



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:27 AM UTC

PDB ID : 6VMI / pdb_00006vmi
EMDB ID : EMD-21242
Title : Structure of the human mitochondrial ribosome-EF-G1 complex (ClassIII)
Authors : Sharma, M.R.; Koripella, R.K.; Agrawal, R.K.
Deposited on : 2020-01-28
Resolution : 2.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

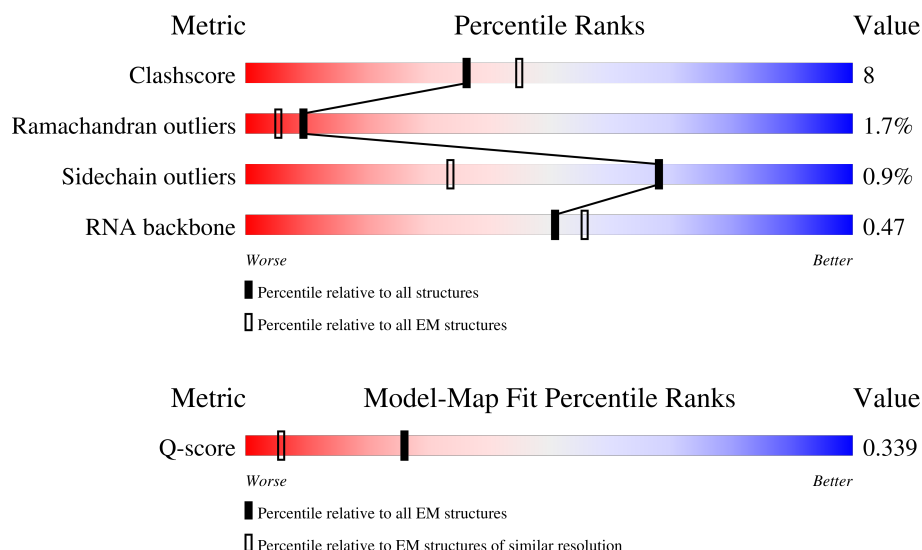
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.96 Å.

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



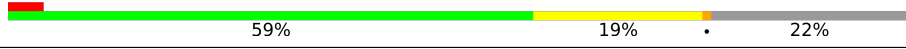
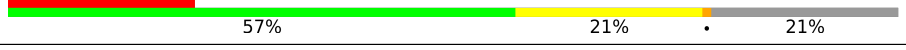
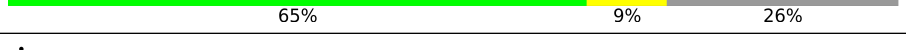
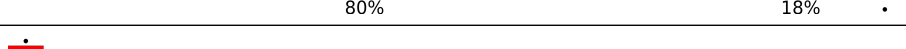
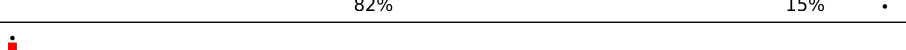
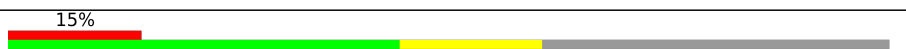
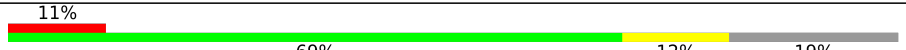
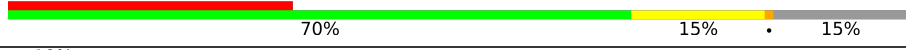
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13155 (2.46 - 3.46)

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

Mol	Chain	Length	Quality of chain
1	AA	954	
2	AB	296	
3	AC	167	

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

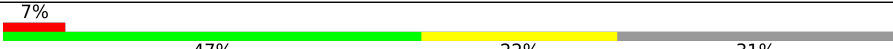
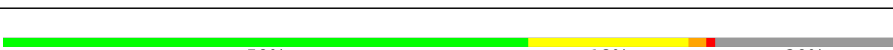
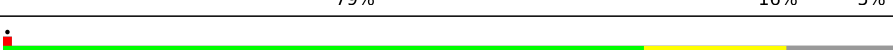
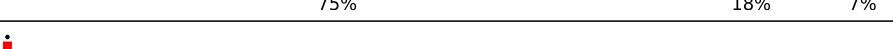
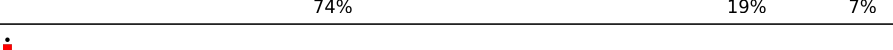
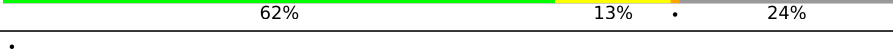
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Mol	Chain	Length	Quality of chain
29	AD	430	
30	AF	242	
31	AG	396	
32	A	1559	
33	B	73	
34	D	305	
35	F	311	
36	H	267	
37	K	178	
38	L	145	
39	M	296	
40	O	175	
41	R	149	
42	S	205	
43	T	212	
44	W	148	
45	X	256	
46	Y	250	
47	Z	161	
48	0	188	
49	1	65	
50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

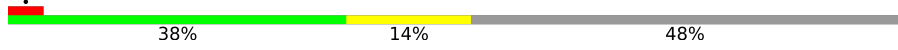
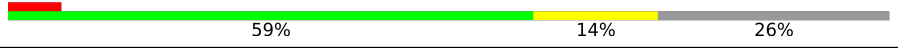
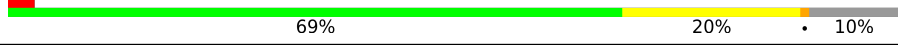
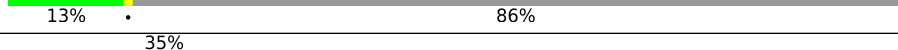
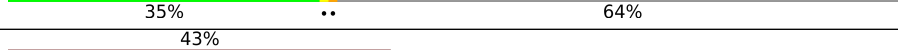
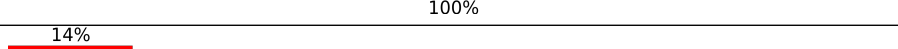
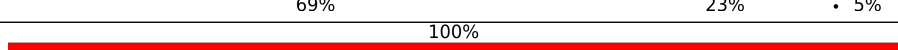
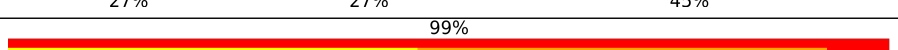
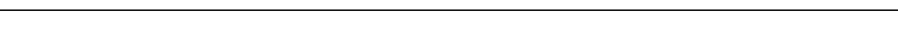
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Mol	Chain	Length	Quality of chain
54	b	155	
55	e	279	
56	g	166	
57	i	128	
58	j	123	
59	m	128	
60	o	102	
61	q	222	
62	r	196	
63	J	192	
64	I	261	
65	N	251	
66	P	179	
67	U	153	
68	V	216	
69	E	348	
70	5	423	
71	6	380	
72	7	338	
73	9	137	
74	a	142	
75	c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

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Mol	Chain	Length	Quality of chain
79	k	112	
80	l	138	
81	p	206	
82	s	439	
83	Q	292	
84	TA	198	
84	TB	198	
84	TC	198	
85	u	65	
86	v	751	
87	A5	11	
88	A6	71	
88	A7	71	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	P5P	A5	2	-	-	X	-
88	Y5P	A6	35	-	-	X	-
88	Y5P	A6	36	-	-	X	-
88	Y5P	A6	69	-	-	X	-
88	Y5P	A6	70	-	-	X	-
88	P5P	A7	71	-	-	X	-
92	GCP	v	802	-	-	X	-

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 176217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 12s rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	variant	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		

- 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	variant	UNP Q13084
X	149	SER	PRO	variant	UNP Q13084
X	150	GLY	LYS	variant	UNP Q13084

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 87 is a DNA chain called mRNA.

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

- Molecule 88 is a DNA chain called P-site and E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	A6	71	Total	C	N	O	P	0	0
			1368	670	204	424	70		

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

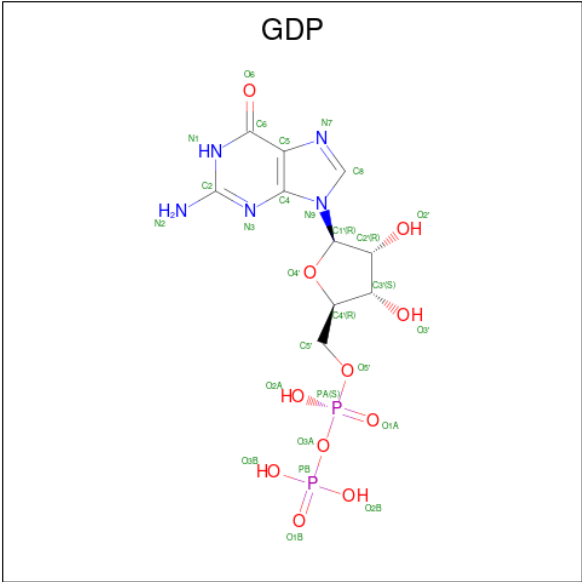
- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	AA	27	Total	Mg	0
			27	27	
89	AC	1	Total	Mg	0
			1	1	
89	A	97	Total	Mg	0
			97	97	
89	D	1	Total	Mg	0
			1	1	
89	W	1	Total	Mg	0
			1	1	
89	g	1	Total	Mg	0
			1	1	
89	E	1	Total	Mg	0
			1	1	
89	v	1	Total	Mg	0
			1	1	

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

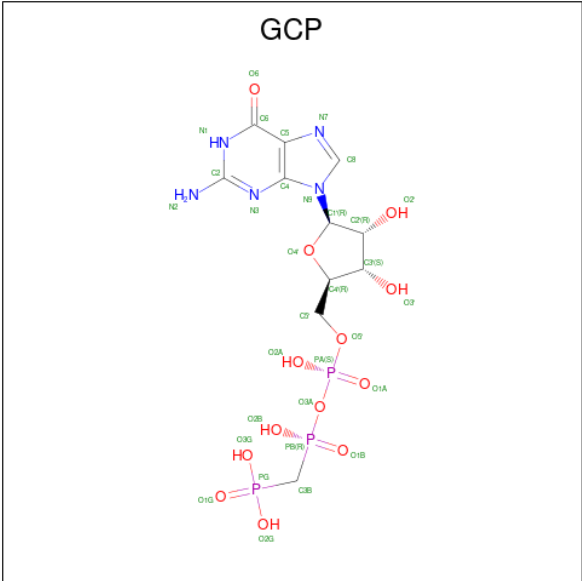
Mol	Chain	Residues	Atoms		AltConf
90	AB	1	Total	Zn	0
			1	1	
90	AO	1	Total	Zn	0
			1	1	
90	AP	1	Total	Zn	0
			1	1	
90	AT	1	Total	Zn	0
			1	1	
90	0	1	Total	Zn	0
			1	1	
90	4	1	Total	Zn	0
			1	1	
90	r	1	Total	Zn	0
			1	1	

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

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

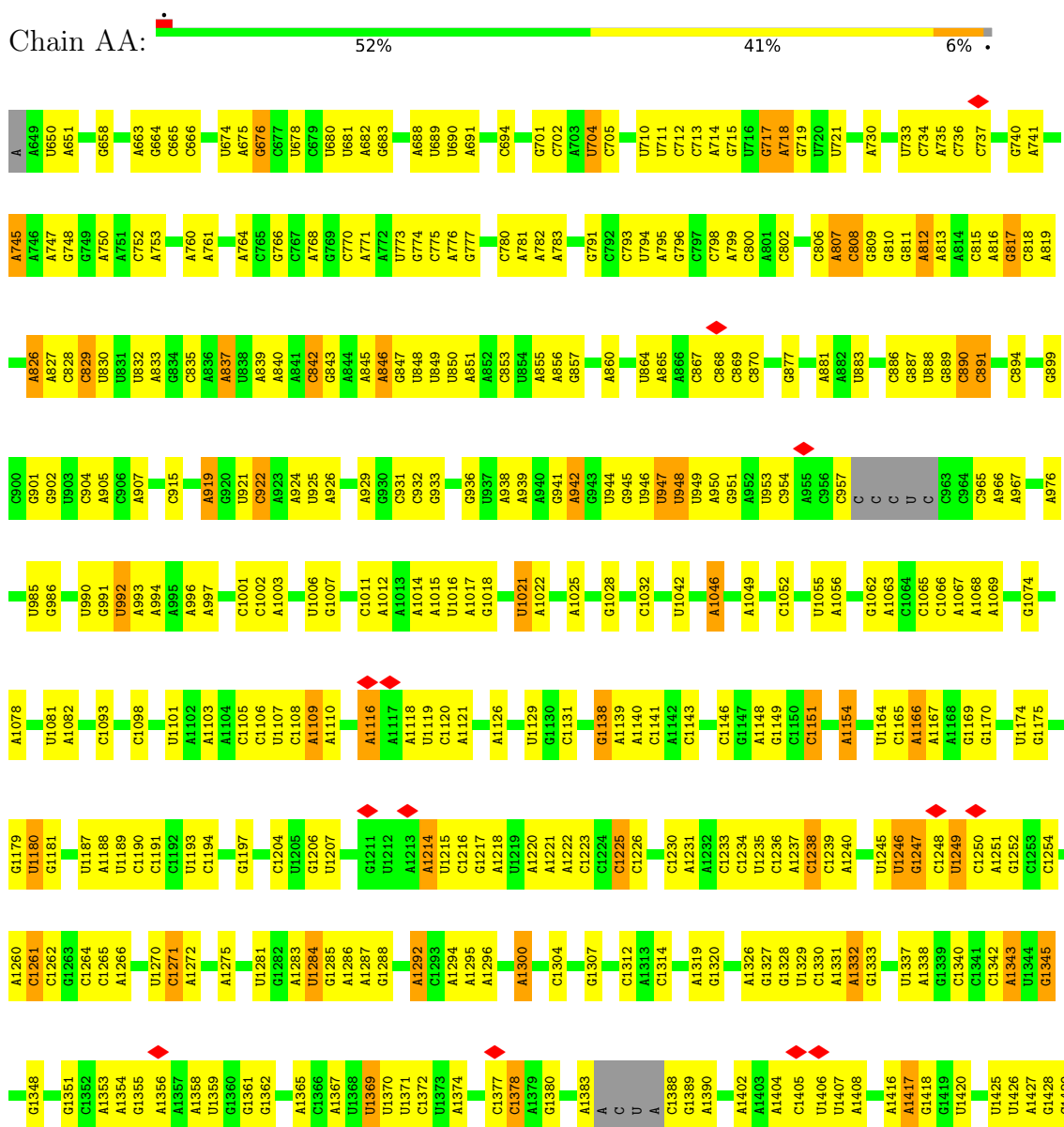


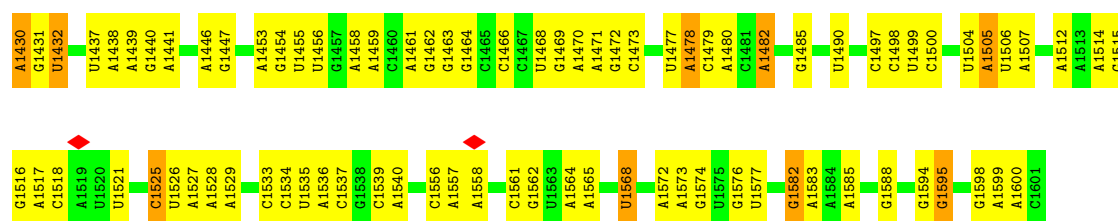
Mol	Chain	Residues	Atoms					AltConf
92	v	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

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

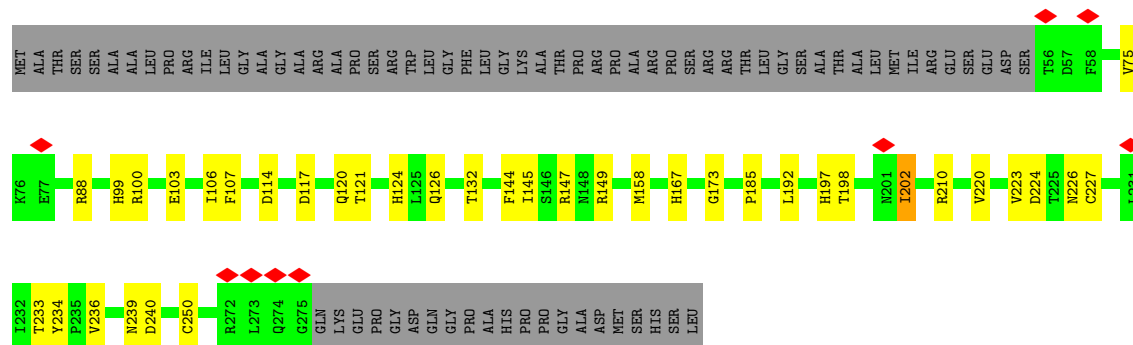
• Molecule 1: 12s rRNA





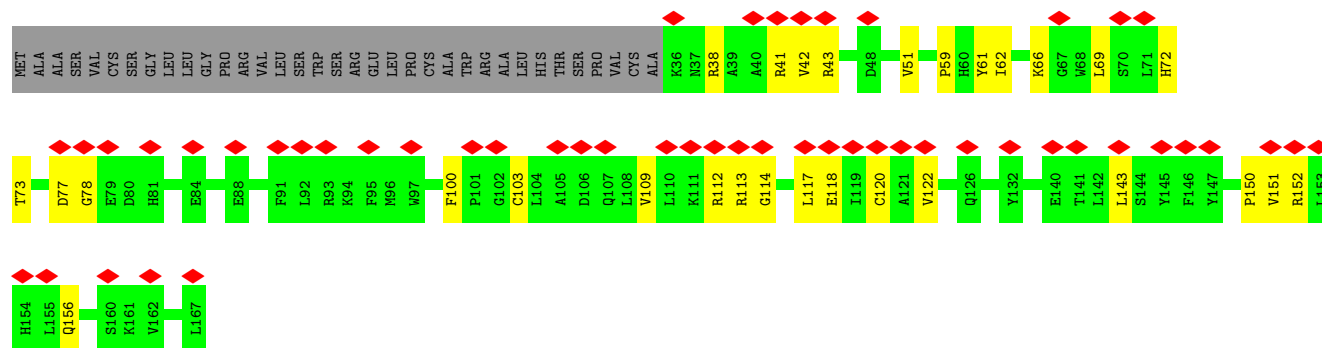
- Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain AB: 61% 12% 26%



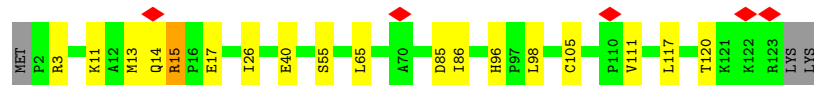
- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC: 31% 62% 17% 21%



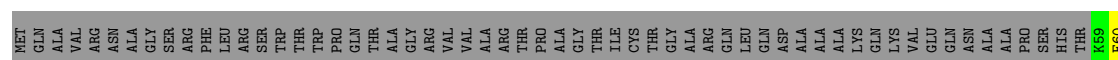
- Molecule 4: 28S ribosomal protein S6, mitochondrial

Chain AE: 83% 14% ..



- Molecule 5: 28S ribosomal protein S11, mitochondrial

Chain AI: 58% 12% 30%

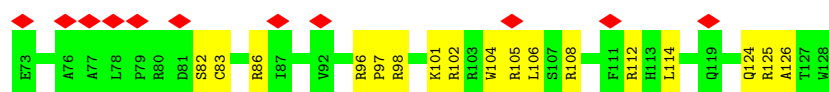
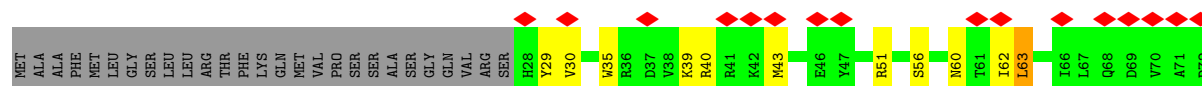




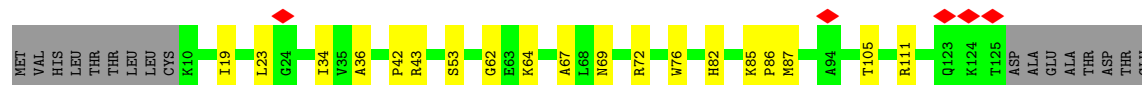
- Molecule 6: 28S ribosomal protein S12, mitochondrial



- Molecule 7: 28S ribosomal protein S14, mitochondrial



- Molecule 8: 28S ribosomal protein S16, mitochondrial

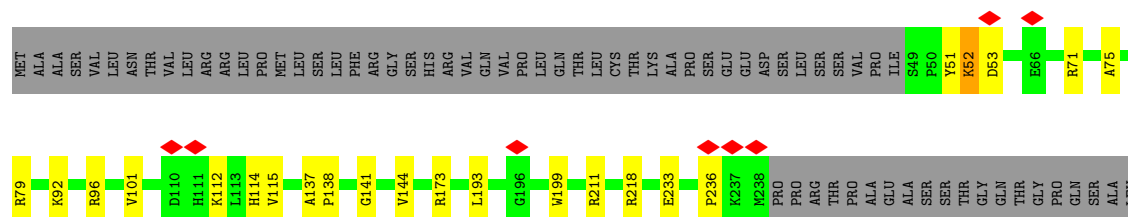


- Molecule 9: 28S ribosomal protein S17, mitochondrial

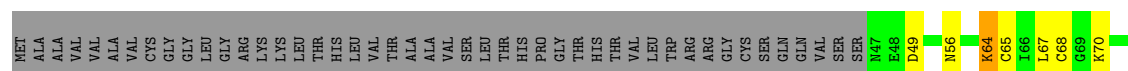


- Molecule 10: 28S ribosomal protein S18b, mitochondrial

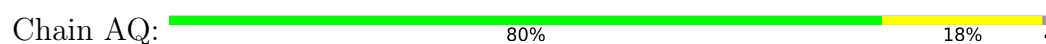




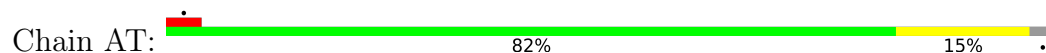
- Molecule 11: 28S ribosomal protein S18c, mitochondrial



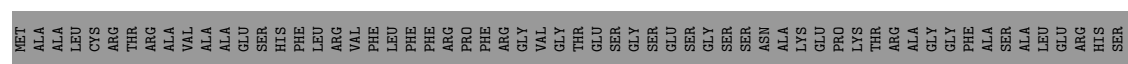
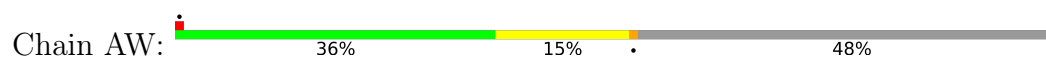
- Molecule 12: 28S ribosomal protein S21, mitochondrial



