wwPDB EM Validation Summary Report (i)

Nov 13, 2022 – 03:24 AM EST

PDB ID	:	6VLZ
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

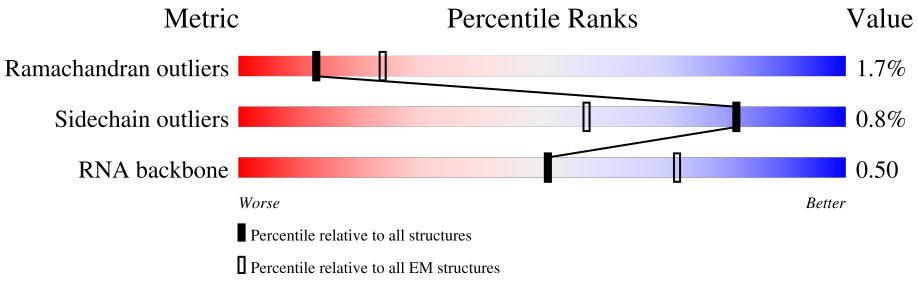
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	AA	954	78% 21%
2	AB	296	6% 73% 26%
3	AC	167	35% 78% 21%
4	AE	125	26% 94%
5	AI	194	13% 68% 30%
6	AJ	138	8% 77% 22%
7	AK	128	19% 77% 21%
8	AM	137	9% 83% 15%

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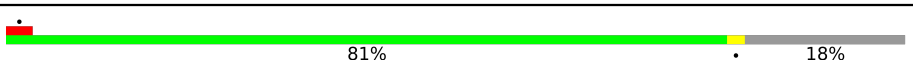
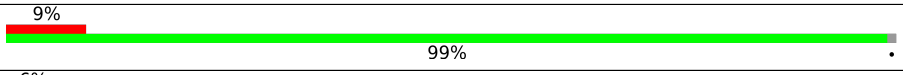
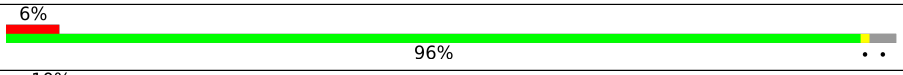
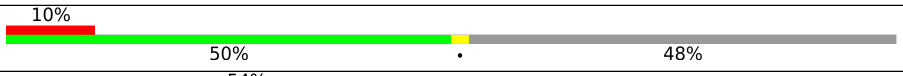
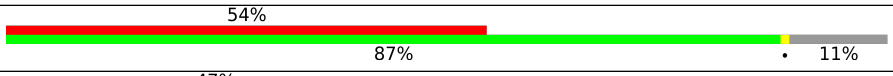
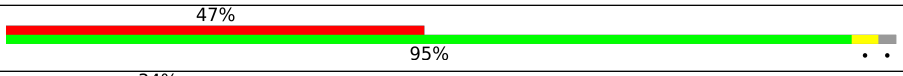
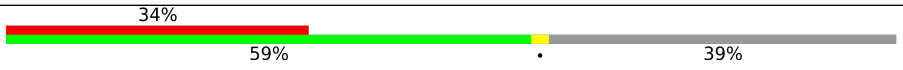
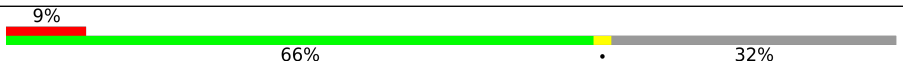
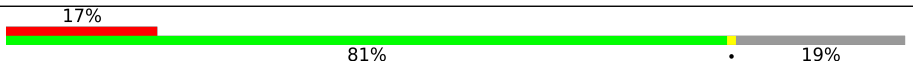
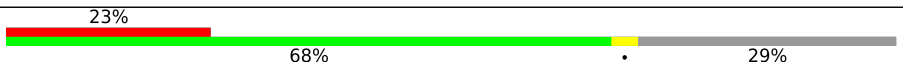
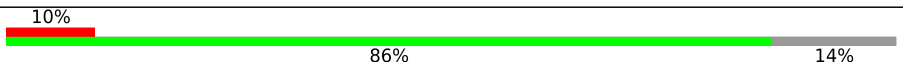
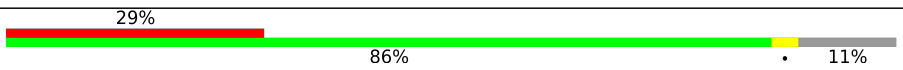
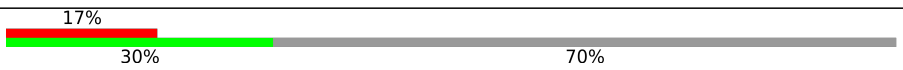
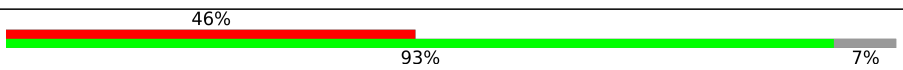
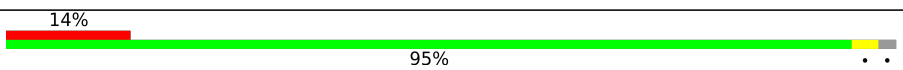
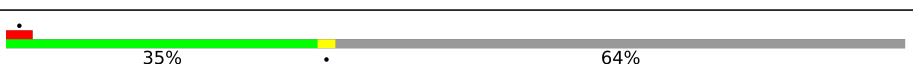
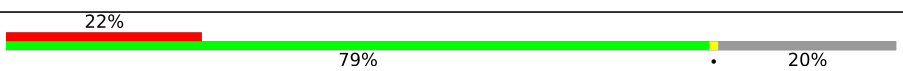
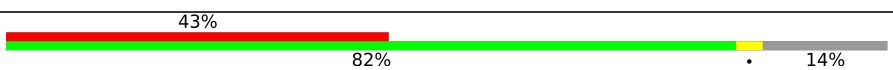
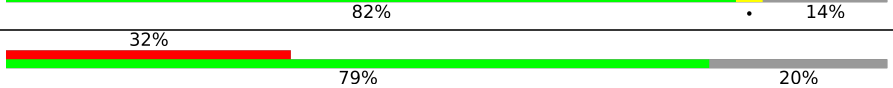
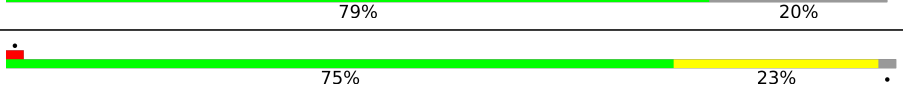
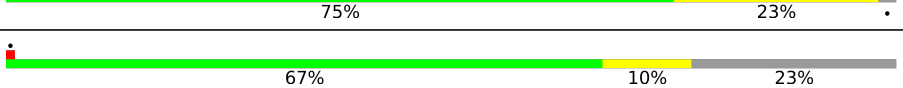
Mol	Chain	Length	Quality of chain
9	AN	130	
10	AO	258	
11	AP	142	
12	AQ	87	
13	AT	173	
14	AW	187	
15	AX	398	
16	A2	118	
17	AH	201	
18	AL	257	
19	AR	360	
20	AS	190	
21	AU	205	
22	AV	414	
23	AY	395	
24	AZ	106	
25	A1	323	
26	A0	218	
27	A3	199	
28	A4	689	
29	AD	430	
30	AF	242	
31	AG	396	
32	A	1559	
33	B	73	

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Mol	Chain	Length	Quality of chain
34	D	305	78% 22%
35	F	311	79% 20%
36	H	267	36% 63%
37	K	178	96%
38	L	145	78% 21%
39	M	296	94%
40	O	175	85% 13%
41	R	149	89% 6%
42	S	205	73% 24%
43	T	212	75% 22%
44	W	148	74% 25%
45	X	256	91% 5%
46	Y	250	68% 30%
47	Z	161	75% 25%
48	0	188	56% 43%
49	1	65	77% 20%
50	2	92	49% 50%
51	3	188	50% 49%
52	4	103	37% 63%
53	8	206	48% 52%
54	b	155	94% 5%
55	e	279	10% 77% 22%
56	g	166	75% 20%
57	i	128	75% 24%
58	j	123	75% 24%

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Mol	Chain	Length	Quality of chain
59	m	128	34% 65%
60	o	102	88% 8%
61	q	222	15% 74% 24%
62	r	196	79% 17%
63	J	192	6% 87% 9%
64	I	261	9% 67% 31%
65	N	251	88% 12%
66	P	179	77% 20%
67	U	153	6% 98%
68	V	216	95% 5%
69	E	348	86% 12%
70	5	423	91% 7%
71	6	380	92% 7%
72	7	338	86% 12%
73	9	137	89% 9%
74	a	142	10% 74% 24%
75	c	332	86% 13%
76	d	306	10% 81% 16%
77	f	194	13% 75% 25%
78	h	158	68% 30%
79	k	112	6% 85% 14%
80	l	138	6% 51% 48%
81	p	206	8% 72% 26%
82	s	439	87% 10%
83	Q	292	6% 79% 18%

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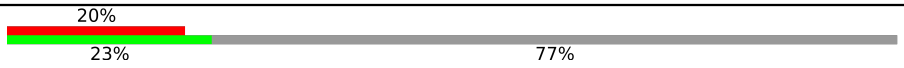
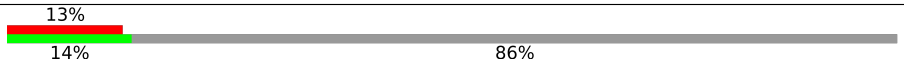
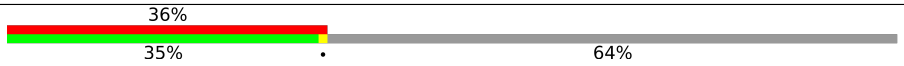
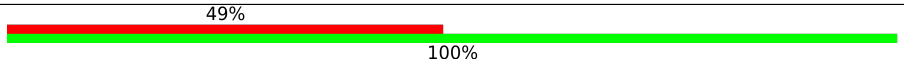
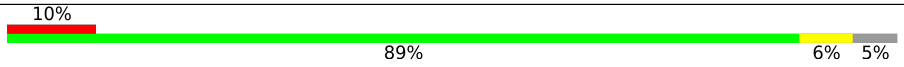
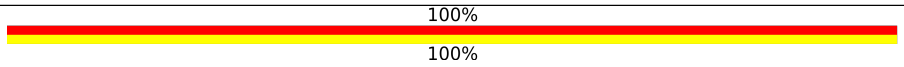
Mol	Chain	Length	Quality of chain
84	TA	198	
84	TB	198	
84	TC	198	
85	u	65	
86	v	751	
87	A5	11	
88	A7	71	

2 Entry composition (i)

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
			Total	C	N	O	P		
1	AA	944	20030	8980	3612	6494	944	0	0

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

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

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

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

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

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

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

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

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

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

- 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 tRNAval.

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 1517	C 970	N 291	O 252	S 4	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

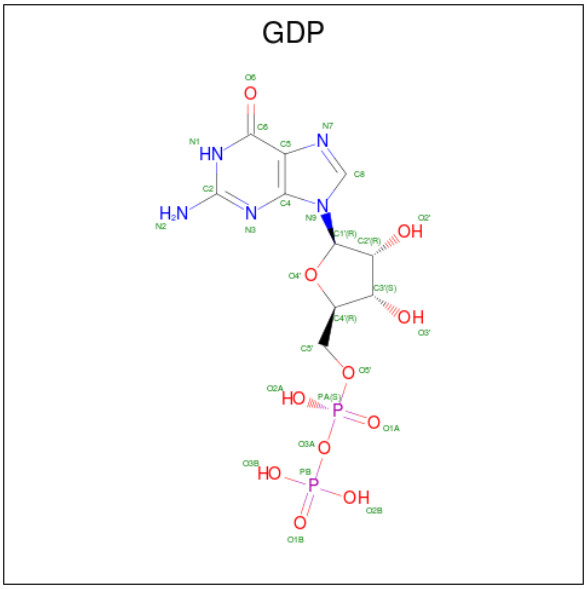
- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: ZN) (formula: Zn).

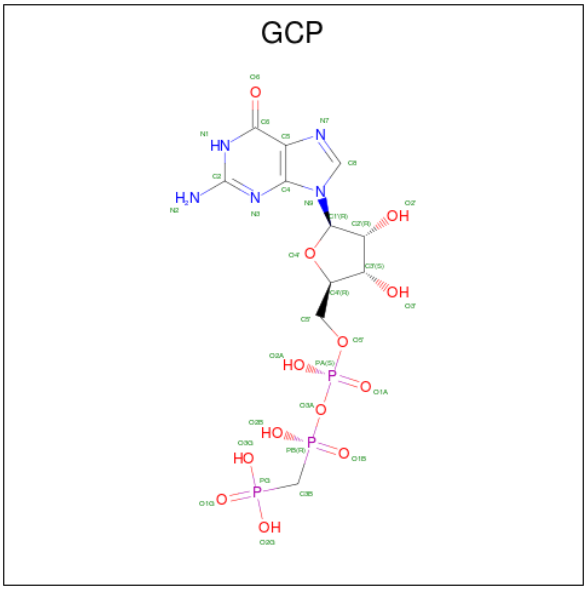
Mol	Chain	Residues	Atoms		AltConf
90	AB	1	Total	Zn	0
			1	1	
90	AO	1	Total	Zn	0
			1	1	
90	AP	1	Total	Zn	0
			1	1	
90	AT	1	Total	Zn	0
			1	1	
90	0	1	Total	Zn	0
			1	1	
90	4	1	Total	Zn	0
			1	1	
90	r	1	Total	Zn	0
			1	1	

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: 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 (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



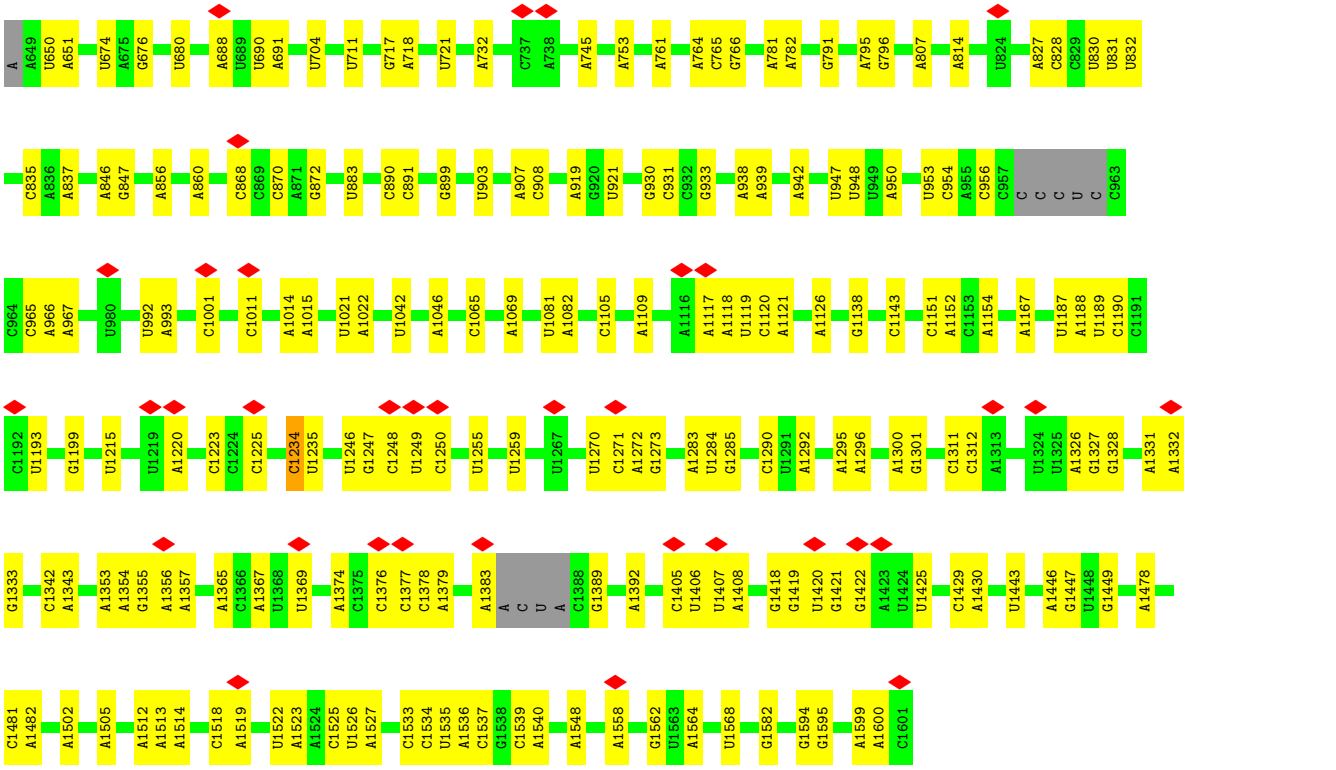
Mol	Chain	Residues	Atoms					AltConf
92	v	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots (i)

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

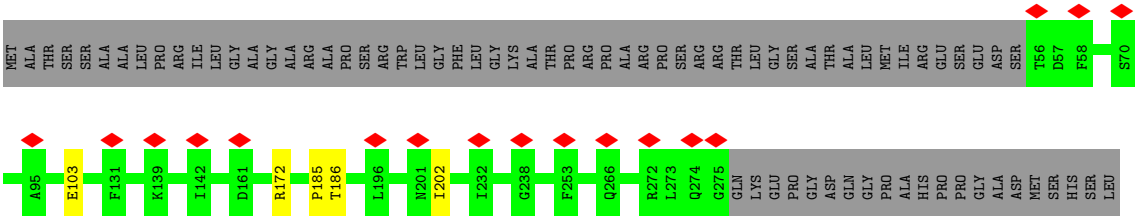
• Molecule 1: 12s rRNA

Chain AA:



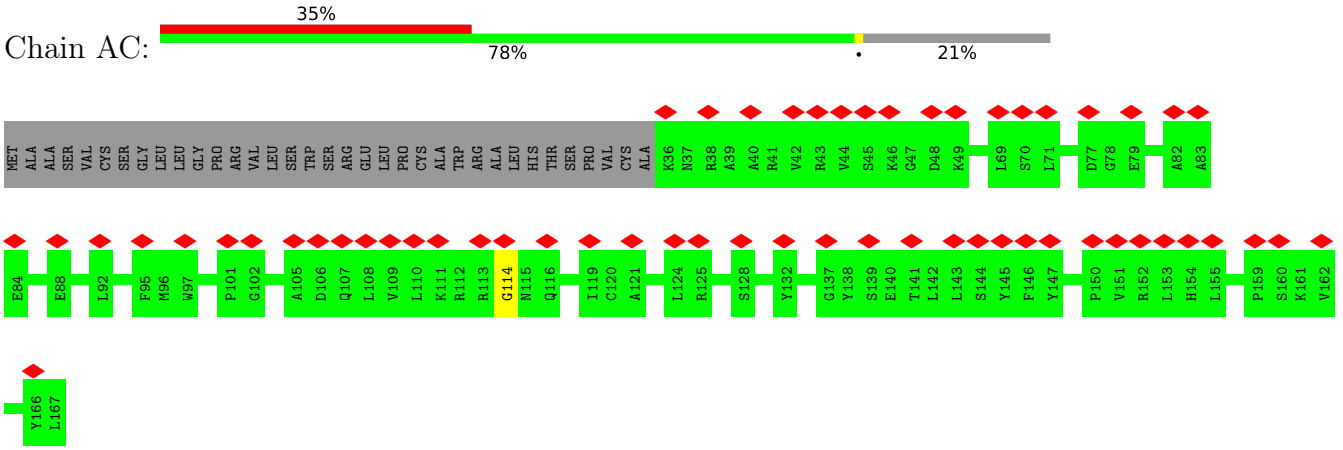
• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain AB:



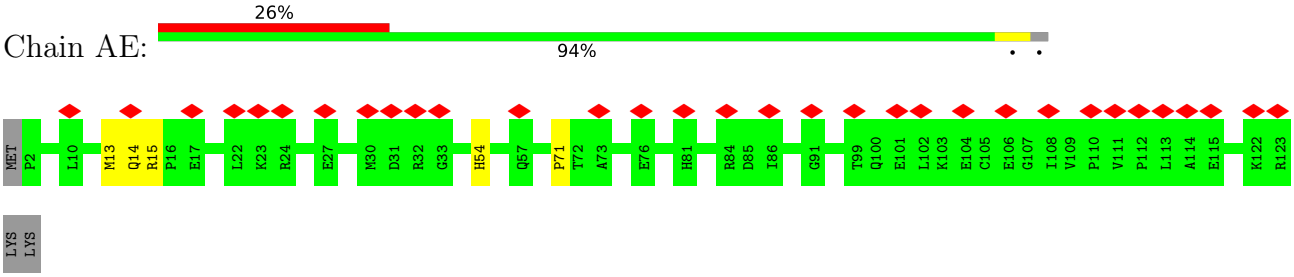
• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC:



