



wwPDB EM Validation Summary Report ⓘ

Aug 17, 2026 – 09:34 PM EDT

PDB ID : 9PG8 / pdb_00009pg8
EMDB ID : EMD-71623
Title : In situ structure of the human mitoribosome in the P-E state
Authors : Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on : 2025-07-07
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

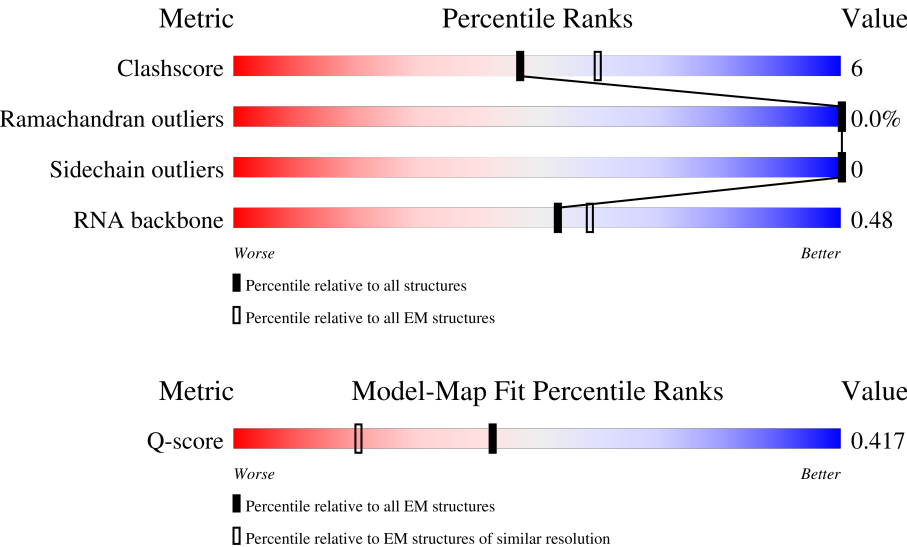
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.06 Å.

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



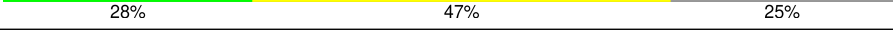
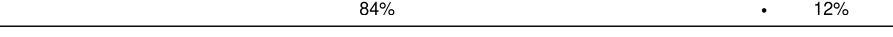
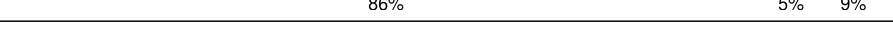
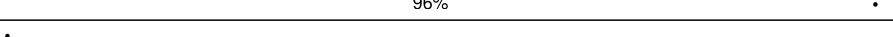
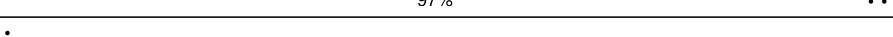
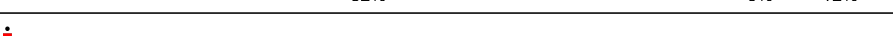
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13976 (2.56 - 3.56)

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

Mol	Chain	Length	Quality of chain
1	0	188	
2	1	65	
3	2	92	

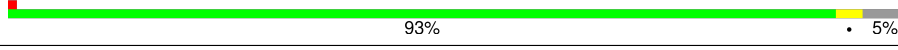
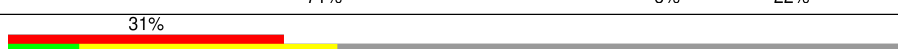
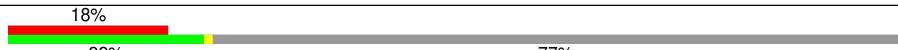
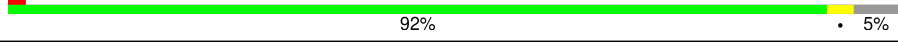
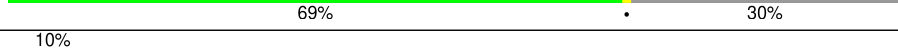
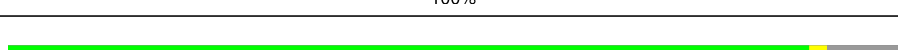
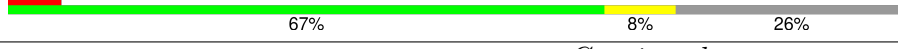
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Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1561	
12	C	297	
13	D	305	
14	E	348	
15	F	311	
16	H	267	
17	J	192	
18	K	178	
19	L	145	
20	M	296	
21	N	251	
22	O	175	
23	P	180	
24	Q	292	
25	R	149	
26	S	205	
27	T	206	
28	U	153	

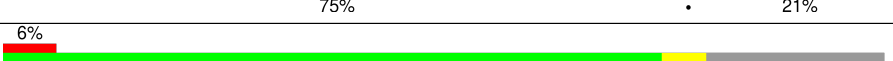
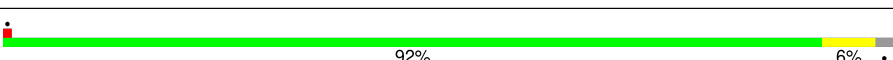
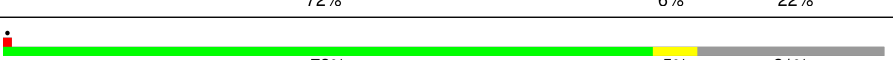
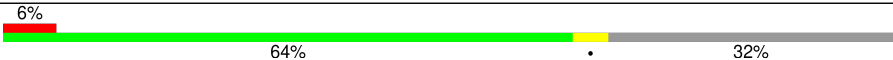
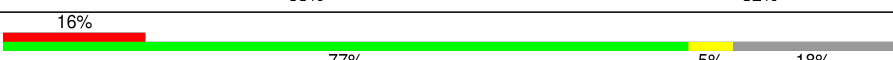
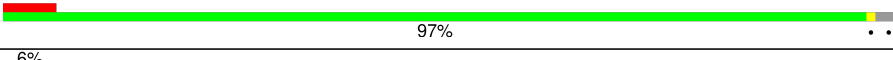
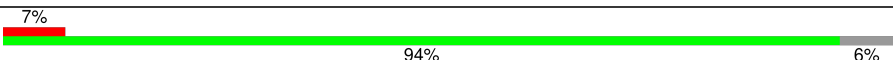
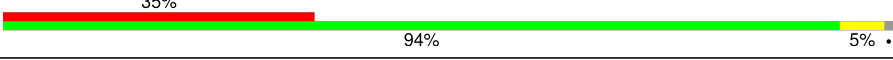
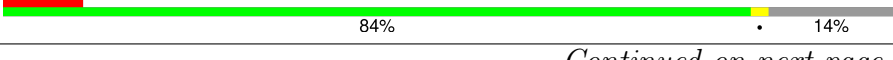
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Mol	Chain	Length	Quality of chain
29	W	148	
30	X	256	
31	Y	250	
32	Z	161	
33	z	325	
34	G	198	
34	t	198	
34	u	198	
35	I	261	
36	V	216	
37	b	215	
38	d	306	
39	e	279	
40	g	166	
41	h	158	
42	i	128	
43	j	123	
44	l	138	
45	m	128	
46	n	43	
47	o	102	
48	q	222	
49	r	196	
50	c	332	
51	f	212	

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Mol	Chain	Length	Quality of chain
52	p	206	
53	s	439	
54	AB	296	
55	AC	167	
56	AD	430	
57	AE	125	
58	AF	242	
59	AG	396	
60	AH	201	
61	AJ	138	
62	AK	128	
63	AL	257	
64	AM	137	
65	AN	130	
66	AO	258	
67	AP	142	
68	AR	360	
69	AS	190	
70	AT	173	
71	AU	205	
72	AV	414	
73	AW	187	
74	AZ	106	
75	A0	217	
76	A1	323	

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Mol	Chain	Length	Quality of chain
77	A3	199	
78	Az	34	
79	AY	395	
80	AA	954	
81	AI	194	
82	OX	435	
83	a	142	
84	Ax	71	
85	Ay	76	
86	A4	689	
87	B	72	
88	AX	398	
89	A2	118	
90	AQ	87	
91	k	112	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
100	SPM	AA	1782	-	-	X	-
100	SPM	AA	1785	-	-	X	-

2 Entry composition

There are 102 unique types of molecules in this entry. The entry contains 321591 atoms, of which 139316 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	110	Total	C	H	N	O	S	0	0
			1815	554	917	176	162	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	56	Total	C	H	N	O	S	0	0
			977	296	513	89	77	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
			784	233	407	83	60	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
			1716	539	884	162	128	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
			704	217	362	72	49	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	394	Total	C	H	N	O	S	0	0
			6419	2073	3209	560	566	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
			5792	1881	2844	525	533	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	294	Total	C	H	N	O	S	0	0
			4789	1529	2399	405	438	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	157	Total	C	H	N	O	S	0	0
			2696	844	1369	235	246	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
			1985	644	988	170	181	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	A	1558	Total	C	H	N	O	P	0	0
			49871	14843	16801	5963	10706	1558		

- Molecule 12 is a protein called Translational activator of cytochrome c oxidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	223	Total	C	N	O	S	0	0
			1732	1072	310	340	10		

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	D	238	Total	C	H	N	O	S	0	0
			3780	1157	1921	376	317	9		

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	E	305	Total	C	H	N	O	S	0	0
			4822	1545	2416	418	432	11		

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	F	252	Total	C	H	N	O	S	0	0
			4097	1305	2066	370	350	6		

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	H	202	Total	C	H	N	O	S	0	0
			3397	1067	1736	304	286	4		

- Molecule 17 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	J	175	Total	C	H	N	O	S	0	0
			2738	847	1408	237	244	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	K	178	Total	C	H	N	O	S	0	0
			2907	936	1452	259	253	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	2	ACE	-	acetylation	UNP H2QWN0
K	132	TYR	ASP	conflict	UNP H2QWN0

- Molecule 19 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	L	115	Total	C	H	N	O	S	0	0
			1832	559	942	171	155	5		

- Molecule 20 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	M	291	Total	C	H	N	O	S	0	0
			4723	1483	2396	430	408	6		

- Molecule 21 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	N	222	Total	C	H	N	O	S	0	0
			3604	1143	1818	326	307	10		

- Molecule 22 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	O	154	Total	C	H	N	O	S	0	0
			2554	792	1295	241	219	7		

- Molecule 23 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	P	144	Total	C	H	N	O	S	0	0
			2339	733	1166	224	211	5		

- Molecule 24 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Q	239	Total	C	H	N	O	S	0	0
			4021	1277	2031	353	351	9		

- Molecule 25 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	R	140	Total	C	H	N	O	S	0	0
			2369	732	1215	231	187	4		

- Molecule 26 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	S	161	Total	C	H	N	O	S	0	0
			2659	835	1366	227	227	4		

- Molecule 27 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	T	166	Total	C	H	N	O	S	0	0
			2781	875	1412	254	233	7		

- Molecule 28 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	U	152	Total	C	H	N	O	S	0	0
			2476	786	1228	234	225	3		

- Molecule 29 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	W	116	Total	C	H	N	O	S	0	0
			1840	577	936	171	153	3		

- Molecule 30 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	X	244	Total	C	H	N	O	S	0	0
			4105	1322	2061	352	365	5		

- Molecule 31 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Y	181	Total	C	H	N	O	S	0	0
			3154	995	1598	298	259	4		

- Molecule 32 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Z	122	Total	C	H	N	O	S	0	0
			2041	636	1045	186	171	3		

- Molecule 33 is a protein called Large ribosomal subunit protein uL1m.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	z	252	Total	C	H	N	O	S	0	0
			4103	1304	2076	336	381	6		

- Molecule 34 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	G	72	Total	C	N	O	0	0
			558	358	97	103		
34	t	46	Total	C	H	N	O	0
			732	228	378	56	70	
34	u	32	Total	C	H	N	O	0
			541	168	284	40	49	

- Molecule 35 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	I	181	Total	C	H	N	O	S	0	0
			2979	932	1533	260	244	10		

- Molecule 36 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	V	205	Total	C	H	N	O	S	0	0
			3365	1068	1689	298	302	8		

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	b	150	Total	C	H	N	O	S	0	0
			2379	742	1186	231	217	3		

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	259	Total	C	N	O	S	0	0
			2124	1357	369	384	14		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
39	e	238	Total	C	H	N	O	S	0	0
			3848	1222	1917	339	364	6		

- Molecule 40 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	g	134	Total	C	H	N	O	S	0	0
			2210	719	1097	193	199	2		

- Molecule 41 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	h	110	Total	C	H	N	O	S	0	0
			1778	568	883	156	168	3		

- Molecule 42 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	i	97	Total	C	H	N	O	S	0	0
			1687	532	859	165	127	4		

- Molecule 43 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	j	94	Total	C	H	N	O	S	0	0
			1492	463	747	144	136	2		

- Molecule 44 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	l	82	Total	C	H	N	O	S	0	0
			1363	437	675	120	128	3		

- Molecule 45 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	m	92	Total	C	H	N	O	S	0	0
			1551	488	760	159	142	2		

- Molecule 46 is a RNA chain called Nascent polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	n	43	Total	C	N	O	0	0
			215	129	43	43		

- Molecule 47 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	o	94	Total	C	H	N	O	S	0	0
			1604	501	806	165	129	3		

- Molecule 48 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	q	177	Total	C	H	N	O	S	0	0
			2437	929	942	292	269	5		

- Molecule 49 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	r	162	Total	C	H	N	O	S	0	0
			2671	839	1349	252	223	8		

- Molecule 50 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	c	286	Total	C	H	N	O	S	0	0
			4621	1470	2322	397	423	9		

- Molecule 51 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	f	157	Total	C	H	N	O	S	0	0
			2523	799	1271	207	242	4		

- Molecule 52 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	p	147	Total	C	H	N	O	S	0	0
			2430	748	1225	228	225	4		

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	s	385	Total	C	H	N	O	S	0	0
			6285	2018	3137	558	558	14		

- Molecule 54 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	AB	225	Total	C	H	N	O	S	0	0
			3644	1164	1816	331	323	10		

- Molecule 55 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	AC	132	Total	C	H	N	O	S	0	0
			2172	699	1089	195	185	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
56	AD	343	Total	C	H	N	O	S	0	0
			5536	1713	2805	518	487	13		

- Molecule 57 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	AE	122	Total	C	H	N	O	S	0	0
			1972	614	1000	177	177	4		

- Molecule 58 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	AF	208	Total	C	H	N	O	S	0	0
			3496	1104	1771	312	298	11		

- Molecule 59 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	AG	327	Total	C	H	N	O	S	0	0
			5377	1710	2689	477	487	14		

- Molecule 60 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	AH	140	Total	C	H	N	O	S	0	0
			2339	745	1187	194	210	3		

- Molecule 61 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	AJ	108	Total	C	H	N	O	S	0	0
			1727	521	888	169	143	6		

- Molecule 62 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	AK	101	Total	C	H	N	O	S	0	0
			1748	537	886	179	141	5		

- Molecule 63 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	AL	174	Total	C	H	N	O	S	0	0
			2994	925	1541	270	251	7		

- Molecule 64 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	AM	119	Total	C	H	N	O	S	0	0
			1908	594	966	185	157	6		

- Molecule 65 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	AN	110	Total	C	H	N	O	S	0	0
			1797	562	929	156	147	3		

- Molecule 66 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	AO	193	Total	C	H	N	O	S	0	0
			3149	1014	1557	294	277	7		

- Molecule 67 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	AP	97	Total	C	H	N	O	S	0	0
			1587	501	806	134	138	8		

- Molecule 68 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	AR	295	Total	C	H	N	O	S	0	0
			4839	1533	2430	413	455	8		

- Molecule 69 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	AS	135	Total	C	H	N	O	S	0	0
			2227	716	1116	198	196	1		

- Molecule 70 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	AT	168	Total	C	H	N	O	S	0	0
			2764	877	1393	239	244	11		

- Molecule 71 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	AU	176	Total	C	H	N	O	S	0	0
			2989	916	1501	301	267	4		

- Molecule 72 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	AV	362	Total	C	H	N	O	S	0	0
			5933	1904	2964	495	558	12		

- Molecule 73 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	AW	100	Total	C	H	N	O	S	0	0
			1593	498	804	141	146	4		

- Molecule 74 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	AZ	100	Total	C	H	N	O	S	0	0
			1698	534	859	153	148	4		

- Molecule 75 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	A0	215	Total	C	H	N	O	S	0	0
			3584	1130	1797	339	313	5		

- Molecule 76 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	A1	279	Total	C	H	N	O	S	0	0
			4561	1435	2296	387	432	11		

- Molecule 77 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	A3	70	Total	C	H	N	O	S	0	0
			1326	401	701	134	89	1		

- Molecule 78 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	Az	34	Total	C	H	N	O	P	0	0
			1079	324	360	123	238	34		

- Molecule 79 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	AY	119	Total	C	H	N	O	S	0	0
			1973	654	963	166	188	2		

- Molecule 80 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	AA	954	Total	C	N	O	P		0	0
			20260	9088	3647	6571	954			

- Molecule 81 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	AI	137	Total	C	H	N	O	S	0	0
			2077	641	1058	193	181	4		

- Molecule 82 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	OX	55	Total	C	H	N	O	S	0	0
			933	292	465	93	81	2		

- Molecule 83 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	a	103	Total	C	H	N	O	S	0	0
			1695	543	830	155	162	5		

- Molecule 84 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	Ax	71	Total	C	H	N	O	P	0	0
			2264	673	766	264	491	70		

- Molecule 85 is a RNA chain called E/E-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	Ay	70	Total	C	H	N	O	P	0	0
			2235	665	752	261	487	70		

- Molecule 86 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	A4	588	Total	C	H	N	O	S	0	0
			9535	3053	4767	808	879	28		

- Molecule 87 is a RNA chain called mitochondrial tRNA^{Val}.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	B	72	Total	C	H	N	O	P	0	0
			2304	685	780	269	498	72		

- Molecule 88 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	AX	352	Total	C	H	N	O	S	0	0
			5693	1822	2844	499	517	11		

- Molecule 89 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	A2	118	Total	C	H	N	O	S	0	0
			1906	579	971	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 90 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
90	AQ	87	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	1	ACE	-	acetylation	UNP P82921
AQ	50	ARG	CYS	variant	UNP P82921

- Molecule 91 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
91	k	102	Total	C	H	N	O	S	0	0
			1559	479	785	148	142	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	2	ACE	-	acetylation	UNP Q96EL3

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
92	0	1	Total	Zn	0
			1	1	
92	4	1	Total	Zn	0
			1	1	
92	AO	1	Total	Zn	0
			1	1	

- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

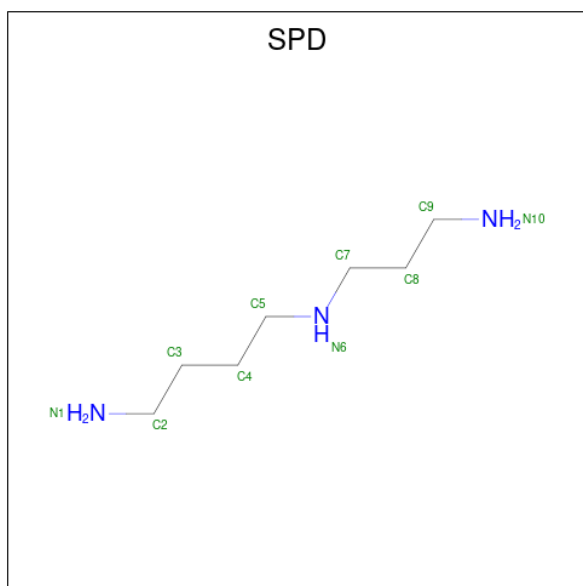
Mol	Chain	Residues	Atoms		AltConf
93	6	1	Total	K	0
			1	1	
93	A	29	Total	K	0
			29	29	

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Mol	Chain	Residues	Atoms		AltConf
93	D	1	Total	K	0
			1	1	
93	M	2	Total	K	0
			2	2	
93	N	1	Total	K	0
			1	1	
93	W	1	Total	K	0
			1	1	
93	o	1	Total	K	0
			1	1	
93	AA	18	Total	K	0
			18	18	

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



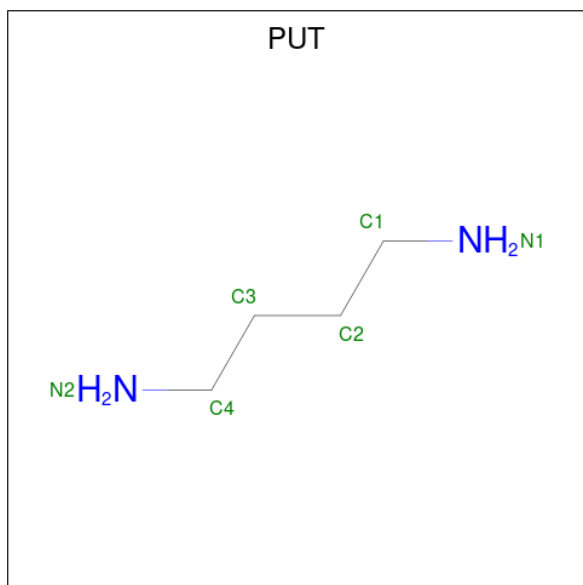
Mol	Chain	Residues	Atoms				AltConf
94	A	1	Total	C	H	N	0
			32	7	22	3	
94	A	1	Total	C	H	N	0
			32	7	22	3	
94	A	1	Total	C	N		0
			10	7	3		
94	A	1	Total	C	N		0
			10	7	3		
94	O	1	Total	C	N		0
			10	7	3		

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Mol	Chain	Residues	Atoms			AltConf
94	AA	1	Total	C	N	0
			10	7	3	
94	AA	1	Total	C	N	0
			10	7	3	
94	AA	1	Total	C	N	0
			10	7	3	

- Molecule 95 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms				AltConf
95	A	1	Total	C	H	N	0
			20	4	14	2	

- Molecule 96 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

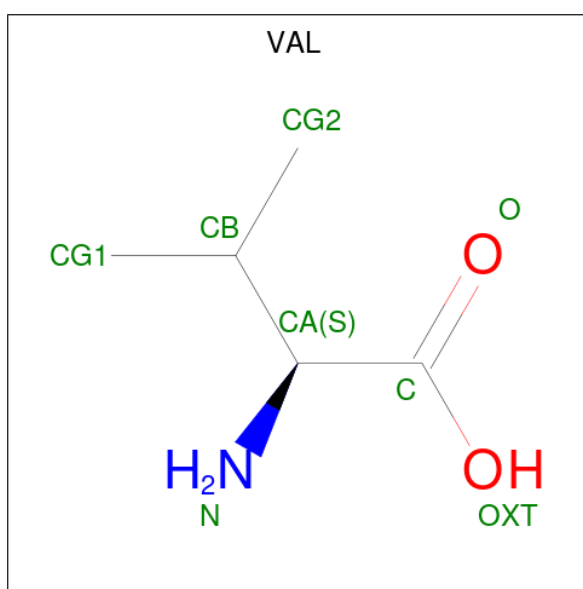
Mol	Chain	Residues	Atoms		AltConf
96	A	136	Total	Mg	0
			136	136	
96	D	2	Total	Mg	0
			2	2	
96	E	1	Total	Mg	0
			1	1	
96	I	1	Total	Mg	0
			1	1	
96	g	1	Total	Mg	0
			1	1	