- Molecule 13: 28S ribosomal protein S25, mitochondrial

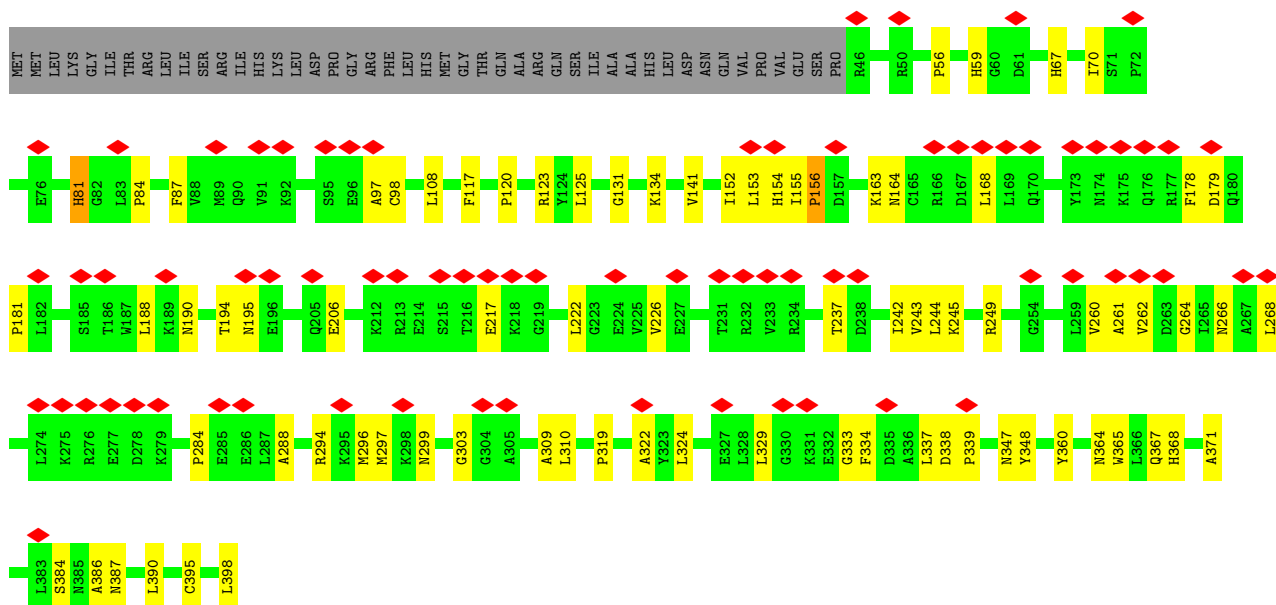


- Molecule 14: 28S ribosomal protein S28, mitochondrial

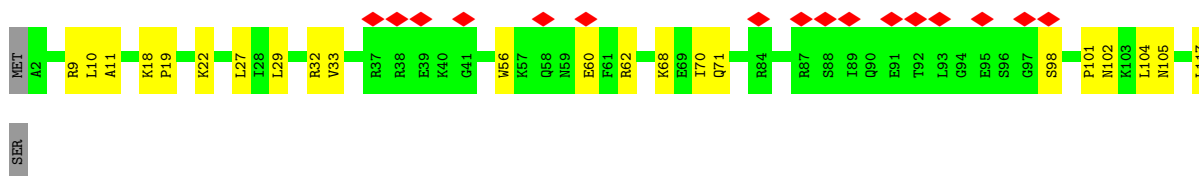
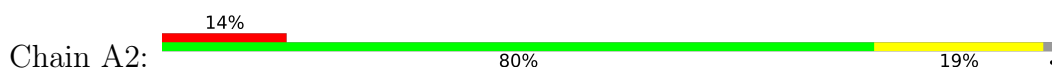


- Molecule 15: 28S ribosomal protein S29, mitochondrial

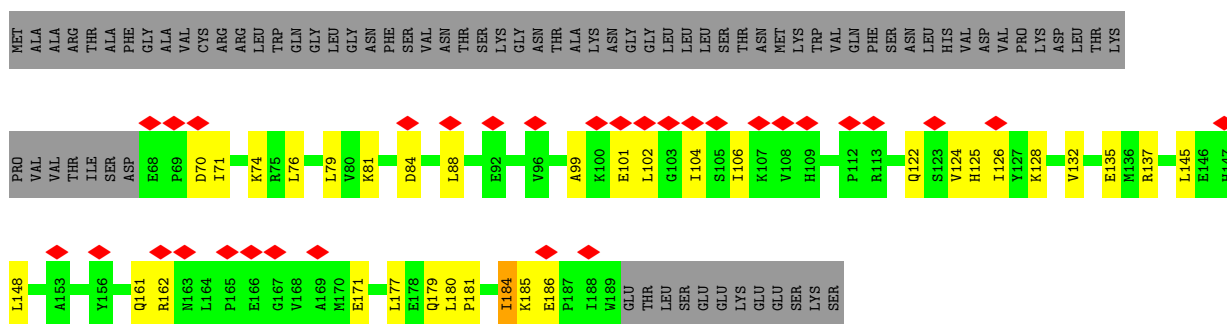




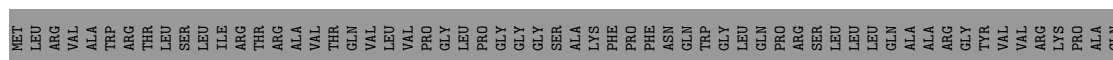
- Molecule 16: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1



- Molecule 17: 28S ribosomal protein S10, mitochondrial

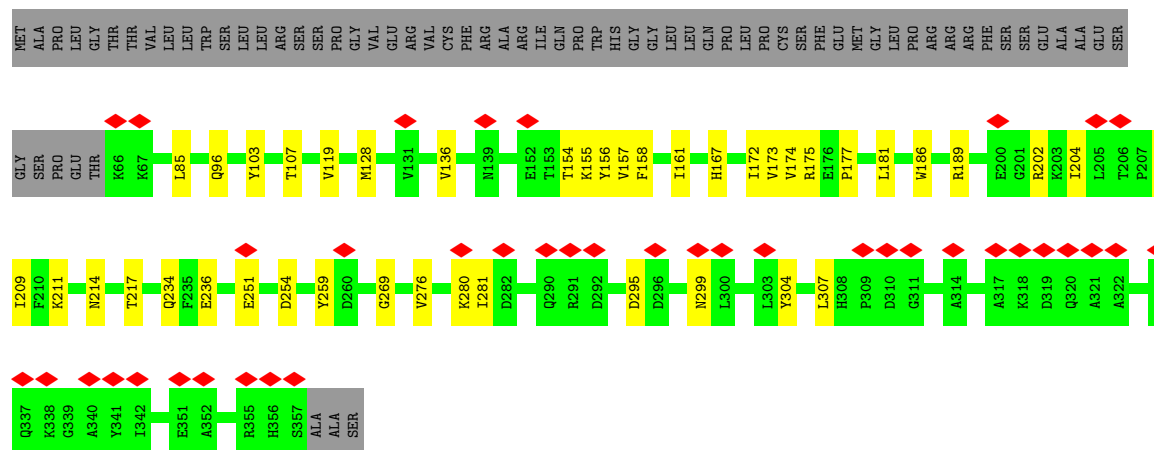


- Molecule 18: 28S ribosomal protein S15, mitochondrial

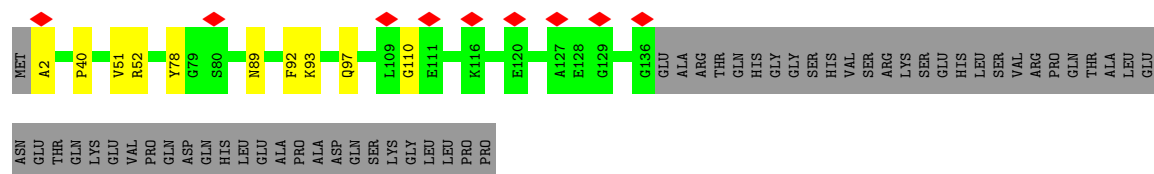




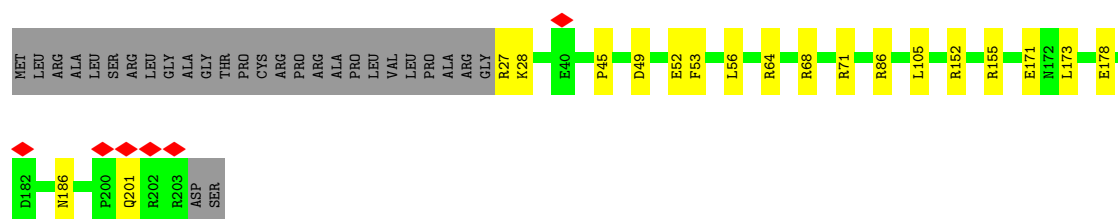
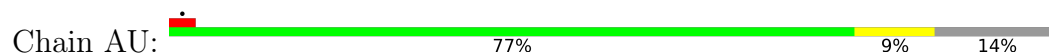
- Molecule 19: 28S ribosomal protein S22, mitochondrial



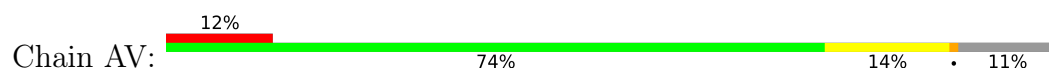
- Molecule 20: 28S ribosomal protein S23, mitochondrial



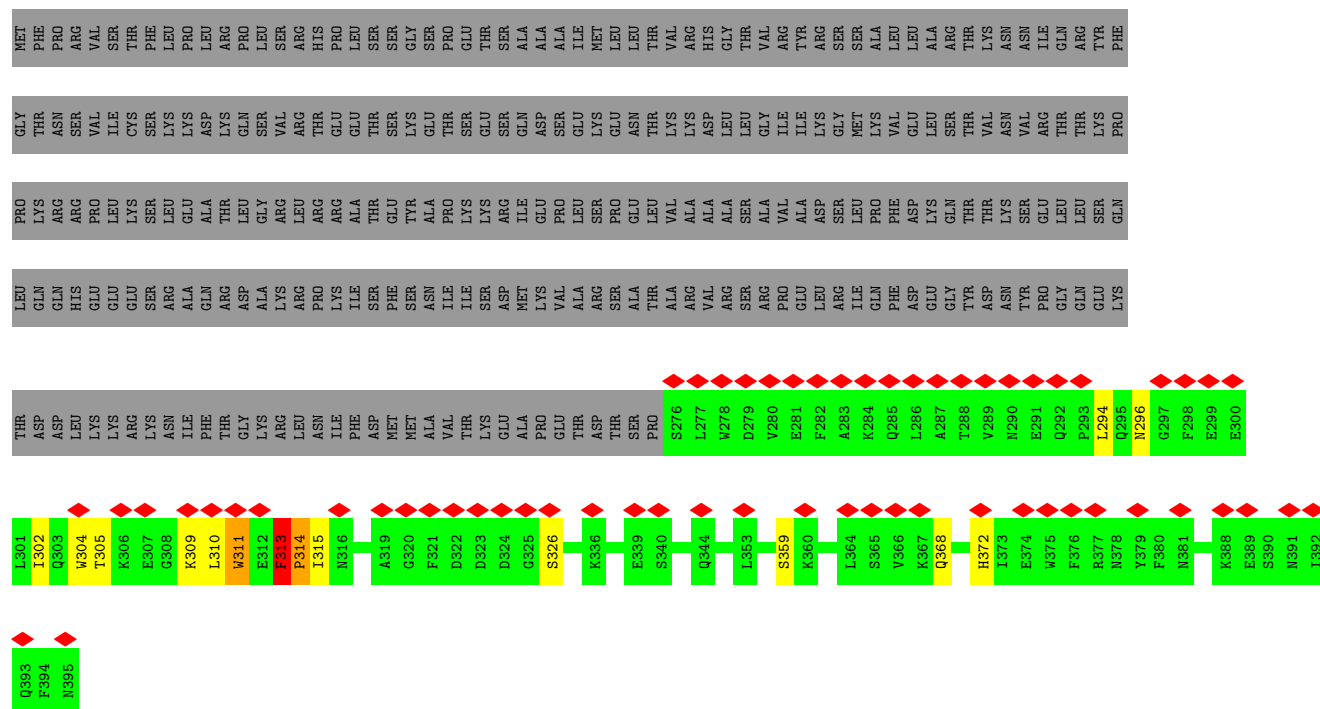
- Molecule 21: 28S ribosomal protein S26, mitochondrial



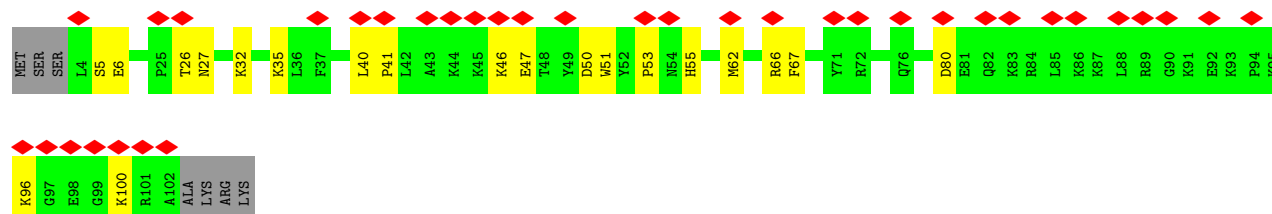
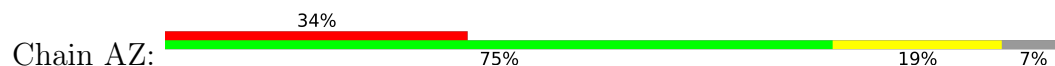
- Molecule 22: 28S ribosomal protein S27, mitochondrial



- Molecule 23: 28S ribosomal protein S31, mitochondrial

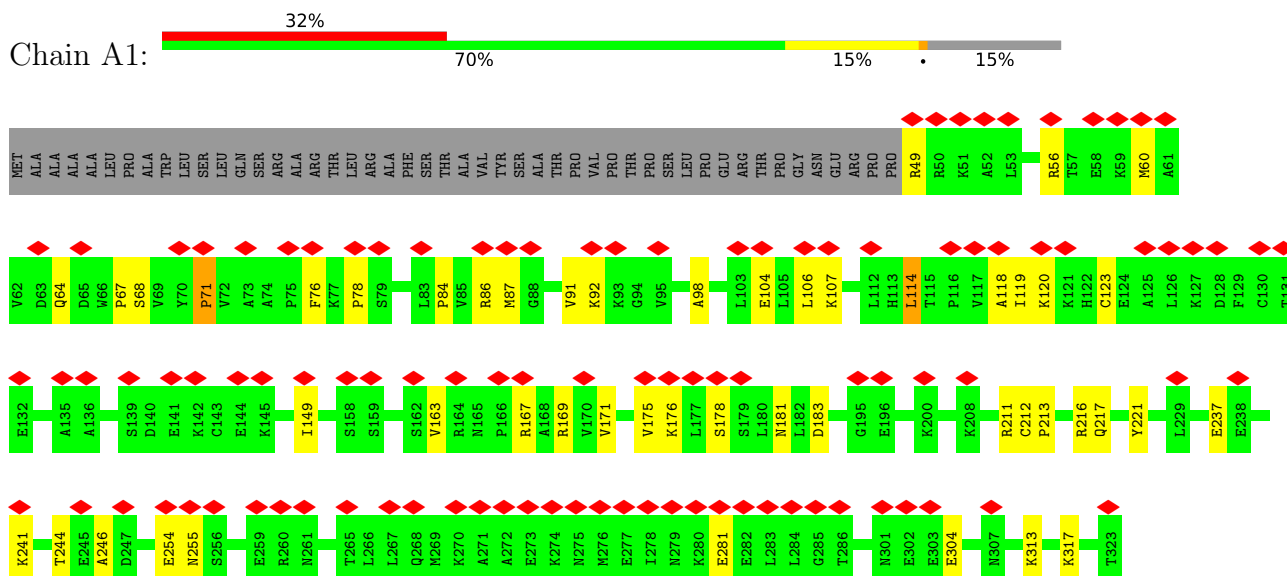


- Molecule 24: 28S ribosomal protein S33, mitochondrial



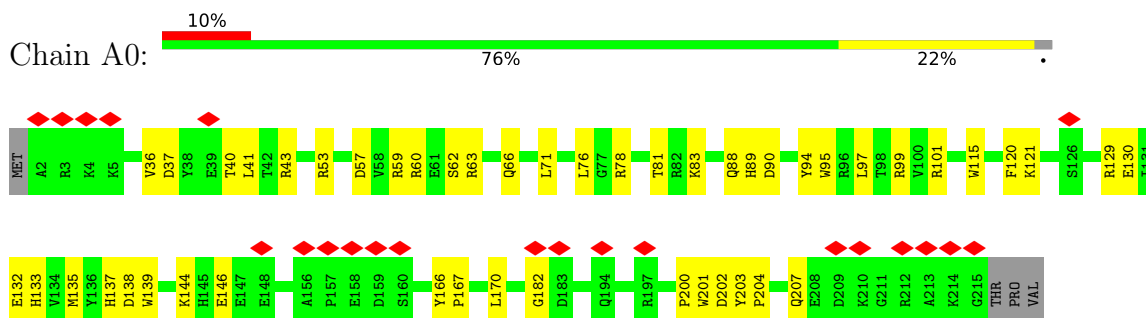
- Molecule 25: 28S ribosomal protein S35, mitochondrial

Chain A1:



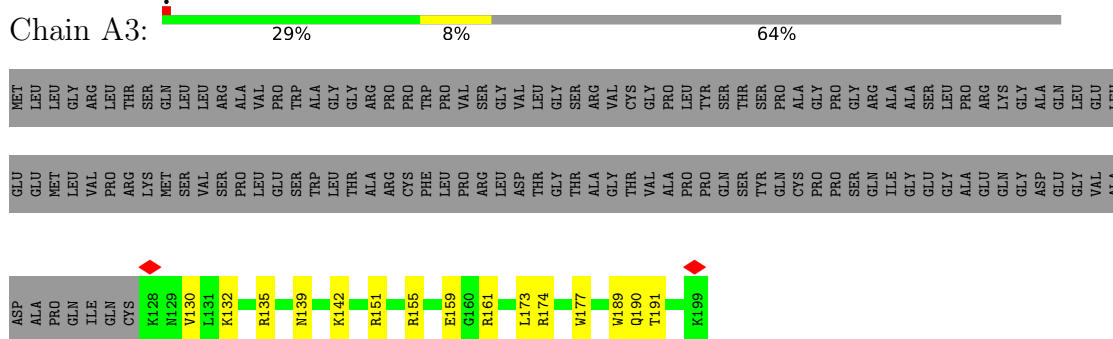
- Molecule 26: 28S ribosomal protein S34, mitochondrial

Chain A0:



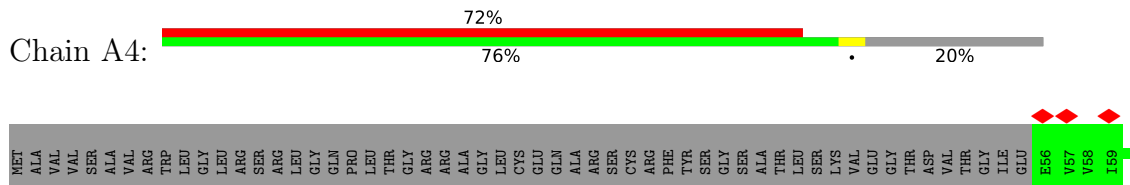
- Molecule 27: Aurora kinase A-interacting protein

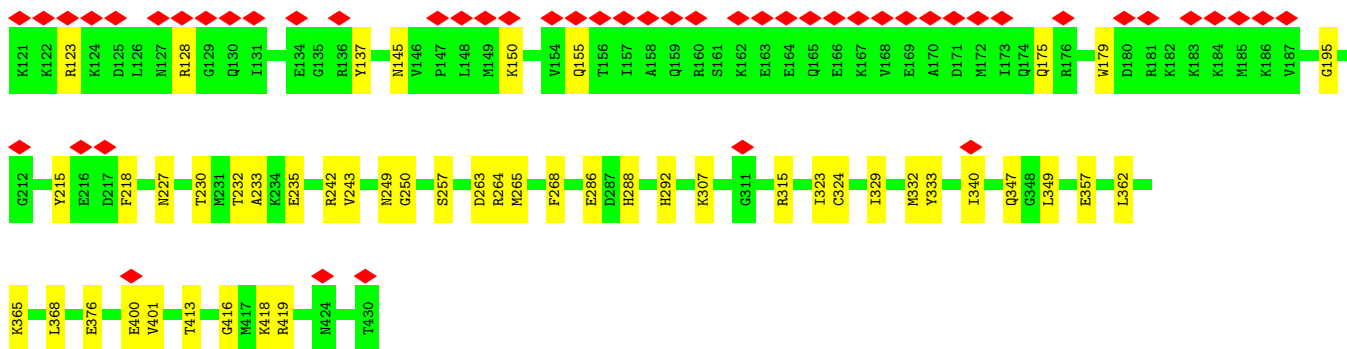
Chain A3:



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

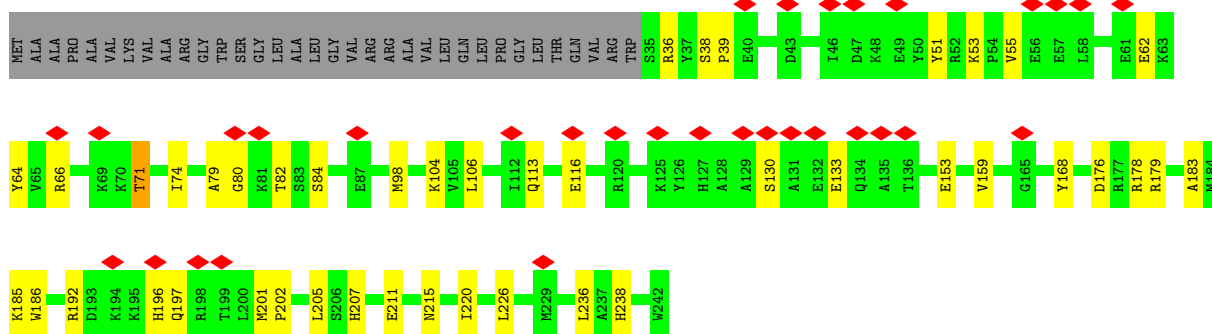
Chain A4:





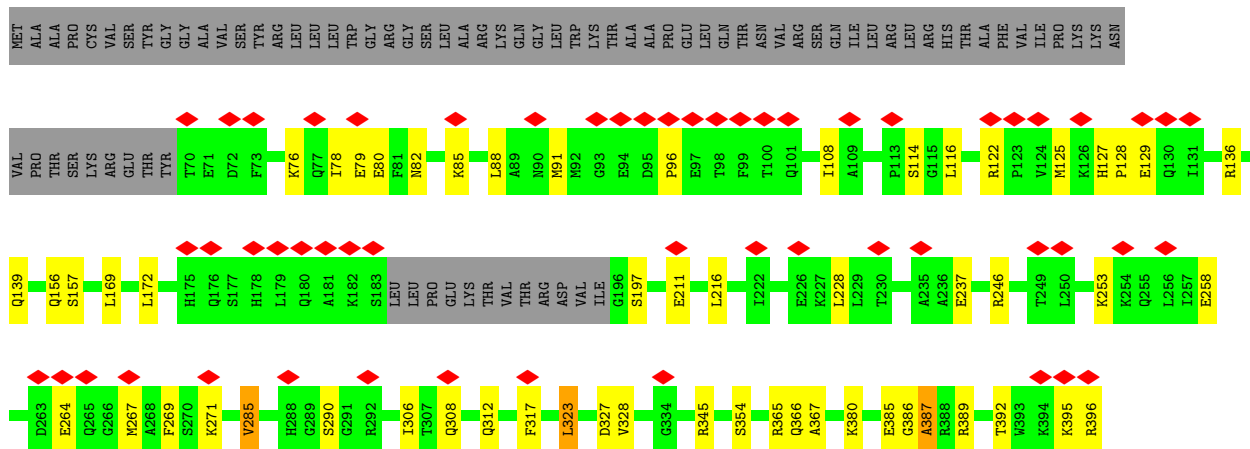
- Molecule 30: 28S ribosomal protein S7, mitochondrial

Chain AF:



- Molecule 31: 28S ribosomal protein S9, mitochondrial

Chain AG:

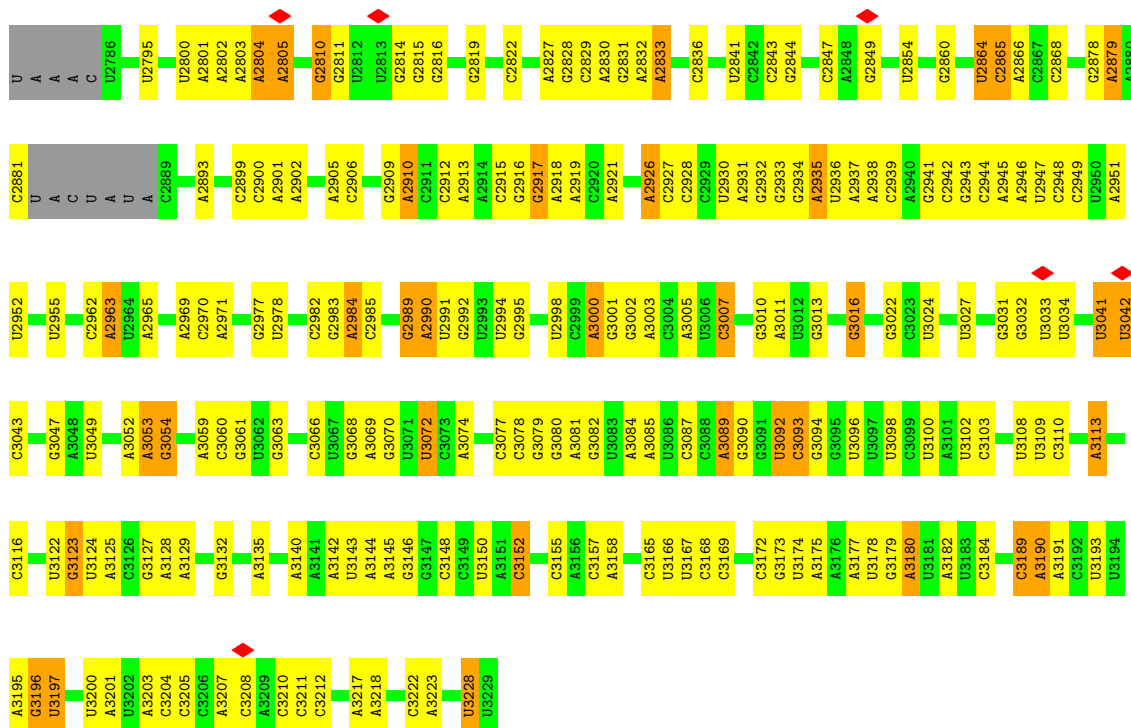


- Molecule 32: 16S rRNA

Chain A:



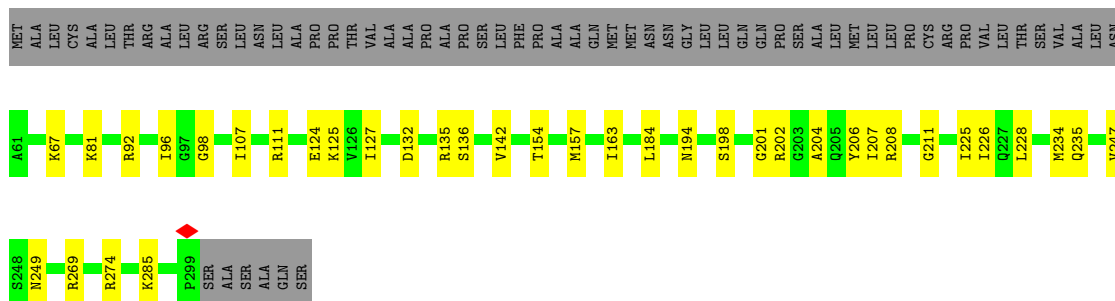
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G2719	A2644	G2571	G2471	G2380	U2301	A2166	A2084	C1903	A1823	A1752
A2723	G2645	A2576	A2473	A2381	A2302	A2167	A2085	A1907	U1824	A1753
G2724	G2646	A2577	A2474	A2382	G2303	U2168	U2086	A1908	C1827	G1754
A2725	G2647	A2578	G2475	U2383	A2304	A2169	U2087	A1909	A1828	A1755
C2726	C2650	A2579	G2476	A2384	G2307	G2170	U2088	C1910	A1829	A1756
U2729	G2651	C2577	U2478	A2388	A2308	U2171	C2092	C1911	G1830	G1760
G2732	G2652	C2578	U2479	C2389	U2311	A2172	G2093	A1912	A1831	A1761
G2733	G2653	C2579	C2484	A2390	A2312	G2173	G2094	C1915	C1833	A1762
A2734	U2654	U2580	G2489	A2393	A2313	G2174	A2097	G1916	A1834	A1763
G2735	G2655	A2581	C2490	C2394	C2314	C2175	G2098	A1917	A1835	G1764
G2736	U2656	C2582	A2394	A2395	A2315	A2180	U2099	G1918	U1836	G1765
C2737	G2657	C2583	A2396	C2396	U2316	A2181	G2098	U1924	C1837	U1766
U2738	U2658	G2584	C2397	C2396	G2317	G2182	C2099	U1925	C1838	G1767
U2739	G2659	G2585	A2404	C2396	A2318	C2183	A2102	A1926	C1839	G1768
A2740	U2660	G2586	U2405	U2404	A2319	A2184	A2103	A1927	C1840	C1769
A2741	U2661	C2587	A2406	U2405	G2320	G2185	A2104	C1930	A1844	G1770
U2742	A2662	A2588	U2407	U2407	A2321	C2186	G2105	A1935	U1848	C1771
U2743	U2663	A2589	C2408	C2414	C2322	C2187	G2106	A1936	U1849	A1772
U2744	A2664	A2590	C2414	C2415	U2325	A2188	G2107	A1937	A1777	A1777
A2745	U2665	G2591	U2414	C2415	G2326	C2189	A2109	A1938	C1882	A1781
U2746	A2666	G2592	U2415	C2415	U2256	A2190	A2110	G1939	A1853	G1782
U2747	U2667	G2593	U2420	U2421	U2257	A2191	G2111	A1940	U1854	U1783
A2748	A2668	A2594	G2421	U2422	A2258	C2192	G2112	C1941	A1855	A1856
U2749	U2669	G2595	A2422	U2422	A2259	U2193	G2113	G1942	A1856	A1857
U2750	G2670	A2601	A2423	A2423	A2260	U2194	U2117	A1943	C1857	G1787
A2753	A2671	C2603	A2424	A2434	G2201	A2195	C2123	C1944	A1858	A1789
A2754	C2672	U2606	C2425	A2434	G2202	A2196	A2124	C1945	A1859	A1789
A2755	C2673	U2607	A2426	C2427	G2203	G2197	A2125	C1946	A1860	A1790
C2756	U2674	C2608	C2427	C2427	U2204	A2198	C2126	A1951	U1952	G1791
A2757	A2675	U2609	A2428	A2432	U2205	A2199	U2126	U1952	U1861	G1792
G2758	C2676	U2610	G2448	A2433	G2206	A2200	A2132	U1953	A1862	G1793
U2759	G2677	U2611	U2449	A2434	U2207	G2201	A2133	U1954	A1863	A1794
A2760	C2678	G2612	G2449	A2444	U2208	G2202	A2134	G1955	A1864	A1795
C	G2679	U2613	A2453	A2444	U2209	G2203	A2135	G1958	A1867	A1798
C	G2680	U2614	G2453	A2444	U2210	U2204	A2136	A1959	G1868	U1799
C	G2681	A2615	A2453	A2444	U2211	U2205	C2136	A1960	A1869	U1800
C	G2682	U2616	A2453	A2444	U2212	A2206	C2137	U1979	A1870	G1800
C	G2683	U2617	A2453	A2444	U2213	A2207	U2138	A1965	A1871	A1803
C	G2684	U2618	A2453	A2444	U2214	A2208	U2139	G1966	U1872	A1804
C	G2685	U2619	A2453	A2444	U2215	A2209	A2142	U1967	A1873	A1805
C	G2686	U2620	A2453	A2444	U2216	G2209	G2143	G1968	U1877	U1806
C	G2687	U2621	A2453	A2444	U2217	U2210	G2144	U1979	U1807	A1808
C	G2688	U2622	A2453	A2444	U2218	U2211	G2145	A1980	A1881	U1809
C	G2689	U2623	A2453	A2444	U2219	U2212	A2146	G1981	A1882	A1810
C	G2690	U2624	A2453	A2444	U2220	U2213	G2147	G1982	A1883	A1811
C	G2691	U2625	A2453	A2444	U2221	U2214	A2151	G1985	A1884	C1812
C	G2692	U2626	A2453	A2444	U2222	U2215	A2152	A1986	A1893	C1813
C	G2693	U2627	A2453	A2444	U2223	U2216	A2153	G1987	A1894	A1814
C	G2694	U2628	A2453	A2444	U2224	U2217	A2154	U1979	A1895	A1815
C	G2695	U2629	A2453	A2444	U2225	U2218	A2155	A1980	A1896	G1816
C	G2696	U2630	A2453	A2444	U2226	U2219	A2156	G1981	A1897	C1817
C	G2697	U2631	A2453	A2444	U2227	U2220	A2157	G1982	A1898	A1900
C	G2698	U2632	A2453	A2444	U2228	U2221	U2158	A1985	A1899	
C	A2706	U2633	A2453	A2444	U2229	U2222	U2159	C1992	A1900	
C	A2707	U2634	A2453	A2444	U2230	U2223		A1994		
C	C2708	U2635	A2453	A2444	U2231	U2224				
C	A2709	U2636	A2453	A2444	U2232	U2225				
C	C2710	U2637	A2453	A2444	U2233	U2226				
C	A2711	U2638	A2453	A2444	U2234	U2227				
C	A2712	U2639	A2453	A2444	U2235	U2228				
C	C2713	U2640	A2453	A2444	U2236	U2229				
C	A2714	U2641	A2453	A2444	U2237	U2230				
C	A2715	U2642	A2453	A2444	U2238	U2231				



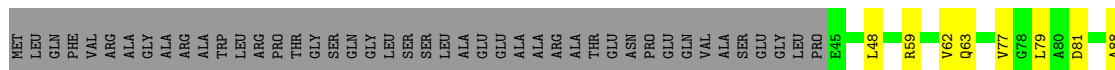
- Molecule 33: tRNA^{Val}

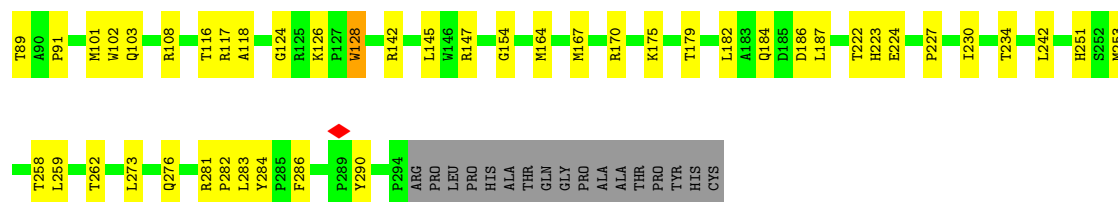


- Molecule 34: 39S ribosomal protein L2, mitochondrial

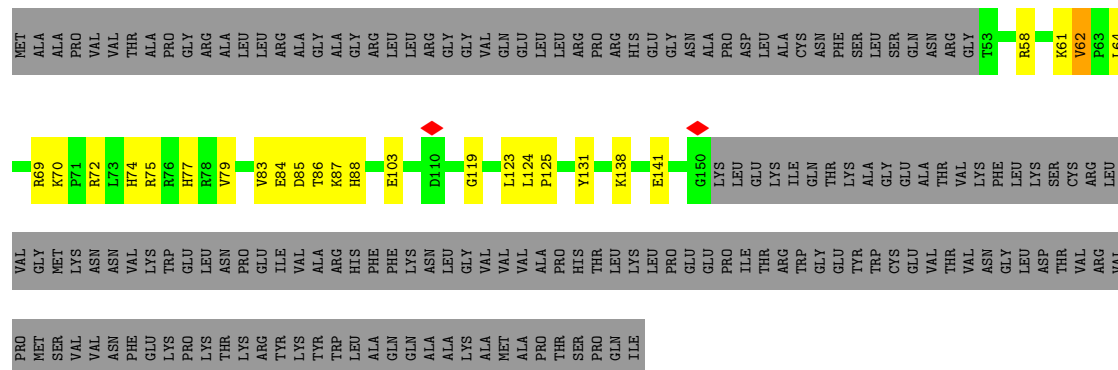


- Molecule 35: 39S ribosomal protein L4, mitochondrial

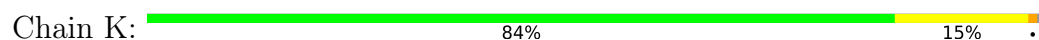




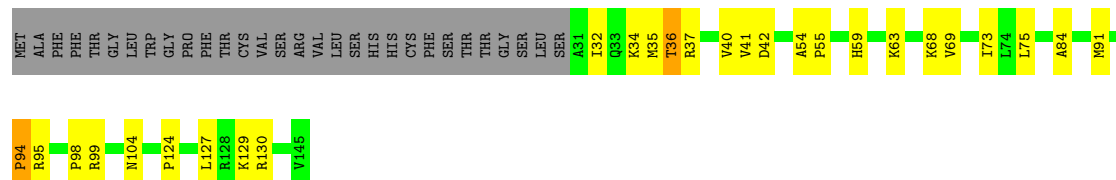
- Molecule 36: 39S ribosomal protein L9, mitochondrial



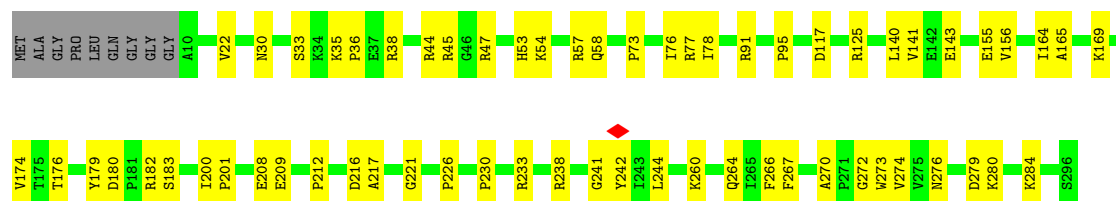
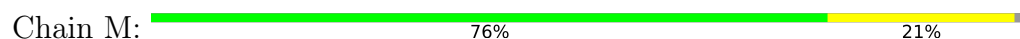
- Molecule 37: 39S ribosomal protein L13, mitochondrial



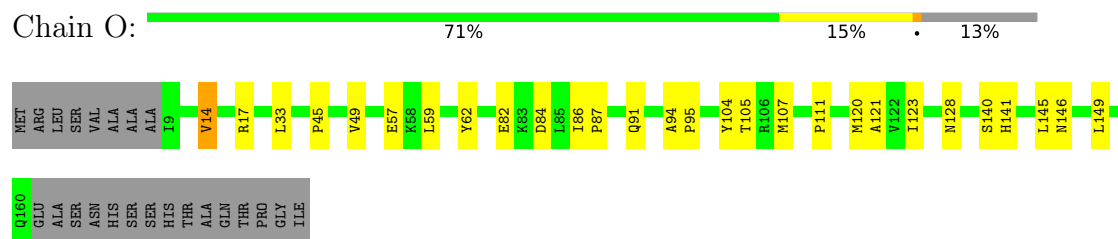
- Molecule 38: 39S ribosomal protein L14, mitochondrial



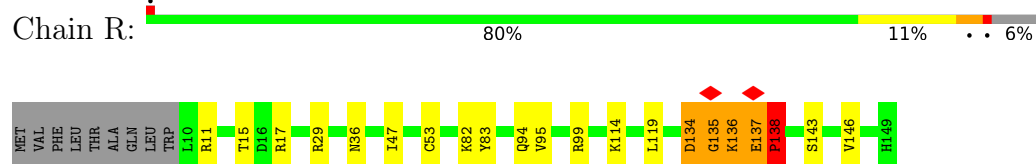
- Molecule 39: 39S ribosomal protein L15, mitochondrial



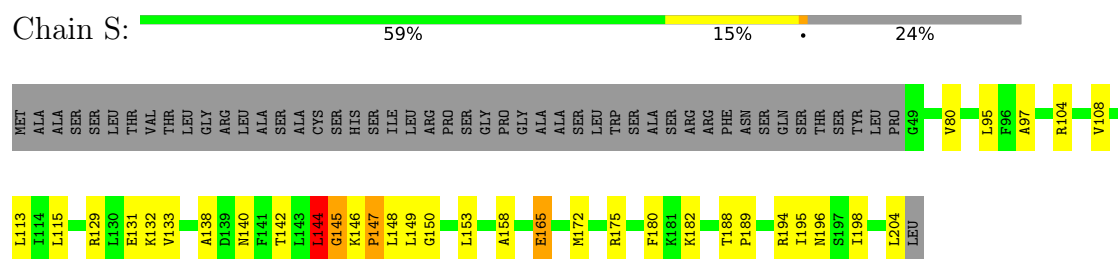
- Molecule 40: 39S ribosomal protein L17, mitochondrial



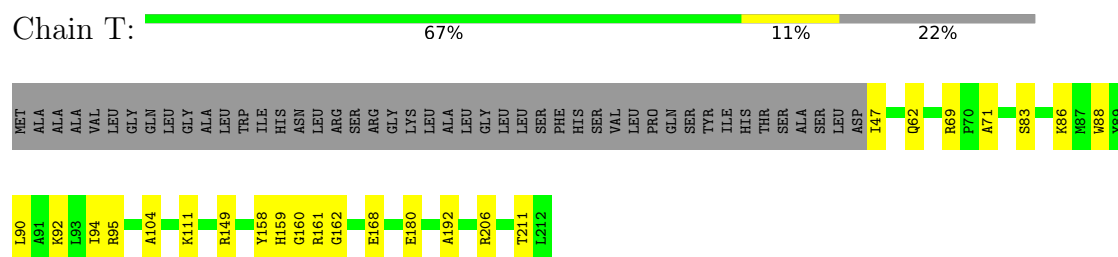
- Molecule 41: 39S ribosomal protein L20, mitochondrial



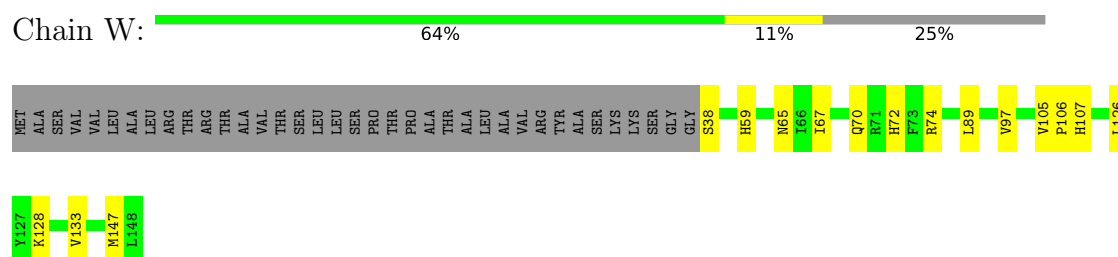
- Molecule 42: 39S ribosomal protein L21, mitochondrial



- Molecule 43: 39S ribosomal protein L22, mitochondrial



- Molecule 44: 39S ribosomal protein L27, mitochondrial



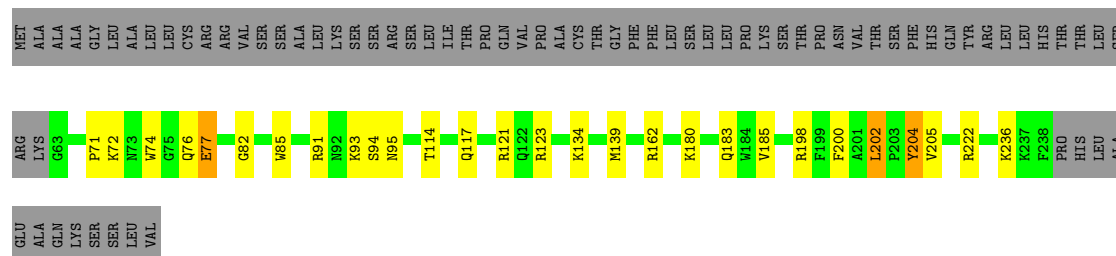
- Molecule 45: 39S ribosomal protein L28, mitochondrial

Chain X: 



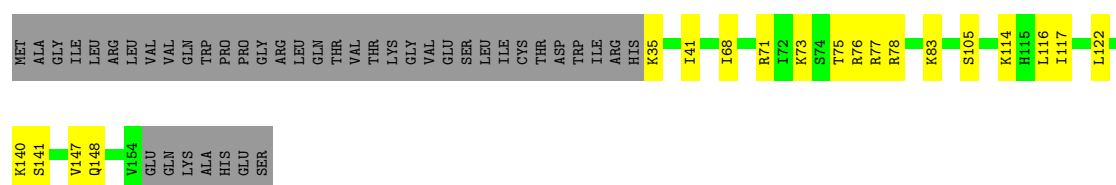
- Molecule 46: 39S ribosomal protein L47, mitochondrial

Chain Y: 



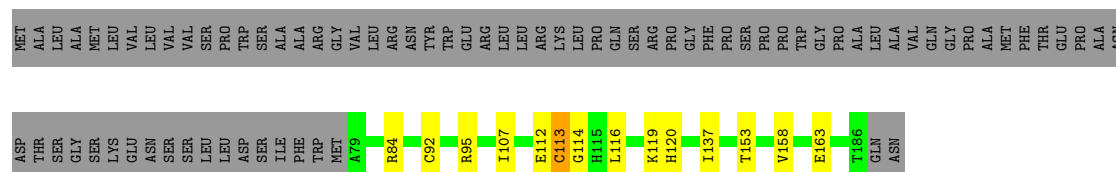
- Molecule 47: 39S ribosomal protein L30, mitochondrial

Chain Z: 



- Molecule 48: 39S ribosomal protein L32, mitochondrial

Chain 0: 



- Molecule 49: 39S ribosomal protein L33, mitochondrial

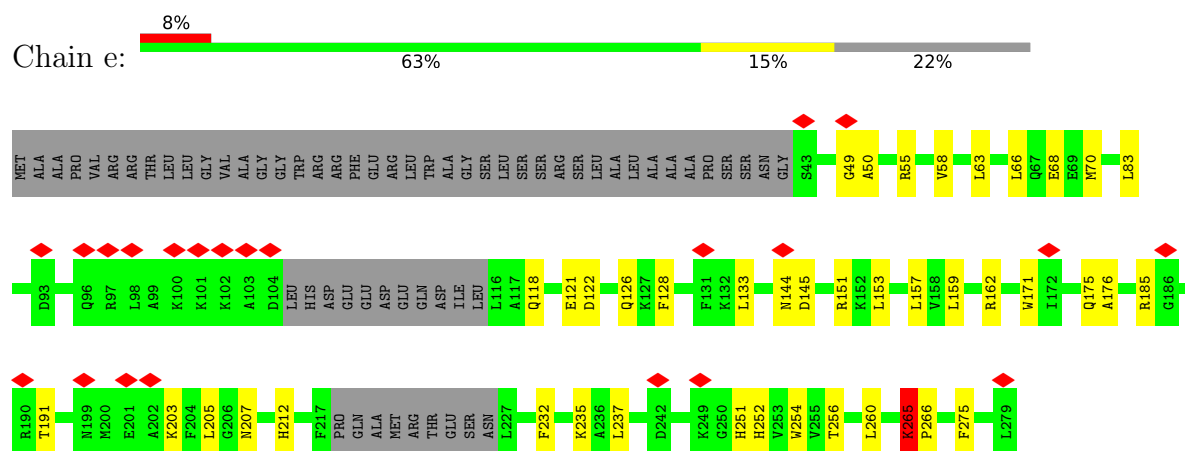
Chain 1: 



