



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2024 – 05:00 pm GMT

PDB ID : 7OG4  
EMDB ID : EMD-12877  
Title : Human mitochondrial ribosome in complex with P/E-tRNA  
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.  
Deposited on : 2021-05-06  
Resolution : 3.80 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](mailto: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>.

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

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

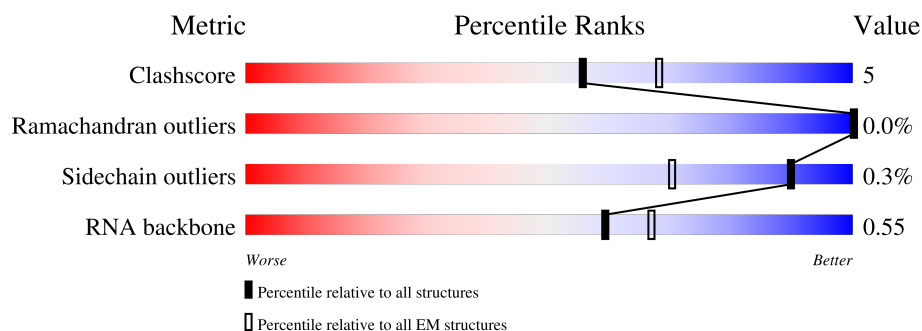
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	0	188	52% 6% 43%
2	1	65	68% 14% 18%
3	2	92	46% 50%
4	3	188	44% 7% 49%
5	4	103	29% 8% 63%
6	5	423	81% 11% 7%
7	6	380	80% 13% 7%

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Mol	Chain	Length	Quality of chain
8	7	338	
9	8	206	
10	9	137	
11	XA	1561	
12	A0	218	
13	A1	323	
14	A2	118	
15	A3	199	
16	A4	689	
17	AA	954	
18	AB	296	
19	AC	167	
20	AD	430	
21	AE	125	
22	AF	242	
23	AG	396	
24	AH	201	
25	AI	194	
26	AJ	138	
27	AK	128	
28	AL	257	
29	AM	137	
30	AN	130	
31	AO	258	
32	AP	142	

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Mol	Chain	Length	Quality of chain
33	AQ	87	
34	AR	360	
35	AS	190	
36	AT	173	
37	AU	205	
38	AV	414	
39	AW	187	
40	AX	398	
41	AY	395	
42	AZ	106	
43	XB	72	
44	XD	305	
45	XE	348	
46	XF	311	
47	XH	267	
48	XI	261	
49	XJ	192	
50	XK	178	
51	XL	145	
52	XM	296	
53	XN	251	
54	XO	175	
55	XP	180	
56	XQ	292	
57	XR	149	

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Mol	Chain	Length	Quality of chain
58	XS	205	
59	XT	206	
60	XU	153	
61	XV	216	
62	XW	148	
63	XX	256	
64	XY	250	
65	XZ	161	
66	a	142	
67	b	215	
68	c	332	
69	d	306	
70	e	279	
71	f	212	
72	g	166	
73	h	158	
74	i	128	
75	j	123	
76	k	112	
77	l	138	
78	m	128	
79	o	102	
80	p	206	
81	q	222	
82	r	196	

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Mol	Chain	Length	Quality of chain
83	r3	75	<div><div></div><div>93%</div><div></div><div>100%</div></div>
84	s	439	<div><div></div><div>84%</div><div>16%</div></div>
85	t1	198	<div><div></div><div>18%</div><div>23%</div><div></div><div>77%</div></div>
85	t2	198	<div><div></div><div>12%</div><div>15%</div><div></div><div>85%</div></div>
85	t3	198	<div><div></div><div>15%</div><div>15%</div><div></div><div>85%</div></div>
85	t4	198	<div><div></div><div>15%</div><div>15%</div><div></div><div>85%</div></div>
85	t5	198	<div><div></div><div>15%</div><div>15%</div><div></div><div>85%</div></div>
85	t6	198	<div><div></div><div>14%</div><div>14%</div><div></div><div>86%</div></div>

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 311905 atoms, of which 143004 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	108	Total	C	H	N	O	S	0	0
			1783	545	903	172	157	6		

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	53	Total	C	H	N	O	S	0	0
			919	281	480	84	72	2		

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	46	Total	C	H	N	O	S	0	0
			782	233	406	83	59	1		

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	95	Total	C	H	N	O	S	0	0
			1714	539	883	162	127	3		

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	38	Total	C	H	N	O	S	0	0
			702	217	361	72	48	4		

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	393	Total	C	H	N	O	S	0	0
			6404	2070	3200	559	564	11		

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	354	Total	C	H	N	O	S	0	0
			5786	1881	2839	525	532	9		

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	291	Total	C	H	N	O	S	0	0
			4738	1514	2373	401	432	18		

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	134	Total	C	H	N	O	S	0	0
			2301	724	1166	201	208	2		

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	9	124	Total	C	H	N	O	S	0	0
			1983	644	987	170	180	2		

- Molecule 11 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	XA	1498	Total	C	H	N	O	P	0	0
			47973	14274	16160	5751	10290	1498		

- Molecule 12 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	A0	201	Total	C	H	N	O	S	0	0
			3369	1065	1685	322	292	5		

- Molecule 13 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	A1	275	Total	C	H	N	O	S	0	0
			4491	1414	2261	380	425	11		

- Molecule 14 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.



Mol	Chain	Residues	Atoms						AltConf	Trace
14	A2	116	Total	C	H	N	O	S	0	0
			1889	574	964	181	162	8		

- Molecule 15 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	A3	69	Total	C	H	N	O	S	0	0
			1292	393	682	130	86	1		

- Molecule 16 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	A4	552	Total	C	H	N	O	S	0	0
			8955	2866	4485	756	820	28		

- Molecule 17 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AA	924	Total	C	H	N	O	P	0	0
			29598	8800	9970	3540	6364	924		

- Molecule 18 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AB	218	Total	C	H	N	O	S	0	0
			3545	1135	1769	322	309	10		

- Molecule 19 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AC	132	Total	C	H	N	O	S	0	0
			2170	699	1088	195	184	4		

- Molecule 20 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AD	343	Total	C	H	N	O	S	0	0
			5501	1706	2785	515	482	13		

- Molecule 21 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 22 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AF	201	Total	C	H	N	O	S	0	0
			3382	1069	1714	305	283	11		

- Molecule 23 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AG	304	Total	C	H	N	O	S	0	0
			4997	1593	2492	444	454	14		

- Molecule 24 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AH	135	Total	C	H	N	O	S	0	0
			2241	712	1136	187	203	3		

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AI	136	Total	C	H	N	O	S	0	0
			2063	637	1052	192	178	4		

- Molecule 26 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AJ	108	Total	C	H	N	O	S	0	0
			1725	521	887	169	142	6		

- Molecule 27 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	AK	101	Total	C	H	N	O	S	0	0
			1746	537	885	179	140	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AL	164	Total	C	H	N	O	S	0	0
			2854	883	1472	257	235	7		

- Molecule 29 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AM	116	Total	C	H	N	O	S	0	0
			1871	582	951	182	150	6		

- Molecule 30 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AN	107	Total	C	H	N	O	S	0	0
			1754	549	908	153	141	3		

- Molecule 31 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AO	185	Total	C	H	N	O	S	0	0
			3018	970	1490	285	267	6		

- Molecule 32 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	AP	95	Total	C	H	N	O	S	0	0
			1561	493	796	132	132	8		

- Molecule 33 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	AQ	85	Total	C	H	N	O	S	0	0
			1483	455	749	149	123	7		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 34 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	AR	250	Total	C	H	N	O	S	0	0
			4134	1314	2074	353	385	8		

- Molecule 35 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	AS	133	Total	C	H	N	O	S	0	0
			2203	709	1103	196	194	1		

- Molecule 36 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	AT	162	Total	C	H	N	O	S	0	0
			2672	850	1342	231	238	11		

- Molecule 37 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	AU	173	Total	C	H	N	O	S	0	0
			2932	900	1471	294	263	4		

- Molecule 38 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	AV	349	Total	C	H	N	O	S	0	0
			5730	1841	2863	478	536	12		

- Molecule 39 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	AW	97	Total	C	H	N	O	S	0	0
			1551	486	785	137	139	4		

- Molecule 40 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	AX	348	Total	C	H	N	O	S	0	0
			5619	1802	2805	491	510	11		

- Molecule 41 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	AY	113	Total	C	H	N	O	S	0	0
			1867	621	911	157	176	2		

- Molecule 42 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	AZ	86	Total	C	H	N	O	S	0	0
			1465	467	734	131	129	4		

- Molecule 43 is a RNA chain called mitochondrial tRNA<sup>Val</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	XB	59	Total	C	H	N	O	P	0	0
			1895	563	640	227	406	59		

- Molecule 44 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	XD	236	Total	C	H	N	O	S	0	0
			3738	1145	1896	373	315	9		

- Molecule 45 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	XE	304	Total	C	H	N	O	S	0	0
			4798	1539	2402	416	430	11		

- Molecule 46 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	XF	250	Total	C	H	N	O	S	0	0
			4058	1294	2045	365	348	6		

- Molecule 47 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	XH	95	Total	C	H	N	O		0	0
			1616	498	832	152	134			

- Molecule 48 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	XI	211	Total	C	H	N	O	S	0	0
			3474	1086	1783	303	291	11		

- Molecule 49 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	XJ	170	Total	C	H	N	O	S	0	0
			2658	825	1367	230	234	2		

- Molecule 50 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	XK	177	Total	C	H	N	O	S	0	0
			2899	934	1448	259	251	7		

- Molecule 51 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	XL	115	Total	C	H	N	O	S	0	0
			1830	559	941	171	154	5		

- Molecule 52 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	XM	287	Total	C	H	N	O	S	0	0
			4683	1472	2378	425	402	6		

- Molecule 53 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	XN	221	Total	C	H	N	O	S	0	0
			3586	1138	1808	325	305	10		

- Molecule 54 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	XO	152	Total	C	H	N	O	S	0	0
			2528	784	1283	239	215	7		

- Molecule 55 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	XP	143	Total	C	H	N	O	S	
			2326	729	1162	223	207	5	
								0	0

- Molecule 56 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	XQ	238	Total	C	H	N	O	S	
			4000	1268	2022	352	349	9	
								0	0

- Molecule 57 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	XR	140	Total	C	H	N	O	S	
			2367	732	1214	231	186	4	
								0	0

- Molecule 58 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	XS	160	Total	C	H	N	O	S	
			2638	829	1354	226	225	4	
								0	0

- Molecule 59 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	XT	166	Total	C	H	N	O	S	
			2778	875	1410	254	232	7	
								0	0

- Molecule 60 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	XU	141	Total	C	H	N	O	S	
			2335	743	1164	222	203	3	
								0	0

- Molecule 61 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	XV	202	Total	C	H	N	O	S	
			3304	1051	1656	294	295	8	
								0	0

- Molecule 62 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	XW	111	Total	C	H	N	O	S	0	0
			1769	558	898	164	146	3		

- Molecule 63 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	XX	243	Total	C	H	N	O	S	0	0
			4089	1317	2054	351	362	5		

- Molecule 64 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	XY	178	Total	C	H	N	O	S	0	0
			3109	981	1575	295	254	4		

- Molecule 65 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	XZ	120	Total	C	H	N	O	S	0	0
			2008	626	1030	183	166	3		

- Molecule 66 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	a	97	Total	C	H	N	O	S	0	0
			1590	512	777	145	151	5		

- Molecule 67 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	b	148	Total	C	H	N	O	S	0	0
			2358	733	1180	229	213	3		

- Molecule 68 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	c	275	Total	C	H	N	O	S	0	0
			4437	1415	2220	383	410	9		

- Molecule 69 is a protein called 39S ribosomal protein L45, mitochondrial.



Mol	Chain	Residues	Atoms						AltConf	Trace
69	d	216	Total	C	H	N	O	S	0	0
			3501	1125	1743	305	315	13		

- Molecule 70 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	e	217	Total	C	H	N	O	S	0	0
			3529	1124	1767	310	323	5		

- Molecule 71 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	f	142	Total	C	H	N	O	S	0	0
			2291	731	1152	185	219	4		

- Molecule 72 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	g	132	Total	C	H	N	O	S	0	0
			2183	710	1086	191	194	2		

- Molecule 73 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	h	108	Total	C	H	N	O	S	0	0
			1748	560	866	154	165	3		

- Molecule 74 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	i	97	Total	C	H	N	O	S	0	0
			1684	532	857	165	126	4		

- Molecule 75 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	j	86	Total	C	H	N	O	S	0	0
			1367	426	678	134	127	2		

- Molecule 76 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	k	95	Total	C	H	N	O	S	0	0
			1477	456	745	139	132	5		

- Molecule 77 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	l	80	Total	C	H	N	O	S	0	0
			1327	427	654	118	125	3		

- Molecule 78 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	m	60	Total	C	H	N	O	S	0	0
			1025	309	525	104	85	2		

- Molecule 79 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	o	94	Total	C	H	N	O	S	0	0
			1601	501	804	165	128	3		

- Molecule 80 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	p	127	Total	C	H	N	O	S	0	0
			2141	661	1083	201	192	4		

- Molecule 81 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	q	164	Total	C	H	N	O	S	0	0
			2738	858	1359	267	249	5		

- Molecule 82 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	r	152	Total	C	H	N	O	S	0	0
			2514	792	1267	239	208	8		

- Molecule 83 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	r3	75	Total	C	N	O	P	0	0
			1468	714	228	451	75		

- Molecule 84 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	s	370	Total	C	H	N	O	S	0	0
			6059	1946	3023	542	534	14		

- Molecule 85 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	t1	46	Total	C	H	N	O	2	0
			733	228	379	56	70		
85	t2	30	Total	C	H	N	O	0	0
			506	154	268	38	46		
85	t3	30	Total	C	H	N	O	0	0
			506	154	268	38	46		
85	t4	29	Total	C	H	N	O	0	0
			484	148	255	36	45		
85	t5	29	Total	C	H	N	O	0	0
			484	148	255	36	45		
85	t6	27	Total	C	H	N	O	0	0
			450	137	236	34	43		

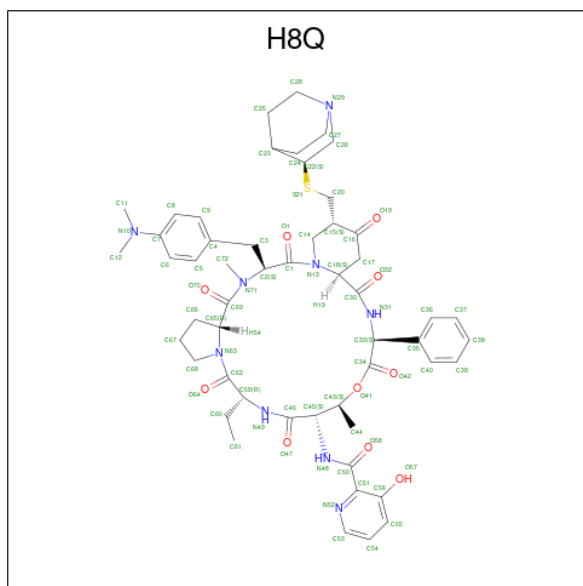
- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	0	1	Total	Zn	0
			1	1	
86	4	1	Total	Zn	0
			1	1	
86	AB	1	Total	Zn	0
			1	1	
86	AO	1	Total	Zn	0
			1	1	
86	AP	1	Total	Zn	0
			1	1	
86	AT	1	Total	Zn	0
			1	1	
86	r	1	Total	Zn	0
			1	1	

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

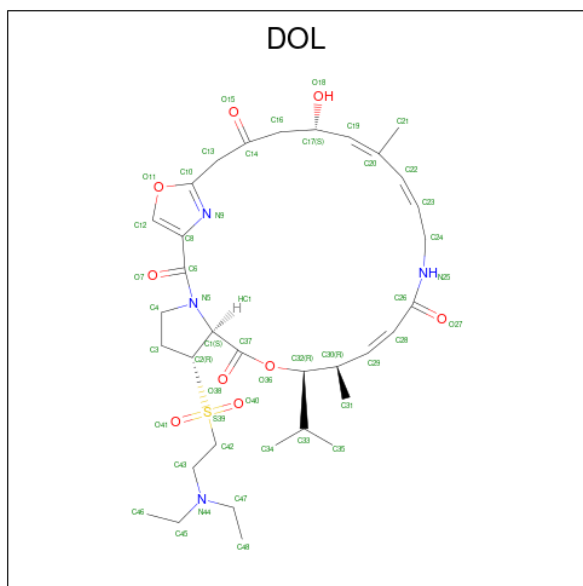
Mol	Chain	Residues	Atoms		AltConf
87	9	1	Total	Mg	0
			1	1	
87	XA	143	Total	Mg	0
			143	143	
87	AA	46	Total	Mg	0
			46	46	
87	XD	1	Total	Mg	0
			1	1	
87	XI	1	Total	Mg	0
			1	1	
87	XM	1	Total	Mg	0
			1	1	
87	XW	1	Total	Mg	0
			1	1	
87	g	1	Total	Mg	0
			1	1	

- Molecule 88 is {N}-[(3 {S},6 {R},12 {R},15 {S},16 {S},19 {S},22 {S},25 {S})-25-[(3 {S})-1-azabicyclo[2.2.2]octan-3-yl)sulfanylmethyl]-3-[[4-(dimethylamino)phenyl)methyl]-12-ethyl-4,16-dimethyl-2,5,11,14,18,21,24-heptakis(oxidanylidene)-19-phenyl-17-oxa-1,4,10,13,20-pentazatricyclo[20.4.0.0<sup>^</sup>{6,10}]hexacosan-15-yl]-3-oxidanyl-pyridine-2-carboxamide (three-letter code: H8Q) (formula: C<sub>53</sub>H<sub>67</sub>N<sub>9</sub>O<sub>10</sub>S).



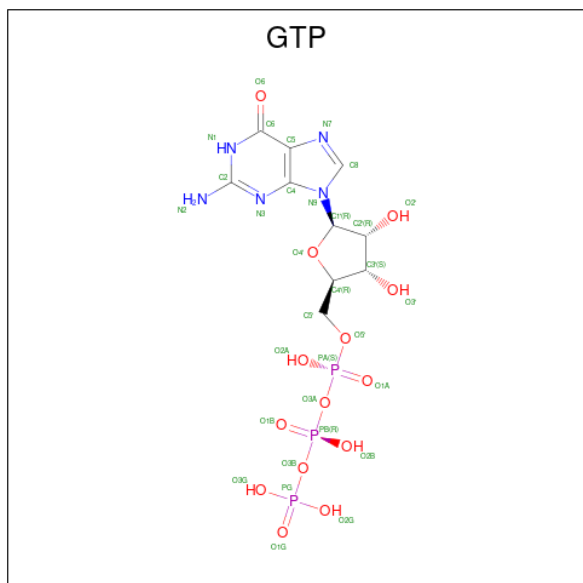
Mol	Chain	Residues	Atoms						AltConf
88	XA	1	Total	C	H	N	O	S	0
			140	53	67	9	10	1	

- Molecule 89 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula:  $C_{34}H_{50}N_4O_9S$ ).