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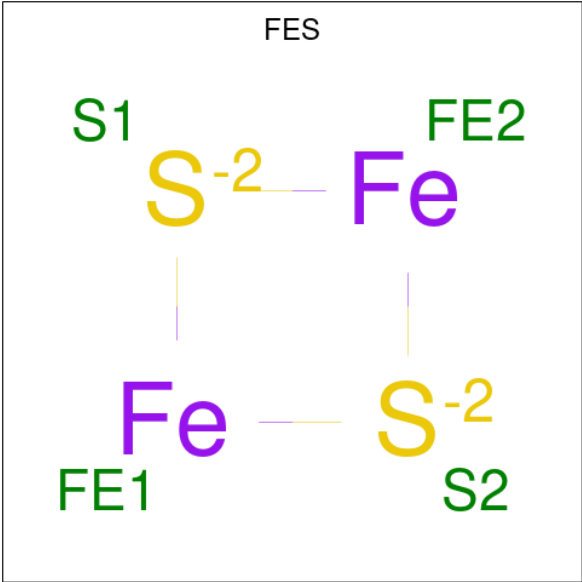
Mol	Chain	Residues	Atoms		AltConf
96	AB	1	Total	Mg	0
			1	1	
96	A3	1	Total	Mg	0
			1	1	
96	AA	61	Total	Mg	0
			61	61	
96	AX	1	Total	Mg	0
			1	1	

- Molecule 97 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



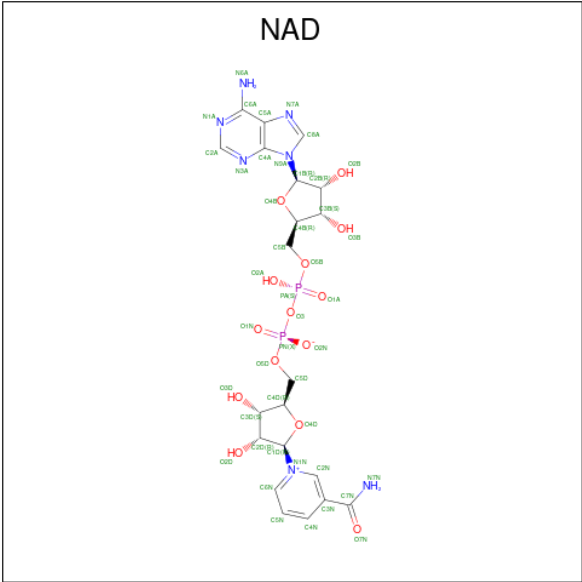
Mol	Chain	Residues	Atoms					AltConf
97	e	1	Total	C	H	N	O	0
			15	5	8	1	1	

- Molecule 98 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



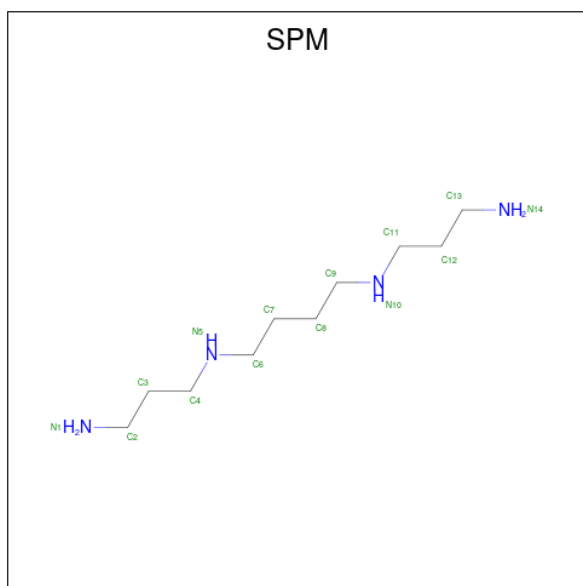
Mol	Chain	Residues	Atoms			AltConf
98	r	1	Total	Fe	S	0
			4	2	2	
98	AP	1	Total	Fe	S	0
			4	2	2	
98	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 99 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



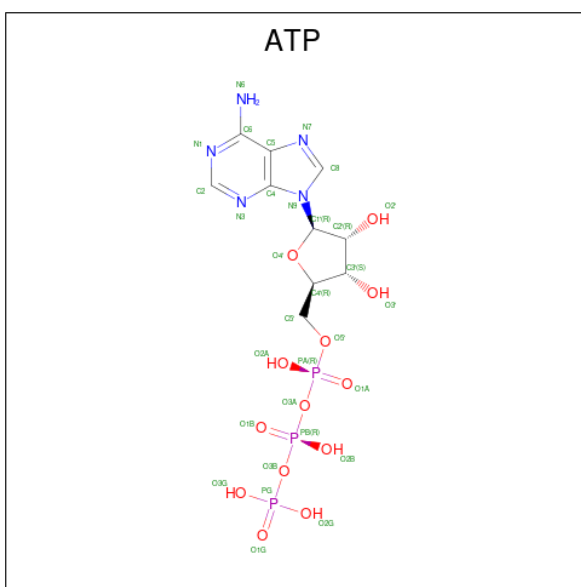
Mol	Chain	Residues	Atoms					AltConf
99	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 100 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



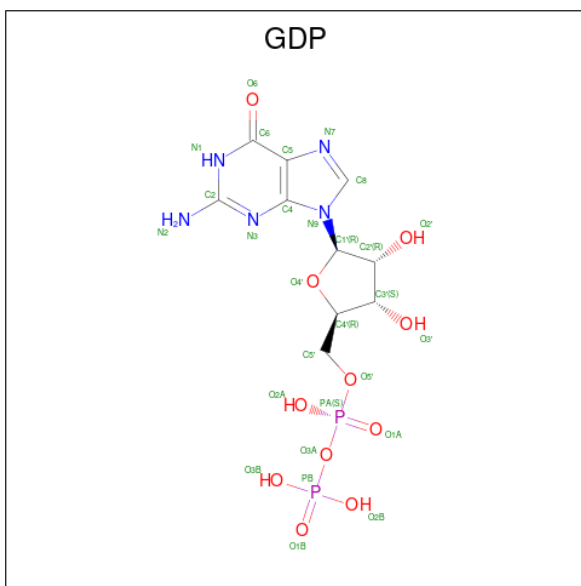
Mol	Chain	Residues	Atoms					AltConf
100	AA	1	Total	C	N			0
			14	10	4			
100	AA	1	Total	C	N			0
			14	10	4			
100	AA	1	Total	C	N			0
			14	10	4			

- Molecule 101 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
101	AX	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 102 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).

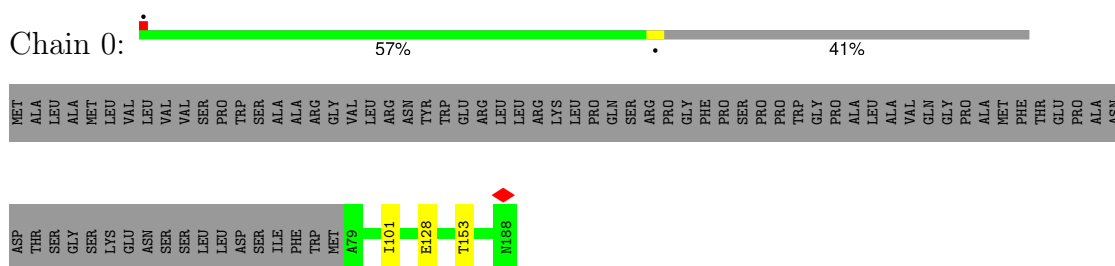


Mol	Chain	Residues	Atoms					AltConf	
102	AX	1	Total	C	H	N	O	P	0
			40	10	12	5	11	2	

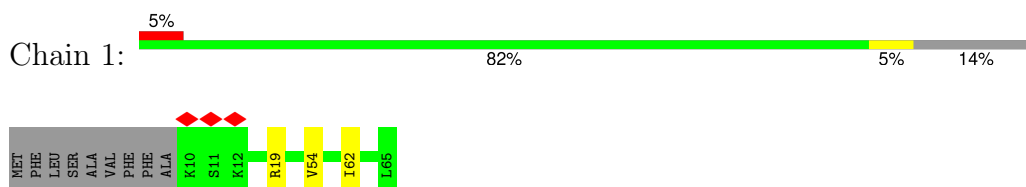
3 Residue-property plots [i](#)

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

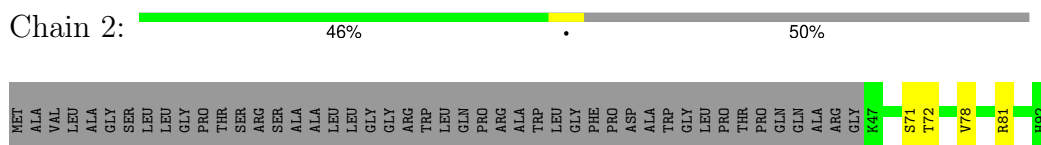
- Molecule 1: 39S ribosomal protein L32, mitochondrial



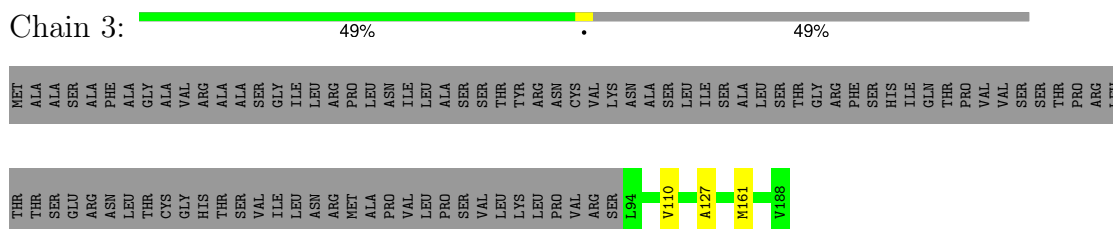
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial



- Molecule 4: 39S ribosomal protein L35, mitochondrial



- Molecule 5: 39S ribosomal protein L36, mitochondrial



MET ALA ALA ASN PHE PHE ARG LYS MET VAL ASN PRO LEU LEU TYR SER LEU ARG HIS THR VAL LYS PRO ARG ALA LEU SER THR PHE LEU PHE GLY SER ILE ARG ILE GLY ALA ALA PRO VAL VAL ALA VAL PRO GLY GLY ALA VAL ARG SER LEU LEU PRO HIS LEU LEU

LEU PRO ALA ALA LEU LEU GLY P66 D78 K83 T94 M103

- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5: 88% 5% 7%

MET ALA ALA LEU LEU ALA SER GLY PRO ARG ALA ARG ALA LEU ALA ALA GLY SER GLY LEU GLN SER LEU GLY THR LEU GLY PHE GLY ARG ALA PRO ARG ARG GLY A30 L98 F107 L113 Q165 T166 T167 R173 Y176 C177 P178 V179 D272 L315 F318 L322 L336 V351

T362 L381 K393 V396 A423

- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 90% 7%

MET ALA ALA PRO TRP TRP ARG ALA ALA LEU CYS CYS ARG TRP ARG TRP ARG GLY PHE SER THR SER ALA VAL LEU GLY R27 N37 Y57 R81 T82 D83 P84 R85 R96 W139 C143 Y206 E210 W214 E283 L293 T328 H332 L335

E339 S372 Y380

- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7: 82% 5% 13%

MET GLU ALA LEU ALA MET GLY SER ARG ALA LEU LEU ARG LEU TRP LEU VAL TRP ALA PRO GLY GLY THR ILE SER TRP PHE ILE THR SER SER ALA SER Q34 L47 R61 K64 R81 R84 T85 S86 N139 V174 V183 V184 E191 K204 A223

L227 E228 L286 Q290 T294 R295 R296 D327 GLN SER LYS ALA THR THR GLU CYS THR THR

- Molecule 9: 39S ribosomal protein L40, mitochondrial

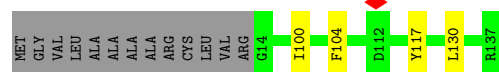
Chain 8: 12% 73% 24%

MET THR ALA SER VAL LEU ARG SER ILE SER LEU LEU ALA ARG PRO THR THR GLY LEU LEU GLY THR TRP GLN THR GLN ARG ALA SER LEU LEU SER PHE TRP GLU LEU ILE PRO MET ARG S47 E48 P49 L50 R51 K52 K53 K54 K55 V56 D57 P58 K59 K60

E63 L68 K77 L92 K97 Q103 V104 E105 D134 T135 I136 E141 E148 S154 L157 L168 T179 N184 E203 PHE LYS ARG

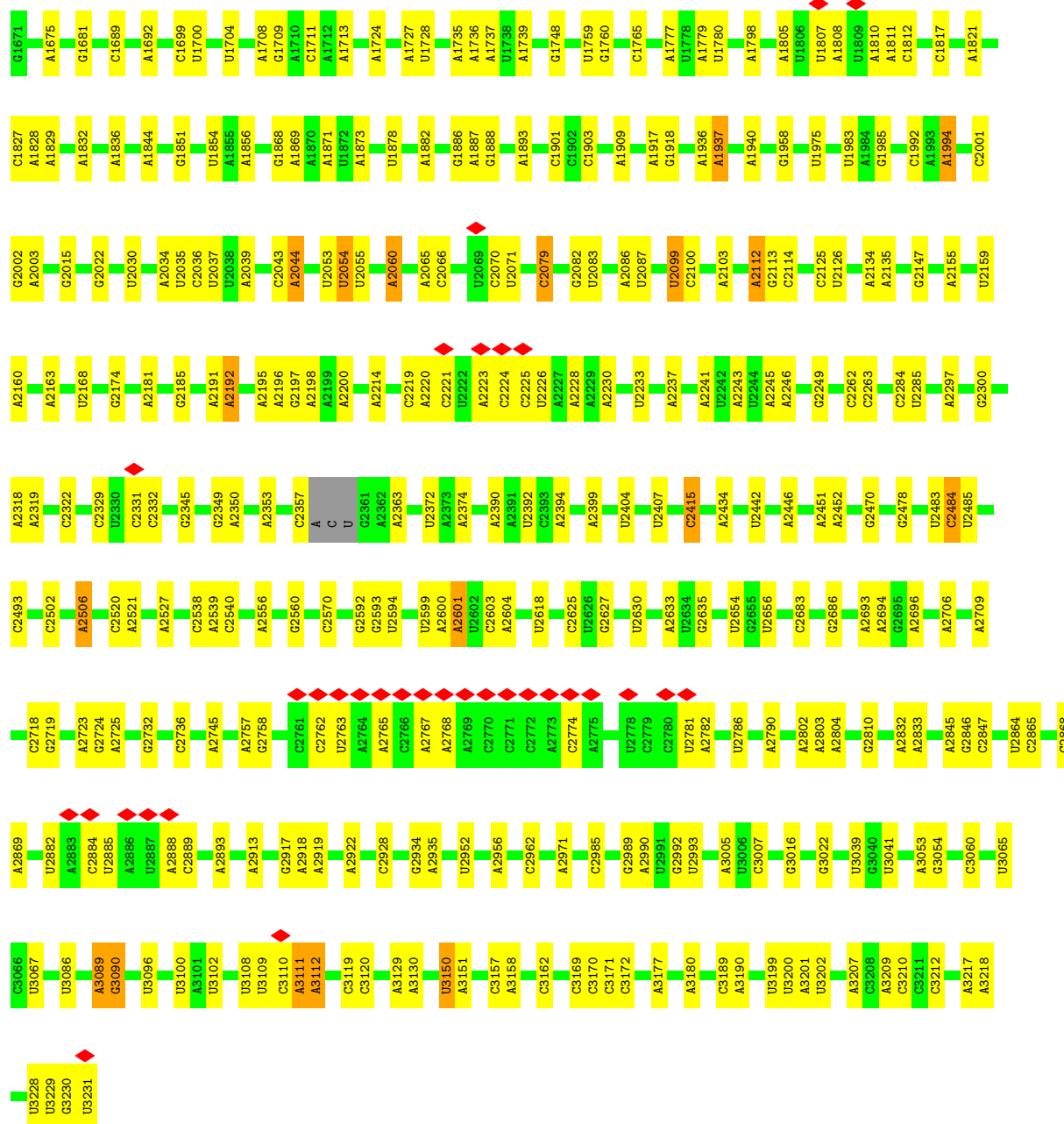
- Molecule 10: 39S ribosomal protein L41, mitochondrial

Chain 9:  88% 9%

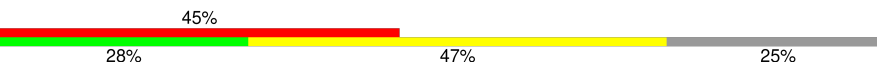


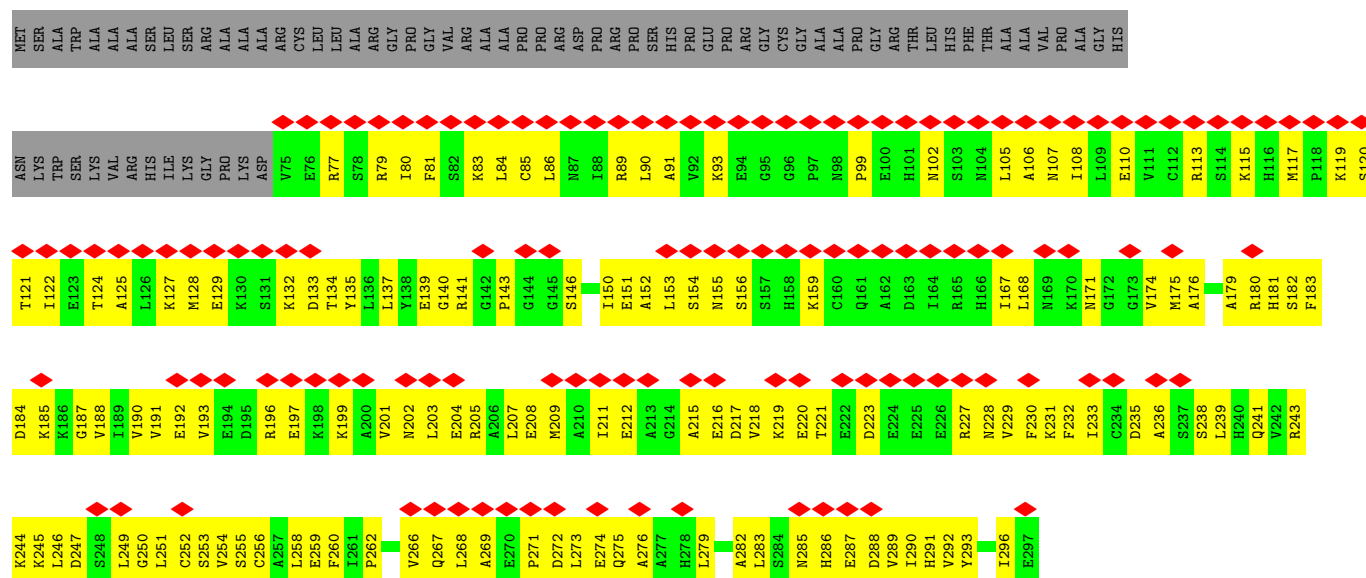
• Molecule 11: 16S mitochondrial rRNA

Chain A:  80% 19%

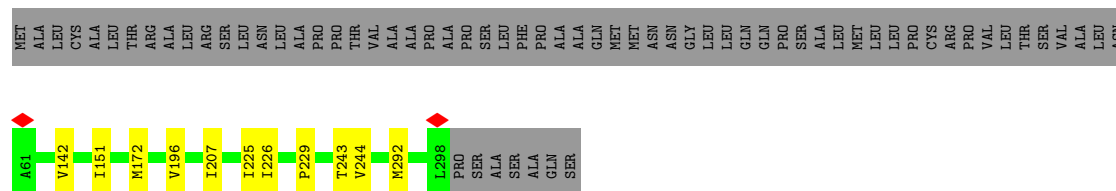


• Molecule 12: Translational activator of cytochrome c oxidase 1

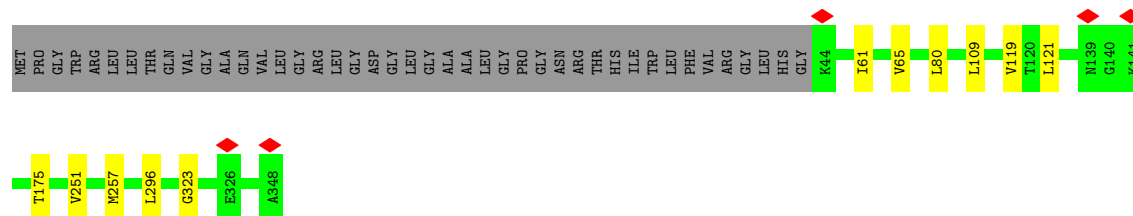
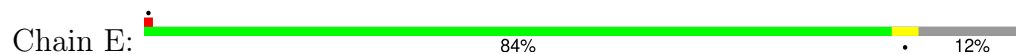
Chain C:  28% 45% 47% 25%



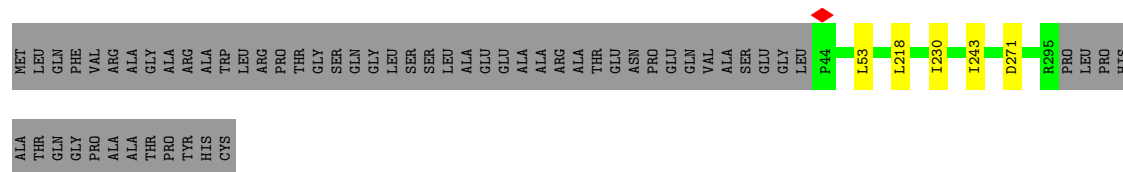
- Molecule 13: 39S ribosomal protein L2, mitochondrial



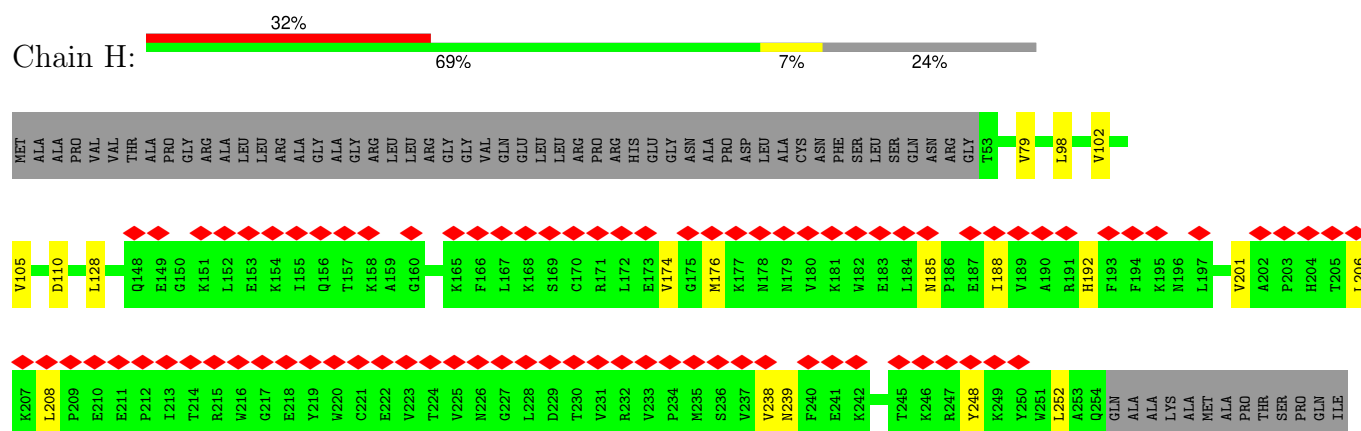
- Molecule 14: 39S ribosomal protein L3, mitochondrial



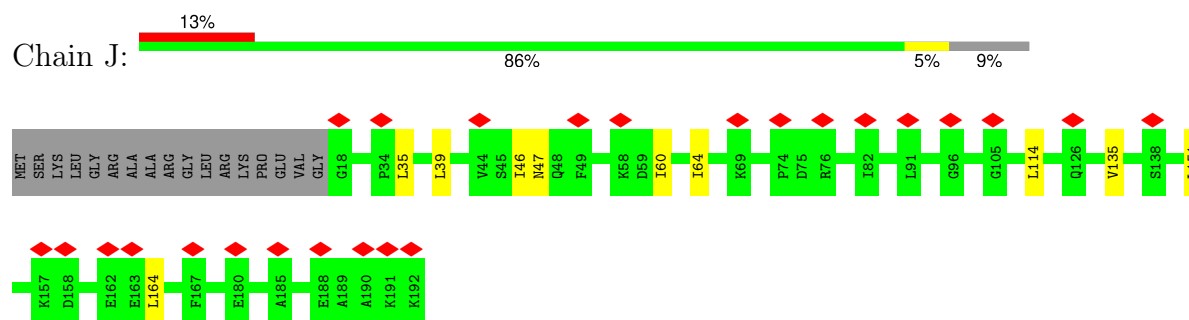
- Molecule 15: 39S ribosomal protein L4, mitochondrial



