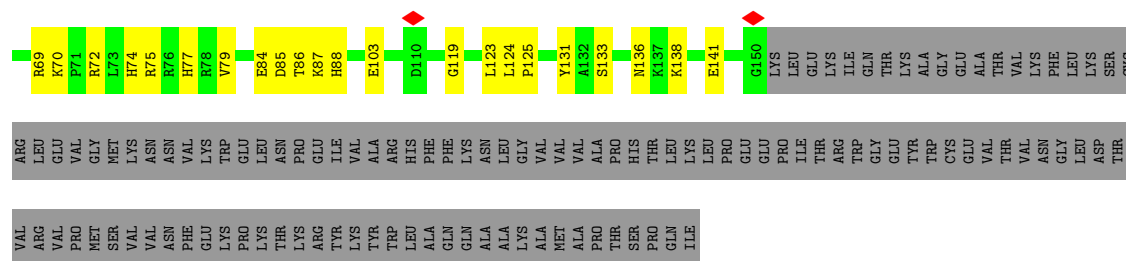


• Molecule 35: 39S ribosomal protein L4, mitochondrial



• Molecule 36: 39S ribosomal protein L9, mitochondrial





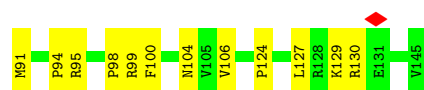
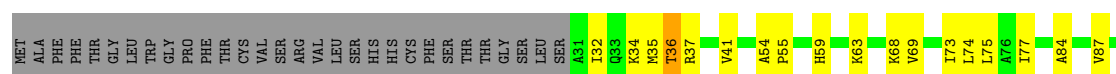
- Molecule 37: 39S ribosomal protein L13, mitochondrial

Chain K: 84% 15% ..



- Molecule 38: 39S ribosomal protein L14, mitochondrial

Chain L: 59% 20% 21%



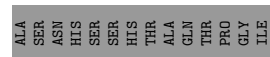
- Molecule 39: 39S ribosomal protein L15, mitochondrial

Chain M: 76% 21%



- Molecule 40: 39S ribosomal protein L17, mitochondrial

Chain O: 71% 15% 13%

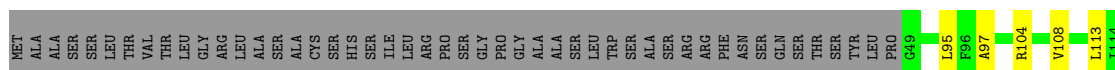


- Molecule 41: 39S ribosomal protein L20, mitochondrial

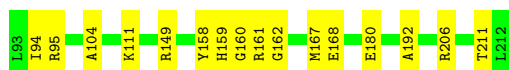
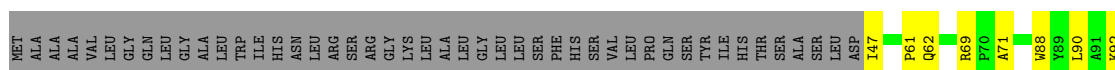
Chain R: 79% 13% 6%



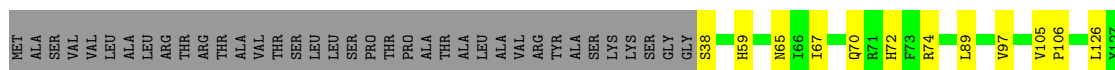
- Molecule 42: 39S ribosomal protein L21, mitochondrial



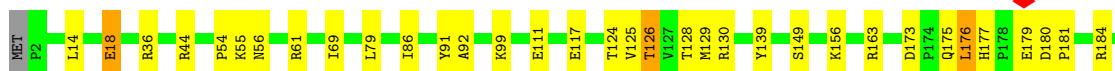
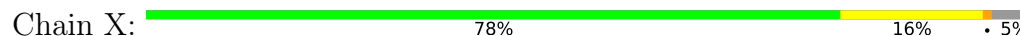
- Molecule 43: 39S ribosomal protein L22, mitochondrial



- Molecule 44: 39S ribosomal protein L27, mitochondrial

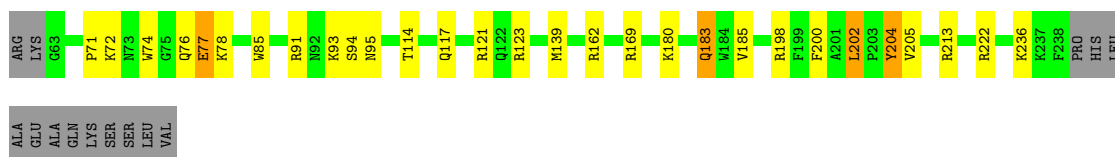


- Molecule 45: 39S ribosomal protein L28, mitochondrial



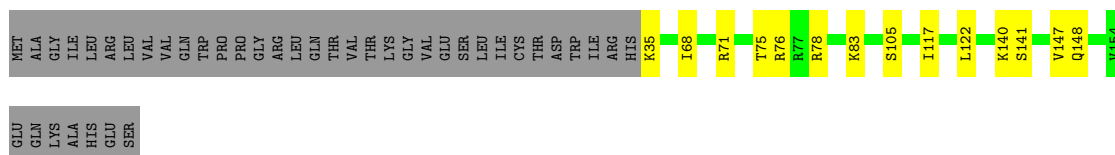
- Molecule 46: 39S ribosomal protein L47, mitochondrial





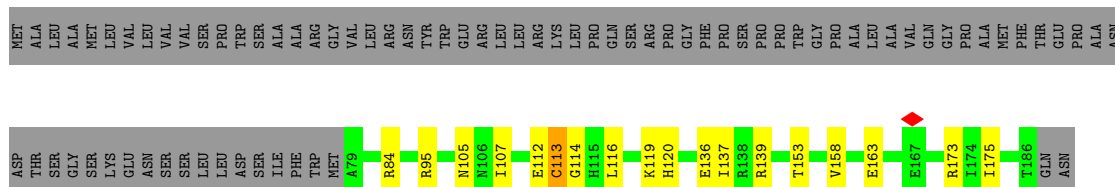
- Molecule 47: 39S ribosomal protein L30, mitochondrial

Chain Z: 66% 9% 25%



- Molecule 48: 39S ribosomal protein L32, mitochondrial

Chain 0: 48% 9% 43%



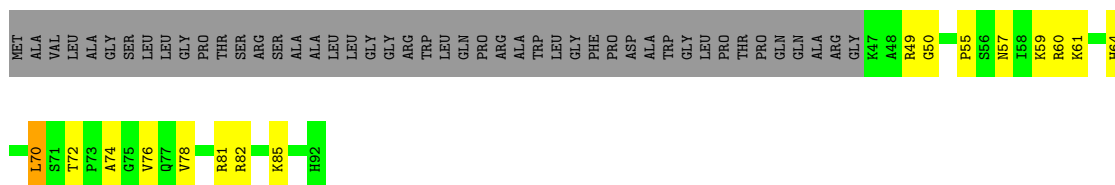
- Molecule 49: 39S ribosomal protein L33, mitochondrial

Chain 1: 58% 22% 20%



- Molecule 50: 39S ribosomal protein L34, mitochondrial

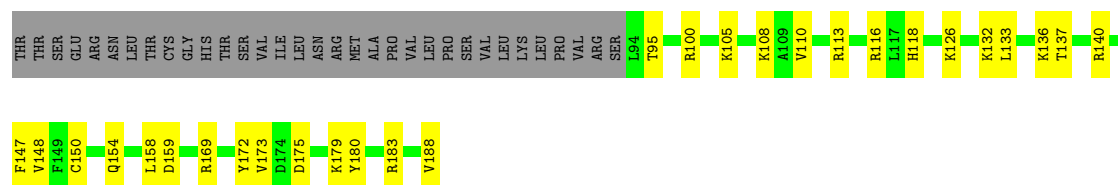
Chain 2: 33% 16% 50%



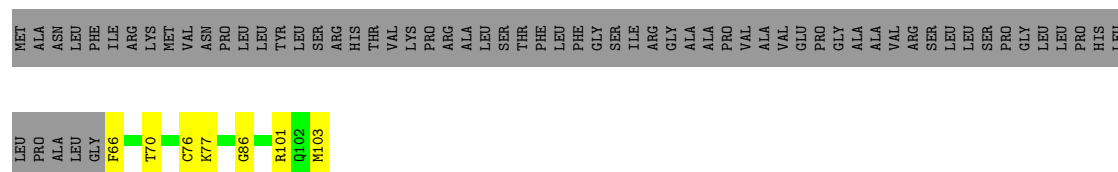
- Molecule 51: 39S ribosomal protein L35, mitochondrial

Chain 3: 36% 15% 49%

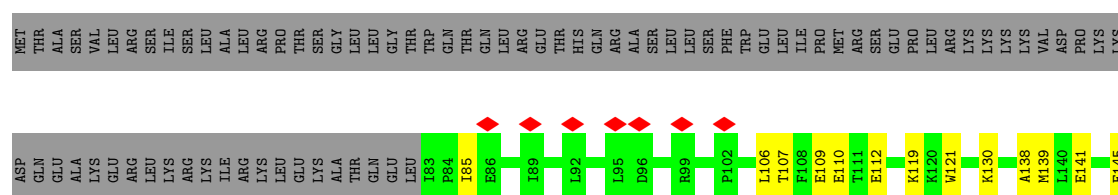
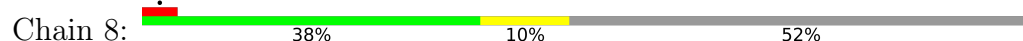




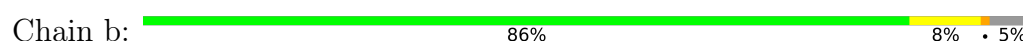
- Molecule 52: 39S ribosomal protein L36, mitochondrial



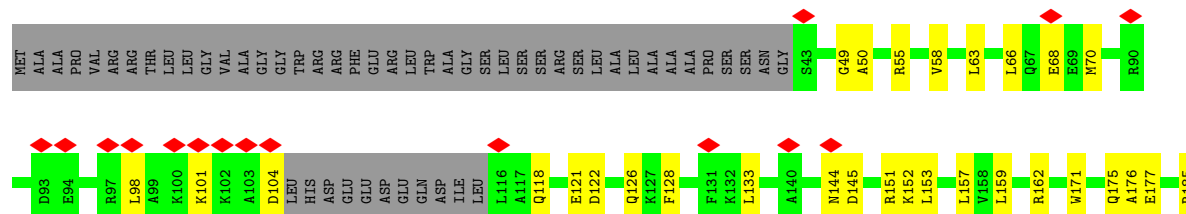
- Molecule 53: 39S ribosomal protein L40, mitochondrial

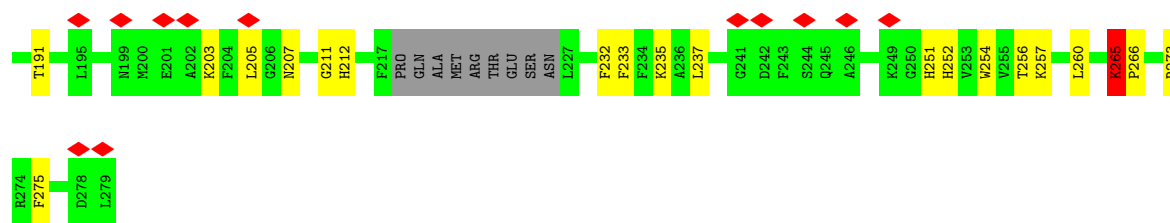


- Molecule 54: 39S ribosomal protein L43, mitochondrial

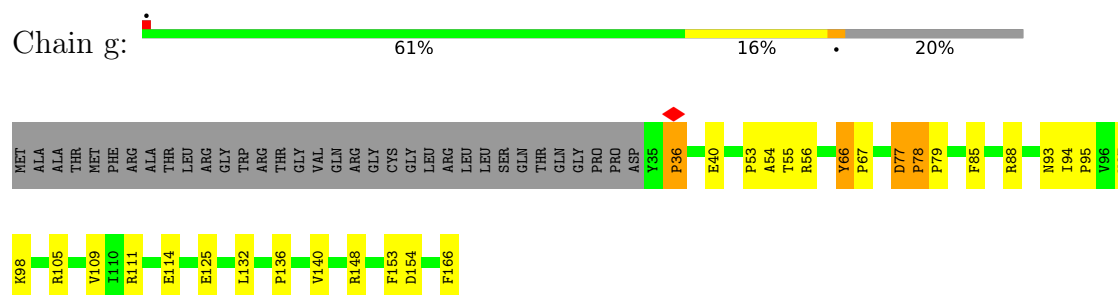


- Molecule 55: 39S ribosomal protein L46, mitochondrial

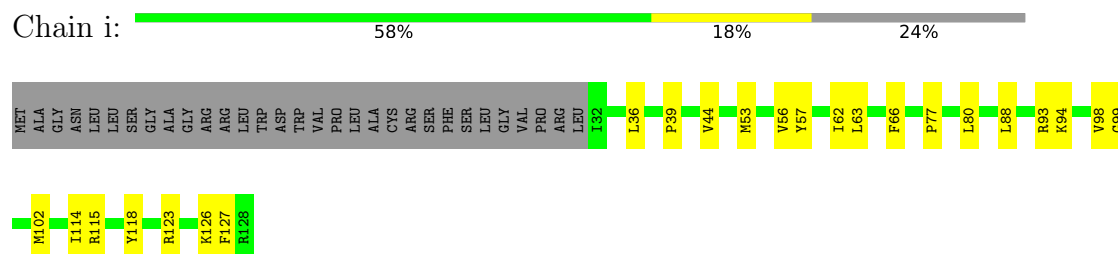




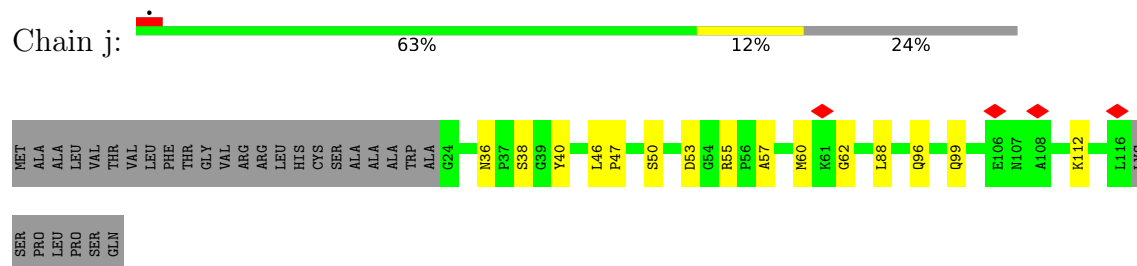
- Molecule 56: 39S ribosomal protein L49, mitochondrial



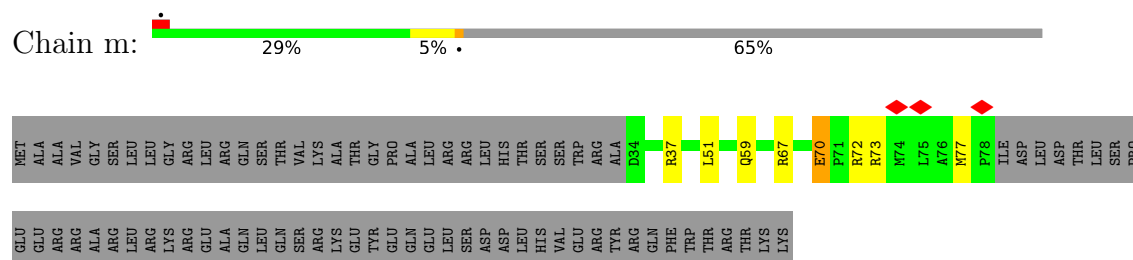
- Molecule 57: 39S ribosomal protein L51, mitochondrial