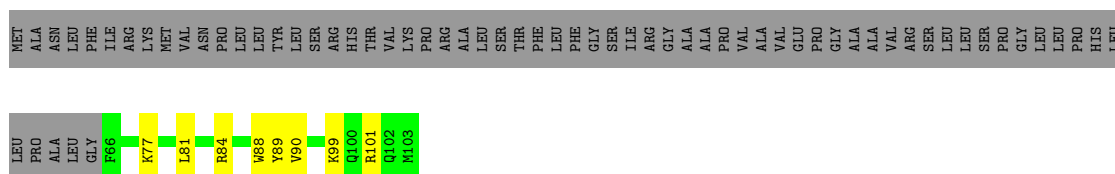
Mol	Chain	Residues	Atoms					AltConf	
89	XA	1	Total	C	H	N	O	S	0
			98	34	50	4	9	1	

- Molecule 90 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

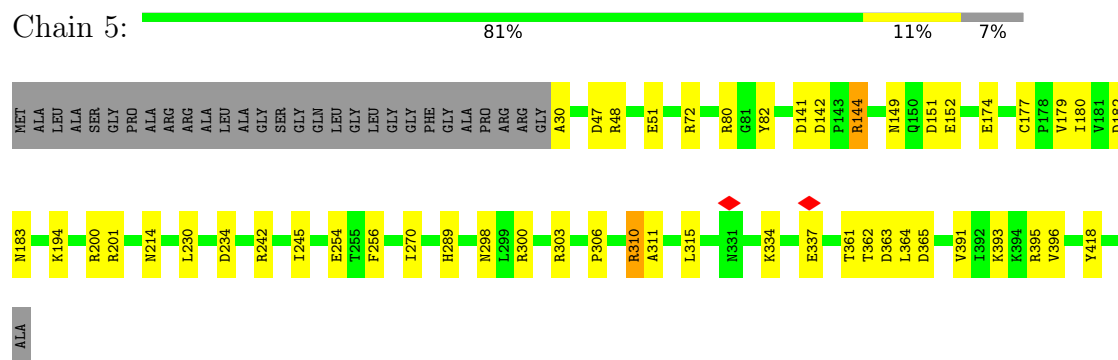


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
90	AX	1	42	10	10	5	14	3	0

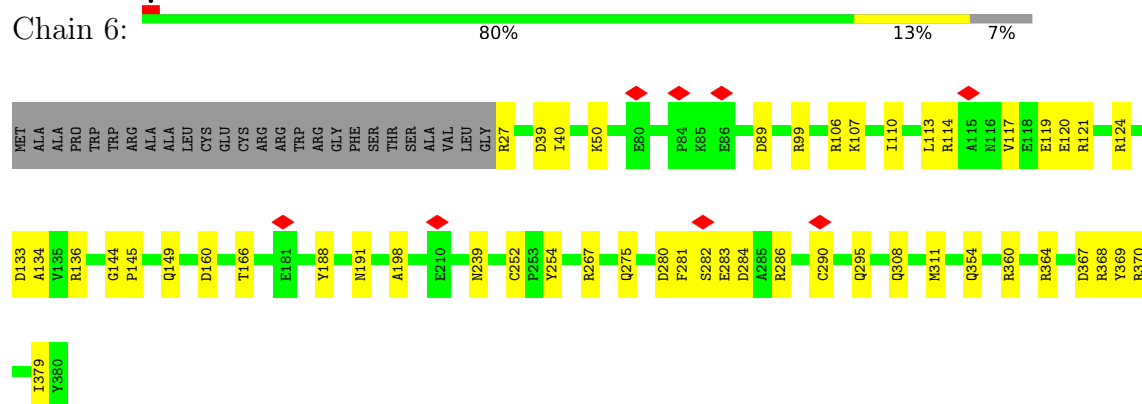




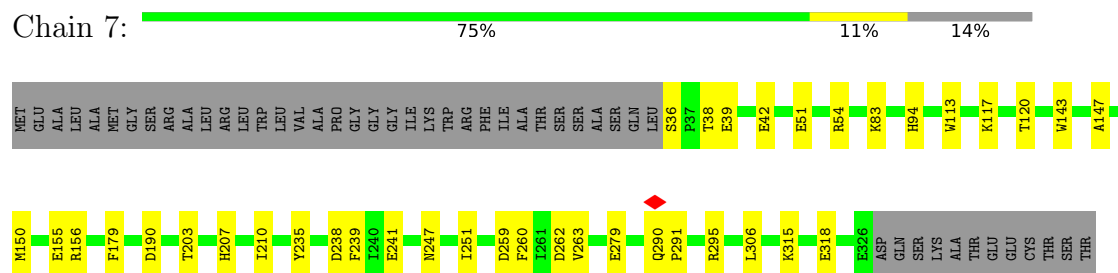
- Molecule 6: 39S ribosomal protein L37, mitochondrial



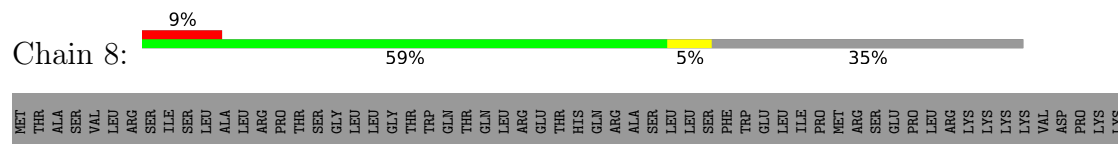
- Molecule 7: 39S ribosomal protein L38, mitochondrial



- Molecule 8: 39S ribosomal protein L39, mitochondrial

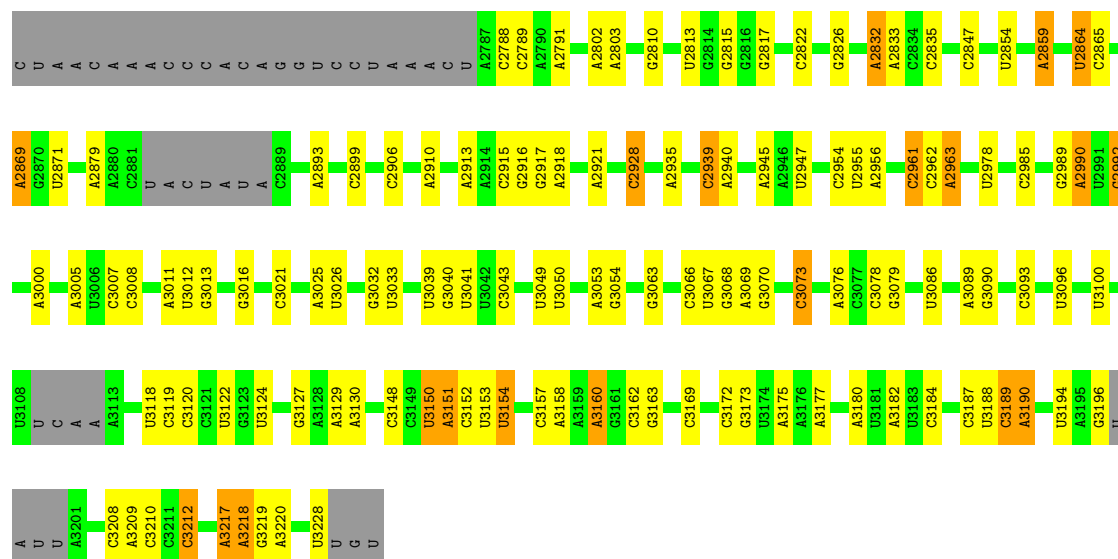


- Molecule 9: 39S ribosomal protein L40, mitochondrial



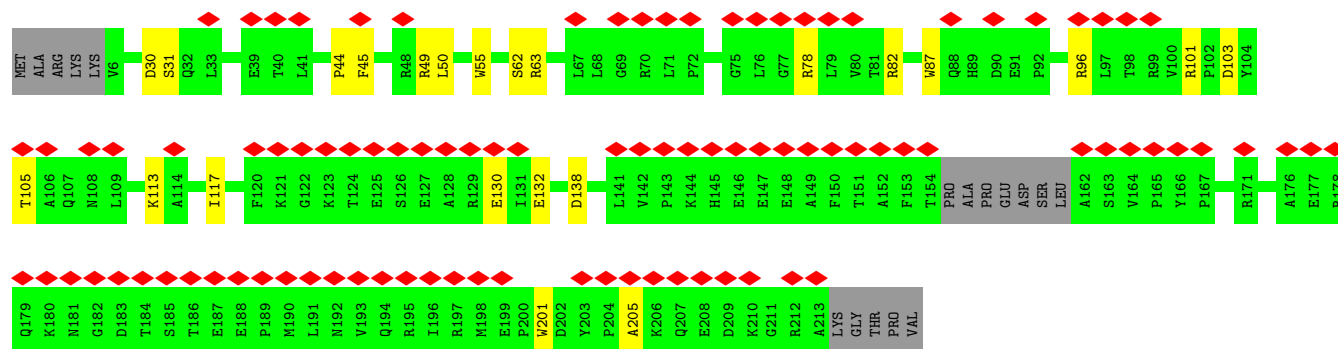






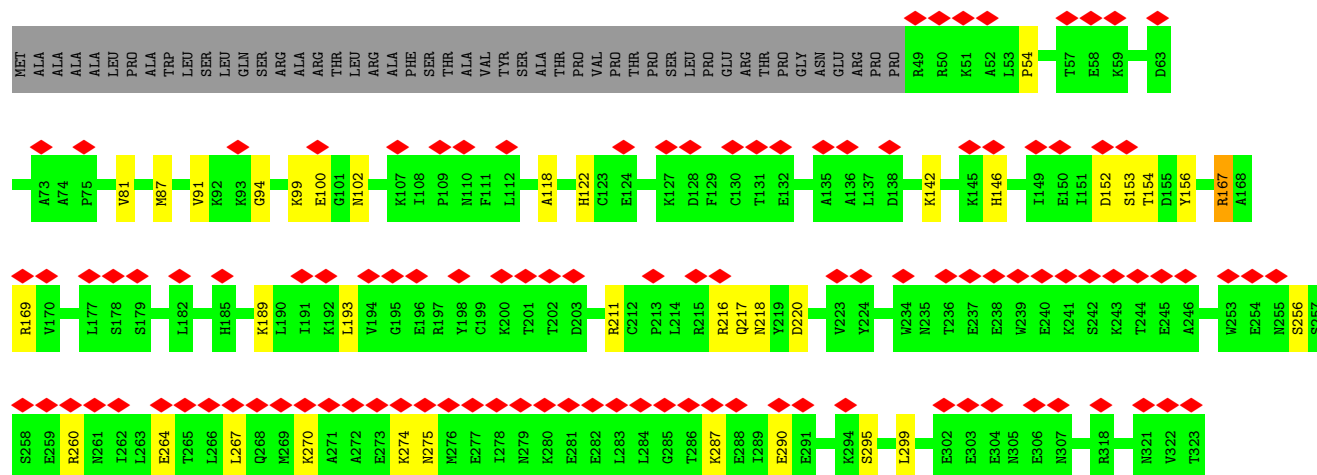
• Molecule 12: 28S ribosomal protein S34, mitochondrial

Chain A0: 44% 82% 11% 8%

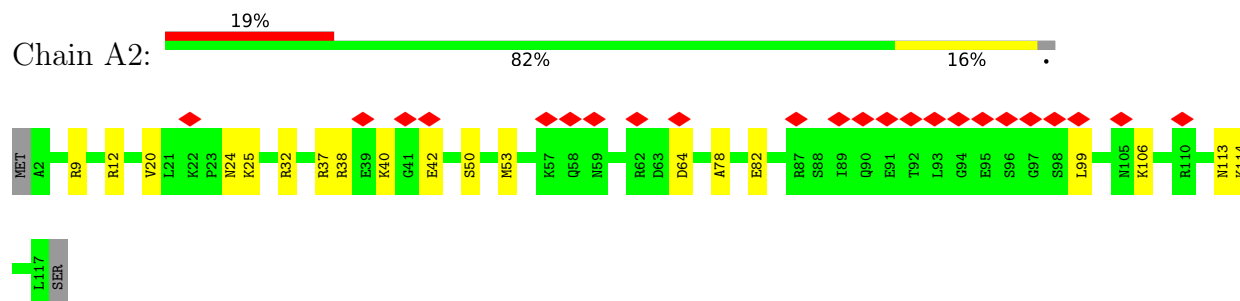


• Molecule 13: 28S ribosomal protein S35, mitochondrial

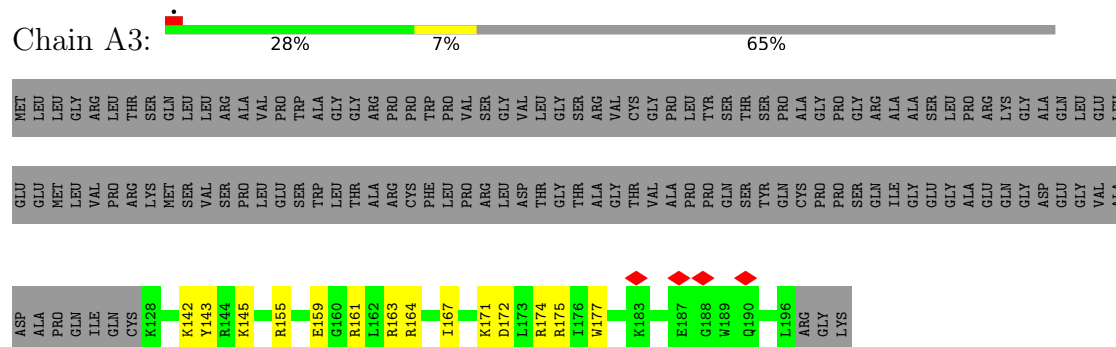
Chain A1: 34% 74% 11% 15%



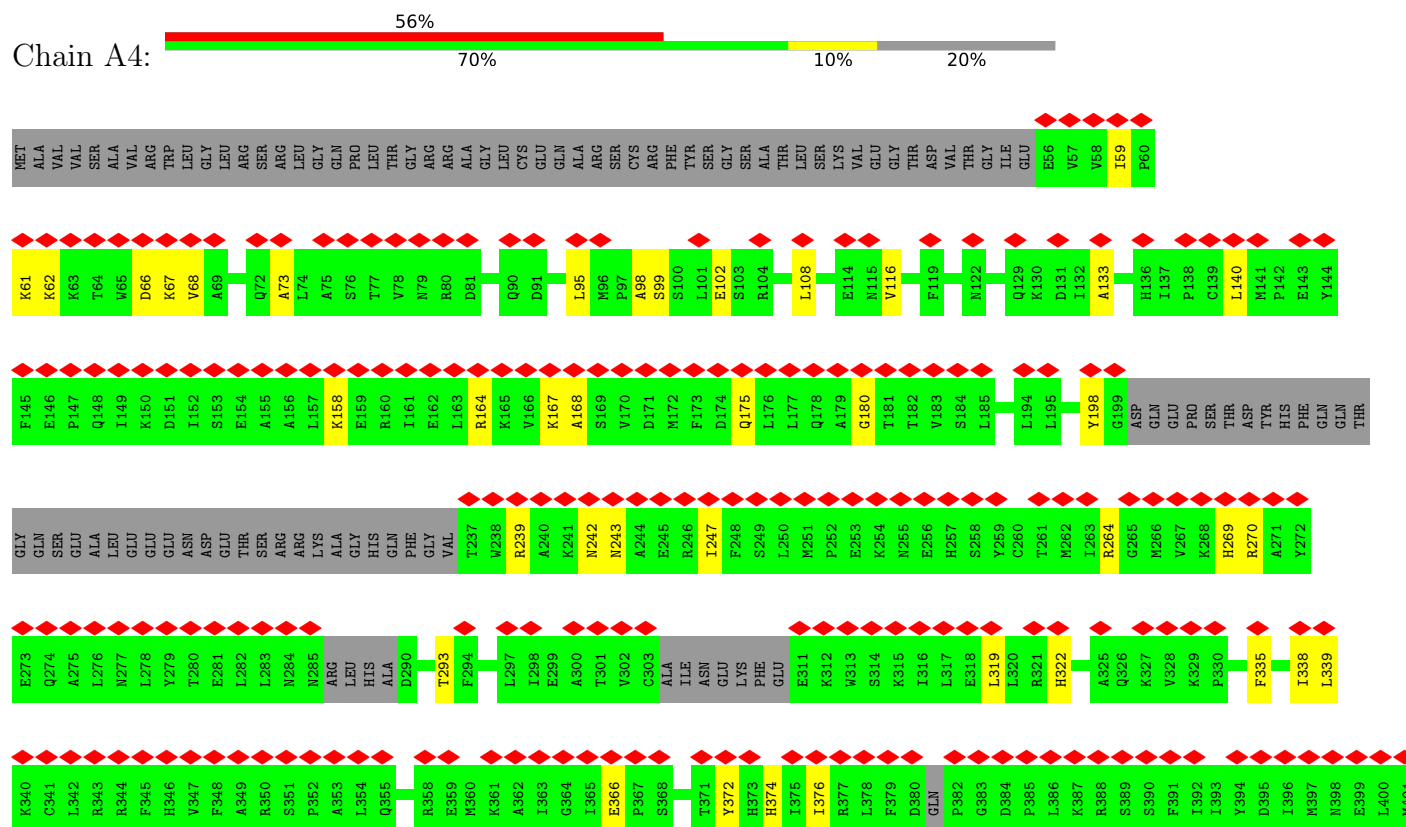
- Chain A2:



- Chain A3:



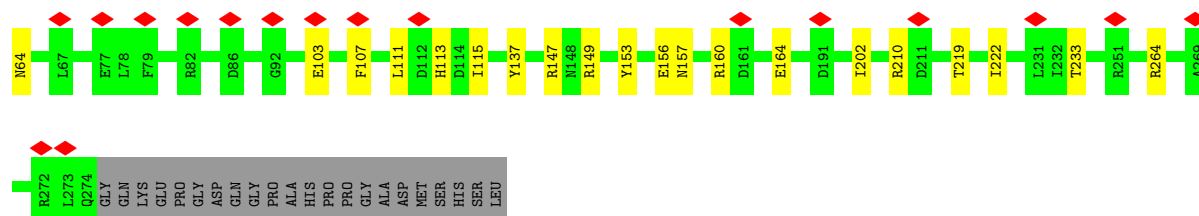
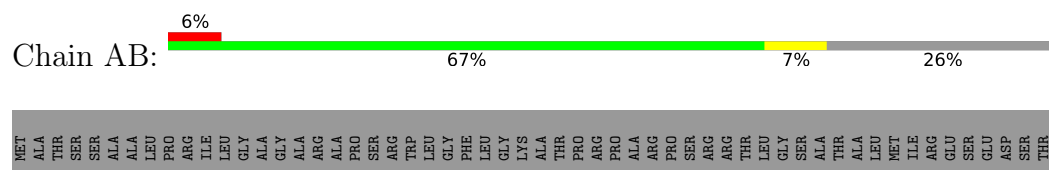
- Chain A4:



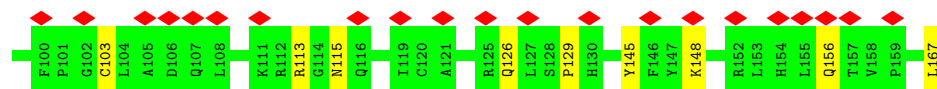
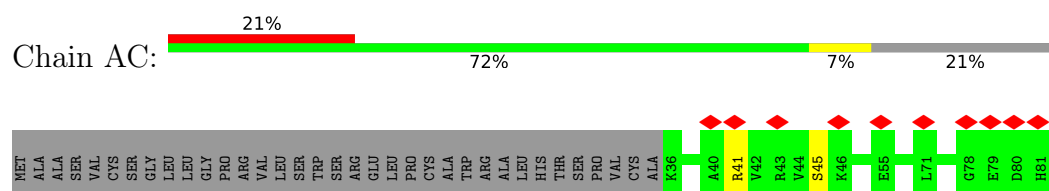




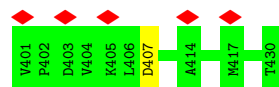
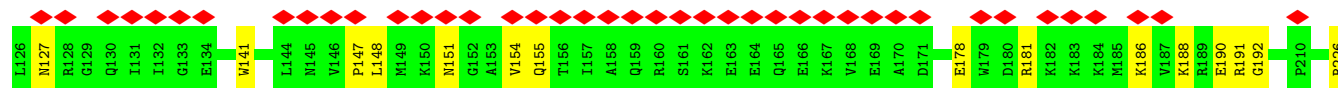
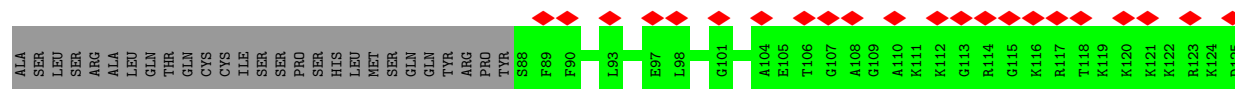
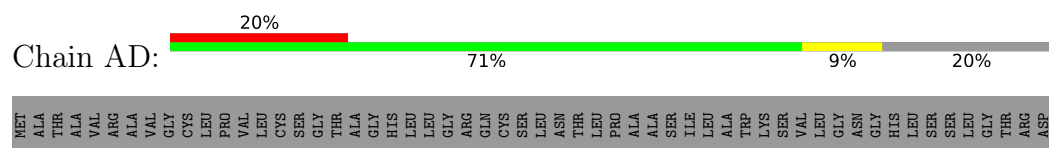
- Molecule 18: 28S ribosomal protein S2, mitochondrial



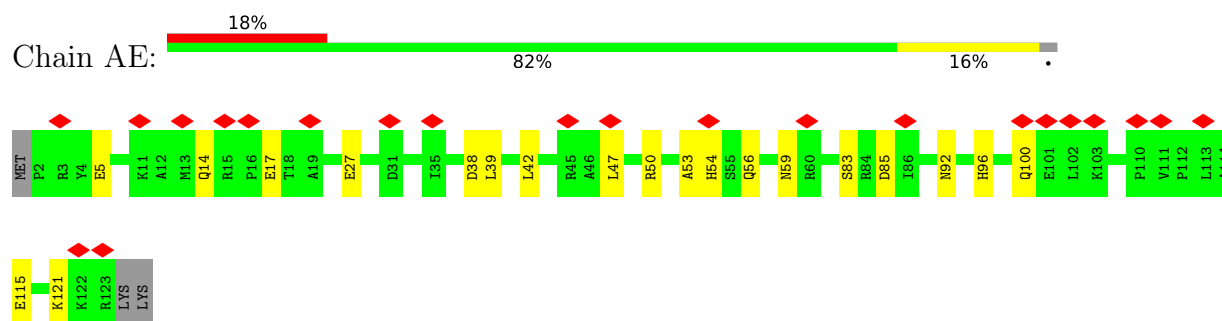
- Molecule 19: 28S ribosomal protein S24, mitochondrial



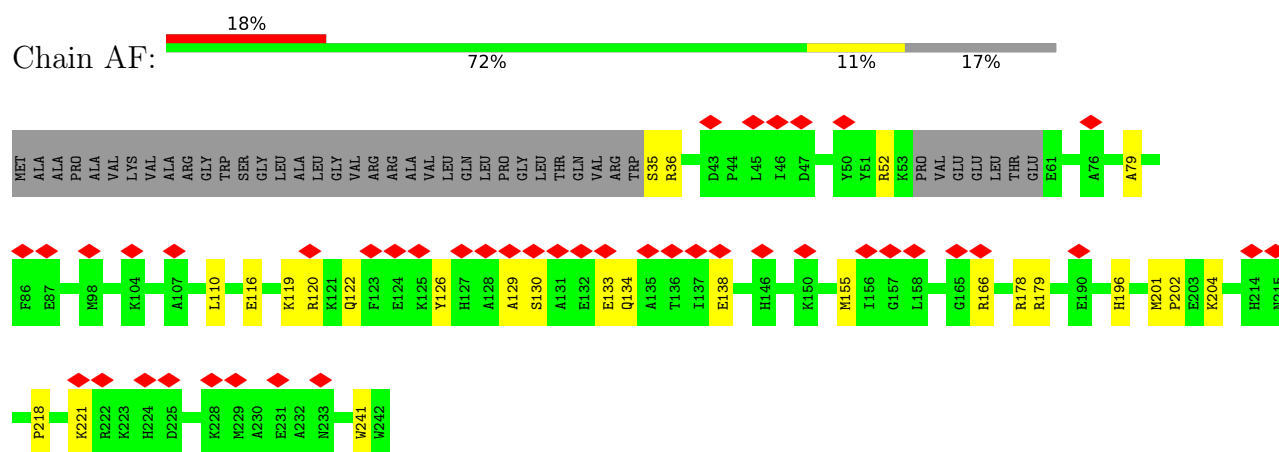
- Molecule 20: 28S ribosomal protein S5, mitochondrial