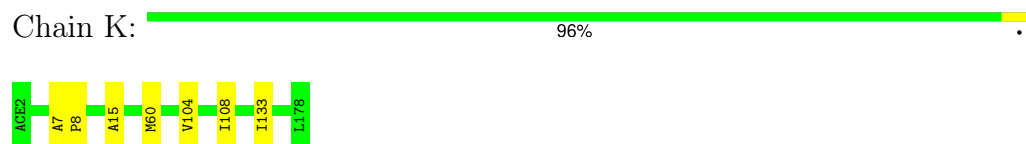
- Molecule 16: 39S ribosomal protein L9, mitochondrial



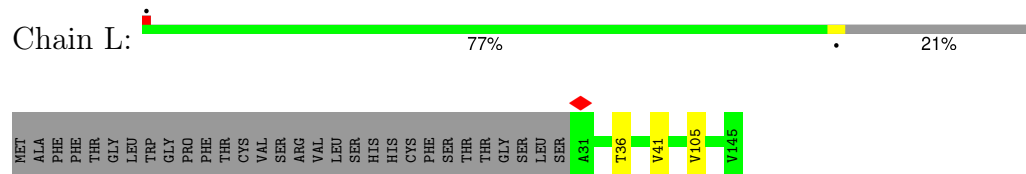
- Molecule 17: 39S ribosomal protein L11, mitochondrial



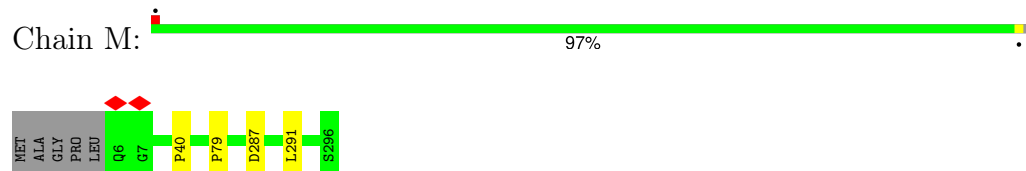
- Molecule 18: Large ribosomal subunit protein uL13m



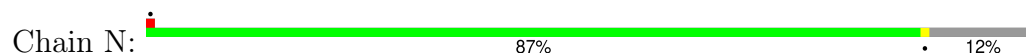
- Molecule 19: 39S ribosomal protein L14, mitochondrial

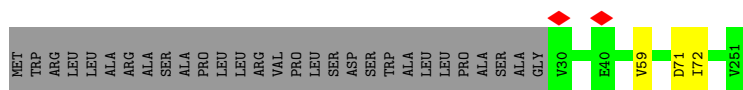


- Molecule 20: 39S ribosomal protein L15, mitochondrial

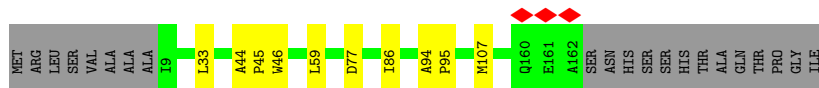
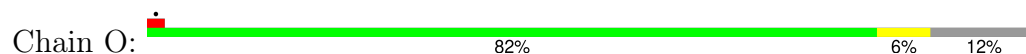


- Molecule 21: 39S ribosomal protein L16, mitochondrial

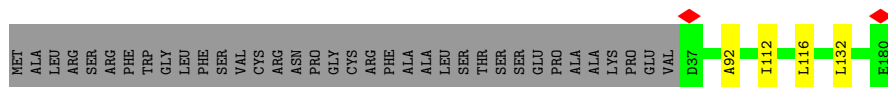
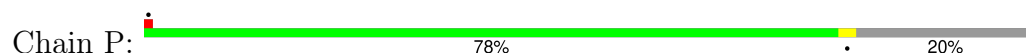




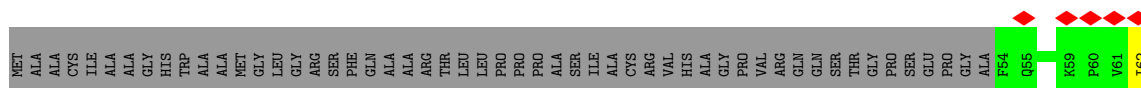
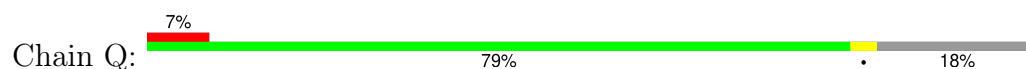
- Molecule 22: 39S ribosomal protein L17, mitochondrial



- Molecule 23: 39S ribosomal protein L18, mitochondrial



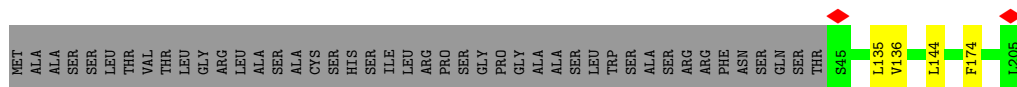
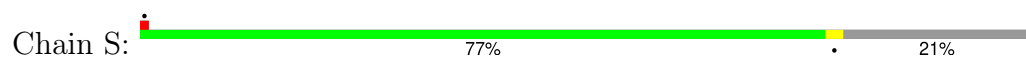
- Molecule 24: 39S ribosomal protein L19, mitochondrial



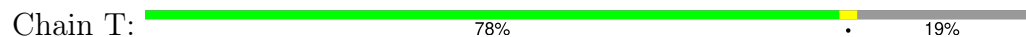
- Molecule 25: 39S ribosomal protein L20, mitochondrial

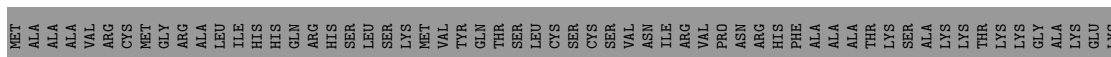


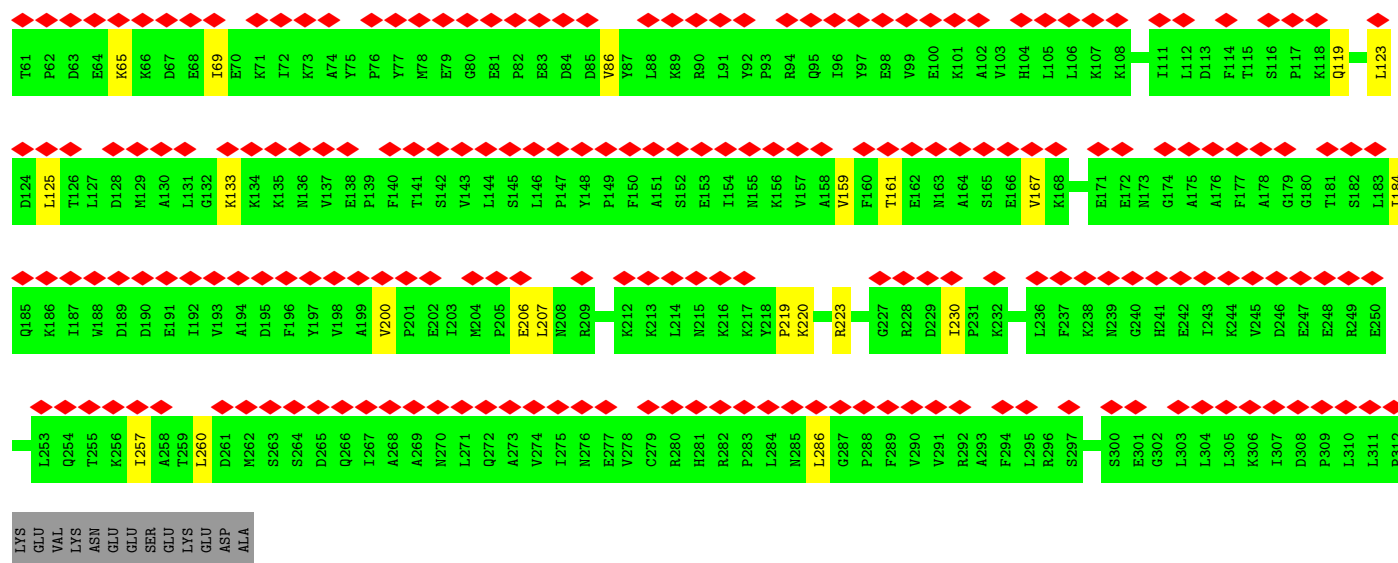
- Molecule 26: 39S ribosomal protein L21, mitochondrial



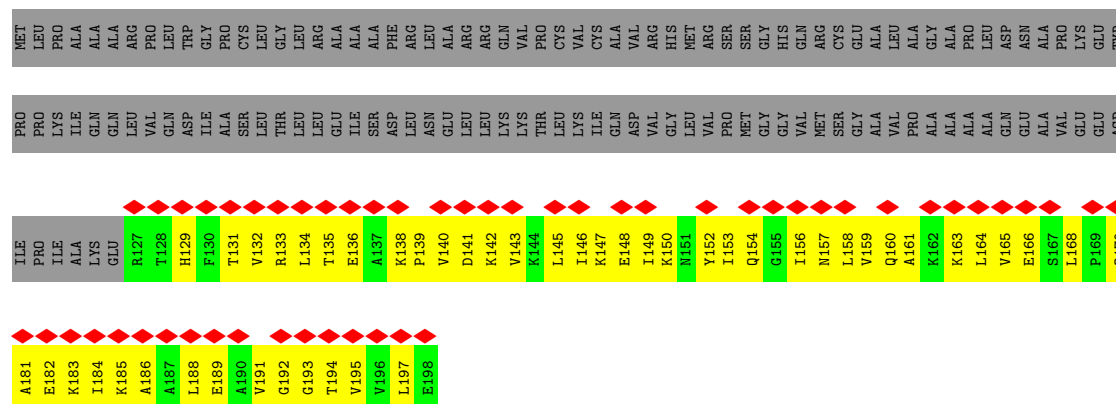
- Molecule 27: 39S ribosomal protein L22, mitochondrial



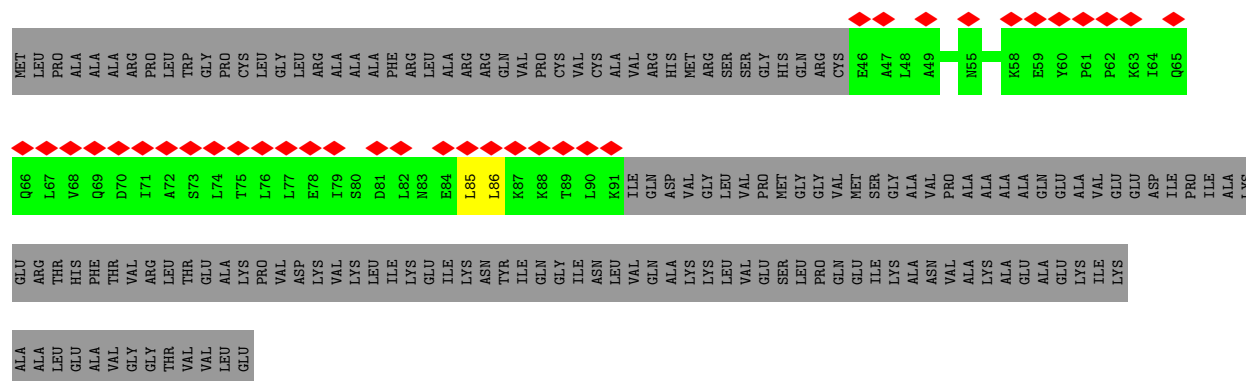




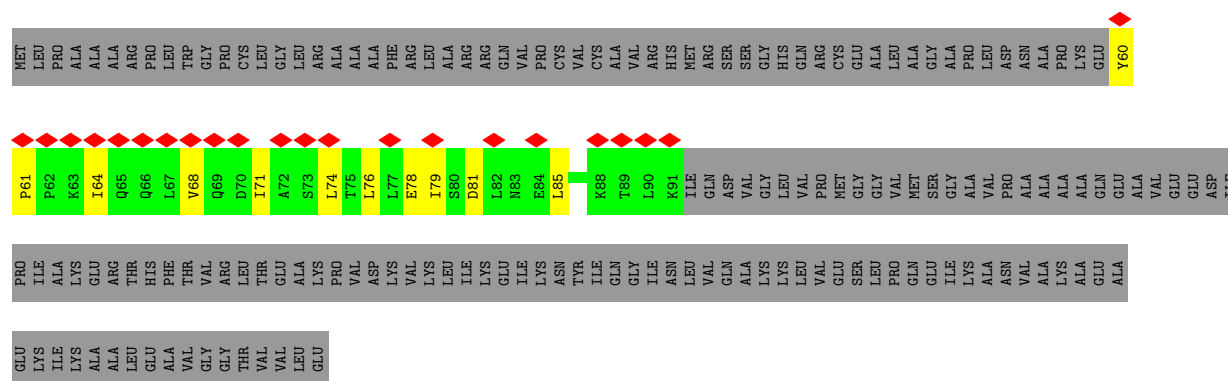
• Molecule 34: 39S ribosomal protein L12, mitochondrial



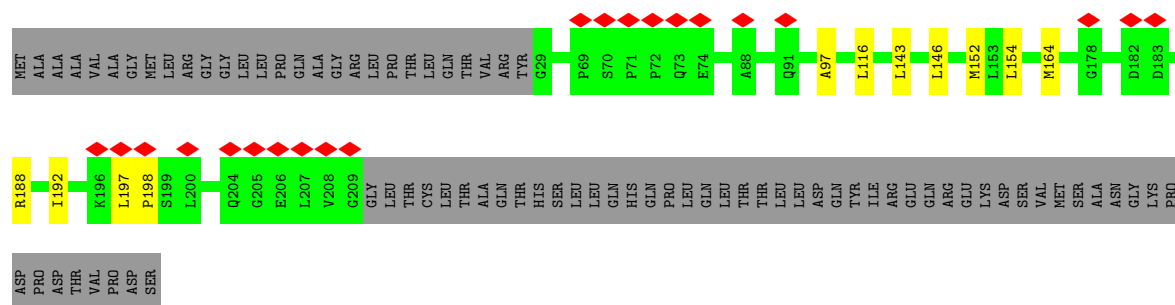
• Molecule 34: 39S ribosomal protein L12, mitochondrial



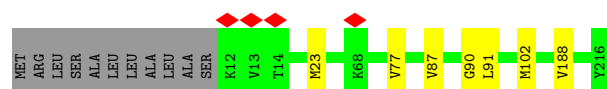
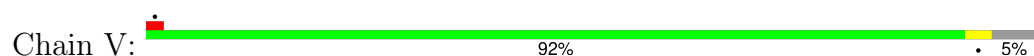
• Molecule 34: 39S ribosomal protein L12, mitochondrial



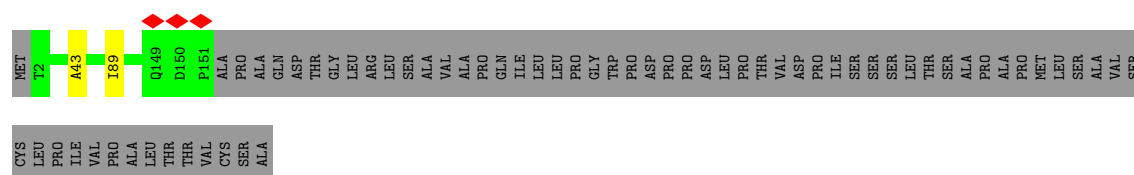
- Molecule 35: 39S ribosomal protein L10, mitochondrial



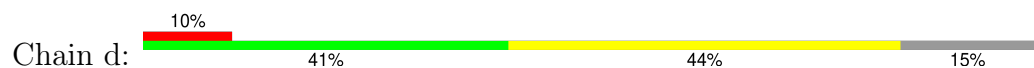
- Molecule 36: 39S ribosomal protein L24, mitochondrial

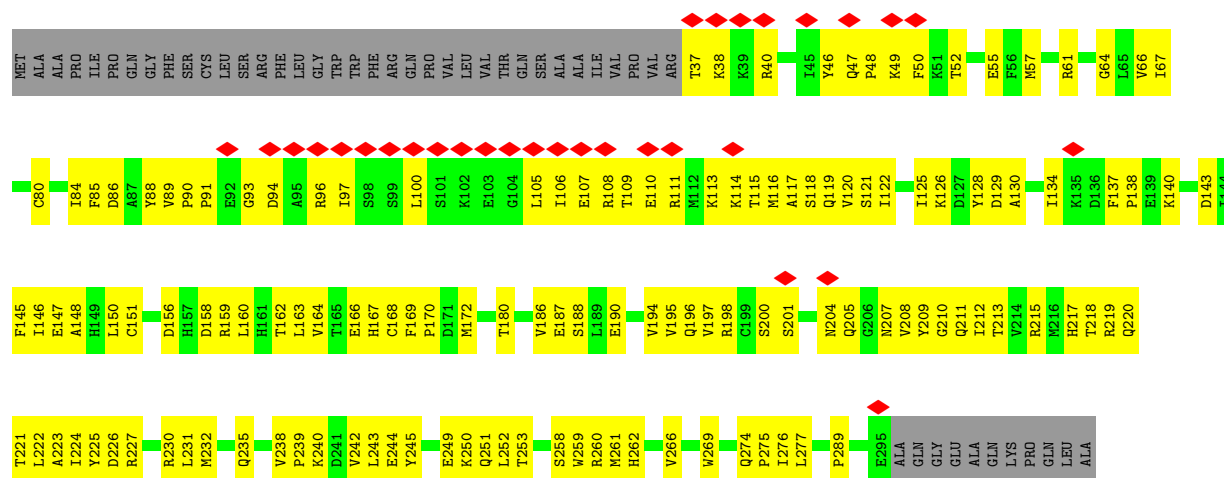


- Molecule 37: 39S ribosomal protein L43, mitochondrial



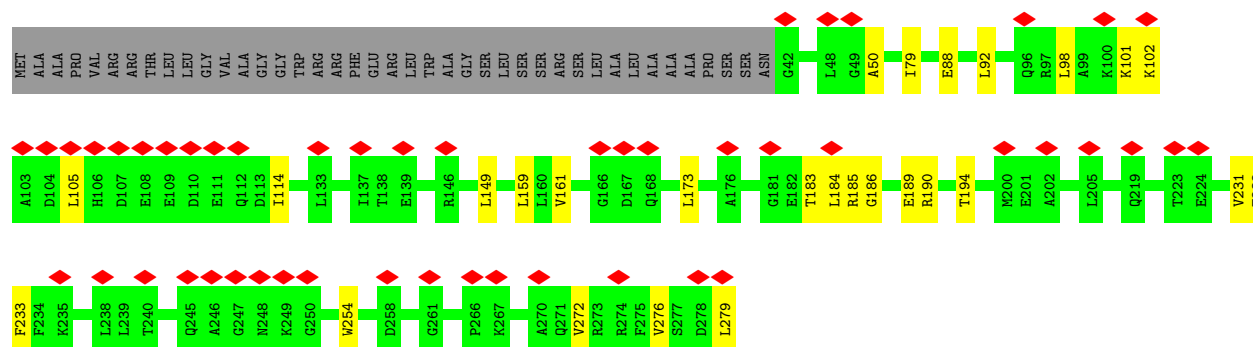
- Molecule 38: 39S ribosomal protein L45, mitochondrial





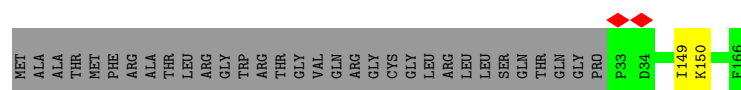
- Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e:



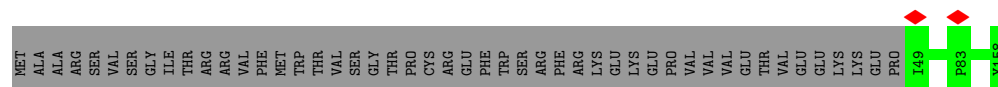
- Molecule 40: 39S ribosomal protein L49, mitochondrial

Chain g:



- Molecule 41: 39S ribosomal protein L50, mitochondrial

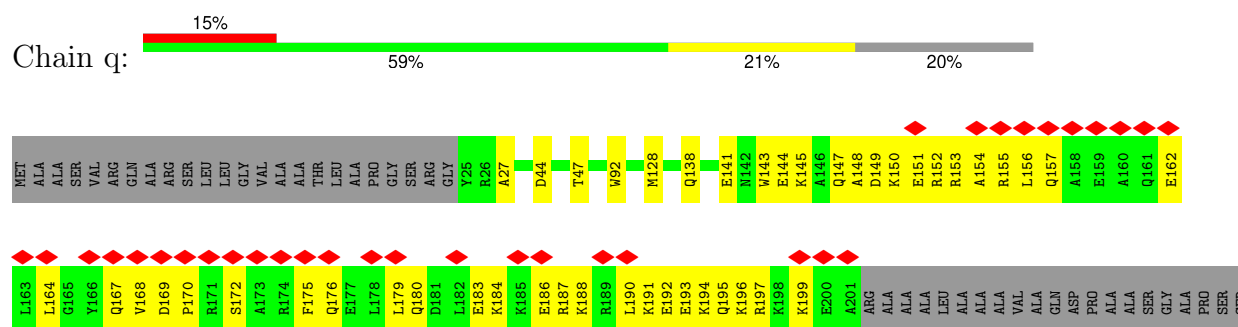
Chain h:



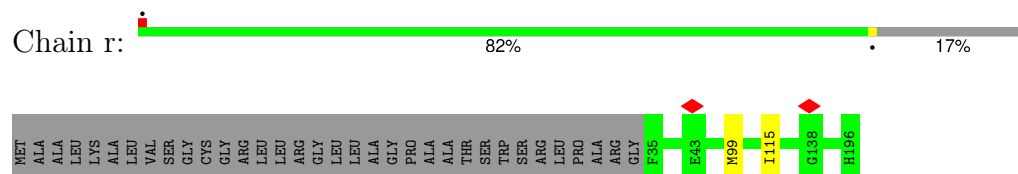
- Molecule 42: 39S ribosomal protein L51, mitochondrial

Chain i:

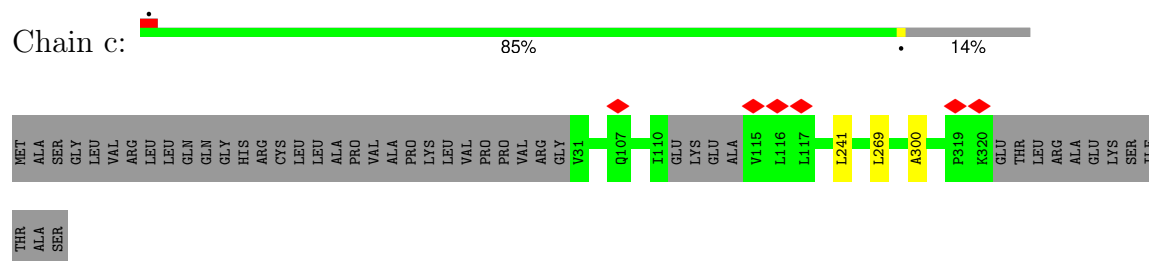




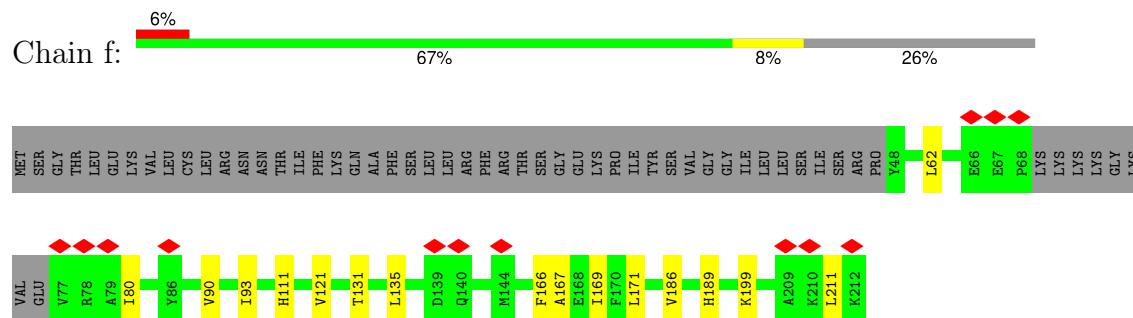
- Molecule 49: 39S ribosomal protein S18a, mitochondrial



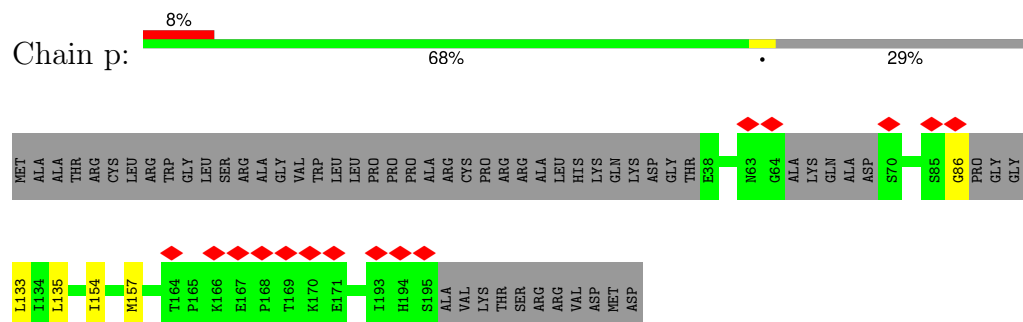
- Molecule 50: 39S ribosomal protein L44, mitochondrial



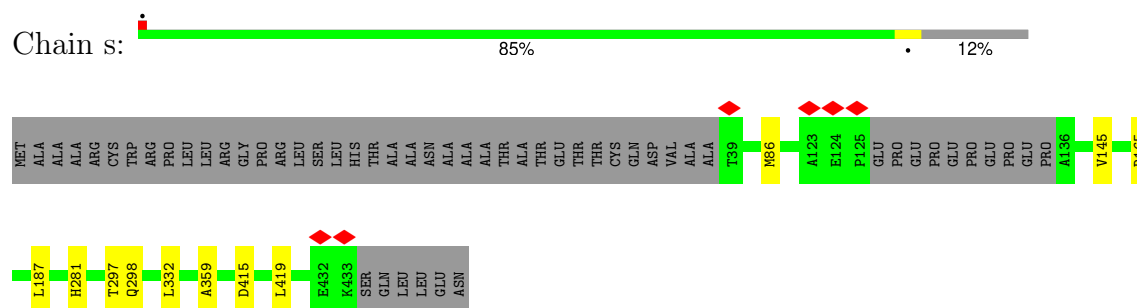
- Molecule 51: 39S ribosomal protein L48, mitochondrial



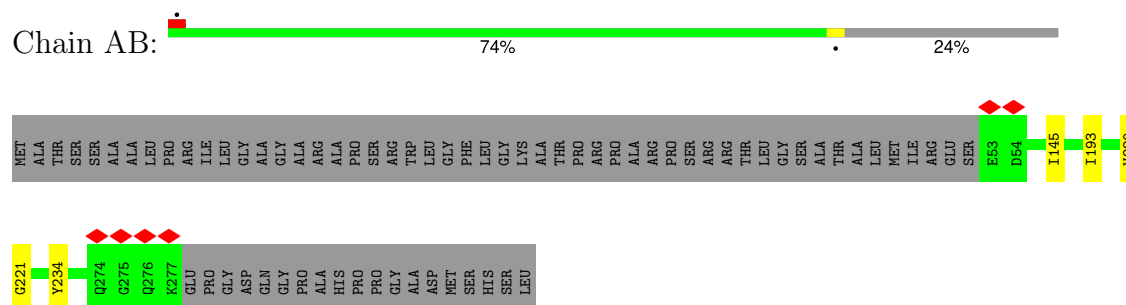
- Molecule 52: Peptidyl-tRNA hydrolase ICT1, mitochondrial



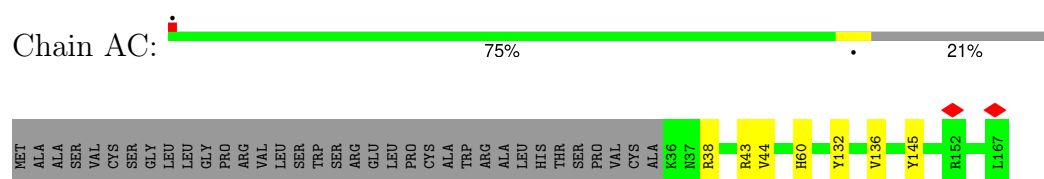
- Molecule 53: 39S ribosomal protein S30, mitochondrial



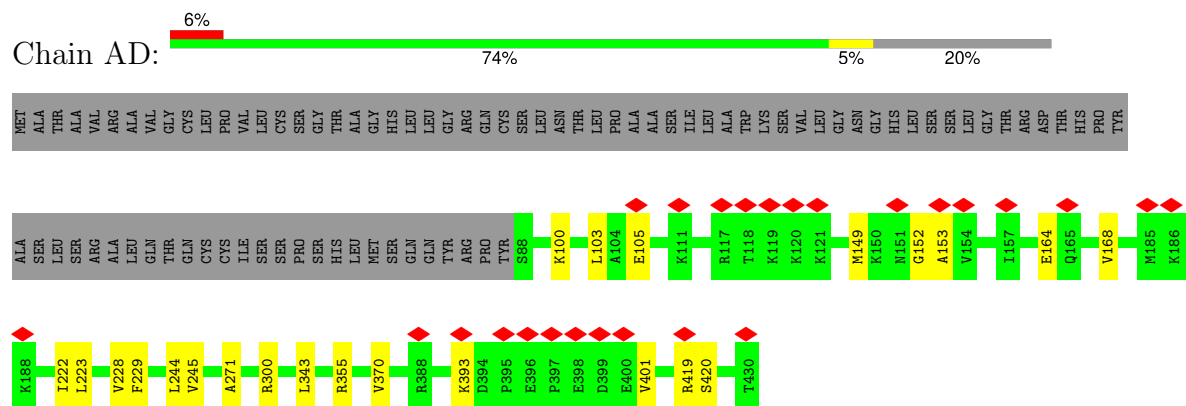
- Molecule 54: 28S ribosomal protein S2, mitochondrial



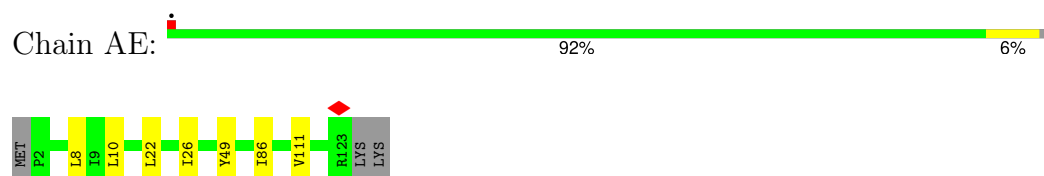
- Molecule 55: 28S ribosomal protein S24, mitochondrial

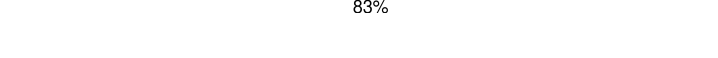


- Molecule 56: 28S ribosomal protein S5, mitochondrial



- Molecule 57: 28S ribosomal protein S6, mitochondrial

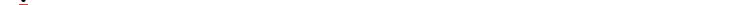


- Chain AF:  83% 14%
- 
- | Amino Acid | Percentage |
|------------|------------|
| MET | 0.00 |
| ALA | 0.00 |
| ALA | 0.00 |
| PRO | 0.00 |
| ALA | 0.00 |
| VAL | 0.00 |
| LYS | 0.00 |
| VAL | 0.00 |
| ALA | 0.00 |
| ARG | 0.00 |
| GLY | 0.00 |
| TRP | 0.00 |
| SER | 0.00 |
| GLY | 0.00 |
| LEU | 0.00 |
| ALA | 0.00 |
| LEU | 0.00 |
| GLY | 0.00 |
| VAL | 0.00 |
| ARG | 0.00 |
| ARG | 0.00 |
| ALA | 0.00 |
| VAL | 0.00 |
| LEU | 0.00 |
| GLN | 0.00 |
| LEU | 0.00 |
| PRO | 0.00 |
| GLY | 0.00 |
| LEU | 0.00 |
| THR | 0.00 |
| GLN | 0.00 |
| VAL | 0.00 |
| ARG | 0.00 |
| TRP | 0.00 |
| S35 | 0.00 |
| E40 | 0.00 |
| R52 | 0.00 |
| E56 | 0.00 |
| Y64 | 0.00 |
| L73 | 0.00 |
| F86 | 0.00 |
| I100 | 0.00 |
| E132 | 0.00 |
| I161 | 0.00 |
| R166 | 0.00 |
| V242 | 0.00 |

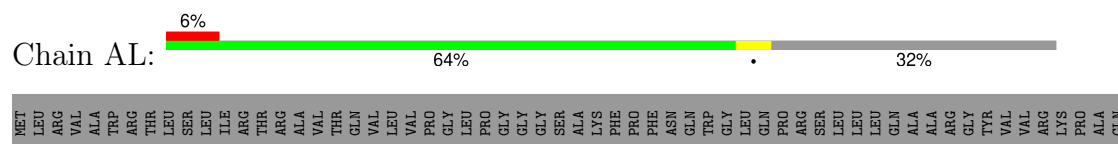
- Chain AG:
-
- 5% 78% 5% 17%
- MET ALA ALA PRO CYS VAL SER THR GLY GLY ALA VAL SER ARG LEU LEU LEU THR GLY ARG GLY SER LEU ALA ARG LYS GLN GLY LEU THR LYS THR ALA ALA ASP PRO GLU LEU GLN THR ASN VAL ARG SER GLN ILE LEU ARG LEU ARG HIS THR A53 P57 K58 K59 N60 V61 P62

- [illegible]

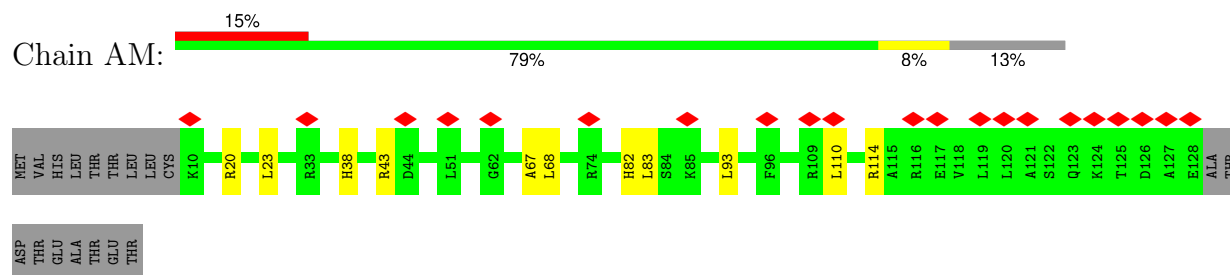
- Chain A.J:
-
- 72% 6% 22%
- MET SER SER TRP SER SER GLY LEU LEU HIS GLY LEU ASN THR SER LEU THR CYS GLY PRO ALA LEU VAL PRO ARG LEU TRP ALA THR CYS MET A31 R44 P45 K59 K72 A76 Y77 R78 E88 E104 I107 G112 K137 K138

- Chain AK: 
- | Residue | Color |
|---------|--------|
| MET | Grey |
| ALA | Grey |
| ALA | Grey |
| PHE | Grey |
| MET | Grey |
| LEU | Grey |
| GLY | Grey |
| SER | Grey |
| LEU | Grey |
| LEU | Grey |
| THR | Grey |
| PHE | Grey |
| LYS | Grey |
| GLN | Grey |
| MET | Grey |
| VAL | Grey |
| PRO | Grey |
| SER | Grey |
| SER | Grey |
| ALA | Grey |
| SER | Grey |
| GLY | Grey |
| GLN | Grey |
| VAL | Grey |
| ARG | Grey |
| SER | Grey |
| P38 | Green |
| Y29 | Yellow |
| M32 | Green |
| R33 | Green |
| M34 | Yellow |
| V38 | Yellow |
| Q68 | Green |
| V92 | Yellow |
| T127 | Yellow |
| M128 | Yellow |

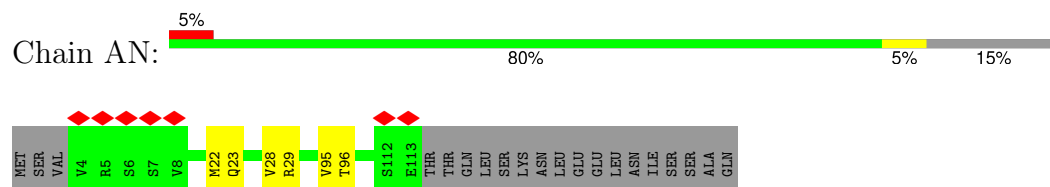
- Molecule 63: 28S ribosomal protein S15, mitochondrial



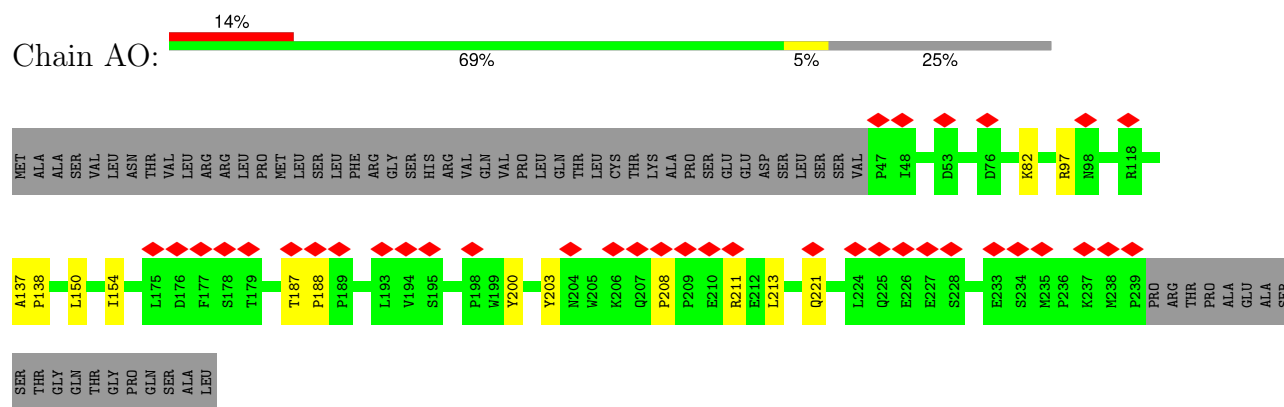
- Molecule 64: 28S ribosomal protein S16, mitochondrial



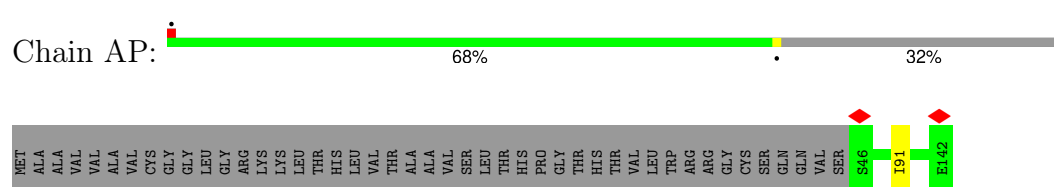
- Molecule 65: 28S ribosomal protein S17, mitochondrial



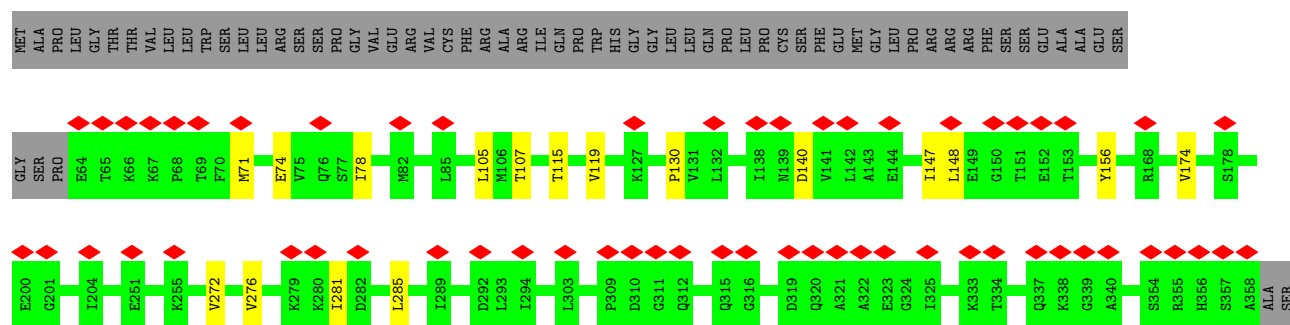
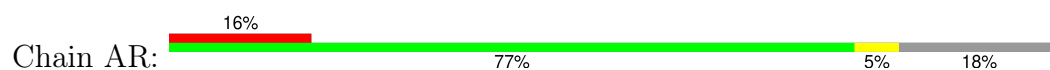
- Molecule 66: 28S ribosomal protein S18b, mitochondrial



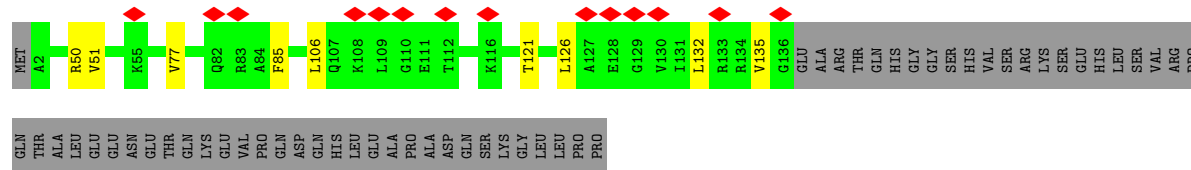
- Molecule 67: 28S ribosomal protein S18c, mitochondrial



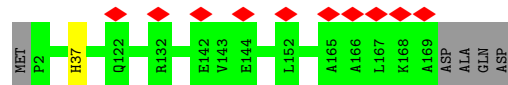
- Molecule 68: 28S ribosomal protein S22, mitochondrial



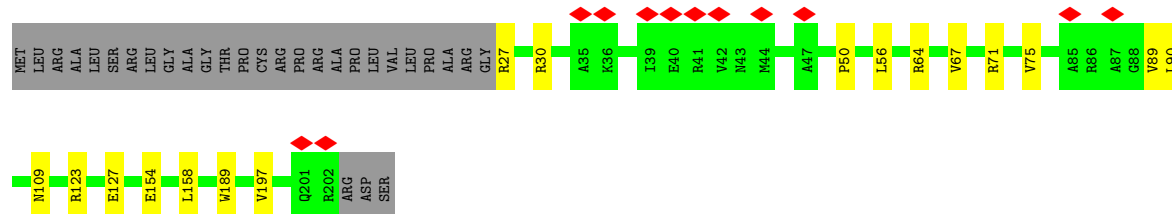
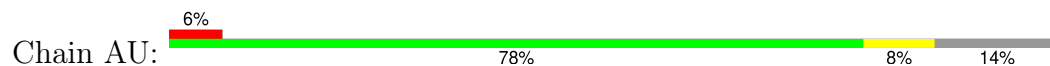
- Molecule 69: 28S ribosomal protein S23, mitochondrial



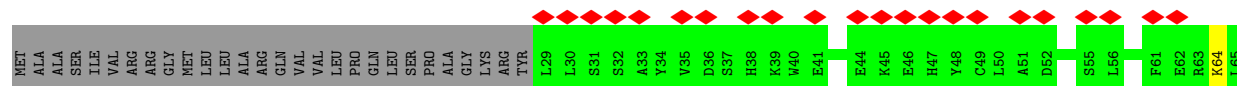
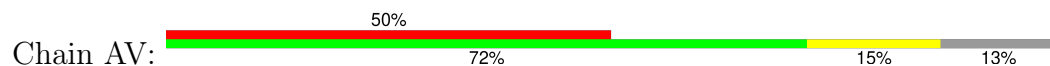
- Molecule 70: 28S ribosomal protein S25, mitochondrial

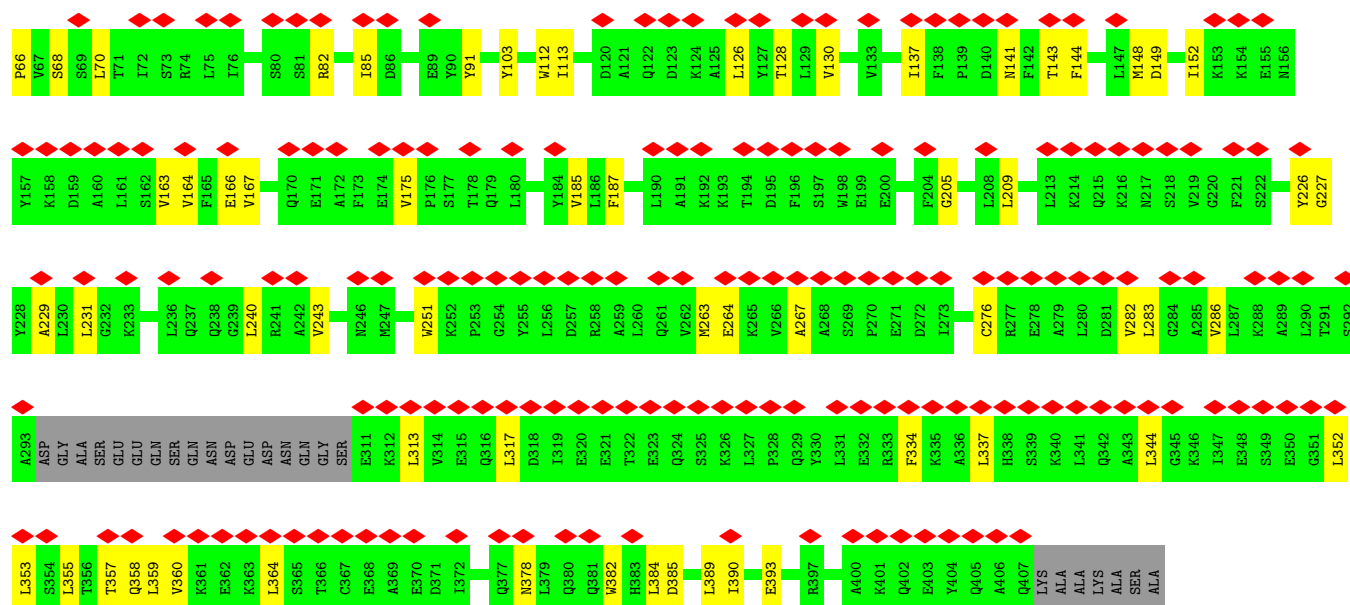


- Molecule 71: 28S ribosomal protein S26, mitochondrial



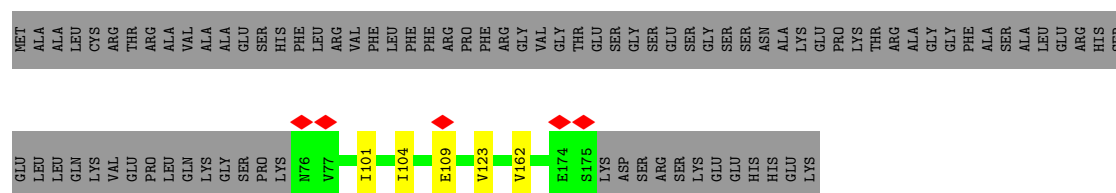
- Molecule 72: 28S ribosomal protein S27, mitochondrial