- Molecule 58: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA



- Molecule 59: 39S ribosomal protein L55, mitochondrial



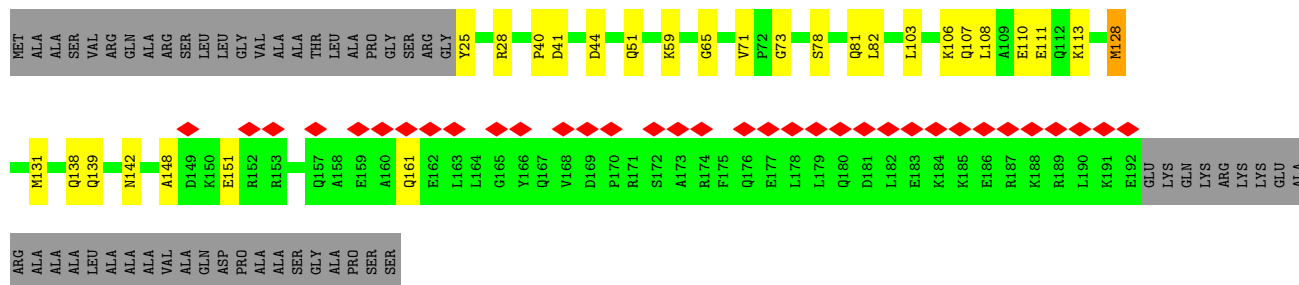
- Molecule 60: Ribosomal protein 63, mitochondrial

Chain o:  71% 21% 8%



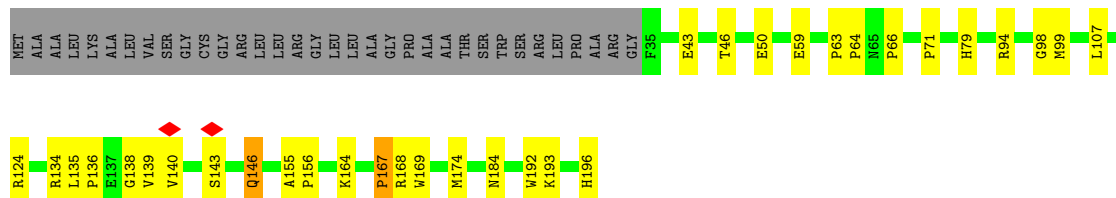
- Molecule 61: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  15% 63% 12% 24%



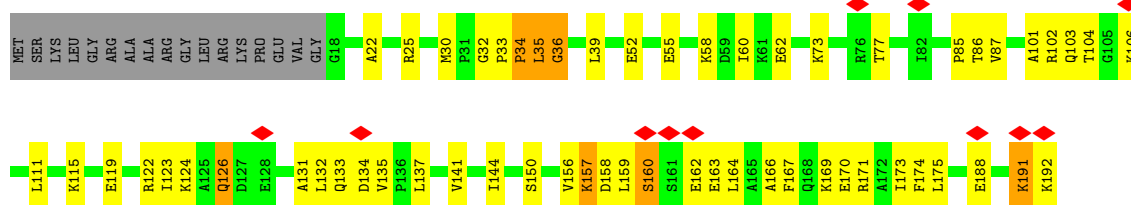
- Molecule 62: 39S ribosomal protein S18a, mitochondrial

Chain r:  66% 16% 17%



- Molecule 63: 39S ribosomal protein L11, mitochondrial

Chain J:  6% 60% 27% 9%



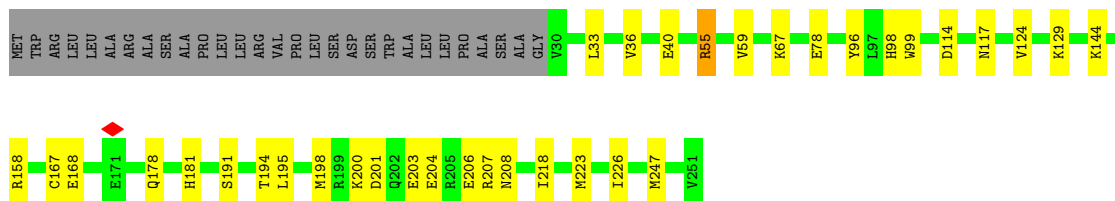
- Molecule 64: 39S ribosomal protein L10, mitochondrial

Chain I:  9% 47% 22% 31%

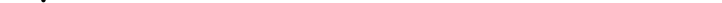


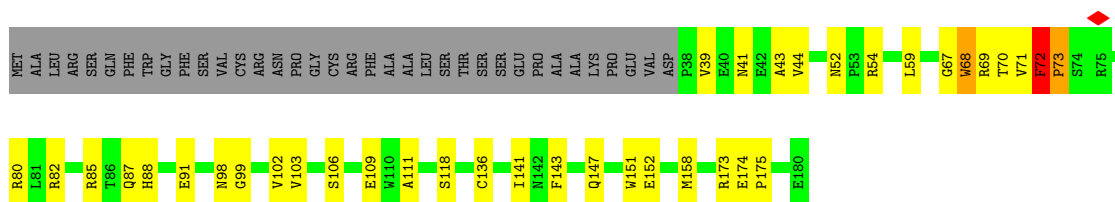
- Molecule 65: 39S ribosomal protein L16, mitochondrial

Chain N: 75% 14% 12%



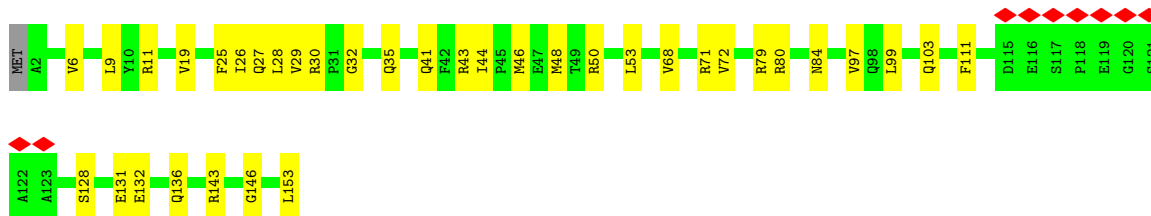
- Molecule 66: Mitochondrial ribosomal protein L18, isoform CRA b

Chain P:  59% 20% 20%



- Molecule 67: 39S ribosomal protein L23, mitochondrial

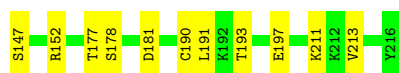
Chain U:  6% 76% 24%



- Molecule 68: 39S ribosomal protein L24, mitochondrial

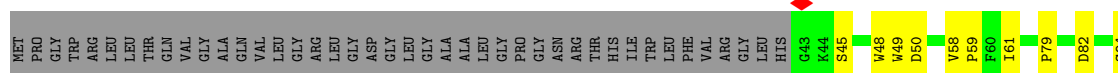
Chain V:





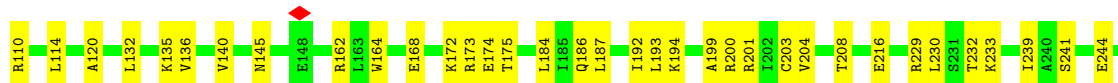
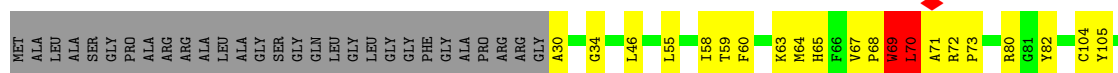
- Molecule 69: 39S ribosomal protein L3, mitochondrial

Chain E: 72% 16% 12%



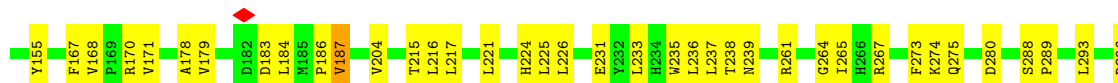
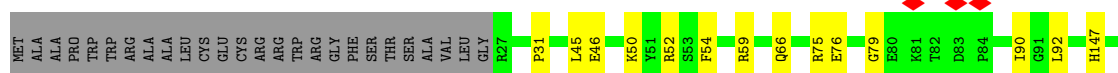
- Molecule 70: 39S ribosomal protein L37, mitochondrial

Chain 5: 73% 20% 7%



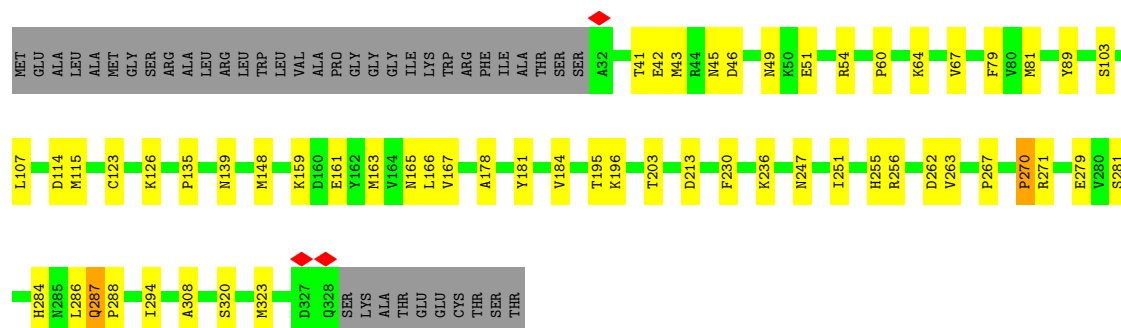
- Molecule 71: 39S ribosomal protein L38, mitochondrial

Chain 6: 73% 19% 7%



- Molecule 72: 39S ribosomal protein L39, mitochondrial

Chain 7: 71% 16% 12%



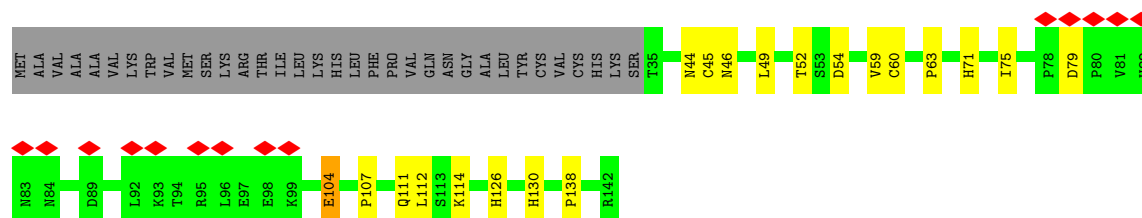
- Molecule 73: 39S ribosomal protein L41, mitochondrial

Chain 9: 78% 12% 9%



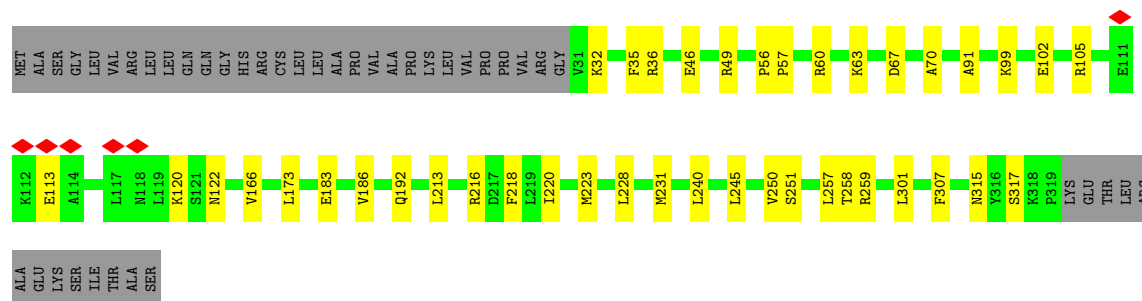
- Molecule 74: 39S ribosomal protein L42, mitochondrial

Chain a: 10% 62% 13% 24%



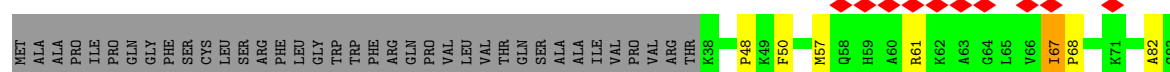
- Molecule 75: 39S ribosomal protein L44, mitochondrial

Chain c: 75% 12% 13%

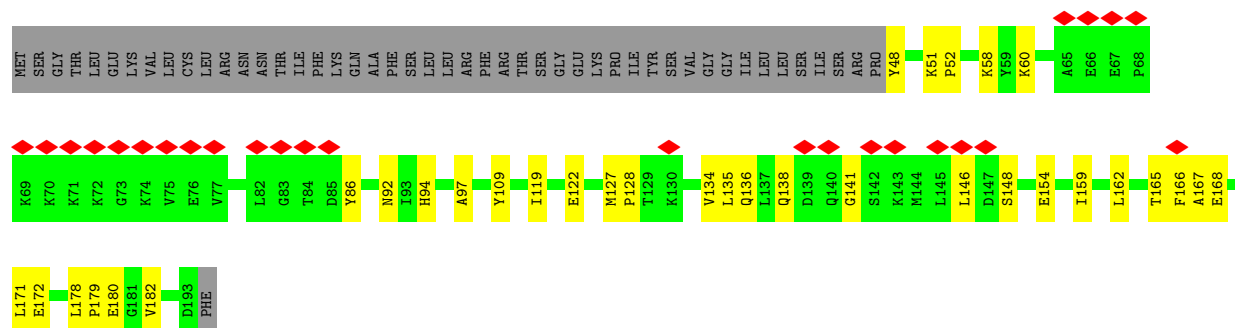


- Molecule 76: 39S ribosomal protein L45, mitochondrial

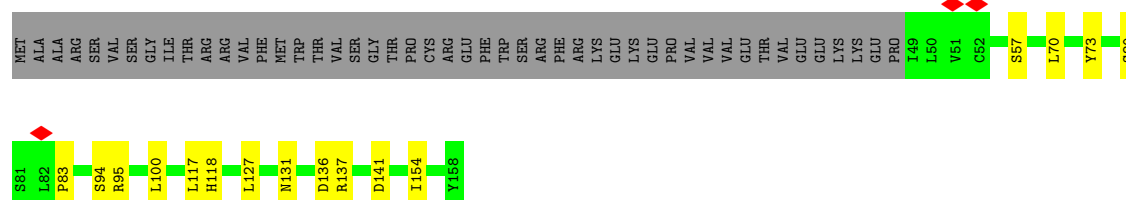
Chain d: 10% 69% 14% 16%



- Molecule 77: 39S ribosomal protein L48, mitochondrial



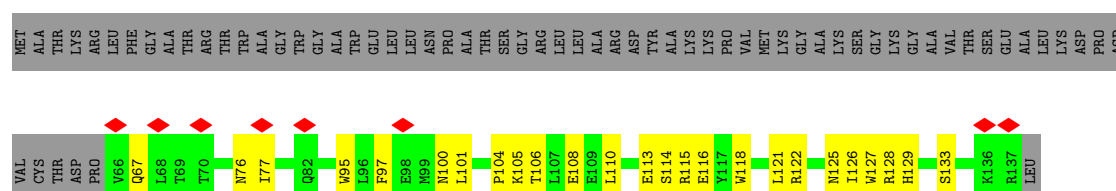
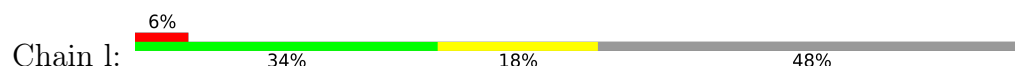
- Molecule 78: 39S ribosomal protein L50, mitochondrial