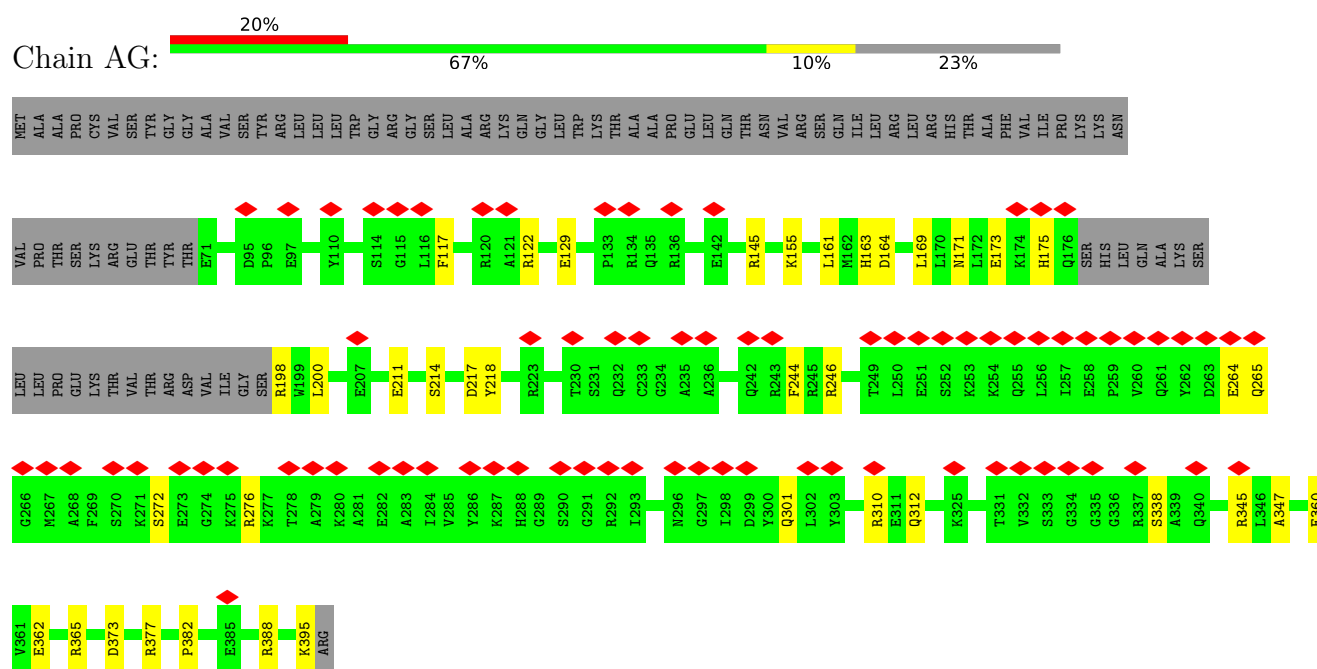
- Molecule 21: 28S ribosomal protein S6, mitochondrial



- Molecule 22: 28S ribosomal protein S7, mitochondrial



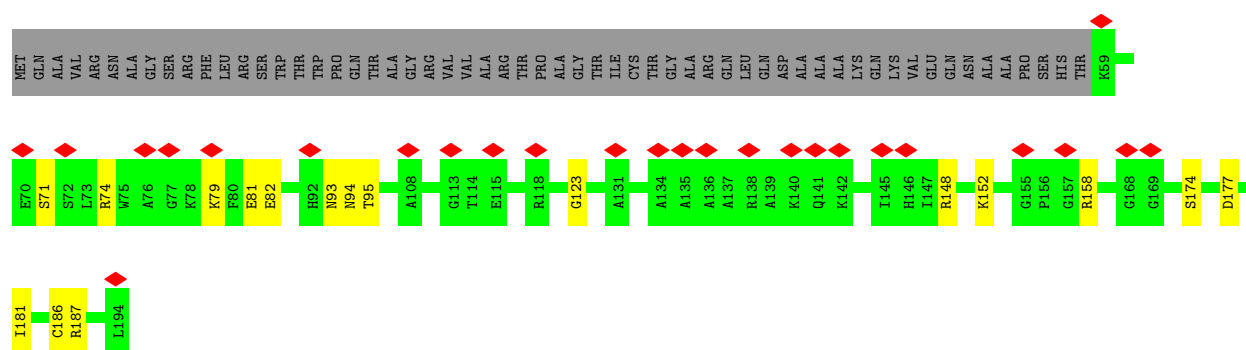
- Molecule 23: 28S ribosomal protein S9, mitochondrial



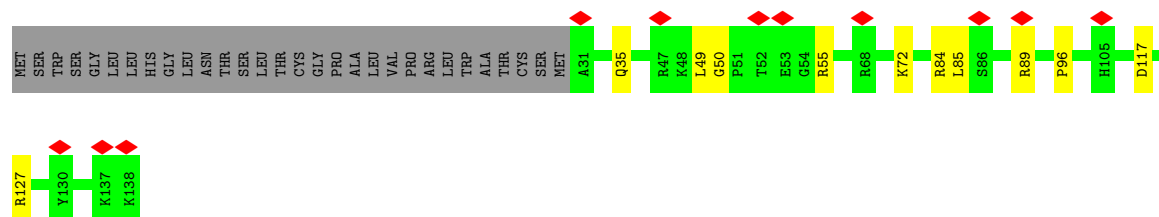
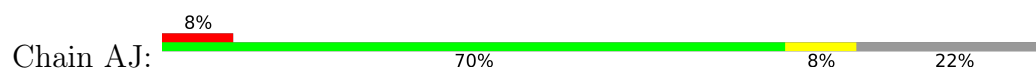
- Molecule 24: 28S ribosomal protein S10, mitochondrial



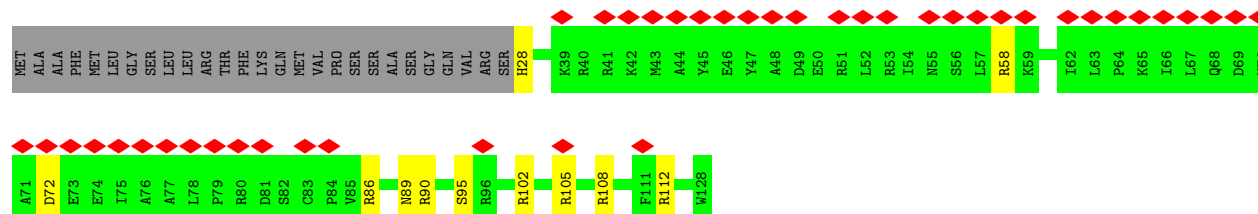
- Molecule 25: 28S ribosomal protein S11, mitochondrial



- Molecule 26: 28S ribosomal protein S12, mitochondrial



- Molecule 27: 28S ribosomal protein S14, mitochondrial



- Molecule 28: 28S ribosomal protein S15, mitochondrial

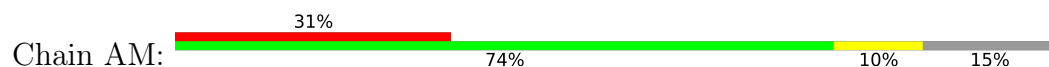


MET LEU ARG VAL ASP ALA TRP ARG THR SER LEU ILE ARG THR ARG ALA VAL THR GLN VAL LEU VAL VAL PRO GLY LEU PRO PRO GLY GLY SER SER ALA LYS PHE PHE ASN GLN TRP GLY LEU GLN GLN PRO ARG SER LEU LEU LEU GLN ALA ALA ARG GLY TYR VAL VAL ARG LYS PRO GLN

SER ARG LEU ASP D86 D75 N78 V79 E83 K84 V85 D86 D87 V88 V89 K90 K100 L104 A117 E120 D121 T122 R123 K135 E140 E141 H142 L143 E144 D149 H152 H153 R154 Q162 M166 N169 L170 F178 W183 E188 Y196

R197 R198 R201 Q218 K219 K222 R223 R224 R225 A226 L227 K228 A229 ALA ALA ALA GLN LYS LYS ALA ARG ARG ASN PRO ASP SER PRO ALA LYS ALA ILE PRO LYS THR LEU LYS ASP SER GLN

- Molecule 29: 28S ribosomal protein S16, mitochondrial



MET VAL HIS LEU THR THR LEU LEU CYS K10 G14 R20 L21 A22 L23 G24 G25 V35 A36 K40 C41 P42 R43 D44 G45 R46 F47 V48 E49 Q50 D55 P58 N59 S60 H61 G62 E63 K64 L68 N69 L70 D71 R72 I73 W76 S84 K85 P86 M87 E88 K89

L90 L91 G92 L93 F96 F97 P98 R111 L119 L120 A121 S122 Q123 K124 T125 ASP ALA GLU THR THR GLU THR THR THR THR THR THR

- Molecule 30: 28S ribosomal protein S17, mitochondrial



MET SER VAL R5 K16 T20 R29 L33 L39 L40 K41 A51 H52 D53 A54 L55 Q56 Q57 G58 T59 D62 L66 R73 H76 H79 A82 V83 D93 T96 C100 A101 T104 Y105 L106 E107 S108 P109 S111 SER GLU THR

THR GLN LEU SER LYS ASN LEU GLU LEU ILE ASN SER SER ALA GLN

- Molecule 31: 28S ribosomal protein S18b, mitochondrial



MET ALA ALA SER VAL LEU ASN THR VAL ARG ARG ARG MET PRO MET LEU SER LEU PHE ARG GLY SER HIS ARG VAL GLN VAL PRO LEU GLN THR CYS THR LYS ALA PRO SER GLU ASP SER LEU SER SER VAL PRO ILE SER PRO TYR K52 E50 S61 E62 Q65 G69

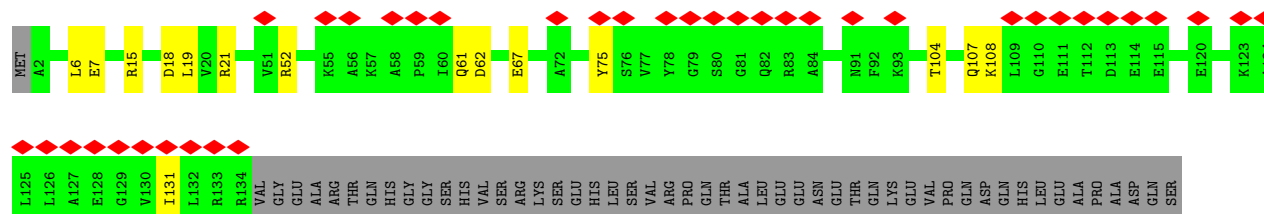
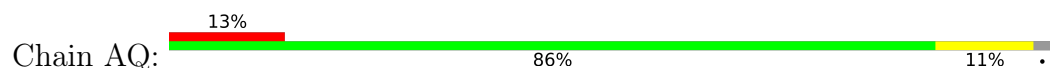
S70 R71 R78 R79 N80 H81 K82 G83 R89 T90 R91 R97 N98 C105 P106 R109 V115 V120 K121 E124 A129 F135 R149 L150 Q151 Q152 A153 I154 D159 H160 G161 L162 L163 I164 P168 Q169 V170 S171 E171 P172 R173 D174 L175 D176 F177 S178 T179 S180

H181 G182 A183 V184 S185 A186 P189 L193 V194 S195 G196 D197 P198 K206 Q207 P208 P209 E210 R211 R215 L216 R217 G222 H223 L224 Q225 E226 E227 S228 G229 P232 E233 S234 M235 P236 LYS MET PRO ARG ARG THR PRO ALA ALA SER THR GLY THR THR PRO GLN

SER ALA LEU




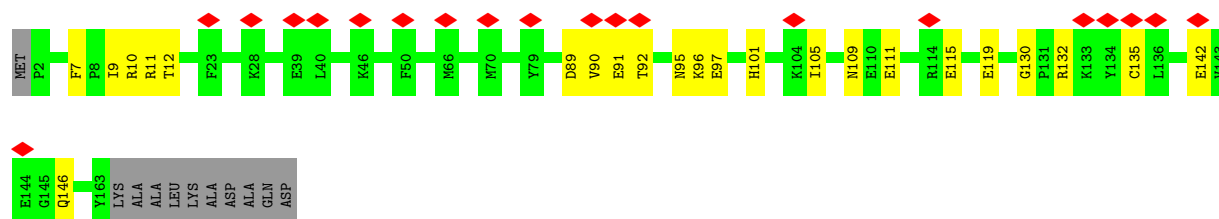
- Chain AP: 




LYS  
GLY  
LEU  
LEU  
PRO  
PRO

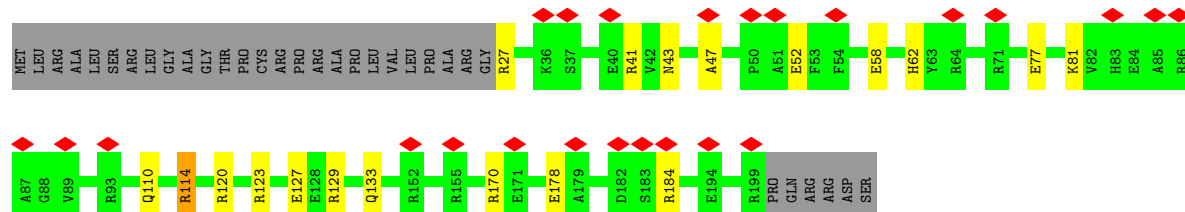
- Molecule 36: 28S ribosomal protein S25, mitochondrial

Chain AT: 




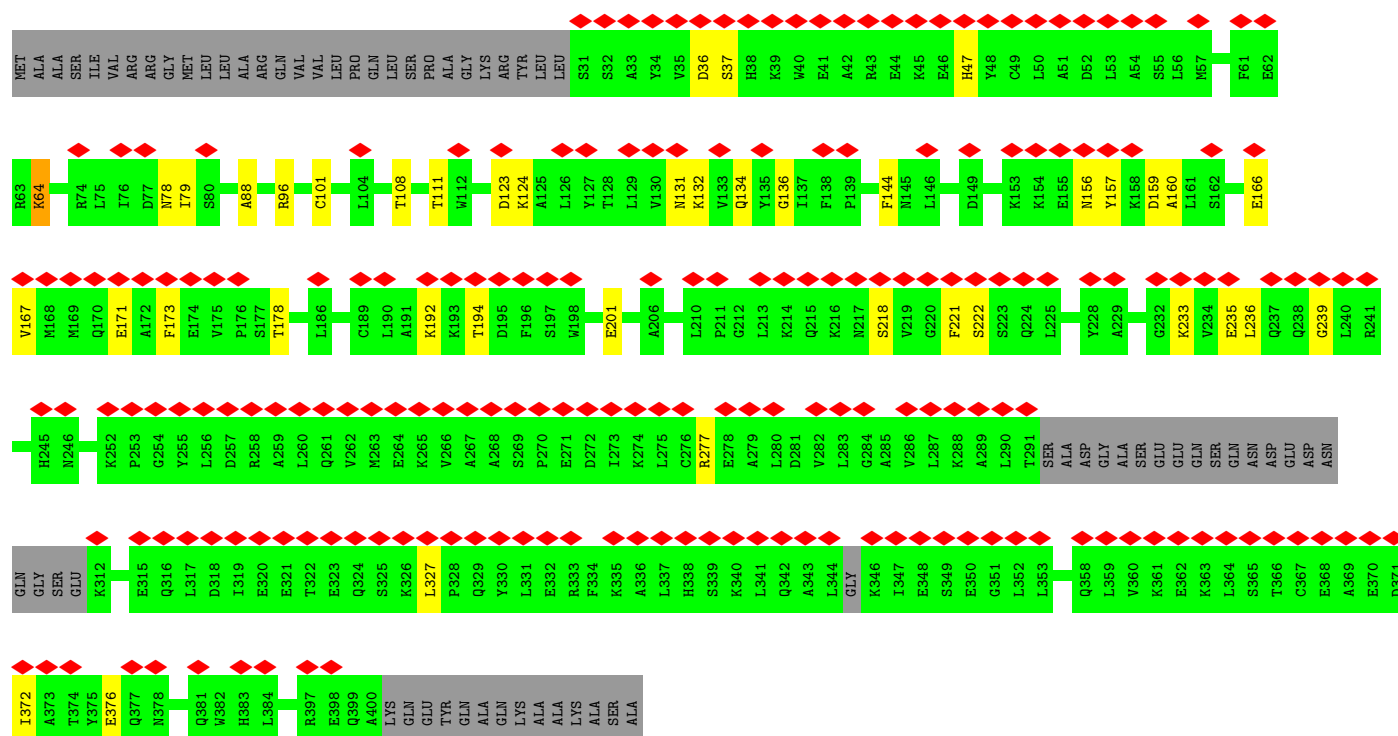
- Molecule 37: 28S ribosomal protein S26, mitochondrial

Chain AU: 



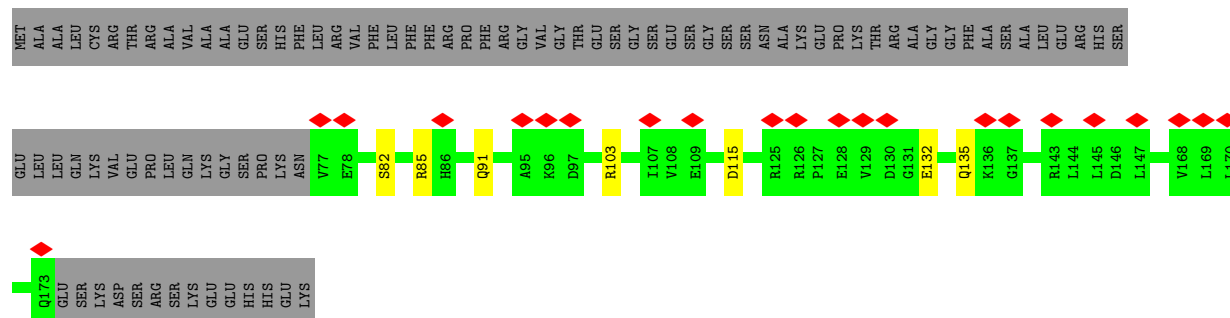
- Molecule 38: 28S ribosomal protein S27, mitochondrial

Chain AV: 



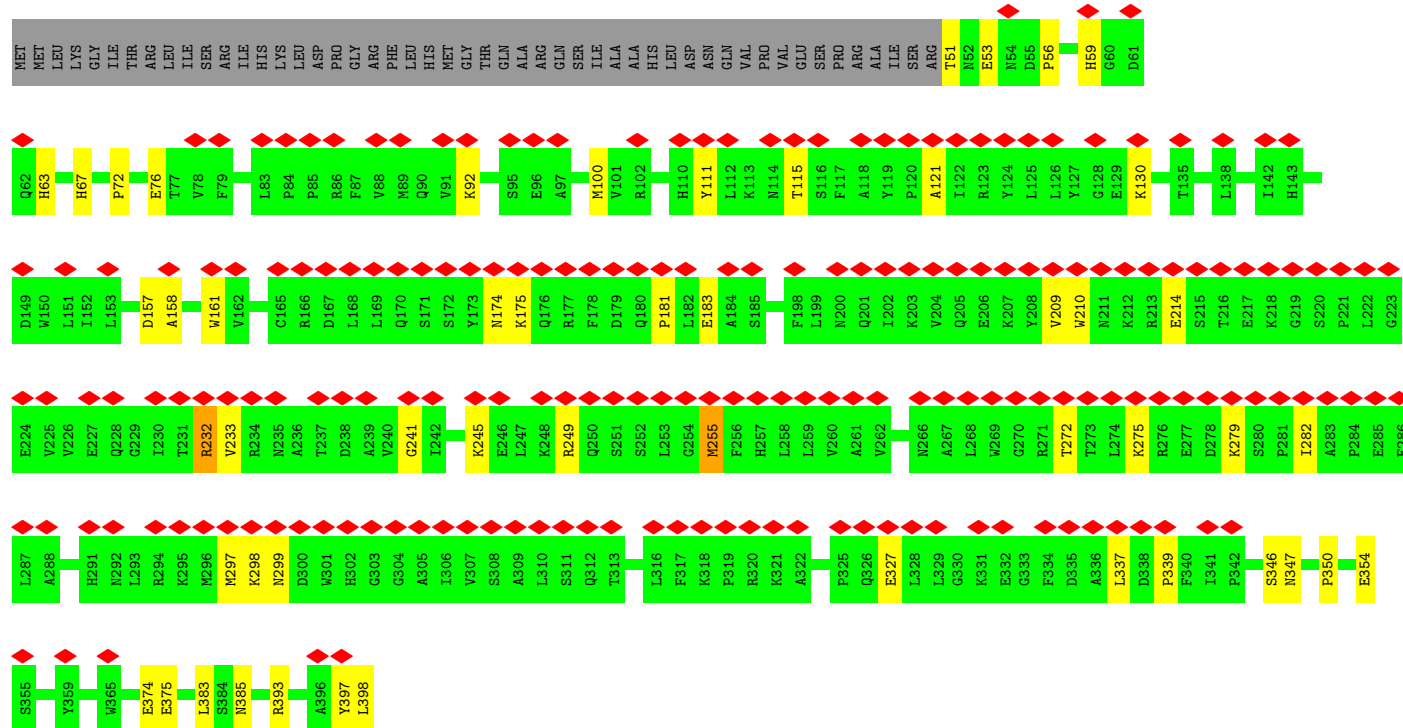
- Molecule 39: 28S ribosomal protein S28, mitochondrial

Chain AW: 