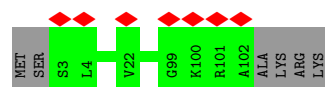
- Molecule 73: 28S ribosomal protein S28, mitochondrial

Chain AW: 51% 47%



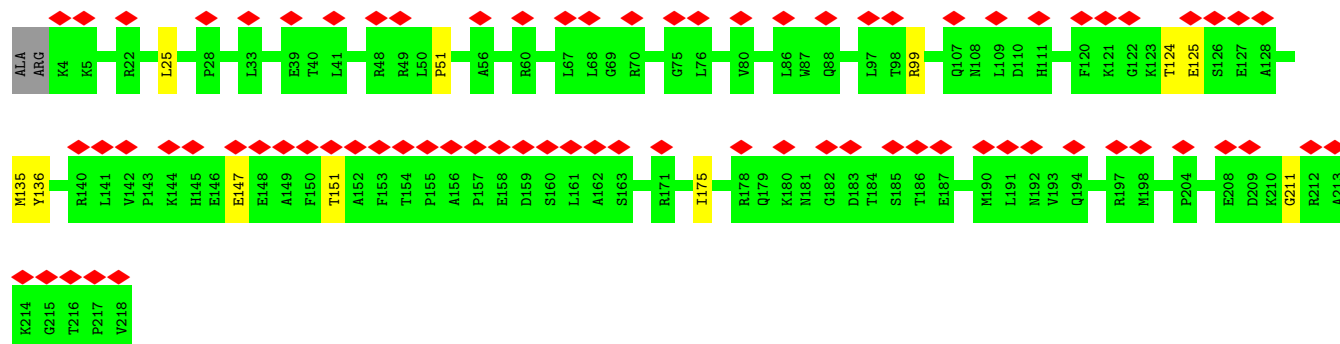
- Molecule 74: 28S ribosomal protein S33, mitochondrial

Chain AZ: 7% 94% 6%

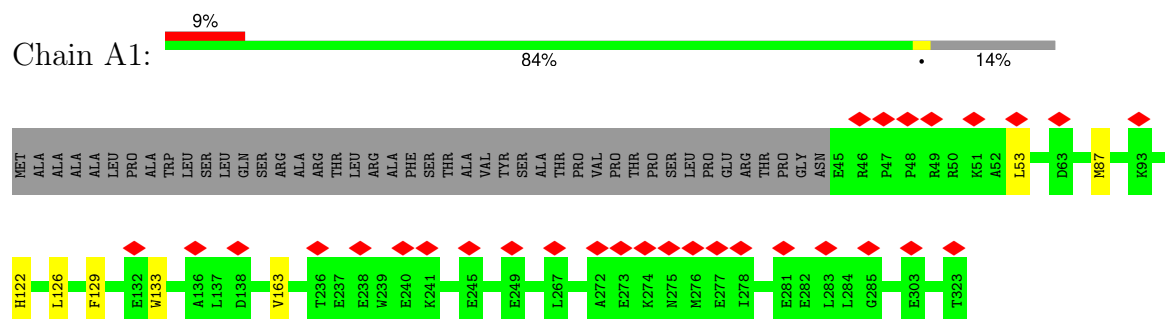


- Molecule 75: Small ribosomal subunit protein mS34

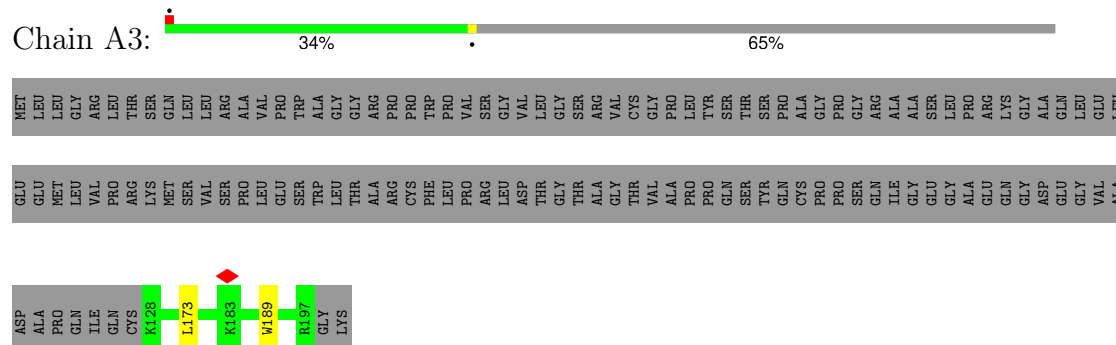
Chain A0: 35% 94% 5%



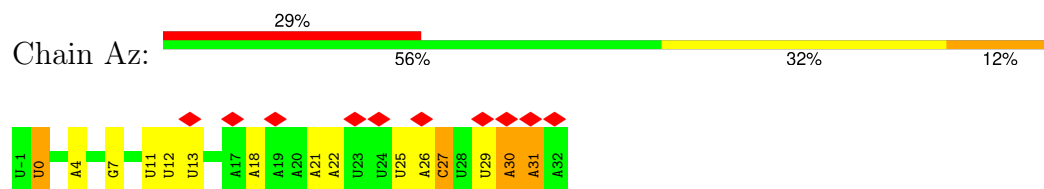
- Chain A1:



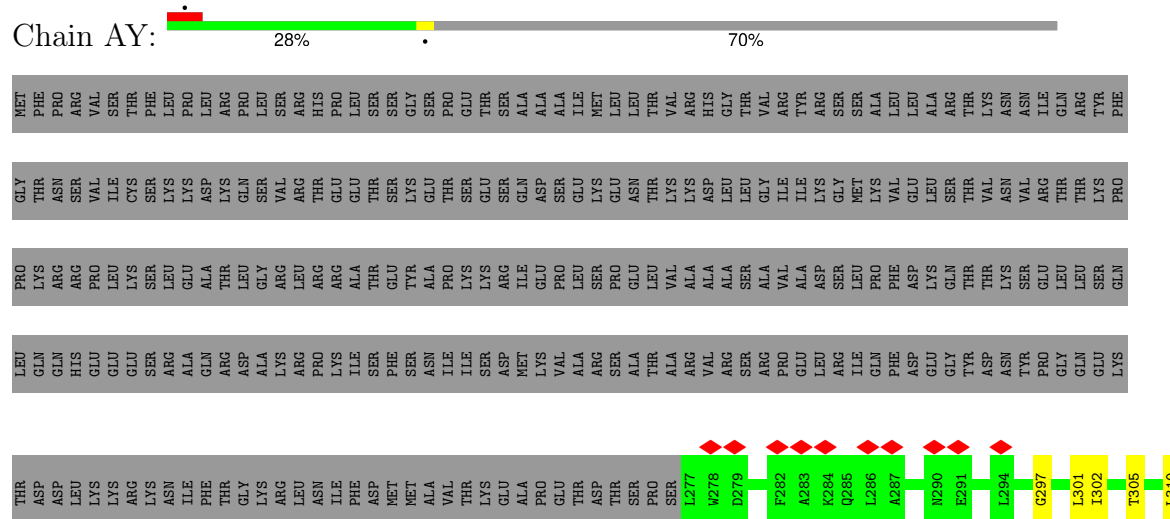
- Chain A3:

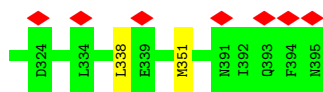


- Chain Az:

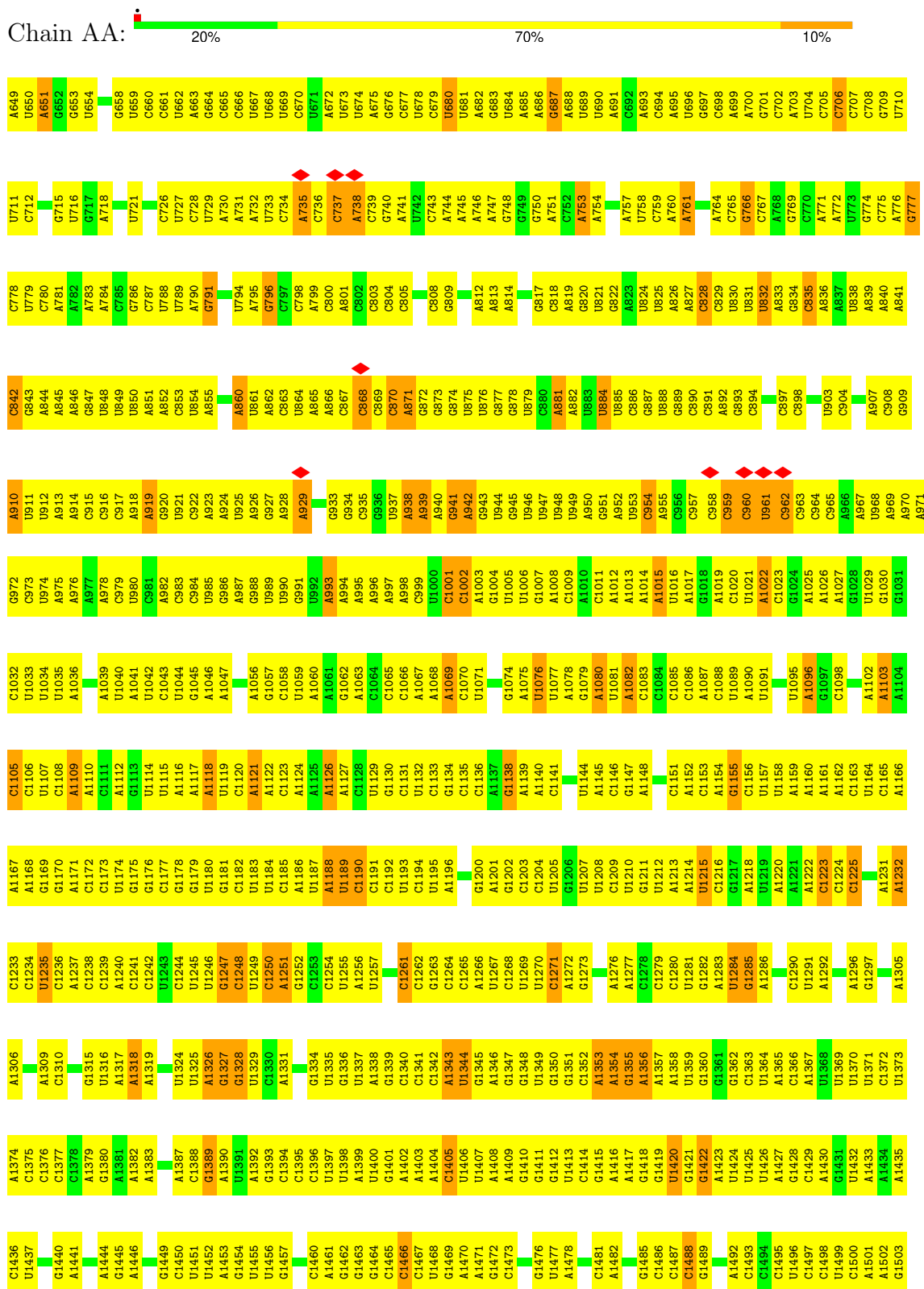


- Chain AY:



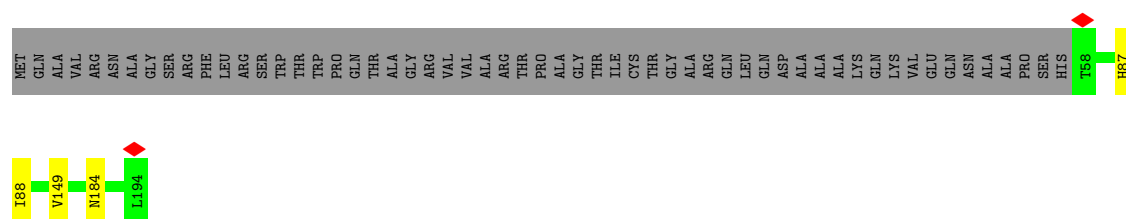


• Molecule 80: 12S mitochondrial rRNA

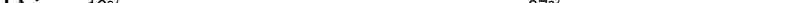


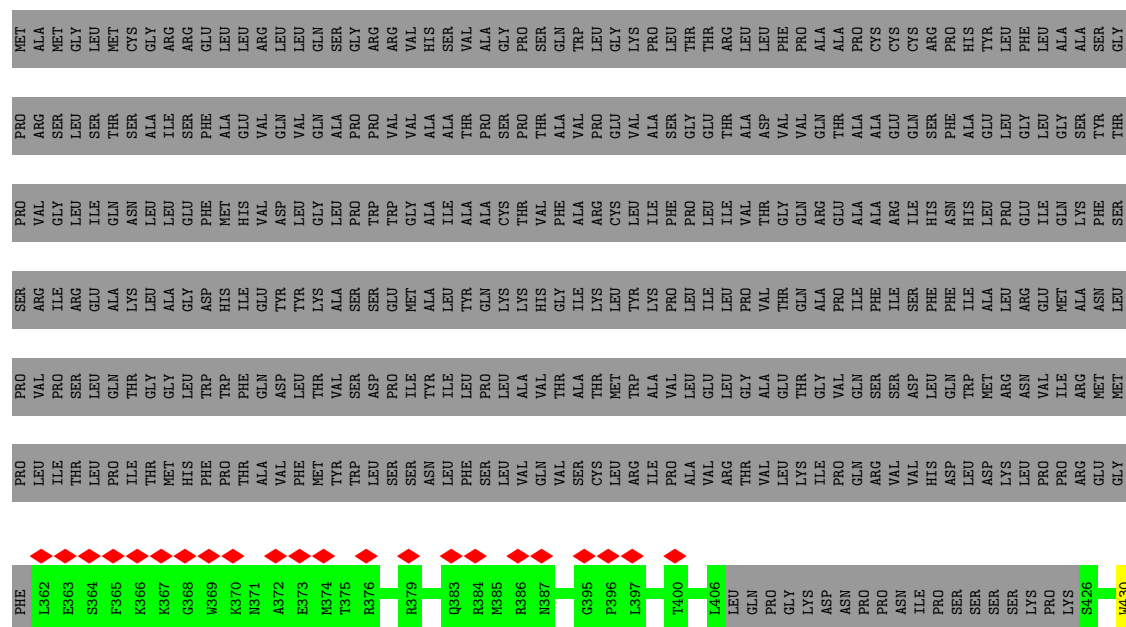
- Molecule 81: 28S ribosomal protein S11, mitochondrial

Chain AI:  69% 29% 2%



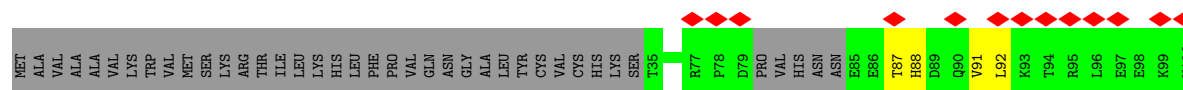
- Molecule 82: Mitochondrial inner membrane protein OXA1L

Chain OX: 



- Molecule 83: 39S ribosomal protein L42, mitochondrial

Chain a:

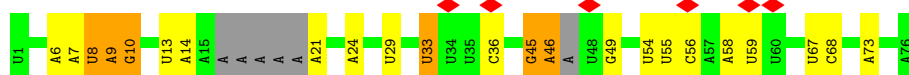




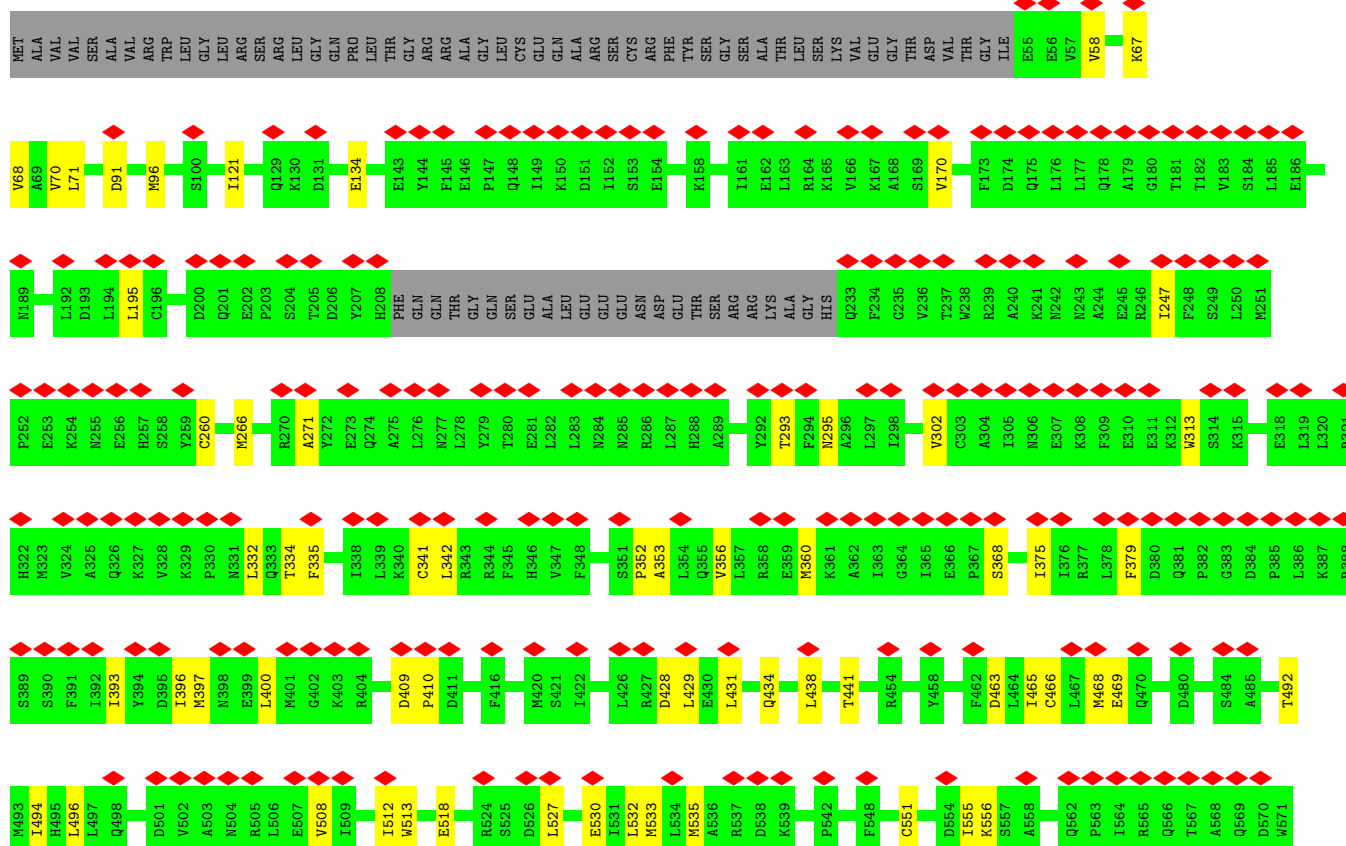
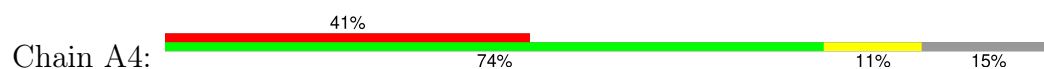
- Molecule 84: P/P-tRNA

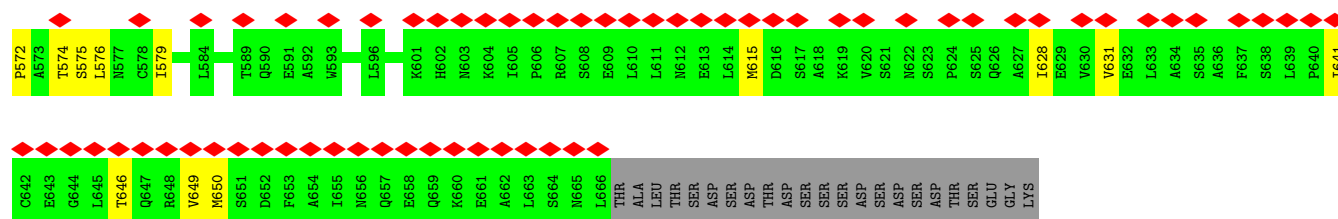


- Molecule 85: E/E-tRNA

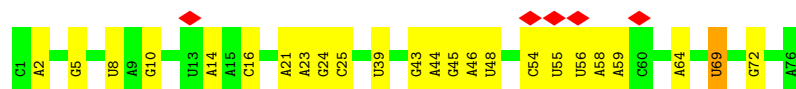


- Molecule 86: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

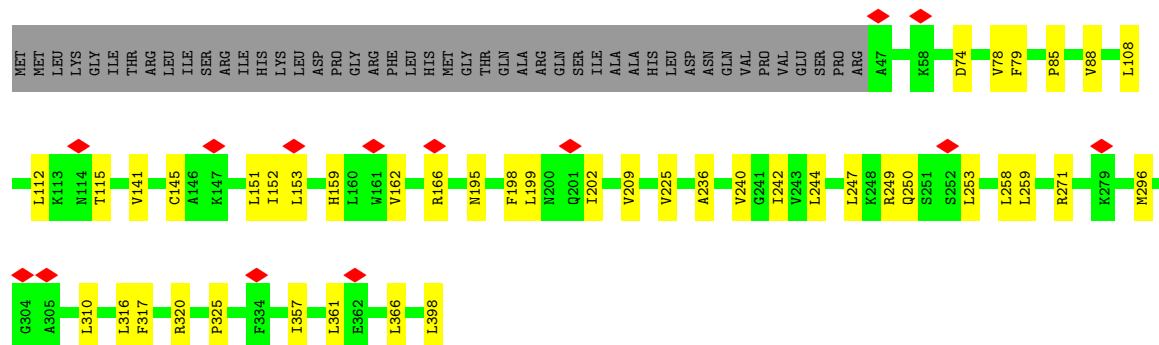
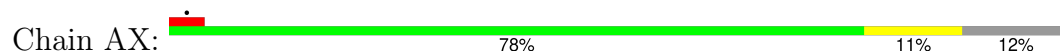




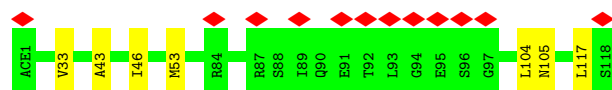
- Molecule 87: mitochondrial tRNAVal



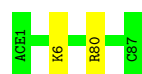
- Molecule 88: 28S ribosomal protein S29, mitochondrial



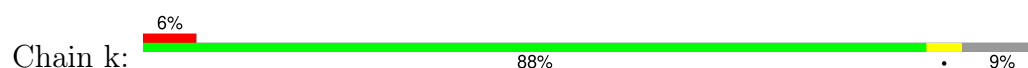
- Molecule 89: Small ribosomal subunit protein mS37

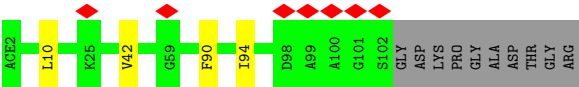


- Molecule 90: Small ribosomal subunit protein bS21m



- Molecule 91: Large ribosomal subunit protein mL53





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, OMG, ZN, K, MG, GDP, 5MC, MA6, PSU, PUT, SPM, B8T, 2MG, OMU, 1MA, NAD, ACE, SPD, ATP, 5MU