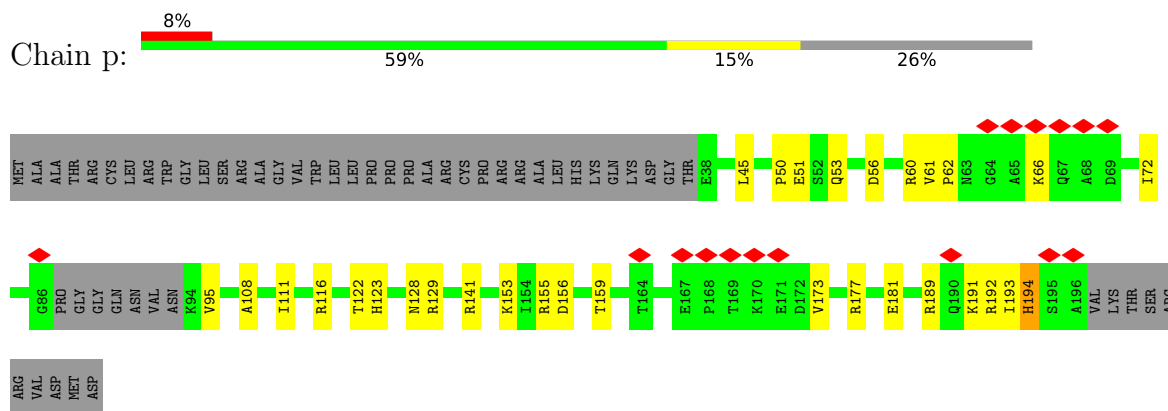
- Molecule 79: 39S ribosomal protein L53, mitochondrial



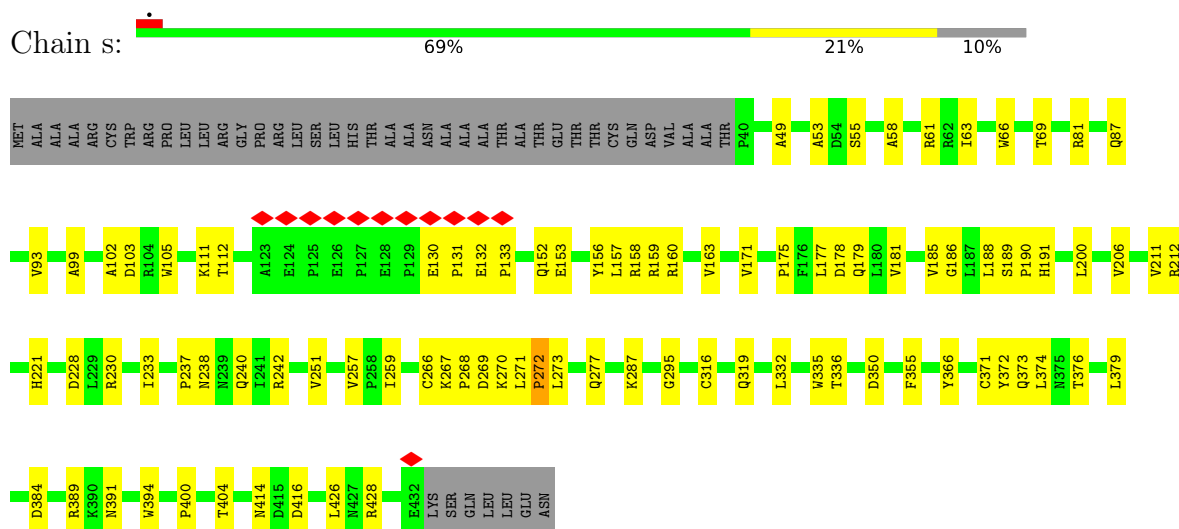
- Molecule 80: 39S ribosomal protein L54, mitochondrial



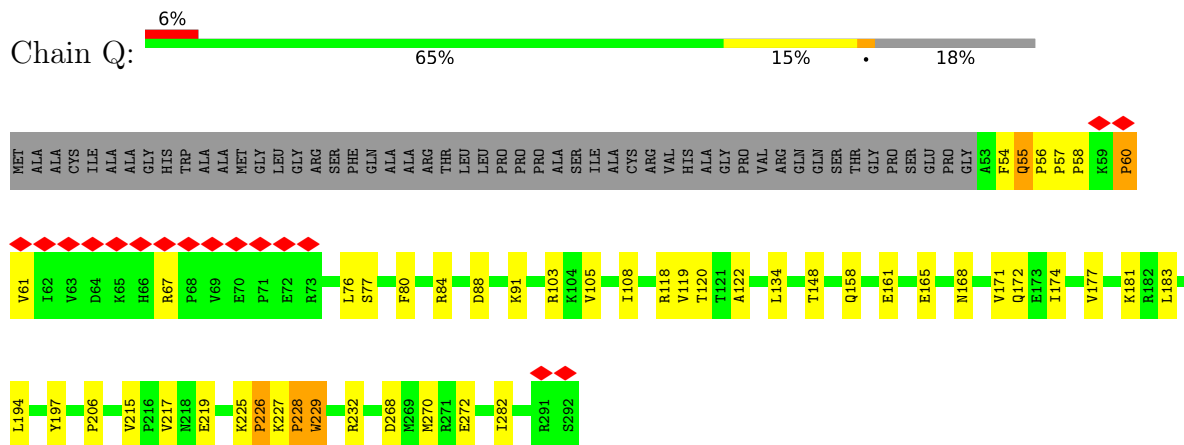
- Molecule 81: Peptidyl-tRNA hydrolase ICT1, mitochondrial



- Molecule 82: 39S ribosomal protein S30, mitochondrial

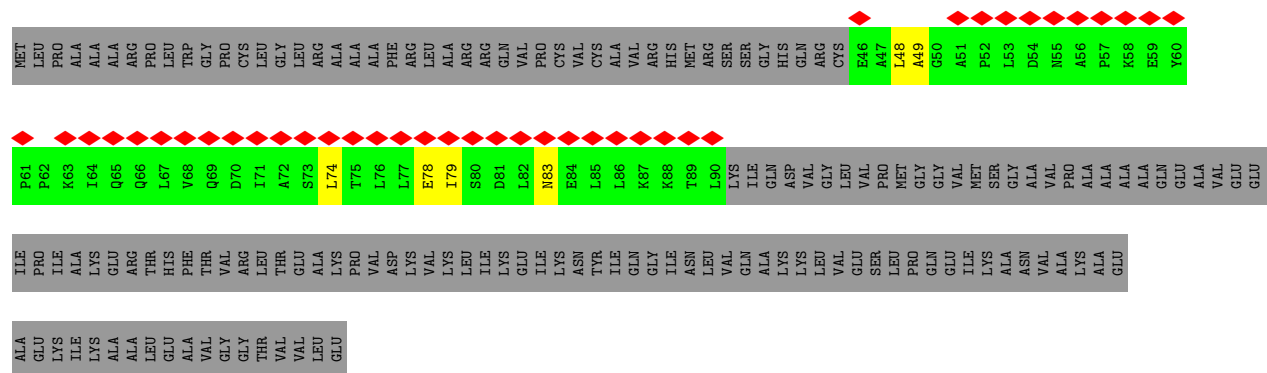


- Molecule 83: 39S ribosomal protein L19, mitochondrial

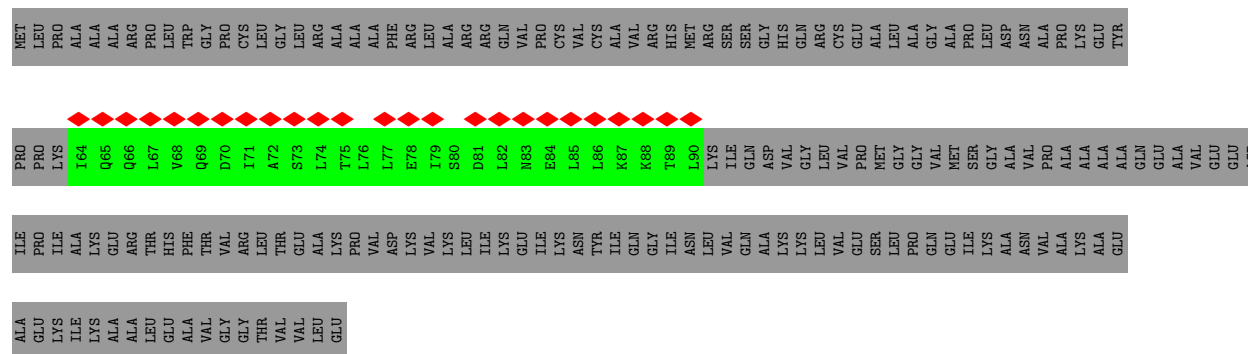


- Molecule 84: 39S ribosomal protein L12, mitochondrial

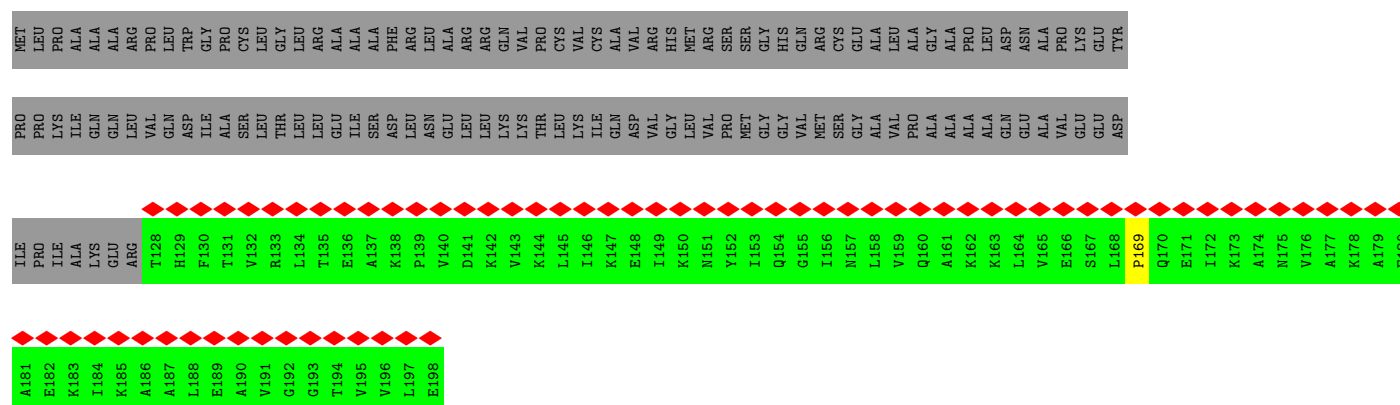




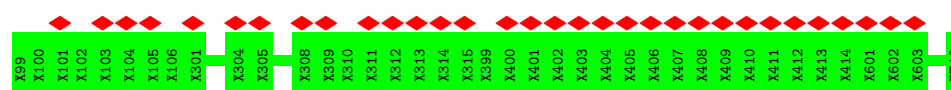
- Molecule 84: 39S ribosomal protein L12, mitochondrial



- Molecule 84: 39S ribosomal protein L12, mitochondrial

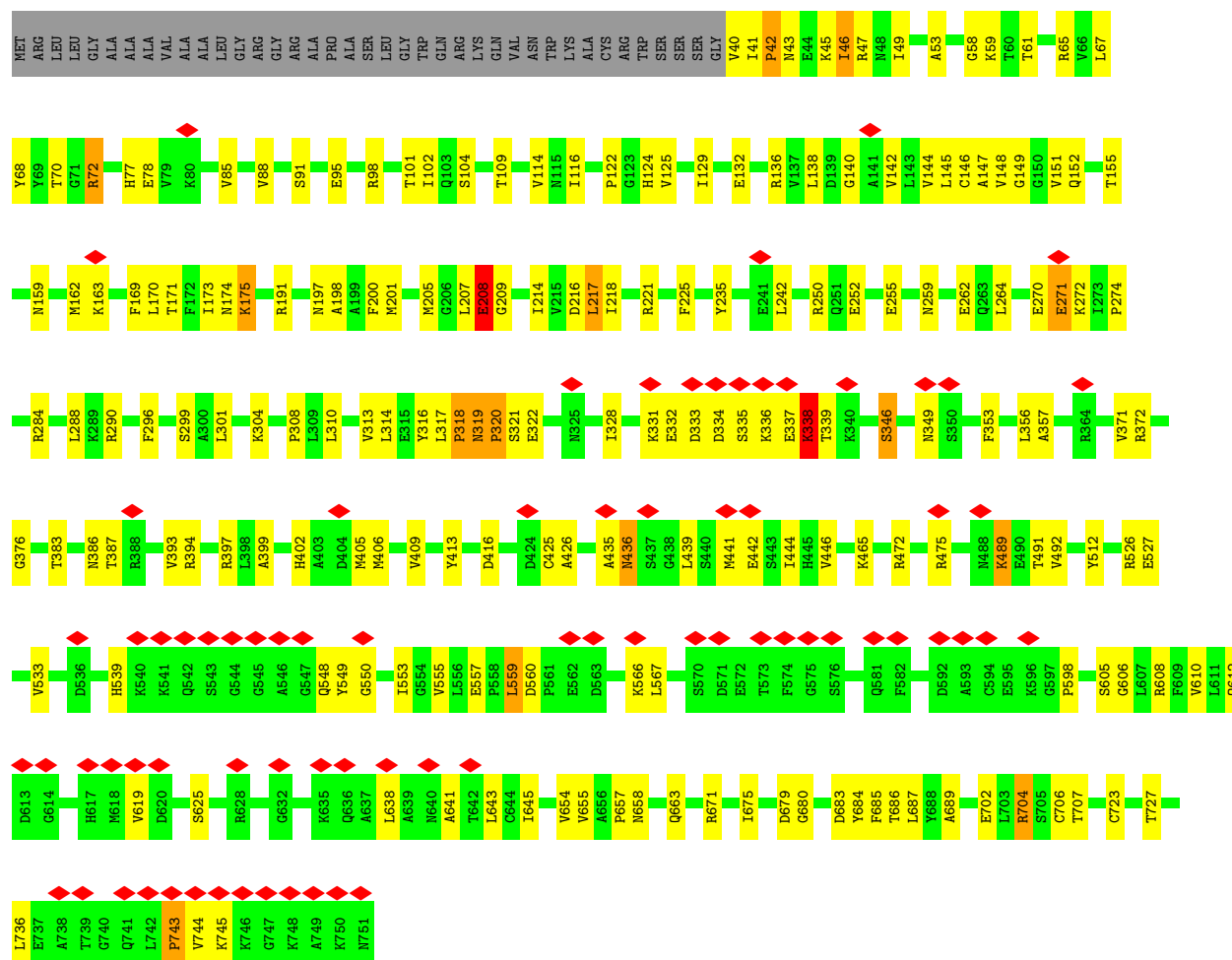


- Molecule 85: P-site finger

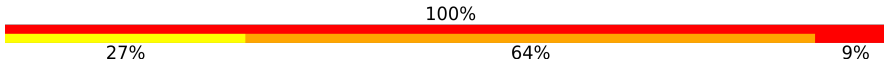


• Molecule 86: Elongation factor G, mitochondrial

Chain v: 