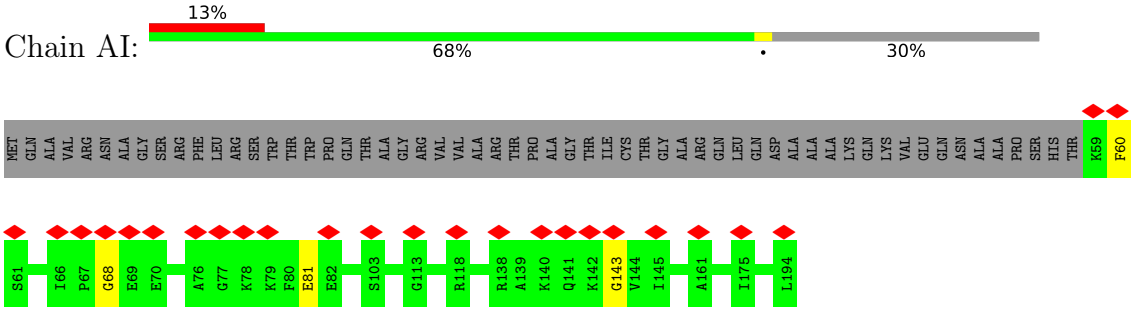
• Molecule 4: 28S ribosomal protein S6, mitochondrial

Chain AE:



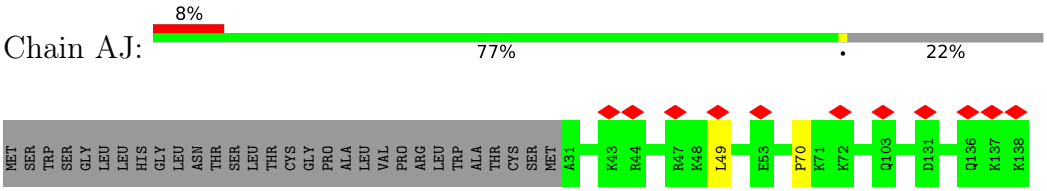
• Molecule 5: 28S ribosomal protein S11, mitochondrial

Chain AI:



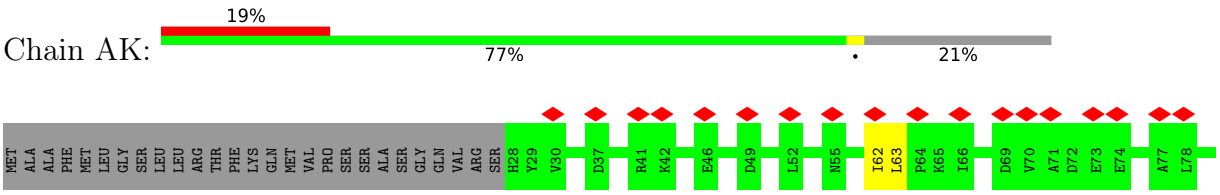
• Molecule 6: 28S ribosomal protein S12, mitochondrial

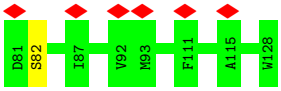
Chain AJ:



• Molecule 7: 28S ribosomal protein S14, mitochondrial

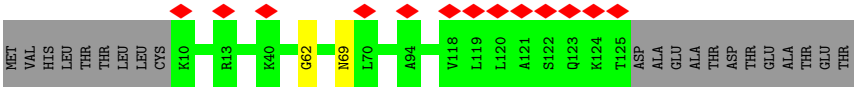
Chain AK:





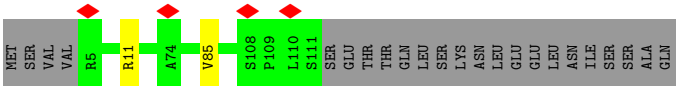
• Molecule 8: 28S ribosomal protein S16, mitochondrial

Chain AM:



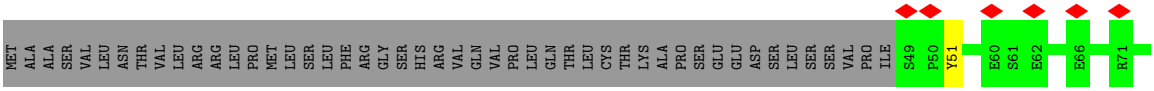
• Molecule 9: 28S ribosomal protein S17, mitochondrial

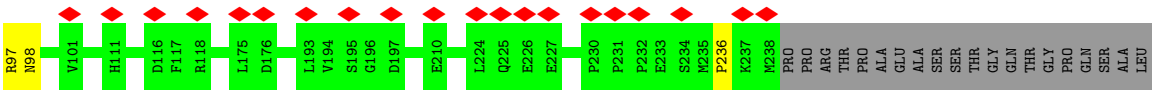
Chain AN:



• Molecule 10: 28S ribosomal protein S18b, mitochondrial

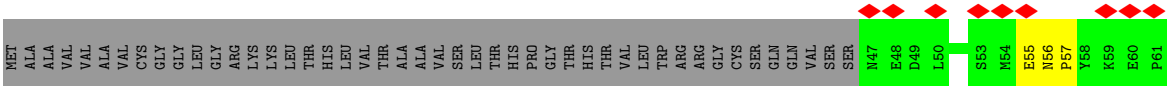
Chain AO:

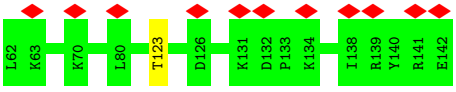




• Molecule 11: 28S ribosomal protein S18c, mitochondrial

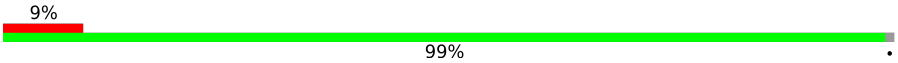
Chain AP:

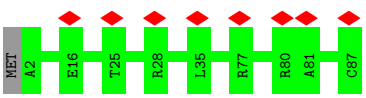




• Molecule 12: 28S ribosomal protein S21, mitochondrial

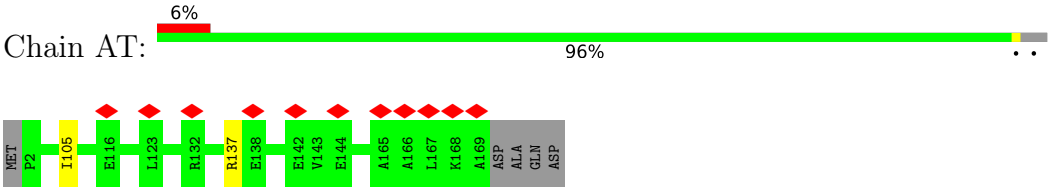
Chain AQ:





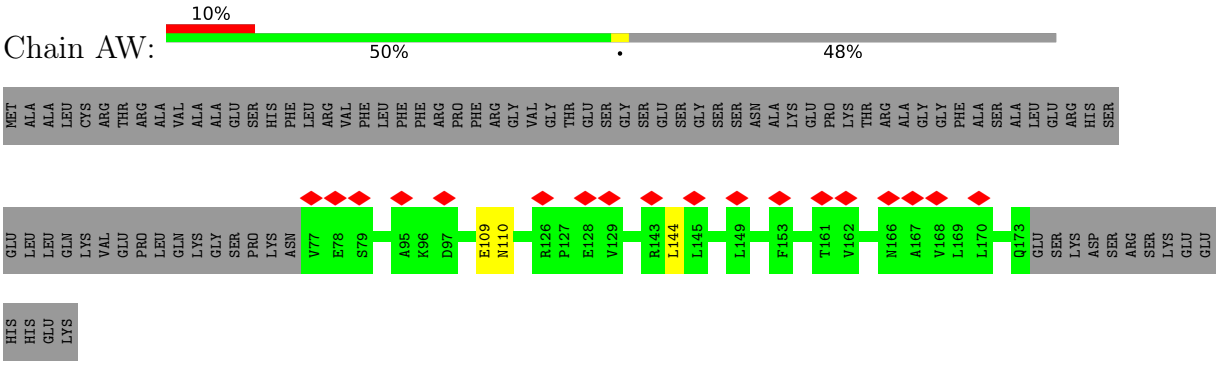
• Molecule 13: 28S ribosomal protein S25, mitochondrial

Chain AT:



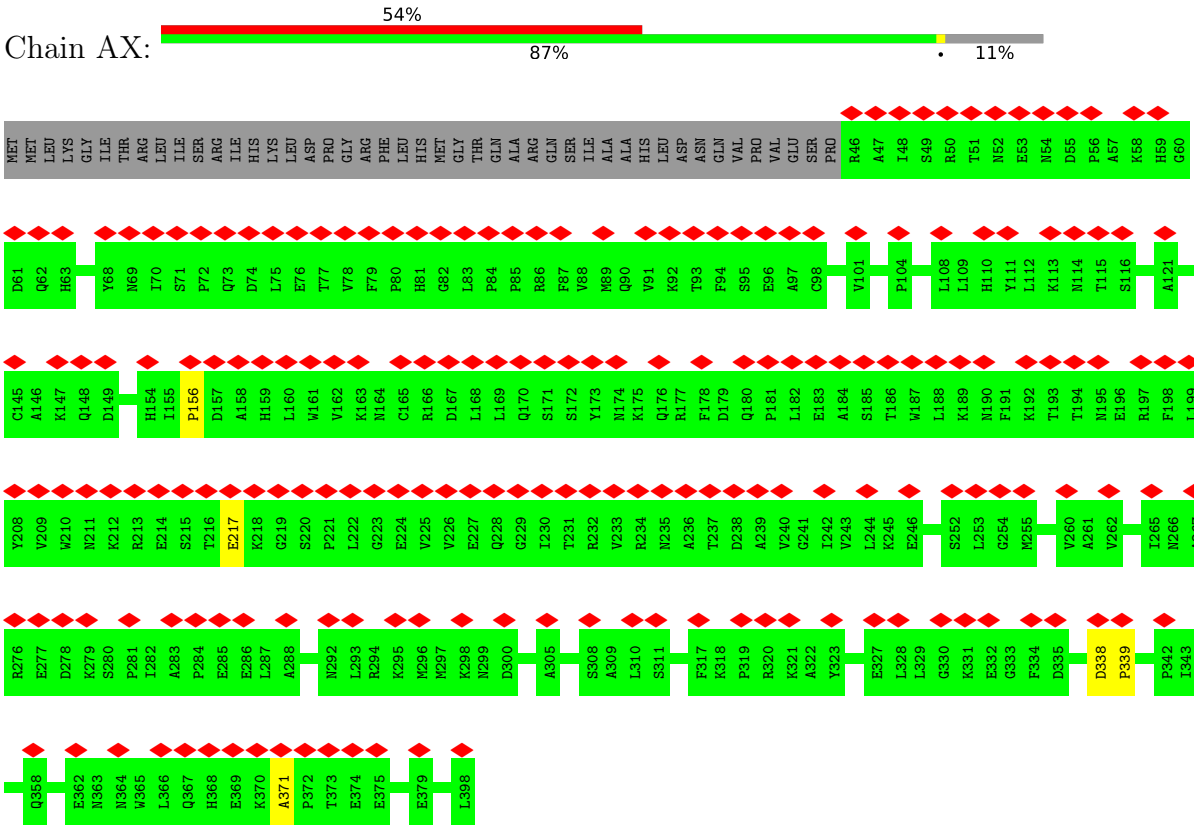
• Molecule 14: 28S ribosomal protein S28, mitochondrial

Chain AW:



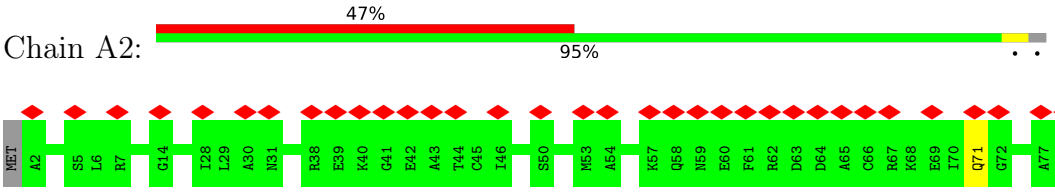
• Molecule 15: 28S ribosomal protein S29, mitochondrial

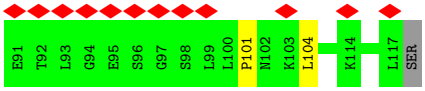
Chain AX:



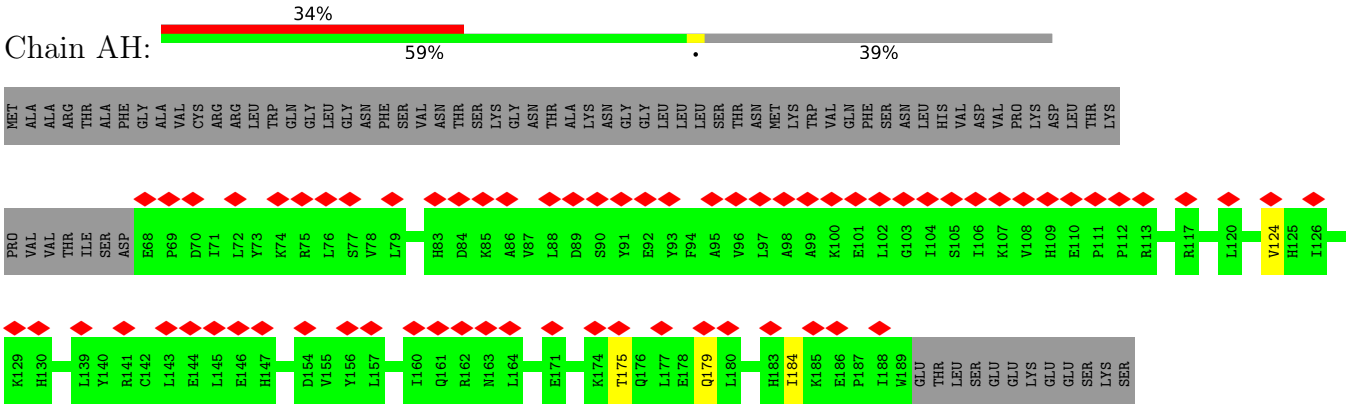
• Molecule 16: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2:

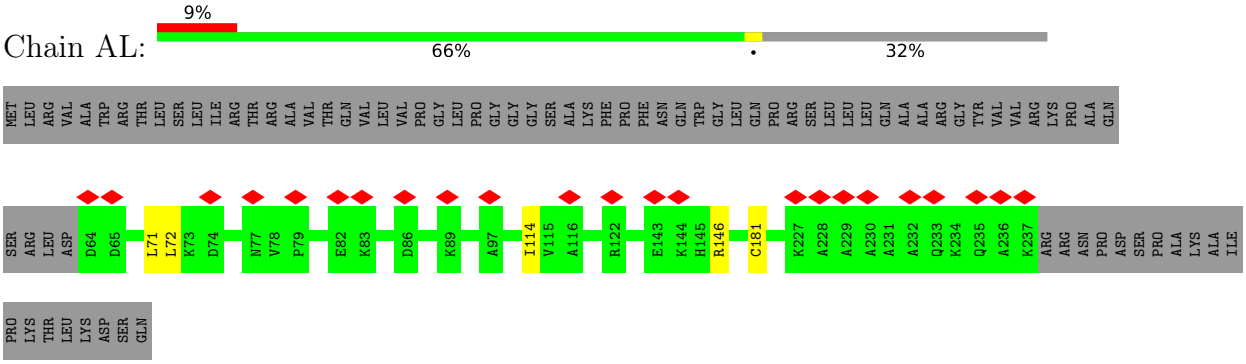




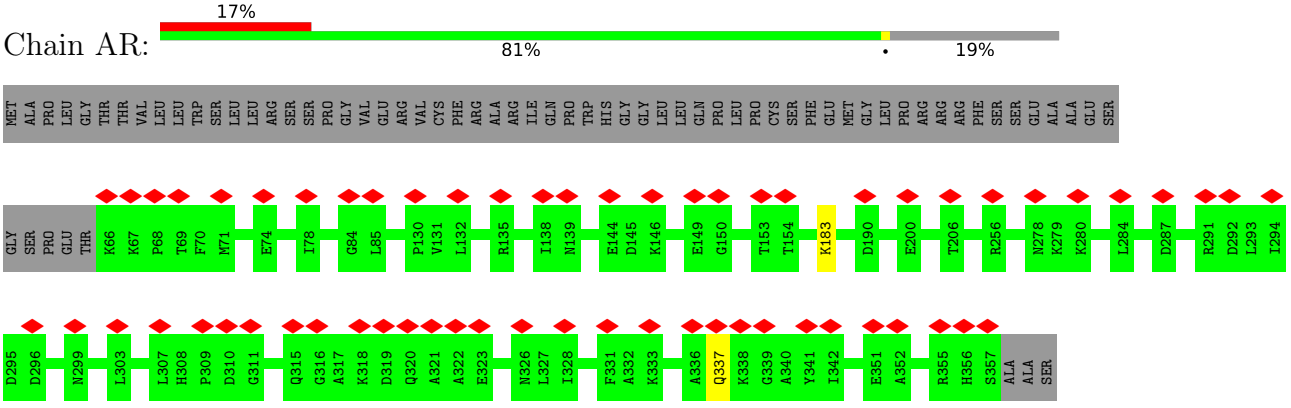
• Molecule 17: 28S ribosomal protein S10, mitochondrial



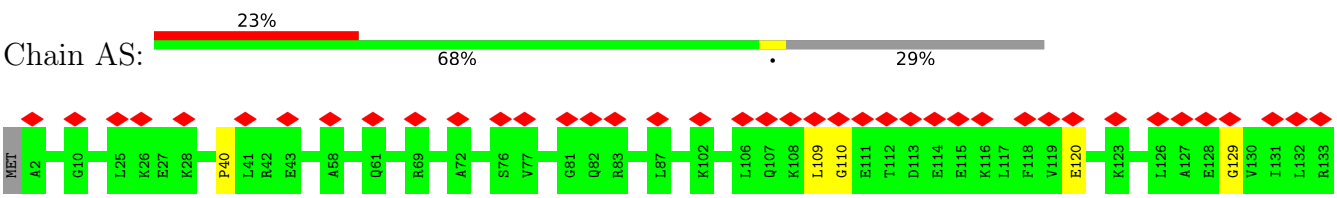
• Molecule 18: 28S ribosomal protein S15, mitochondrial

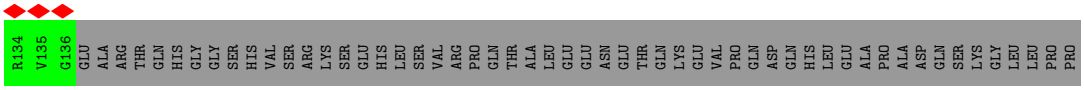


• Molecule 19: 28S ribosomal protein S22, mitochondrial

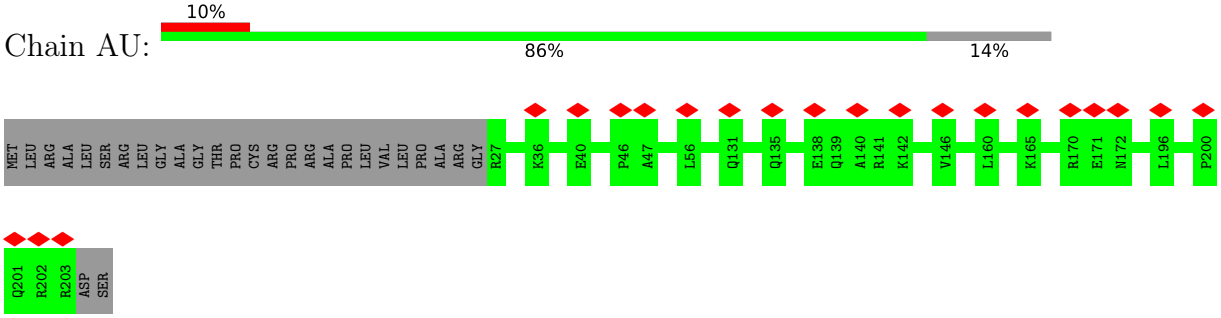


• Molecule 20: 28S ribosomal protein S23, mitochondrial

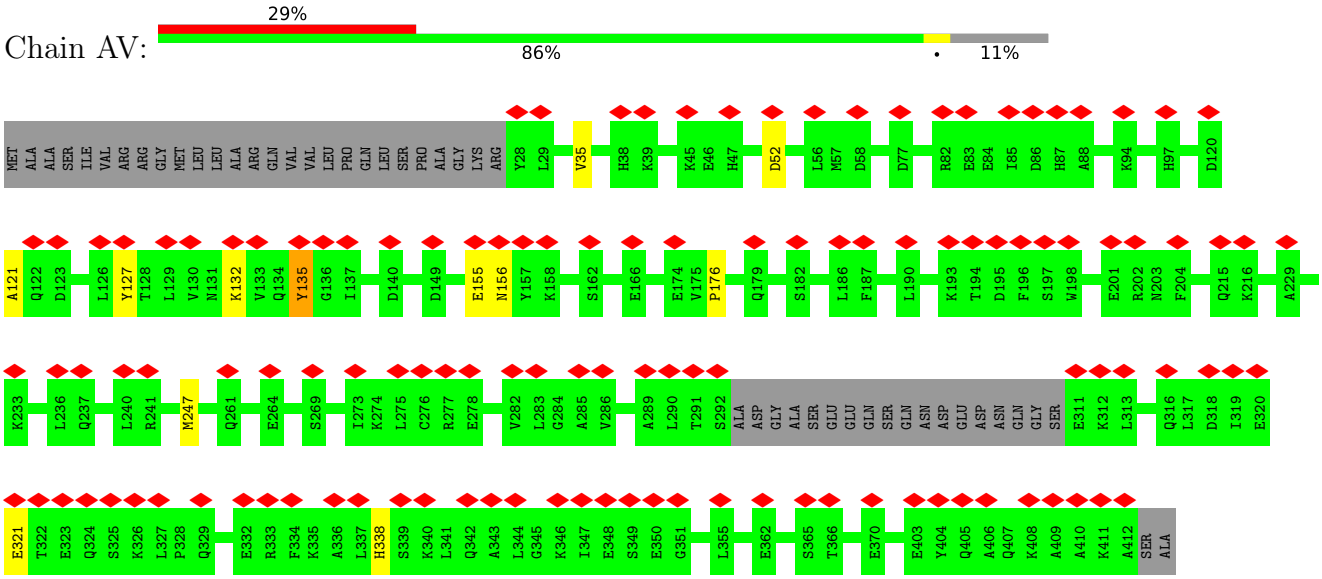




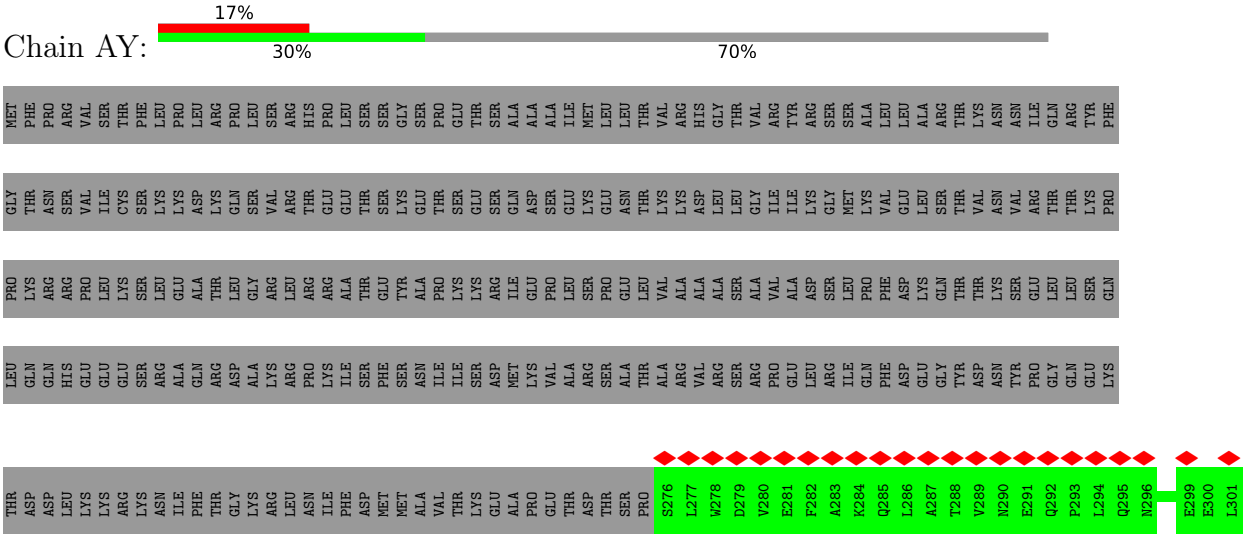
• Molecule 21: 28S ribosomal protein S26, mitochondrial