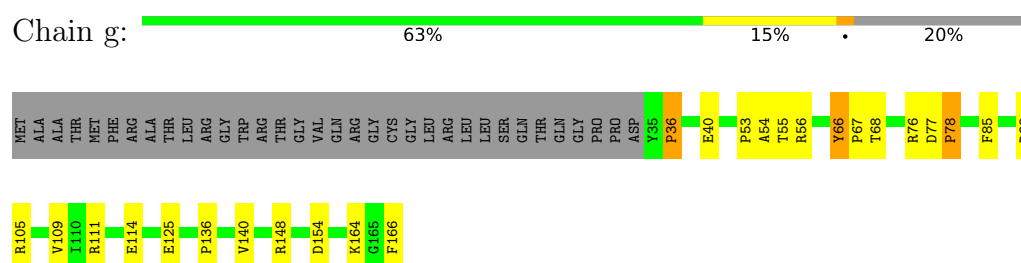
- Molecule 50: 39S ribosomal protein L34, mitochondrial



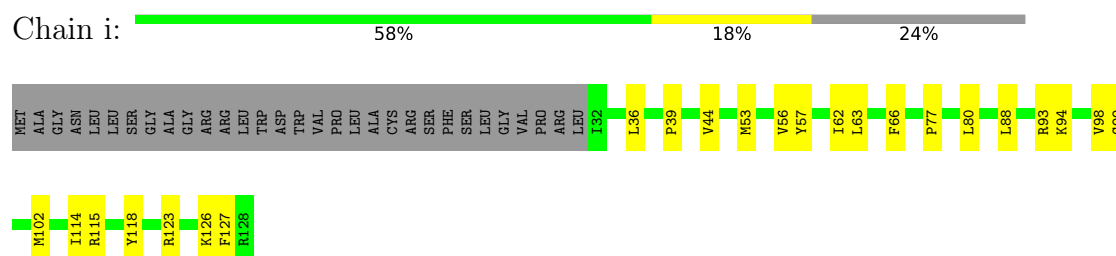
- Molecule 55: 39S ribosomal protein L46, mitochondrial



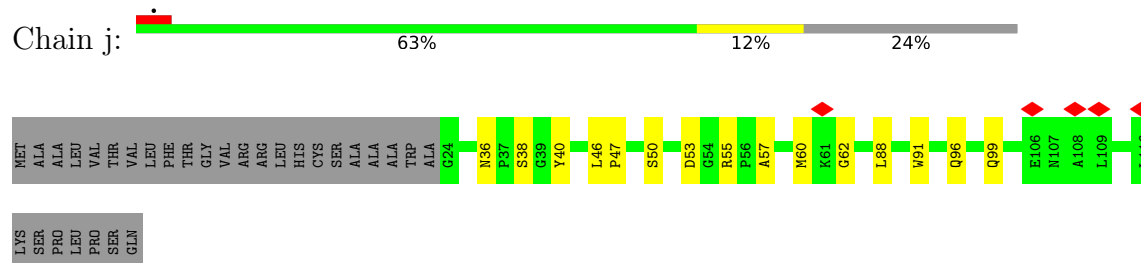
- Molecule 56: 39S ribosomal protein L49, mitochondrial



- Molecule 57: 39S ribosomal protein L51, mitochondrial

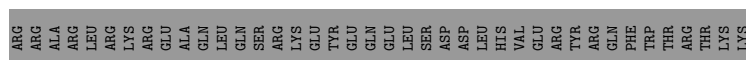
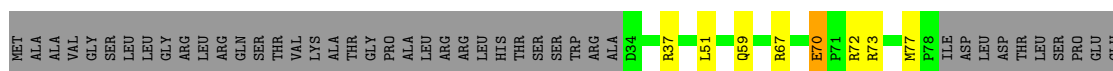


- Molecule 58: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA



- Molecule 59: 39S ribosomal protein L55, mitochondrial

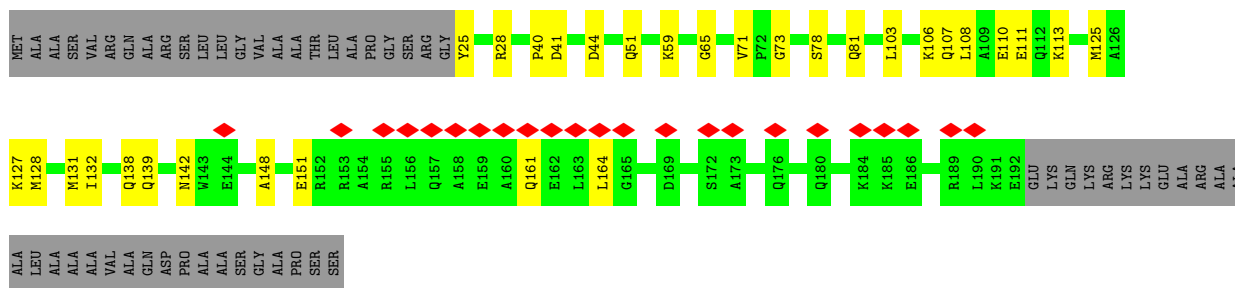




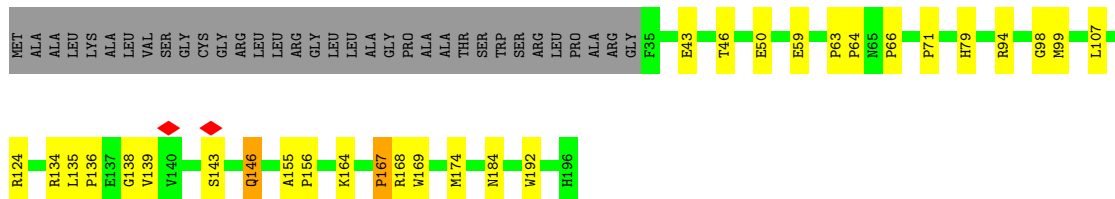
- Molecule 60: Ribosomal protein 63, mitochondrial



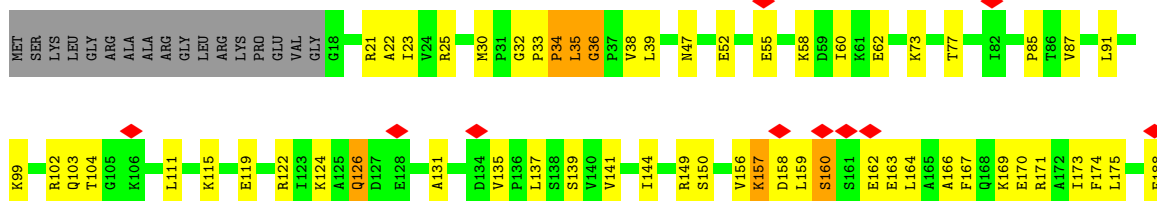
- Molecule 61: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 62: 39S ribosomal protein S18a, mitochondrial

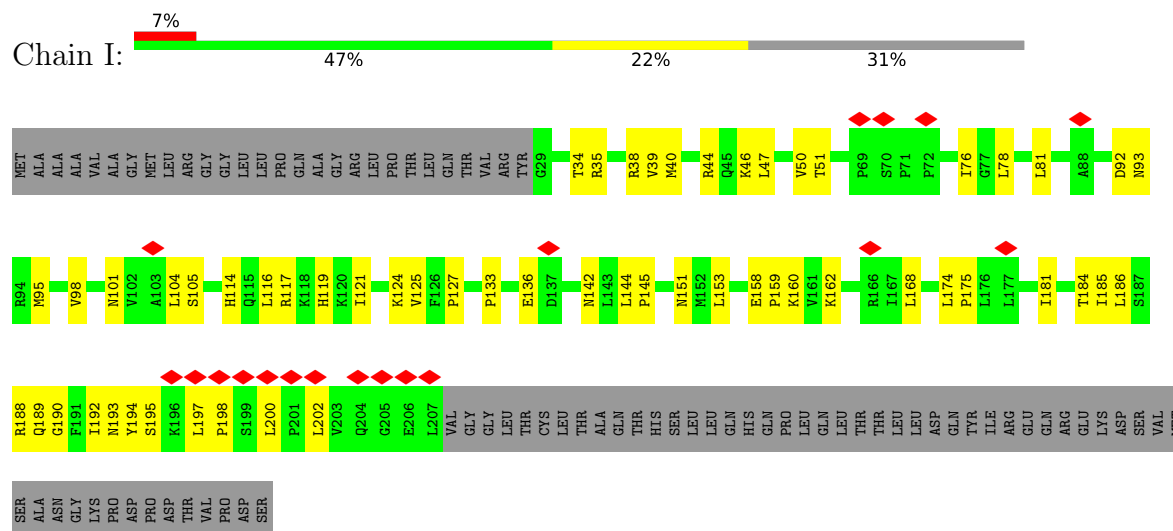


- Molecule 63: 39S ribosomal protein L11, mitochondrial

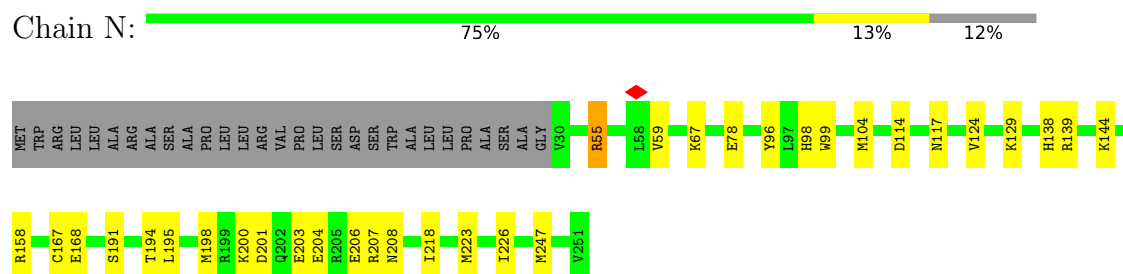




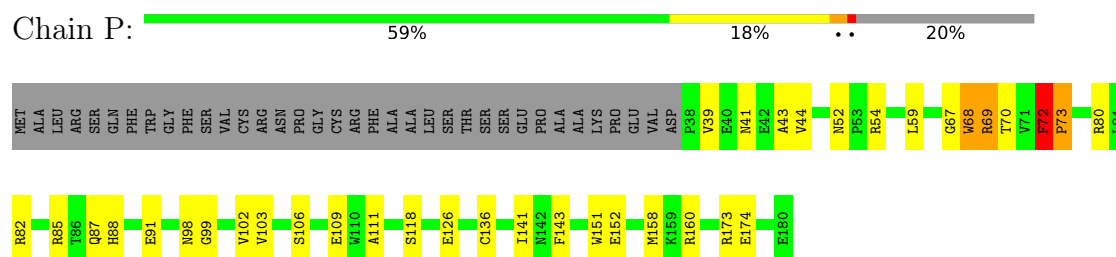
- Molecule 64: 39S ribosomal protein L10, mitochondrial



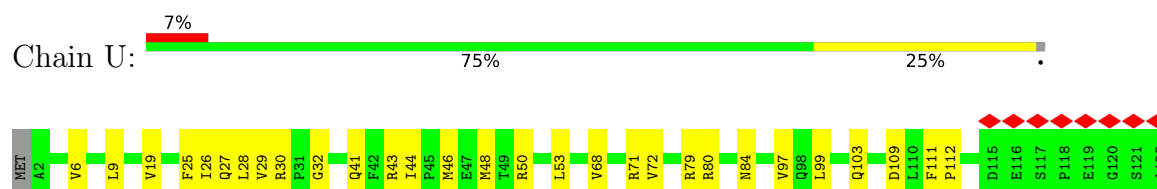
- Molecule 65: 39S ribosomal protein L16, mitochondrial



- Molecule 66: Mitochondrial ribosomal protein L18, isoform CRA_b



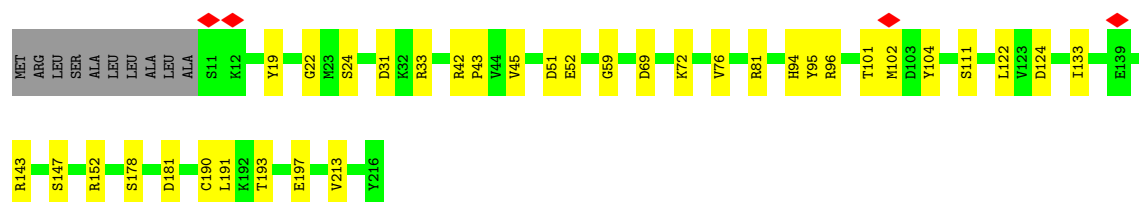
- Molecule 67: 39S ribosomal protein L23, mitochondrial





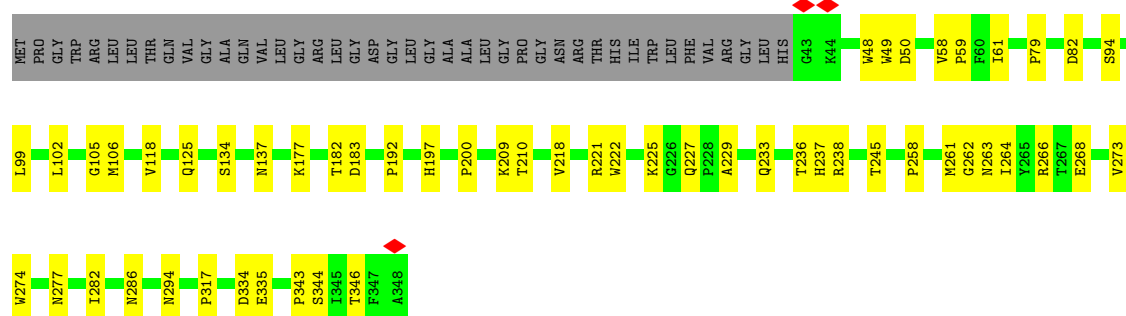
- Molecule 68: 39S ribosomal protein L24, mitochondrial

Chain V: 79% 16% 5%



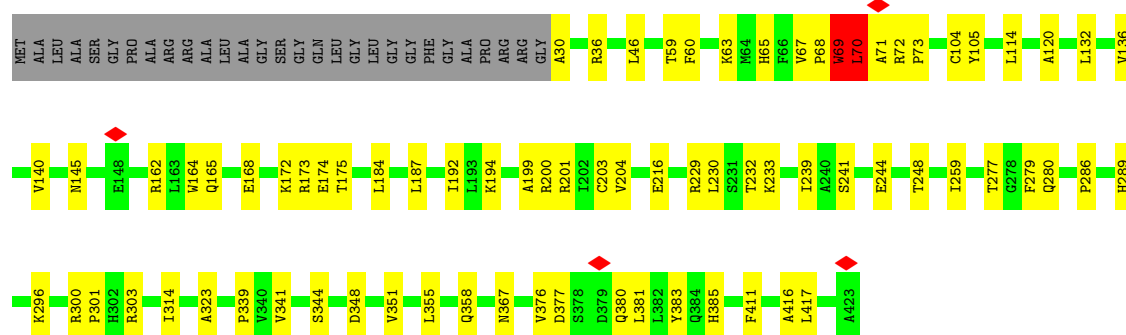
- Molecule 69: 39S ribosomal protein L3, mitochondrial

Chain E: 72% 16% 12%



- Molecule 70: 39S ribosomal protein L37, mitochondrial

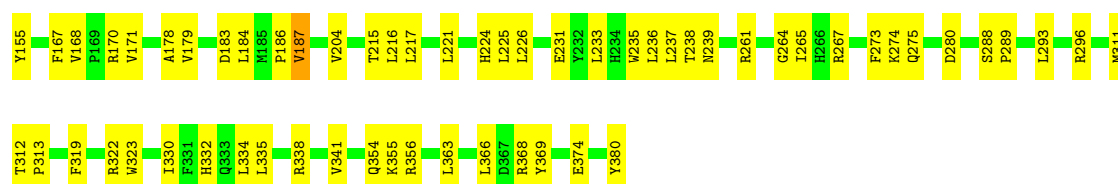
Chain 5: 75% 18% 7%



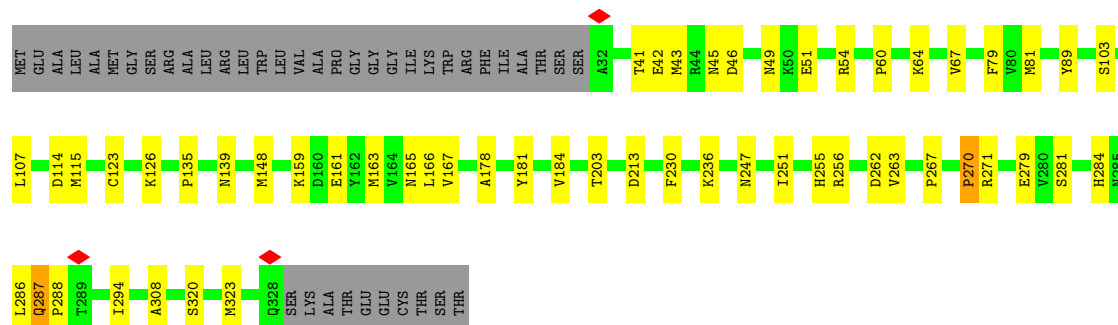
- Molecule 71: 39S ribosomal protein L38, mitochondrial

Chain 6: 74% 19% 7%

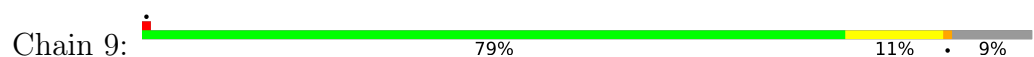




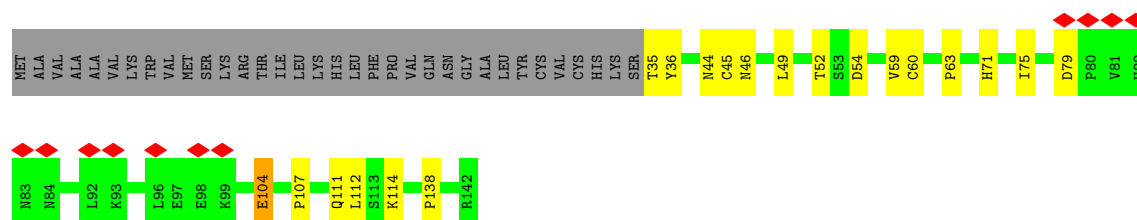
- Molecule 72: 39S ribosomal protein L39, mitochondrial



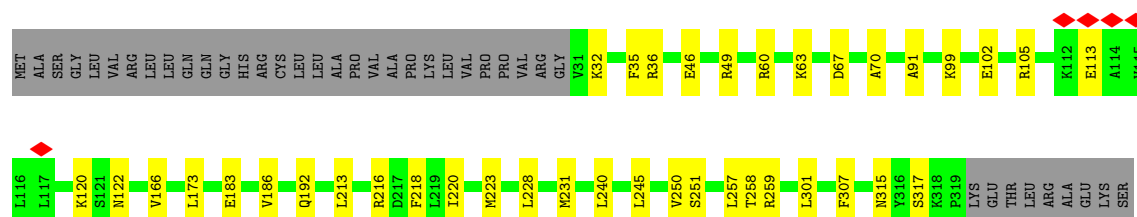
- Molecule 73: 39S ribosomal protein L41, mitochondrial



- Molecule 74: 39S ribosomal protein L42, mitochondrial



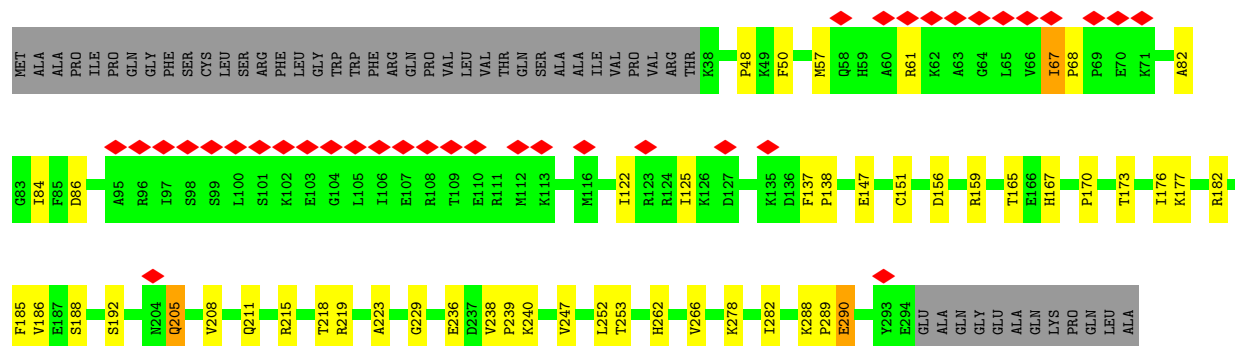
- Molecule 75: 39S ribosomal protein L44, mitochondrial



ILE
THR
ALA
SER

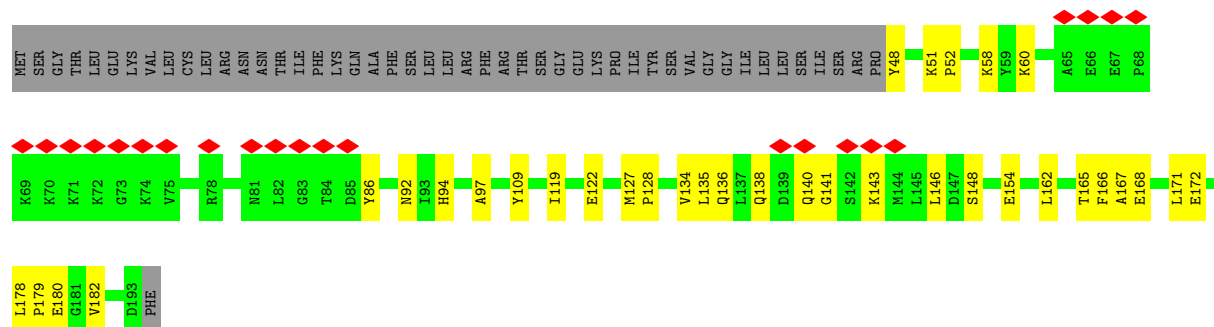
- Molecule 76: 39S ribosomal protein L45, mitochondrial

Chain d: 



- Molecule 77: 39S ribosomal protein L48, mitochondrial

Chain f: 



- Molecule 78: 39S ribosomal protein L50, mitochondrial

Chain h: 

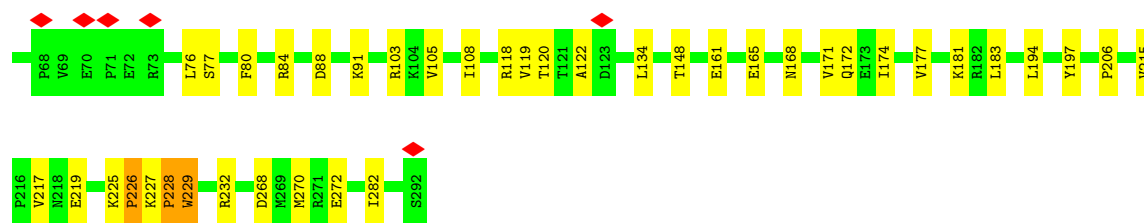


- Molecule 79: 39S ribosomal protein L53, mitochondrial

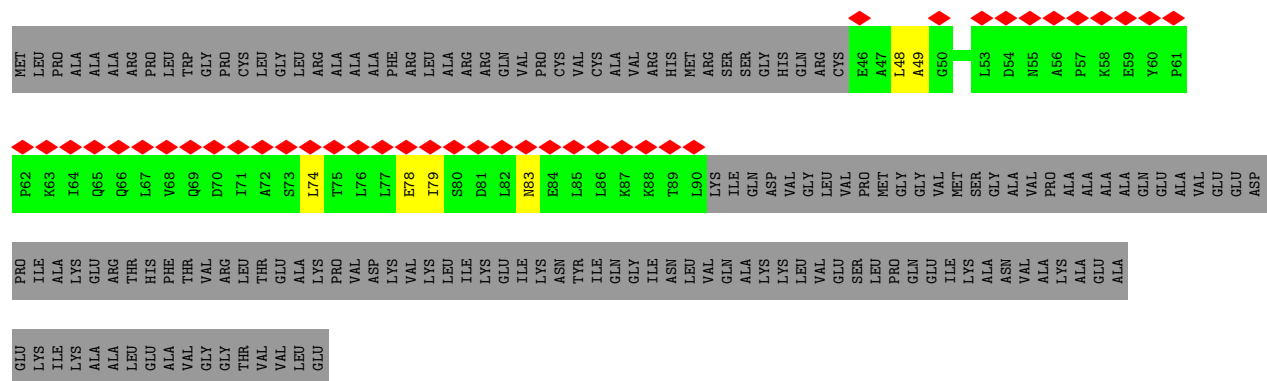
Chain k: 