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	0.28	0/913	0.31	0/1224
2	1	0.25	0/469	0.30	0/621
3	2	0.34	0/383	0.31	0/507
4	3	0.32	0/853	0.30	0/1136
5	4	0.30	0/350	0.30	0/461
6	5	0.26	0/3305	0.30	0/4502
7	6	0.23	0/3043	0.31	0/4140
8	7	0.22	0/2447	0.30	0/3310
9	8	0.19	0/1354	0.32	0/1819
10	9	0.26	0/1025	0.29	0/1379
11	A	0.33	0/36876	0.30	0/57402
12	C	0.12	0/1754	0.26	0/2357
13	D	0.28	0/1896	0.29	0/2549
14	E	0.29	0/2475	0.31	0/3355
15	F	0.30	0/2090	0.31	0/2842
16	H	0.18	0/1698	0.27	0/2292
17	J	0.15	0/1348	0.29	0/1813
18	K	0.30	0/1497	0.32	0/2031
19	L	0.27	0/905	0.32	0/1218
20	M	0.29	0/2381	0.31	0/3212
21	N	0.28	0/1833	0.30	0/2468
22	O	0.29	0/1283	0.32	0/1727
23	P	0.25	0/1199	0.29	0/1623
24	Q	0.26	0/2039	0.30	0/2750
25	R	0.32	0/1175	0.30	0/1572
26	S	0.30	0/1320	0.31	0/1789
27	T	0.30	0/1403	0.31	0/1886
28	U	0.27	0/1279	0.31	0/1730
29	W	0.29	0/926	0.31	0/1244
30	X	0.26	0/2099	0.27	0/2837
31	Y	0.29	0/1593	0.27	0/2136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.29	0/1021	0.32	0/1378
33	z	0.14	0/2067	0.32	0/2793
34	G	0.15	0/562	0.35	0/754
34	t	0.13	0/358	0.27	0/486
34	u	0.14	0/259	0.32	0/350
35	I	0.19	0/1478	0.31	0/1999
36	V	0.23	0/1721	0.29	0/2333
37	b	0.30	0/1218	0.29	0/1649
38	d	0.20	0/2181	0.30	0/2949
39	e	0.16	0/1970	0.31	0/2658
40	g	0.28	0/1151	0.31	0/1569
41	h	0.22	0/918	0.27	0/1249
42	i	0.33	0/850	0.31	0/1135
43	j	0.26	0/760	0.27	0/1023
44	l	0.16	0/707	0.27	0/960
45	m	0.15	0/805	0.31	0/1081
47	o	0.30	0/819	0.31	0/1097
48	q	0.20	0/1529	0.28	0/2055
49	r	0.27	0/1362	0.31	0/1846
50	c	0.26	0/2347	0.28	0/3171
51	f	0.21	0/1273	0.34	0/1716
52	p	0.20	0/1223	0.28	0/1641
53	s	0.28	0/3231	0.31	0/4389
54	AB	0.20	0/1871	0.27	0/2531
55	AC	0.24	0/1113	0.35	0/1505
56	AD	0.19	0/2783	0.27	0/3724
57	AE	0.21	0/989	0.31	0/1335
58	AF	0.18	0/1767	0.27	0/2373
59	AG	0.18	0/2746	0.27	0/3681
60	AH	0.19	0/1178	0.29	0/1598
61	AJ	0.18	0/855	0.30	0/1148
62	AK	0.18	0/880	0.27	0/1182
63	AL	0.20	0/1477	0.26	0/1974
64	AM	0.15	0/963	0.30	0/1295
65	AN	0.18	0/886	0.28	0/1199
66	AO	0.15	0/1648	0.28	0/2243
67	AP	0.22	0/798	0.30	0/1070
68	AR	0.14	0/2456	0.27	0/3317
69	AS	0.18	0/1138	0.26	0/1533
70	AT	0.18	0/1402	0.29	0/1883
71	AU	0.16	0/1510	0.28	0/2025
72	AV	0.17	0/3030	0.33	0/4093
73	AW	0.18	0/801	0.27	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	AZ	0.17	0/857	0.28	0/1141
75	A0	0.14	0/1834	0.28	0/2484
76	A1	0.17	0/2313	0.30	0/3129
77	A3	0.24	0/636	0.29	0/839
78	Az	0.16	0/804	0.29	0/1248
79	AY	0.16	0/1040	0.25	0/1402
80	AA	0.24	0/22537	0.26	0/35085
81	AI	0.21	0/1039	0.27	0/1400
82	OX	0.21	0/478	0.36	0/639
83	a	0.27	0/891	0.33	0/1208
84	Ax	0.21	0/1673	0.32	0/2602
85	Ay	0.17	0/1655	0.27	0/2567
86	A4	0.16	0/4877	0.31	0/6598
87	B	0.18	0/1627	0.25	0/2527
88	AX	0.16	0/2921	0.31	0/3954
89	A2	0.20	0/947	0.28	0/1266
90	AQ	0.24	0/754	0.27	0/1003
91	k	0.18	0/783	0.25	0/1057
All	All	0.25	0/190978	0.29	0/271150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	898	917	916	3	0
2	1	464	513	511	3	0
3	2	377	407	406	2	0
4	3	832	884	883	3	0
5	4	342	362	361	4	0
6	5	3210	3209	3206	13	0
7	6	2948	2844	2841	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	7	2390	2399	2397	11	0
9	8	1327	1369	1368	7	0
10	9	997	988	987	5	0
11	A	33070	16801	16793	49	0
12	C	1732	0	1740	197	0
13	D	1859	1921	1920	6	0
14	E	2406	2416	2415	7	0
15	F	2031	2066	2065	4	0
16	H	1661	1736	1734	13	0
17	J	1330	1408	1407	8	0
18	K	1455	1452	1452	5	0
19	L	890	942	941	2	0
20	M	2327	2396	2395	3	0
21	N	1786	1818	1817	2	0
22	O	1259	1295	1294	6	0
23	P	1173	1166	1165	3	0
24	Q	1990	2031	2031	5	0
25	R	1154	1215	1214	2	0
26	S	1293	1366	1365	3	0
27	T	1369	1412	1410	5	0
28	U	1248	1228	1228	3	0
29	W	904	936	935	6	0
30	X	2044	2061	2060	6	0
31	Y	1556	1598	1597	7	0
32	Z	996	1045	1044	1	0
33	z	2027	2076	2076	19	0
34	G	558	0	612	123	0
34	t	354	378	377	6	0
34	u	257	284	283	13	0
35	I	1446	1533	1532	8	0
36	V	1676	1689	1687	6	0
37	b	1193	1186	1191	1	0
38	d	2124	0	2125	127	0
39	e	1931	1917	1916	17	0
40	g	1113	1097	1097	1	0
41	h	895	883	881	0	0
42	i	828	859	857	1	0
43	j	745	747	746	1	0
44	l	688	675	674	5	0
45	m	791	760	796	6	0
46	n	215	0	53	0	0
47	o	798	806	804	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	q	1495	942	1492	64	0
49	r	1322	1349	1348	1	0
50	c	2299	2322	2320	3	0
51	f	1252	1271	1269	13	0
52	p	1205	1225	1223	5	0
53	s	3148	3137	3131	9	0
54	AB	1828	1816	1815	3	0
55	AC	1083	1089	1088	5	0
56	AD	2731	2805	2804	19	0
57	AE	972	1000	1000	6	0
58	AF	1725	1771	1769	8	0
59	AG	2688	2689	2687	14	0
60	AH	1152	1187	1183	23	0
61	AJ	839	888	887	9	0
62	AK	862	886	885	6	0
63	AL	1453	1541	1540	10	0
64	AM	942	966	965	9	0
65	AN	868	929	928	5	0
66	AO	1592	1557	1557	14	0
67	AP	781	806	806	1	0
68	AR	2409	2430	2428	13	0
69	AS	1111	1116	1115	8	0
70	AT	1371	1393	1393	2	0
71	AU	1488	1501	1499	14	0
72	AV	2969	2964	2961	48	0
73	AW	789	804	802	4	0
74	AZ	839	859	858	0	0
75	A0	1787	1797	1796	10	0
76	A1	2265	2296	2294	11	0
77	A3	625	701	698	3	0
78	Az	719	360	360	5	0
79	AY	1010	963	957	6	0
80	AA	20260	0	10284	986	0
81	AI	1019	1058	1059	6	0
82	OX	468	465	464	2	0
83	a	865	830	829	3	0
84	Ax	1498	766	766	4	0
85	Ay	1483	752	754	10	0
86	A4	4768	4767	4766	61	0
87	B	1524	780	779	4	0
88	AX	2849	2844	2844	31	0
89	A2	935	971	971	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	AQ	744	758	758	2	0
91	k	774	785	784	2	0
92	0	1	0	0	0	0
92	4	1	0	0	0	0
92	AO	1	0	0	0	0
93	6	1	0	0	0	0
93	A	29	0	0	0	0
93	AA	18	0	0	0	0
93	D	1	0	0	0	0
93	M	2	0	0	0	0
93	N	1	0	0	0	0
93	W	1	0	0	0	0
93	o	1	0	0	0	0
94	A	40	44	76	1	0
94	AA	30	0	53	8	0
94	O	10	0	19	0	0
95	A	6	14	12	0	0
96	A	136	0	0	0	0
96	A3	1	0	0	0	0
96	AA	61	0	0	0	0
96	AB	1	0	0	0	0
96	AX	1	0	0	0	0
96	D	2	0	0	0	0
96	E	1	0	0	0	0
96	I	1	0	0	0	0
96	g	1	0	0	0	0
97	e	7	8	8	0	0
98	AP	4	0	0	0	0
98	AT	4	0	0	0	0
98	r	4	0	0	0	0
99	AA	44	0	26	2	0
100	AA	42	0	75	23	0
101	AX	31	11	12	0	0
102	AX	28	12	12	1	0
All	All	182275	139316	154814	2022	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 6.

The worst 5 of 2022 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)
12:C:211:ILE:HD12	34:G:143:VAL:HG12	1.21	1.16
12:C:239:LEU:HD11	12:C:256:CYS:HB2	1.44	0.98
80:AA:1562:G:H1'	80:AA:1583:MA6:H2	1.45	0.96
80:AA:1414:C:H3'	80:AA:1415:G:H21	1.30	0.96
34:G:134:LEU:HB2	34:G:195:VAL:HG22	1.47	0.96

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	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
2	1	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
3	2	44/92 (48%)	41 (93%)	3 (7%)	0	100	100
4	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	370 (94%)	22 (6%)	0	100	100
7	6	352/380 (93%)	339 (96%)	13 (4%)	0	100	100
8	7	292/338 (86%)	284 (97%)	8 (3%)	0	100	100
9	8	155/206 (75%)	150 (97%)	5 (3%)	0	100	100
10	9	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
12	C	221/297 (74%)	209 (95%)	12 (5%)	0	100	100
13	D	236/305 (77%)	223 (94%)	13 (6%)	0	100	100
14	E	303/348 (87%)	291 (96%)	12 (4%)	0	100	100
15	F	250/311 (80%)	242 (97%)	8 (3%)	0	100	100
16	H	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
17	J	173/192 (90%)	168 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	K	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
19	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
20	M	289/296 (98%)	277 (96%)	12 (4%)	0	100	100
21	N	220/251 (88%)	214 (97%)	6 (3%)	0	100	100
22	O	152/175 (87%)	146 (96%)	6 (4%)	0	100	100
23	P	142/180 (79%)	132 (93%)	10 (7%)	0	100	100
24	Q	237/292 (81%)	234 (99%)	3 (1%)	0	100	100
25	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
26	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
27	T	164/206 (80%)	159 (97%)	5 (3%)	0	100	100
28	U	150/153 (98%)	145 (97%)	5 (3%)	0	100	100
29	W	114/148 (77%)	110 (96%)	4 (4%)	0	100	100
30	X	242/256 (94%)	236 (98%)	6 (2%)	0	100	100
31	Y	179/250 (72%)	174 (97%)	5 (3%)	0	100	100
32	Z	120/161 (74%)	115 (96%)	5 (4%)	0	100	100
33	z	250/325 (77%)	229 (92%)	21 (8%)	0	100	100
34	G	70/198 (35%)	67 (96%)	3 (4%)	0	100	100
34	t	44/198 (22%)	42 (96%)	2 (4%)	0	100	100
34	u	30/198 (15%)	30 (100%)	0	0	100	100
35	I	179/261 (69%)	172 (96%)	7 (4%)	0	100	100
36	V	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
37	b	148/215 (69%)	139 (94%)	9 (6%)	0	100	100
38	d	257/306 (84%)	235 (91%)	22 (9%)	0	100	100
39	e	236/279 (85%)	218 (92%)	18 (8%)	0	100	100
40	g	132/166 (80%)	128 (97%)	4 (3%)	0	100	100
41	h	108/158 (68%)	100 (93%)	8 (7%)	0	100	100
42	i	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
43	j	92/123 (75%)	88 (96%)	4 (4%)	0	100	100
44	l	80/138 (58%)	76 (95%)	4 (5%)	0	100	100
45	m	90/128 (70%)	86 (96%)	4 (4%)	0	100	100
47	o	92/102 (90%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	q	175/222 (79%)	173 (99%)	2 (1%)	0	100	100
49	r	160/196 (82%)	155 (97%)	5 (3%)	0	100	100
50	c	282/332 (85%)	275 (98%)	7 (2%)	0	100	100
51	f	153/212 (72%)	143 (94%)	10 (6%)	0	100	100
52	p	141/206 (68%)	135 (96%)	6 (4%)	0	100	100
53	s	381/439 (87%)	373 (98%)	8 (2%)	0	100	100
54	AB	223/296 (75%)	216 (97%)	7 (3%)	0	100	100
55	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
56	AD	341/430 (79%)	330 (97%)	11 (3%)	0	100	100
57	AE	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
58	AF	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
59	AG	323/396 (82%)	314 (97%)	9 (3%)	0	100	100
60	AH	138/201 (69%)	134 (97%)	3 (2%)	1 (1%)	18	45
61	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
62	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
63	AL	172/257 (67%)	170 (99%)	2 (1%)	0	100	100
64	AM	117/137 (85%)	110 (94%)	7 (6%)	0	100	100
65	AN	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
66	AO	191/258 (74%)	185 (97%)	6 (3%)	0	100	100
67	AP	95/142 (67%)	91 (96%)	4 (4%)	0	100	100
68	AR	293/360 (81%)	284 (97%)	9 (3%)	0	100	100
69	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
70	AT	166/173 (96%)	161 (97%)	5 (3%)	0	100	100
71	AU	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
72	AV	358/414 (86%)	342 (96%)	16 (4%)	0	100	100
73	AW	98/187 (52%)	92 (94%)	5 (5%)	1 (1%)	12	37
74	AZ	98/106 (92%)	95 (97%)	3 (3%)	0	100	100
75	A0	213/217 (98%)	206 (97%)	7 (3%)	0	100	100
76	A1	277/323 (86%)	266 (96%)	11 (4%)	0	100	100
77	A3	68/199 (34%)	65 (96%)	3 (4%)	0	100	100
79	AY	117/395 (30%)	115 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	AI	135/194 (70%)	127 (94%)	8 (6%)	0	100	100
82	OX	51/435 (12%)	47 (92%)	4 (8%)	0	100	100
83	a	99/142 (70%)	93 (94%)	6 (6%)	0	100	100
86	A4	584/689 (85%)	558 (96%)	26 (4%)	0	100	100
88	AX	350/398 (88%)	328 (94%)	22 (6%)	0	100	100
89	A2	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
90	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
91	k	100/112 (89%)	97 (97%)	3 (3%)	0	100	100
All	All	14908/19622 (76%)	14356 (96%)	550 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	AH	126	ILE
73	AW	109	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (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%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	146/190 (77%)	146 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	C	193/245 (79%)	193 (100%)	0	100	100
13	D	192/245 (78%)	192 (100%)	0	100	100
14	E	260/290 (90%)	260 (100%)	0	100	100
15	F	219/262 (84%)	219 (100%)	0	100	100
16	H	182/228 (80%)	182 (100%)	0	100	100
17	J	138/150 (92%)	138 (100%)	0	100	100
18	K	155/155 (100%)	155 (100%)	0	100	100
19	L	98/124 (79%)	98 (100%)	0	100	100
20	M	246/249 (99%)	246 (100%)	0	100	100
21	N	189/211 (90%)	189 (100%)	0	100	100
22	O	134/150 (89%)	134 (100%)	0	100	100
23	P	126/155 (81%)	126 (100%)	0	100	100
24	Q	221/256 (86%)	221 (100%)	0	100	100
25	R	118/126 (94%)	118 (100%)	0	100	100
26	S	146/180 (81%)	146 (100%)	0	100	100
27	T	146/176 (83%)	146 (100%)	0	100	100
28	U	134/135 (99%)	134 (100%)	0	100	100
29	W	94/119 (79%)	94 (100%)	0	100	100
30	X	220/229 (96%)	220 (100%)	0	100	100
31	Y	163/223 (73%)	163 (100%)	0	100	100
32	Z	113/147 (77%)	113 (100%)	0	100	100
33	z	226/287 (79%)	226 (100%)	0	100	100
34	G	60/158 (38%)	60 (100%)	0	100	100
34	t	40/158 (25%)	40 (100%)	0	100	100
34	u	31/158 (20%)	31 (100%)	0	100	100
35	I	165/232 (71%)	165 (100%)	0	100	100
36	V	183/191 (96%)	183 (100%)	0	100	100
37	b	132/186 (71%)	132 (100%)	0	100	100
38	d	237/274 (86%)	237 (100%)	0	100	100
39	e	207/236 (88%)	207 (100%)	0	100	100
40	g	124/148 (84%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	h	104/148 (70%)	104 (100%)	0	100	100
42	i	86/110 (78%)	86 (100%)	0	100	100
43	j	74/97 (76%)	74 (100%)	0	100	100
44	l	76/116 (66%)	76 (100%)	0	100	100
45	m	85/113 (75%)	85 (100%)	0	100	100
47	o	80/87 (92%)	80 (100%)	0	100	100
48	q	153/178 (86%)	153 (100%)	0	100	100
49	r	147/169 (87%)	147 (100%)	0	100	100
50	c	251/288 (87%)	251 (100%)	0	100	100
51	f	139/188 (74%)	139 (100%)	0	100	100
52	p	135/181 (75%)	135 (100%)	0	100	100
53	s	339/381 (89%)	339 (100%)	0	100	100
54	AB	198/249 (80%)	198 (100%)	0	100	100
55	AC	115/143 (80%)	115 (100%)	0	100	100
56	AD	286/357 (80%)	286 (100%)	0	100	100
57	AE	104/107 (97%)	104 (100%)	0	100	100
58	AF	185/209 (88%)	185 (100%)	0	100	100
59	AG	285/342 (83%)	285 (100%)	0	100	100
60	AH	130/180 (72%)	130 (100%)	0	100	100
61	AJ	93/118 (79%)	93 (100%)	0	100	100
62	AK	91/113 (80%)	91 (100%)	0	100	100
63	AL	158/226 (70%)	158 (100%)	0	100	100
64	AM	97/113 (86%)	97 (100%)	0	100	100
65	AN	96/115 (84%)	96 (100%)	0	100	100
66	AO	174/230 (76%)	174 (100%)	0	100	100
67	AP	88/123 (72%)	88 (100%)	0	100	100
68	AR	264/318 (83%)	264 (100%)	0	100	100
69	AS	116/164 (71%)	116 (100%)	0	100	100
70	AT	153/157 (98%)	153 (100%)	0	100	100
71	AU	152/174 (87%)	152 (100%)	0	100	100
72	AV	325/364 (89%)	325 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	AW	87/158 (55%)	87 (100%)	0	100	100
74	AZ	90/95 (95%)	90 (100%)	0	100	100
75	A0	188/189 (100%)	188 (100%)	0	100	100
76	A1	257/291 (88%)	257 (100%)	0	100	100
77	A3	65/166 (39%)	65 (100%)	0	100	100
79	AY	110/357 (31%)	110 (100%)	0	100	100
81	AI	105/147 (71%)	105 (100%)	0	100	100
82	OX	49/372 (13%)	49 (100%)	0	100	100
83	a	99/133 (74%)	99 (100%)	0	100	100
86	A4	526/609 (86%)	526 (100%)	0	100	100
88	AX	311/351 (89%)	311 (100%)	0	100	100
89	A2	100/100 (100%)	100 (100%)	0	100	100
90	AQ	78/78 (100%)	78 (100%)	0	100	100
91	k	83/89 (93%)	83 (100%)	0	100	100
All	All	13322/16932 (79%)	13322 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
55	AC	75	ASN
66	AO	160	HIS
57	AE	92	ASN
62	AK	68	GLN
70	AT	101	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1561 (99%)	250 (16%)	4 (0%)
46	n	0/43	-	-
78	Az	33/34 (97%)	14 (42%)	0
80	AA	953/954 (99%)	149 (15%)	1 (0%)
84	Ax	70/71 (98%)	16 (22%)	0
85	Ay	67/76 (88%)	13 (19%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
87	B	71/72 (98%)	16 (22%)	0
All	All	2750/2811 (97%)	458 (16%)	5 (0%)

5 of 458 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1689	C
11	A	1692	A
11	A	1699	C
11	A	1700	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1779	A
11	A	2112	A
11	A	2245	A
11	A	2484	C
80	AA	1520	U

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

13 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	$\# Z > 2$
87	1MA	B	9	87	21,25,26	0.40	0	30,37,40	0.58	0
80	MA6	AA	1584	80	23,26,27	0.33	0	33,38,41	0.65	1 (3%)
80	5MC	AA	1488	80	19,22,23	0.83	1 (5%)	26,32,35	0.50	0
11	OMG	A	2815	84,11,93	23,26,27	0.37	0	32,38,41	0.39	0
11	OMG	A	3040	11	23,26,27	0.35	0	32,38,41	0.38	0
87	2MG	B	10	87	23,26,27	0.36	0	33,38,41	0.43	0
87	PSU	B	39	87	18,21,22	1.06	1 (5%)	21,30,33	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	5MU	AA	1076	80	19,22,23	0.36	0	27,32,35	0.39	0
80	MA6	AA	1583	80	23,26,27	0.34	0	33,38,41	0.65	1 (3%)
80	B8T	AA	1486	96,80	19,22,23	0.42	0	25,31,34	0.38	0
11	1MA	A	2617	11	21,25,26	0.45	0	30,37,40	0.61	0
11	OMU	A	3039	11,93	19,22,23	0.32	0	25,31,34	0.62	1 (4%)
11	PSU	A	3067	11	18,21,22	1.16	2 (11%)	21,30,33	0.74	1 (4%)

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
87	1MA	B	9	87	-	2/7/25/26	0/3/3/3
80	MA6	AA	1584	80	-	1/11/29/30	0/3/3/3
80	5MC	AA	1488	80	-	0/7/25/26	0/2/2/2
11	OMG	A	2815	84,11,93	-	0/9/27/28	0/3/3/3
11	OMG	A	3040	11	-	0/9/27/28	0/3/3/3
87	2MG	B	10	87	-	0/9/27/28	0/3/3/3
87	PSU	B	39	87	-	0/7/25/26	0/2/2/2
80	5MU	AA	1076	80	-	5/7/25/26	0/2/2/2
80	MA6	AA	1583	80	-	0/11/29/30	0/3/3/3
80	B8T	AA	1486	96,80	-	0/7/27/28	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
11	OMU	A	3039	11,93	-	0/9/27/28	0/2/2/2
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	B	39	PSU	C6-C5	3.61	1.39	1.35
11	A	3067	PSU	C6-C5	3.56	1.39	1.35
80	AA	1488	5MC	C5-C4	-3.28	1.41	1.44
11	A	3067	PSU	O4'-C1'	-2.61	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	AA	1583	MA6	C2-N1-C6	2.70	118.41	111.83
80	AA	1584	MA6	C2-N1-C6	2.68	118.39	111.83
11	A	3039	OMU	C2'-C1'-N1	-2.27	109.92	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	3067	PSU	O4'-C1'-C2'	2.23	108.24	105.15