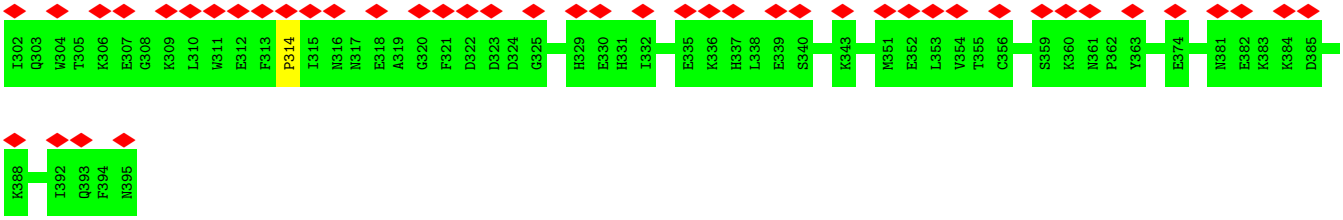


• Molecule 22: 28S ribosomal protein S27, mitochondrial



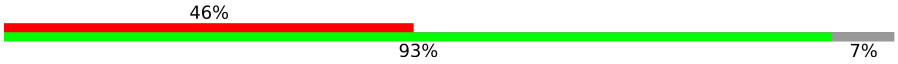
• Molecule 23: 28S ribosomal protein S31, mitochondrial

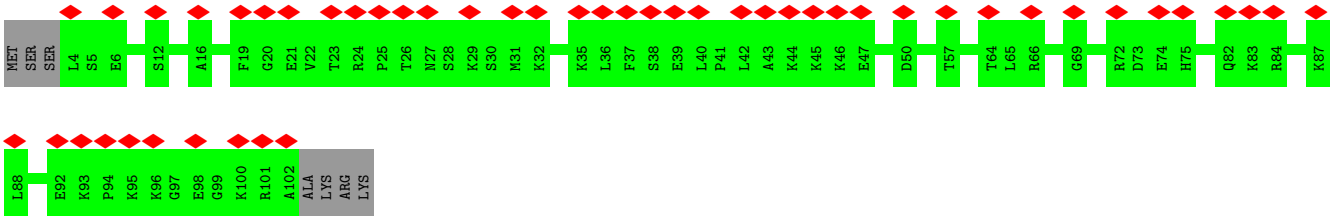




• Molecule 24: 28S ribosomal protein S33, mitochondrial

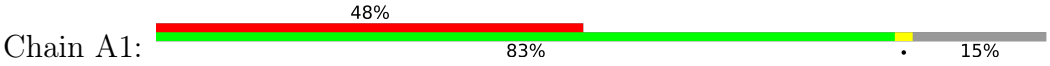
Chain AZ:

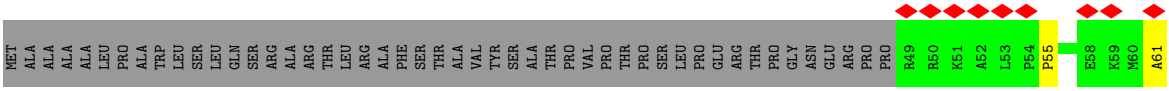


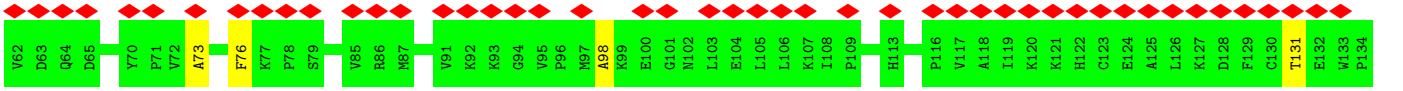


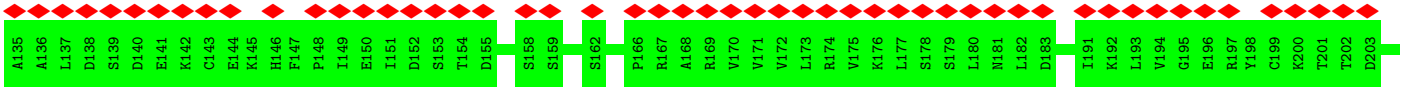
• Molecule 25: 28S ribosomal protein S35, mitochondrial

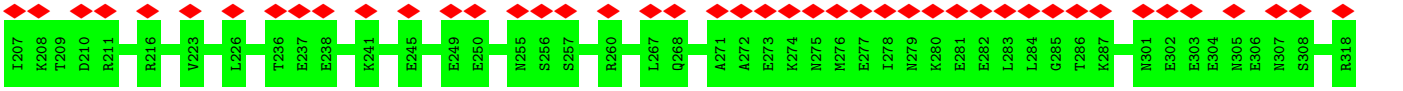
Chain A1:





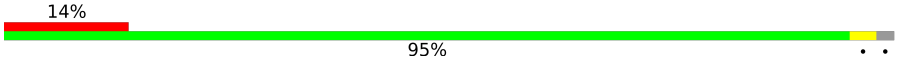


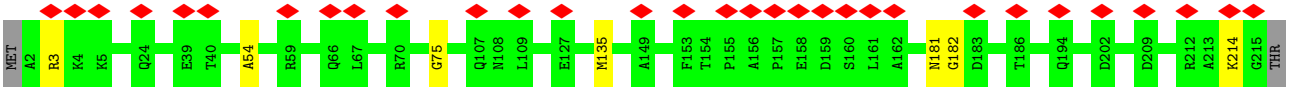




• Molecule 26: 28S ribosomal protein S34, mitochondrial

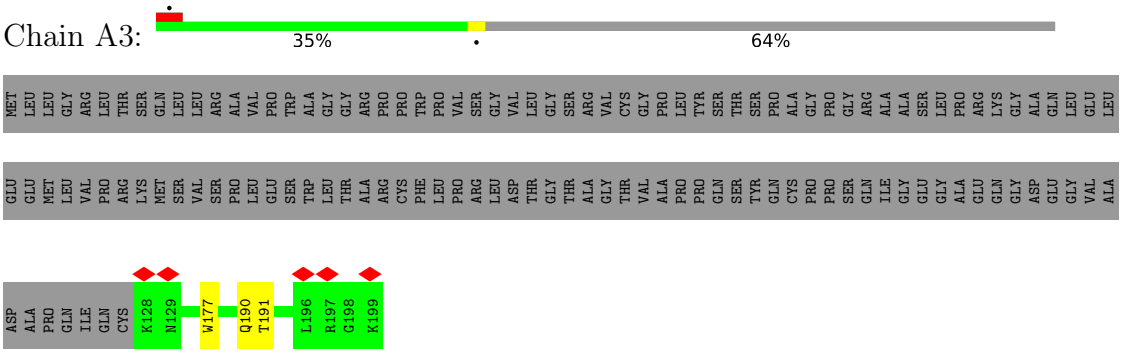
Chain A0:





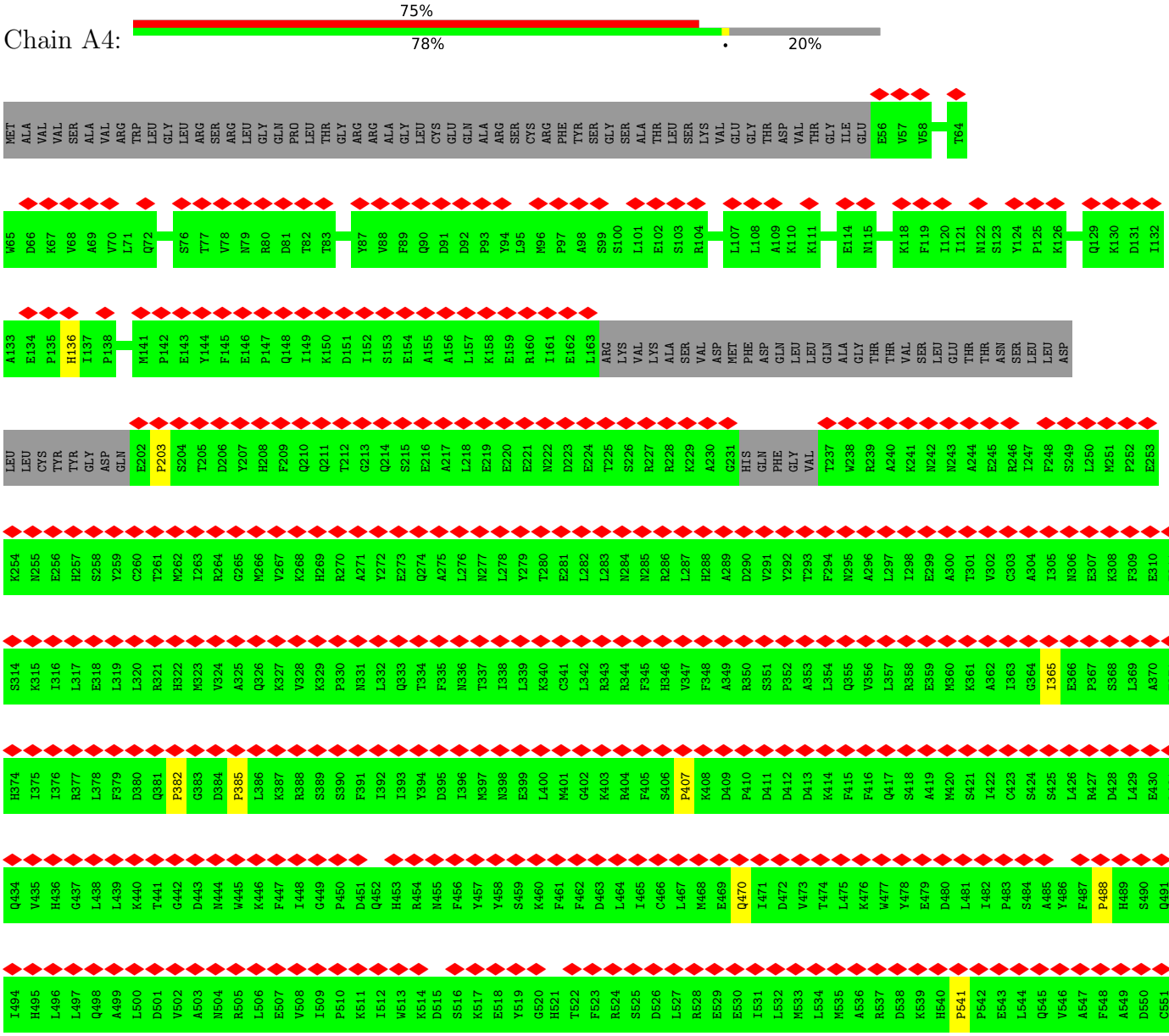
• Molecule 27: Aurora kinase A-interacting protein

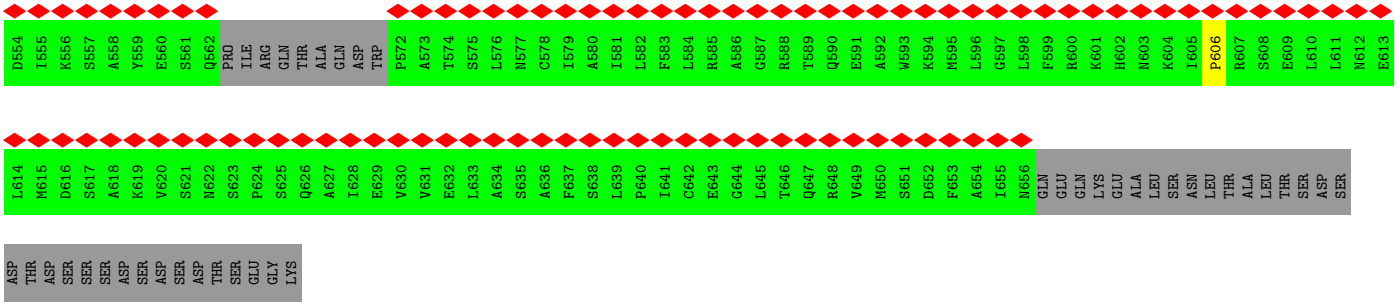
Chain A3:



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

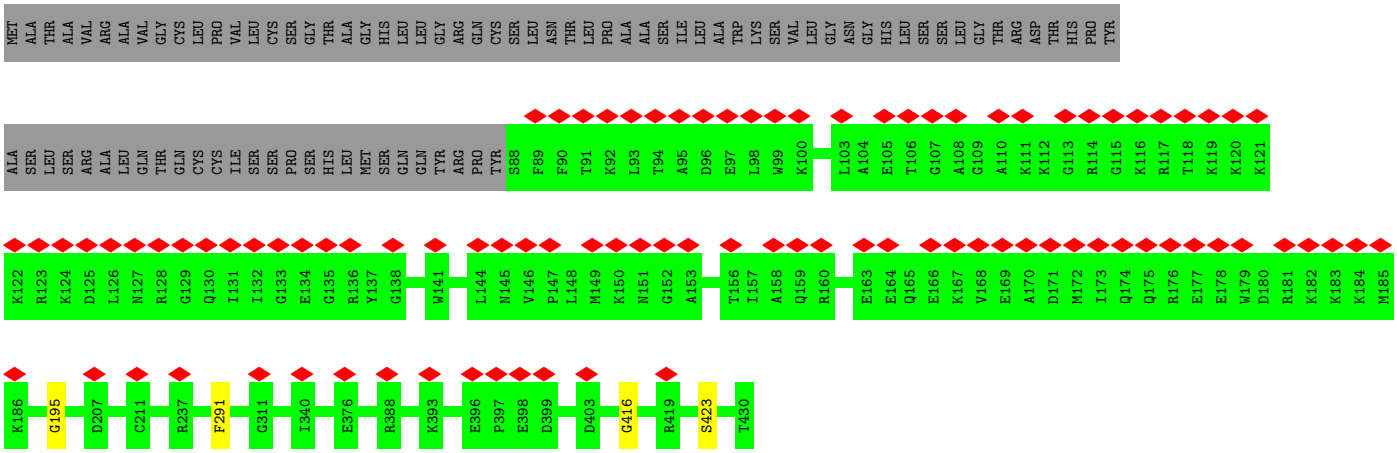
Chain A4:





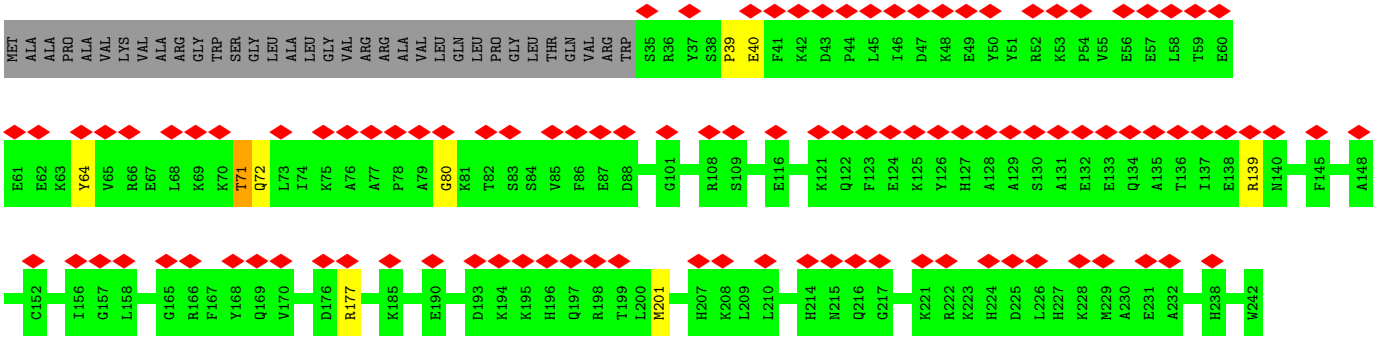
• Molecule 29: 28S ribosomal protein S5, mitochondrial

Chain AD:



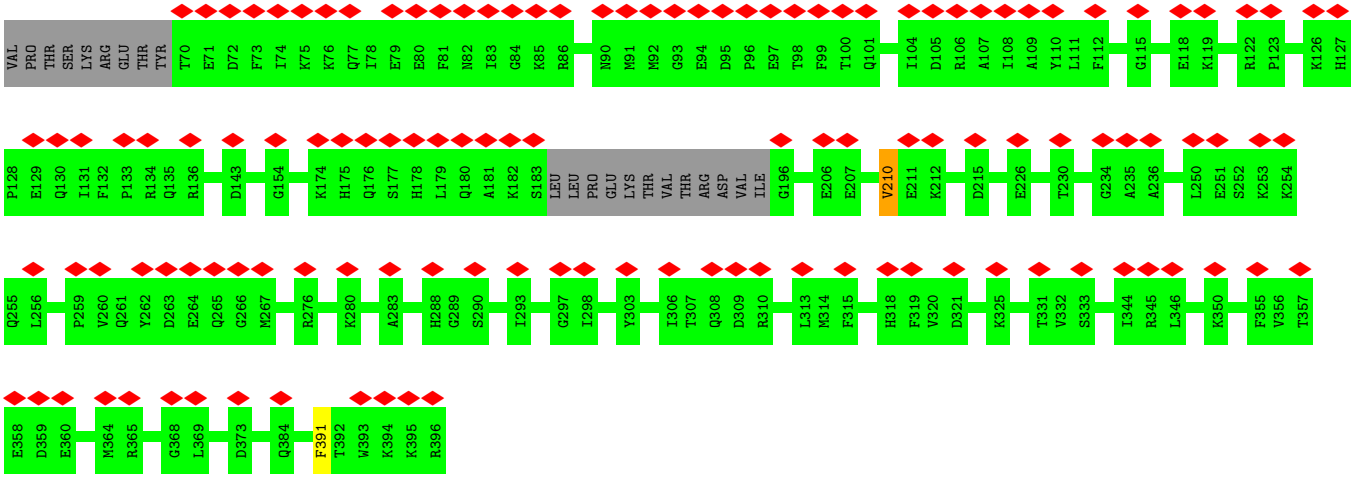
• Molecule 30: 28S ribosomal protein S7, mitochondrial

Chain AF:



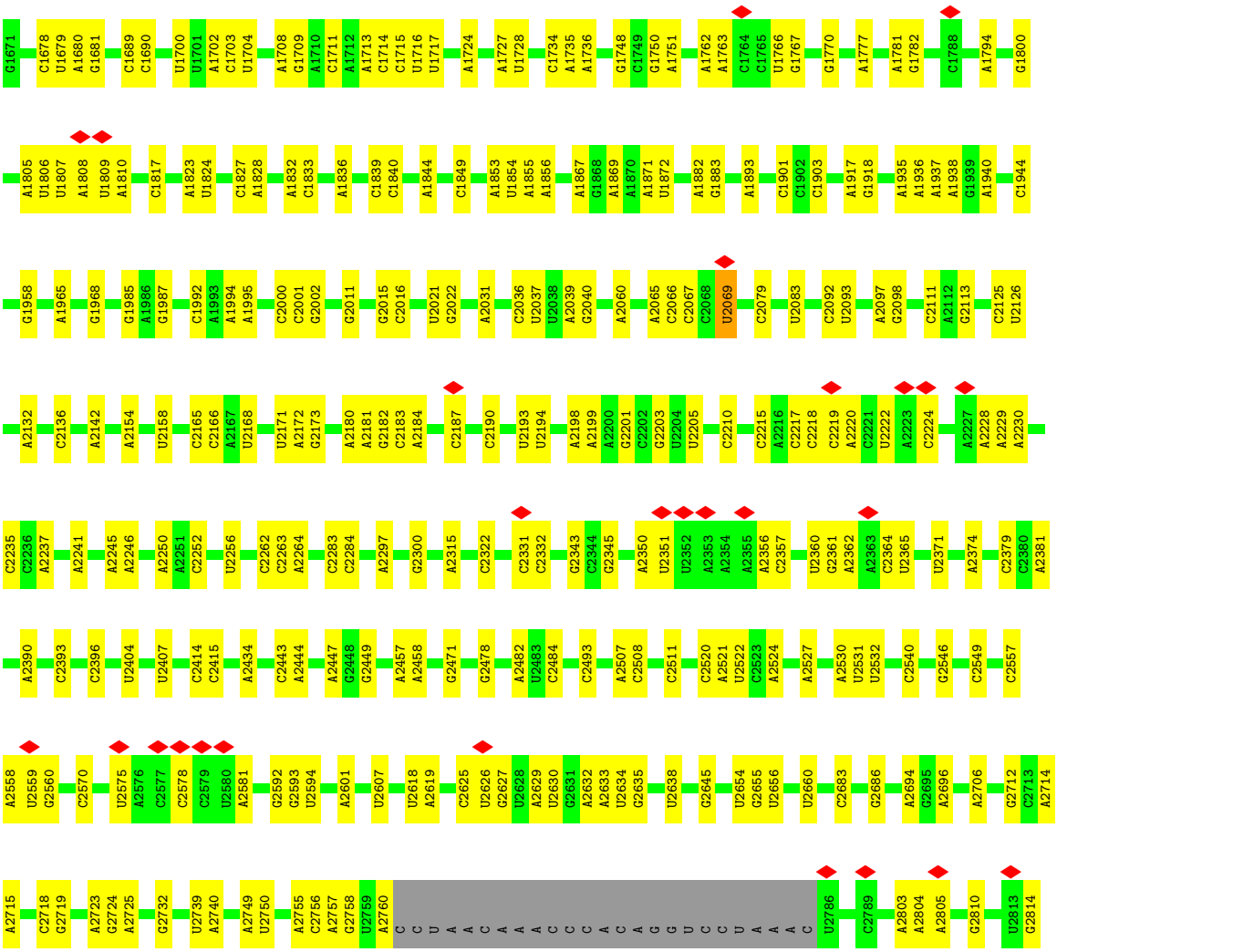
• Molecule 31: 28S ribosomal protein S9, mitochondrial

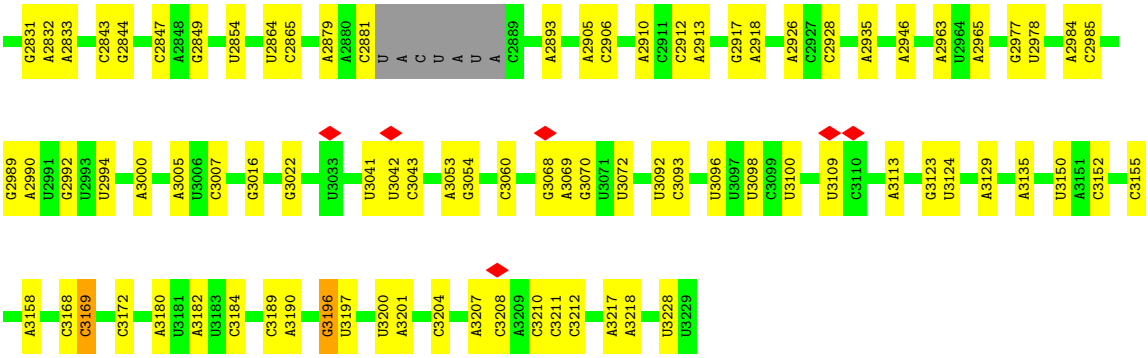
Chain AG:



- Molecule 32: 16s rRNA

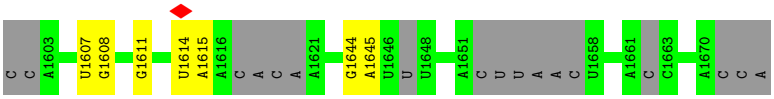
Chain A:





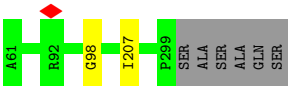
• Molecule 33: tRNAval

Chain B:



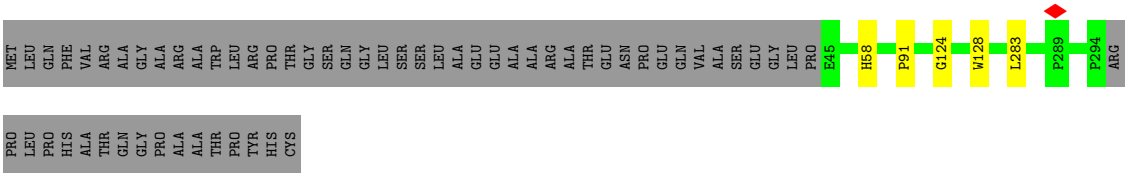
• Molecule 34: 39S ribosomal protein L2, mitochondrial

Chain D:



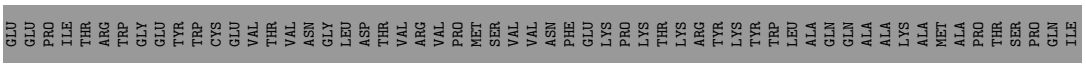
• Molecule 35: 39S ribosomal protein L4, mitochondrial

Chain F:



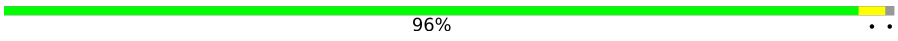
• Molecule 36: 39S ribosomal protein L9, mitochondrial

Chain H:



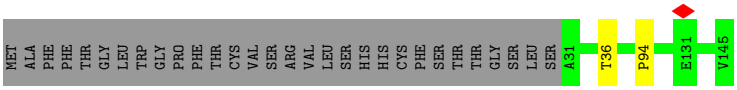
• Molecule 37: 39S ribosomal protein L13, mitochondrial

Chain K:



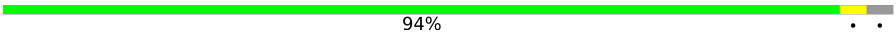
• Molecule 38: 39S ribosomal protein L14, mitochondrial

Chain L:



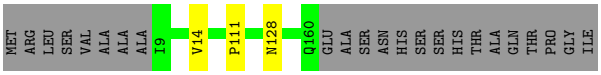
• Molecule 39: 39S ribosomal protein L15, mitochondrial

Chain M:



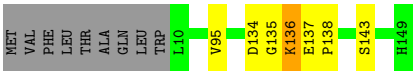
• Molecule 40: 39S ribosomal protein L17, mitochondrial

Chain O:



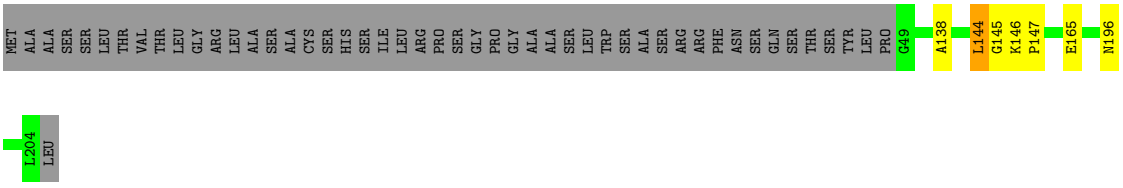
• Molecule 41: 39S ribosomal protein L20, mitochondrial

Chain R:



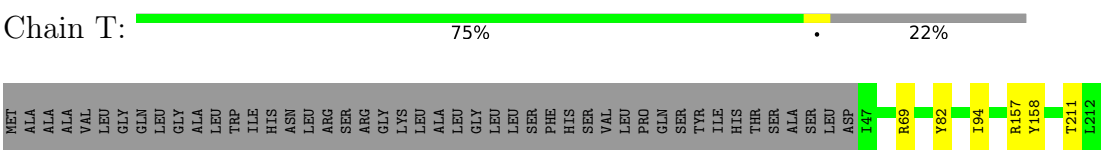
• Molecule 42: 39S ribosomal protein L21, mitochondrial

Chain S:



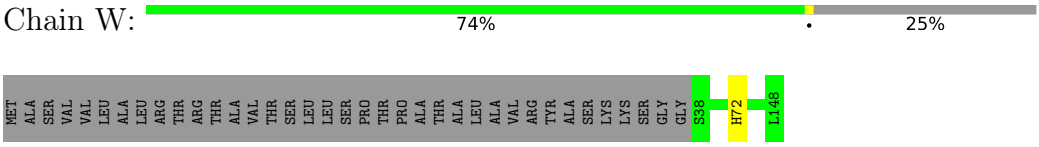
• Molecule 43: 39S ribosomal protein L22, mitochondrial

Chain T:



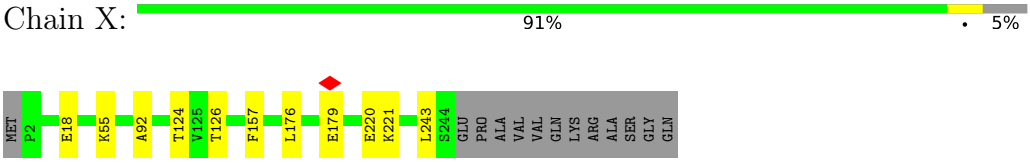
• Molecule 44: 39S ribosomal protein L27, mitochondrial

Chain W:



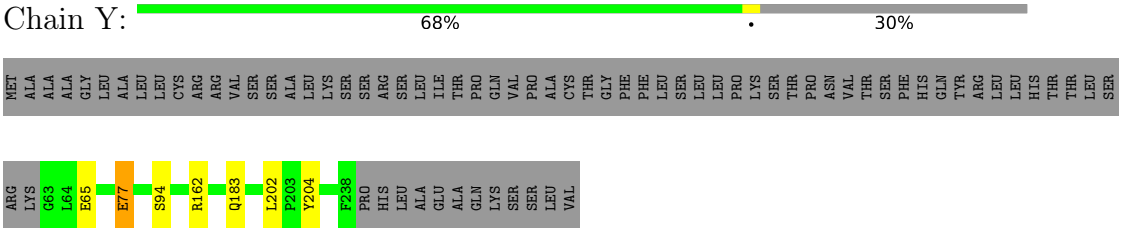
• Molecule 45: 39S ribosomal protein L28, mitochondrial

Chain X:



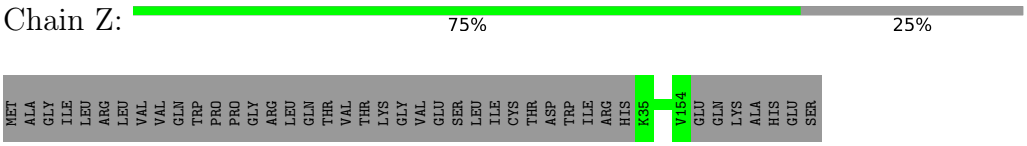
• Molecule 46: 39S ribosomal protein L47, mitochondrial

Chain Y:



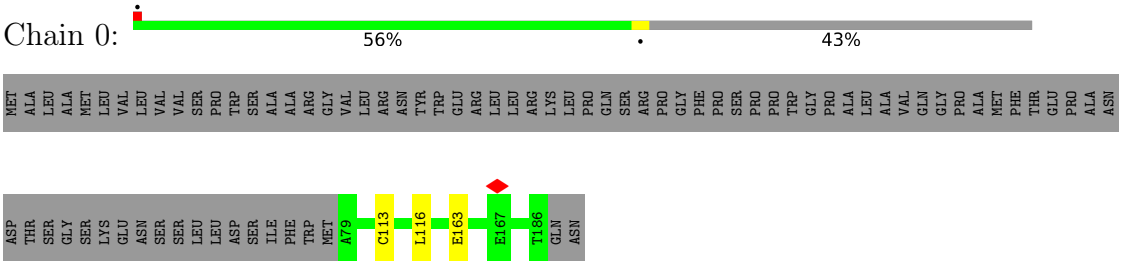
• Molecule 47: 39S ribosomal protein L30, mitochondrial

Chain Z:



• Molecule 48: 39S ribosomal protein L32, mitochondrial

Chain 0:

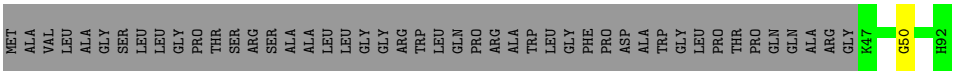


• Molecule 49: 39S ribosomal protein L33, mitochondrial

Chain 1:

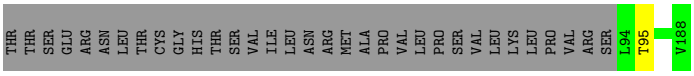
• Molecule 50: 39S ribosomal protein L34, mitochondrial

Chain 2:



• Molecule 51: 39S ribosomal protein L35, mitochondrial

Chain 3:

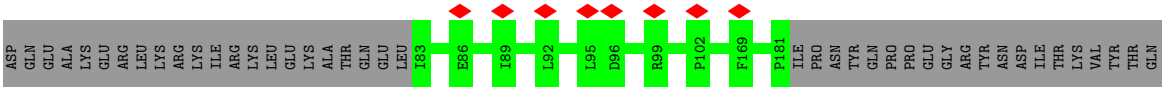


• Molecule 52: 39S ribosomal protein L36, mitochondrial

Chain 4:

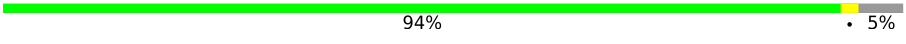
• Molecule 53: 39S ribosomal protein L40, mitochondrial

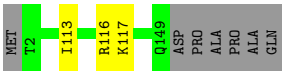
Chain 8:



• Molecule 54: 39S ribosomal protein L43, mitochondrial

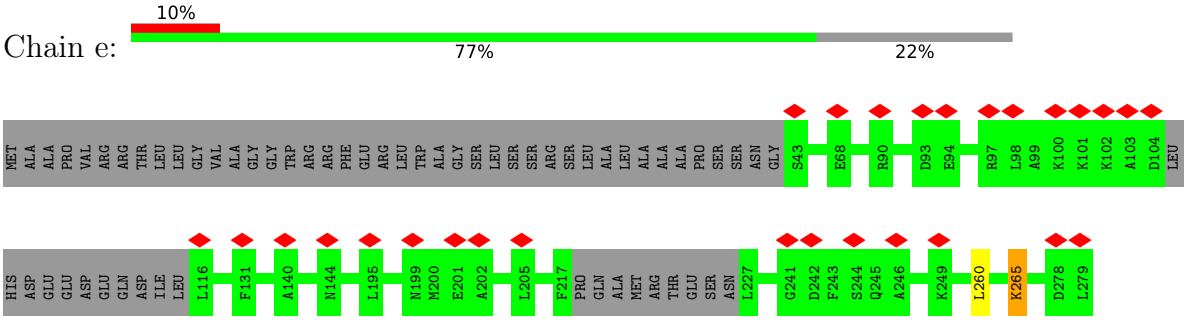
Chain b:





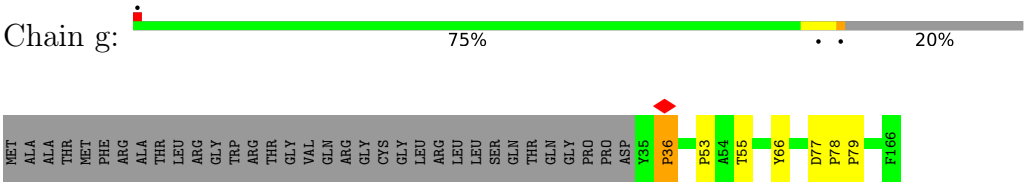
• Molecule 55: 39S ribosomal protein L46, mitochondrial

Chain e:



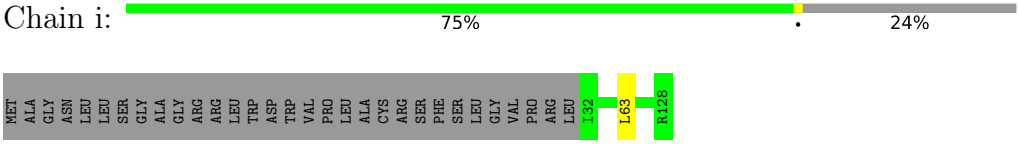
• Molecule 56: 39S ribosomal protein L49, mitochondrial

Chain g:



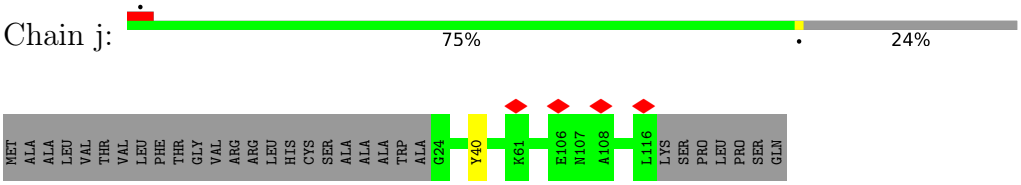
• Molecule 57: 39S ribosomal protein L51, mitochondrial

Chain i:



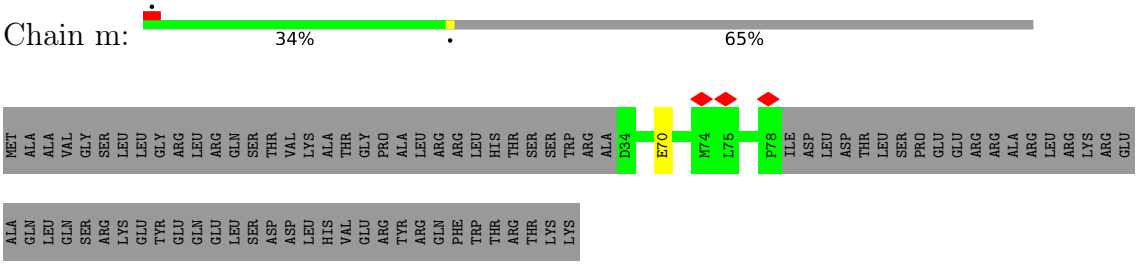
• Molecule 58: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA

Chain j:



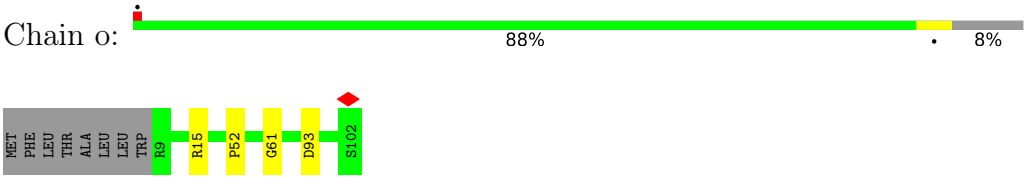
• Molecule 59: 39S ribosomal protein L55, mitochondrial

Chain m:



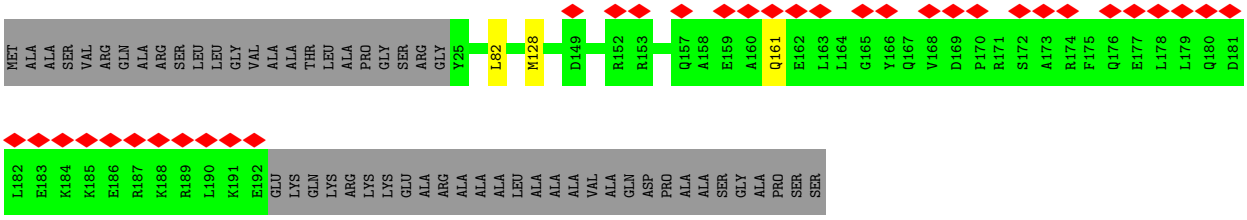
• Molecule 60: Ribosomal protein 63, mitochondrial

Chain o:



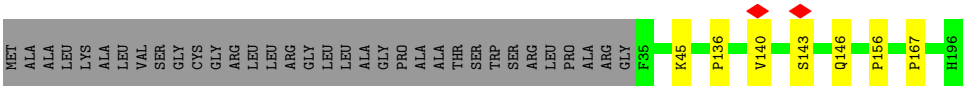
• Molecule 61: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



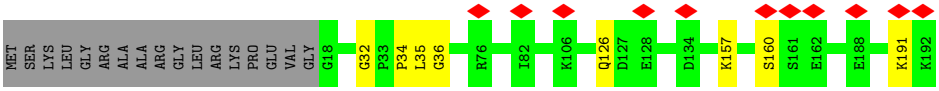
• Molecule 62: 39S ribosomal protein S18a, mitochondrial

Chain r:



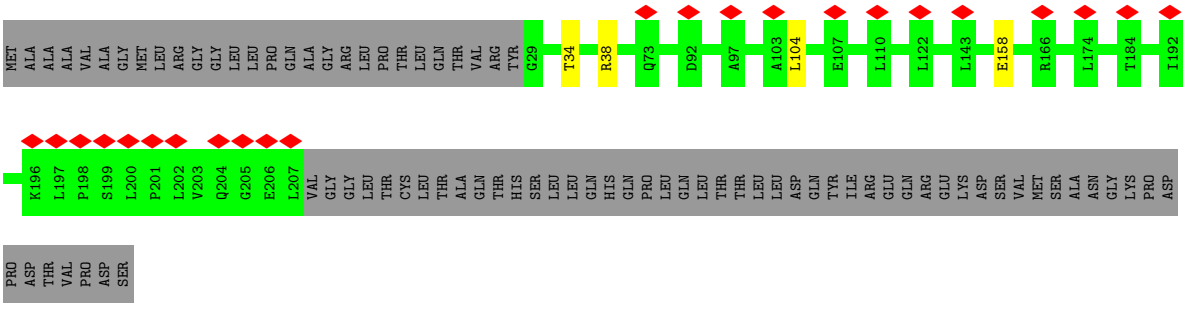
• Molecule 63: 39S ribosomal protein L11, mitochondrial

Chain J:



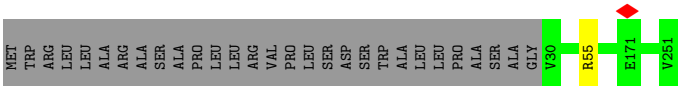
• Molecule 64: 39S ribosomal protein L10, mitochondrial

Chain I:



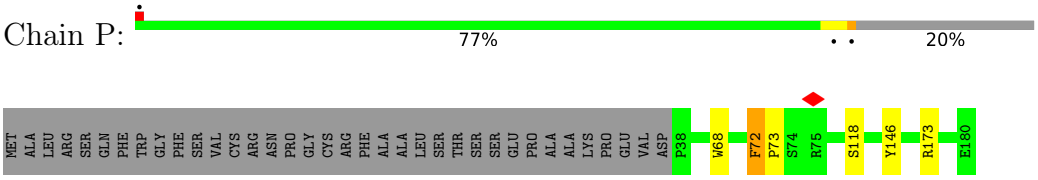
• Molecule 65: 39S ribosomal protein L16, mitochondrial

Chain N:



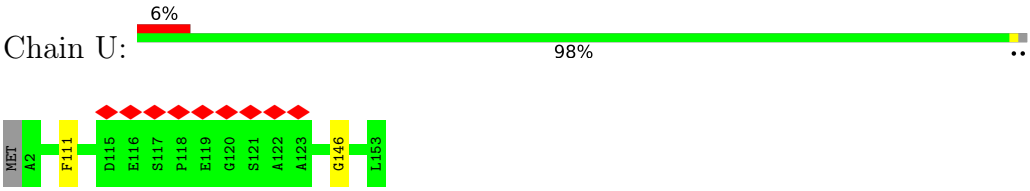
• Molecule 66: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain P:



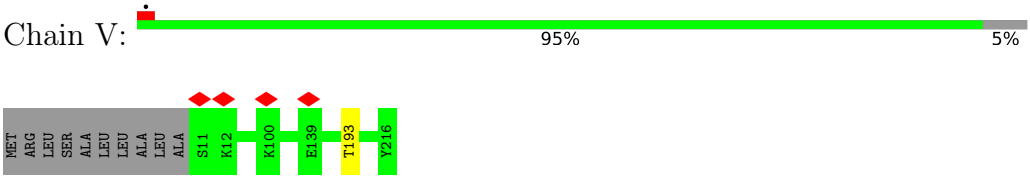
• Molecule 67: 39S ribosomal protein L23, mitochondrial

Chain U:



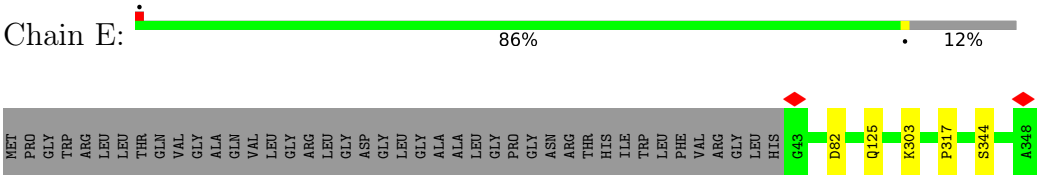
• Molecule 68: 39S ribosomal protein L24, mitochondrial

Chain V:



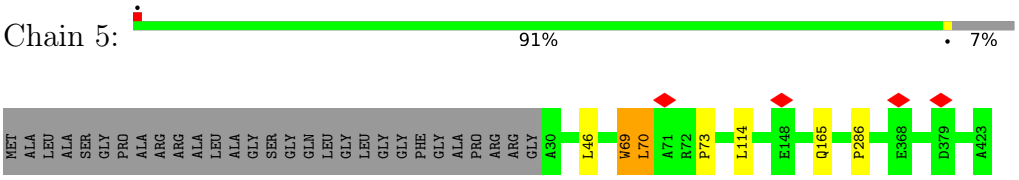
• Molecule 69: 39S ribosomal protein L3, mitochondrial

Chain E:



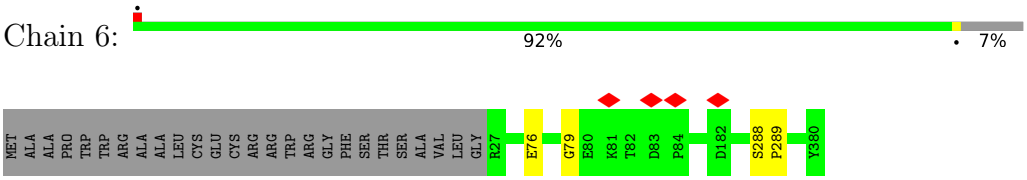
• Molecule 70: 39S ribosomal protein L37, mitochondrial

Chain 5:



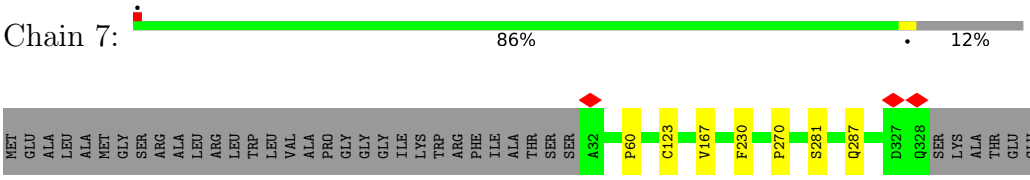
• Molecule 71: 39S ribosomal protein L38, mitochondrial

Chain 6:



• Molecule 72: 39S ribosomal protein L39, mitochondrial

Chain 7:

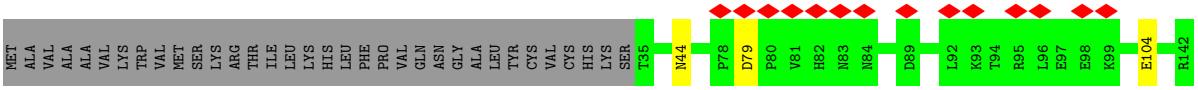


• Molecule 73: 39S ribosomal protein L41, mitochondrial

Chain 9:

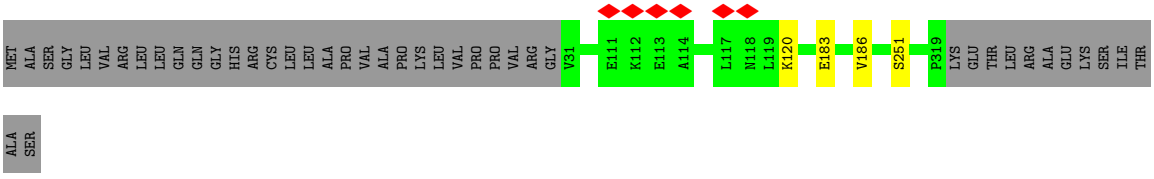
• Molecule 74: 39S ribosomal protein L42, mitochondrial

Chain a:



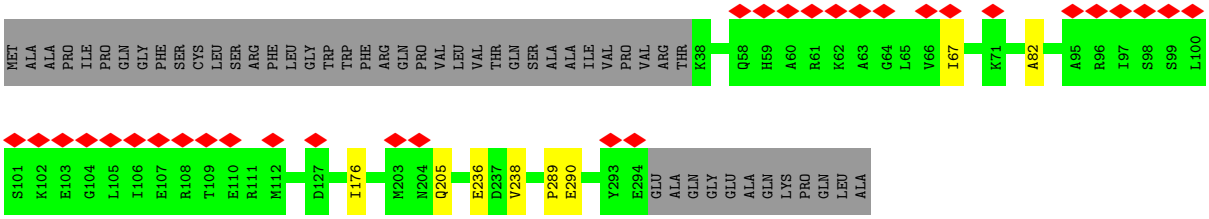
• Molecule 75: 39S ribosomal protein L44, mitochondrial

Chain c:



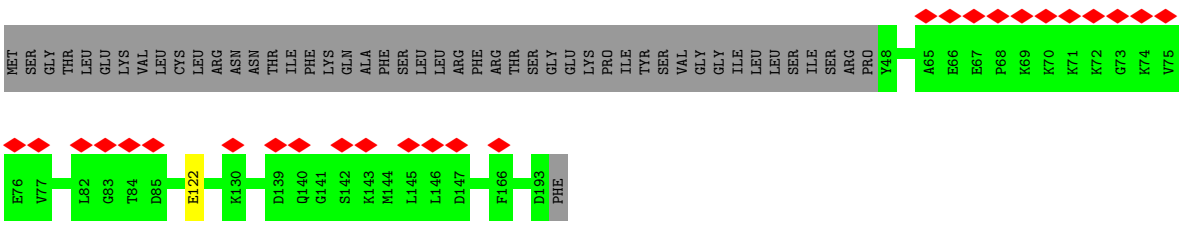
• Molecule 76: 39S ribosomal protein L45, mitochondrial

Chain d:



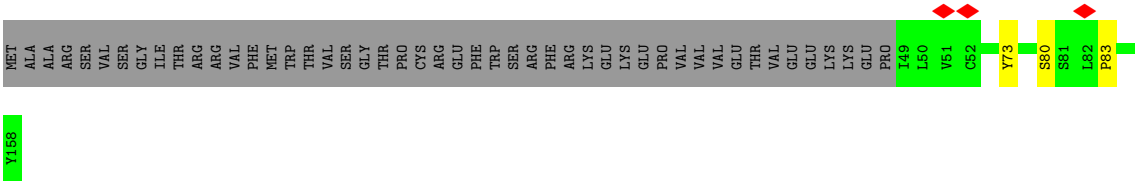
• Molecule 77: 39S ribosomal protein L48, mitochondrial

Chain f:



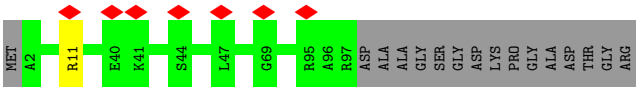
• Molecule 78: 39S ribosomal protein L50, mitochondrial

Chain h:



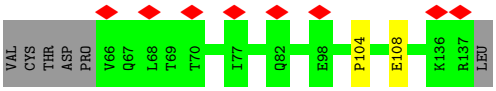
• Molecule 79: 39S ribosomal protein L53, mitochondrial

Chain k:



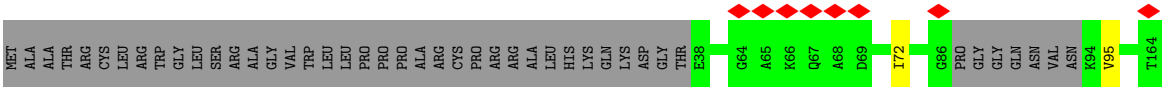
• Molecule 80: 39S ribosomal protein L54, mitochondrial

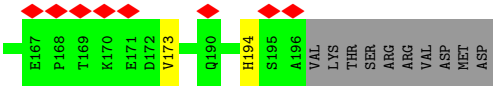
Chain l:



• Molecule 81: Peptidyl-tRNA hydrolase ICT1, mitochondrial

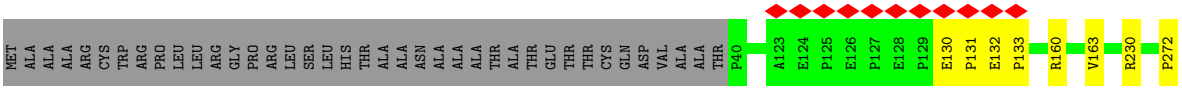
Chain p:

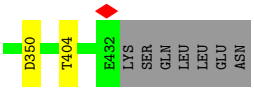




• Molecule 82: 39S ribosomal protein S30, mitochondrial

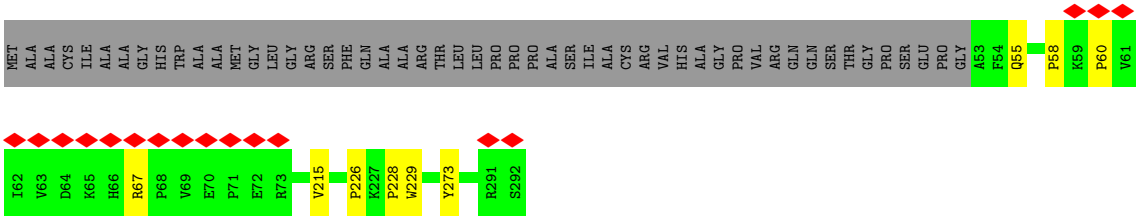
Chain s:





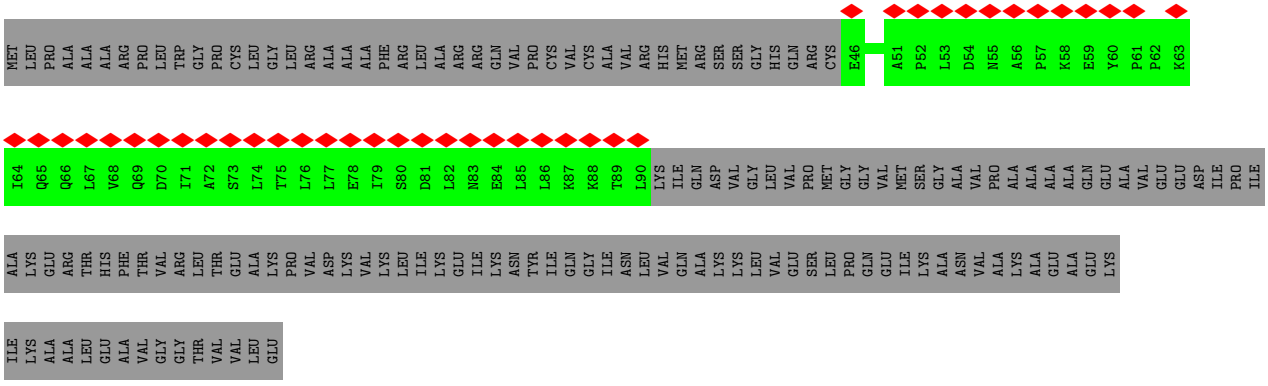
• Molecule 83: 39S ribosomal protein L19, mitochondrial

Chain Q:



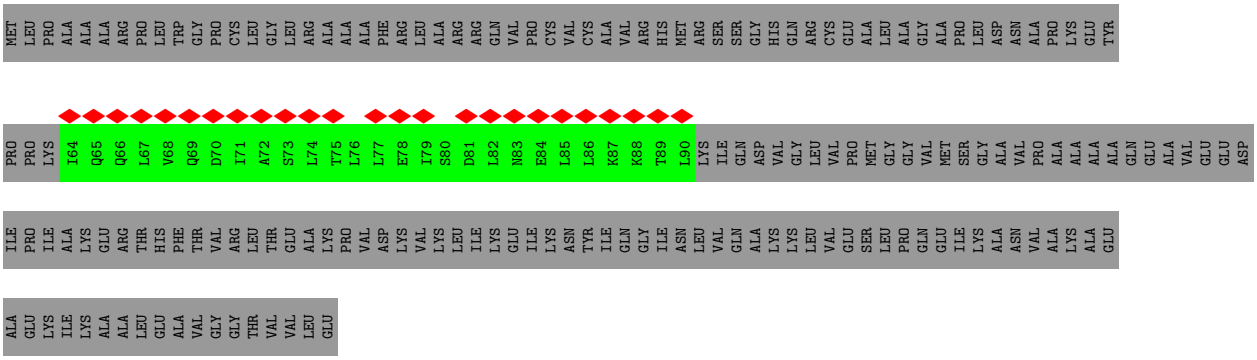
• Molecule 84: 39S ribosomal protein L12, mitochondrial

Chain TA:



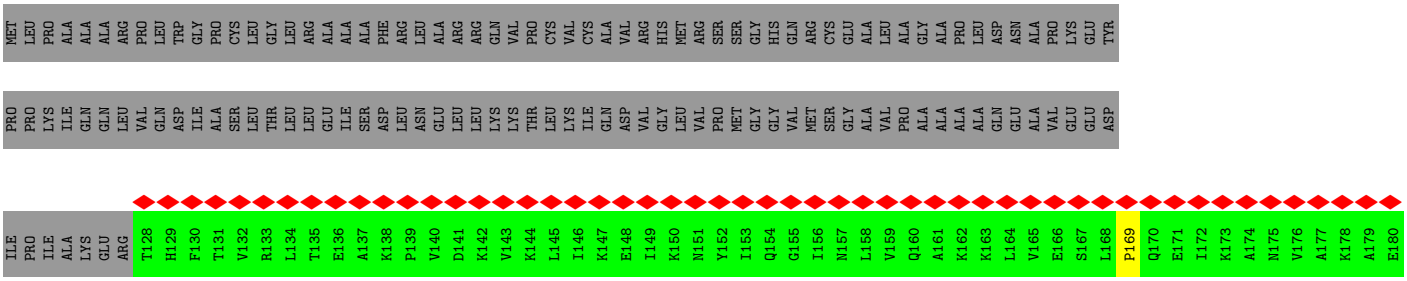
• Molecule 84: 39S ribosomal protein L12, mitochondrial

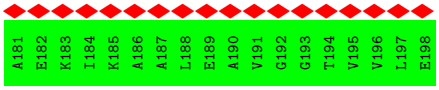
Chain TB:



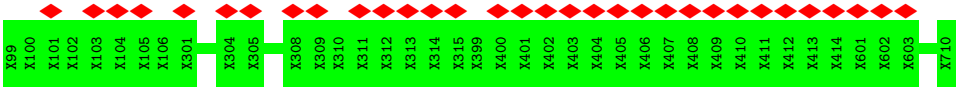
• Molecule 84: 39S ribosomal protein L12, mitochondrial

Chain TC:

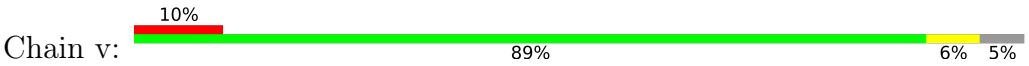


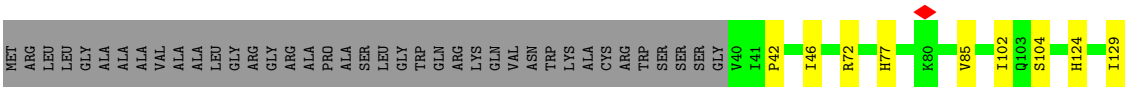


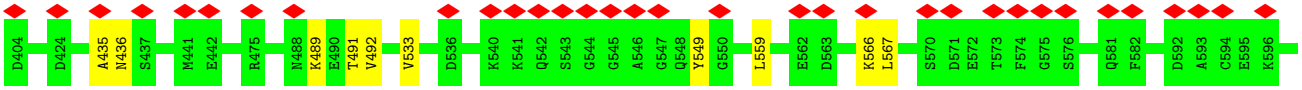
• Molecule 85: P-site finger

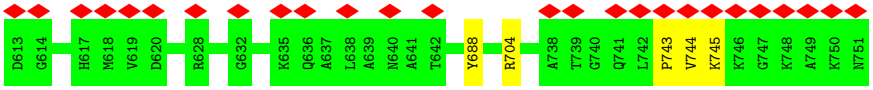


• Molecule 86: Elongation factor G, mitochondrial



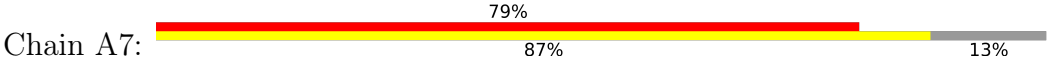


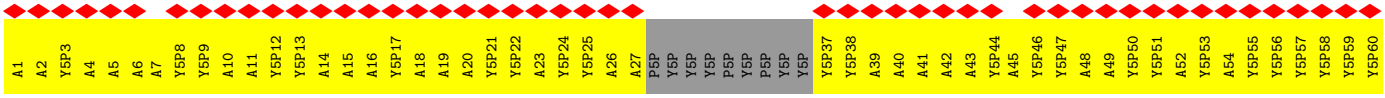




• Molecule 87: mRNA

• Molecule 88: E-tRNA





4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	438.44, 438.44, 438.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN, GCP, P5P, MG, Y5P, GDP