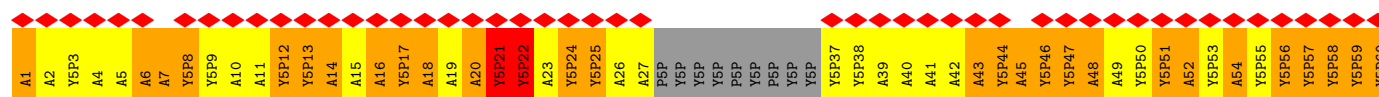
• Molecule 87: mRNA

Chain A5: 



• Molecule 88: E-tRNA

Chain A7: 



Y5P61	◆
Y5P62	◆
Y5P63	◆
Y5P64	◆
Y5P65	◆
Y5P66	◆
Y5P67	◆
Y5P68	◆
Y5P69	◆
Y5P70	◆
471	◆

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99804	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 ($e^-/\text{\AA}^2$)	69.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.725	Depositor
Minimum map value	-1.810	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.267	Depositor
Map size ($\text{\AA}$)	438.44, 438.44, 438.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, Y5P, P5P, GDP, GCP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.06	0/22406	0.16	0/34881
2	AB	0.07	0/1830	0.23	0/2477
3	AC	0.07	0/1112	0.24	0/1505
4	AE	0.09	0/989	0.37	0/1335
5	AI	0.08	0/1031	0.34	0/1390
6	AJ	0.09	0/854	0.27	0/1148
7	AK	0.09	0/879	0.29	0/1182
8	AM	0.08	0/941	0.25	0/1265
9	AN	0.07	0/864	0.22	0/1169
10	AO	0.08	0/1624	0.22	0/2209
11	AP	0.07	0/791	0.21	0/1062
12	AQ	0.09	0/752	0.27	0/1001
13	AT	0.08	0/1402	0.21	0/1883
14	AW	0.08	0/778	0.27	0/1048
15	AX	0.08	0/2932	0.22	0/3968
16	A2	0.09	0/939	0.27	0/1256
17	AH	0.07	0/1037	0.21	0/1403
18	AL	0.09	0/1475	0.24	0/1970
19	AR	0.07	0/2435	0.21	0/3288
20	AS	0.09	0/1138	0.24	0/1533
21	AU	0.10	0/1521	0.26	0/2039
22	AV	0.08	0/3071	0.22	0/4147
23	AY	0.10	0/1046	0.34	0/1410
24	AZ	0.07	0/851	0.22	0/1133
25	A1	0.08	0/2277	0.24	0/3079
26	A0	0.08	0/1827	0.26	0/2473
27	A3	0.10	0/650	0.31	0/855
28	A4	0.06	0/3028	0.16	0/4197
29	AD	0.07	0/2783	0.23	0/3724
30	AF	0.09	0/1765	0.27	0/2369
31	AG	0.07	0/2642	0.23	0/3538
32	A	0.07	0/36246	0.18	0/56422

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B	0.06	0/1328	0.15	0/2056
34	D	0.08	0/1904	0.25	0/2561
35	F	0.08	0/2071	0.26	0/2817
36	H	0.10	0/820	0.29	0/1102
37	K	0.07	0/1495	0.24	0/2029
38	L	0.07	0/904	0.24	0/1218
39	M	0.09	0/2359	0.27	0/3185
40	O	0.10	0/1269	0.29	0/1708
41	R	0.10	0/1174	0.44	2/1572 (0.1%)
42	S	0.10	0/1276	0.40	3/1729 (0.2%)
43	T	0.07	0/1402	0.24	0/1886
44	W	0.07	0/893	0.22	0/1204
45	X	0.07	0/2081	0.23	0/2812
46	Y	0.08	0/1552	0.25	0/2079
47	Z	0.07	0/1003	0.23	0/1354
48	0	0.08	0/895	0.26	0/1201
49	1	0.07	0/438	0.26	0/583
50	2	0.08	0/382	0.27	0/507
51	3	0.08	0/852	0.24	0/1136
52	4	0.09	0/350	0.30	0/461
53	8	0.09	0/855	0.24	0/1152
54	b	0.08	0/1202	0.26	0/1626
55	e	0.08	0/1797	0.25	0/2422
56	g	0.12	0/1132	0.30	0/1543
57	i	0.09	0/849	0.27	0/1135
58	j	0.08	0/755	0.25	0/1016
59	m	0.09	0/379	0.28	0/510
60	o	0.11	0/818	0.36	0/1097
61	q	0.10	0/1325	0.33	0/1799
62	r	0.09	0/1362	0.25	0/1846
63	J	0.27	1/1348 (0.1%)	0.38	0/1813
64	I	0.09	0/1467	0.28	0/1984
65	N	0.08	0/1833	0.25	0/2468
66	P	0.15	0/1191	0.38	0/1611
67	U	0.10	0/1254	0.27	0/1700
68	V	0.09	0/1727	0.25	0/2341
69	E	0.07	0/2479	0.20	0/3360
70	5	0.17	1/3305 (0.0%)	0.31	0/4502
71	6	0.08	0/3043	0.24	0/4140
72	7	0.07	0/2467	0.22	0/3337
73	9	0.08	0/1025	0.24	0/1379
74	a	0.08	0/923	0.22	0/1254
75	c	0.08	0/2371	0.23	0/3205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	d	0.09	0/2132	0.25	0/2887
77	f	0.06	0/1144	0.21	0/1551
78	h	0.08	0/917	0.24	0/1249
79	k	0.10	0/754	0.27	0/1017
80	l	0.08	0/636	0.23	0/860
81	p	0.09	0/1246	0.25	0/1675
82	s	0.09	0/3262	0.29	0/4435
83	Q	0.11	0/2044	0.27	0/2757
84	TA	0.12	0/349	0.39	0/475
84	TB	0.06	0/212	0.16	0/286
84	TC	0.07	0/351	0.27	0/488
86	v	0.14	0/5647	0.34	0/7623
All	All	0.09	2/181965 (0.0%)	0.24	5/258102 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
41	R	0	1
42	S	0	1
56	g	0	1
66	P	0	1
82	s	0	1
86	v	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	J	188	GLU	C-N	8.15	1.45	1.34
70	5	69	TRP	NE1-CE2	-5.47	1.31	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	S	144	LEU	CA-C-N	-6.20	109.27	121.41
42	S	144	LEU	C-N-CA	-6.20	109.27	121.41
42	S	145	GLY	N-CA-C	5.96	127.31	113.18
41	R	136	LYS	CA-C-N	5.65	135.58	121.80
41	R	136	LYS	C-N-CA	5.65	135.58	121.80

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	P	72	PHE	Peptide
41	R	134	ASP	Peptide
42	S	144	LEU	Peptide
56	g	79	PRO	Peptide
82	s	160	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	20030	0	10171	256	0
2	AB	1787	0	1779	27	0
3	AC	1082	0	1088	25	0
4	AE	972	0	1001	13	0
5	AI	1011	0	1052	14	0
6	AJ	838	0	887	17	0
7	AK	861	0	885	23	0
8	AM	920	0	951	13	0
9	AN	846	0	908	14	0
10	AO	1570	0	1534	18	0
11	AP	774	0	803	11	0
12	AQ	740	0	754	12	0
13	AT	1371	0	1396	14	0
14	AW	766	0	785	13	0
15	AX	2860	0	2856	43	0
16	A2	925	0	964	15	0
17	AH	1014	0	1036	20	0
18	AL	1451	0	1543	15	0
19	AR	2388	0	2410	28	0
20	AS	1111	0	1115	7	0
21	AU	1499	0	1512	13	0
22	AV	3009	0	3006	51	0
23	AY	1016	0	962	17	0
24	AZ	833	0	853	13	0
25	A1	2231	0	2261	28	0
26	A0	1781	0	1791	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A3	639	0	715	5	0
28	A4	3010	0	1760	14	0
29	AD	2731	0	2802	48	0
30	AF	1724	0	1765	17	0
31	AG	2587	0	2572	24	0
32	A	32395	0	16450	525	0
33	B	1191	0	607	12	0
34	D	1866	0	1927	30	0
35	F	2013	0	2044	35	0
36	H	806	0	849	18	0
37	K	1451	0	1448	15	0
38	L	889	0	941	18	0
39	M	2305	0	2378	44	0
40	O	1245	0	1283	17	0
41	R	1153	0	1214	16	0
42	S	1251	0	1322	27	0
43	T	1368	0	1410	16	0
44	W	871	0	897	12	0
45	X	2027	0	2040	30	0
46	Y	1517	0	1561	27	0
47	Z	978	0	1030	10	0
48	0	880	0	904	11	0
49	1	433	0	475	20	0
50	2	376	0	406	13	0
51	3	831	0	883	20	0
52	4	342	0	362	6	0
53	8	836	0	844	17	0
54	b	1178	0	1180	10	0
55	e	1762	0	1767	33	0
56	g	1096	0	1081	22	0
57	i	827	0	857	17	0
58	j	740	0	741	9	0
59	m	372	0	387	5	0
60	o	797	0	804	14	0
61	q	1294	0	1178	20	0
62	r	1322	0	1350	22	0
63	J	1330	0	1405	129	0
64	I	1435	0	1519	81	0
65	N	1786	0	1817	33	0
66	P	1165	0	1162	32	0
67	U	1224	0	1191	26	0
68	V	1682	0	1692	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	E	2410	0	2418	37	0
70	5	3210	0	3206	111	0
71	6	2948	0	2841	53	0
72	7	2410	0	2415	32	0
73	9	997	0	987	12	0
74	a	896	0	847	15	0
75	c	2322	0	2338	23	0
76	d	2075	0	2037	30	0
77	f	1126	0	1106	24	0
78	h	894	0	881	9	0
79	k	743	0	758	13	0
80	l	619	0	611	47	0
81	p	1227	0	1239	23	0
82	s	3178	0	3124	65	0
83	Q	1995	0	2036	37	0
84	TA	345	0	364	5	0
84	TB	213	0	234	0	0
84	TC	352	0	169	0	0
85	u	325	0	76	0	0
86	v	5546	0	5505	142	0
87	A5	213	0	122	14	0
88	A7	1197	0	690	33	0
89	A	97	0	0	0	0
89	A2	1	0	0	0	0
89	AA	26	0	0	0	0
89	AH	1	0	0	0	0
89	D	1	0	0	0	0
89	E	1	0	0	0	0
89	W	1	0	0	0	0
89	g	1	0	0	0	0
89	v	1	0	0	0	0
90	0	1	0	0	0	0
90	4	1	0	0	0	0
90	AB	1	0	0	0	0
90	AO	1	0	0	0	0
90	AP	1	0	0	0	0
90	AT	1	0	0	0	0
90	r	1	0	0	0	0
91	AX	28	0	9	0	0
92	v	32	0	14	33	0
All	All	174849	0	147350	2370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2370 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:5:60:PHE:CD1	70:5:71:ALA:HB1	1.25	1.65
63:J:171:ARG:HA	63:J:174:PHE:CE2	1.29	1.65
70:5:68:PRO:HG2	70:5:69:TRP:CE3	1.24	1.63
63:J:132:LEU:HG	64:I:114:HIS:CG	1.40	1.52
45:X:156:LYS:NZ	70:5:70:LEU:HD23	1.25	1.47

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	218/296 (74%)	187 (86%)	27 (12%)	4 (2%)	6	28
3	AC	130/167 (78%)	107 (82%)	22 (17%)	1 (1%)	16	47
4	AE	120/125 (96%)	98 (82%)	18 (15%)	4 (3%)	3	15
5	AI	134/194 (69%)	113 (84%)	18 (13%)	3 (2%)	5	24
6	AJ	106/138 (77%)	92 (87%)	12 (11%)	2 (2%)	6	27
7	AK	99/128 (77%)	88 (89%)	8 (8%)	3 (3%)	3	17
8	AM	114/137 (83%)	103 (90%)	10 (9%)	1 (1%)	14	45
9	AN	105/130 (81%)	85 (81%)	18 (17%)	2 (2%)	6	27
10	AO	188/258 (73%)	166 (88%)	18 (10%)	4 (2%)	5	25
11	AP	94/142 (66%)	82 (87%)	10 (11%)	2 (2%)	5	25
12	AQ	84/87 (97%)	71 (84%)	13 (16%)	0	100	100
13	AT	166/173 (96%)	149 (90%)	16 (10%)	1 (1%)	21	53
14	AW	95/187 (51%)	77 (81%)	15 (16%)	3 (3%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AX	351/398 (88%)	319 (91%)	28 (8%)	4 (1%)	11	40
16	A2	114/118 (97%)	96 (84%)	17 (15%)	1 (1%)	14	45
17	AH	120/201 (60%)	101 (84%)	16 (13%)	3 (2%)	4	21
18	AL	172/257 (67%)	154 (90%)	15 (9%)	3 (2%)	7	30
19	AR	290/360 (81%)	263 (91%)	26 (9%)	1 (0%)	36	67
20	AS	133/190 (70%)	119 (90%)	10 (8%)	4 (3%)	3	17
21	AU	175/205 (85%)	163 (93%)	12 (7%)	0	100	100
22	AV	363/414 (88%)	319 (88%)	36 (10%)	8 (2%)	5	24
23	AY	118/395 (30%)	107 (91%)	10 (8%)	1 (1%)	16	47
24	AZ	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
25	A1	273/323 (84%)	242 (89%)	25 (9%)	6 (2%)	5	24
26	A0	212/218 (97%)	185 (87%)	22 (10%)	5 (2%)	4	22
27	A3	70/199 (35%)	64 (91%)	6 (9%)	0	100	100
28	A4	541/689 (78%)	465 (86%)	66 (12%)	10 (2%)	6	28
29	AD	341/430 (79%)	306 (90%)	31 (9%)	4 (1%)	10	38
30	AF	206/242 (85%)	180 (87%)	23 (11%)	3 (2%)	8	33
31	AG	311/396 (78%)	272 (88%)	37 (12%)	2 (1%)	21	53
34	D	237/305 (78%)	208 (88%)	27 (11%)	2 (1%)	16	47
35	F	248/311 (80%)	217 (88%)	27 (11%)	4 (2%)	7	31
36	H	96/267 (36%)	84 (88%)	10 (10%)	2 (2%)	5	25
37	K	175/178 (98%)	153 (87%)	16 (9%)	6 (3%)	3	15
38	L	113/145 (78%)	102 (90%)	10 (9%)	1 (1%)	14	45
39	M	285/296 (96%)	252 (88%)	26 (9%)	7 (2%)	4	21
40	O	150/175 (86%)	128 (85%)	19 (13%)	3 (2%)	6	26
41	R	138/149 (93%)	123 (89%)	10 (7%)	5 (4%)	2	14
42	S	154/205 (75%)	135 (88%)	15 (10%)	4 (3%)	4	20
43	T	164/212 (77%)	148 (90%)	13 (8%)	3 (2%)	6	28
44	W	109/148 (74%)	97 (89%)	11 (10%)	1 (1%)	14	45
45	X	241/256 (94%)	212 (88%)	24 (10%)	5 (2%)	5	25
46	Y	174/250 (70%)	161 (92%)	7 (4%)	6 (3%)	3	15
47	Z	118/161 (73%)	106 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	0	106/188 (56%)	93 (88%)	10 (9%)	3 (3%)	4	19
49	1	50/65 (77%)	42 (84%)	7 (14%)	1 (2%)	6	26
50	2	44/92 (48%)	41 (93%)	2 (4%)	1 (2%)	5	23
51	3	93/188 (50%)	84 (90%)	8 (9%)	1 (1%)	11	40
52	4	36/103 (35%)	34 (94%)	2 (6%)	0	100	100
53	8	97/206 (47%)	85 (88%)	12 (12%)	0	100	100
54	b	146/155 (94%)	129 (88%)	14 (10%)	3 (2%)	5	25
55	e	211/279 (76%)	188 (89%)	22 (10%)	1 (0%)	24	58
56	g	130/166 (78%)	109 (84%)	17 (13%)	4 (3%)	3	16
57	i	95/128 (74%)	75 (79%)	20 (21%)	0	100	100
58	j	91/123 (74%)	84 (92%)	6 (7%)	1 (1%)	11	40
59	m	43/128 (34%)	34 (79%)	8 (19%)	1 (2%)	5	23
60	o	92/102 (90%)	79 (86%)	10 (11%)	3 (3%)	3	15
61	q	166/222 (75%)	154 (93%)	10 (6%)	2 (1%)	10	38
62	r	160/196 (82%)	139 (87%)	16 (10%)	5 (3%)	3	16
63	J	173/192 (90%)	152 (88%)	15 (9%)	6 (4%)	3	14
64	I	177/261 (68%)	164 (93%)	12 (7%)	1 (1%)	21	53
65	N	220/251 (88%)	203 (92%)	16 (7%)	1 (0%)	24	58
66	P	141/179 (79%)	123 (87%)	14 (10%)	4 (3%)	4	19
67	U	150/153 (98%)	122 (81%)	26 (17%)	2 (1%)	9	36
68	V	204/216 (94%)	179 (88%)	25 (12%)	0	100	100
69	E	304/348 (87%)	268 (88%)	32 (10%)	4 (1%)	9	36
70	5	392/423 (93%)	347 (88%)	41 (10%)	4 (1%)	12	42
71	6	352/380 (93%)	302 (86%)	47 (13%)	3 (1%)	14	45
72	7	295/338 (87%)	260 (88%)	28 (10%)	7 (2%)	4	22
73	9	122/137 (89%)	106 (87%)	15 (12%)	1 (1%)	16	47
74	a	106/142 (75%)	95 (90%)	8 (8%)	3 (3%)	4	19
75	c	287/332 (86%)	265 (92%)	18 (6%)	4 (1%)	9	34
76	d	255/306 (83%)	216 (85%)	33 (13%)	6 (2%)	4	22
77	f	144/194 (74%)	121 (84%)	22 (15%)	1 (1%)	18	50
78	h	108/158 (68%)	93 (86%)	13 (12%)	2 (2%)	6	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	k	94/112 (84%)	85 (90%)	9 (10%)	0	100	100
80	l	70/138 (51%)	62 (89%)	7 (10%)	1 (1%)	9	34
81	p	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	34
82	s	391/439 (89%)	342 (88%)	41 (10%)	8 (2%)	6	26
83	Q	238/292 (82%)	211 (89%)	20 (8%)	7 (3%)	3	18
84	TA	43/198 (22%)	32 (74%)	11 (26%)	0	100	100
84	TB	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
84	TC	69/198 (35%)	57 (83%)	11 (16%)	1 (1%)	9	34
86	v	710/751 (94%)	566 (80%)	117 (16%)	27 (4%)	2	13
All	All	14720/19244 (76%)	12876 (88%)	1589 (11%)	255 (2%)	9	30