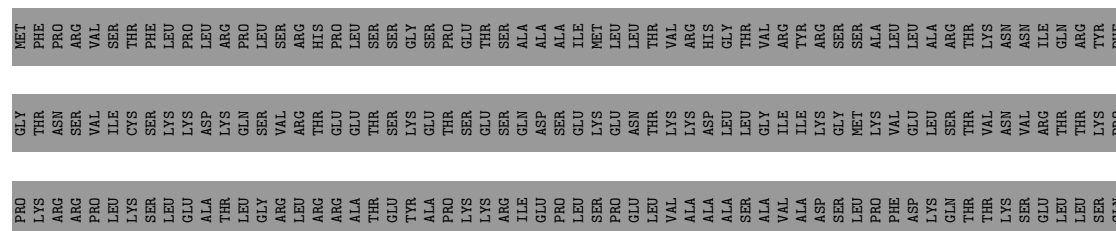
- Molecule 40: 28S ribosomal protein S29, mitochondrial

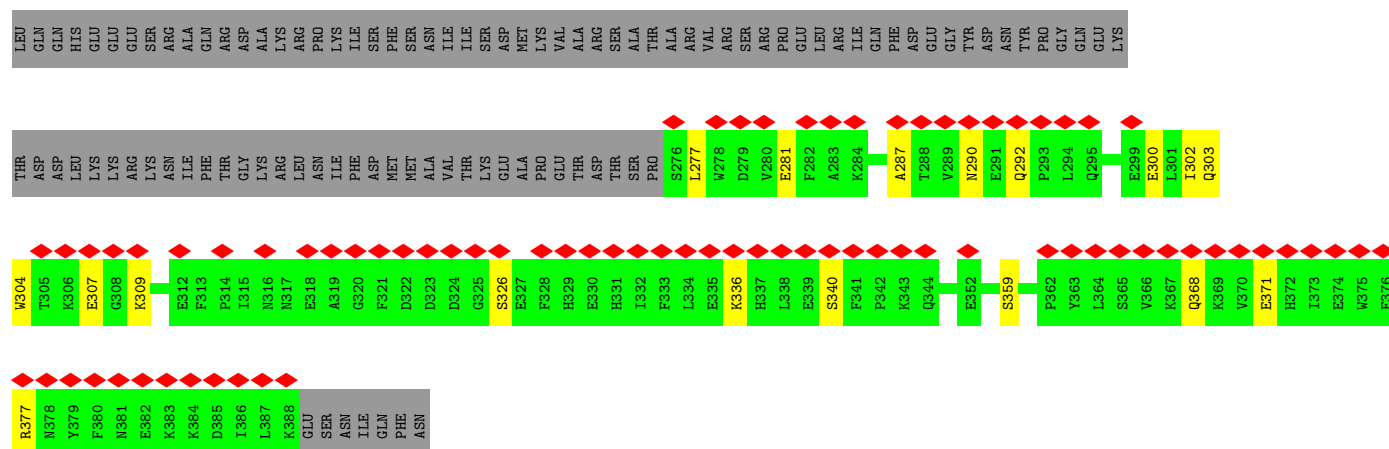
Chain AX: 



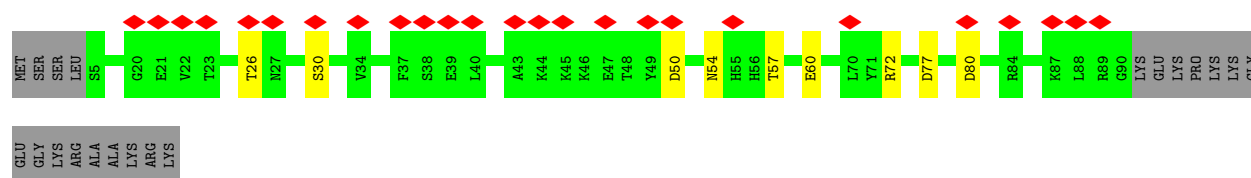
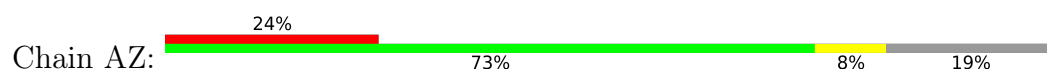
- Molecule 41: 28S ribosomal protein S31, mitochondrial

Chain AY: 

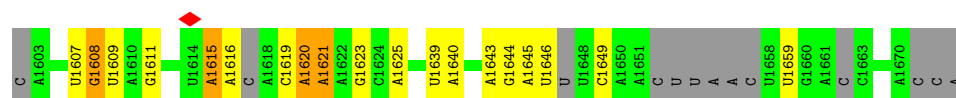




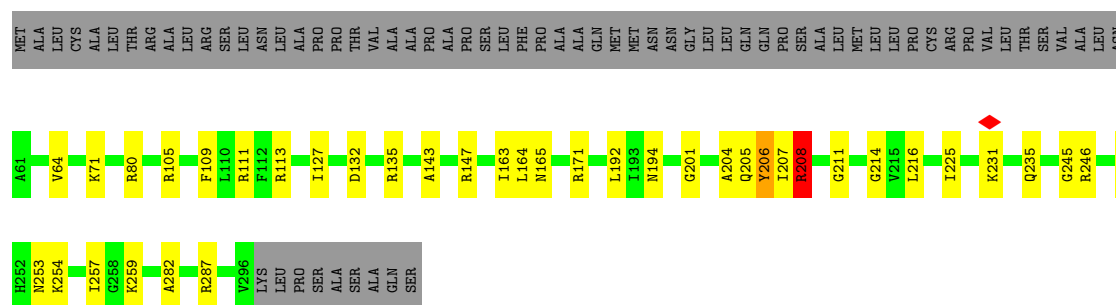
- Molecule 42: 28S ribosomal protein S33, mitochondrial



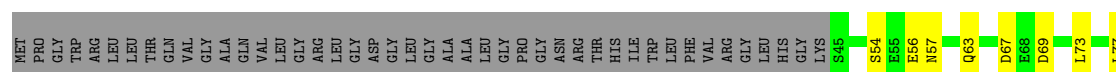
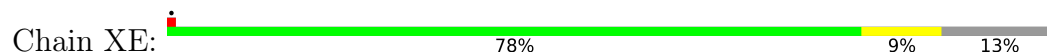
- Molecule 43: mitochondrial tRNAVal

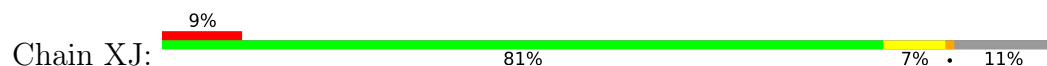


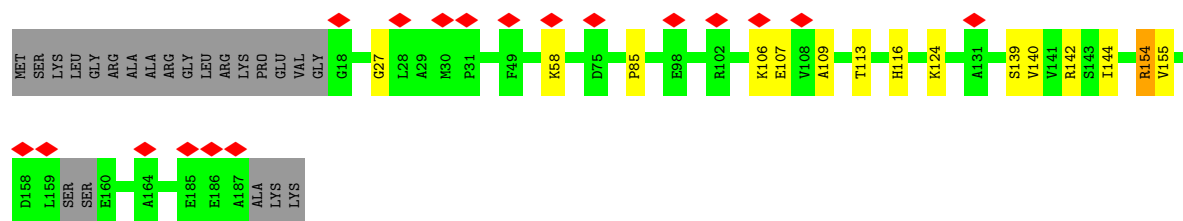
- Molecule 44: 39S ribosomal protein L2, mitochondrial



- Molecule 45: 39S ribosomal protein L3, mitochondrial







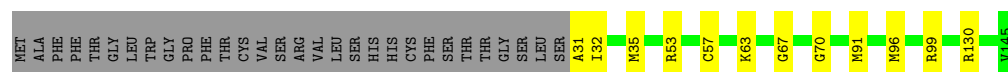
- Molecule 50: 39S ribosomal protein L13, mitochondrial

Chain XK: 85% 14% .



- Molecule 51: 39S ribosomal protein L14, mitochondrial

Chain XL: 71% 8% 21%



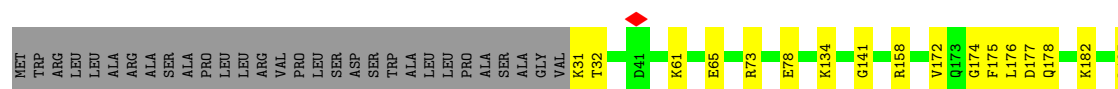
- Molecule 52: 39S ribosomal protein L15, mitochondrial

Chain XM: 83% 14% .



- Molecule 53: 39S ribosomal protein L16, mitochondrial

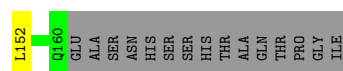
Chain XN: 78% 10% 12%



- Molecule 54: 39S ribosomal protein L17, mitochondrial

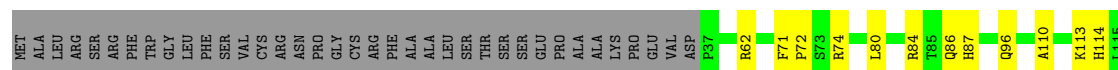
Chain XO: 69% 18% 13%





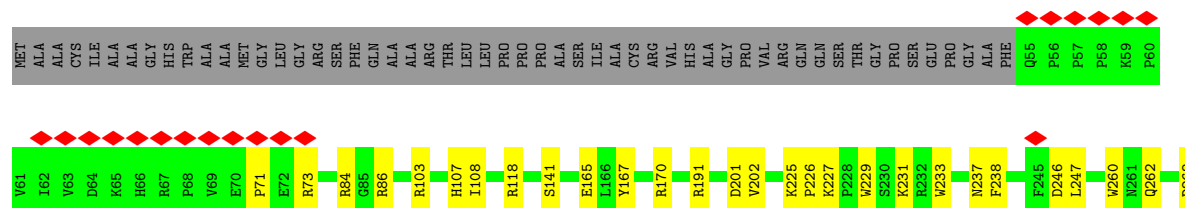
- Molecule 55: 39S ribosomal protein L18, mitochondrial

Chain XP: 69% 10% 21%



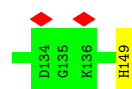
- Molecule 56: 39S ribosomal protein L19, mitochondrial

Chain XQ: 7% 70% 12% 18%



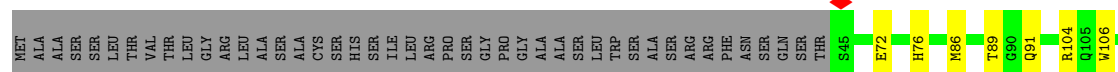
- Molecule 57: 39S ribosomal protein L20, mitochondrial

Chain XR: 75% 19% 6%



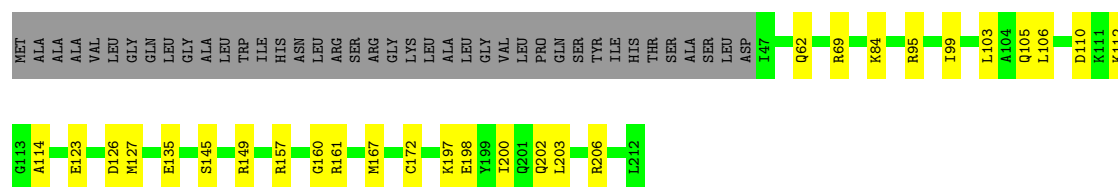
- Molecule 58: 39S ribosomal protein L21, mitochondrial

Chain XS: 69% 9% 22%




- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT:  67% 14% 19%




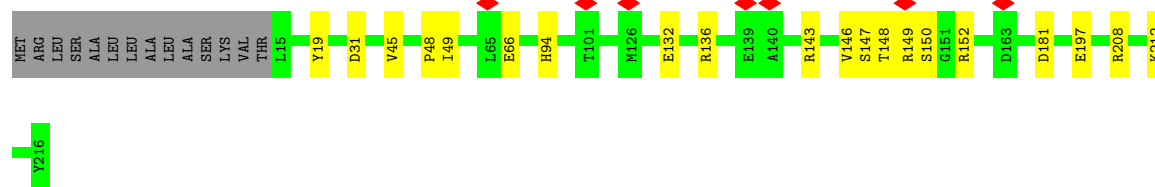
- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU:  79% 13% 8%



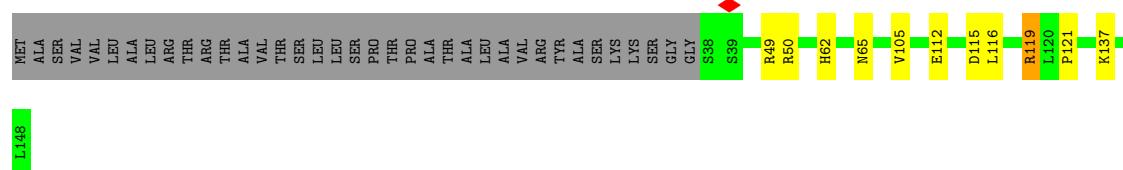
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV:  84% 9% 6%




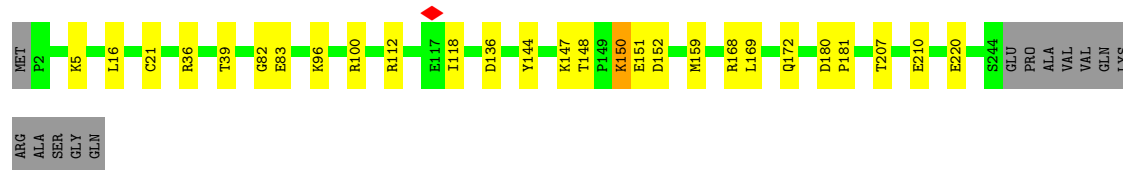
- Molecule 62: 39S ribosomal protein L27, mitochondrial

Chain XW:  68% 7% 25%



- Molecule 63: 39S ribosomal protein L28, mitochondrial

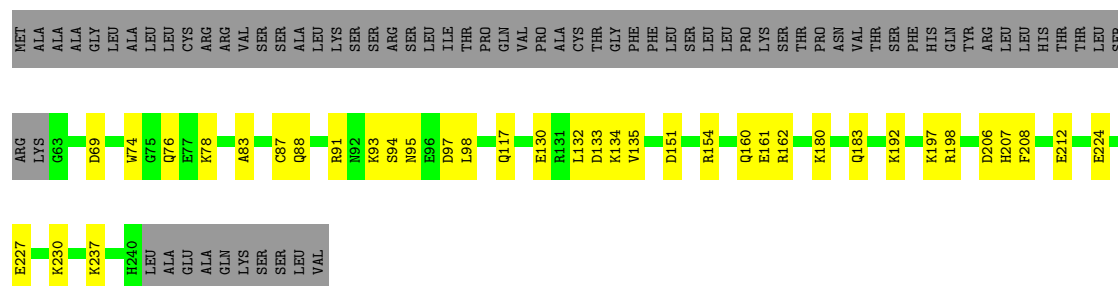
Chain XX:  84% 10% 5%



- Molecule 64: 39S ribosomal protein L47, mitochondrial

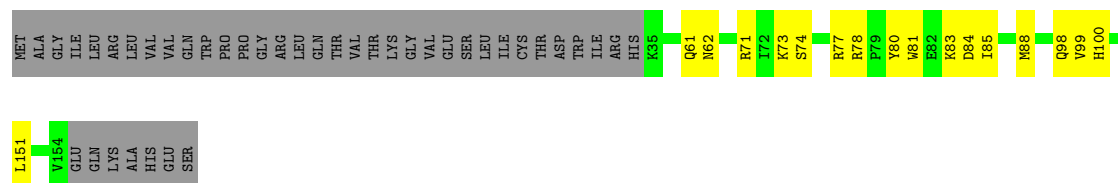
Chain XY:  56% 15% 29%





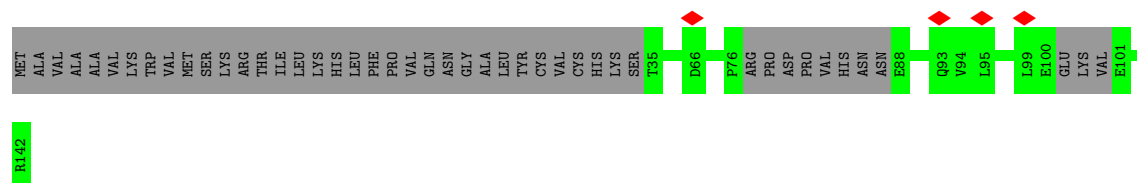
- Molecule 65: 39S ribosomal protein L30, mitochondrial

Chain XZ: 64% 11% 25%



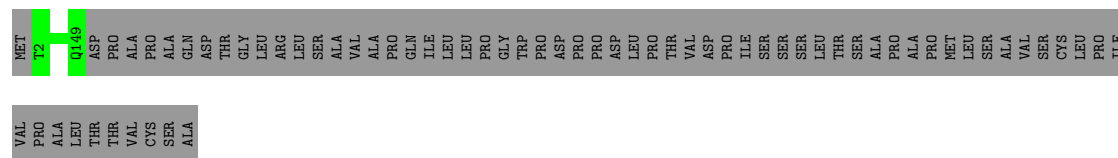
- Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a: 68% 32%



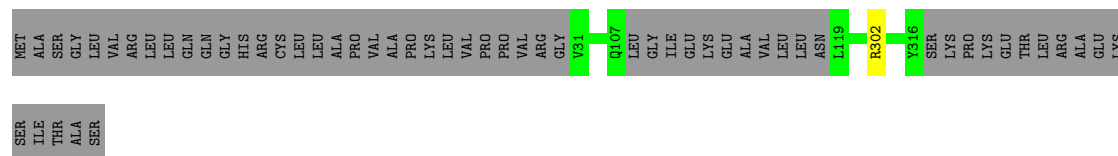
- Molecule 67: 39S ribosomal protein L43, mitochondrial

Chain b: 69% 31%



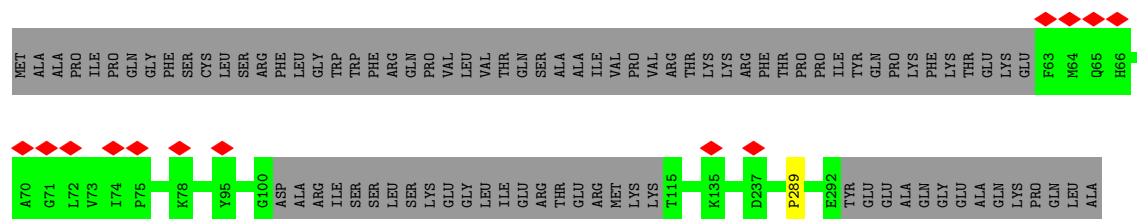
- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c: 83% 17%




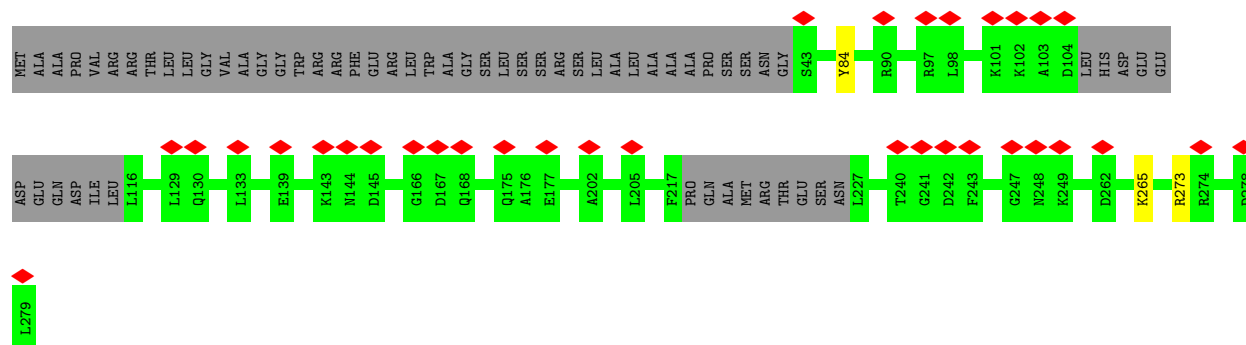
- Molecule 69: 39S ribosomal protein L45, mitochondrial

Chain d:  70% 29%



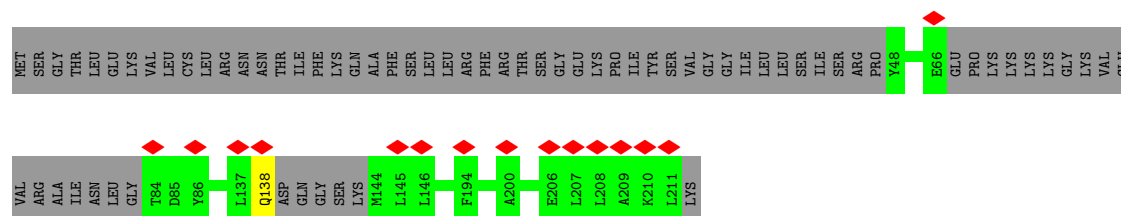
- Molecule 70: 39S ribosomal protein L46, mitochondrial

Chain e:  12% 77% 22%




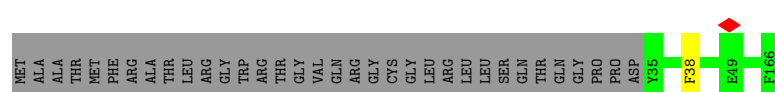
- Molecule 71: 39S ribosomal protein L48, mitochondrial

Chain f:  7% 67% 33%



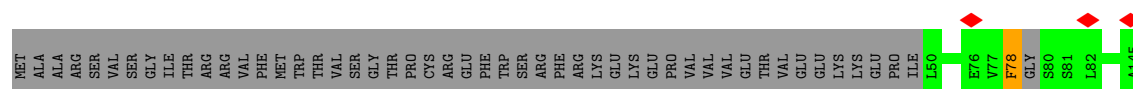
- Molecule 72: 39S ribosomal protein L49, mitochondrial