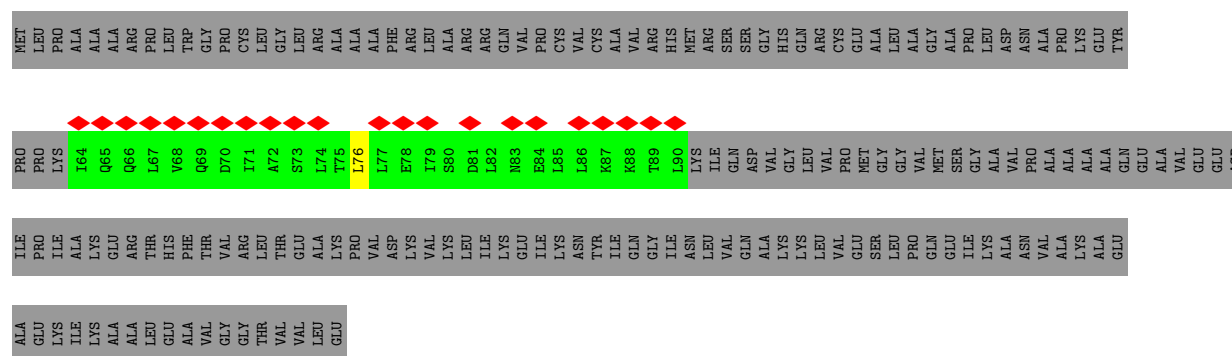
- [illegible]



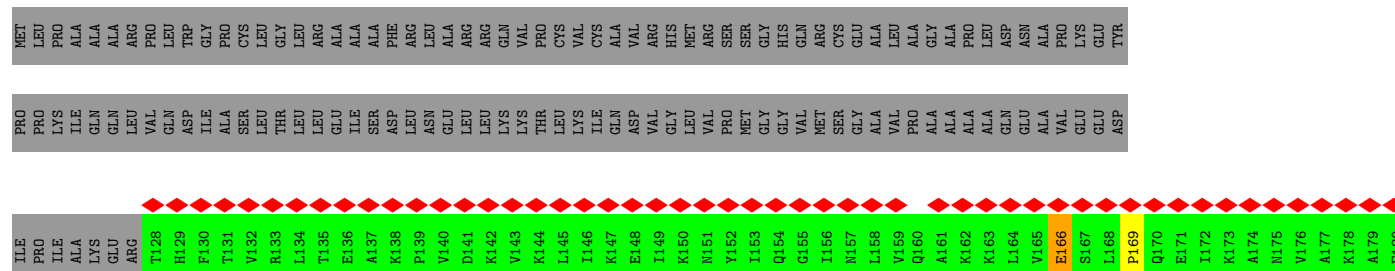
• Molecule 84: 39S ribosomal protein L12, mitochondrial

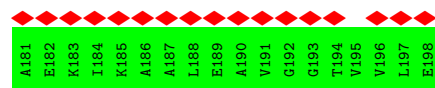


• Molecule 84: 39S ribosomal protein L12, mitochondrial

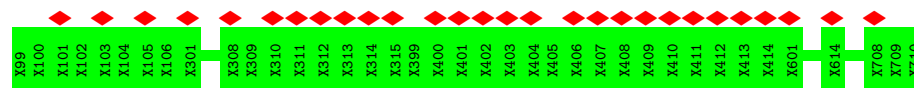
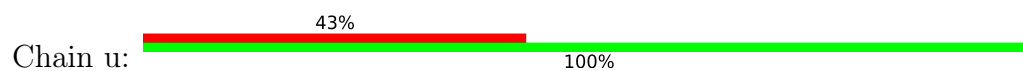


• Molecule 84: 39S ribosomal protein L12, mitochondrial

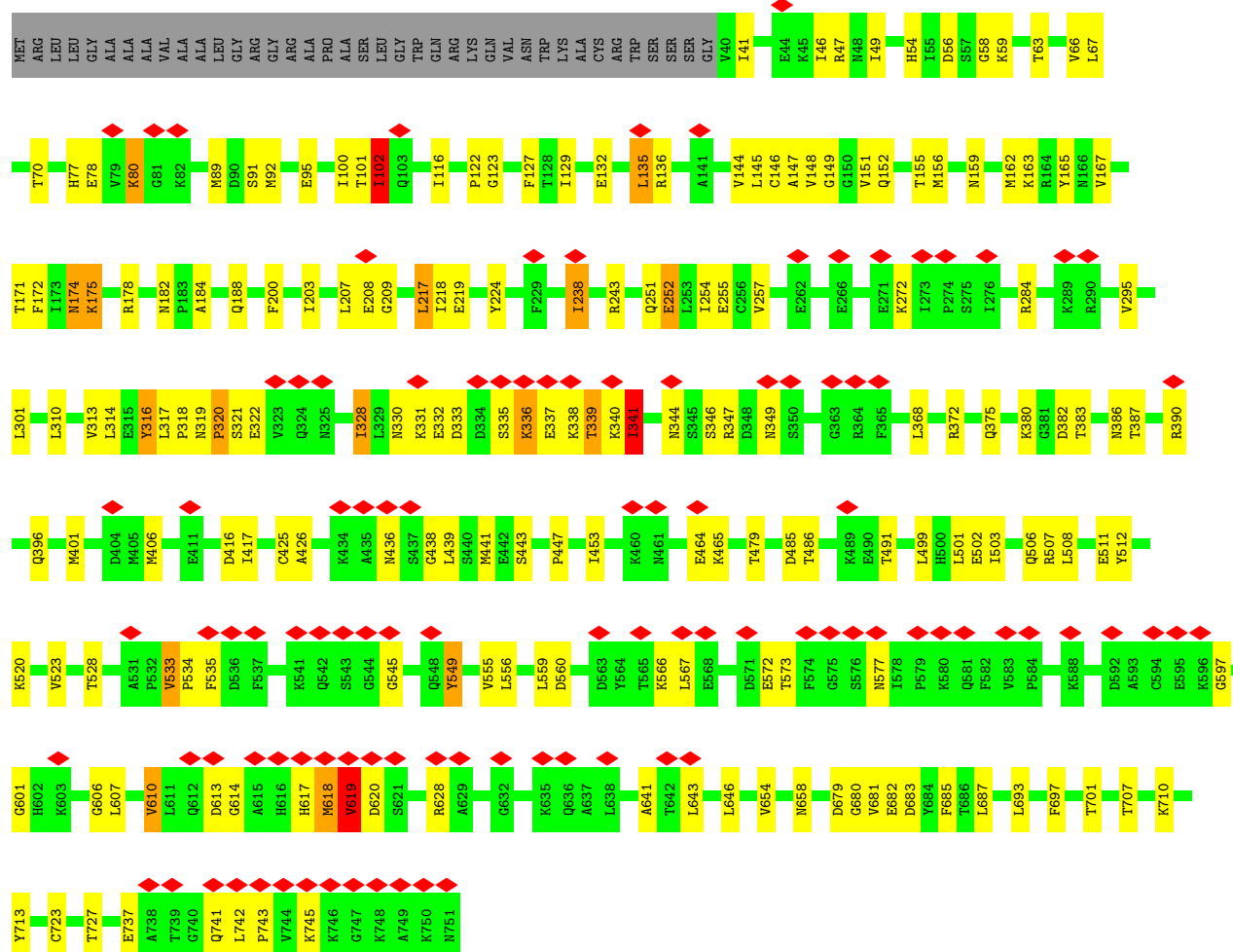




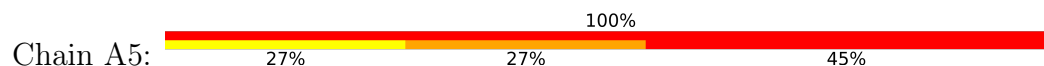
• Molecule 85: P-site finger



• Molecule 86: Elongation factor G, mitochondrial

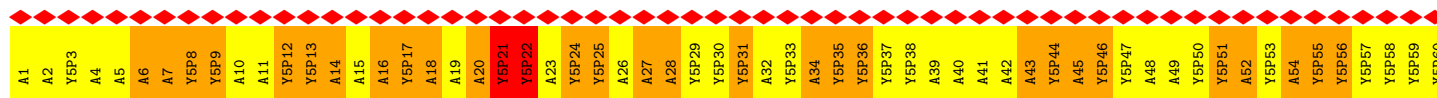


• Molecule 87: mRNA

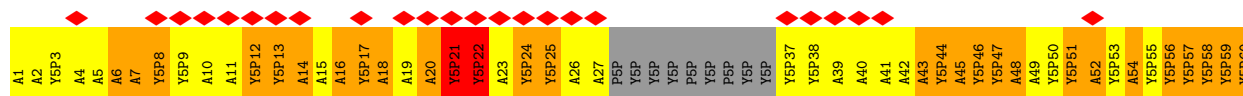
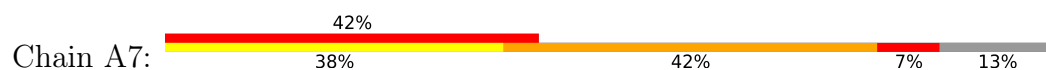




- Molecule 88: P-site and E-site tRNA



- Molecule 88: P-site and E-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.076	Depositor
Minimum map value	-1.966	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.267	Depositor
Map size ($\text{\AA}$)	438.44, 438.44, 438.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.07	0/22406	0.17	0/34881
2	AB	0.07	0/1830	0.22	0/2477
3	AC	0.08	0/1112	0.28	0/1505
4	AE	0.09	0/989	0.33	0/1335
5	AI	0.07	0/1031	0.25	0/1390
6	AJ	0.09	0/854	0.27	0/1148
7	AK	0.09	0/879	0.30	0/1182
8	AM	0.10	0/941	0.34	0/1265
9	AN	0.07	0/864	0.22	0/1169
10	AO	0.07	0/1624	0.23	0/2209
11	AP	0.07	0/791	0.21	0/1062
12	AQ	0.09	0/752	0.26	0/1001
13	AT	0.07	0/1402	0.20	0/1883
14	AW	0.08	0/778	0.27	0/1048
15	AX	0.08	0/2932	0.23	0/3968
16	A2	0.08	0/939	0.26	0/1256
17	AH	0.08	0/1037	0.22	0/1403
18	AL	0.09	0/1475	0.25	0/1970
19	AR	0.07	0/2435	0.20	0/3288
20	AS	0.08	0/1138	0.22	0/1533
21	AU	0.10	0/1521	0.26	0/2039
22	AV	0.08	0/3071	0.21	0/4147
23	AY	0.14	0/1046	0.41	4/1410 (0.3%)
24	AZ	0.07	0/851	0.20	0/1133
25	A1	0.07	0/2277	0.21	0/3079
26	A0	0.08	0/1827	0.26	0/2473
27	A3	0.10	0/650	0.29	0/855
28	A4	0.06	0/3028	0.18	0/4197
29	AD	0.07	0/2783	0.22	0/3724
30	AF	0.09	0/1765	0.25	0/2369
31	AG	0.08	0/2642	0.23	0/3538
32	A	0.10	2/36246 (0.0%)	0.21	2/56422 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B	0.06	0/1328	0.15	0/2056
34	D	0.07	0/1904	0.24	0/2561
35	F	0.08	0/2071	0.26	0/2817
36	H	0.10	0/820	0.28	0/1102
37	K	0.07	0/1495	0.24	0/2029
38	L	0.07	0/904	0.24	0/1218
39	M	0.09	0/2359	0.28	0/3185
40	O	0.10	0/1269	0.28	0/1708
41	R	0.12	0/1174	0.54	7/1572 (0.4%)
42	S	0.11	0/1276	0.47	3/1729 (0.2%)
43	T	0.08	0/1402	0.24	0/1886
44	W	0.07	0/893	0.22	0/1204
45	X	0.08	0/2081	0.24	0/2812
46	Y	0.08	0/1552	0.25	0/2079
47	Z	0.07	0/1003	0.24	0/1354
48	0	0.08	0/895	0.26	0/1201
49	1	0.07	0/438	0.26	0/583
50	2	0.08	0/382	0.26	0/507
51	3	0.08	0/852	0.24	0/1136
52	4	0.09	0/350	0.30	0/461
53	8	0.09	0/855	0.25	0/1152
54	b	0.08	0/1202	0.27	0/1626
55	e	0.08	0/1797	0.25	0/2422
56	g	0.12	0/1132	0.31	0/1543
57	i	0.10	0/849	0.28	0/1135
58	j	0.09	0/755	0.25	0/1016
59	m	0.09	0/379	0.28	0/510
60	o	0.10	0/818	0.34	0/1097
61	q	0.11	0/1325	0.41	2/1799 (0.1%)
62	r	0.08	0/1362	0.25	0/1846
63	J	0.27	1/1348 (0.1%)	0.37	0/1813
64	I	0.09	0/1467	0.28	0/1984
65	N	0.08	0/1833	0.25	0/2468
66	P	0.22	0/1191	0.41	1/1611 (0.1%)
67	U	0.11	0/1254	0.27	0/1700
68	V	0.08	0/1727	0.24	0/2341
69	E	0.07	0/2479	0.20	0/3360
70	5	0.17	1/3305 (0.0%)	0.31	0/4502
71	6	0.08	0/3043	0.24	0/4140
72	7	0.07	0/2467	0.22	0/3337
73	9	0.08	0/1025	0.24	0/1379
74	a	0.07	0/923	0.23	0/1254
75	c	0.08	0/2371	0.24	0/3205

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	d	0.09	0/2132	0.25	0/2887
77	f	0.06	0/1144	0.21	0/1551
78	h	0.08	0/917	0.23	0/1249
79	k	0.10	0/754	0.26	0/1017
80	l	0.08	0/636	0.23	0/860
81	p	0.09	0/1246	0.25	0/1675
82	s	0.11	0/3262	0.42	5/4435 (0.1%)
83	Q	0.12	0/2044	0.29	0/2757
84	TA	0.12	0/349	0.38	0/475
84	TB	0.05	0/212	0.16	0/286
84	TC	0.10	0/351	0.59	2/488 (0.4%)
86	v	0.26	3/5647 (0.1%)	0.51	15/7623 (0.2%)
All	All	0.10	7/181965 (0.0%)	0.26	41/258102 (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
23	AY	0	1
41	R	0	1
42	S	0	1
66	P	0	1
82	s	0	1
84	TC	0	1
86	v	0	1
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	v	174	ASN	C-N	12.20	1.50	1.33
63	J	188	GLU	C-N	8.20	1.45	1.34
86	v	175	LYS	N-CA	8.11	1.56	1.46
32	A	3089	A	C3'-O3'	-6.20	1.32	1.42
86	v	175	LYS	CA-C	5.54	1.60	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	s	160	ARG	CA-C-N	-11.64	105.31	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	s	160	ARG	C-N-CA	-11.64	105.31	121.84
86	v	339	THR	N-CA-C	10.60	125.52	109.41
32	A	3089	A	C4'-C3'-O3'	10.54	128.80	113.00
42	S	144	LEU	CA-C-N	-9.37	103.04	121.41

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	AY	313	PHE	Peptide
66	P	72	PHE	Peptide
41	R	134	ASP	Peptide
42	S	144	LEU	Peptide
82	s	160	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	20030	0	10172	283	0
2	AB	1787	0	1779	24	0
3	AC	1082	0	1088	20	0
4	AE	972	0	1001	11	0
5	AI	1011	0	1052	14	0
6	AJ	838	0	887	18	0
7	AK	861	0	885	22	0
8	AM	920	0	951	12	0
9	AN	846	0	908	12	0
10	AO	1570	0	1533	14	0
11	AP	774	0	803	15	0
12	AQ	740	0	754	14	0
13	AT	1371	0	1395	14	0
14	AW	766	0	785	19	0
15	AX	2860	0	2856	45	0
16	A2	925	0	962	16	0
17	AH	1014	0	1036	23	0
18	AL	1451	0	1543	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AR	2388	0	2410	28	0
20	AS	1111	0	1115	5	0
21	AU	1499	0	1512	20	0
22	AV	3009	0	3006	32	0
23	AY	1016	0	962	15	0
24	AZ	833	0	853	13	0
25	A1	2231	0	2261	37	0
26	A0	1781	0	1791	34	0
27	A3	639	0	715	10	0
28	A4	3010	0	1760	10	0
29	AD	2731	0	2804	52	0
30	AF	1724	0	1765	25	0
31	AG	2587	0	2570	36	0
32	A	32395	0	16450	608	0
33	B	1191	0	607	12	0
34	D	1866	0	1927	26	0
35	F	2013	0	2044	34	0
36	H	806	0	849	16	0
37	K	1451	0	1448	15	0
38	L	889	0	941	17	0
39	M	2305	0	2378	44	0
40	O	1245	0	1283	16	0
41	R	1153	0	1214	14	0
42	S	1251	0	1322	28	0
43	T	1368	0	1410	16	0
44	W	871	0	897	13	0
45	X	2027	0	2040	24	0
46	Y	1517	0	1561	25	0
47	Z	978	0	1030	13	0
48	0	880	0	904	9	0
49	1	433	0	475	6	0
50	2	376	0	406	13	0
51	3	831	0	883	20	0
52	4	342	0	362	7	0
53	8	836	0	844	18	0
54	b	1178	0	1180	10	0
55	e	1762	0	1767	28	0
56	g	1096	0	1081	18	0
57	i	827	0	857	18	0
58	j	740	0	741	9	0
59	m	372	0	387	5	0
60	o	797	0	804	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	q	1294	0	1178	20	0
62	r	1322	0	1350	21	0
63	J	1330	0	1407	103	0
64	I	1435	0	1521	41	0
65	N	1786	0	1817	21	0
66	P	1165	0	1162	35	0
67	U	1224	0	1191	25	0
68	V	1682	0	1692	23	0
69	E	2410	0	2418	37	0
70	5	3210	0	3206	94	0
71	6	2948	0	2841	53	0
72	7	2410	0	2415	31	0
73	9	997	0	987	11	0
74	a	896	0	847	15	0
75	c	2322	0	2338	22	0
76	d	2075	0	2037	30	0
77	f	1126	0	1106	24	0
78	h	894	0	881	8	0
79	k	743	0	758	11	0
80	l	619	0	611	24	0
81	p	1227	0	1239	22	0
82	s	3178	0	3124	53	0
83	Q	1995	0	2036	29	0
84	TA	345	0	364	5	0
84	TB	213	0	234	1	0
84	TC	352	0	169	0	0
85	u	325	0	76	0	0
86	v	5546	0	5501	170	0
87	A5	213	0	122	29	0
88	A6	1368	0	790	73	0
88	A7	1197	0	690	39	0
89	A	97	0	0	0	0
89	AA	27	0	0	0	0
89	AC	1	0	0	0	0
89	D	1	0	0	0	0
89	E	1	0	0	0	0
89	W	1	0	0	0	0
89	g	1	0	0	0	0
89	v	1	0	0	0	0
90	0	1	0	0	0	0
90	4	1	0	0	0	0
90	AB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	AO	1	0	0	0	0
90	AP	1	0	0	0	0
90	AT	1	0	0	0	0
90	r	1	0	0	0	0
91	AX	28	0	10	3	0
92	v	32	0	14	44	0
All	All	176217	0	148138	2448	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2448 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:J:171:ARG:HA	63:J:174:PHE:CE2	1.29	1.66
70:5:60:PHE:CD1	70:5:71:ALA:HB1	1.25	1.63
70:5:68:PRO:HG2	70:5:69:TRP:CE3	1.24	1.62
86:v:175:LYS:HE2	92:v:802:GCP:C4	1.38	1.51
45:X:156:LYS:NZ	70:5:70:LEU:HD23	1.24	1.44