5 of 255 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AI	68	GLY
22	AV	35	VAL
28	A4	203	PRO
40	O	111	PRO
41	R	137	GLU

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	
2	AB	193/249 (78%)	191 (99%)	2 (1%)	68	83
3	AC	115/143 (80%)	115 (100%)	0	100	100
4	AE	104/107 (97%)	103 (99%)	1 (1%)	68	83
5	AI	104/147 (71%)	102 (98%)	2 (2%)	50	75
6	AJ	93/118 (79%)	93 (100%)	0	100	100
7	AK	91/113 (80%)	91 (100%)	0	100	100
8	AM	95/113 (84%)	94 (99%)	1 (1%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AN	93/115 (81%)	92 (99%)	1 (1%)	65	82
10	AO	171/230 (74%)	170 (99%)	1 (1%)	78	88
11	AP	87/123 (71%)	86 (99%)	1 (1%)	65	82
12	AQ	78/79 (99%)	78 (100%)	0	100	100
13	AT	153/157 (98%)	152 (99%)	1 (1%)	76	87
14	AW	84/158 (53%)	84 (100%)	0	100	100
15	AX	312/351 (89%)	311 (100%)	1 (0%)	86	91
16	A2	99/101 (98%)	97 (98%)	2 (2%)	48	75
17	AH	112/180 (62%)	111 (99%)	1 (1%)	70	85
18	AL	157/226 (70%)	156 (99%)	1 (1%)	78	88
19	AR	262/318 (82%)	260 (99%)	2 (1%)	73	86
20	AS	116/164 (71%)	114 (98%)	2 (2%)	53	77
21	AU	153/174 (88%)	153 (100%)	0	100	100
22	AV	328/364 (90%)	324 (99%)	4 (1%)	63	82
23	AY	111/357 (31%)	110 (99%)	1 (1%)	70	85
24	AZ	89/95 (94%)	89 (100%)	0	100	100
25	A1	253/291 (87%)	253 (100%)	0	100	100
26	A0	186/190 (98%)	186 (100%)	0	100	100
27	A3	66/166 (40%)	64 (97%)	2 (3%)	36	67
28	A4	83/609 (14%)	83 (100%)	0	100	100
29	AD	286/357 (80%)	286 (100%)	0	100	100
30	AF	185/209 (88%)	181 (98%)	4 (2%)	45	73
31	AG	273/342 (80%)	272 (100%)	1 (0%)	84	90
34	D	193/245 (79%)	193 (100%)	0	100	100
35	F	217/262 (83%)	215 (99%)	2 (1%)	70	85
36	H	88/228 (39%)	88 (100%)	0	100	100
37	K	155/156 (99%)	155 (100%)	0	100	100
38	L	98/124 (79%)	97 (99%)	1 (1%)	68	83
39	M	245/249 (98%)	245 (100%)	0	100	100
40	O	133/150 (89%)	132 (99%)	1 (1%)	73	86
41	R	118/126 (94%)	117 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	S	141/180 (78%)	141 (100%)	0	100	100
43	T	146/182 (80%)	145 (99%)	1 (1%)	76	87
44	W	91/119 (76%)	91 (100%)	0	100	100
45	X	217/227 (96%)	212 (98%)	5 (2%)	44	72
46	Y	159/223 (71%)	157 (99%)	2 (1%)	61	81
47	Z	111/147 (76%)	111 (100%)	0	100	100
48	0	97/164 (59%)	97 (100%)	0	100	100
49	1	49/60 (82%)	48 (98%)	1 (2%)	48	75
50	2	40/72 (56%)	39 (98%)	1 (2%)	42	71
51	3	88/166 (53%)	86 (98%)	2 (2%)	44	72
52	4	37/89 (42%)	37 (100%)	0	100	100
53	8	91/190 (48%)	91 (100%)	0	100	100
54	b	130/135 (96%)	130 (100%)	0	100	100
55	e	188/236 (80%)	186 (99%)	2 (1%)	65	82
56	g	122/148 (82%)	119 (98%)	3 (2%)	42	71
57	i	86/110 (78%)	84 (98%)	2 (2%)	44	72
58	j	74/97 (76%)	74 (100%)	0	100	100
59	m	40/113 (35%)	40 (100%)	0	100	100
60	o	80/87 (92%)	79 (99%)	1 (1%)	61	81
61	q	114/178 (64%)	113 (99%)	1 (1%)	70	85
62	r	147/169 (87%)	146 (99%)	1 (1%)	76	87
63	J	138/150 (92%)	135 (98%)	3 (2%)	45	73
64	I	164/232 (71%)	160 (98%)	4 (2%)	43	72
65	N	189/211 (90%)	188 (100%)	1 (0%)	81	89
66	P	125/154 (81%)	124 (99%)	1 (1%)	73	86
67	U	126/135 (93%)	125 (99%)	1 (1%)	73	86
68	V	184/191 (96%)	182 (99%)	2 (1%)	65	82
69	E	260/290 (90%)	259 (100%)	1 (0%)	84	90
70	5	353/368 (96%)	350 (99%)	3 (1%)	73	86
71	6	313/332 (94%)	308 (98%)	5 (2%)	55	78
72	7	272/303 (90%)	272 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	9	104/112 (93%)	103 (99%)	1 (1%)	68	83
74	a	101/133 (76%)	101 (100%)	0	100	100
75	c	253/288 (88%)	253 (100%)	0	100	100
76	d	224/274 (82%)	220 (98%)	4 (2%)	51	76
77	f	122/173 (70%)	122 (100%)	0	100	100
78	h	104/148 (70%)	103 (99%)	1 (1%)	68	83
79	k	81/90 (90%)	79 (98%)	2 (2%)	42	71
80	l	67/116 (58%)	67 (100%)	0	100	100
81	p	134/181 (74%)	131 (98%)	3 (2%)	45	73
82	s	336/381 (88%)	335 (100%)	1 (0%)	86	91
83	Q	221/256 (86%)	220 (100%)	1 (0%)	81	89
84	TA	39/158 (25%)	39 (100%)	0	100	100
84	TB	26/158 (16%)	26 (100%)	0	100	100
86	v	598/630 (95%)	576 (96%)	22 (4%)	30	62
All	All	12561/16442 (76%)	12447 (99%)	114 (1%)	68	85

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
62	r	146	GLN
86	v	492	VAL
70	5	46	LEU
86	v	491	THR
86	v	145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 262 such sidechains are listed below:

Mol	Chain	Res	Type
80	l	129	HIS
82	s	207	HIS
86	v	622	ASN
35	F	58	HIS
34	D	195	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	940/954 (98%)	191 (20%)	7 (0%)
32	A	1523/1559 (97%)	347 (22%)	18 (1%)
33	B	51/73 (69%)	6 (11%)	1 (1%)
All	All	2514/2586 (97%)	544 (21%)	26 (1%)

5 of 544 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	650	U
1	AA	651	A
1	AA	674	U
1	AA	676	G
1	AA	680	U

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	A	2165	C
32	A	2457	A
32	A	3196	G
32	A	2245	A
32	A	2507	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	P5P	A7	18	88	20,23,24	1.00	3 (15%)	27,33,36	2.04	4 (14%)
88	P5P	A7	20	88	20,23,24	0.98	3 (15%)	27,33,36	2.01	5 (18%)
87	P5P	A5	6	87	20,23,24	1.05	3 (15%)	27,33,36	2.03	5 (18%)
88	P5P	A7	14	88	20,23,24	1.01	2 (10%)	27,33,36	1.99	3 (11%)
87	Y5P	A5	4	87	14,19,20	4.80	2 (14%)	18,26,29	1.83	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	P5P	A7	15	88	20,23,24	1.06	3 (15%)	27,33,36	1.99	5 (18%)
88	Y5P	A7	25	88	14,19,20	4.33	2 (14%)	18,26,29	1.39	3 (16%)
88	P5P	A7	27	88	20,23,24	0.99	2 (10%)	27,33,36	2.08	4 (14%)
88	P5P	A7	52	88	20,23,24	1.13	3 (15%)	27,33,36	1.97	5 (18%)
88	Y5P	A7	53	88	14,19,20	4.65	2 (14%)	18,26,29	1.55	3 (16%)
88	Y5P	A7	55	88	14,19,20	4.46	2 (14%)	18,26,29	1.50	3 (16%)
88	Y5P	A7	66	88	14,19,20	4.60	2 (14%)	18,26,29	1.48	2 (11%)
88	Y5P	A7	9	88	14,19,20	4.65	2 (14%)	18,26,29	1.78	3 (16%)
88	Y5P	A7	61	88	14,19,20	4.46	2 (14%)	18,26,29	1.42	3 (16%)
88	Y5P	A7	21	88	14,19,20	4.38	2 (14%)	18,26,29	1.45	3 (16%)
88	Y5P	A7	70	88	14,19,20	4.48	2 (14%)	18,26,29	1.45	2 (11%)
88	P5P	A7	6	88	20,23,24	1.02	3 (15%)	27,33,36	2.10	5 (18%)
88	Y5P	A7	59	88	14,19,20	4.76	2 (14%)	18,26,29	1.46	3 (16%)
88	Y5P	A7	58	88	14,19,20	4.57	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A7	24	88	14,19,20	4.17	2 (14%)	18,26,29	1.36	2 (11%)
87	Y5P	A5	8	87	14,19,20	4.66	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A7	42	88	20,23,24	0.97	3 (15%)	27,33,36	2.03	4 (14%)
88	Y5P	A7	44	88	14,19,20	4.69	2 (14%)	18,26,29	1.45	2 (11%)
88	Y5P	A7	37	88	14,19,20	4.37	2 (14%)	18,26,29	1.41	3 (16%)
88	P5P	A7	10	88	20,23,24	0.99	2 (10%)	27,33,36	1.98	4 (14%)
87	P5P	A5	5	87	20,23,24	1.07	3 (15%)	27,33,36	1.97	4 (14%)
87	Y5P	A5	7	87	14,19,20	4.60	2 (14%)	18,26,29	1.43	3 (16%)
88	P5P	A7	40	88	20,23,24	1.00	3 (15%)	27,33,36	2.05	5 (18%)
88	P5P	A7	1	88	20,20,24	0.97	1 (5%)	28,29,36	1.95	4 (14%)
88	Y5P	A7	56	88	14,19,20	4.55	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A7	46	88	14,19,20	4.53	2 (14%)	18,26,29	1.49	3 (16%)
87	P5P	A5	2	87	20,23,24	1.10	2 (10%)	27,33,36	1.98	4 (14%)
88	P5P	A7	26	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
88	P5P	A7	16	88	20,23,24	1.08	3 (15%)	27,33,36	2.14	6 (22%)
88	P5P	A7	45	88	20,23,24	1.05	2 (10%)	27,33,36	2.15	4 (14%)
88	Y5P	A7	47	88	14,19,20	4.57	2 (14%)	18,26,29	1.52	3 (16%)
87	P5P	A5	9	87	20,23,24	1.01	3 (15%)	27,33,36	1.96	4 (14%)
88	Y5P	A7	22	88	14,19,20	4.28	2 (14%)	18,26,29	1.42	3 (16%)
88	P5P	A7	41	88	20,23,24	1.04	3 (15%)	27,33,36	1.94	5 (18%)
88	P5P	A7	48	88	20,23,24	1.02	3 (15%)	27,33,36	2.08	5 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	Y5P	A7	50	88	14,19,20	4.53	2 (14%)	18,26,29	1.39	2 (11%)
88	P5P	A7	54	88	20,23,24	1.08	3 (15%)	27,33,36	1.93	3 (11%)
88	Y5P	A7	68	88	14,19,20	4.73	2 (14%)	18,26,29	1.69	4 (22%)
88	P5P	A7	43	88	20,23,24	1.11	2 (10%)	27,33,36	2.08	4 (14%)
88	Y5P	A7	63	88	14,19,20	4.55	2 (14%)	18,26,29	1.49	3 (16%)
88	P5P	A7	11	88	20,23,24	0.98	3 (15%)	27,33,36	2.09	5 (18%)
88	Y5P	A7	51	88	14,19,20	4.35	2 (14%)	18,26,29	1.44	3 (16%)
88	P5P	A7	5	88	20,23,24	1.00	2 (10%)	27,33,36	2.02	4 (14%)
88	P5P	A7	39	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
88	Y5P	A7	12	88	14,19,20	4.28	2 (14%)	18,26,29	1.39	3 (16%)
87	Y5P	A5	3	87	14,19,20	4.47	2 (14%)	18,26,29	1.63	3 (16%)
88	P5P	A7	4	88	20,23,24	1.07	3 (15%)	27,33,36	2.13	5 (18%)
88	P5P	A7	23	88	20,23,24	1.03	3 (15%)	27,33,36	1.92	4 (14%)
88	P5P	A7	71	32,88	20,23,24	0.96	3 (15%)	27,33,36	1.91	3 (11%)
87	Y5P	A5	10	87	14,19,20	4.50	2 (14%)	18,26,29	1.46	3 (16%)
88	P5P	A7	2	88	20,23,24	1.02	2 (10%)	27,33,36	2.12	4 (14%)
88	Y5P	A7	17	88	14,19,20	4.60	2 (14%)	18,26,29	1.42	2 (11%)
87	Y5P	A5	1	87	14,19,20	4.81	2 (14%)	18,26,29	1.85	3 (16%)
88	Y5P	A7	3	88	14,19,20	4.38	2 (14%)	18,26,29	1.50	3 (16%)
88	Y5P	A7	65	88	14,19,20	4.62	2 (14%)	18,26,29	1.46	3 (16%)
88	Y5P	A7	67	88	14,19,20	4.64	2 (14%)	18,26,29	1.61	3 (16%)
88	P5P	A7	49	88	20,23,24	1.01	3 (15%)	27,33,36	2.05	5 (18%)
88	Y5P	A7	60	88	14,19,20	4.45	2 (14%)	18,26,29	1.57	2 (11%)
88	Y5P	A7	13	88	14,19,20	4.19	2 (14%)	18,26,29	1.28	2 (11%)
88	Y5P	A7	38	88	14,19,20	4.37	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A7	64	88	14,19,20	4.52	2 (14%)	18,26,29	1.35	2 (11%)
88	Y5P	A7	69	88	14,19,20	4.64	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A7	19	88	20,23,24	1.04	3 (15%)	27,33,36	2.15	5 (18%)
88	Y5P	A7	57	88	14,19,20	4.47	2 (14%)	18,26,29	1.45	3 (16%)
88	Y5P	A7	62	88	14,19,20	4.41	2 (14%)	18,26,29	1.49	3 (16%)
88	P5P	A7	7	88	20,23,24	0.97	2 (10%)	27,33,36	2.07	4 (14%)
88	Y5P	A7	8	88	14,19,20	4.65	2 (14%)	18,26,29	1.41	3 (16%)
87	P5P	A5	11	87	20,23,24	1.01	3 (15%)	27,33,36	1.97	5 (18%)