Chain g:  79% 20%



- Molecule 73: 39S ribosomal protein L50, mitochondrial

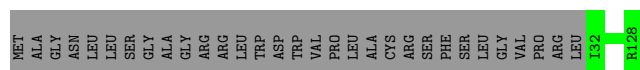
Chain h:  68% 32%





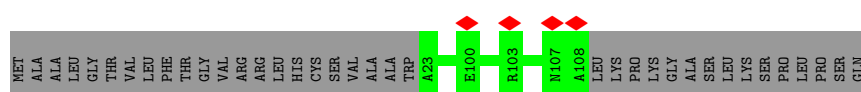
- Molecule 74: 39S ribosomal protein L51, mitochondrial

Chain i: 76% 24%



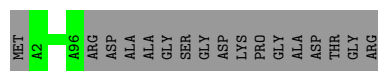
- Molecule 75: 39S ribosomal protein L52, mitochondrial

Chain j: 70% 30%



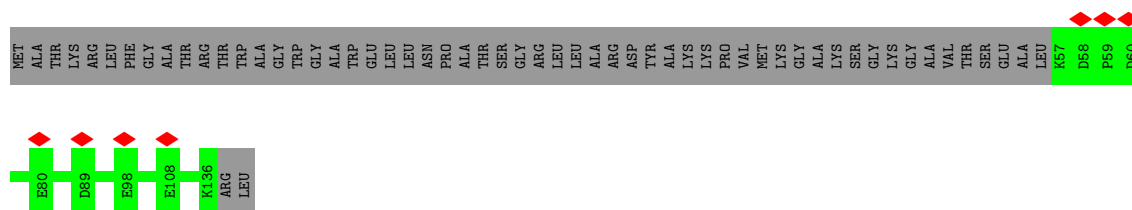
- Molecule 76: 39S ribosomal protein L53, mitochondrial

Chain k: 85% 15%



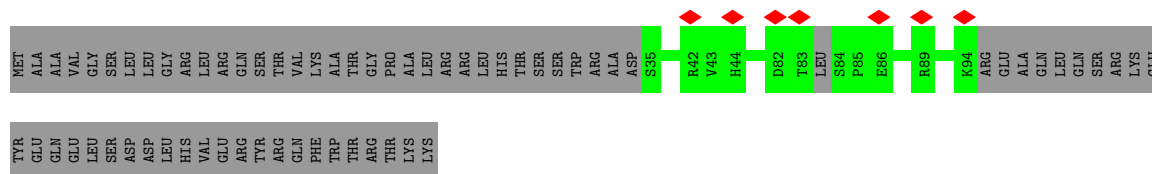
- Molecule 77: 39S ribosomal protein L54, mitochondrial

Chain l: 5% 58% 42%



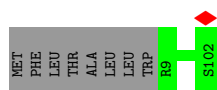
- Molecule 78: 39S ribosomal protein L55, mitochondrial

Chain m: 5% 47% 53%



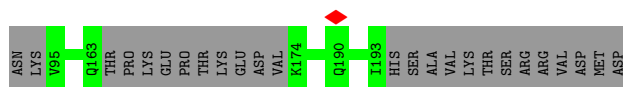
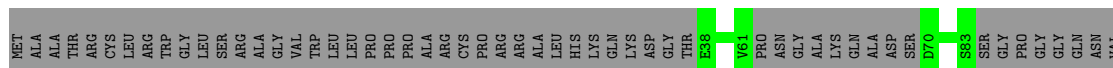
- Molecule 79: Ribosomal protein 63, mitochondrial

Chain o: 92% 8%



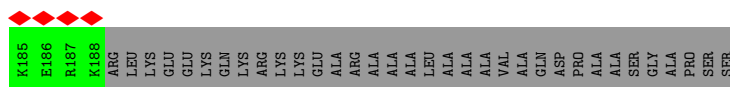
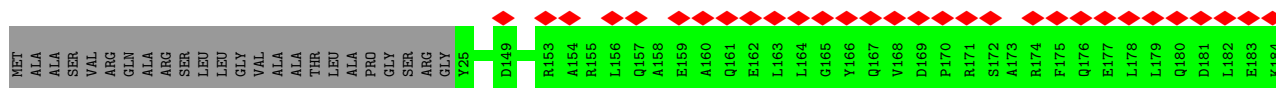
- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p: 62% 38%



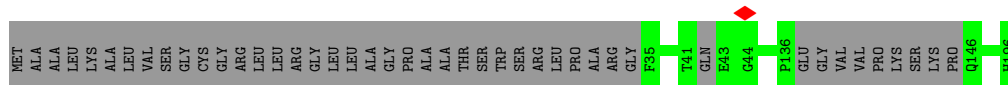
- Molecule 81: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q: 15% 74% 26%

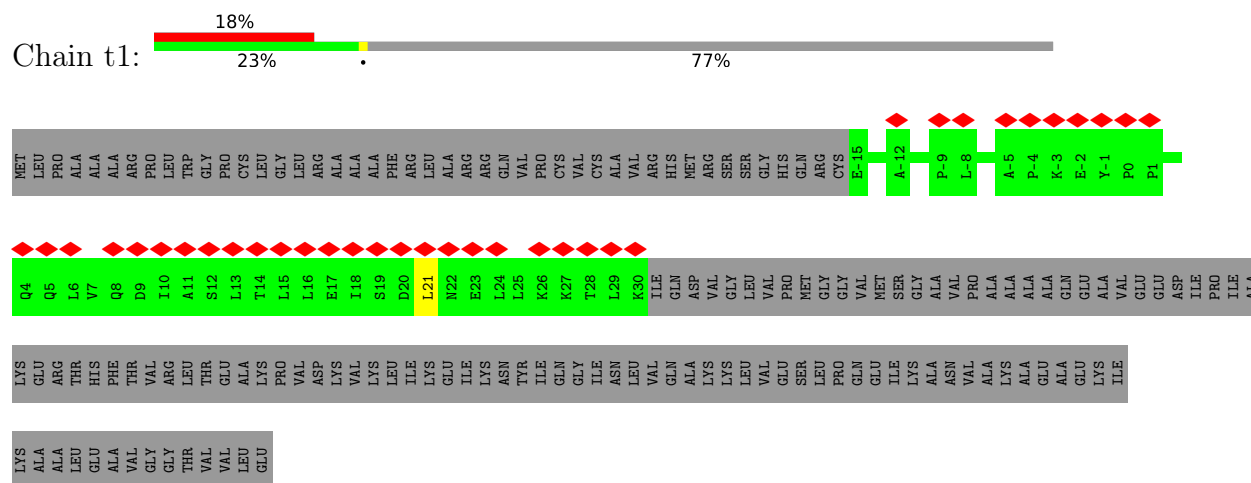


- Molecule 82: 39S ribosomal protein S18a, mitochondrial

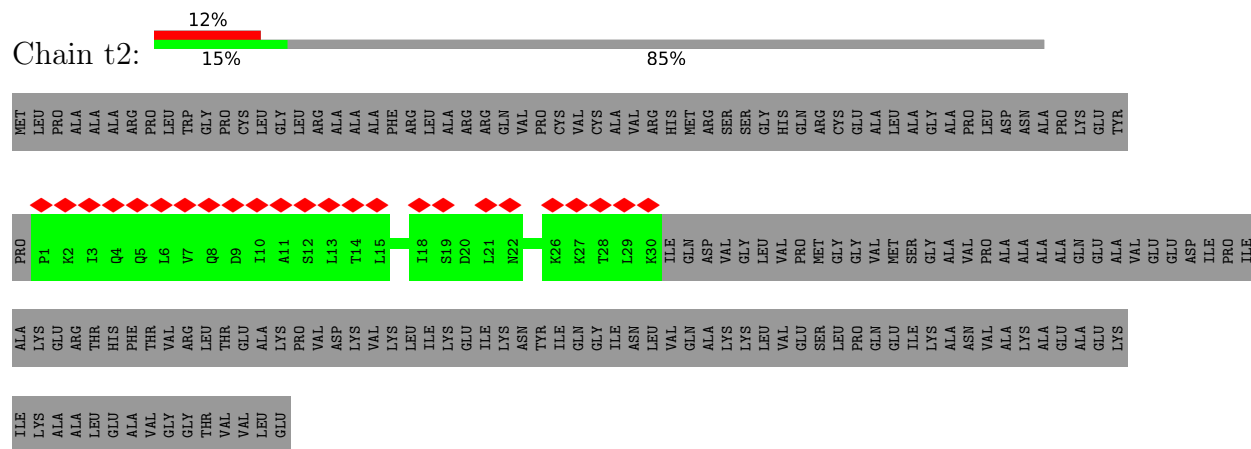
Chain r: 78% 22%



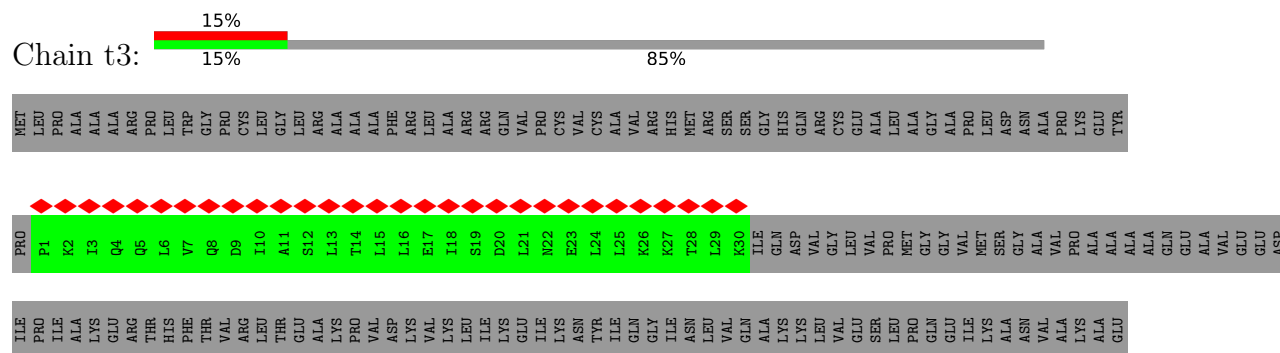
- Molecule 85: 39S ribosomal protein L12, mitochondrial



- Molecule 85: 39S ribosomal protein L12, mitochondrial



- Molecule 85: 39S ribosomal protein L12, mitochondrial



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• Molecule 85: 39S ribosomal protein L12, mitochondrial



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• Molecule 85: 39S ribosomal protein L12, mitochondrial



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• Molecule 85: 39S ribosomal protein L12, mitochondrial



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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19968	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 ( $e^-/\text{\AA}^2$ )	30	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	0.244	Depositor
Minimum map value	-0.124	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H8Q, MG, DOL, Y5P, ZN, P5P, GTP

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	0	0.31	0/895	0.46	0/1201
2	1	0.28	0/444	0.49	0/591
3	2	0.34	0/382	0.45	0/507
4	3	0.35	0/852	0.45	0/1136
5	4	0.32	0/349	0.45	0/461
6	5	0.28	0/3298	0.42	0/4492
7	6	0.28	0/3040	0.42	0/4134
8	7	0.27	0/2420	0.43	0/3270
9	8	1.84	1/1159 (0.1%)	0.46	2/1559 (0.1%)
10	9	0.29	0/1024	0.42	0/1379
11	XA	0.40	2/35592 (0.0%)	0.78	0/55390
12	A0	0.23	0/1727	0.43	0/2338
13	A1	0.24	0/2276	0.40	0/3079
14	A2	0.25	0/939	0.42	0/1256
15	A3	0.27	0/621	0.44	0/820
16	A4	0.25	0/4559	0.41	0/6149
17	AA	0.21	0/21952	0.75	1/34164 (0.0%)
18	AB	0.24	0/1819	0.40	0/2462
19	AC	0.24	0/1112	0.41	0/1505
20	AD	0.24	0/2768	0.44	0/3707
21	AE	0.24	0/989	0.44	0/1335
22	AF	0.24	0/1708	0.39	0/2291
23	AG	0.25	0/2559	0.41	0/3429
24	AH	0.24	0/1128	0.43	0/1529
25	AI	0.25	0/1031	0.43	0/1390
26	AJ	0.25	0/854	0.45	0/1148
27	AK	0.22	0/879	0.40	0/1182
28	AL	0.25	0/1406	0.40	0/1878
29	AM	0.24	0/941	0.42	0/1265
30	AN	0.25	0/864	0.43	0/1169
31	AO	0.24	0/1580	0.39	0/2150
32	AP	0.25	0/782	0.38	0/1050



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	AQ	0.24	0/746	0.42	0/993
34	AR	0.68	1/2103 (0.0%)	0.52	3/2842 (0.1%)
35	AS	0.25	0/1127	0.40	0/1518
36	AT	0.26	0/1361	0.42	0/1829
37	AU	0.23	0/1482	0.41	0/1987
38	AV	0.24	0/2925	0.40	0/3948
39	AW	0.25	0/778	0.44	0/1048
40	AX	0.25	0/2886	0.44	0/3909
41	AY	0.25	0/985	0.39	0/1329
42	AZ	0.24	0/748	0.38	0/1000
43	XB	0.21	0/1400	0.73	0/2168
44	XD	0.30	0/1879	0.48	0/2527
45	XE	0.31	0/2465	0.45	0/3344
46	XF	0.34	0/2071	0.47	0/2817
47	XH	0.27	0/798	0.46	0/1073
48	XI	0.26	0/1727	0.45	0/2340
49	XJ	0.24	0/1309	0.40	0/1764
50	XK	0.33	0/1495	0.44	0/2029
51	XL	0.30	0/904	0.46	0/1218
52	XM	0.32	0/2359	0.45	0/3185
53	XN	0.31	0/1825	0.45	0/2458
54	XO	0.28	0/1269	0.46	0/1708
55	XP	0.27	0/1190	0.46	0/1611
56	XQ	0.27	0/2026	0.44	0/2734
57	XR	0.36	0/1174	0.48	0/1572
58	XS	0.33	0/1311	0.47	0/1778
59	XT	0.35	0/1402	0.45	0/1886
60	XU	0.32	0/1200	0.43	0/1623
61	XV	0.29	0/1693	0.45	0/2297
62	XW	0.33	0/893	0.45	0/1204
63	XX	0.37	2/2090 (0.1%)	0.56	4/2825 (0.1%)
64	XY	0.29	0/1571	0.41	0/2106
65	XZ	0.32	0/1003	0.44	0/1354
66	a	0.30	0/838	0.46	0/1138
67	b	0.33	0/1202	0.45	0/1626
68	c	0.28	0/2264	0.44	0/3059
69	d	0.27	0/1807	0.42	0/2450
70	e	1.43	6/1797 (0.3%)	0.43	0/2422
71	f	0.27	0/1159	0.42	0/1565
72	g	0.33	0/1134	0.49	0/1547
73	h	0.26	0/905	0.45	0/1233
74	i	0.34	0/849	0.48	0/1135
75	j	0.29	0/703	0.44	0/947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	k	0.24	0/743	0.45	0/1003
77	l	0.24	0/692	0.37	0/939
78	m	0.23	0/508	0.45	0/682
79	o	0.32	0/818	0.45	0/1097
80	p	0.24	0/1071	0.43	0/1433
81	q	0.26	0/1413	0.42	0/1906
82	r	0.29	0/1282	0.43	0/1734
84	s	0.29	0/3114	0.44	0/4225
85	t1	0.24	0/366	0.36	0/497
85	t2	0.22	0/238	0.38	0/319
85	t3	0.23	0/238	0.37	0/319
85	t4	0.22	0/229	0.36	0/308
85	t5	0.23	0/229	0.40	0/308
85	t6	0.25	0/213	0.42	0/286
All	All	0.37	12/175956 (0.0%)	0.58	10/249618 (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
44	XD	0	1
48	XI	0	2
70	e	0	1
71	f	0	1
73	h	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	99	ARG	CG-CD	61.76	3.06	1.51
70	e	84	TYR	CD2-CE2	31.77	1.87	1.39
70	e	84	TYR	CD1-CE1	31.12	1.86	1.39
34	AR	308	HIS	C-N	28.79	1.89	1.34
70	e	84	TYR	CE2-CZ	21.80	1.66	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	XX	147	LYS	O-C-N	13.68	144.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AR	309	PRO	O-C-N	11.64	141.32	122.70
63	XX	147	LYS	CA-C-N	-9.85	95.52	117.20
34	AR	309	PRO	CA-C-N	-8.79	97.86	117.20
63	XX	150	LYS	O-C-N	-6.82	111.78	122.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	XD	206	TYR	Peptide
48	XI	197	LEU	Peptide
48	XI	90	PHE	Peptide
70	e	265	LYS	Peptide
71	f	138	GLN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	880	903	903	9	0
2	1	439	480	480	5	0
3	2	376	406	406	3	0
4	3	831	883	883	10	0
5	4	341	361	361	6	0
6	5	3204	3200	3200	31	0
7	6	2947	2839	2839	36	0
8	7	2365	2373	2372	22	0
9	8	1135	1166	1166	7	0
10	9	996	987	987	11	0
11	XA	31813	16160	16160	230	0
12	A0	1684	1685	1685	15	0
13	A1	2230	2261	2261	25	0
14	A2	925	964	964	13	0
15	A3	610	682	682	11	0
16	A4	4470	4485	4486	64	0
17	AA	19628	9970	9971	144	0
18	AB	1776	1769	1769	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AC	1082	1088	1088	12	0
20	AD	2716	2785	2785	36	0
21	AE	972	1001	1001	14	0
22	AF	1668	1714	1716	18	0
23	AG	2505	2492	2490	27	0
24	AH	1105	1136	1136	23	0
25	AI	1011	1052	1052	13	0
26	AJ	838	887	887	10	0
27	AK	861	885	885	10	0
28	AL	1382	1472	1472	15	0
29	AM	920	951	951	11	0
30	AN	846	908	908	12	0
31	AO	1528	1490	1490	19	0
32	AP	765	796	796	6	0
33	AQ	734	749	749	7	0
34	AR	2060	2074	2074	20	0
35	AS	1100	1103	1103	12	0
36	AT	1330	1342	1342	15	0
37	AU	1461	1471	1471	14	0
38	AV	2867	2863	2862	22	0
39	AW	766	785	785	5	0
40	AX	2814	2805	2804	32	0
41	AY	956	911	911	12	0
42	AZ	731	734	734	6	0
43	XB	1255	640	640	9	0
44	XD	1842	1896	1896	27	0
45	XE	2396	2402	2402	23	0
46	XF	2013	2045	2044	26	0
47	XH	784	832	832	14	0
48	XI	1691	1783	1783	16	0
49	XJ	1291	1367	1364	11	0
50	XK	1451	1448	1448	15	0
51	XL	889	941	941	8	0
52	XM	2305	2378	2378	30	0
53	XN	1778	1808	1808	16	0
54	XO	1245	1283	1283	23	0
55	XP	1164	1162	1162	18	0
56	XQ	1978	2022	2022	23	0
57	XR	1153	1214	1214	25	0
58	XS	1284	1354	1354	13	0
59	XT	1368	1410	1410	20	0
60	XU	1171	1164	1164	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	XV	1648	1656	1654	14	0
62	XW	871	898	898	10	0
63	XX	2035	2054	2054	26	0
64	XY	1534	1575	1575	27	0
65	XZ	978	1030	1030	12	0
66	a	813	777	777	0	0
67	b	1178	1180	1180	0	0
68	c	2217	2220	2220	0	0
69	d	1758	1743	1742	0	0
70	e	1762	1767	1767	0	0
71	f	1139	1152	1152	0	0
72	g	1097	1086	1085	0	0
73	h	882	866	867	0	0
74	i	827	857	857	0	0
75	j	689	678	678	0	0
76	k	732	745	745	0	0
77	l	673	654	653	0	0
78	m	500	525	525	0	0
79	o	797	804	804	0	0
80	p	1058	1083	1083	0	0
81	q	1379	1359	1359	0	0
82	r	1247	1267	1267	0	0
83	r3	1468	0	823	0	0
84	s	3036	3023	3022	0	0
85	t1	354	379	374	0	0
85	t2	238	268	270	0	0
85	t3	238	268	270	0	0
85	t4	229	255	257	0	0
85	t5	229	255	257	0	0
85	t6	214	236	236	0	0
86	0	1	0	0	0	0
86	4	1	0	0	0	0
86	AB	1	0	0	0	0
86	AO	1	0	0	0	0
86	AP	1	0	0	0	0
86	AT	1	0	0	0	0
86	r	1	0	0	0	0
87	9	1	0	0	0	0
87	AA	46	0	0	0	0
87	XA	143	0	0	0	0
87	XD	1	0	0	0	0
87	XI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	XM	1	0	0	0	0
87	XW	1	0	0	0	0
87	g	1	0	0	0	0
88	XA	73	67	0	2	0
89	XA	48	50	50	0	0
90	AX	32	10	12	1	0
All	All	168901	143004	143755	1148	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 5.