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	0.14	0/22406	0.73	11/34881 (0.0%)
2	AB	0.23	0/1830	0.38	0/2477
3	AC	0.23	0/1112	0.38	0/1505
4	AE	0.23	0/989	0.43	0/1335
5	AI	0.24	0/1031	0.45	0/1390
6	AJ	0.23	0/854	0.41	0/1148
7	AK	0.21	0/879	0.37	0/1182
8	AM	0.23	0/941	0.39	0/1265
9	AN	0.23	0/864	0.40	0/1169
10	AO	0.23	0/1624	0.37	0/2209
11	AP	0.23	0/791	0.36	0/1062
12	AQ	0.22	0/752	0.36	0/1001
13	AT	0.24	0/1402	0.39	0/1883
14	AW	0.23	0/778	0.42	0/1048
15	AX	0.23	0/2932	0.39	0/3968
16	A2	0.23	0/939	0.38	0/1256
17	AH	0.23	0/1037	0.40	0/1403
18	AL	0.23	0/1475	0.34	0/1970
19	AR	0.23	0/2435	0.37	0/3288
20	AS	0.24	0/1138	0.37	0/1533
21	AU	0.23	0/1521	0.34	0/2039
22	AV	0.23	0/3071	0.36	0/4147
23	AY	0.24	0/1046	0.40	0/1410
24	AZ	0.24	0/851	0.37	0/1133
25	A1	0.23	0/2277	0.36	0/3079
26	A0	0.22	0/1827	0.38	0/2473
27	A3	0.23	0/650	0.36	0/855
28	A4	0.23	0/3028	0.36	0/4197
29	AD	0.23	0/2783	0.39	0/3724
30	AF	0.23	0/1765	0.38	0/2369
31	AG	0.23	0/2642	0.39	0/3538
32	A	0.14	0/36246	0.74	6/56422 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	B	0.13	0/1328	0.71	0/2056
34	D	0.23	0/1904	0.41	0/2561
35	F	0.23	0/2071	0.39	0/2817
36	H	0.22	0/820	0.41	0/1102
37	K	0.23	0/1495	0.38	0/2029
38	L	0.23	0/904	0.41	0/1218
39	M	0.24	0/2359	0.38	0/3185
40	O	0.23	0/1269	0.39	0/1708
41	R	0.23	0/1174	0.42	1/1572 (0.1%)
42	S	0.23	0/1276	0.47	2/1729 (0.1%)
43	T	0.23	0/1402	0.38	0/1886
44	W	0.24	0/893	0.42	0/1204
45	X	0.23	0/2081	0.37	0/2812
46	Y	0.23	0/1552	0.35	0/2079
47	Z	0.23	0/1003	0.39	0/1354
48	0	0.22	0/895	0.40	0/1201
49	1	0.23	0/438	0.41	0/583
50	2	0.22	0/382	0.38	0/507
51	3	0.23	0/852	0.38	0/1136
52	4	0.22	0/350	0.39	0/461
53	8	0.23	0/855	0.38	0/1152
54	b	0.23	0/1202	0.40	0/1626
55	e	0.24	0/1797	0.40	0/2422
56	g	0.25	0/1132	0.41	0/1543
57	i	0.23	0/849	0.36	0/1135
58	j	0.23	0/755	0.38	0/1016
59	m	0.21	0/379	0.41	0/510
60	o	0.22	0/818	0.36	0/1097
61	q	0.23	0/1325	0.39	0/1799
62	r	0.22	0/1362	0.37	0/1846
63	J	0.30	0/1348	0.47	0/1813
64	I	0.24	0/1467	0.42	0/1984
65	N	0.24	0/1833	0.40	0/2468
66	P	0.25	0/1191	0.48	0/1611
67	U	0.24	0/1254	0.39	0/1700
68	V	0.23	0/1727	0.40	0/2341
69	E	0.24	0/2479	0.40	0/3360
70	5	0.29	1/3305 (0.0%)	0.43	0/4502
71	6	0.23	0/3043	0.39	0/4140
72	7	0.23	0/2467	0.39	0/3337
73	9	0.25	0/1025	0.39	0/1379
74	a	0.22	0/923	0.39	0/1254
75	c	0.24	0/2371	0.37	0/3205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	d	0.24	0/2132	0.40	0/2887
77	f	0.23	0/1144	0.43	0/1551
78	h	0.23	0/917	0.38	0/1249
79	k	0.23	0/754	0.40	0/1017
80	l	0.23	0/636	0.37	0/860
81	p	0.22	0/1246	0.39	0/1675
82	s	0.24	0/3262	0.40	0/4435
83	Q	0.24	0/2044	0.39	0/2757
84	TA	0.23	0/349	0.41	0/475
84	TB	0.21	0/212	0.39	0/286
84	TC	0.24	0/351	0.41	0/488
86	v	0.25	0/5647	0.44	0/7623
All	All	0.21	1/181965 (0.0%)	0.54	20/258102 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	5	69	TRP	CD2-CE2	-6.57	1.33	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	765	C	C2-N1-C1'	8.18	127.80	118.80
1	AA	1443	U	C2-N1-C1'	7.01	126.12	117.70
32	A	3169	C	C2-N1-C1'	6.91	126.40	118.80
1	AA	765	C	N1-C2-O2	6.87	123.02	118.90
32	A	3169	C	N1-C2-O2	6.45	122.77	118.90

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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	218/296 (74%)	187 (86%)	27 (12%)	4 (2%)	8 35
3	AC	130/167 (78%)	107 (82%)	22 (17%)	1 (1%)	19 55
4	AE	120/125 (96%)	98 (82%)	18 (15%)	4 (3%)	4 19
5	AI	134/194 (69%)	113 (84%)	18 (13%)	3 (2%)	6 29
6	AJ	106/138 (77%)	92 (87%)	12 (11%)	2 (2%)	8 33
7	AK	99/128 (77%)	88 (89%)	8 (8%)	3 (3%)	4 21
8	AM	114/137 (83%)	103 (90%)	10 (9%)	1 (1%)	17 53
9	AN	105/130 (81%)	85 (81%)	18 (17%)	2 (2%)	8 33
10	AO	188/258 (73%)	166 (88%)	18 (10%)	4 (2%)	7 30
11	AP	94/142 (66%)	82 (87%)	10 (11%)	2 (2%)	7 30
12	AQ	84/87 (97%)	71 (84%)	13 (16%)	0	100 100
13	AT	166/173 (96%)	149 (90%)	16 (10%)	1 (1%)	25 61
14	AW	95/187 (51%)	77 (81%)	15 (16%)	3 (3%)	4 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	AX	351/398 (88%)	319 (91%)	28 (8%)	4 (1%)	14 47
16	A2	114/118 (97%)	96 (84%)	17 (15%)	1 (1%)	17 53
17	AH	120/201 (60%)	101 (84%)	16 (13%)	3 (2%)	5 26
18	AL	172/257 (67%)	154 (90%)	15 (9%)	3 (2%)	9 36
19	AR	290/360 (81%)	263 (91%)	26 (9%)	1 (0%)	41 74
20	AS	133/190 (70%)	119 (90%)	10 (8%)	4 (3%)	4 21
21	AU	175/205 (85%)	163 (93%)	12 (7%)	0	100 100
22	AV	363/414 (88%)	319 (88%)	36 (10%)	8 (2%)	6 29
23	AY	118/395 (30%)	107 (91%)	10 (8%)	1 (1%)	19 55
24	AZ	97/106 (92%)	82 (84%)	15 (16%)	0	100 100
25	A1	273/323 (84%)	242 (89%)	25 (9%)	6 (2%)	6 29
26	A0	212/218 (97%)	185 (87%)	22 (10%)	5 (2%)	6 27
27	A3	70/199 (35%)	64 (91%)	6 (9%)	0	100 100
28	A4	541/689 (78%)	465 (86%)	66 (12%)	10 (2%)	8 35
29	AD	341/430 (79%)	306 (90%)	31 (9%)	4 (1%)	13 45
30	AF	206/242 (85%)	180 (87%)	23 (11%)	3 (2%)	10 39
31	AG	311/396 (78%)	272 (88%)	37 (12%)	2 (1%)	25 61
34	D	237/305 (78%)	208 (88%)	27 (11%)	2 (1%)	19 55
35	F	248/311 (80%)	217 (88%)	27 (11%)	4 (2%)	9 38
36	H	96/267 (36%)	84 (88%)	10 (10%)	2 (2%)	7 30
37	K	175/178 (98%)	153 (87%)	16 (9%)	6 (3%)	3 18
38	L	113/145 (78%)	102 (90%)	10 (9%)	1 (1%)	17 53
39	M	285/296 (96%)	252 (88%)	26 (9%)	7 (2%)	5 26
40	O	150/175 (86%)	128 (85%)	19 (13%)	3 (2%)	7 32
41	R	138/149 (93%)	123 (89%)	10 (7%)	5 (4%)	3 17
42	S	154/205 (75%)	135 (88%)	15 (10%)	4 (3%)	5 25
43	T	164/212 (77%)	148 (90%)	13 (8%)	3 (2%)	8 35
44	W	109/148 (74%)	97 (89%)	11 (10%)	1 (1%)	17 53
45	X	241/256 (94%)	212 (88%)	24 (10%)	5 (2%)	7 30
46	Y	174/250 (70%)	161 (92%)	7 (4%)	6 (3%)	3 18
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%)	5 23
49	1	50/65 (77%)	42 (84%)	7 (14%)	1 (2%)	7 32
50	2	44/92 (48%)	41 (93%)	2 (4%)	1 (2%)	6 28
51	3	93/188 (50%)	84 (90%)	8 (9%)	1 (1%)	14 47
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%)	7 30
55	e	211/279 (76%)	188 (89%)	22 (10%)	1 (0%)	29 66
56	g	130/166 (78%)	109 (84%)	17 (13%)	4 (3%)	4 20
57	i	95/128 (74%)	75 (79%)	20 (21%)	0	100 100
58	j	91/123 (74%)	84 (92%)	6 (7%)	1 (1%)	14 47
59	m	43/128 (34%)	34 (79%)	8 (19%)	1 (2%)	6 28
60	o	92/102 (90%)	79 (86%)	10 (11%)	3 (3%)	4 19
61	q	166/222 (75%)	154 (93%)	10 (6%)	2 (1%)	13 45
62	r	160/196 (82%)	139 (87%)	16 (10%)	5 (3%)	4 20
63	J	173/192 (90%)	152 (88%)	15 (9%)	6 (4%)	3 18
64	I	177/261 (68%)	164 (93%)	12 (7%)	1 (1%)	25 61
65	N	220/251 (88%)	203 (92%)	16 (7%)	1 (0%)	29 66
66	P	141/179 (79%)	123 (87%)	14 (10%)	4 (3%)	5 23
67	U	150/153 (98%)	122 (81%)	26 (17%)	2 (1%)	12 43
68	V	204/216 (94%)	179 (88%)	25 (12%)	0	100 100
69	E	304/348 (87%)	268 (88%)	32 (10%)	4 (1%)	12 43
70	5	392/423 (93%)	347 (88%)	41 (10%)	4 (1%)	15 50
71	6	352/380 (93%)	302 (86%)	47 (13%)	3 (1%)	17 53
72	7	295/338 (87%)	260 (88%)	28 (10%)	7 (2%)	6 27
73	9	122/137 (89%)	106 (87%)	15 (12%)	1 (1%)	19 55
74	a	106/142 (75%)	95 (90%)	8 (8%)	3 (3%)	5 23
75	c	287/332 (86%)	265 (92%)	18 (6%)	4 (1%)	11 41
76	d	255/306 (83%)	216 (85%)	33 (13%)	6 (2%)	6 27
77	f	144/194 (74%)	121 (84%)	22 (15%)	1 (1%)	22 58
78	h	108/158 (68%)	93 (86%)	13 (12%)	2 (2%)	8 33

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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%)	11 41
81	p	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	11 41
82	s	391/439 (89%)	342 (88%)	41 (10%)	8 (2%)	7 32
83	Q	238/292 (82%)	211 (89%)	20 (8%)	7 (3%)	4 22
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%)	11 41
86	v	710/751 (94%)	566 (80%)	117 (16%)	27 (4%)	3 16
All	All	14720/19244 (76%)	12876 (88%)	1589 (11%)	255 (2%)	13 36

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	193/249 (78%)	192 (100%)	1 (0%)	88 95
3	AC	115/143 (80%)	115 (100%)	0	100 100
4	AE	104/107 (97%)	103 (99%)	1 (1%)	76 91
5	AI	104/147 (71%)	103 (99%)	1 (1%)	76 91
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%)	73 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AN	93/115 (81%)	93 (100%)	0	100	100
10	AO	171/230 (74%)	171 (100%)	0	100	100
11	AP	87/123 (71%)	85 (98%)	2 (2%)	50	79
12	AQ	78/79 (99%)	78 (100%)	0	100	100
13	AT	153/157 (98%)	152 (99%)	1 (1%)	84	93
14	AW	84/158 (53%)	84 (100%)	0	100	100
15	AX	312/351 (89%)	311 (100%)	1 (0%)	92	97
16	A2	99/101 (98%)	96 (97%)	3 (3%)	41	73
17	AH	112/180 (62%)	111 (99%)	1 (1%)	78	91
18	AL	157/226 (70%)	155 (99%)	2 (1%)	69	88
19	AR	262/318 (82%)	261 (100%)	1 (0%)	91	97
20	AS	116/164 (71%)	115 (99%)	1 (1%)	78	91
21	AU	153/174 (88%)	153 (100%)	0	100	100
22	AV	328/364 (90%)	323 (98%)	5 (2%)	65	86
23	AY	111/357 (31%)	111 (100%)	0	100	100
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%)	184 (99%)	2 (1%)	73	90
27	A3	66/166 (40%)	63 (96%)	3 (4%)	27	62
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%)	178 (96%)	7 (4%)	33	67
31	AG	273/342 (80%)	272 (100%)	1 (0%)	91	97
34	D	193/245 (79%)	193 (100%)	0	100	100
35	F	217/262 (83%)	216 (100%)	1 (0%)	88	95
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%)	76	91
39	M	245/249 (98%)	242 (99%)	3 (1%)	71	89
40	O	133/150 (89%)	133 (100%)	0	100	100
41	R	118/126 (94%)	117 (99%)	1 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	S	141/180 (78%)	140 (99%)	1 (1%)	84 93
43	T	146/182 (80%)	143 (98%)	3 (2%)	53 80
44	W	91/119 (76%)	91 (100%)	0	100 100
45	X	217/227 (96%)	211 (97%)	6 (3%)	43 75
46	Y	159/223 (71%)	157 (99%)	2 (1%)	69 88
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%)	55 81
50	2	40/72 (56%)	40 (100%)	0	100 100
51	3	88/166 (53%)	88 (100%)	0	100 100
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%)	73 90
56	g	122/148 (82%)	119 (98%)	3 (2%)	47 77
57	i	86/110 (78%)	85 (99%)	1 (1%)	71 89
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%)	69 88
61	q	114/178 (64%)	113 (99%)	1 (1%)	78 91
62	r	147/169 (87%)	145 (99%)	2 (1%)	67 86
63	J	138/150 (92%)	136 (99%)	2 (1%)	67 86
64	I	164/232 (71%)	161 (98%)	3 (2%)	59 83
65	N	189/211 (90%)	189 (100%)	0	100 100
66	P	125/154 (81%)	123 (98%)	2 (2%)	62 85
67	U	126/135 (93%)	126 (100%)	0	100 100
68	V	184/191 (96%)	183 (100%)	1 (0%)	88 95
69	E	260/290 (90%)	259 (100%)	1 (0%)	91 97
70	5	353/368 (96%)	349 (99%)	4 (1%)	73 90
71	6	313/332 (94%)	312 (100%)	1 (0%)	92 97
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%)	76 91
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%)	222 (99%)	2 (1%)	78 91
77	f	122/173 (70%)	122 (100%)	0	100 100
78	h	104/148 (70%)	103 (99%)	1 (1%)	76 91
79	k	81/90 (90%)	80 (99%)	1 (1%)	71 89
80	l	67/116 (58%)	66 (98%)	1 (2%)	65 86
81	p	134/181 (74%)	132 (98%)	2 (2%)	65 86
82	s	336/381 (88%)	335 (100%)	1 (0%)	92 97
83	Q	221/256 (86%)	219 (99%)	2 (1%)	78 91
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%)	580 (97%)	18 (3%)	41 73
All	All	12561/16442 (76%)	12455 (99%)	106 (1%)	82 92

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	g	77	ASP
69	E	303	LYS
86	v	393	VAL
60	o	93	ASP
64	I	34	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 200 such sidechains are listed below:

Mol	Chain	Res	Type
58	j	63	GLN
69	E	313	ASN
86	v	678	GLN
61	q	81	GLN
64	I	91	GLN

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	Y5P	A7	51	88	14,19,20	3.49	1 (7%)	18,26,29	1.04	2 (11%)
88	Y5P	A7	12	88	14,19,20	3.31	1 (7%)	18,26,29	1.00	1 (5%)
88	Y5P	A7	62	88	14,19,20	3.49	1 (7%)	18,26,29	1.08	1 (5%)
87	P5P	A5	6	87	16,23,24	1.37	2 (12%)	14,33,36	2.17	3 (21%)
88	P5P	A7	18	88	16,23,24	1.43	3 (18%)	14,33,36	2.17	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	Y5P	A7	55	88	14,19,20	3.44	1 (7%)	18,26,29	1.10	1 (5%)
88	P5P	A7	16	88	16,23,24	1.54	4 (25%)	14,33,36	2.29	3 (21%)
88	Y5P	A7	13	88	14,19,20	3.33	1 (7%)	18,26,29	0.85	1 (5%)
87	Y5P	A5	3	87	14,19,20	3.47	1 (7%)	18,26,29	1.29	2 (11%)
88	Y5P	A7	57	88	14,19,20	3.51	1 (7%)	18,26,29	1.02	1 (5%)
88	P5P	A7	15	88	16,23,24	1.54	4 (25%)	14,33,36	2.04	2 (14%)
88	Y5P	A7	67	88	14,19,20	3.75	1 (7%)	18,26,29	1.15	1 (5%)
88	P5P	A7	45	88	16,23,24	1.34	2 (12%)	14,33,36	2.28	2 (14%)
88	Y5P	A7	64	88	14,19,20	3.68	1 (7%)	18,26,29	0.95	1 (5%)
88	P5P	A7	14	88	16,23,24	1.41	3 (18%)	14,33,36	1.98	2 (14%)
88	Y5P	A7	17	88	14,19,20	3.53	1 (7%)	18,26,29	0.93	1 (5%)
88	Y5P	A7	38	88	14,19,20	3.49	1 (7%)	18,26,29	0.97	1 (5%)
88	Y5P	A7	66	88	14,19,20	3.70	1 (7%)	18,26,29	1.02	1 (5%)
88	Y5P	A7	68	88	14,19,20	3.58	1 (7%)	18,26,29	1.30	3 (16%)
88	P5P	A7	52	88	16,23,24	1.42	2 (12%)	14,33,36	2.16	3 (21%)
87	Y5P	A5	1	87	14,19,20	3.76	2 (14%)	18,26,29	1.55	2 (11%)
88	Y5P	A7	25	88	14,19,20	3.40	1 (7%)	18,26,29	0.96	1 (5%)
87	Y5P	A5	8	87	14,19,20	3.51	1 (7%)	18,26,29	1.01	2 (11%)
88	Y5P	A7	63	88	14,19,20	3.50	1 (7%)	18,26,29	1.08	2 (11%)
88	Y5P	A7	50	88	14,19,20	3.46	1 (7%)	18,26,29	0.99	1 (5%)
88	P5P	A7	7	88	16,23,24	1.41	2 (12%)	14,33,36	2.23	2 (14%)
87	Y5P	A5	10	87	14,19,20	3.45	1 (7%)	18,26,29	0.99	1 (5%)
88	P5P	A7	2	88	16,23,24	1.54	3 (18%)	14,33,36	2.22	2 (14%)
88	P5P	A7	39	88	16,23,24	1.35	2 (12%)	14,33,36	2.21	2 (14%)
88	Y5P	A7	3	88	14,19,20	3.58	1 (7%)	18,26,29	1.09	1 (5%)
88	P5P	A7	43	88	16,23,24	1.54	3 (18%)	14,33,36	2.43	4 (28%)
88	P5P	A7	5	88	16,23,24	1.36	1 (6%)	14,33,36	2.14	2 (14%)
88	Y5P	A7	22	88	14,19,20	3.48	1 (7%)	18,26,29	1.02	1 (5%)
88	P5P	A7	19	88	16,23,24	1.43	2 (12%)	14,33,36	2.19	3 (21%)
88	P5P	A7	42	88	16,23,24	1.32	2 (12%)	14,33,36	2.16	2 (14%)
88	P5P	A7	20	88	16,23,24	1.37	1 (6%)	14,33,36	2.10	2 (14%)
88	P5P	A7	48	88	16,23,24	1.35	2 (12%)	14,33,36	2.16	2 (14%)
88	P5P	A7	49	88	16,23,24	1.39	2 (12%)	14,33,36	2.13	2 (14%)
88	Y5P	A7	24	88	14,19,20	3.35	1 (7%)	18,26,29	0.95	1 (5%)
88	P5P	A7	71	88,32	16,23,24	1.32	3 (18%)	14,33,36	1.99	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	Y5P	A7	59	88	14,19,20	3.62	1 (7%)	18,26,29	1.02	1 (5%)
88	Y5P	A7	8	88	14,19,20	3.65	1 (7%)	18,26,29	0.96	2 (11%)
88	Y5P	A7	70	88	14,19,20	3.68	1 (7%)	18,26,29	0.93	2 (11%)
88	P5P	A7	54	88	16,23,24	1.40	2 (12%)	14,33,36	2.05	2 (14%)
88	Y5P	A7	65	88	14,19,20	3.63	1 (7%)	18,26,29	1.04	1 (5%)
88	Y5P	A7	69	88	14,19,20	3.50	1 (7%)	18,26,29	1.00	2 (11%)
88	Y5P	A7	60	88	14,19,20	3.59	1 (7%)	18,26,29	1.15	1 (5%)
88	P5P	A7	1	88	16,20,24	1.44	1 (6%)	14,29,36	2.06	2 (14%)
88	P5P	A7	26	88	16,23,24	1.38	2 (12%)	14,33,36	2.20	2 (14%)
87	P5P	A5	11	87	16,23,24	1.35	2 (12%)	14,33,36	2.01	2 (14%)
87	P5P	A5	9	87	16,23,24	1.34	2 (12%)	14,33,36	2.00	2 (14%)
88	Y5P	A7	9	88	14,19,20	3.65	1 (7%)	18,26,29	1.47	2 (11%)
88	Y5P	A7	37	88	14,19,20	3.44	1 (7%)	18,26,29	0.99	2 (11%)
87	P5P	A5	5	87	16,23,24	1.38	2 (12%)	14,33,36	2.07	2 (14%)
88	Y5P	A7	47	88	14,19,20	3.59	1 (7%)	18,26,29	1.12	1 (5%)
88	P5P	A7	4	88	16,23,24	1.36	2 (12%)	14,33,36	2.21	3 (21%)
88	P5P	A7	40	88	16,23,24	1.36	2 (12%)	14,33,36	2.13	2 (14%)
87	P5P	A5	2	87	16,23,24	1.50	2 (12%)	14,33,36	2.09	2 (14%)
88	Y5P	A7	56	88	14,19,20	3.42	1 (7%)	18,26,29	1.08	1 (5%)
87	Y5P	A5	4	87	14,19,20	3.75	2 (14%)	18,26,29	1.53	3 (16%)
88	P5P	A7	6	88	16,23,24	1.34	1 (6%)	14,33,36	2.21	2 (14%)
88	P5P	A7	27	88	16,23,24	1.34	1 (6%)	14,33,36	2.20	2 (14%)
88	Y5P	A7	46	88	14,19,20	3.59	1 (7%)	18,26,29	1.08	2 (11%)
88	Y5P	A7	21	88	14,19,20	3.50	1 (7%)	18,26,29	1.14	1 (5%)
88	P5P	A7	41	88	16,23,24	1.41	2 (12%)	14,33,36	1.94	2 (14%)
88	Y5P	A7	44	88	14,19,20	3.72	1 (7%)	18,26,29	0.94	1 (5%)
87	Y5P	A5	7	87	14,19,20	3.57	1 (7%)	18,26,29	1.03	2 (11%)
88	Y5P	A7	61	88	14,19,20	3.44	1 (7%)	18,26,29	1.00	1 (5%)
88	Y5P	A7	53	88	14,19,20	3.80	1 (7%)	18,26,29	1.18	2 (11%)
88	P5P	A7	11	88	16,23,24	1.36	2 (12%)	14,33,36	2.18	2 (14%)
88	P5P	A7	23	88	16,23,24	1.38	2 (12%)	14,33,36	1.99	2 (14%)
88	P5P	A7	10	88	16,23,24	1.35	2 (12%)	14,33,36	2.10	2 (14%)
88	Y5P	A7	58	88	14,19,20	3.61	1 (7%)	18,26,29	1.05	1 (5%)