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
88	P5P	A7	18	88	-	1/7/25/26	0/3/3/3
88	P5P	A7	20	88	-	0/7/25/26	0/3/3/3
87	P5P	A5	6	87	-	0/7/25/26	0/3/3/3
88	P5P	A7	14	88	-	2/7/25/26	0/3/3/3
87	Y5P	A5	4	87	-	7/7/33/34	0/2/2/2
88	P5P	A7	15	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	25	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	27	88	-	1/7/25/26	0/3/3/3
88	P5P	A7	52	88	-	6/7/25/26	0/3/3/3
88	Y5P	A7	53	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	55	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	66	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	9	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	61	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	21	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	70	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	6	88	-	4/7/25/26	0/3/3/3
88	Y5P	A7	59	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	58	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	24	88	-	1/7/33/34	0/2/2/2
87	Y5P	A5	8	87	-	3/7/33/34	0/2/2/2
88	P5P	A7	42	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	44	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	37	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	10	88	-	0/7/25/26	0/3/3/3
87	P5P	A5	5	87	-	2/7/25/26	0/3/3/3
87	Y5P	A5	7	87	-	3/7/33/34	0/2/2/2
88	P5P	A7	40	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	1	88	-	0/6/22/26	0/3/3/3
88	Y5P	A7	56	88	-	4/7/33/34	0/2/2/2
88	Y5P	A7	46	88	-	3/7/33/34	0/2/2/2
87	P5P	A5	2	87	-	2/7/25/26	0/3/3/3
88	P5P	A7	26	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	16	88	-	2/7/25/26	0/3/3/3
88	P5P	A7	45	88	-	2/7/25/26	0/3/3/3
88	Y5P	A7	47	88	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	P5P	A5	9	87	-	0/7/25/26	0/3/3/3
88	Y5P	A7	22	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	41	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	48	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	50	88	-	4/7/33/34	0/2/2/2
88	P5P	A7	54	88	-	1/7/25/26	0/3/3/3
88	Y5P	A7	68	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	43	88	-	5/7/25/26	0/3/3/3
88	Y5P	A7	63	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	11	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	51	88	-	2/7/33/34	0/2/2/2
88	P5P	A7	5	88	-	2/7/25/26	0/3/3/3
88	P5P	A7	39	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	12	88	-	3/7/33/34	0/2/2/2
87	Y5P	A5	3	87	-	4/7/33/34	0/2/2/2
88	P5P	A7	4	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	23	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	71	32,88	-	1/7/25/26	0/3/3/3
87	Y5P	A5	10	87	-	1/7/33/34	0/2/2/2
88	P5P	A7	2	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	17	88	-	2/7/33/34	0/2/2/2
87	Y5P	A5	1	87	-	7/7/33/34	0/2/2/2
88	Y5P	A7	3	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	65	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	67	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	49	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	60	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	13	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	38	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	64	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	69	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	19	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	57	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	62	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	7	88	-	3/7/25/26	0/3/3/3
88	Y5P	A7	8	88	-	1/7/33/34	0/2/2/2
87	P5P	A5	11	87	-	0/7/25/26	0/3/3/3

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	53	Y5P	C4-N3	-13.51	1.33	1.46
88	A7	67	Y5P	C4-N3	-13.44	1.33	1.46
88	A7	44	Y5P	C4-N3	-13.31	1.33	1.46
87	A5	1	Y5P	C4-N3	-13.23	1.33	1.46
88	A7	66	Y5P	C4-N3	-13.23	1.33	1.46

The worst 5 of 258 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	45	P5P	C6-N1-C2	8.80	126.18	115.80
88	A7	27	P5P	C6-N1-C2	8.66	126.02	115.80
88	A7	2	P5P	C6-N1-C2	8.60	125.95	115.80
88	A7	11	P5P	C6-N1-C2	8.58	125.93	115.80
88	A7	7	P5P	C6-N1-C2	8.52	125.85	115.80

There are no chirality outliers.

5 of 122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	A5	1	Y5P	O4'-C4'-C5'-O5'
87	A5	1	Y5P	C3'-C4'-C5'-O5'
87	A5	2	P5P	O4'-C4'-C5'-O5'
87	A5	4	Y5P	O4'-C4'-C5'-O5'
87	A5	4	Y5P	C3'-C4'-C5'-O5'

There are no ring outliers.

25 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A7	20	P5P	1	0
87	A5	4	Y5P	3	0
88	A7	25	Y5P	1	0
88	A7	61	Y5P	1	0
88	A7	21	Y5P	2	0
88	A7	70	Y5P	4	0
88	A7	59	Y5P	1	0
88	A7	58	Y5P	1	0
88	A7	24	Y5P	1	0
88	A7	1	P5P	9	0
88	A7	47	Y5P	1	0
88	A7	22	Y5P	1	0
88	A7	48	P5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A7	63	Y5P	1	0
88	A7	12	Y5P	1	0
88	A7	71	P5P	6	0
87	A5	10	Y5P	4	0
87	A5	1	Y5P	7	0
88	A7	65	Y5P	2	0
88	A7	60	Y5P	4	0
88	A7	13	Y5P	1	0
88	A7	64	Y5P	3	0
88	A7	69	Y5P	2	0
88	A7	57	Y5P	1	0
88	A7	62	Y5P	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 139 ligands modelled in this entry, 137 are monoatomic - leaving 2 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	$\# Z > 2$
92	GCP	v	802	89	32,34,34	1.67	6 (18%)	49,54,54	1.87	10 (20%)
91	GDP	AX	500	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (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
92	GCP	v	802	89	-	5/19/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	GDP	AX	500	-	-	1/16/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	v	802	GCP	PG-O1G	5.53	1.61	1.50
91	AX	500	GDP	C5-C4	3.22	1.47	1.38
92	v	802	GCP	PG-O3G	3.06	1.61	1.55
92	v	802	GCP	C5-C4	3.03	1.47	1.38
92	v	802	GCP	PG-O2G	-2.61	1.49	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	AX	500	GDP	C5-C4-N3	-6.34	118.30	128.39
92	v	802	GCP	PB-O3A-PA	-5.90	113.13	132.37
91	AX	500	GDP	C2-N3-C4	5.15	121.17	112.30
92	v	802	GCP	C2-N3-C4	4.82	120.60	112.30
91	AX	500	GDP	N9-C4-N3	4.71	135.37	125.95

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	v	802	GCP	PG-C3B-PB-O1B
92	v	802	GCP	PG-C3B-PB-O3A
92	v	802	GCP	O4'-C4'-C5'-O5'
92	v	802	GCP	C3'-C4'-C5'-O5'
92	v	802	GCP	PG-C3B-PB-O2B

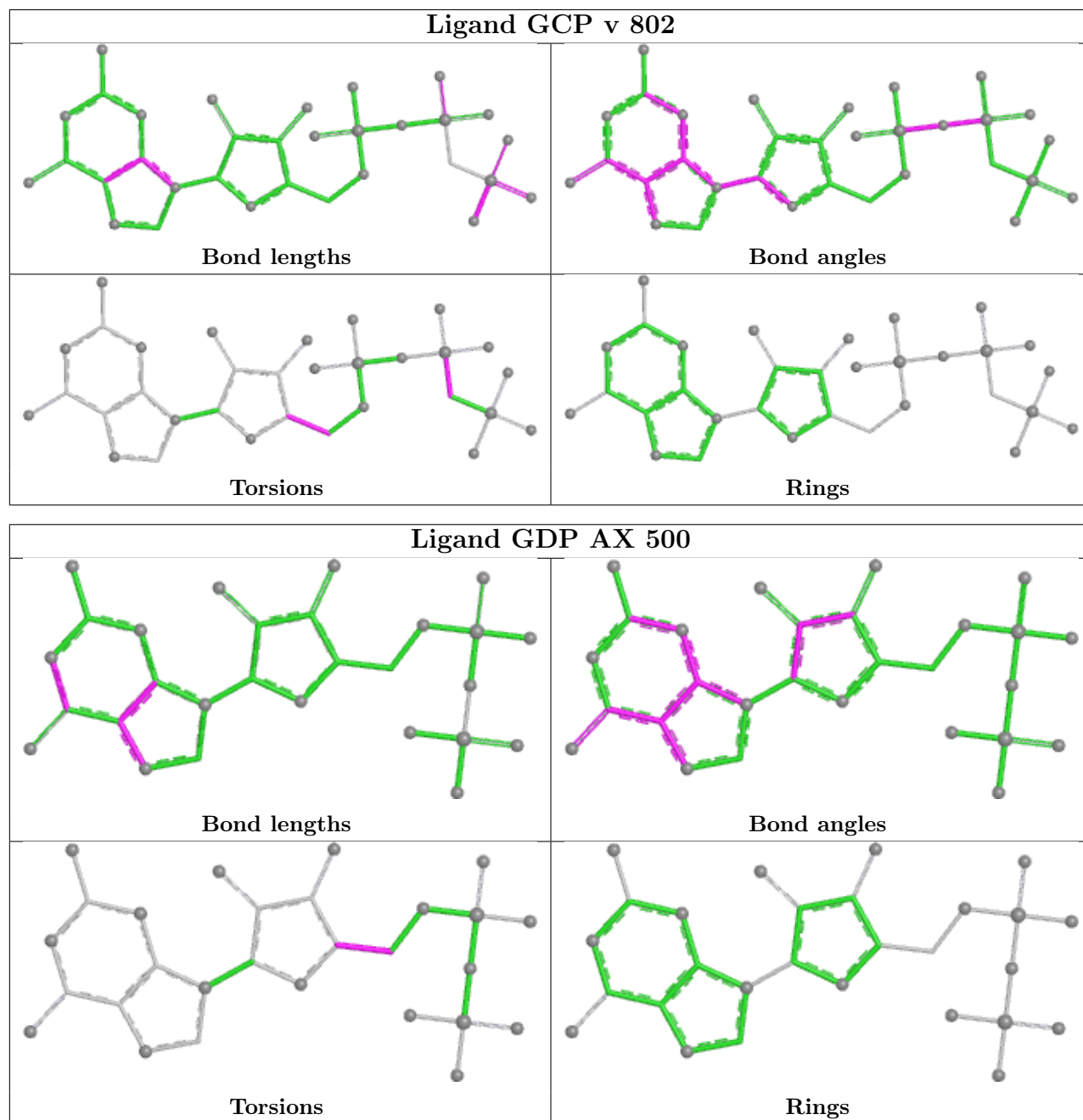
There are no ring outliers.

1 monomer is involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	v	802	GCP	33	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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
85	u	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	u	414:UNK	C	601:UNK	N	48.04
1	u	106:UNK	C	301:UNK	N	30.89
1	u	315:UNK	C	399:UNK	N	19.09
1	u	615:UNK	C	700:UNK	N	18.25

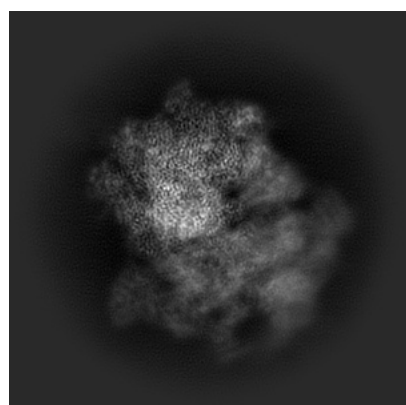
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21233. These allow visual inspection of the internal detail of the map and identification of artifacts.