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	AA	1076	5MU	O4'-C4'-C5'-O5'
80	AA	1076	5MU	C3'-C4'-C5'-O5'
80	AA	1076	5MU	C2'-C1'-N1-C2
87	B	9	1MA	O4'-C4'-C5'-O5'
80	AA	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
80	AA	1488	5MC	2	0
80	AA	1076	5MU	4	0
80	AA	1583	MA6	4	0
80	AA	1486	B8T	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 281 ligands modelled in this entry, 262 are monoatomic - leaving 19 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
100	SPM	AA	1782	100	13,13,13	0.36	0	12,12,12	0.98	0
99	NAD	AA	1701	96	46,48,48	2.63	19 (41%)	64,73,73	1.65	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
102	GDP	AX	503	-	29,30,30	2.84	13 (44%)	45,47,47	1.52	9 (20%)
94	SPD	O	301	-	9,9,9	0.32	0	8,8,8	0.90	0
100	SPM	AA	1785	100	13,13,13	0.36	0	12,12,12	0.84	0
98	FES	r	201	49,35	0,4,4	-	-	-	-	-
101	ATP	AX	501	96	32,33,33	0.52	0	48,52,52	0.59	0
94	SPD	A	3301	96	9,9,9	0.34	0	8,8,8	0.73	0
94	SPD	A	3469	-	9,9,9	0.30	0	8,8,8	0.86	0
94	SPD	A	3470	-	9,9,9	0.32	0	8,8,8	0.87	0
100	SPM	AA	1702	-	13,13,13	0.37	0	12,12,12	1.12	0
95	PUT	A	3303	-	5,5,5	0.20	0	4,4,4	0.55	0
98	FES	AP	201	67,57	0,4,4	-	-	-	-	-
94	SPD	AA	1786	94	9,9,9	0.33	0	8,8,8	0.72	0
94	SPD	A	3302	-	9,9,9	0.32	0	8,8,8	0.88	0
98	FES	AT	201	64,70	0,4,4	-	-	-	-	-
97	VAL	e	301	-	4,6,7	0.56	0	6,7,9	0.89	0
94	SPD	AA	1703	-	9,9,9	0.33	0	8,8,8	0.89	0
94	SPD	AA	1784	94	9,9,9	0.31	0	8,8,8	0.96	0

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
100	SPM	AA	1782	100	-	8/11/11/11	-
99	NAD	AA	1701	96	-	10/30/62/62	0/5/5/5
102	GDP	AX	503	-	-	5/16/32/32	0/3/3/3
94	SPD	O	301	-	-	2/7/7/7	-
100	SPM	AA	1785	100	-	6/11/11/11	-
98	FES	r	201	49,35	-	-	0/1/1/1
101	ATP	AX	501	96	-	0/22/38/38	0/3/3/3
94	SPD	A	3301	96	-	3/7/7/7	-
94	SPD	A	3469	-	-	1/7/7/7	-
94	SPD	A	3470	-	-	0/7/7/7	-
100	SPM	AA	1702	-	-	1/11/11/11	-
95	PUT	A	3303	-	-	0/3/3/3	-
98	FES	AP	201	67,57	-	-	0/1/1/1
94	SPD	AA	1786	94	-	3/7/7/7	-
94	SPD	A	3302	-	-	3/7/7/7	-
98	FES	AT	201	64,70	-	-	0/1/1/1
97	VAL	e	301	-	-	1/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	SPD	AA	1703	-	-	2/7/7/7	-
94	SPD	AA	1784	94	-	4/7/7/7	-

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
102	AX	503	GDP	O6-C6	8.75	1.40	1.23
99	AA	1701	NAD	C7N-N7N	7.10	1.46	1.33
99	AA	1701	NAD	O4D-C1D	6.35	1.49	1.40
99	AA	1701	NAD	PN-O3	5.77	1.65	1.59
99	AA	1701	NAD	C6A-N6A	5.47	1.48	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
99	AA	1701	NAD	C4A-N9A-C8A	8.48	114.64	105.74
102	AX	503	GDP	C8-N9-C4	4.37	114.22	106.03
102	AX	503	GDP	C3'-C2'-C1'	2.95	107.05	101.46
102	AX	503	GDP	C2-N1-C6	-2.92	119.81	125.11
99	AA	1701	NAD	C4D-O4D-C1D	-2.90	107.27	109.92

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
97	e	301	VAL	O-C-CA-CB
99	AA	1701	NAD	C5D-O5D-PN-O3
99	AA	1701	NAD	C5D-O5D-PN-O1N
99	AA	1701	NAD	C5D-O5D-PN-O2N
102	AX	503	GDP	PA-O3A-PB-O3B

There are no ring outliers.

9 monomers are involved in 35 short contacts:

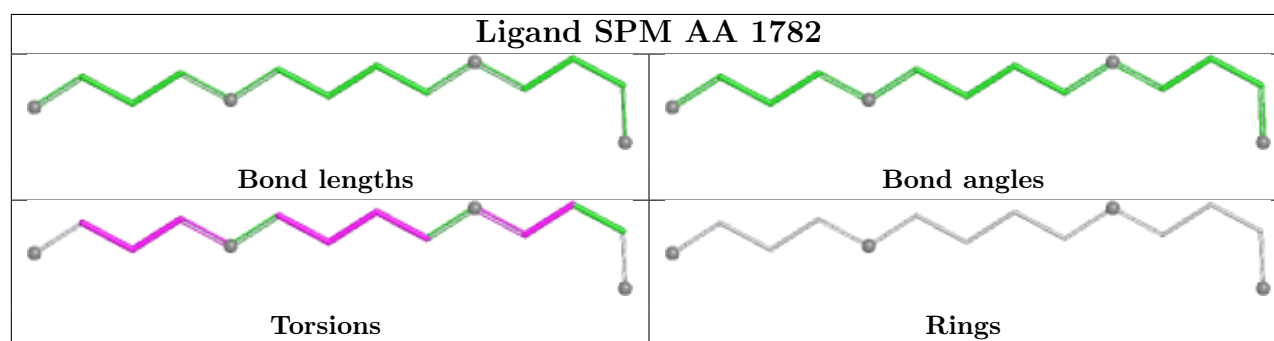
Mol	Chain	Res	Type	Clashes	Symm-Clashes
100	AA	1782	SPM	16	0
99	AA	1701	NAD	2	0
102	AX	503	GDP	1	0
100	AA	1785	SPM	19	0
94	A	3470	SPD	1	0

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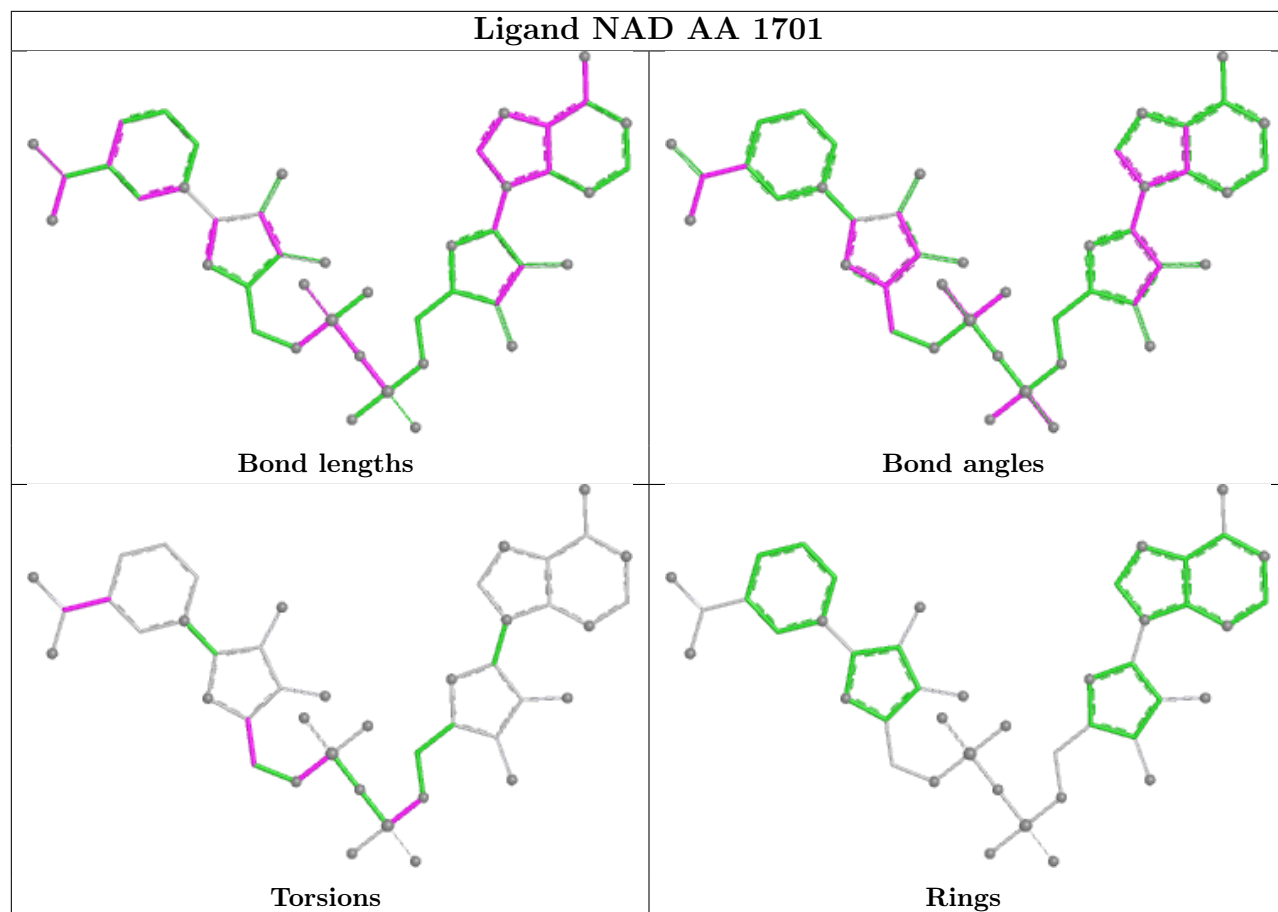
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
100	AA	1702	SPM	2	0
94	AA	1786	SPD	5	0
94	AA	1703	SPD	1	0
94	AA	1784	SPD	5	0

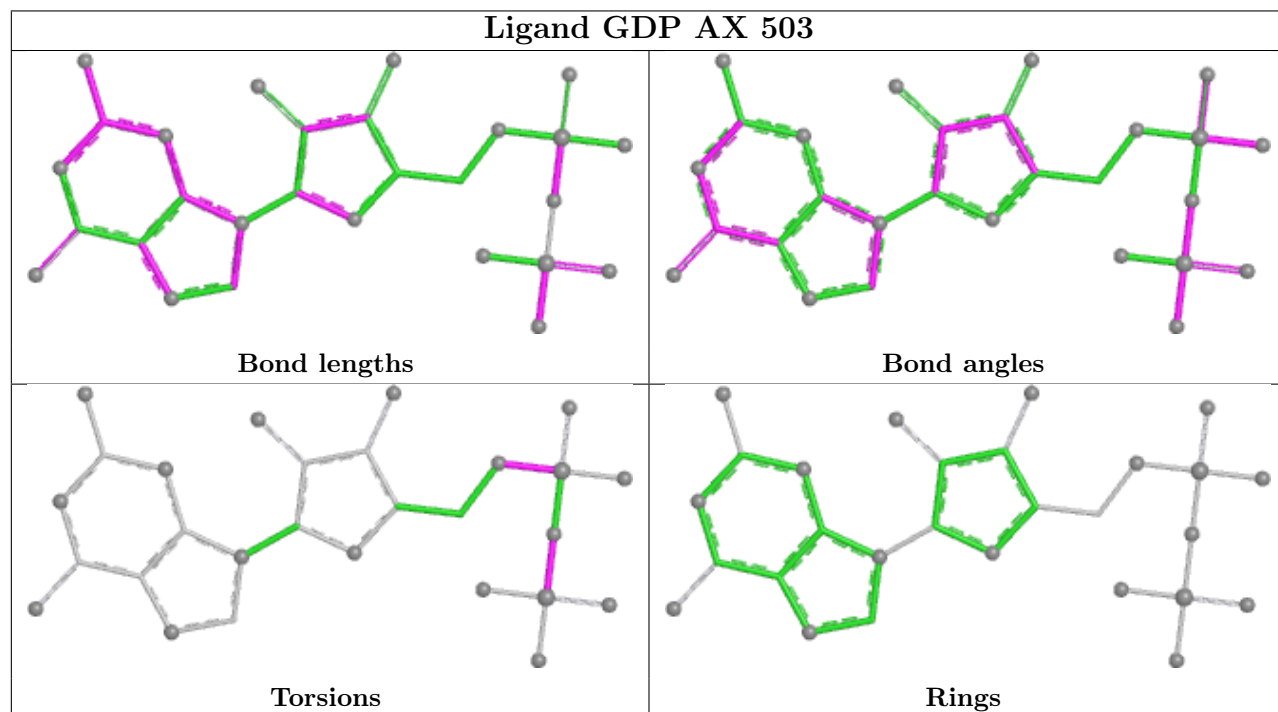
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