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	Y5P	A7	51	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	12	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	62	88	-	1/7/33/34	0/2/2/2
87	P5P	A5	6	87	-	0/3/25/26	0/3/3/3
88	P5P	A7	18	88	-	1/3/25/26	0/3/3/3
88	Y5P	A7	55	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	16	88	-	2/3/25/26	0/3/3/3
88	Y5P	A7	13	88	-	1/7/33/34	0/2/2/2
87	Y5P	A5	3	87	-	4/7/33/34	0/2/2/2
88	Y5P	A7	57	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	15	88	-	0/3/25/26	0/3/3/3
88	Y5P	A7	67	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	45	88	-	2/3/25/26	0/3/3/3
88	Y5P	A7	64	88	-	2/7/33/34	0/2/2/2
88	P5P	A7	14	88	-	2/3/25/26	0/3/3/3
88	Y5P	A7	17	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	38	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	66	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	68	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	52	88	-	3/3/25/26	0/3/3/3
87	Y5P	A5	1	87	-	7/7/33/34	0/2/2/2
88	Y5P	A7	25	88	-	1/7/33/34	0/2/2/2
87	Y5P	A5	8	87	-	3/7/33/34	0/2/2/2
88	Y5P	A7	63	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	50	88	-	4/7/33/34	0/2/2/2
88	P5P	A7	7	88	-	3/3/25/26	0/3/3/3
87	Y5P	A5	10	87	-	1/7/33/34	0/2/2/2
88	P5P	A7	2	88	-	0/3/25/26	0/3/3/3
88	P5P	A7	39	88	-	0/3/25/26	0/3/3/3
88	Y5P	A7	3	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	43	88	-	3/3/25/26	0/3/3/3
88	P5P	A7	5	88	-	2/3/25/26	0/3/3/3
88	Y5P	A7	22	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	19	88	-	0/3/25/26	0/3/3/3
88	P5P	A7	42	88	-	0/3/25/26	0/3/3/3
88	P5P	A7	20	88	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	P5P	A7	48	88	-	0/3/25/26	0/3/3/3
88	P5P	A7	49	88	-	0/3/25/26	0/3/3/3
88	Y5P	A7	24	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	71	88,32	-	1/3/25/26	0/3/3/3
88	Y5P	A7	59	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	8	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	70	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	54	88	-	1/3/25/26	0/3/3/3
88	Y5P	A7	65	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	69	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	60	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	1	88	-	0/2/22/26	0/3/3/3
88	P5P	A7	26	88	-	0/3/25/26	0/3/3/3
87	P5P	A5	11	87	-	0/3/25/26	0/3/3/3
87	P5P	A5	9	87	-	0/3/25/26	0/3/3/3
88	Y5P	A7	9	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	37	88	-	1/7/33/34	0/2/2/2
87	P5P	A5	5	87	-	2/3/25/26	0/3/3/3
88	Y5P	A7	47	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	4	88	-	0/3/25/26	0/3/3/3
88	P5P	A7	40	88	-	0/3/25/26	0/3/3/3
87	P5P	A5	2	87	-	2/3/25/26	0/3/3/3
88	Y5P	A7	56	88	-	3/7/33/34	0/2/2/2
87	Y5P	A5	4	87	-	7/7/33/34	0/2/2/2
88	P5P	A7	6	88	-	3/3/25/26	0/3/3/3
88	P5P	A7	27	88	-	0/3/25/26	0/3/3/3
88	Y5P	A7	46	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	21	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	41	88	-	0/3/25/26	0/3/3/3
88	Y5P	A7	44	88	-	3/7/33/34	0/2/2/2
87	Y5P	A5	7	87	-	3/7/33/34	0/2/2/2
88	Y5P	A7	61	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	53	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	11	88	-	0/3/25/26	0/3/3/3
88	P5P	A7	23	88	-	0/3/25/26	0/3/3/3
88	P5P	A7	10	88	-	0/3/25/26	0/3/3/3
88	Y5P	A7	58	88	-	3/7/33/34	0/2/2/2

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A7	53	Y5P	C4-N3	-13.91	1.33	1.46
88	A7	67	Y5P	C4-N3	-13.84	1.33	1.46
88	A7	44	Y5P	C4-N3	-13.71	1.33	1.46
87	A5	1	Y5P	C4-N3	-13.62	1.33	1.46
88	A7	66	Y5P	C4-N3	-13.62	1.33	1.46

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	A7	45	P5P	C6-N1-C2	7.22	126.18	115.84
88	A7	27	P5P	C6-N1-C2	7.10	126.02	115.84
88	A7	2	P5P	C6-N1-C2	7.06	125.95	115.84
88	A7	11	P5P	C6-N1-C2	7.04	125.93	115.84
88	A7	7	P5P	C6-N1-C2	6.99	125.85	115.84

There are no chirality outliers.

5 of 114 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.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	27,34,34	1.82	6 (22%)	34,54,54	2.36	8 (23%)
91	GDP	AX	500	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)

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	-	5/15/38/38	0/3/3/3
91	GDP	AX	500	-	-	1/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	v	802	GCP	PG-O1G	5.34	1.61	1.50
92	v	802	GCP	C5-C6	4.49	1.49	1.41
92	v	802	GCP	PG-O3G	3.01	1.61	1.54
92	v	802	GCP	PG-O2G	-2.53	1.49	1.54
91	AX	500	GDP	C6-N1	-2.36	1.34	1.37

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
92	v	802	GCP	PB-O3A-PA	-6.13	113.13	132.56
92	v	802	GCP	C4-C5-C6	-5.86	115.20	120.80
92	v	802	GCP	C2-N1-C6	4.66	123.34	115.93
92	v	802	GCP	C2-N3-C4	4.59	120.60	115.36
92	v	802	GCP	N3-C2-N1	-4.02	121.86	127.22

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'

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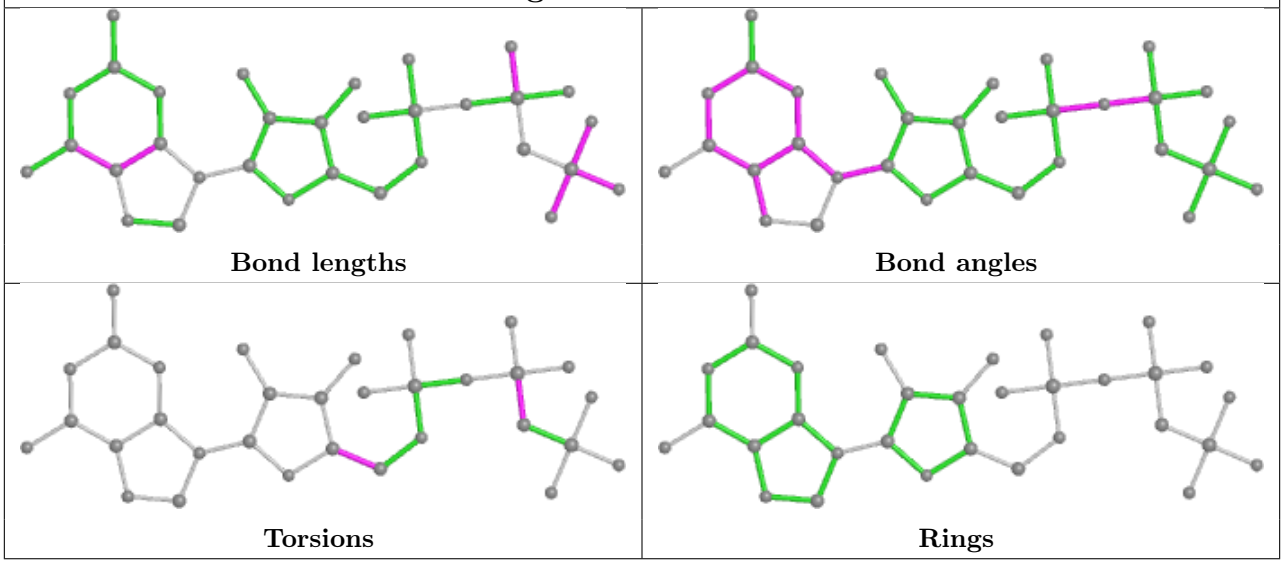
Mol	Chain	Res	Type	Atoms
92	v	802	GCP	PG-C3B-PB-O2B

There are no ring outliers.

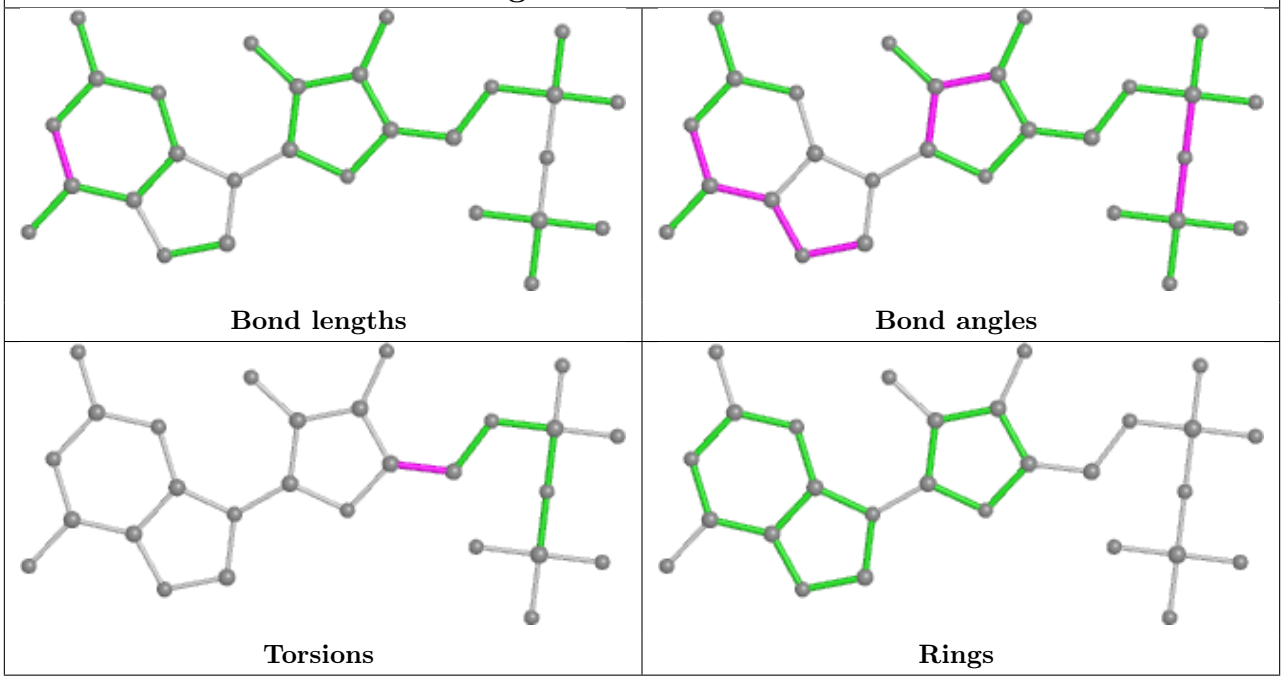
No monomer is involved in short contacts.

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

Ligand GCP v 802



Ligand GDP AX 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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

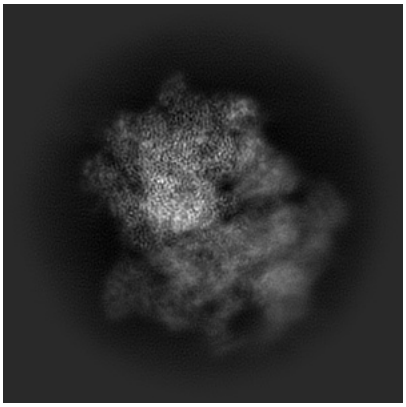
6 Map visualisation

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.

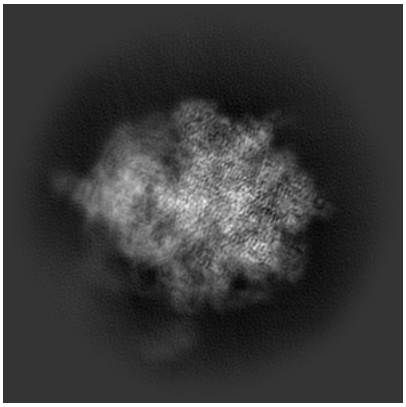
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

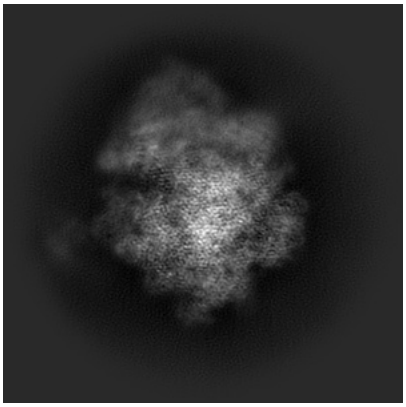
6.1.1 Primary map



X



Y

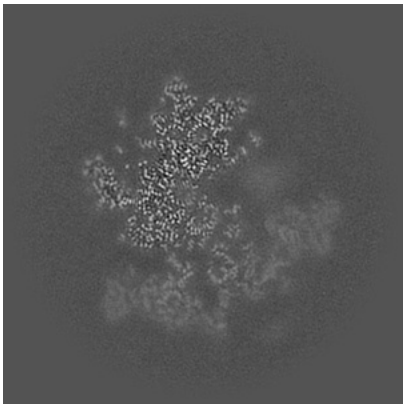


Z

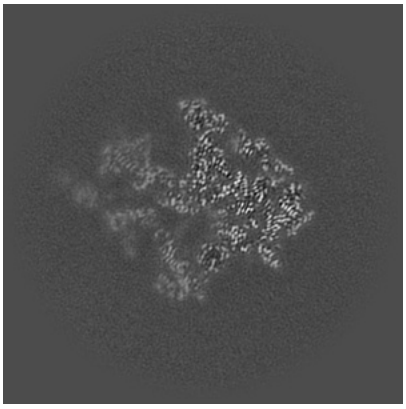
The images above show the map projected in three orthogonal directions.

6.2 Central slices

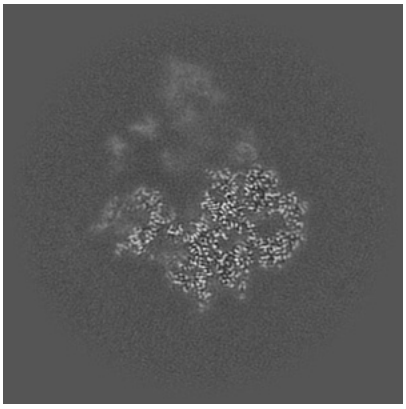
6.2.1 Primary map



X Index: 200



Y Index: 200

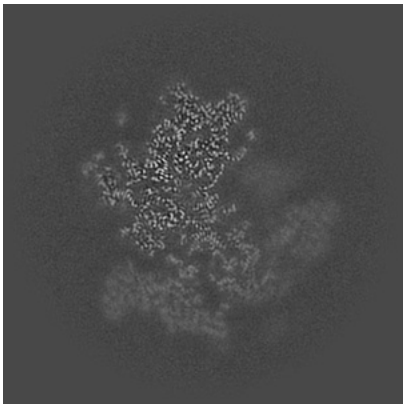


Z Index: 200

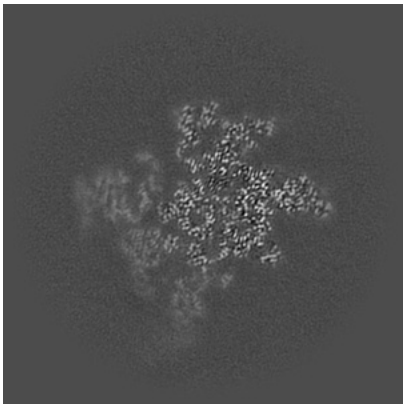
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

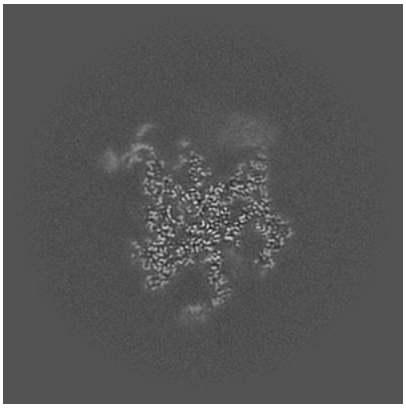
6.3.1 Primary map



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 surface views (i)