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	218/296 (74%)	193 (88%)	21 (10%)	4 (2%)	6	19
3	AC	130/167 (78%)	110 (85%)	19 (15%)	1 (1%)	16	37
4	AE	120/125 (96%)	102 (85%)	15 (12%)	3 (2%)	4	13
5	AI	134/194 (69%)	117 (87%)	12 (9%)	5 (4%)	2	6
6	AJ	106/138 (77%)	88 (83%)	15 (14%)	3 (3%)	4	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AK	99/128 (77%)	87 (88%)	10 (10%)	2 (2%)	6	16
8	AM	114/137 (83%)	101 (89%)	12 (10%)	1 (1%)	14	34
9	AN	105/130 (81%)	83 (79%)	21 (20%)	1 (1%)	12	32
10	AO	188/258 (73%)	170 (90%)	15 (8%)	3 (2%)	7	21
11	AP	94/142 (66%)	79 (84%)	12 (13%)	3 (3%)	3	8
12	AQ	84/87 (97%)	75 (89%)	9 (11%)	0	100	100
13	AT	166/173 (96%)	149 (90%)	17 (10%)	0	100	100
14	AW	95/187 (51%)	78 (82%)	15 (16%)	2 (2%)	5	16
15	AX	351/398 (88%)	318 (91%)	27 (8%)	6 (2%)	7	20
16	A2	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
17	AH	120/201 (60%)	96 (80%)	20 (17%)	4 (3%)	3	7
18	AL	172/257 (67%)	151 (88%)	17 (10%)	4 (2%)	5	14
19	AR	290/360 (81%)	253 (87%)	36 (12%)	1 (0%)	36	59
20	AS	133/190 (70%)	122 (92%)	8 (6%)	3 (2%)	5	14
21	AU	175/205 (85%)	164 (94%)	11 (6%)	0	100	100
22	AV	363/414 (88%)	312 (86%)	42 (12%)	9 (2%)	4	13
23	AY	118/395 (30%)	105 (89%)	12 (10%)	1 (1%)	16	37
24	AZ	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
25	A1	273/323 (84%)	247 (90%)	23 (8%)	3 (1%)	11	29
26	A0	212/218 (97%)	183 (86%)	27 (13%)	2 (1%)	14	34
27	A3	70/199 (35%)	65 (93%)	4 (6%)	1 (1%)	9	24
28	A4	541/689 (78%)	468 (86%)	61 (11%)	12 (2%)	5	15
29	AD	341/430 (79%)	298 (87%)	38 (11%)	5 (2%)	8	23
30	AF	206/242 (85%)	184 (89%)	19 (9%)	3 (2%)	8	23
31	AG	311/396 (78%)	274 (88%)	35 (11%)	2 (1%)	21	45
34	D	237/305 (78%)	207 (87%)	28 (12%)	2 (1%)	16	37
35	F	248/311 (80%)	217 (88%)	26 (10%)	5 (2%)	6	16
36	H	96/267 (36%)	83 (86%)	11 (12%)	2 (2%)	5	16
37	K	175/178 (98%)	153 (87%)	16 (9%)	6 (3%)	3	7
38	L	113/145 (78%)	101 (89%)	11 (10%)	1 (1%)	14	34
39	M	285/296 (96%)	252 (88%)	26 (9%)	7 (2%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	O	150/175 (86%)	128 (85%)	19 (13%)	3 (2%)	6	16
41	R	138/149 (93%)	124 (90%)	9 (6%)	5 (4%)	2	6
42	S	154/205 (75%)	135 (88%)	15 (10%)	4 (3%)	4	12
43	T	164/212 (77%)	148 (90%)	13 (8%)	3 (2%)	6	19
44	W	109/148 (74%)	96 (88%)	12 (11%)	1 (1%)	14	34
45	X	241/256 (94%)	213 (88%)	22 (9%)	6 (2%)	4	13
46	Y	174/250 (70%)	161 (92%)	8 (5%)	5 (3%)	3	10
47	Z	118/161 (73%)	106 (90%)	12 (10%)	0	100	100
48	0	106/188 (56%)	93 (88%)	10 (9%)	3 (3%)	4	11
49	1	50/65 (77%)	42 (84%)	7 (14%)	1 (2%)	6	16
50	2	44/92 (48%)	41 (93%)	2 (4%)	1 (2%)	5	14
51	3	93/188 (50%)	84 (90%)	8 (9%)	1 (1%)	11	29
52	4	36/103 (35%)	33 (92%)	3 (8%)	0	100	100
53	8	97/206 (47%)	84 (87%)	13 (13%)	0	100	100
54	b	146/155 (94%)	129 (88%)	14 (10%)	3 (2%)	5	16
55	e	211/279 (76%)	188 (89%)	22 (10%)	1 (0%)	24	49
56	g	130/166 (78%)	111 (85%)	14 (11%)	5 (4%)	2	6
57	i	95/128 (74%)	75 (79%)	20 (21%)	0	100	100
58	j	91/123 (74%)	83 (91%)	7 (8%)	1 (1%)	11	29
59	m	43/128 (34%)	34 (79%)	8 (19%)	1 (2%)	5	14
60	o	92/102 (90%)	78 (85%)	11 (12%)	3 (3%)	3	7
61	q	166/222 (75%)	154 (93%)	10 (6%)	2 (1%)	10	28
62	r	160/196 (82%)	139 (87%)	17 (11%)	4 (2%)	4	13
63	J	173/192 (90%)	152 (88%)	15 (9%)	6 (4%)	3	7
64	I	177/261 (68%)	164 (93%)	12 (7%)	1 (1%)	21	45
65	N	220/251 (88%)	203 (92%)	16 (7%)	1 (0%)	24	49
66	P	141/179 (79%)	123 (87%)	13 (9%)	5 (4%)	3	7
67	U	150/153 (98%)	121 (81%)	27 (18%)	2 (1%)	9	26
68	V	204/216 (94%)	179 (88%)	25 (12%)	0	100	100
69	E	304/348 (87%)	268 (88%)	32 (10%)	4 (1%)	9	26
70	5	392/423 (93%)	347 (88%)	41 (10%)	4 (1%)	12	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	6	352/380 (93%)	302 (86%)	47 (13%)	3 (1%)	14	34
72	7	295/338 (87%)	260 (88%)	28 (10%)	7 (2%)	4	13
73	9	122/137 (89%)	106 (87%)	15 (12%)	1 (1%)	16	37
74	a	106/142 (75%)	95 (90%)	8 (8%)	3 (3%)	4	11
75	c	287/332 (86%)	266 (93%)	17 (6%)	4 (1%)	9	24
76	d	255/306 (83%)	215 (84%)	34 (13%)	6 (2%)	4	13
77	f	144/194 (74%)	122 (85%)	21 (15%)	1 (1%)	18	40
78	h	108/158 (68%)	93 (86%)	13 (12%)	2 (2%)	6	17
79	k	94/112 (84%)	86 (92%)	8 (8%)	0	100	100
80	l	70/138 (51%)	62 (89%)	7 (10%)	1 (1%)	9	24
81	p	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	24
82	s	391/439 (89%)	342 (88%)	40 (10%)	9 (2%)	5	14
83	Q	238/292 (82%)	216 (91%)	16 (7%)	6 (2%)	4	13
84	TA	43/198 (22%)	32 (74%)	11 (26%)	0	100	100
84	TB	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
84	TC	69/198 (35%)	57 (83%)	11 (16%)	1 (1%)	9	24
86	v	710/751 (94%)	565 (80%)	128 (18%)	17 (2%)	4	13
All	All	14720/19244 (76%)	12885 (88%)	1589 (11%)	246 (2%)	9	20

5 of 246 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	AL	71	LEU
23	AY	314	PRO
28	A4	252	PRO
28	A4	450	PRO
28	A4	542	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	193/249 (78%)	192 (100%)	1 (0%)	81	90
3	AC	115/143 (80%)	114 (99%)	1 (1%)	70	83
4	AE	104/107 (97%)	103 (99%)	1 (1%)	68	82
5	AI	104/147 (71%)	103 (99%)	1 (1%)	68	82
6	AJ	93/118 (79%)	93 (100%)	0	100	100
7	AK	91/113 (80%)	90 (99%)	1 (1%)	65	80
8	AM	95/113 (84%)	95 (100%)	0	100	100
9	AN	93/115 (81%)	92 (99%)	1 (1%)	65	80
10	AO	171/230 (74%)	170 (99%)	1 (1%)	78	89
11	AP	87/123 (71%)	87 (100%)	0	100	100
12	AQ	78/79 (99%)	78 (100%)	0	100	100
13	AT	153/157 (98%)	151 (99%)	2 (1%)	61	78
14	AW	84/158 (53%)	84 (100%)	0	100	100
15	AX	312/351 (89%)	311 (100%)	1 (0%)	86	92
16	A2	99/101 (98%)	99 (100%)	0	100	100
17	AH	112/180 (62%)	111 (99%)	1 (1%)	70	83
18	AL	157/226 (70%)	156 (99%)	1 (1%)	78	89
19	AR	262/318 (82%)	262 (100%)	0	100	100
20	AS	116/164 (71%)	116 (100%)	0	100	100
21	AU	153/174 (88%)	153 (100%)	0	100	100
22	AV	328/364 (90%)	325 (99%)	3 (1%)	70	83
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%)	250 (99%)	3 (1%)	63	79
26	A0	186/190 (98%)	186 (100%)	0	100	100
27	A3	66/166 (40%)	64 (97%)	2 (3%)	36	60
28	A4	83/609 (14%)	83 (100%)	0	100	100
29	AD	286/357 (80%)	285 (100%)	1 (0%)	86	92
30	AF	185/209 (88%)	180 (97%)	5 (3%)	39	64
31	AG	273/342 (80%)	269 (98%)	4 (2%)	57	76
34	D	193/245 (79%)	193 (100%)	0	100	100
35	F	217/262 (83%)	215 (99%)	2 (1%)	70	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	H	88/228 (39%)	86 (98%)	2 (2%)	44	67
37	K	155/156 (99%)	155 (100%)	0	100	100
38	L	98/124 (79%)	97 (99%)	1 (1%)	68	82
39	M	245/249 (98%)	244 (100%)	1 (0%)	84	92
40	O	133/150 (89%)	132 (99%)	1 (1%)	73	85
41	R	118/126 (94%)	117 (99%)	1 (1%)	73	85
42	S	141/180 (78%)	141 (100%)	0	100	100
43	T	146/182 (80%)	145 (99%)	1 (1%)	76	87
44	W	91/119 (76%)	91 (100%)	0	100	100
45	X	217/227 (96%)	212 (98%)	5 (2%)	44	67
46	Y	159/223 (71%)	157 (99%)	2 (1%)	61	78
47	Z	111/147 (76%)	111 (100%)	0	100	100
48	0	97/164 (59%)	97 (100%)	0	100	100
49	1	49/60 (82%)	48 (98%)	1 (2%)	48	71
50	2	40/72 (56%)	39 (98%)	1 (2%)	42	66
51	3	88/166 (53%)	86 (98%)	2 (2%)	44	67
52	4	37/89 (42%)	37 (100%)	0	100	100
53	8	91/190 (48%)	91 (100%)	0	100	100
54	b	130/135 (96%)	130 (100%)	0	100	100
55	e	188/236 (80%)	186 (99%)	2 (1%)	65	80
56	g	122/148 (82%)	120 (98%)	2 (2%)	55	75
57	i	86/110 (78%)	84 (98%)	2 (2%)	44	67
58	j	74/97 (76%)	74 (100%)	0	100	100
59	m	40/113 (35%)	40 (100%)	0	100	100
60	o	80/87 (92%)	79 (99%)	1 (1%)	61	78
61	q	114/178 (64%)	114 (100%)	0	100	100
62	r	147/169 (87%)	146 (99%)	1 (1%)	76	87
63	J	138/150 (92%)	135 (98%)	3 (2%)	45	69
64	I	164/232 (71%)	160 (98%)	4 (2%)	43	67
65	N	189/211 (90%)	188 (100%)	1 (0%)	81	90
66	P	125/154 (81%)	124 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	U	126/135 (93%)	125 (99%)	1 (1%)	73	85
68	V	184/191 (96%)	182 (99%)	2 (1%)	65	80
69	E	260/290 (90%)	259 (100%)	1 (0%)	84	92
70	5	353/368 (96%)	350 (99%)	3 (1%)	73	85
71	6	313/332 (94%)	308 (98%)	5 (2%)	55	75
72	7	272/303 (90%)	272 (100%)	0	100	100
73	9	104/112 (93%)	103 (99%)	1 (1%)	68	82
74	a	101/133 (76%)	101 (100%)	0	100	100
75	c	253/288 (88%)	253 (100%)	0	100	100
76	d	224/274 (82%)	220 (98%)	4 (2%)	51	72
77	f	122/173 (70%)	121 (99%)	1 (1%)	73	85
78	h	104/148 (70%)	103 (99%)	1 (1%)	68	82
79	k	81/90 (90%)	79 (98%)	2 (2%)	42	66
80	l	67/116 (58%)	67 (100%)	0	100	100
81	p	134/181 (74%)	131 (98%)	3 (2%)	45	69
82	s	336/381 (88%)	335 (100%)	1 (0%)	86	92
83	Q	221/256 (86%)	221 (100%)	0	100	100
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%)	582 (97%)	16 (3%)	39	64
All	All	12561/16442 (76%)	12453 (99%)	108 (1%)	68	83

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
62	r	146	GLN
70	5	46	LEU
86	v	178	ARG
63	J	135	VAL
65	N	59	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 266 such sidechains are listed below:

Mol	Chain	Res	Type
79	k	93	HIS
82	s	154	HIS
86	v	349	ASN
34	D	165	ASN
31	AG	308	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	940/954 (98%)	190 (20%)	10 (1%)
32	A	1523/1559 (97%)	345 (22%)	18 (1%)
33	B	51/73 (69%)	6 (11%)	1 (1%)
All	All	2514/2586 (97%)	541 (21%)	29 (1%)

5 of 541 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	650	U
1	AA	651	A
1	AA	663	A
1	AA	676	G
1	AA	680	U

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	A	1823	A
32	A	3196	G
32	A	2165	C
32	A	2989	G
32	A	1994	A

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

144 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	A6	70	88	14,19,20	4.52	2 (14%)	18,26,29	1.46	2 (11%)
88	P5P	A7	42	88	20,23,24	0.98	3 (15%)	27,33,36	2.04	4 (14%)
88	Y5P	A6	61	88	14,19,20	4.57	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A6	25	88	14,19,20	4.34	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A7	24	88	14,19,20	4.16	2 (14%)	18,26,29	1.36	2 (11%)
88	P5P	A6	43	88	20,23,24	1.09	3 (15%)	27,33,36	2.01	4 (14%)
88	Y5P	A6	65	88	14,19,20	4.42	2 (14%)	18,26,29	1.42	3 (16%)
88	P5P	A6	32	88	20,23,24	0.96	3 (15%)	27,33,36	1.93	4 (14%)
88	Y5P	A7	21	88	14,19,20	4.36	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A6	1	88	20,20,24	0.97	2 (10%)	28,29,36	1.97	4 (14%)
88	Y5P	A6	24	88	14,19,20	4.16	2 (14%)	18,26,29	1.36	2 (11%)
88	P5P	A6	23	88	20,23,24	1.01	3 (15%)	27,33,36	1.94	4 (14%)
88	P5P	A6	71	32,88	20,23,24	1.00	3 (15%)	27,33,36	1.96	4 (14%)
88	P5P	A7	5	88	20,23,24	1.00	2 (10%)	27,33,36	2.02	4 (14%)
88	P5P	A7	41	88	20,23,24	1.04	3 (15%)	27,33,36	1.94	5 (18%)
88	P5P	A6	15	88	20,23,24	1.08	3 (15%)	27,33,36	2.02	5 (18%)
88	P5P	A6	18	88	20,23,24	1.03	3 (15%)	27,33,36	1.97	4 (14%)
88	P5P	A6	48	88	20,23,24	1.02	3 (15%)	27,33,36	2.04	5 (18%)
87	Y5P	A5	1	87	14,19,20	4.80	2 (14%)	18,26,29	1.85	3 (16%)
88	Y5P	A6	66	88	14,19,20	4.54	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A7	51	88	14,19,20	4.36	2 (14%)	18,26,29	1.43	3 (16%)
88	P5P	A7	43	88	20,23,24	1.11	2 (10%)	27,33,36	2.08	4 (14%)
88	P5P	A6	14	88	20,23,24	1.00	2 (10%)	27,33,36	1.99	3 (11%)
88	Y5P	A7	44	88	14,19,20	4.69	2 (14%)	18,26,29	1.45	2 (11%)
88	Y5P	A7	9	88	14,19,20	4.67	2 (14%)	18,26,29	1.78	3 (16%)
88	P5P	A6	49	88	20,23,24	1.01	3 (15%)	27,33,36	2.09	5 (18%)
88	Y5P	A7	69	88	14,19,20	4.66	2 (14%)	18,26,29	1.46	3 (16%)
88	P5P	A6	26	88	20,23,24	1.00	3 (15%)	27,33,36	2.07	5 (18%)
88	Y5P	A7	37	88	14,19,20	4.37	2 (14%)	18,26,29	1.41	3 (16%)
88	Y5P	A6	55	88	14,19,20	4.52	2 (14%)	18,26,29	1.52	3 (16%)
88	Y5P	A7	17	88	14,19,20	4.61	2 (14%)	18,26,29	1.42	2 (11%)
88	Y5P	A6	36	88	14,19,20	4.42	2 (14%)	18,26,29	1.36	3 (16%)
87	P5P	A5	6	87	20,23,24	1.05	3 (15%)	27,33,36	2.04	5 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	Y5P	A6	69	88	14,19,20	4.64	2 (14%)	18,26,29	1.96	6 (33%)
88	P5P	A7	10	88	20,23,24	0.99	2 (10%)	27,33,36	1.97	4 (14%)
88	P5P	A7	4	88	20,23,24	1.07	3 (15%)	27,33,36	2.13	4 (14%)
88	Y5P	A6	37	88	14,19,20	4.37	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	46	88	14,19,20	4.49	2 (14%)	18,26,29	1.46	3 (16%)
88	P5P	A6	20	88	20,23,24	1.00	3 (15%)	27,33,36	1.96	5 (18%)
88	P5P	A6	41	88	20,23,24	1.02	2 (10%)	27,33,36	1.95	4 (14%)
88	Y5P	A6	3	88	14,19,20	4.43	2 (14%)	18,26,29	1.50	3 (16%)
88	P5P	A7	11	88	20,23,24	0.99	3 (15%)	27,33,36	2.10	5 (18%)
88	P5P	A6	4	88	20,23,24	1.00	3 (15%)	27,33,36	1.95	5 (18%)
88	Y5P	A7	64	88	14,19,20	4.53	2 (14%)	18,26,29	1.34	2 (11%)
88	Y5P	A6	30	88	14,19,20	4.48	2 (14%)	18,26,29	1.47	3 (16%)
88	Y5P	A7	63	88	14,19,20	4.53	2 (14%)	18,26,29	1.49	3 (16%)
88	Y5P	A6	53	88	14,19,20	4.69	2 (14%)	18,26,29	1.50	4 (22%)
88	Y5P	A7	67	88	14,19,20	4.66	2 (14%)	18,26,29	1.61	3 (16%)
88	P5P	A6	52	88	20,23,24	1.14	3 (15%)	27,33,36	1.98	5 (18%)
88	Y5P	A6	63	88	14,19,20	4.62	2 (14%)	18,26,29	1.52	3 (16%)
88	P5P	A7	19	88	20,23,24	1.03	3 (15%)	27,33,36	2.14	5 (18%)
88	Y5P	A6	22	88	14,19,20	4.29	2 (14%)	18,26,29	1.40	3 (16%)
88	P5P	A7	52	88	20,23,24	1.13	3 (15%)	27,33,36	1.98	5 (18%)
88	P5P	A7	14	88	20,23,24	1.01	2 (10%)	27,33,36	1.99	3 (11%)
88	Y5P	A6	67	88	14,19,20	4.68	2 (14%)	18,26,29	1.52	3 (16%)
88	P5P	A7	7	88	20,23,24	0.98	2 (10%)	27,33,36	2.07	4 (14%)
88	Y5P	A6	8	88	14,19,20	4.63	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	12	88	14,19,20	4.33	2 (14%)	18,26,29	1.40	3 (16%)
88	P5P	A6	42	88	20,23,24	0.98	2 (10%)	27,33,36	2.00	4 (14%)
88	P5P	A7	39	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
87	P5P	A5	2	87	20,23,24	1.10	2 (10%)	27,33,36	1.98	4 (14%)
88	Y5P	A6	21	88	14,19,20	4.38	2 (14%)	18,26,29	1.38	3 (16%)
88	Y5P	A7	8	88	14,19,20	4.65	2 (14%)	18,26,29	1.41	3 (16%)
88	Y5P	A6	58	88	14,19,20	4.55	2 (14%)	18,26,29	1.41	3 (16%)
88	P5P	A7	48	88	20,23,24	1.02	3 (15%)	27,33,36	2.08	5 (18%)
88	Y5P	A7	25	88	14,19,20	4.31	2 (14%)	18,26,29	1.39	3 (16%)
88	Y5P	A7	50	88	14,19,20	4.54	2 (14%)	18,26,29	1.39	2 (11%)
88	Y5P	A6	64	88	14,19,20	4.52	2 (14%)	18,26,29	1.41	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	Y5P	A6	68	88	14,19,20	4.78	2 (14%)	18,26,29	1.71	4 (22%)
88	Y5P	A7	13	88	14,19,20	4.20	2 (14%)	18,26,29	1.28	2 (11%)
88	Y5P	A7	62	88	14,19,20	4.40	2 (14%)	18,26,29	1.49	3 (16%)
88	Y5P	A6	59	88	14,19,20	4.79	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A6	5	88	20,23,24	1.02	3 (15%)	27,33,36	1.96	4 (14%)
88	Y5P	A7	65	88	14,19,20	4.61	2 (14%)	18,26,29	1.46	3 (16%)
87	P5P	A5	9	87	20,23,24	1.00	3 (15%)	27,33,36	1.95	4 (14%)
88	Y5P	A7	53	88	14,19,20	4.66	2 (14%)	18,26,29	1.55	3 (16%)
87	Y5P	A5	10	87	14,19,20	4.49	2 (14%)	18,26,29	1.46	3 (16%)
88	P5P	A7	6	88	20,23,24	1.02	3 (15%)	27,33,36	2.11	5 (18%)
88	P5P	A6	40	88	20,23,24	1.02	3 (15%)	27,33,36	2.05	5 (18%)
87	Y5P	A5	3	87	14,19,20	4.49	2 (14%)	18,26,29	1.62	3 (16%)
88	Y5P	A7	57	88	14,19,20	4.46	2 (14%)	18,26,29	1.45	3 (16%)
88	P5P	A6	7	88	20,23,24	1.03	3 (15%)	27,33,36	1.96	4 (14%)
88	Y5P	A6	47	88	14,19,20	4.58	2 (14%)	18,26,29	1.51	3 (16%)
88	P5P	A7	71	88	20,23,24	0.99	3 (15%)	27,33,36	1.96	4 (14%)
88	Y5P	A7	61	88	14,19,20	4.46	2 (14%)	18,26,29	1.42	3 (16%)
87	Y5P	A5	8	87	14,19,20	4.64	2 (14%)	18,26,29	1.45	3 (16%)
88	Y5P	A6	9	88	14,19,20	4.66	2 (14%)	18,26,29	1.78	4 (22%)
88	P5P	A6	39	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
88	P5P	A7	18	88	20,23,24	1.00	3 (15%)	27,33,36	2.04	4 (14%)
88	Y5P	A7	70	88	14,19,20	4.51	2 (14%)	18,26,29	1.45	2 (11%)
88	P5P	A7	54	88	20,23,24	1.08	3 (15%)	27,33,36	1.94	3 (11%)
88	Y5P	A7	56	88	14,19,20	4.54	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A7	12	88	14,19,20	4.27	2 (14%)	18,26,29	1.39	3 (16%)
88	Y5P	A6	17	88	14,19,20	4.65	2 (14%)	18,26,29	1.42	2 (11%)
88	P5P	A7	1	88	20,20,24	0.99	2 (10%)	28,29,36	1.96	4 (14%)
88	P5P	A7	23	88	20,23,24	1.02	3 (15%)	27,33,36	1.92	4 (14%)
88	P5P	A7	2	88	20,23,24	1.03	2 (10%)	27,33,36	2.11	4 (14%)
88	P5P	A6	10	88	20,23,24	1.03	3 (15%)	27,33,36	1.98	4 (14%)
88	Y5P	A6	31	88	14,19,20	4.59	2 (14%)	18,26,29	1.45	3 (16%)
87	Y5P	A5	7	87	14,19,20	4.58	2 (14%)	18,26,29	1.43	3 (16%)
88	P5P	A7	15	88	20,23,24	1.06	3 (15%)	27,33,36	2.00	5 (18%)
88	P5P	A7	40	88	20,23,24	1.00	3 (15%)	27,33,36	2.05	5 (18%)
88	P5P	A6	34	88	20,23,24	0.98	3 (15%)	27,33,36	1.91	4 (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	4.47	2 (14%)	18,26,29	1.50	3 (16%)
88	Y5P	A7	66	88	14,19,20	4.58	2 (14%)	18,26,29	1.47	2 (11%)
88	Y5P	A6	29	88	14,19,20	4.37	2 (14%)	18,26,29	1.40	3 (16%)
88	P5P	A6	45	88	20,23,24	1.08	3 (15%)	27,33,36	2.03	4 (14%)
88	Y5P	A7	59	88	14,19,20	4.76	2 (14%)	18,26,29	1.46	3 (16%)
88	Y5P	A6	57	88	14,19,20	4.48	2 (14%)	18,26,29	1.42	3 (16%)
88	Y5P	A6	50	88	14,19,20	4.60	2 (14%)	18,26,29	1.38	2 (11%)
88	P5P	A7	49	88	20,23,24	1.01	3 (15%)	27,33,36	2.06	5 (18%)
88	P5P	A7	26	88	20,23,24	1.01	3 (15%)	27,33,36	2.07	5 (18%)
87	Y5P	A5	4	87	14,19,20	4.79	2 (14%)	18,26,29	1.82	3 (16%)
87	P5P	A5	5	87	20,23,24	1.07	3 (15%)	27,33,36	1.97	4 (14%)
88	Y5P	A6	33	88	14,19,20	4.41	2 (14%)	18,26,29	1.44	3 (16%)
88	P5P	A7	27	88	20,23,24	0.99	3 (15%)	27,33,36	2.07	4 (14%)
88	P5P	A7	45	88	20,23,24	1.05	3 (15%)	27,33,36	2.16	4 (14%)
88	P5P	A6	11	88	20,23,24	0.97	2 (10%)	27,33,36	2.09	4 (14%)
88	Y5P	A7	58	88	14,19,20	4.59	2 (14%)	18,26,29	1.48	3 (16%)
88	Y5P	A6	56	88	14,19,20	4.56	2 (14%)	18,26,29	1.45	3 (16%)
88	Y5P	A7	60	88	14,19,20	4.45	2 (14%)	18,26,29	1.56	2 (11%)
88	P5P	A6	6	88	20,23,24	1.04	3 (15%)	27,33,36	1.98	4 (14%)
88	Y5P	A7	68	88	14,19,20	4.72	2 (14%)	18,26,29	1.69	4 (22%)
88	P5P	A6	2	88	20,23,24	0.95	2 (10%)	27,33,36	1.96	4 (14%)
88	P5P	A6	27	88	20,23,24	0.99	2 (10%)	27,33,36	2.08	4 (14%)
88	Y5P	A7	46	88	14,19,20	4.51	2 (14%)	18,26,29	1.48	3 (16%)
87	P5P	A5	11	87	20,23,24	1.00	3 (15%)	27,33,36	1.97	5 (18%)
88	P5P	A6	16	88	20,23,24	1.11	3 (15%)	27,33,36	2.14	6 (22%)
88	Y5P	A6	60	88	14,19,20	4.51	2 (14%)	18,26,29	1.54	3 (16%)
88	Y5P	A7	3	88	14,19,20	4.38	2 (14%)	18,26,29	1.50	3 (16%)
88	P5P	A6	28	88	20,23,24	1.01	3 (15%)	27,33,36	2.09	4 (14%)
88	P5P	A6	54	88	20,23,24	1.07	3 (15%)	27,33,36	1.95	4 (14%)
88	P5P	A7	20	88	20,23,24	0.98	3 (15%)	27,33,36	2.01	5 (18%)
88	P5P	A6	19	88	20,23,24	0.99	2 (10%)	27,33,36	2.11	5 (18%)
88	P5P	A7	16	88	20,23,24	1.07	3 (15%)	27,33,36	2.14	6 (22%)
88	Y5P	A6	51	88	14,19,20	4.42	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	38	88	14,19,20	4.33	2 (14%)	18,26,29	1.41	3 (16%)
88	Y5P	A6	13	88	14,19,20	4.26	2 (14%)	18,26,29	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	Y5P	A6	35	88	14,19,20	4.40	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	62	88	14,19,20	4.57	2 (14%)	18,26,29	1.50	3 (16%)
88	Y5P	A7	47	88	14,19,20	4.59	2 (14%)	18,26,29	1.53	3 (16%)
88	Y5P	A7	22	88	14,19,20	4.29	2 (14%)	18,26,29	1.42	3 (16%)
88	Y5P	A7	38	88	14,19,20	4.36	2 (14%)	18,26,29	1.40	3 (16%)
88	Y5P	A6	44	88	14,19,20	4.68	2 (14%)	18,26,29	1.46	2 (11%)