The worst 5 of 1148 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)
34:AR:308:HIS:C	34:AR:309:PRO:N	1.88	1.27
63:XX:144:TYR:O	63:XX:148:THR:HB	1.64	0.98
42:AZ:26:THR:HG1	42:AZ:30:SER:HG	1.04	0.97
16:A4:108:LEU:HD21	20:AD:154:VAL:CG1	1.98	0.92
11:XA:2954:C:O2	53:XN:182:LYS:NZ	2.03	0.92

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	
1	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
2	1	51/65 (78%)	50 (98%)	1 (2%)	0	100	100
3	2	44/92 (48%)	44 (100%)	0	0	100	100
4	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
5	4	36/103 (35%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	5	389/423 (92%)	366 (94%)	23 (6%)	0	100	100
7	6	348/380 (92%)	321 (92%)	27 (8%)	0	100	100
8	7	285/338 (84%)	262 (92%)	23 (8%)	0	100	100
9	8	132/206 (64%)	126 (96%)	6 (4%)	0	100	100
10	9	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
12	A0	197/218 (90%)	188 (95%)	9 (5%)	0	100	100
13	A1	273/323 (84%)	255 (93%)	18 (7%)	0	100	100
14	A2	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
15	A3	67/199 (34%)	67 (100%)	0	0	100	100
16	A4	526/689 (76%)	493 (94%)	33 (6%)	0	100	100
18	AB	216/296 (73%)	214 (99%)	2 (1%)	0	100	100
19	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
20	AD	341/430 (79%)	324 (95%)	17 (5%)	0	100	100
21	AE	120/125 (96%)	115 (96%)	5 (4%)	0	100	100
22	AF	197/242 (81%)	192 (98%)	5 (2%)	0	100	100
23	AG	300/396 (76%)	288 (96%)	12 (4%)	0	100	100
24	AH	133/201 (66%)	124 (93%)	9 (7%)	0	100	100
25	AI	134/194 (69%)	130 (97%)	4 (3%)	0	100	100
26	AJ	106/138 (77%)	99 (93%)	7 (7%)	0	100	100
27	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
28	AL	162/257 (63%)	157 (97%)	5 (3%)	0	100	100
29	AM	114/137 (83%)	113 (99%)	1 (1%)	0	100	100
30	AN	105/130 (81%)	101 (96%)	4 (4%)	0	100	100
31	AO	183/258 (71%)	179 (98%)	4 (2%)	0	100	100
32	AP	93/142 (66%)	87 (94%)	6 (6%)	0	100	100
33	AQ	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
34	AR	248/360 (69%)	238 (96%)	10 (4%)	0	100	100
35	AS	131/190 (69%)	123 (94%)	8 (6%)	0	100	100
36	AT	160/173 (92%)	147 (92%)	13 (8%)	0	100	100
37	AU	171/205 (83%)	169 (99%)	2 (1%)	0	100	100
38	AV	341/414 (82%)	322 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	AW	95/187 (51%)	90 (95%)	5 (5%)	0	100	100
40	AX	346/398 (87%)	329 (95%)	17 (5%)	0	100	100
41	AY	111/395 (28%)	104 (94%)	7 (6%)	0	100	100
42	AZ	84/106 (79%)	83 (99%)	1 (1%)	0	100	100
44	XD	234/305 (77%)	219 (94%)	13 (6%)	2 (1%)	14	45
45	XE	302/348 (87%)	288 (95%)	14 (5%)	0	100	100
46	XF	248/311 (80%)	239 (96%)	9 (4%)	0	100	100
47	XH	93/267 (35%)	87 (94%)	6 (6%)	0	100	100
48	XI	209/261 (80%)	193 (92%)	16 (8%)	0	100	100
49	XJ	168/192 (88%)	156 (93%)	12 (7%)	0	100	100
50	XK	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
51	XL	113/145 (78%)	106 (94%)	7 (6%)	0	100	100
52	XM	285/296 (96%)	277 (97%)	8 (3%)	0	100	100
53	XN	219/251 (87%)	208 (95%)	11 (5%)	0	100	100
54	XO	150/175 (86%)	145 (97%)	5 (3%)	0	100	100
55	XP	141/180 (78%)	130 (92%)	11 (8%)	0	100	100
56	XQ	236/292 (81%)	226 (96%)	10 (4%)	0	100	100
57	XR	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
58	XS	158/205 (77%)	153 (97%)	5 (3%)	0	100	100
59	XT	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
60	XU	137/153 (90%)	130 (95%)	7 (5%)	0	100	100
61	XV	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
62	XW	109/148 (74%)	105 (96%)	4 (4%)	0	100	100
63	XX	241/256 (94%)	234 (97%)	7 (3%)	0	100	100
64	XY	176/250 (70%)	173 (98%)	3 (2%)	0	100	100
65	XZ	118/161 (73%)	114 (97%)	4 (3%)	0	100	100
66	a	93/142 (66%)	87 (94%)	6 (6%)	0	100	100
67	b	146/215 (68%)	135 (92%)	11 (8%)	0	100	100
68	c	271/332 (82%)	260 (96%)	11 (4%)	0	100	100
69	d	212/306 (69%)	201 (95%)	10 (5%)	1 (0%)	25	58
70	e	211/279 (76%)	202 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	f	138/212 (65%)	132 (96%)	6 (4%)	0	100	100
72	g	130/166 (78%)	122 (94%)	7 (5%)	1 (1%)	16	49
73	h	106/158 (67%)	103 (97%)	2 (2%)	1 (1%)	14	45
74	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
75	j	84/123 (68%)	83 (99%)	1 (1%)	0	100	100
76	k	93/112 (83%)	90 (97%)	3 (3%)	0	100	100
77	l	78/138 (56%)	73 (94%)	5 (6%)	0	100	100
78	m	58/128 (45%)	53 (91%)	5 (9%)	0	100	100
79	o	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
80	p	119/206 (58%)	113 (95%)	6 (5%)	0	100	100
81	q	162/222 (73%)	157 (97%)	5 (3%)	0	100	100
82	r	144/196 (74%)	137 (95%)	7 (5%)	0	100	100
84	s	366/439 (83%)	351 (96%)	15 (4%)	0	100	100
85	t1	45/198 (23%)	40 (89%)	5 (11%)	0	100	100
85	t2	28/198 (14%)	28 (100%)	0	0	100	100
85	t3	28/198 (14%)	28 (100%)	0	0	100	100
85	t4	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
85	t5	27/198 (14%)	26 (96%)	1 (4%)	0	100	100
85	t6	25/198 (13%)	25 (100%)	0	0	100	100
All	All	13778/19160 (72%)	13145 (95%)	628 (5%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
72	g	38	PHE
44	XD	207	ILE
44	XD	208	ARG
73	h	78	PHE
69	d	289	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	50/60 (83%)	50 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	350 (99%)	3 (1%)	79	84
7	6	313/332 (94%)	312 (100%)	1 (0%)	91	92
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	124/190 (65%)	123 (99%)	1 (1%)	79	84
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	176/190 (93%)	175 (99%)	1 (1%)	84	88
13	A1	253/291 (87%)	251 (99%)	2 (1%)	79	84
14	A2	99/101 (98%)	97 (98%)	2 (2%)	50	68
15	A3	63/166 (38%)	63 (100%)	0	100	100
16	A4	494/609 (81%)	490 (99%)	4 (1%)	79	84
18	AB	192/249 (77%)	192 (100%)	0	100	100
19	AC	115/143 (80%)	115 (100%)	0	100	100
20	AD	283/357 (79%)	281 (99%)	2 (1%)	81	86
21	AE	104/107 (97%)	104 (100%)	0	100	100
22	AF	178/209 (85%)	178 (100%)	0	100	100
23	AG	264/342 (77%)	264 (100%)	0	100	100
24	AH	125/180 (69%)	125 (100%)	0	100	100
25	AI	104/147 (71%)	104 (100%)	0	100	100
26	AJ	93/118 (79%)	93 (100%)	0	100	100
27	AK	91/113 (80%)	91 (100%)	0	100	100
28	AL	152/226 (67%)	151 (99%)	1 (1%)	81	86
29	AM	95/113 (84%)	95 (100%)	0	100	100
30	AN	93/115 (81%)	93 (100%)	0	100	100
31	AO	166/230 (72%)	166 (100%)	0	100	100
32	AP	86/123 (70%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	AQ	77/79 (98%)	77 (100%)	0	100	100
34	AR	229/318 (72%)	228 (100%)	1 (0%)	89	91
35	AS	115/164 (70%)	115 (100%)	0	100	100
36	AT	150/157 (96%)	150 (100%)	0	100	100
37	AU	149/174 (86%)	148 (99%)	1 (1%)	81	86
38	AV	315/364 (86%)	314 (100%)	1 (0%)	91	92
39	AW	84/158 (53%)	84 (100%)	0	100	100
40	AX	307/351 (88%)	302 (98%)	5 (2%)	58	73
41	AY	104/357 (29%)	104 (100%)	0	100	100
42	AZ	79/95 (83%)	79 (100%)	0	100	100
44	XD	190/245 (78%)	188 (99%)	2 (1%)	70	79
45	XE	259/290 (89%)	259 (100%)	0	100	100
46	XF	217/262 (83%)	217 (100%)	0	100	100
47	XH	86/228 (38%)	86 (100%)	0	100	100
48	XI	194/232 (84%)	194 (100%)	0	100	100
49	XJ	133/150 (89%)	132 (99%)	1 (1%)	79	84
50	XK	155/156 (99%)	155 (100%)	0	100	100
51	XL	98/124 (79%)	98 (100%)	0	100	100
52	XM	245/249 (98%)	244 (100%)	1 (0%)	89	91
53	XN	188/211 (89%)	188 (100%)	0	100	100
54	XO	133/150 (89%)	133 (100%)	0	100	100
55	XP	125/155 (81%)	124 (99%)	1 (1%)	79	84
56	XQ	220/256 (86%)	220 (100%)	0	100	100
57	XR	118/126 (94%)	118 (100%)	0	100	100
58	XS	145/180 (81%)	145 (100%)	0	100	100
59	XT	146/176 (83%)	146 (100%)	0	100	100
60	XU	126/135 (93%)	126 (100%)	0	100	100
61	XV	179/191 (94%)	178 (99%)	1 (1%)	84	88
62	XW	91/119 (76%)	90 (99%)	1 (1%)	70	79
63	XX	219/229 (96%)	219 (100%)	0	100	100
64	XY	161/223 (72%)	161 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	XZ	111/147 (76%)	111 (100%)	0	100	100
66	a	93/133 (70%)	93 (100%)	0	100	100
67	b	130/186 (70%)	130 (100%)	0	100	100
68	c	241/288 (84%)	240 (100%)	1 (0%)	89	91
69	d	196/274 (72%)	196 (100%)	0	100	100
70	e	188/236 (80%)	187 (100%)	1 (0%)	86	90
71	f	127/188 (68%)	127 (100%)	0	100	100
72	g	122/148 (82%)	122 (100%)	0	100	100
73	h	103/148 (70%)	103 (100%)	0	100	100
74	i	86/110 (78%)	86 (100%)	0	100	100
75	j	68/97 (70%)	68 (100%)	0	100	100
76	k	80/90 (89%)	80 (100%)	0	100	100
77	l	74/116 (64%)	74 (100%)	0	100	100
78	m	54/113 (48%)	54 (100%)	0	100	100
79	o	80/87 (92%)	80 (100%)	0	100	100
80	p	117/181 (65%)	117 (100%)	0	100	100
81	q	141/178 (79%)	141 (100%)	0	100	100
82	r	138/169 (82%)	138 (100%)	0	100	100
84	s	326/381 (86%)	326 (100%)	0	100	100
85	t1	41/158 (26%)	40 (98%)	1 (2%)	44	62
85	t2	29/158 (18%)	29 (100%)	0	100	100
85	t3	29/158 (18%)	29 (100%)	0	100	100
85	t4	28/158 (18%)	28 (100%)	0	100	100
85	t5	28/158 (18%)	28 (100%)	0	100	100
85	t6	26/158 (16%)	26 (100%)	0	100	100
All	All	12392/16507 (75%)	12357 (100%)	35 (0%)	90	92

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	XM	44	ARG
55	XP	164	MET
68	c	302	ARG

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Mol	Chain	Res	Type
16	A4	403	LYS
16	A4	242	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
40	AX	347	ASN
76	k	15	GLN
41	AY	378	ASN
56	XQ	158	GLN
77	l	135	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	XA	1489/1561 (95%)	262 (17%)	7 (0%)
17	AA	916/954 (96%)	161 (17%)	3 (0%)
43	XB	54/72 (75%)	11 (20%)	0
83	r3	0/75	-	-
All	All	2459/2662 (92%)	434 (17%)	10 (0%)

5 of 434 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	XA	1681	G
11	XA	1685	C
11	XA	1689	C
11	XA	1692	A
11	XA	1693	C

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	AA	770	C
17	AA	1048	C
17	AA	1234	C
11	XA	2558	A
11	XA	2574	G

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

75 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$
83	Y5P	r3	55	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	P5P	r3	65	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	14	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	27	83	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	28	83	16,23,24	0.94	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	30	83	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	43	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	49	83	14,19,20	3.15	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	25	83	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
83	Y5P	r3	13	83	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
83	P5P	r3	71	83	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	23	83	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	60	83	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	P5P	r3	31	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	54	83	14,19,20	3.13	3 (21%)	18,26,29	0.56	0
83	P5P	r3	70	83	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	74	83,11	16,23,24	0.96	1 (6%)	14,33,36	2.11	3 (21%)
83	P5P	r3	37	83	20,24,24	0.87	1 (5%)	21,36,36	4.65	9 (42%)
83	P5P	r3	7	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	68	83	14,19,20	3.16	3 (21%)	18,26,29	0.58	0
83	P5P	r3	46	83	16,23,24	0.95	1 (6%)	14,33,36	1.96	3 (21%)
83	Y5P	r3	67	83	14,19,20	3.13	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	2	83	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
83	P5P	r3	24	83	16,23,24	0.95	1 (6%)	14,33,36	1.97	3 (21%)
83	P5P	r3	57	83	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	18	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
83	Y5P	r3	45	83	14,19,20	3.14	3 (21%)	18,26,29	0.56	0
83	Y5P	r3	42	83	14,19,20	3.14	3 (21%)	18,26,29	0.54	0
83	Y5P	r3	75	83	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
83	P5P	r3	19	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	15	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	9	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	52	83	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	6	83	16,23,24	0.95	1 (6%)	14,33,36	2.01	3 (21%)
83	P5P	r3	44	83	16,23,24	0.94	1 (6%)	14,33,36	2.00	3 (21%)
83	Y5P	r3	62	83	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	Y5P	r3	50	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	32	83	14,19,20	3.14	3 (21%)	18,26,29	0.61	0
83	Y5P	r3	33	83	14,19,20	3.14	3 (21%)	18,26,29	0.53	0
83	Y5P	r3	8	83	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
83	Y5P	r3	72	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	3	83	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
83	P5P	r3	21	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	5	83	16,23,24	0.95	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	69	83	16,23,24	0.94	1 (6%)	14,33,36	1.97	3 (21%)
83	P5P	r3	1	83	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
83	P5P	r3	26	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	38	83	16,23,24	0.95	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	41	83	14,19,20	3.14	3 (21%)	18,26,29	0.58	0
83	Y5P	r3	12	83	14,19,20	3.15	3 (21%)	18,26,29	0.56	0
83	Y5P	r3	39	83	14,19,20	3.15	3 (21%)	18,26,29	0.55	0
83	Y5P	r3	56	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	P5P	r3	73	83	16,23,24	0.97	1 (6%)	14,33,36	2.00	3 (21%)
83	Y5P	r3	17	83	14,19,20	3.15	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	16	83	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	Y5P	r3	47	83	14,19,20	3.13	3 (21%)	18,26,29	0.61	0
83	Y5P	r3	66	83	14,19,20	3.15	3 (21%)	18,26,29	0.54	0
83	P5P	r3	53	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	P5P	r3	35	83	16,23,24	0.95	1 (6%)	14,33,36	2.00	3 (21%)
83	Y5P	r3	4	83	14,19,20	3.12	3 (21%)	18,26,29	0.60	0
83	P5P	r3	58	83	16,23,24	0.94	1 (6%)	14,33,36	1.98	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
83	P5P	r3	29	83	16,23,24	0.94	1 (6%)	14,33,36	2.01	3 (21%)
83	Y5P	r3	51	83	14,19,20	3.13	3 (21%)	18,26,29	0.59	0
83	P5P	r3	63	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	P5P	r3	10	83	16,23,24	0.96	1 (6%)	14,33,36	1.98	3 (21%)
83	Y5P	r3	59	83	14,19,20	3.14	3 (21%)	18,26,29	0.59	0
83	Y5P	r3	40	83	14,19,20	3.15	3 (21%)	18,26,29	0.57	0
83	Y5P	r3	61	83	14,19,20	3.15	3 (21%)	18,26,29	0.54	0
83	P5P	r3	34	83	16,23,24	0.96	1 (6%)	14,33,36	2.02	3 (21%)
83	P5P	r3	22	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	48	83	14,19,20	3.14	3 (21%)	18,26,29	0.55	0
83	P5P	r3	36	83	16,23,24	0.97	1 (6%)	14,33,36	1.99	3 (21%)
83	Y5P	r3	20	83	14,19,20	3.14	4 (28%)	18,26,29	0.59	0
83	Y5P	r3	11	83	14,19,20	3.14	3 (21%)	18,26,29	0.57	0
83	P5P	r3	64	83	16,23,24	0.96	1 (6%)	14,33,36	1.99	3 (21%)

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
83	Y5P	r3	55	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	65	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	14	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	27	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	28	83	-	2/3/25/26	0/3/3/3
83	P5P	r3	30	83	-	1/3/25/26	0/3/3/3
83	Y5P	r3	43	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	49	83	-	3/7/33/34	0/2/2/2
83	Y5P	r3	25	83	-	3/7/33/34	0/2/2/2
83	Y5P	r3	13	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	71	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	23	83	-	3/3/25/26	0/3/3/3
83	Y5P	r3	60	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	31	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	54	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	70	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	74	83,11	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	P5P	r3	37	83	-	2/6/26/26	0/3/3/3
83	P5P	r3	7	83	-	2/3/25/26	0/3/3/3
83	Y5P	r3	68	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	46	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	67	83	-	3/7/33/34	0/2/2/2
83	Y5P	r3	2	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	24	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	57	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	18	83	-	2/3/25/26	0/3/3/3
83	Y5P	r3	45	83	-	4/7/33/34	0/2/2/2
83	Y5P	r3	42	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	75	83	-	6/7/33/34	0/2/2/2
83	P5P	r3	19	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	15	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	9	83	-	2/3/25/26	0/3/3/3
83	P5P	r3	52	83	-	3/3/25/26	0/3/3/3
83	P5P	r3	6	83	-	2/3/25/26	0/3/3/3
83	P5P	r3	44	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	62	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	50	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	32	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	33	83	-	2/7/33/34	0/2/2/2
83	Y5P	r3	8	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	72	83	-	3/7/33/34	0/2/2/2
83	Y5P	r3	3	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	21	83	-	1/3/25/26	0/3/3/3
83	P5P	r3	5	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	69	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	1	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	26	83	-	2/3/25/26	0/3/3/3
83	P5P	r3	38	83	-	1/3/25/26	0/3/3/3
83	Y5P	r3	41	83	-	3/7/33/34	0/2/2/2
83	Y5P	r3	12	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	39	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	56	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	73	83	-	2/3/25/26	0/3/3/3
83	Y5P	r3	17	83	-	3/7/33/34	0/2/2/2
83	Y5P	r3	16	83	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	Y5P	r3	47	83	-	4/7/33/34	0/2/2/2
83	Y5P	r3	66	83	-	3/7/33/34	0/2/2/2
83	P5P	r3	53	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	35	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	4	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	58	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	29	83	-	2/3/25/26	0/3/3/3
83	Y5P	r3	51	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	63	83	-	0/3/25/26	0/3/3/3
83	P5P	r3	10	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	59	83	-	2/7/33/34	0/2/2/2
83	Y5P	r3	40	83	-	1/7/33/34	0/2/2/2
83	Y5P	r3	61	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	34	83	-	1/3/25/26	0/3/3/3
83	P5P	r3	22	83	-	3/3/25/26	0/3/3/3
83	Y5P	r3	48	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	36	83	-	0/3/25/26	0/3/3/3
83	Y5P	r3	20	83	-	2/7/33/34	0/2/2/2
83	Y5P	r3	11	83	-	1/7/33/34	0/2/2/2
83	P5P	r3	64	83	-	2/3/25/26	0/3/3/3

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	r3	68	Y5P	C6-C5	10.61	1.52	1.33
83	r3	17	Y5P	C6-C5	10.58	1.52	1.33
83	r3	39	Y5P	C6-C5	10.58	1.52	1.33
83	r3	66	Y5P	C6-C5	10.58	1.52	1.33
83	r3	3	Y5P	C6-C5	10.58	1.52	1.33

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	r3	37	P5P	OP2-P-O5'	-10.25	79.46	106.73
83	r3	37	P5P	O5'-P-OP1	-9.37	80.20	106.47
83	r3	37	P5P	OP2-P-OP1	8.11	142.42	110.68
83	r3	37	P5P	OP3-P-O5'	7.05	125.48	106.73
83	r3	37	P5P	OP3-P-OP1	-6.90	83.67	110.68

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	r3	9	P5P	O4'-C4'-C5'-O5'
83	r3	13	Y5P	C3'-C4'-C5'-O5'
83	r3	13	Y5P	O4'-C1'-N1-C2
83	r3	16	Y5P	O4'-C1'-N1-C2
83	r3	17	Y5P	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 205 ligands modelled in this entry, 202 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
90	GTP	AX	500	-	26,34,34	1.12	2 (7%)	32,54,54	1.51	6 (18%)
89	DOL	XA	5145	-	43,50,50	3.50	17 (39%)	51,70,70	2.67	9 (17%)
88	H8Q	XA	5144	-	77,80,80	1.08	5 (6%)	103,115,115	1.34	15 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	GTP	AX	500	-	-	8/18/38/38	0/3/3/3
89	DOL	XA	5145	-	-	14/58/77/77	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	H8Q	XA	5144	-	-	31/83/127/127	0/8/8/8

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	XA	5145	DOL	C28-C29	10.06	1.56	1.32
89	XA	5145	DOL	C22-C23	9.59	1.57	1.32
89	XA	5145	DOL	C19-C20	7.17	1.57	1.34
89	XA	5145	DOL	C6-N5	6.56	1.49	1.34
89	XA	5145	DOL	C26-N25	6.40	1.48	1.34

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	XA	5145	DOL	O40-S39-O41	-15.14	100.93	118.19
89	XA	5145	DOL	C24-N25-C26	-5.45	113.21	122.03
89	XA	5145	DOL	C23-C22-C20	-3.87	120.04	125.89
88	XA	5144	H8Q	O41-C34-C33	3.84	122.03	110.83
90	AX	500	GTP	PA-O3A-PB	-3.70	120.14	132.83