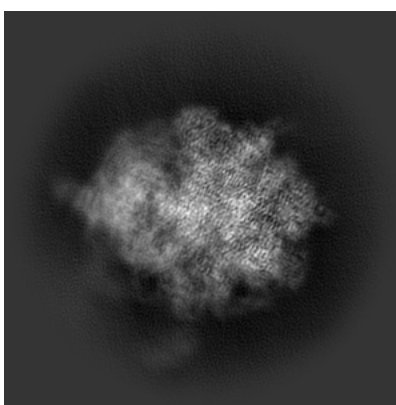
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

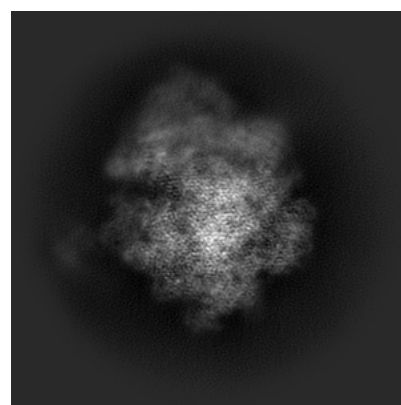
6.1.1 Primary map



X



Y

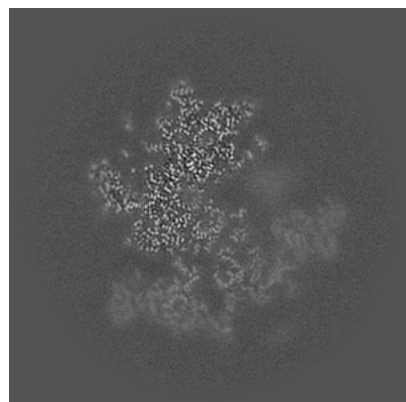


Z

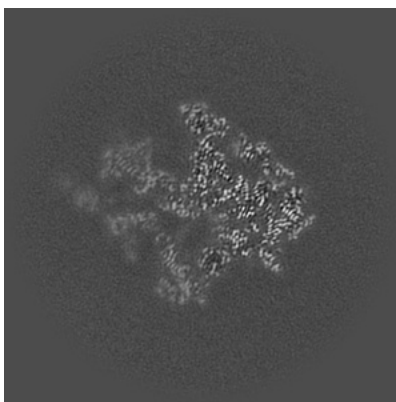
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

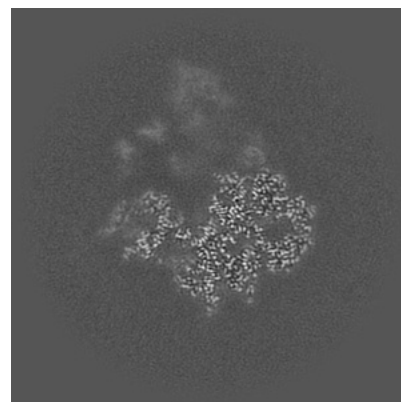
6.2.1 Primary map



X Index: 200



Y Index: 200

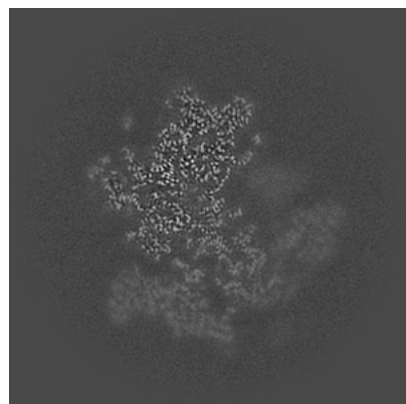


Z Index: 200

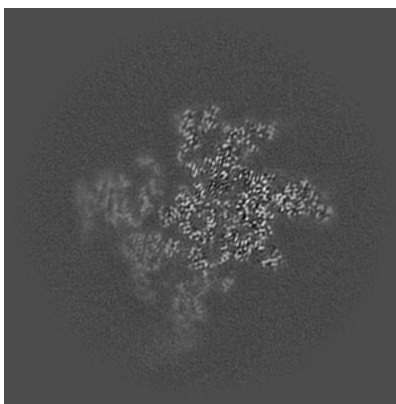
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

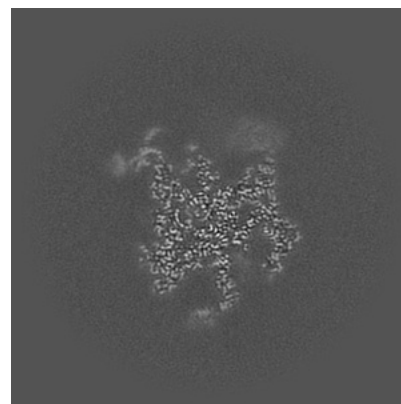
6.3.1 Primary map



X Index: 205



Y Index: 172

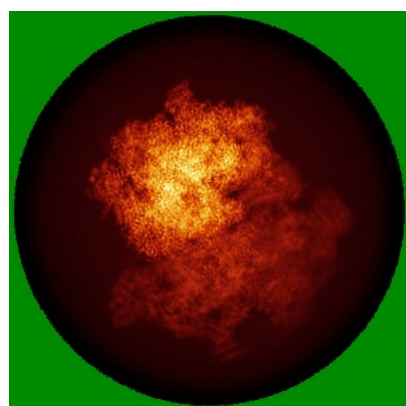


Z Index: 243

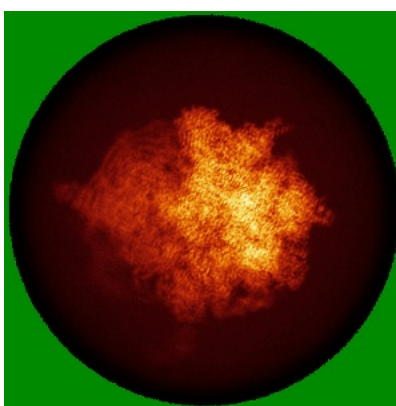
The images above show the largest variance slices of the map in three orthogonal directions.

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

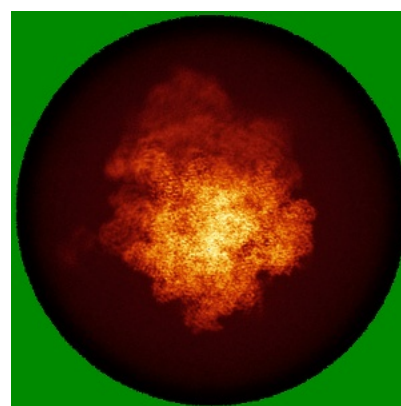
6.4.1 Primary map



X



Y

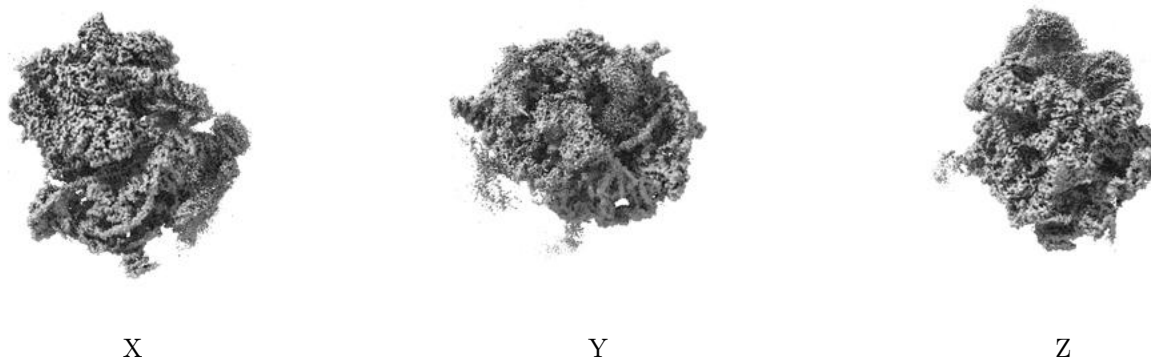


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

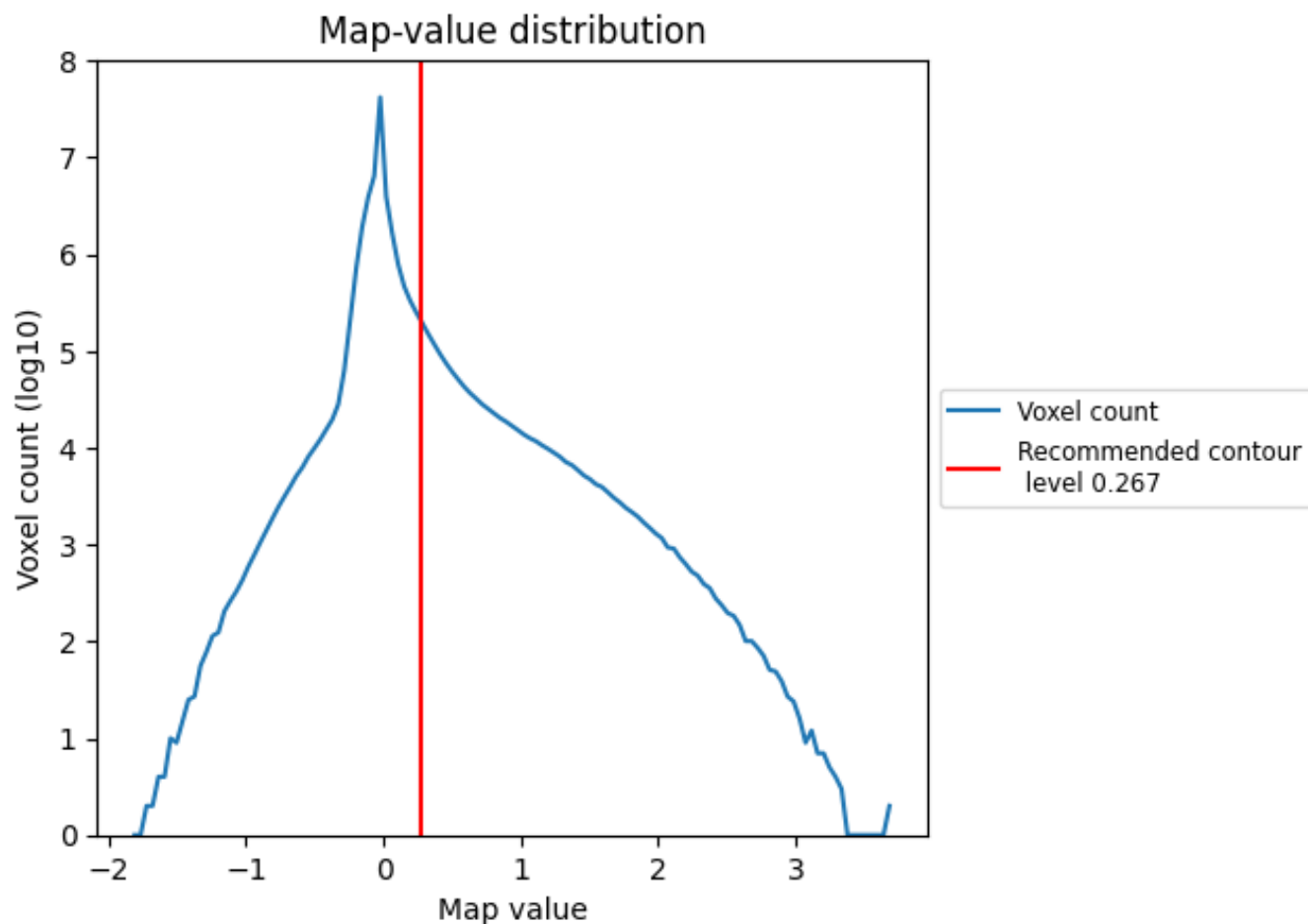
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

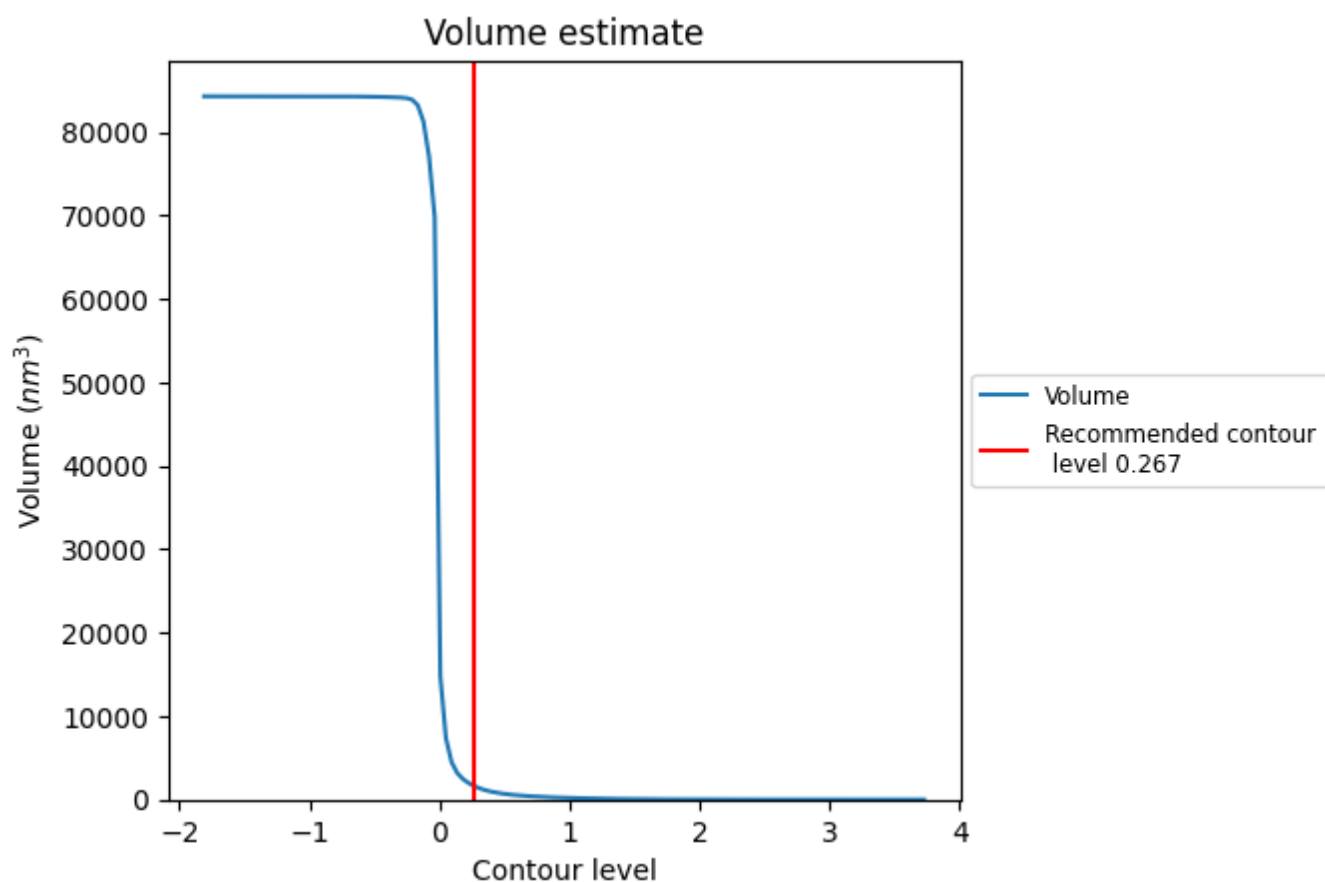
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