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	A6	70	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	42	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	61	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	25	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	24	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	43	88	-	4/7/25/26	0/3/3/3
88	Y5P	A6	65	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	32	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	21	88	-	3/7/33/34	0/2/2/2
88	P5P	A6	1	88	-	0/6/22/26	0/3/3/3
88	Y5P	A6	24	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	23	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	71	32,88	-	1/7/25/26	0/3/3/3
88	P5P	A7	5	88	-	2/7/25/26	0/3/3/3
88	P5P	A7	41	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	15	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	18	88	-	1/7/25/26	0/3/3/3
88	P5P	A6	48	88	-	0/7/25/26	0/3/3/3
87	Y5P	A5	1	87	-	7/7/33/34	0/2/2/2
88	Y5P	A6	66	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	51	88	-	2/7/33/34	0/2/2/2
88	P5P	A7	43	88	-	5/7/25/26	0/3/3/3
88	P5P	A6	14	88	-	2/7/25/26	0/3/3/3
88	Y5P	A7	44	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	9	88	-	3/7/33/34	0/2/2/2
88	P5P	A6	49	88	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A7	69	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	26	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	37	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	55	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	17	88	-	2/7/33/34	0/2/2/2
88	Y5P	A6	36	88	-	1/7/33/34	0/2/2/2
87	P5P	A5	6	87	-	0/7/25/26	0/3/3/3
88	Y5P	A6	69	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	10	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	4	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	37	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	46	88	-	3/7/33/34	0/2/2/2
88	P5P	A6	20	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	41	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	3	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	11	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	4	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	64	88	-	3/7/33/34	0/2/2/2
88	Y5P	A6	30	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	63	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	53	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	67	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	52	88	-	6/7/25/26	0/3/3/3
88	Y5P	A6	63	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	19	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	22	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	52	88	-	6/7/25/26	0/3/3/3
88	P5P	A7	14	88	-	2/7/25/26	0/3/3/3
88	Y5P	A6	67	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	7	88	-	3/7/25/26	0/3/3/3
88	Y5P	A6	8	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	12	88	-	3/7/33/34	0/2/2/2
88	P5P	A6	42	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	39	88	-	0/7/25/26	0/3/3/3
87	P5P	A5	2	87	-	2/7/25/26	0/3/3/3
88	Y5P	A6	21	88	-	3/7/33/34	0/2/2/2
88	Y5P	A7	8	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	58	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	48	88	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A7	25	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	50	88	-	4/7/33/34	0/2/2/2
88	Y5P	A6	64	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	68	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	13	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	62	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	59	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	5	88	-	2/7/25/26	0/3/3/3
88	Y5P	A7	65	88	-	2/7/33/34	0/2/2/2
87	P5P	A5	9	87	-	0/7/25/26	0/3/3/3
88	Y5P	A7	53	88	-	4/7/33/34	0/2/2/2
87	Y5P	A5	10	87	-	1/7/33/34	0/2/2/2
88	P5P	A7	6	88	-	4/7/25/26	0/3/3/3
88	P5P	A6	40	88	-	0/7/25/26	0/3/3/3
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	A6	7	88	-	3/7/25/26	0/3/3/3
88	Y5P	A6	47	88	-	1/7/33/34	0/2/2/2
88	P5P	A7	71	88	-	1/7/25/26	0/3/3/3
88	Y5P	A7	61	88	-	1/7/33/34	0/2/2/2
87	Y5P	A5	8	87	-	3/7/33/34	0/2/2/2
88	Y5P	A6	9	88	-	5/7/33/34	0/2/2/2
88	P5P	A6	39	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	18	88	-	1/7/25/26	0/3/3/3
88	Y5P	A7	70	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	54	88	-	1/7/25/26	0/3/3/3
88	Y5P	A7	56	88	-	4/7/33/34	0/2/2/2
88	Y5P	A7	12	88	-	3/7/33/34	0/2/2/2
88	Y5P	A6	17	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	1	88	-	0/6/22/26	0/3/3/3
88	P5P	A7	23	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	2	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	10	88	-	0/7/25/26	0/3/3/3
88	Y5P	A6	31	88	-	1/7/33/34	0/2/2/2
87	Y5P	A5	7	87	-	3/7/33/34	0/2/2/2
88	P5P	A7	15	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	40	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	34	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	55	88	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A7	66	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	29	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	45	88	-	2/7/25/26	0/3/3/3
88	Y5P	A7	59	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	57	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	50	88	-	4/7/33/34	0/2/2/2
88	P5P	A7	49	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	26	88	-	0/7/25/26	0/3/3/3
87	Y5P	A5	4	87	-	7/7/33/34	0/2/2/2
87	P5P	A5	5	87	-	2/7/25/26	0/3/3/3
88	Y5P	A6	33	88	-	3/7/33/34	0/2/2/2
88	P5P	A7	27	88	-	1/7/25/26	0/3/3/3
88	P5P	A7	45	88	-	2/7/25/26	0/3/3/3
88	P5P	A6	11	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	58	88	-	3/7/33/34	0/2/2/2
88	Y5P	A6	56	88	-	4/7/33/34	0/2/2/2
88	Y5P	A7	60	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	6	88	-	3/7/25/26	0/3/3/3
88	Y5P	A7	68	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	2	88	-	1/7/25/26	0/3/3/3
88	P5P	A6	27	88	-	0/7/25/26	0/3/3/3
88	Y5P	A7	46	88	-	3/7/33/34	0/2/2/2
87	P5P	A5	11	87	-	0/7/25/26	0/3/3/3
88	P5P	A6	16	88	-	2/7/25/26	0/3/3/3
88	Y5P	A6	60	88	-	2/7/33/34	0/2/2/2
88	Y5P	A7	3	88	-	1/7/33/34	0/2/2/2
88	P5P	A6	28	88	-	2/7/25/26	0/3/3/3
88	P5P	A6	54	88	-	1/7/25/26	0/3/3/3
88	P5P	A7	20	88	-	0/7/25/26	0/3/3/3
88	P5P	A6	19	88	-	0/7/25/26	0/3/3/3
88	P5P	A7	16	88	-	2/7/25/26	0/3/3/3
88	Y5P	A6	51	88	-	2/7/33/34	0/2/2/2
88	Y5P	A6	38	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	13	88	-	3/7/33/34	0/2/2/2
88	Y5P	A6	35	88	-	1/7/33/34	0/2/2/2
88	Y5P	A6	62	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	47	88	-	1/7/33/34	0/2/2/2
88	Y5P	A7	22	88	-	3/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	Y5P	A7	38	88	-	2/7/33/34	0/2/2/2
88	Y5P	A6	44	88	-	2/7/33/34	0/2/2/2

The worst 5 of 336 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A6	69	Y5P	C4-N3	-14.56	1.32	1.46
88	A6	53	Y5P	C4-N3	-13.91	1.33	1.46
88	A6	8	Y5P	C4-N3	-13.70	1.33	1.46
88	A7	53	Y5P	C4-N3	-13.56	1.33	1.46
88	A7	67	Y5P	C4-N3	-13.50	1.33	1.46

The worst 5 of 513 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	A7	45	P5P	C6-N1-C2	8.85	126.25	115.80
88	A6	27	P5P	C6-N1-C2	8.68	126.05	115.80
88	A6	28	P5P	C6-N1-C2	8.65	126.01	115.80
88	A7	27	P5P	C6-N1-C2	8.63	125.98	115.80
88	A7	11	P5P	C6-N1-C2	8.61	125.97	115.80

There are no chirality outliers.

5 of 230 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.

45 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A6	70	Y5P	12	0
88	A6	61	Y5P	1	0
88	A6	25	Y5P	2	0
88	A7	24	Y5P	1	0
88	A7	21	Y5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	A6	24	Y5P	1	0
88	A6	71	P5P	1	0
87	A5	1	Y5P	2	0
88	A6	36	Y5P	13	0
88	A6	69	Y5P	23	0
88	A6	20	P5P	1	0
88	A7	64	Y5P	3	0
88	A7	63	Y5P	1	0
88	A6	63	Y5P	1	0
88	A6	22	Y5P	1	0
88	A6	12	Y5P	1	0
87	A5	2	P5P	7	0
88	A6	21	Y5P	2	0
88	A7	48	P5P	1	0
88	A7	25	Y5P	1	0
88	A6	68	Y5P	4	0
88	A7	13	Y5P	1	0
88	A7	62	Y5P	1	0
88	A7	65	Y5P	2	0
87	A5	3	Y5P	6	0
88	A7	57	Y5P	1	0
88	A7	71	P5P	27	0
88	A7	61	Y5P	1	0
87	A5	8	Y5P	1	0
88	A7	70	Y5P	1	0
88	A7	12	Y5P	1	0
88	A6	31	Y5P	5	0
87	A5	7	Y5P	1	0
88	A6	34	P5P	4	0
88	A7	59	Y5P	1	0
87	A5	4	Y5P	6	0
88	A7	58	Y5P	1	0
88	A7	60	Y5P	1	0
88	A6	27	P5P	2	0
87	A5	11	P5P	6	0
88	A7	20	P5P	1	0
88	A6	35	Y5P	9	0
88	A6	62	Y5P	2	0
88	A7	47	Y5P	1	0
88	A7	22	Y5P	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 139 ligands modelled in this entry, 137 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
91	GDP	AX	500	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
92	GCP	v	802	89	32,34,34	1.67	6 (18%)	49,54,54	1.87	10 (20%)

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
91	GDP	AX	500	-	-	1/16/32/32	0/3/3/3
92	GCP	v	802	89	-	5/19/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	v	802	GCP	PG-O1G	5.57	1.61	1.50
91	AX	500	GDP	C5-C4	3.18	1.47	1.38
92	v	802	GCP	C5-C4	3.05	1.47	1.38
92	v	802	GCP	PG-O3G	3.04	1.61	1.55
92	v	802	GCP	PG-O2G	-2.64	1.49	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	AX	500	GDP	C5-C4-N3	-6.32	118.32	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	v	802	GCP	PB-O3A-PA	-5.90	113.11	132.37
91	AX	500	GDP	C2-N3-C4	5.20	121.25	112.30
92	v	802	GCP	C2-N3-C4	4.83	120.62	112.30
92	v	802	GCP	C5-C4-N3	-4.69	120.92	128.39

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

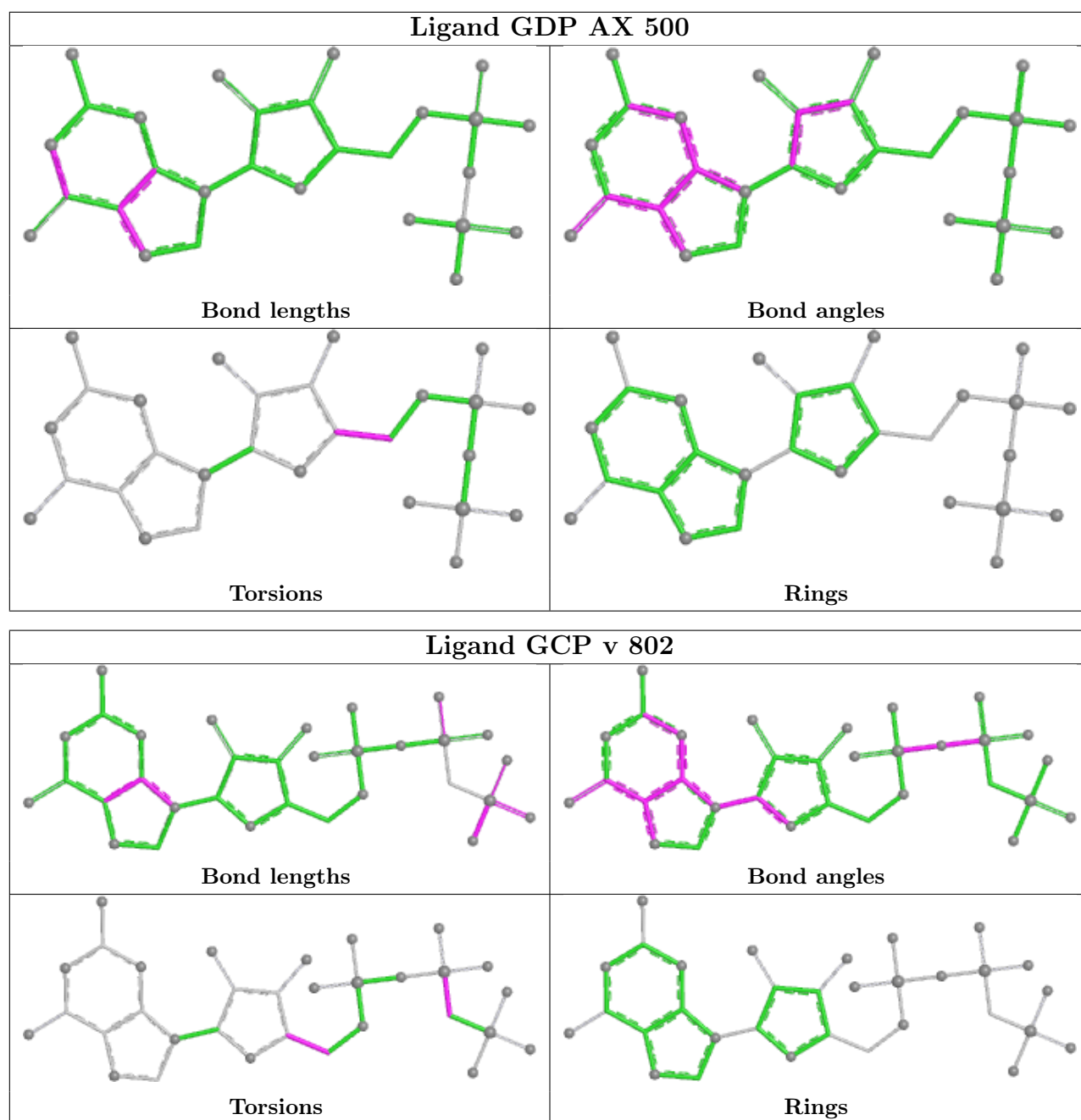
Mol	Chain	Res	Type	Atoms
92	v	802	GCP	PG-C3B-PB-O1B
92	v	802	GCP	PG-C3B-PB-O3A
92	v	802	GCP	O4'-C4'-C5'-O5'
92	v	802	GCP	C3'-C4'-C5'-O5'
92	v	802	GCP	PG-C3B-PB-O2B

There are no ring outliers.

2 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	AX	500	GDP	3	0
92	v	802	GCP	44	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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Mol	Chain	Number of breaks
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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	30.88
1	u	315:UNK	C	399:UNK	N	19.09
1	u	615:UNK	C	700:UNK	N	18.25

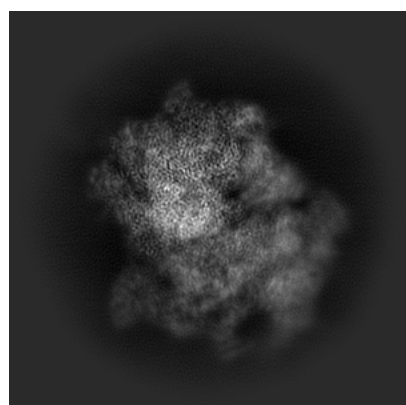
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21242. These allow visual inspection of the internal detail of the map and identification of artifacts.

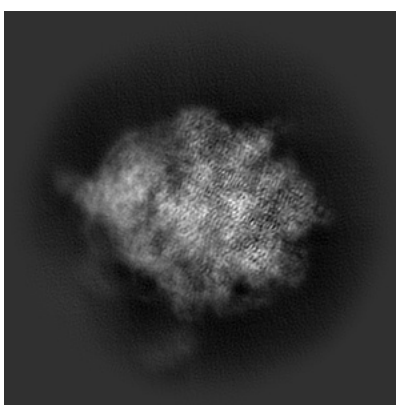
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

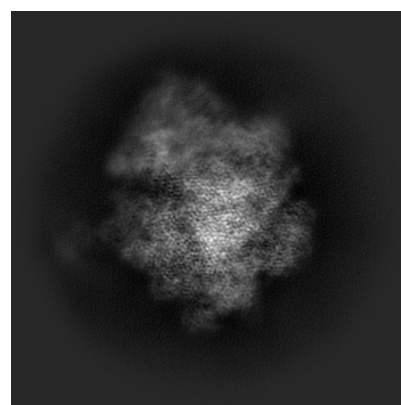
6.1.1 Primary map



X



Y

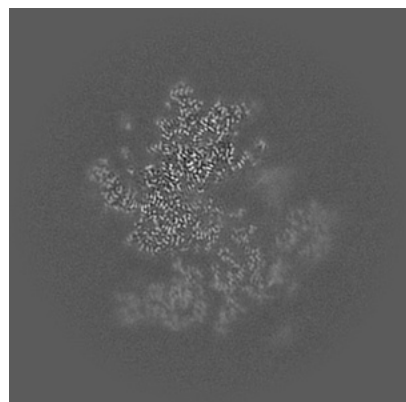


Z

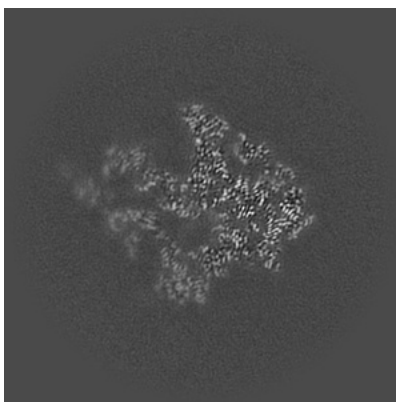
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

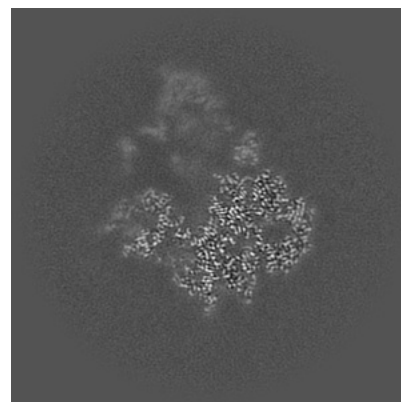
6.2.1 Primary map



X Index: 200



Y Index: 200

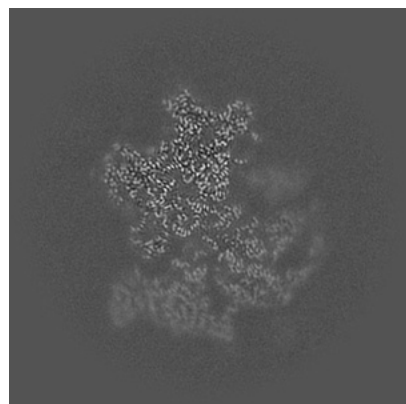


Z Index: 200

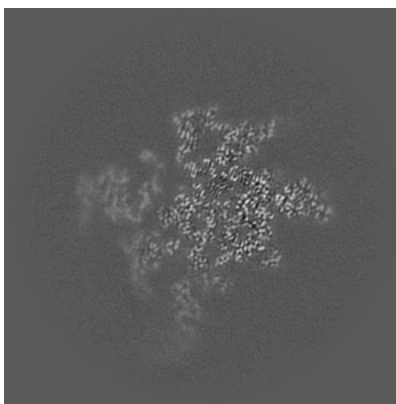
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

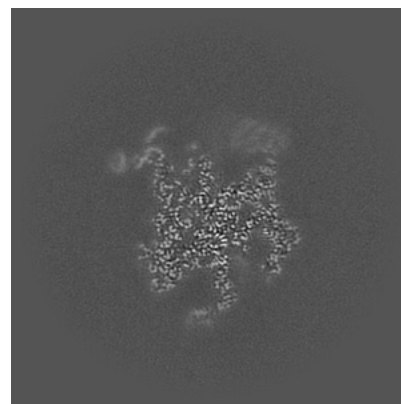
6.3.1 Primary map



X Index: 210



Y Index: 172

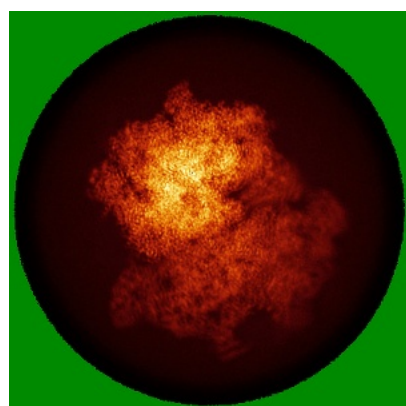


Z Index: 242

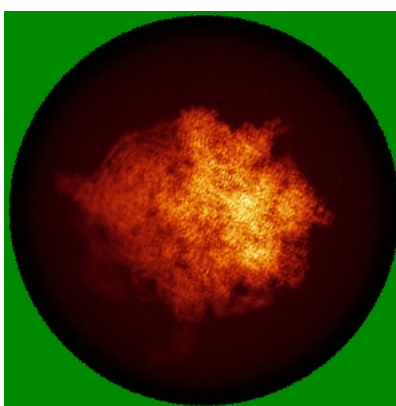
The images above show the largest variance slices of the map in three orthogonal directions.