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	XA	5144	H8Q	C2-C1-N13-C14
88	XA	5144	H8Q	C2-C1-N13-C18
88	XA	5144	H8Q	O1-C1-N13-C14
88	XA	5144	H8Q	O1-C1-N13-C18
88	XA	5144	H8Q	C33-C34-O41-C43

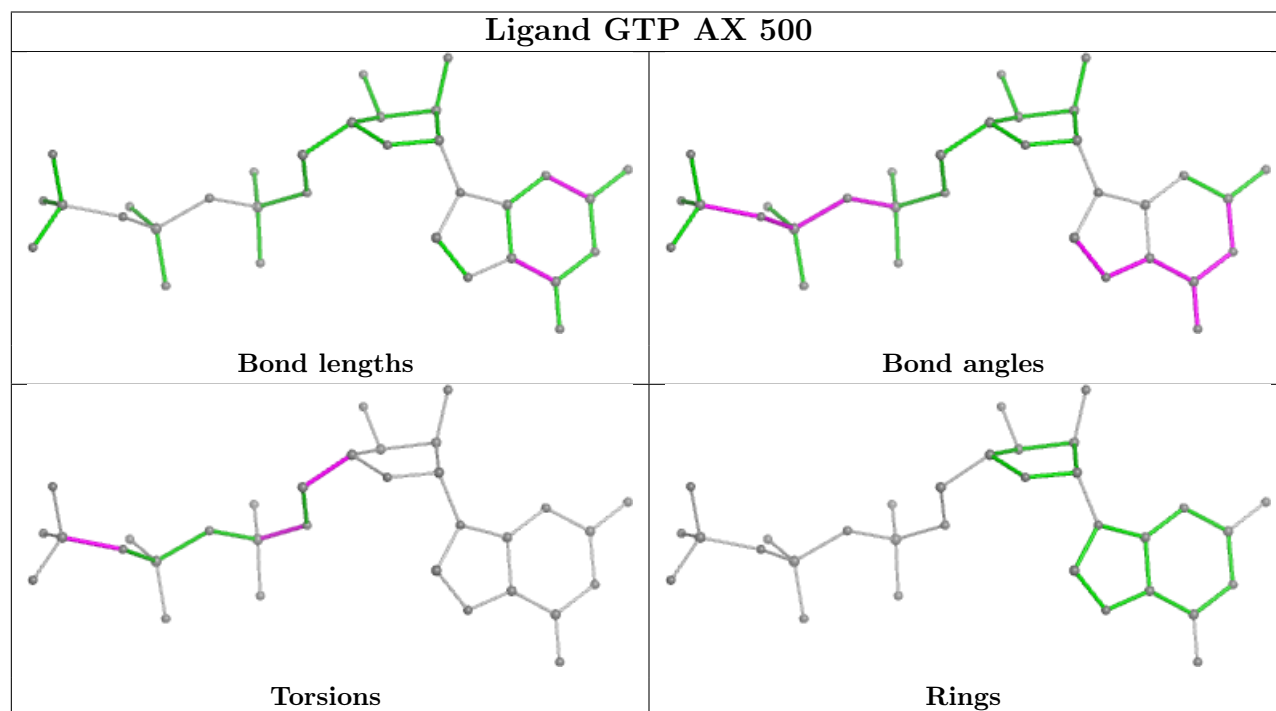
There are no ring outliers.

2 monomers are involved in 3 short contacts:

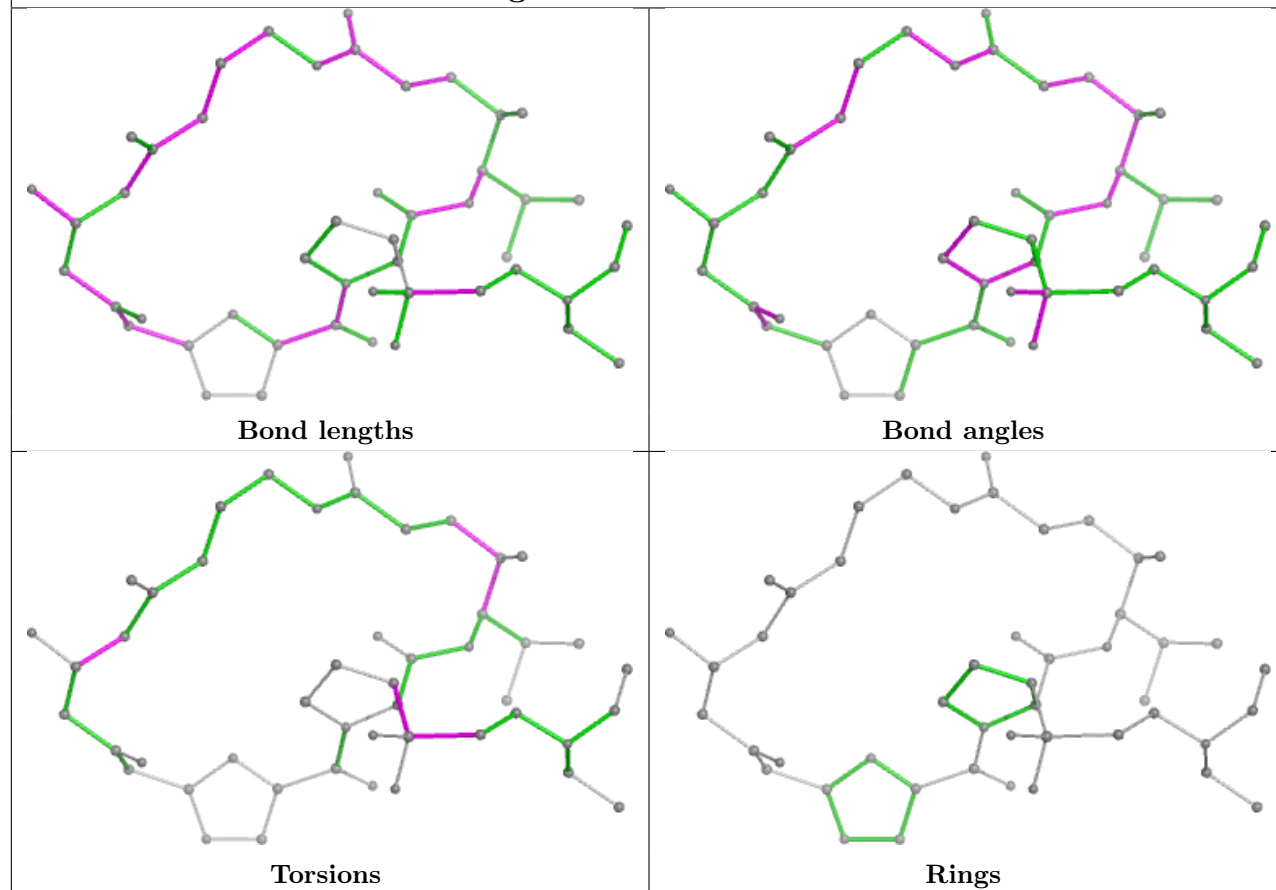
Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	AX	500	GTP	1	0
88	XA	5144	H8Q	2	0

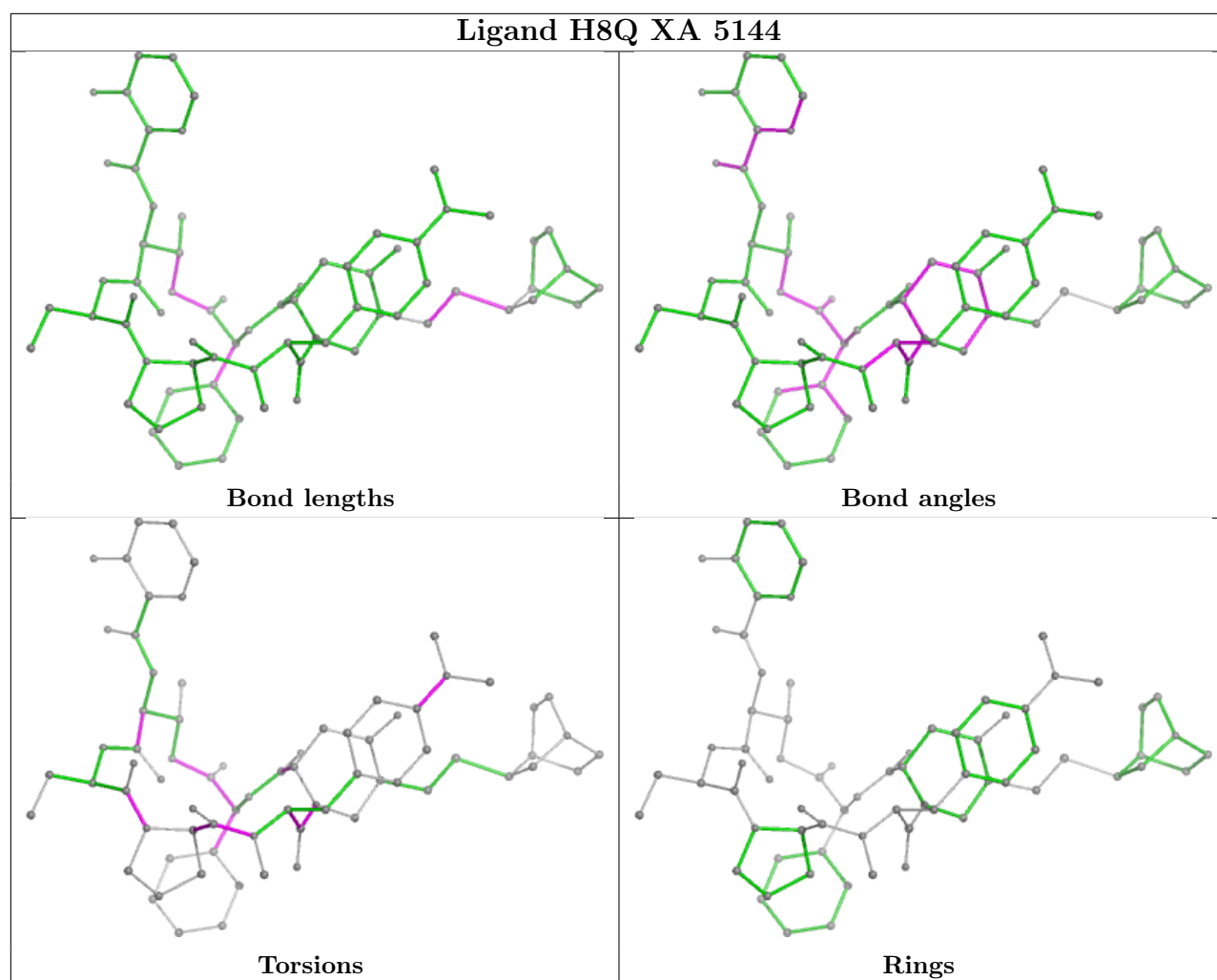
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand DOL XA 5145





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	A4	2
8	7	2
7	6	2
82	r	1
38	AV	1
6	5	1
34	AR	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A4	537:ARG	C	538:ASP	N	6.17
1	7	285:ASN	C	286:LEU	N	5.98
1	r	134:ARG	C	135:LEU	N	5.26
1	AV	269:SER	C	270:PRO	N	4.49
1	7	185:LEU	C	186:ASP	N	3.31



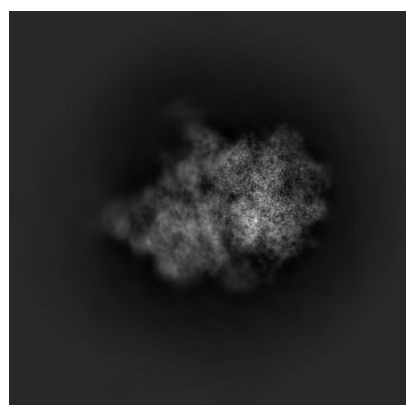
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12877. These allow visual inspection of the internal detail of the map and identification of artifacts.

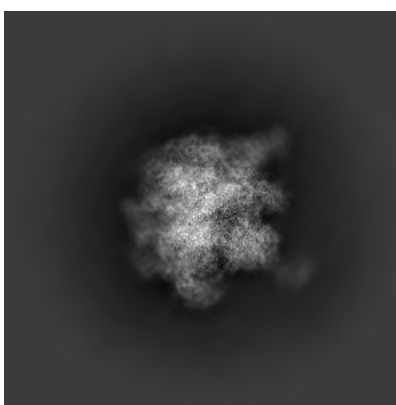
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

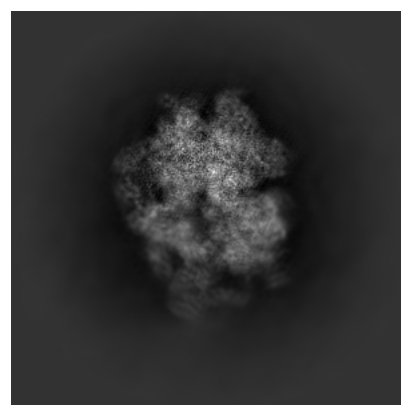
#### 6.1.1 Primary map



X



Y

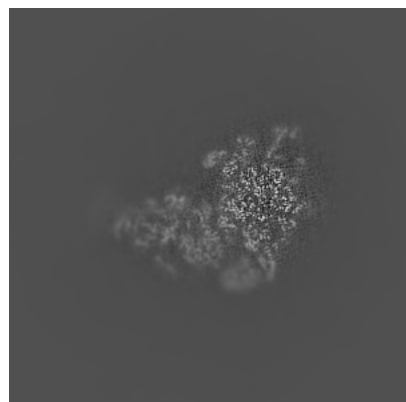


Z

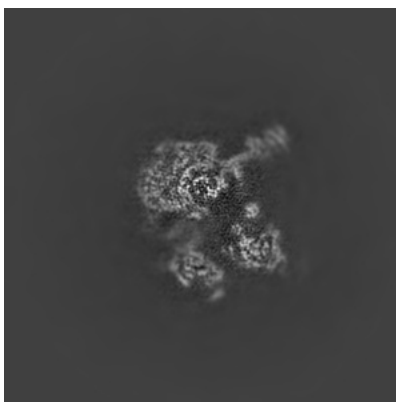
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

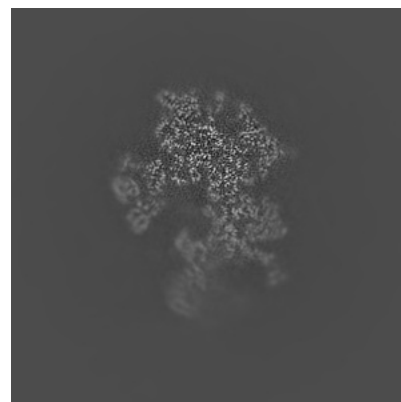
#### 6.2.1 Primary map



X Index: 260



Y Index: 260

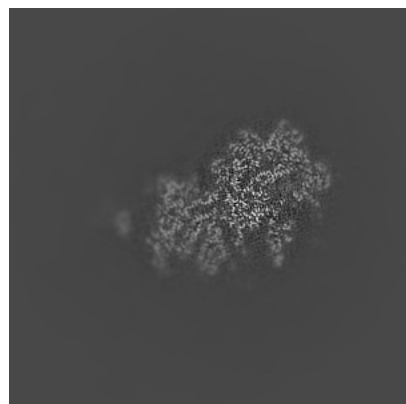


Z Index: 260

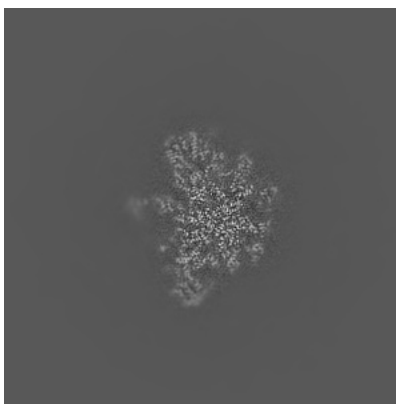
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

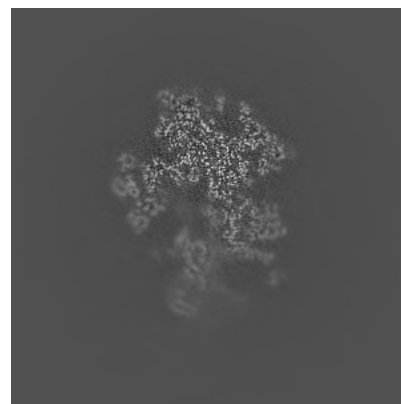
### 6.3.1 Primary map



X Index: 282



Y Index: 321

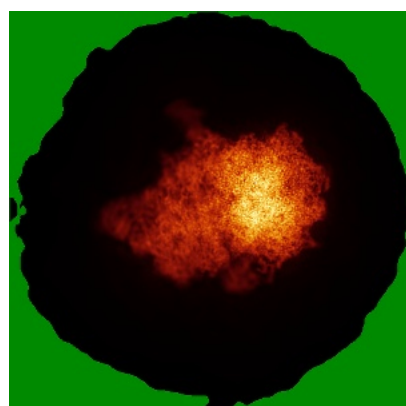


Z Index: 257

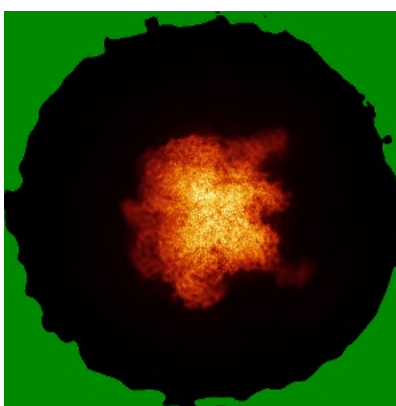
The images above show the largest variance slices of the map in three orthogonal directions.

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

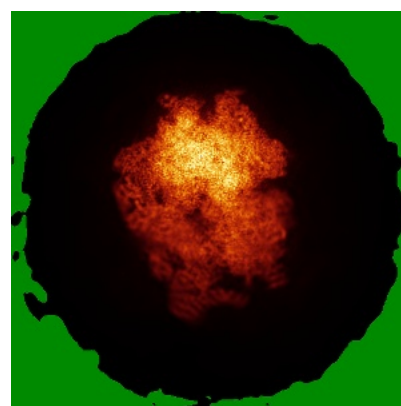
### 6.4.1 Primary map



X



Y

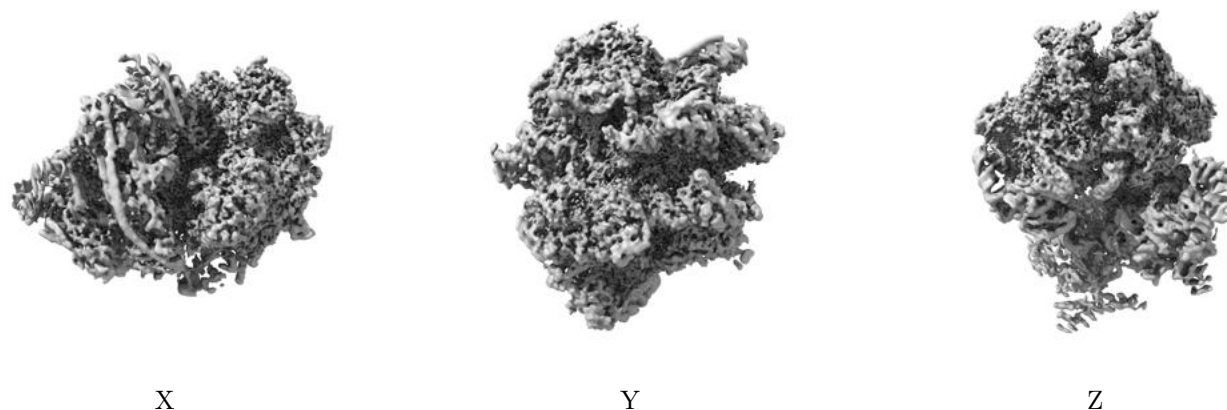


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

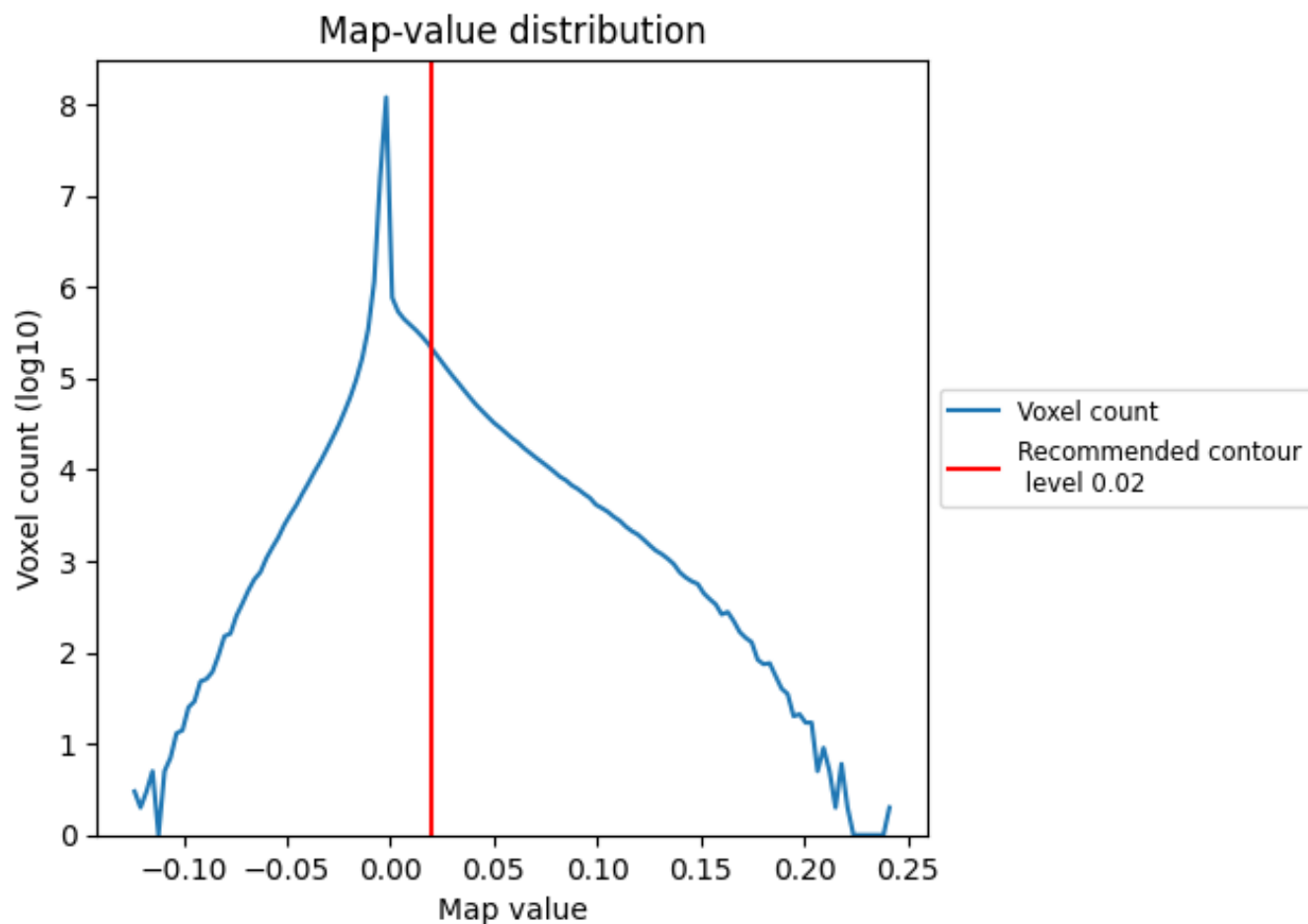
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