6.4.1 Primary map

X

Y

Z

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

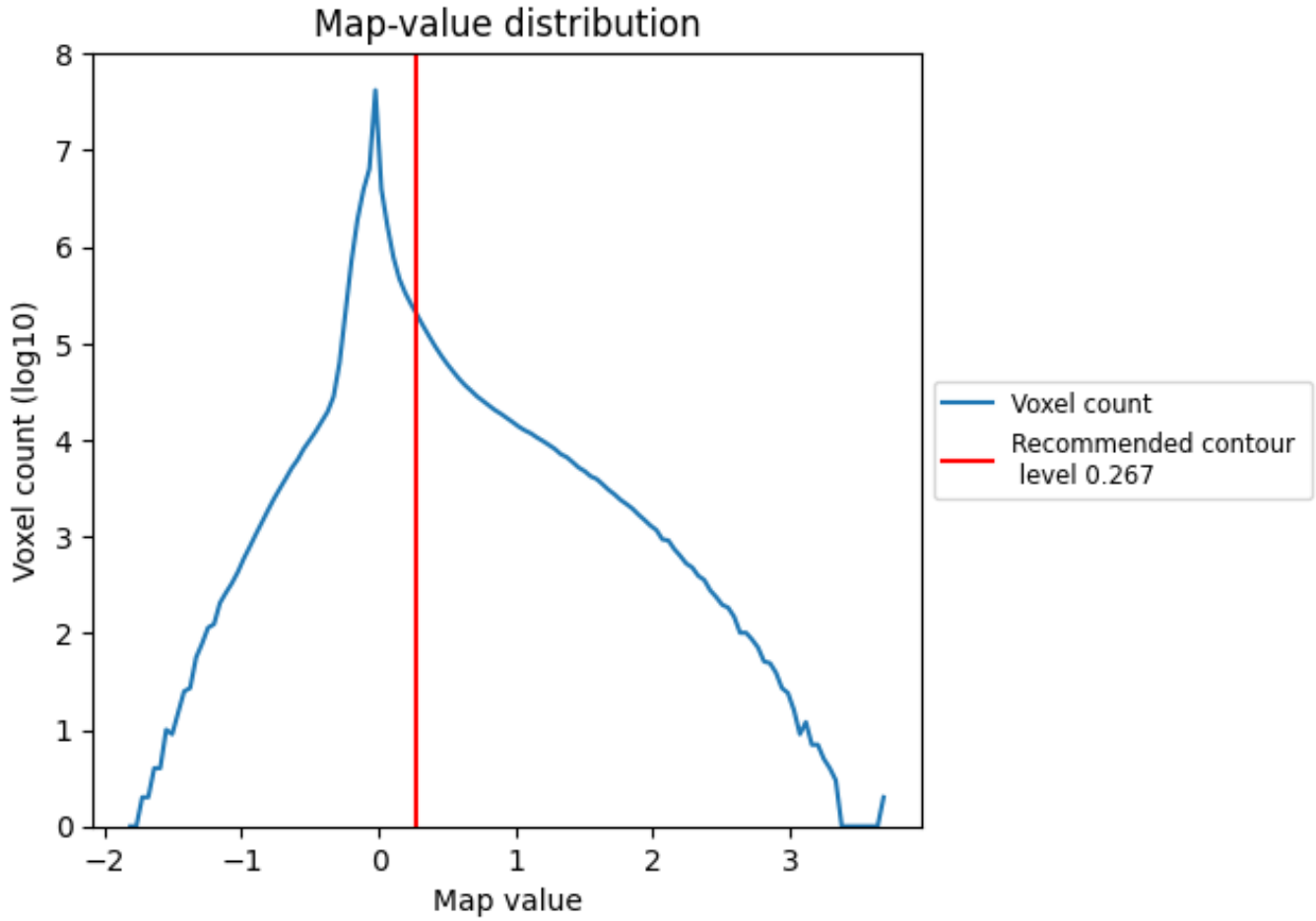
6.5 Mask visualisation (i)

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

7 Map analysis

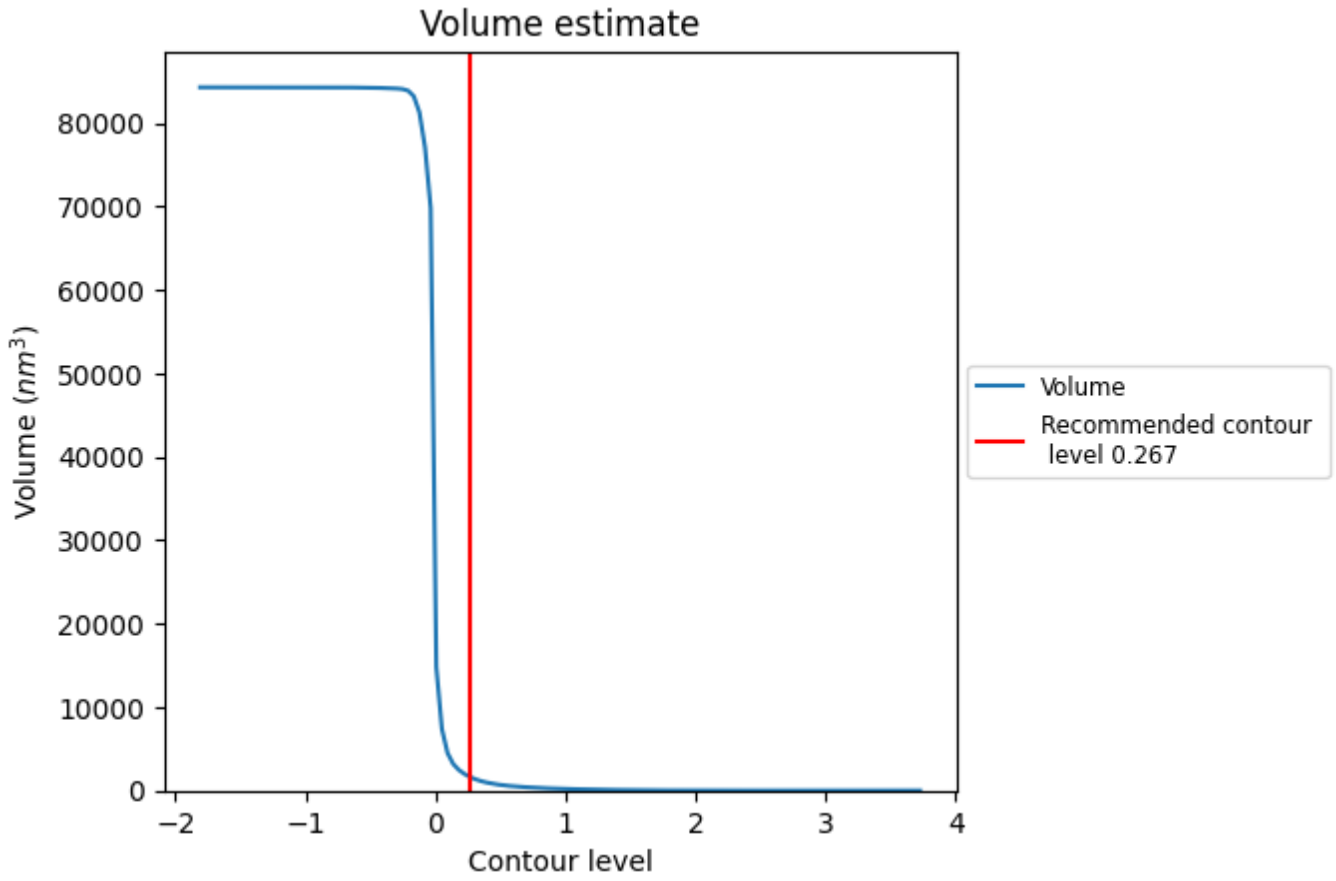
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

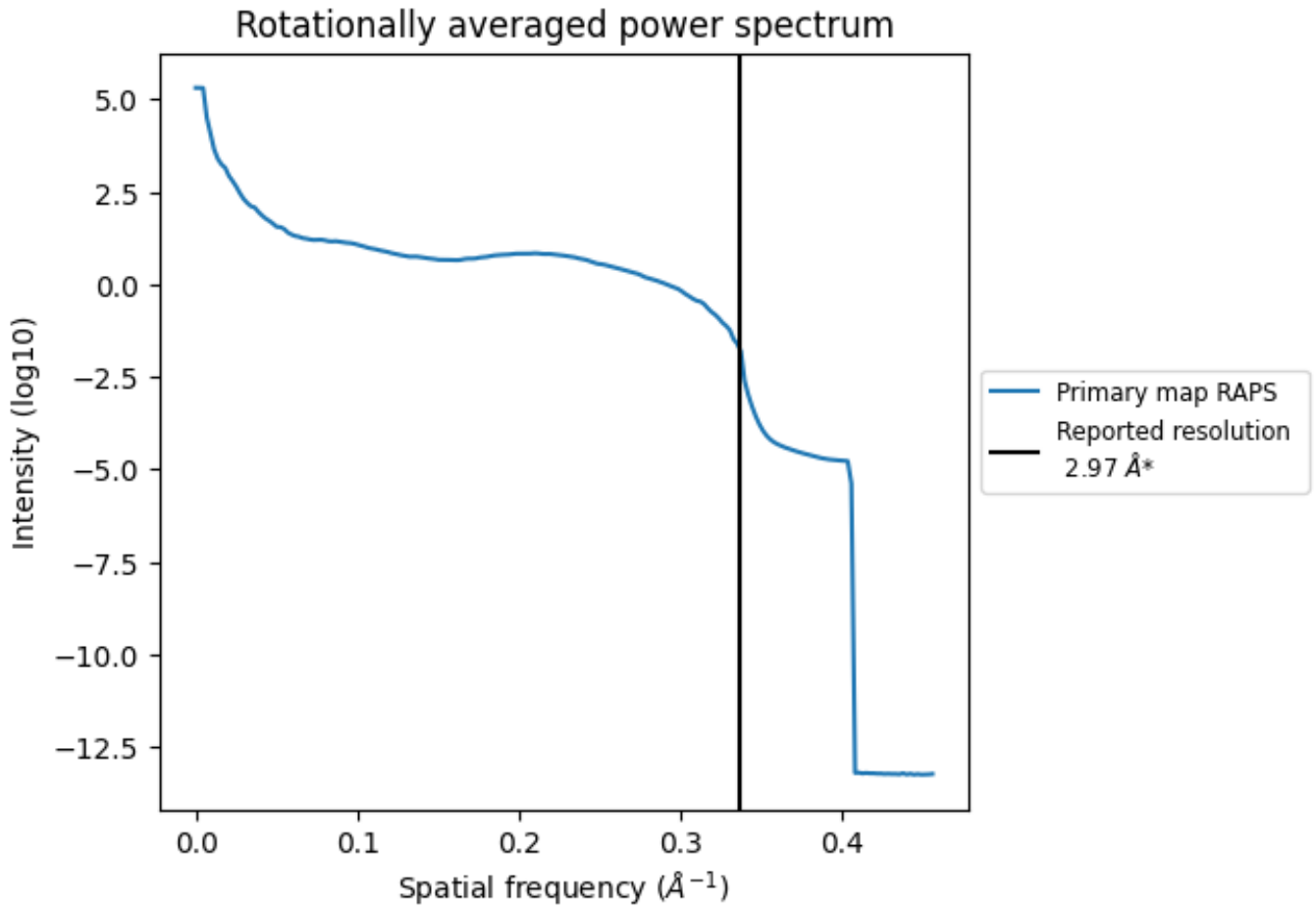
7.2 Volume estimate (i)



The volume at the recommended contour level is 1618 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.337 $Å^{-1}$

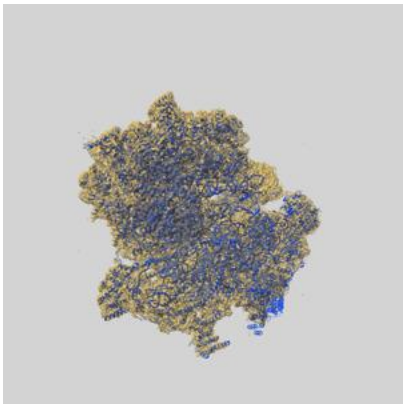
8 Fourier-Shell correlation (i)

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

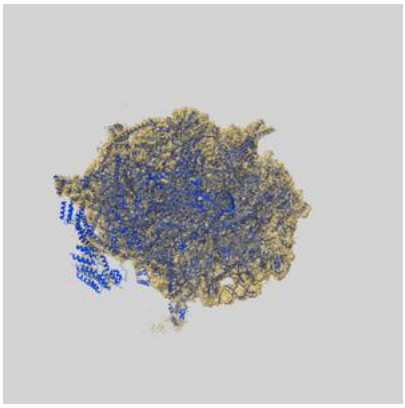
9 Map-model fit

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.

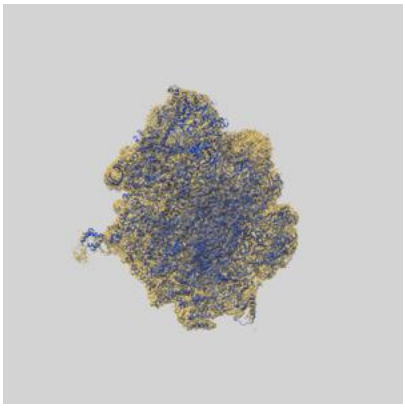
9.1 Map-model overlay



X



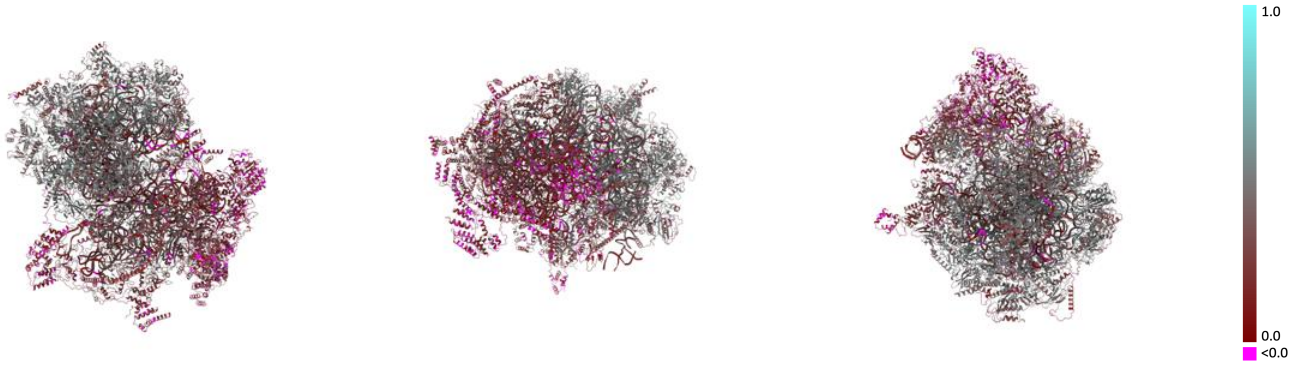
Y



Z

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.

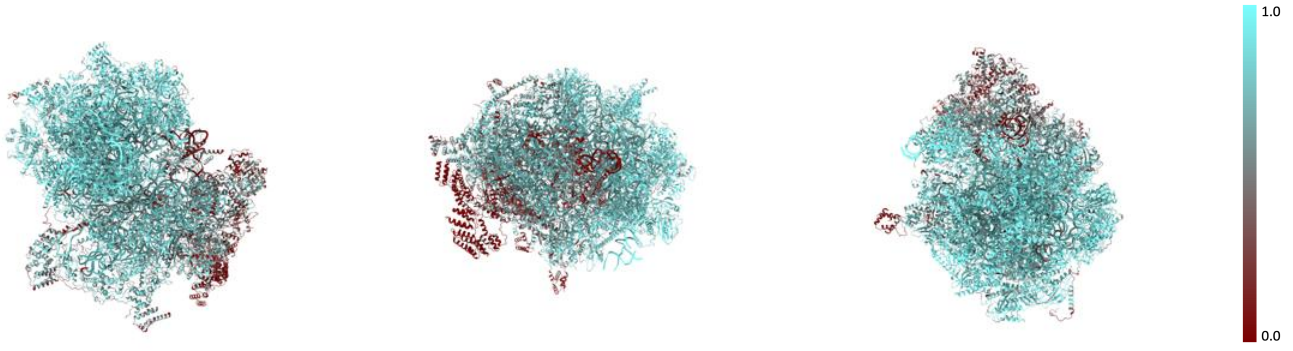
9.2 Q-score mapped to coordinate model



X Y Z

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

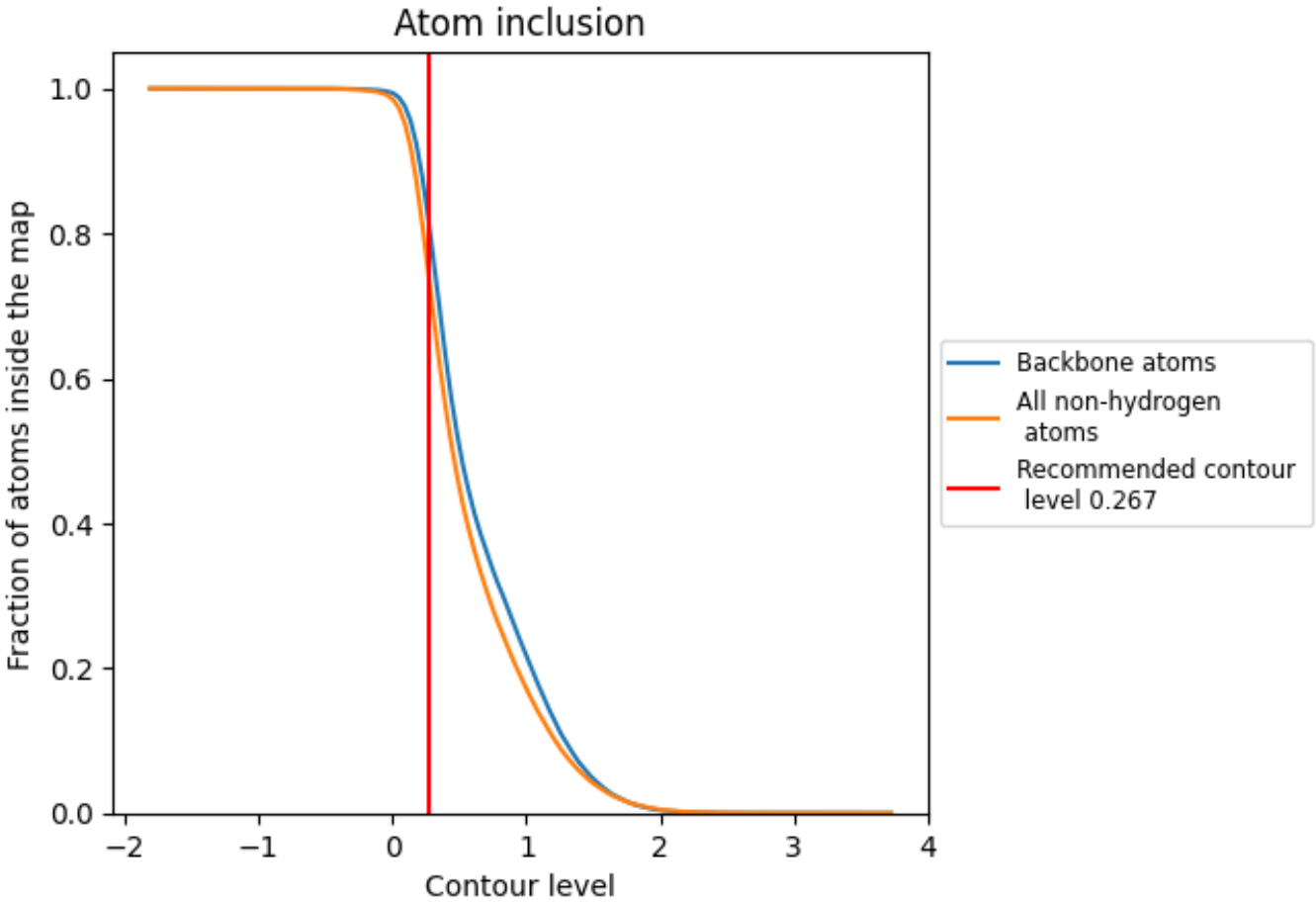
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (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	0.7474	0.3170
0	0.8581	0.4350
1	0.8405	0.4250
2	0.9111	0.4820
3	0.8972	0.4990
4	0.8593	0.4400
5	0.8878	0.4360
6	0.8751	0.4050
7	0.8608	0.4030
8	0.7271	0.2300
9	0.8715	0.4070
A	0.8442	0.3320
A0	0.6793	0.2400
A1	0.3653	0.1370
A2	0.4453	0.2950
A3	0.7274	0.3200
A4	0.1017	0.1390
A5	0.0235	0.0310
A7	0.1287	0.0240
AA	0.8172	0.2590
AB	0.6755	0.2520
AC	0.4548	0.1700
AD	0.5847	0.2880
AE	0.5545	0.2510
AF	0.4057	0.2070
AG	0.5008	0.1720
AH	0.4083	0.1910
AI	0.6405	0.2880
AJ	0.6969	0.3530
AK	0.6189	0.1700
AL	0.6747	0.3090
AM	0.7236	0.2890
AN	0.7956	0.3620
AO	0.6785	0.2530
AP	0.6307	0.2770

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Chain	Atom inclusion	Q-score
AQ	0.7188	0.3230
AR	0.6152	0.2080
AS	0.5479	0.2090
AT	0.7509	0.3280
AU	0.6653	0.2020
AV	0.5191	0.1380
AW	0.6123	0.2510
AX	0.3531	0.0800
AY	0.3588	0.1320
AZ	0.4079	0.1530
B	0.9479	0.2870
D	0.8645	0.4350
E	0.8819	0.4590
F	0.8880	0.4590
H	0.8359	0.3920
I	0.6885	0.2600
J	0.7397	0.2690
K	0.9052	0.4740
L	0.8514	0.4540
M	0.8911	0.4500
N	0.8539	0.4300
O	0.8742	0.4370
P	0.8810	0.4120
Q	0.8074	0.4040
R	0.8890	0.4660
S	0.9018	0.4580
T	0.8907	0.4670
TA	0.1308	0.0810
TB	0.1549	0.0700
TC	0.0341	0.1480
U	0.8678	0.4330
V	0.8587	0.4160
W	0.8826	0.4550
X	0.8799	0.4430
Y	0.8901	0.4430
Z	0.8802	0.4520
a	0.7984	0.3920
b	0.8998	0.4710
c	0.8610	0.4180
d	0.7528	0.3680
e	0.6991	0.1610
f	0.7005	0.2860

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Chain	Atom inclusion	Q-score
g	0.8717	0.4180
h	0.8211	0.3580
i	0.9006	0.4680
j	0.8452	0.4100
k	0.7427	0.2880
l	0.7676	0.2830
m	0.7422	0.2190
o	0.8583	0.4220
p	0.7951	0.3700
q	0.7480	0.3460
r	0.8751	0.4280
s	0.8804	0.4360
u	0.4738	0.1660
v	0.6950	0.2920