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

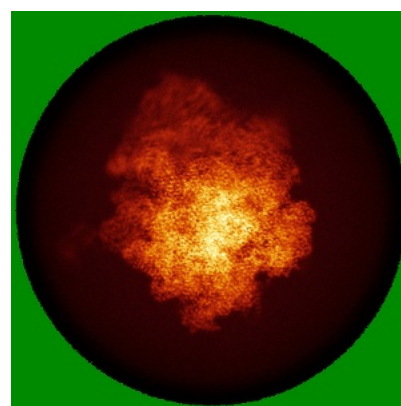
6.4.1 Primary map



X



Y

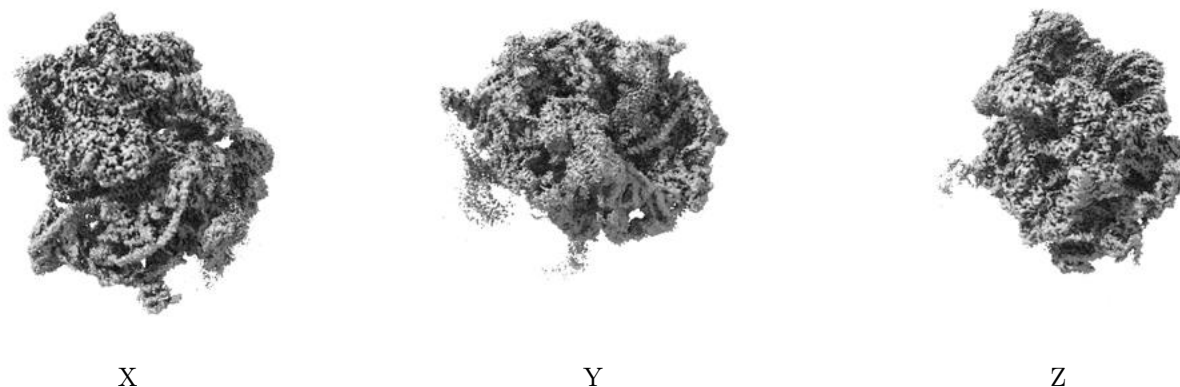


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

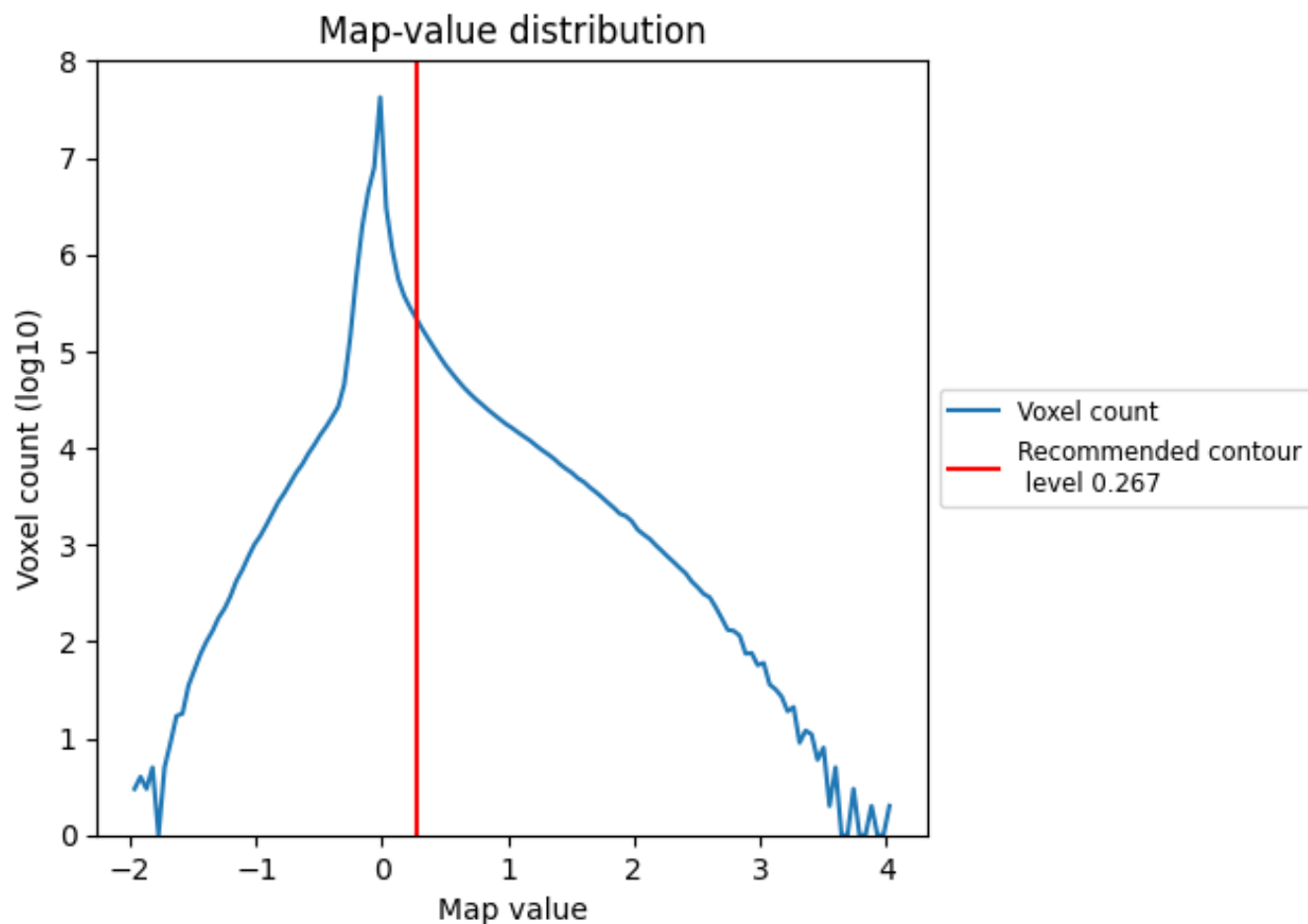
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

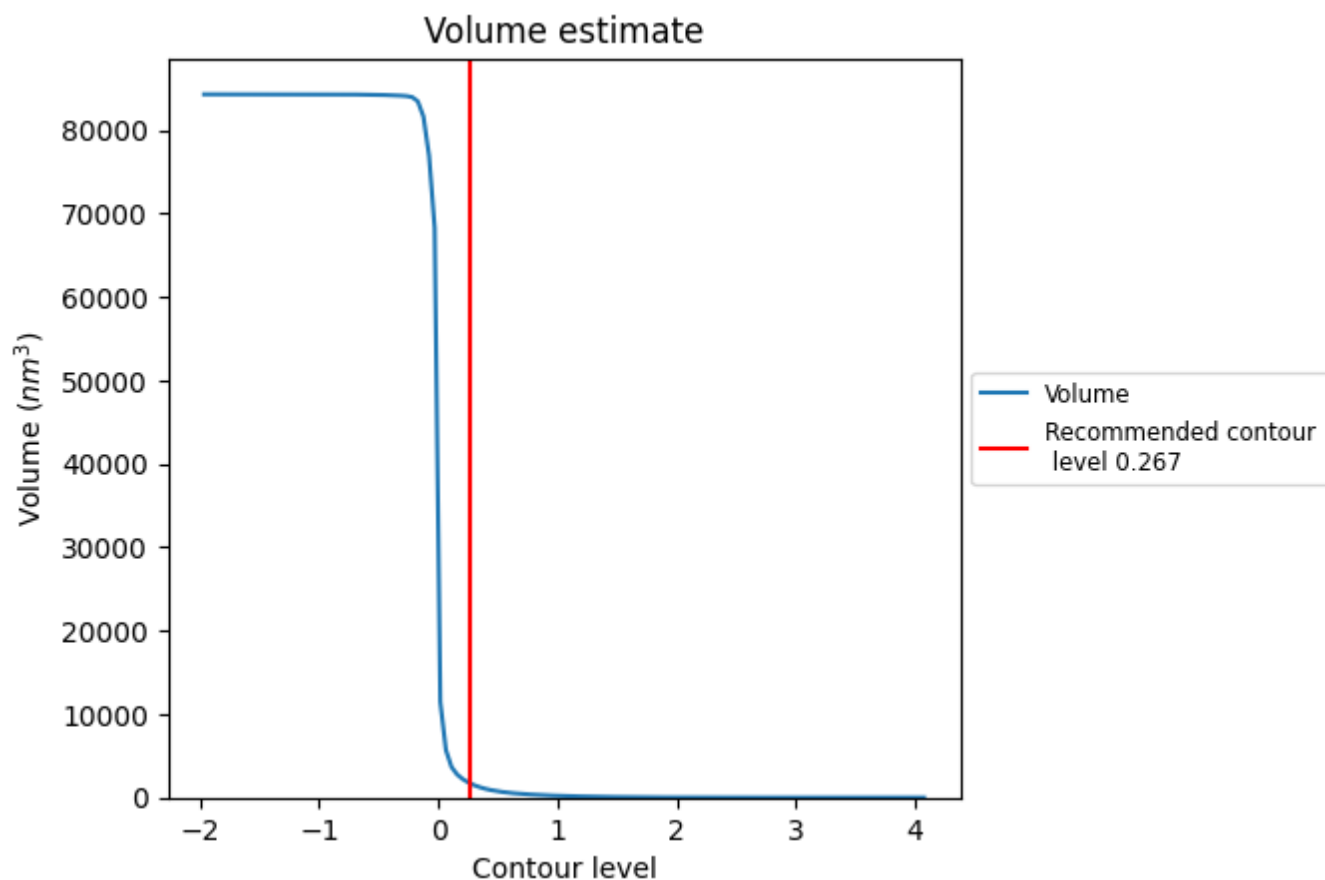
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

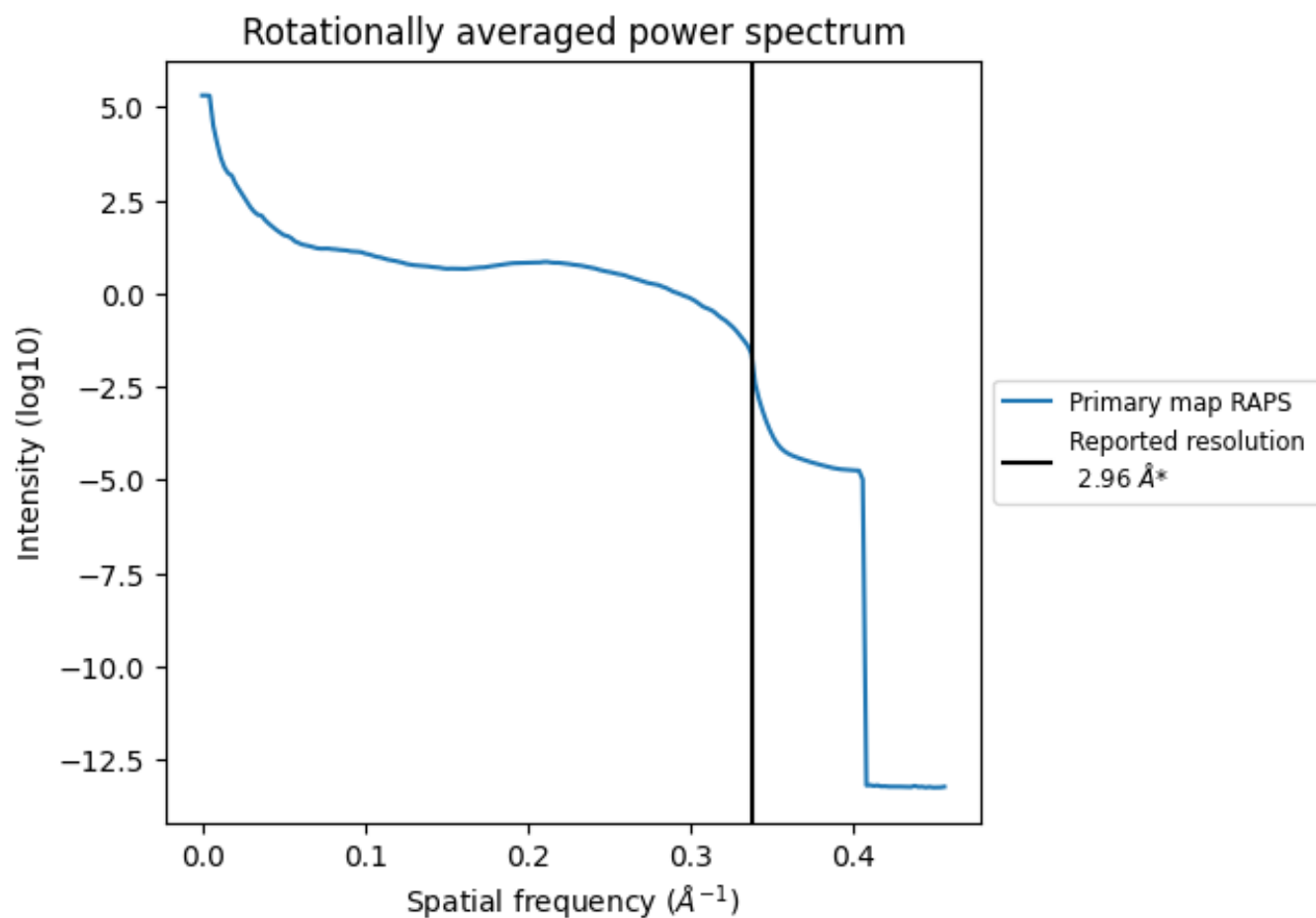
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1709 nm^3 ; this corresponds to an approximate mass of 1544 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8 Fourier-Shell correlation

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

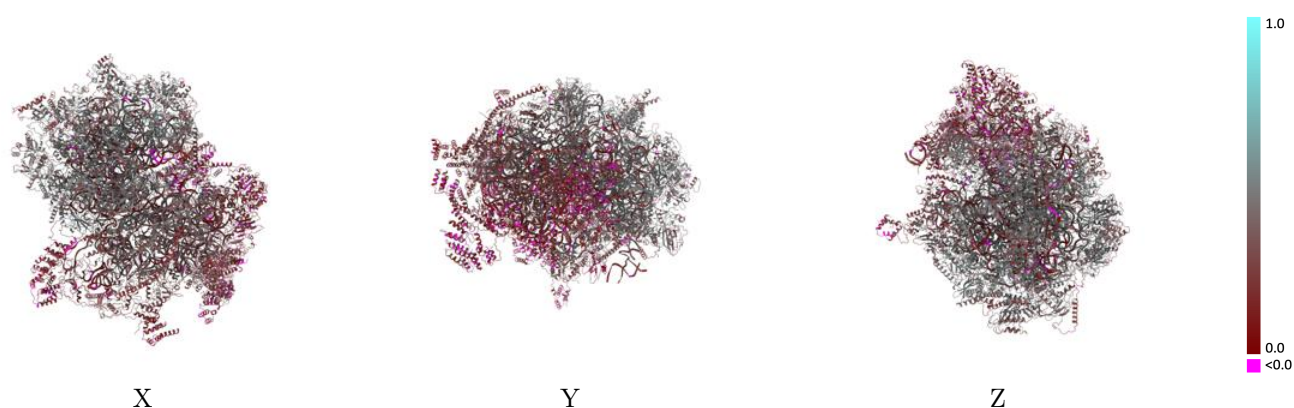
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21242 and PDB model 6VMI. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)

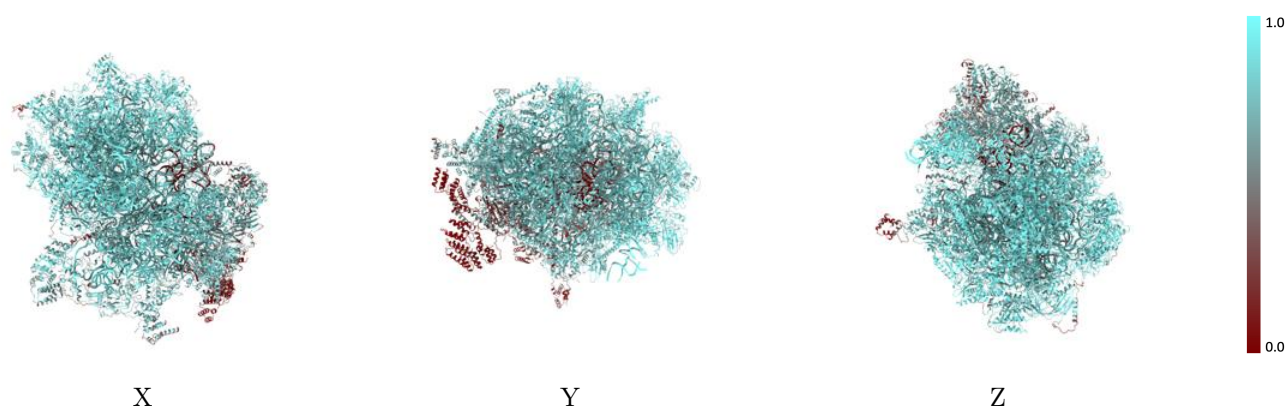
This section was not generated.

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



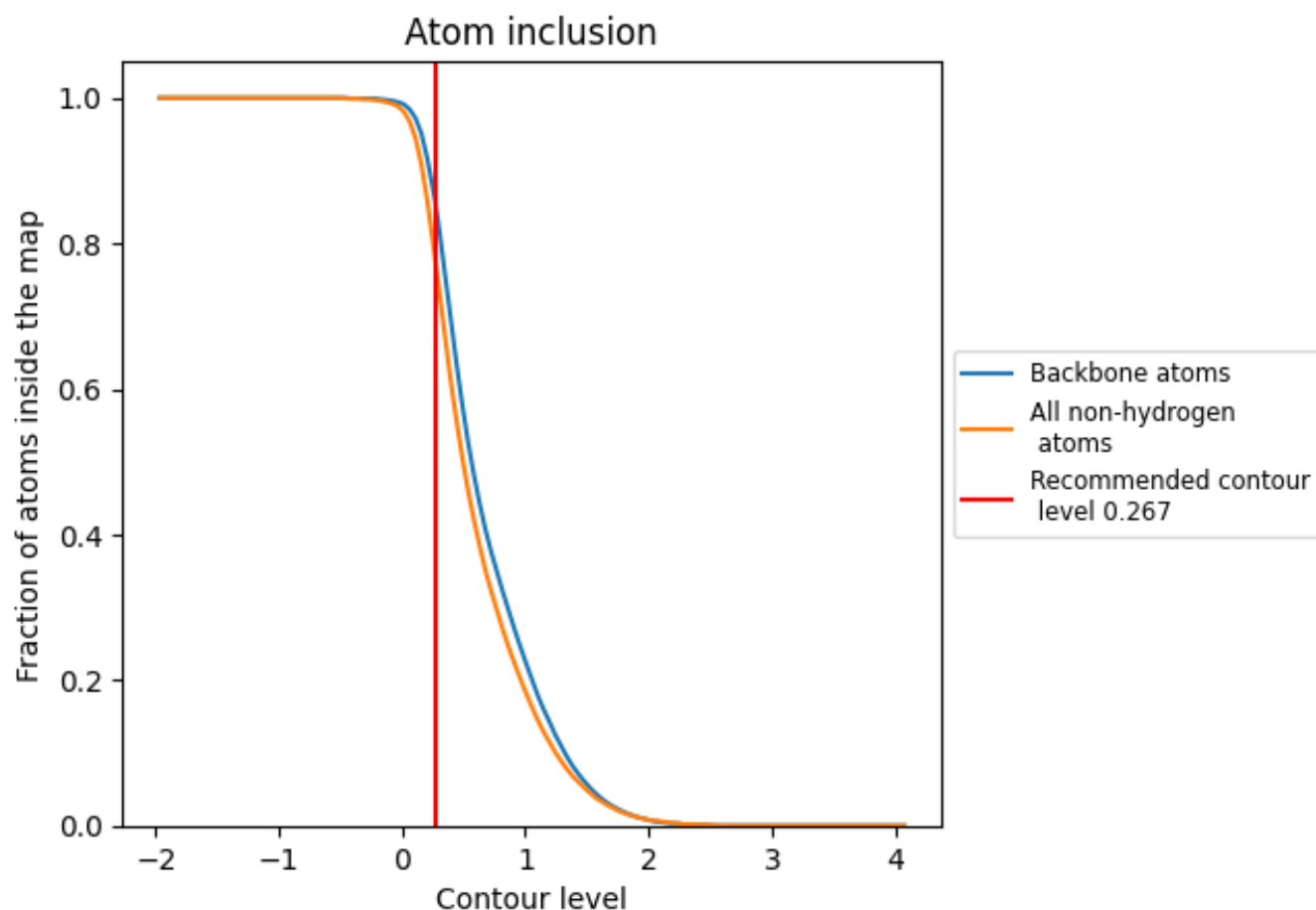
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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	 0.7820	 0.3390
0	 0.8790	 0.4430
1	 0.8550	 0.4410
2	 0.9060	 0.4680
3	 0.9010	 0.5010
4	 0.8990	 0.4740
5	 0.8980	 0.4400
6	 0.8850	 0.4090
7	 0.8660	 0.4100
8	 0.7540	 0.2460
9	 0.8800	 0.4210
A	 0.8460	 0.3360
A0	 0.7340	 0.2560
A1	 0.5090	 0.1810
A2	 0.6550	 0.3320
A3	 0.8090	 0.4300
A4	 0.1430	 0.1650
A5	 0.0470	 0.0780
A6	 0.0270	 0.0710
A7	 0.3890	 0.1280
AA	 0.8650	 0.2980
AB	 0.7760	 0.3190
AC	 0.5070	 0.1970
AD	 0.6200	 0.3110
AE	 0.7640	 0.3890
AF	 0.6420	 0.2680
AG	 0.6450	 0.2300
AH	 0.5830	 0.2180
AI	 0.8290	 0.4060
AJ	 0.7630	 0.3750
AK	 0.5980	 0.1710
AL	 0.7890	 0.3790
AM	 0.7740	 0.2970
AN	 0.8510	 0.4030
AO	 0.7700	 0.2930



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Chain	Atom inclusion	Q-score
AP	 0.7740	 0.3830
AQ	 0.8310	 0.4000
AR	 0.6720	 0.2350
AS	 0.7050	 0.2830
AT	 0.8030	 0.3480
AU	 0.7520	 0.2540
AV	 0.6780	 0.1770
AW	 0.7610	 0.3350
AX	 0.6230	 0.1760
AY	 0.4180	 0.1470
AZ	 0.4910	 0.1800
B	 0.9460	 0.2990
D	 0.8780	 0.4520
E	 0.8940	 0.4620
F	 0.8950	 0.4560
H	 0.8530	 0.4040
I	 0.7190	 0.3300
J	 0.7350	 0.2970
K	 0.9040	 0.4710
L	 0.8610	 0.4600
M	 0.8910	 0.4540
N	 0.8760	 0.4560
O	 0.8870	 0.4420
P	 0.9120	 0.4350
Q	 0.8490	 0.4350
R	 0.8930	 0.4580
S	 0.9030	 0.4520
T	 0.8850	 0.4580
TA	 0.1570	 0.1180
TB	 0.1830	 0.1980
TC	 0.0740	 0.1600
U	 0.8740	 0.4430
V	 0.8570	 0.4170
W	 0.8790	 0.4580
X	 0.8860	 0.4460
Y	 0.8940	 0.4480
Z	 0.8880	 0.4580
a	 0.7940	 0.3920
b	 0.8970	 0.4720
c	 0.8700	 0.4230
d	 0.7510	 0.3760
e	 0.7240	 0.2060

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Chain	Atom inclusion	Q-score
f	 0.7180	 0.3210
g	 0.8820	 0.4300
h	 0.8410	 0.3600
i	 0.9070	 0.4580
j	 0.8450	 0.4020
k	 0.8040	 0.3520
l	 0.7710	 0.3130
m	 0.8020	 0.2930
o	 0.8560	 0.4260
p	 0.8200	 0.3850
q	 0.7930	 0.3470
r	 0.8850	 0.4230
s	 0.8910	 0.4470
u	 0.5290	 0.1420
v	 0.6750	 0.3110