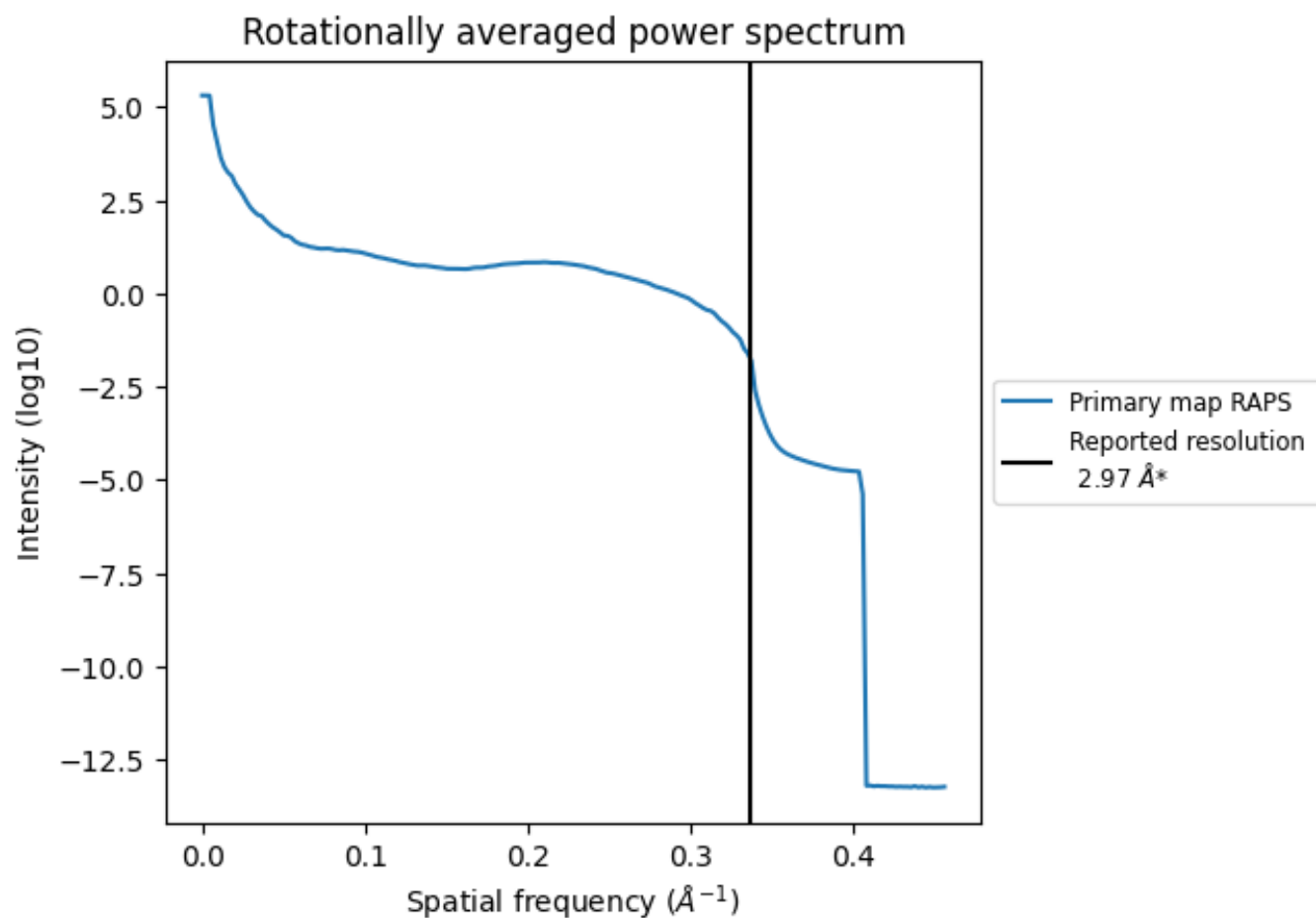
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1618 nm³; this corresponds to an approximate mass of 1461 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 0.337 Å⁻¹

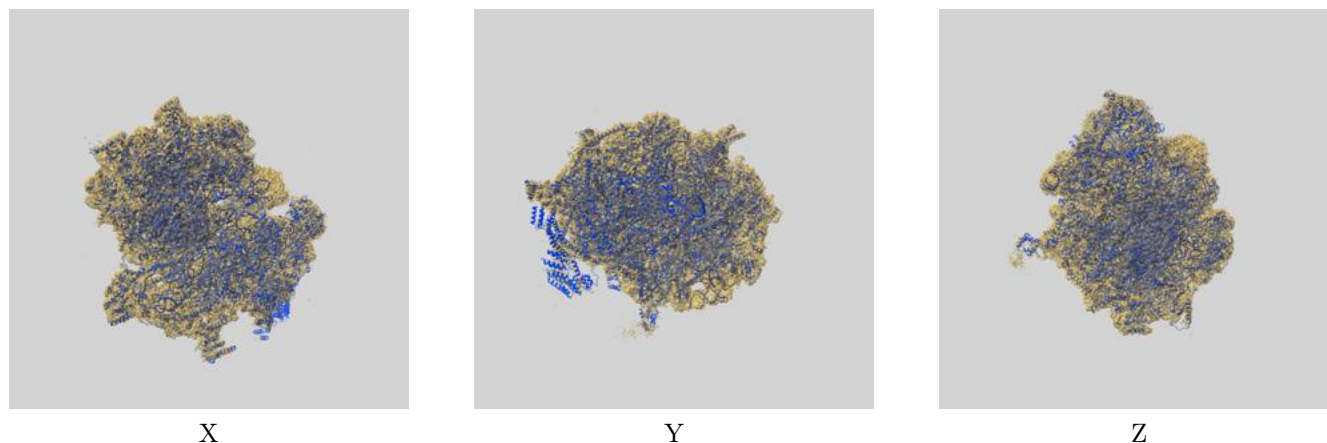
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

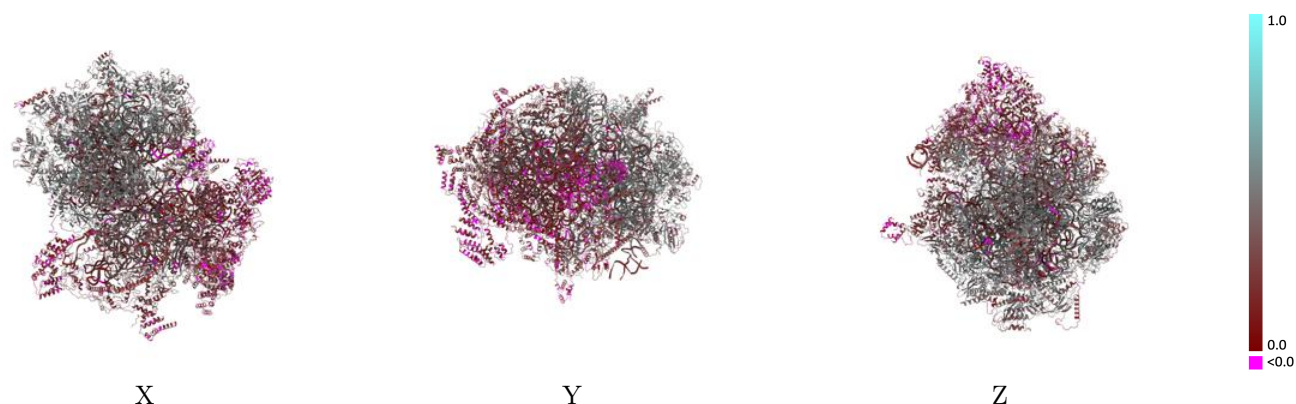
This section contains information regarding the fit between EMDB map EMD-21233 and PDB model 6VLZ. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



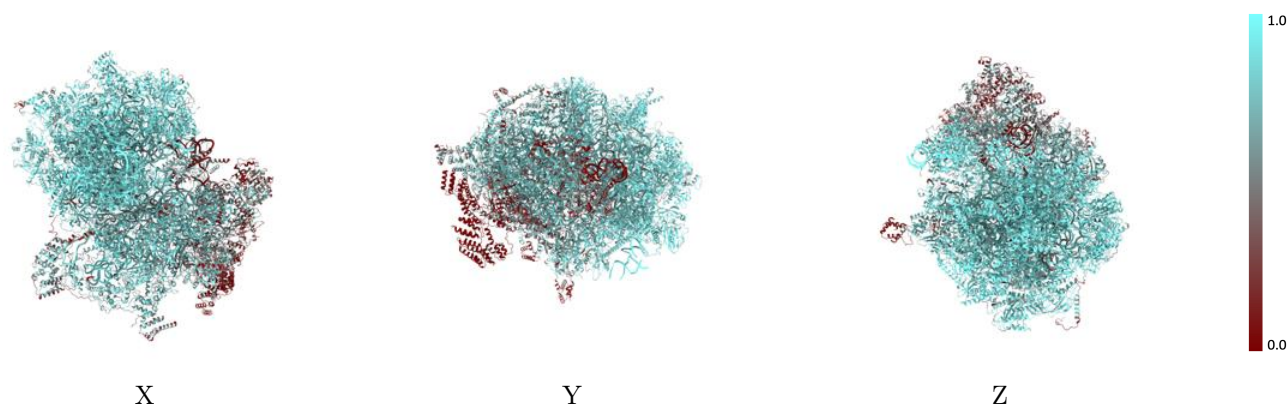
The images above show the 3D surface view of the map at the recommended contour level 0.267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



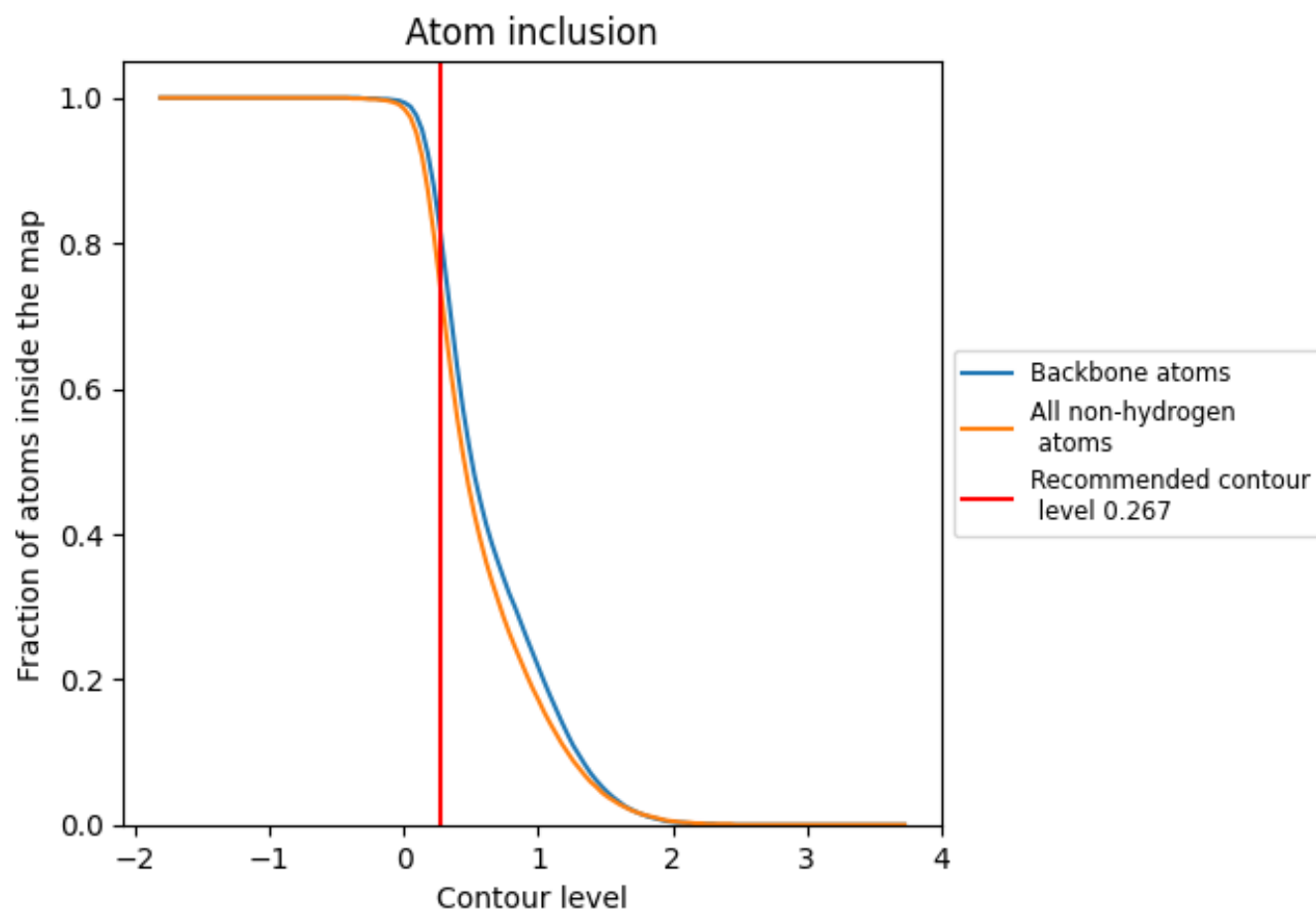
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.267).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.267) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.3170
0	 0.8580	 0.4350
1	 0.8410	 0.4250
2	 0.9110	 0.4820
3	 0.8970	 0.4990
4	 0.8590	 0.4400
5	 0.8880	 0.4360
6	 0.8750	 0.4050
7	 0.8610	 0.4030
8	 0.7270	 0.2300
9	 0.8720	 0.4070
A	 0.8440	 0.3320
A0	 0.6790	 0.2400
A1	 0.3650	 0.1370
A2	 0.4450	 0.2500
A3	 0.7270	 0.3760
A4	 0.1020	 0.1390
A5	 0.0240	 0.0310
A7	 0.1290	 0.0240
AA	 0.8170	 0.2590
AB	 0.6750	 0.2520
AC	 0.4550	 0.1700
AD	 0.5850	 0.2880
AE	 0.5540	 0.2510
AF	 0.4060	 0.2070
AG	 0.5010	 0.1720
AH	 0.4080	 0.1910
AI	 0.6400	 0.2880
AJ	 0.6970	 0.3530
AK	 0.6190	 0.1700
AL	 0.6750	 0.3090
AM	 0.7240	 0.2890
AN	 0.7960	 0.3620
AO	 0.6780	 0.2530
AP	 0.6310	 0.2770



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Chain	Atom inclusion	Q-score
AQ	 0.7190	 0.3230
AR	 0.6150	 0.2080
AS	 0.5480	 0.2090
AT	 0.7510	 0.3280
AU	 0.6650	 0.2020
AV	 0.5190	 0.1380
AW	 0.6120	 0.2510
AX	 0.3530	 0.0800
AY	 0.3590	 0.1320
AZ	 0.4080	 0.1530
B	 0.9480	 0.2870
D	 0.8650	 0.4350
E	 0.8820	 0.4590
F	 0.8880	 0.4590
H	 0.8360	 0.3920
I	 0.6890	 0.2600
J	 0.7400	 0.2690
K	 0.9050	 0.4740
L	 0.8510	 0.4540
M	 0.8910	 0.4500
N	 0.8540	 0.4300
O	 0.8740	 0.4370
P	 0.8810	 0.4120
Q	 0.8070	 0.4040
R	 0.8890	 0.4660
S	 0.9020	 0.4580
T	 0.8910	 0.4670
TA	 0.1310	 0.0810
TB	 0.1550	 0.0700
TC	 0.0340	 0.1480
U	 0.8680	 0.4330
V	 0.8590	 0.4160
W	 0.8830	 0.4550
X	 0.8800	 0.4430
Y	 0.8900	 0.4430
Z	 0.8800	 0.4520
a	 0.7980	 0.3920
b	 0.9000	 0.4710
c	 0.8610	 0.4180
d	 0.7530	 0.3680
e	 0.6990	 0.1610
f	 0.7010	 0.2860

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Chain	Atom inclusion	Q-score
g	 0.8720	 0.4180
h	 0.8210	 0.3580
i	 0.9010	 0.4680
j	 0.8450	 0.4100
k	 0.7430	 0.2880
l	 0.7680	 0.2830
m	 0.7420	 0.2190
o	 0.8580	 0.4220
p	 0.7950	 0.3700
q	 0.7480	 0.3460
r	 0.8750	 0.4280
s	 0.8800	 0.4360
u	 0.4740	 0.1660
v	 0.6950	 0.2920