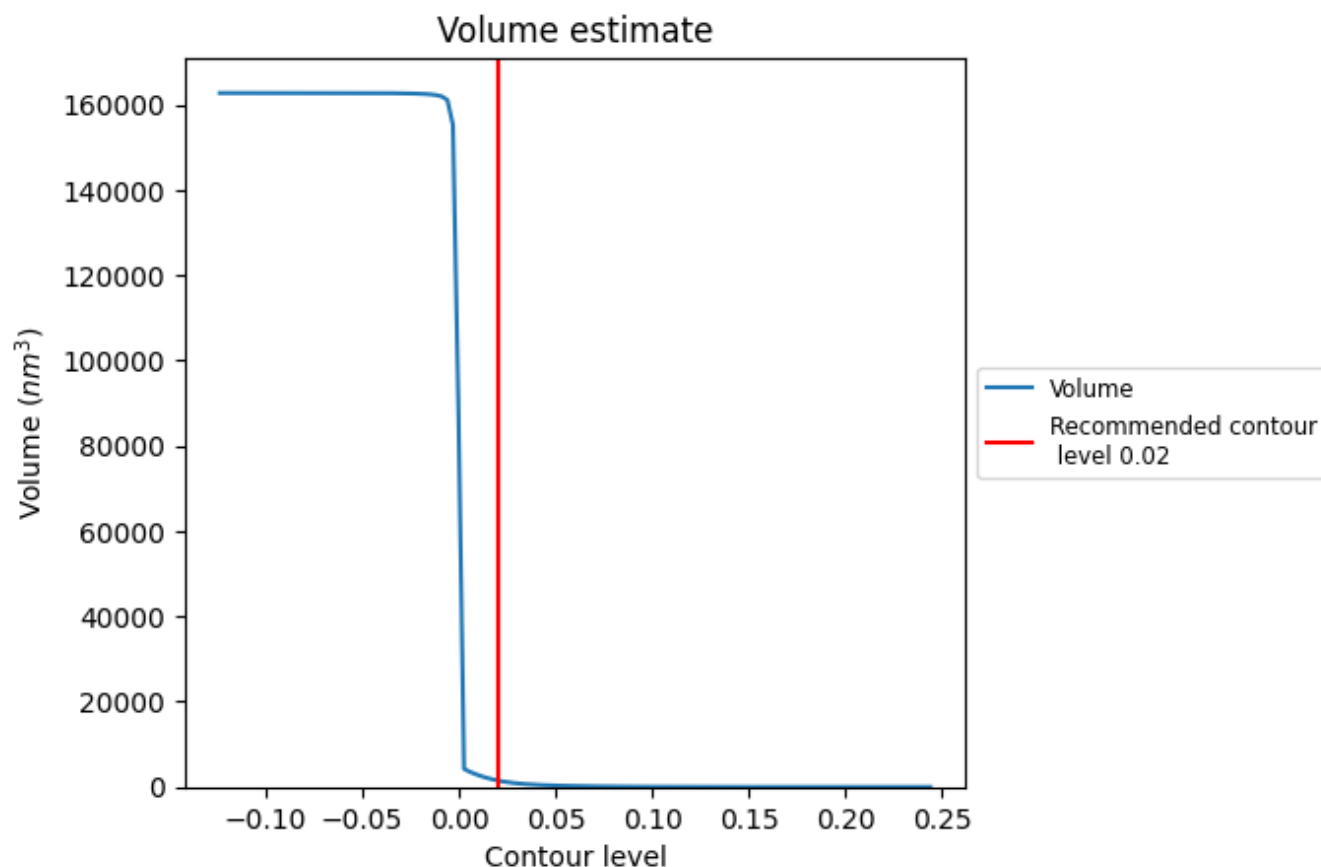
This section contains the results of statistical analysis of the map.

### 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.

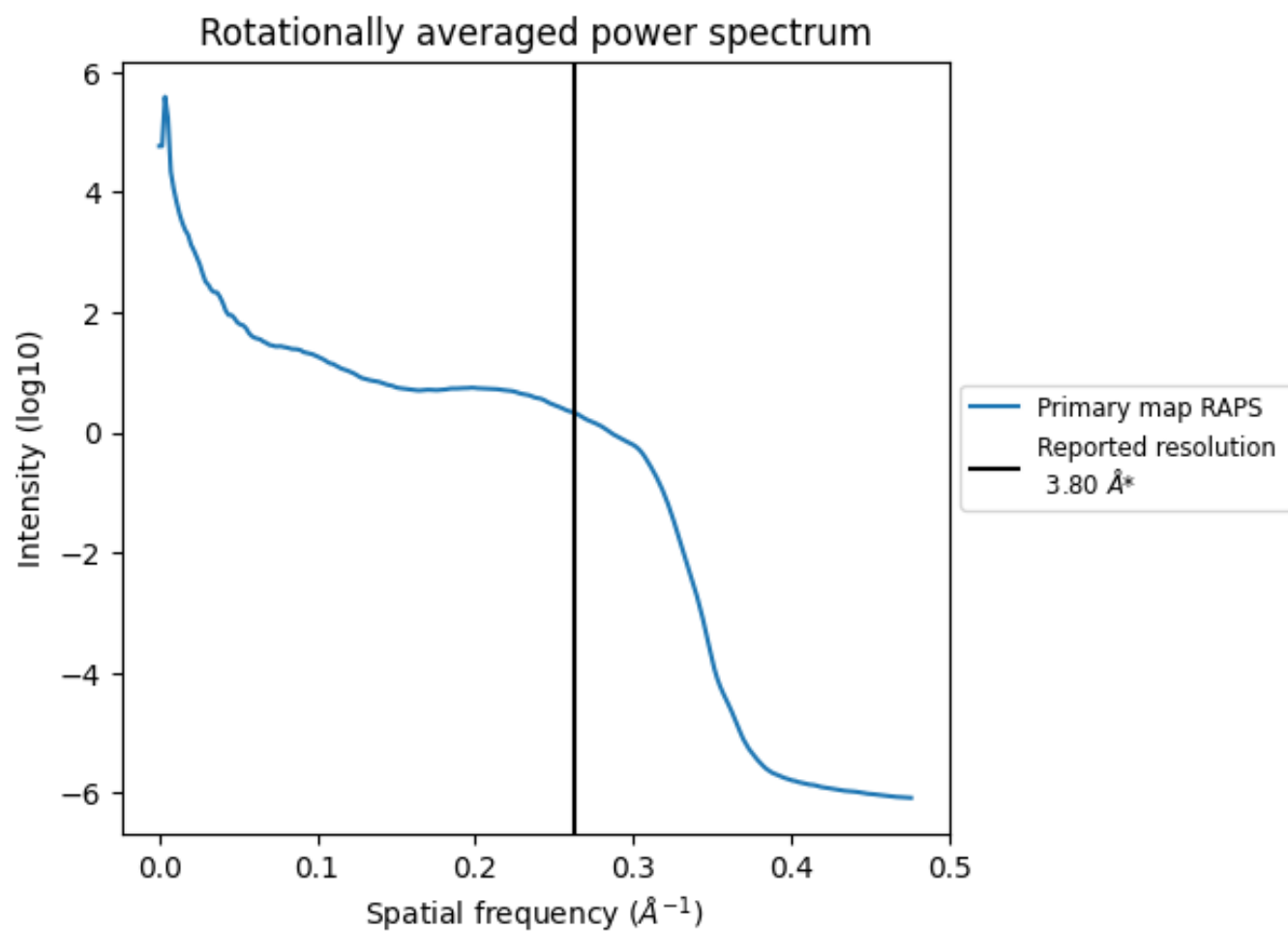
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1527  $\text{nm}^3$ ; this corresponds to an approximate mass of 1379 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 0.263 Å<sup>-1</sup>

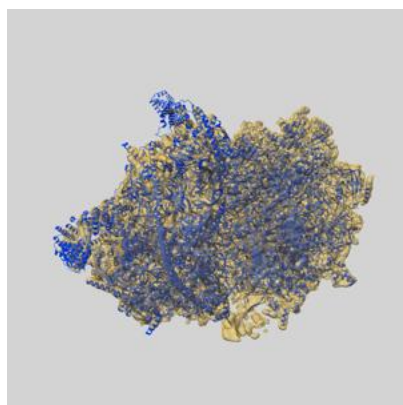
## 8 Fourier-Shell correlation

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

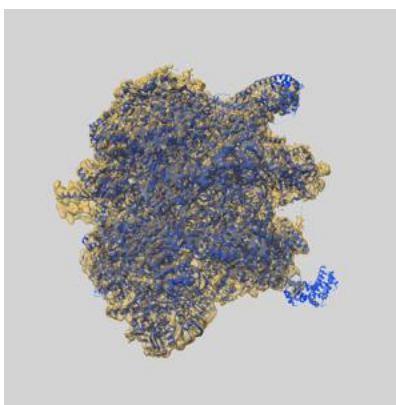
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12877 and PDB model 7OG4. Per-residue inclusion information can be found in section [3](#) on page [23](#).

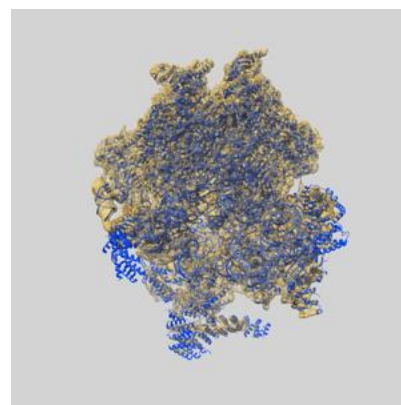
### 9.1 Map-model overlay [i](#)



X



Y

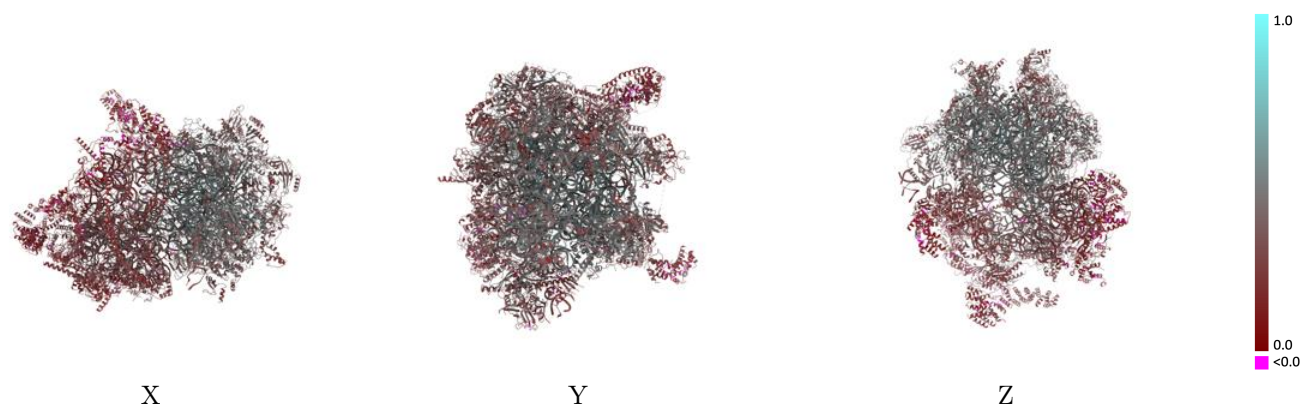


Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

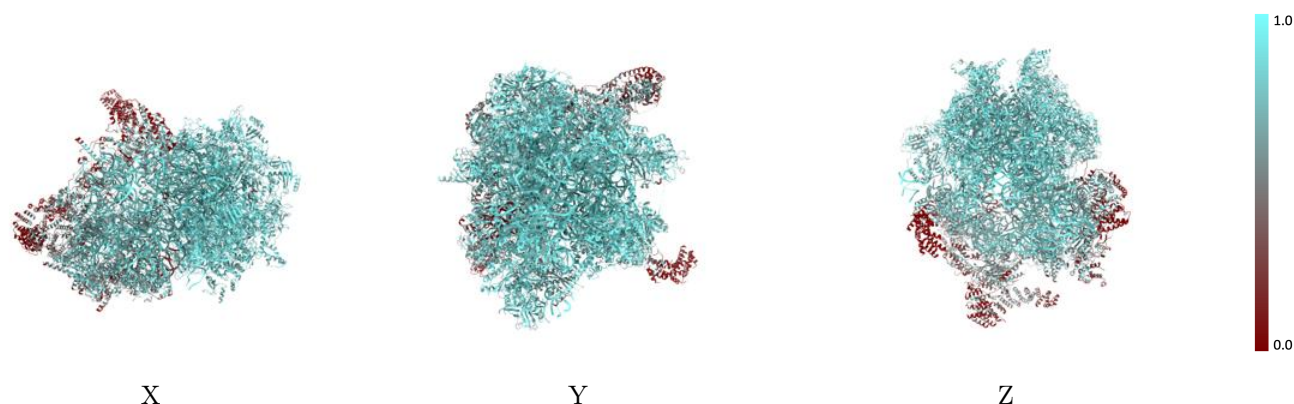


## 9.2 Q-score mapped to coordinate model [i](#)



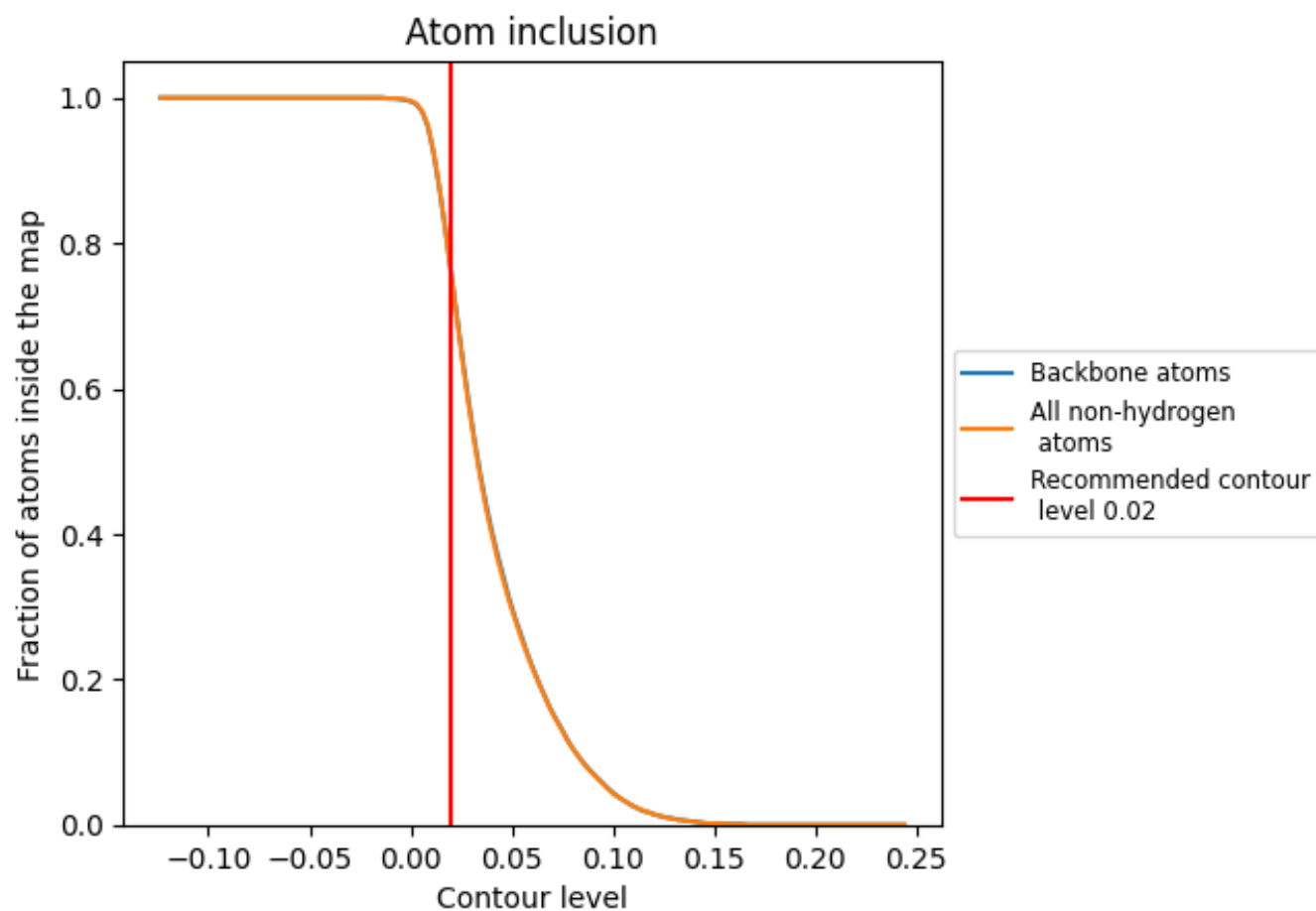
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.3480
0	 0.8310	 0.4140
1	 0.8520	 0.4090
2	 0.9110	 0.5090
3	 0.9000	 0.5010
4	 0.9230	 0.4730
5	 0.8510	 0.4010
6	 0.8100	 0.3530
7	 0.8160	 0.3660
8	 0.6130	 0.2280
9	 0.8210	 0.3930
A0	 0.4230	 0.1660
A1	 0.4360	 0.1900
A2	 0.6190	 0.2530
A3	 0.7610	 0.3660
A4	 0.2550	 0.1590
AA	 0.9010	 0.3120
AB	 0.7040	 0.2630
AC	 0.5440	 0.2180
AD	 0.5760	 0.2700
AE	 0.6670	 0.3280
AF	 0.5720	 0.2160
AG	 0.5560	 0.2180
AH	 0.4310	 0.1890
AI	 0.6470	 0.2900
AJ	 0.7070	 0.2690
AK	 0.4610	 0.1940
AL	 0.6610	 0.2720
AM	 0.5650	 0.1930
AN	 0.6070	 0.2600
AO	 0.5460	 0.2210
AP	 0.6940	 0.3120
AQ	 0.6960	 0.3220
AR	 0.4620	 0.1700
AS	 0.5840	 0.2390































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Chain	Atom inclusion	Q-score
AT	 0.6490	 0.2540
AU	 0.6340	 0.2070
AV	 0.3560	 0.1550
AW	 0.5900	 0.2570
AX	 0.3540	 0.1600
AY	 0.2540	 0.1750
AZ	 0.5460	 0.1760
XA	 0.9600	 0.4830
XB	 0.9550	 0.3170
XD	 0.8790	 0.4480
XE	 0.8620	 0.4440
XF	 0.8870	 0.4530
XH	 0.8090	 0.3640
XI	 0.6040	 0.2720
XJ	 0.6600	 0.2230
XK	 0.8740	 0.4570
XL	 0.8820	 0.4540
XM	 0.8590	 0.4430
XN	 0.8530	 0.4370
XO	 0.8670	 0.4240
XP	 0.8360	 0.3850
XQ	 0.7730	 0.3860
XR	 0.8740	 0.4730
XS	 0.8680	 0.4600
XT	 0.8890	 0.4680
XU	 0.8780	 0.4400
XV	 0.8090	 0.3720
XW	 0.9010	 0.4750
XX	 0.8210	 0.3930
XY	 0.8680	 0.4270
XZ	 0.8880	 0.4660
a	 0.8280	 0.4140
b	 0.8870	 0.4540
c	 0.8410	 0.3890
d	 0.7830	 0.3510
e	 0.6590	 0.1920
f	 0.6870	 0.2630
g	 0.8650	 0.4310
h	 0.7990	 0.3490
i	 0.8890	 0.4810
j	 0.8380	 0.4150
k	 0.7840	 0.3040

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Chain	Atom inclusion	Q-score
l	 0.7130	 0.2600
m	 0.6960	 0.2260
o	 0.9020	 0.4730
p	 0.8170	 0.3490
q	 0.6530	 0.3050
r	 0.8810	 0.4210
r3	 0.0760	 0.0780
s	 0.8620	 0.4190
t1	 0.2180	 0.1990
t2	 0.1810	 0.1860
t3	 0.0000	 0.1740
t4	 0.0000	 0.1200
t5	 0.0000	 0.1370
t6	 0.0000	 0.1020