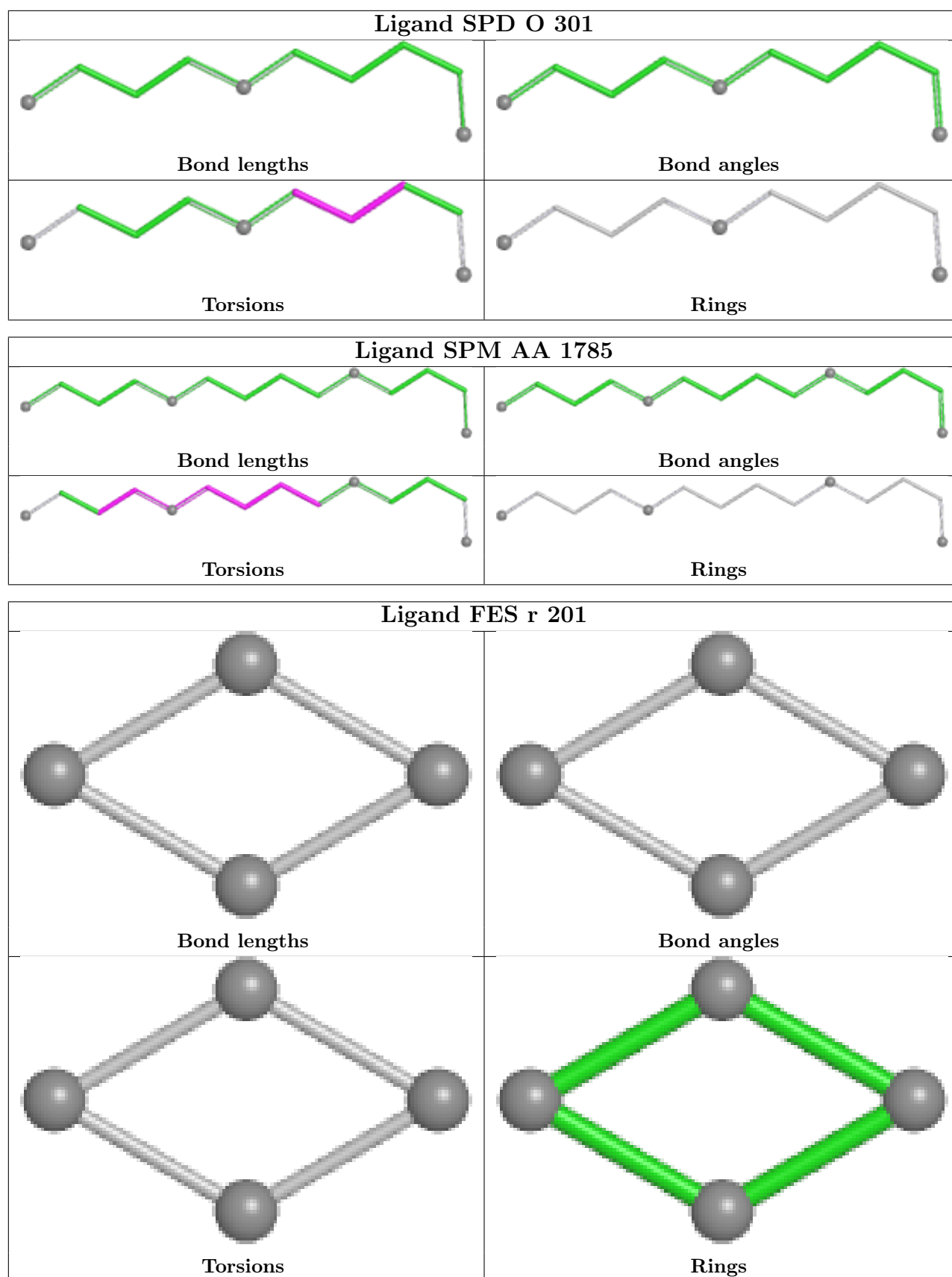


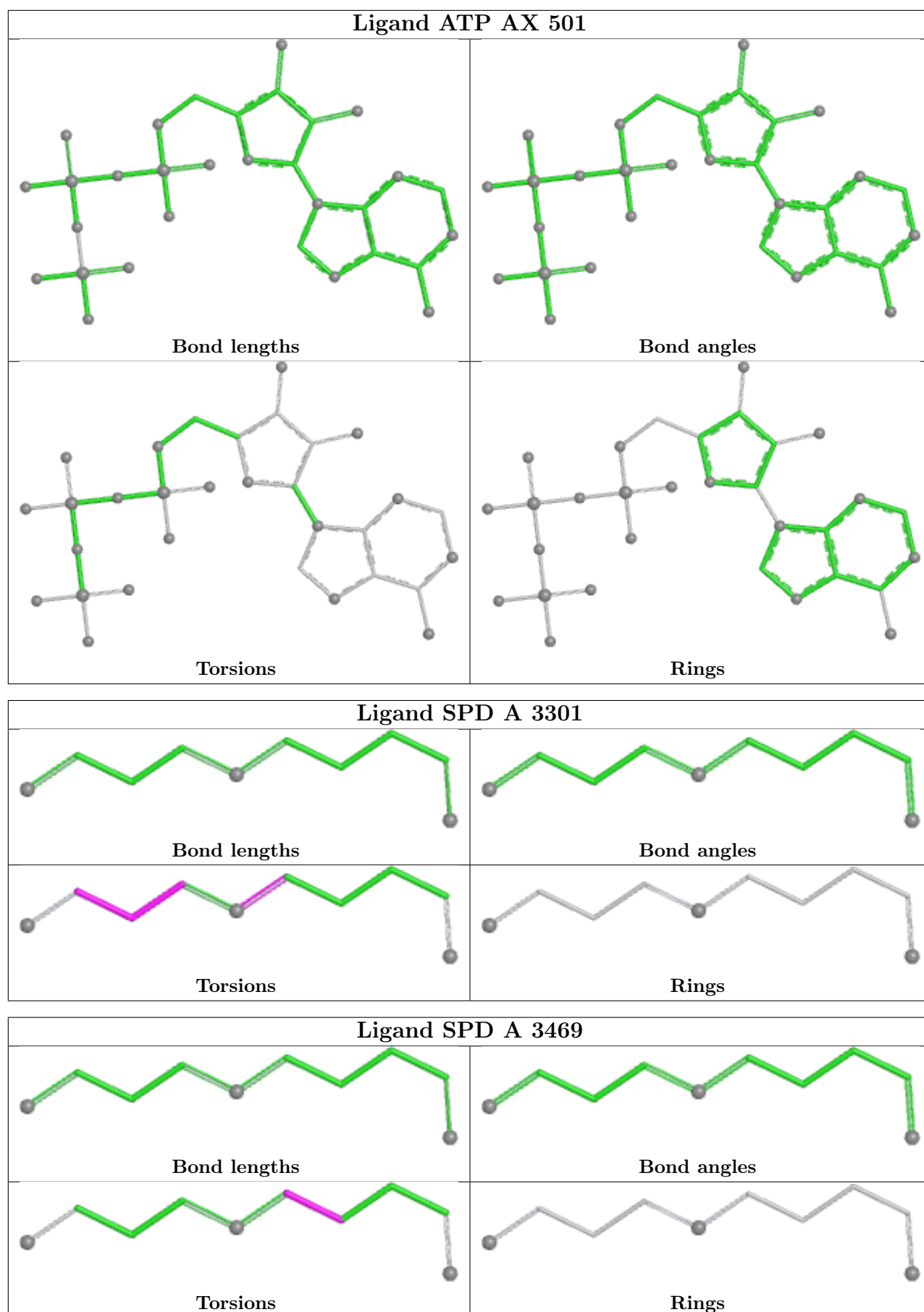
Ligand NAD AA 1701

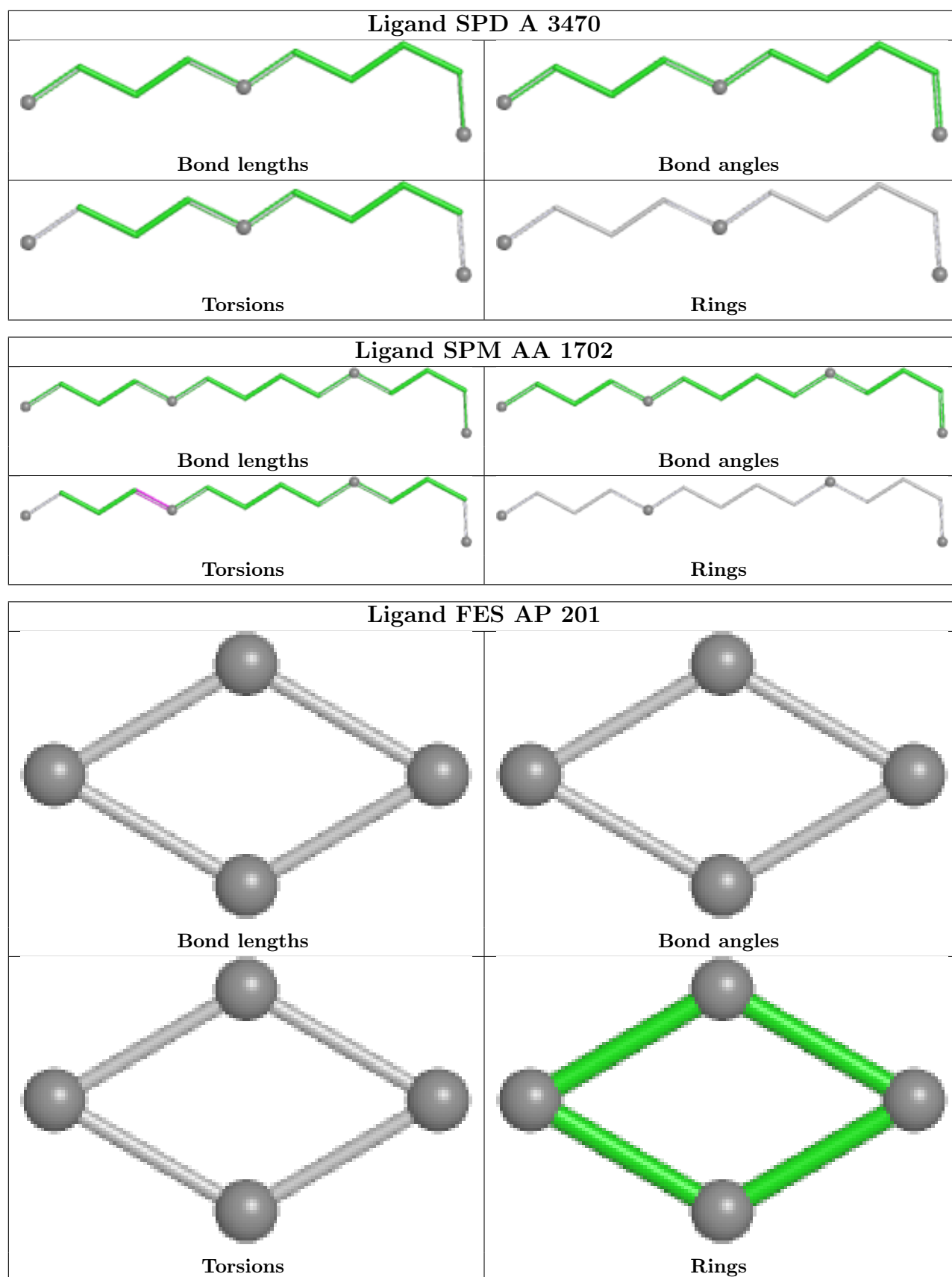


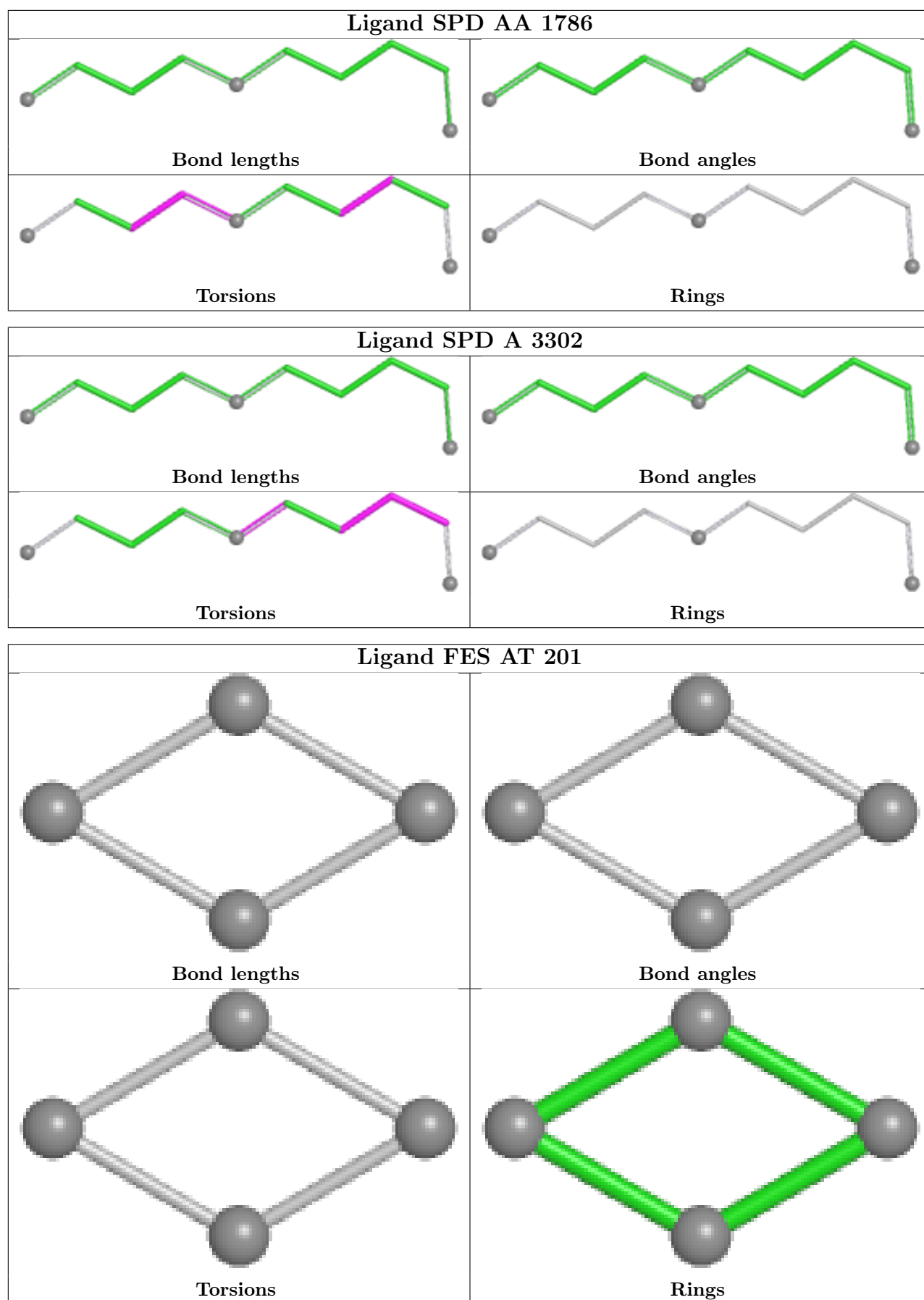
Ligand GDP AX 503

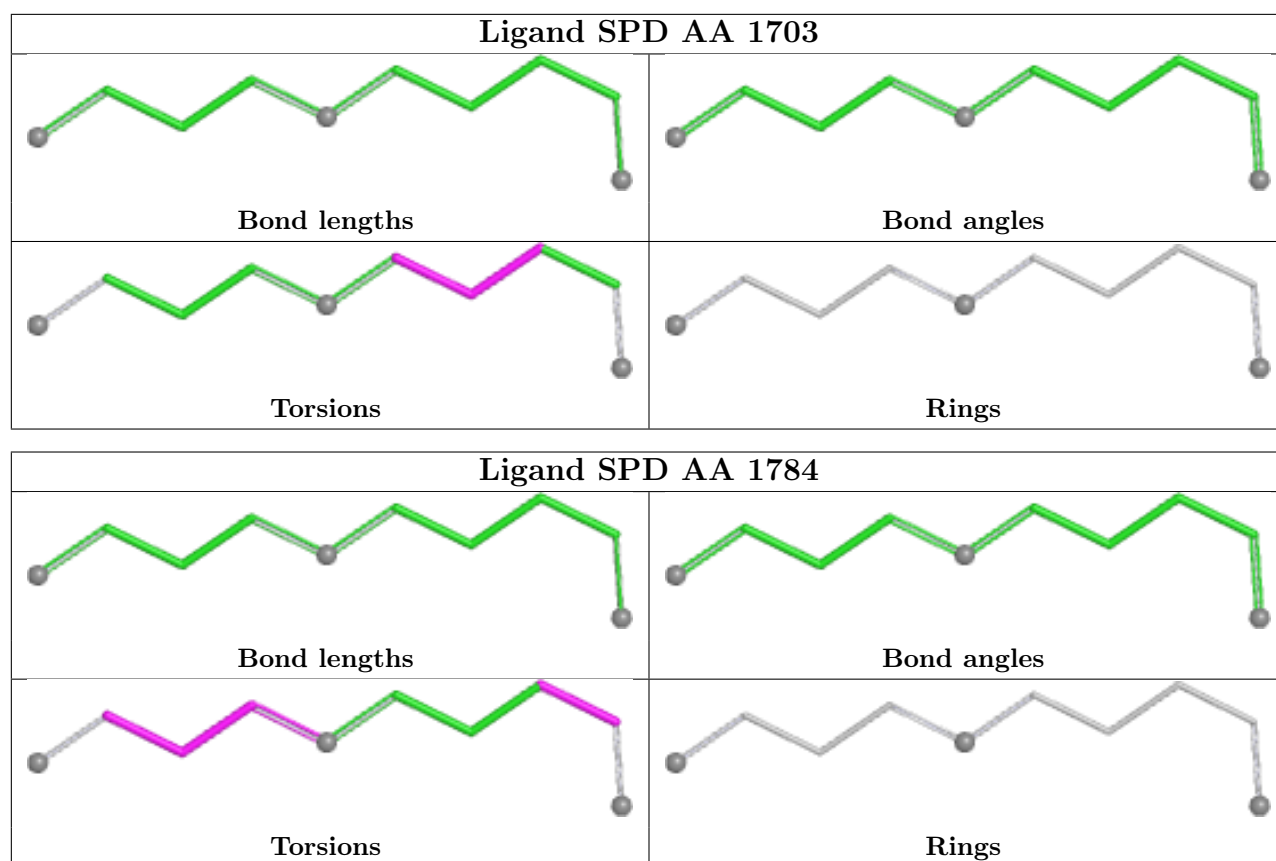












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

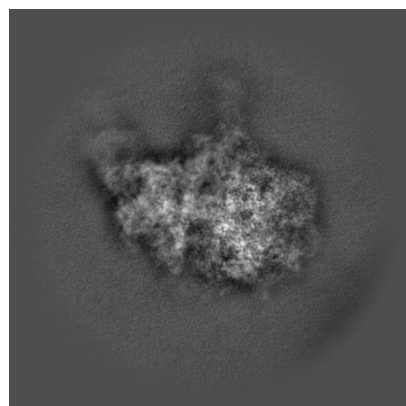
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71623. These allow visual inspection of the internal detail of the map and identification of artifacts.

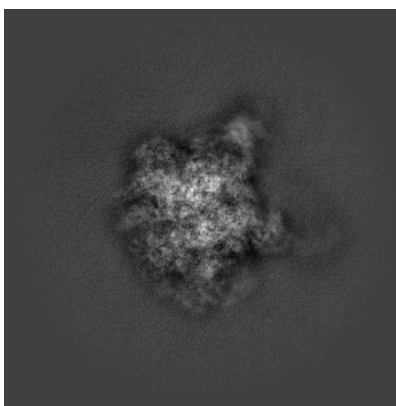
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

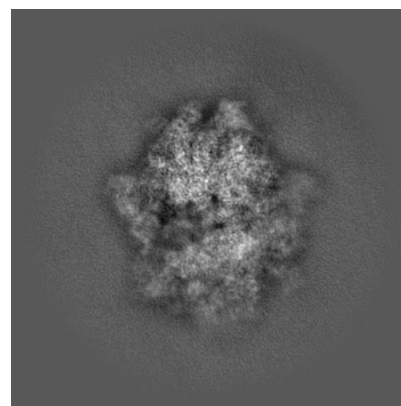
6.1.1 Primary map



X

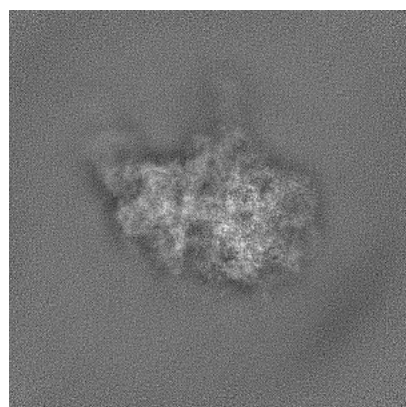


Y

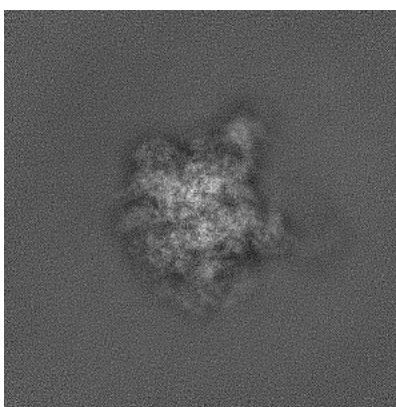


Z

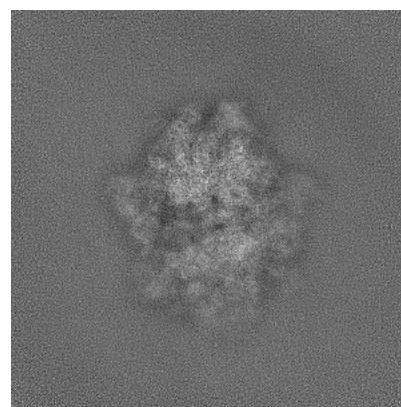
6.1.2 Raw map



X



Y

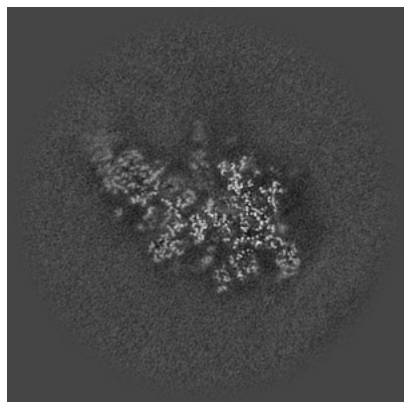


Z

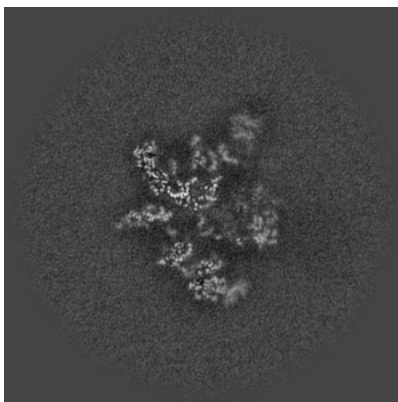
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

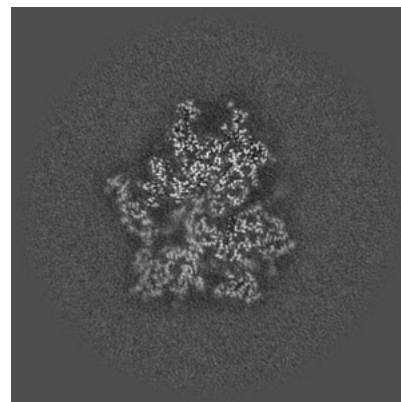
6.2.1 Primary map



X Index: 240

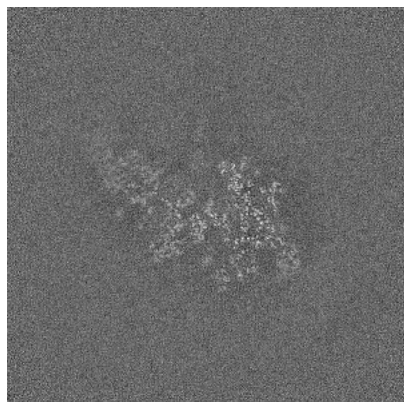


Y Index: 240

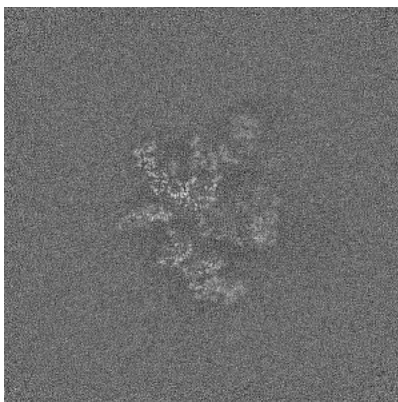


Z Index: 240

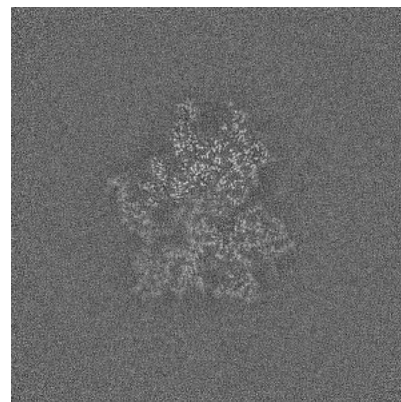
6.2.2 Raw map



X Index: 240



Y Index: 240

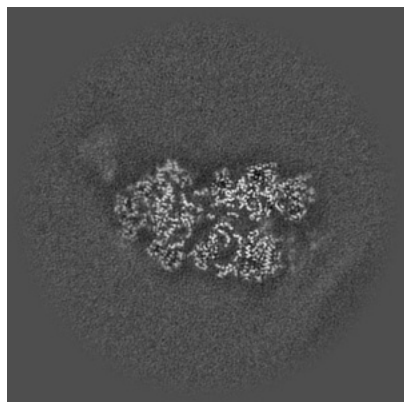


Z Index: 240

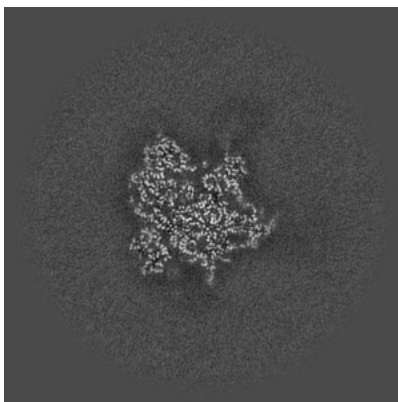
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

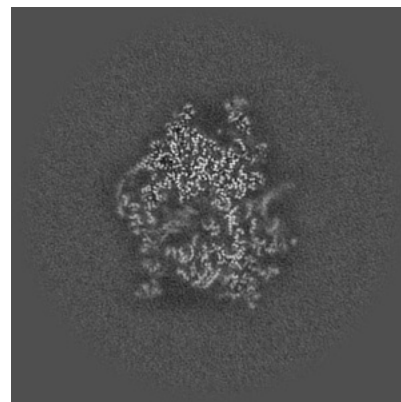
6.3.1 Primary map



X Index: 275

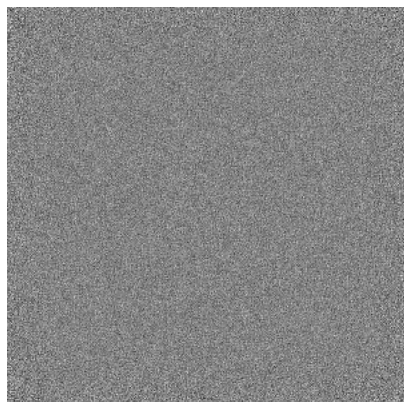


Y Index: 287

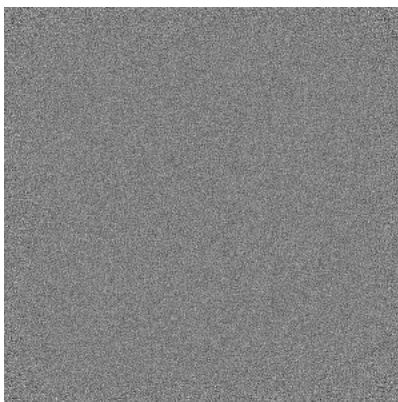


Z Index: 249

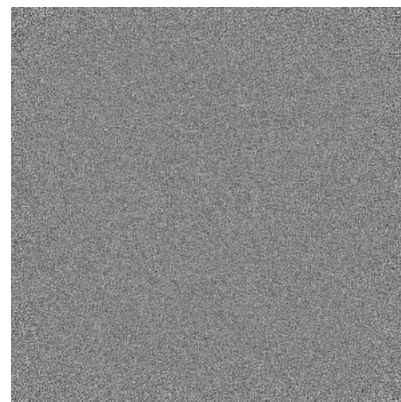
6.3.2 Raw map



X Index: 0



Y Index: 0

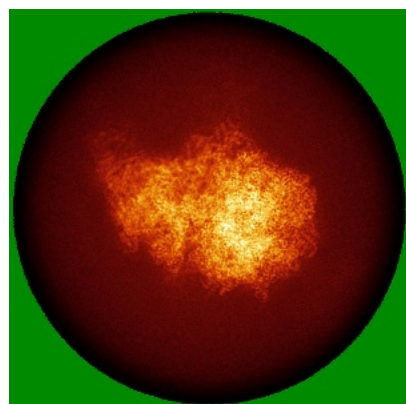


Z Index: 0

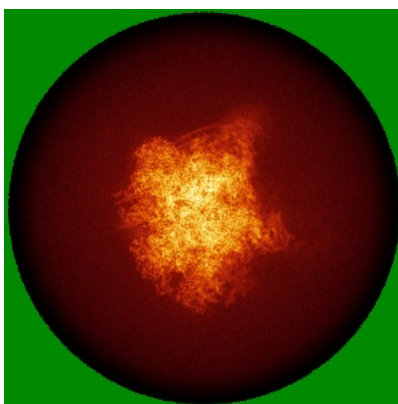
The images above show the largest variance slices of the map in three orthogonal directions.

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

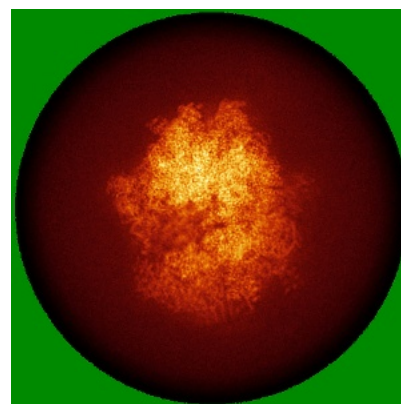
6.4.1 Primary map



X

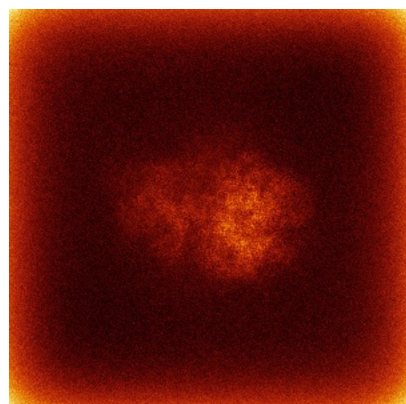


Y

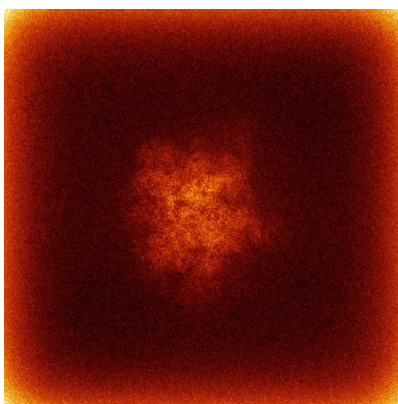


Z

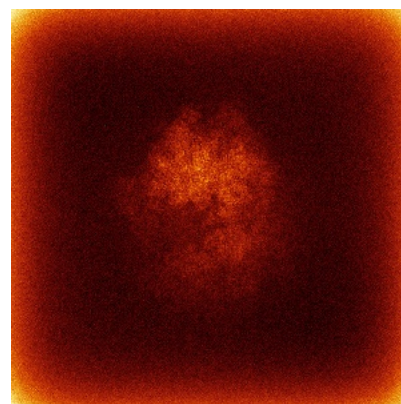
6.4.2 Raw map



X



Y

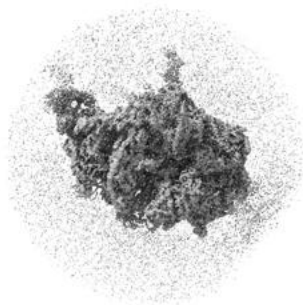


Z

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

6.5 Orthogonal surface views [i](#)

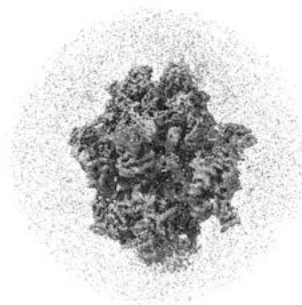
6.5.1 Primary map



X



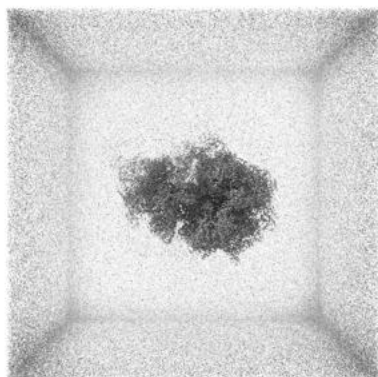
Y



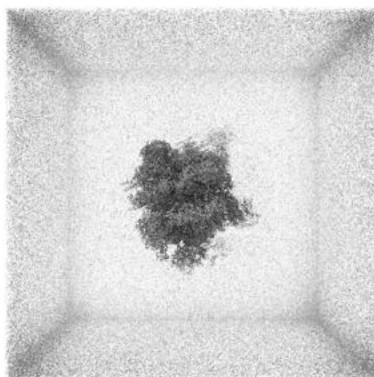
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

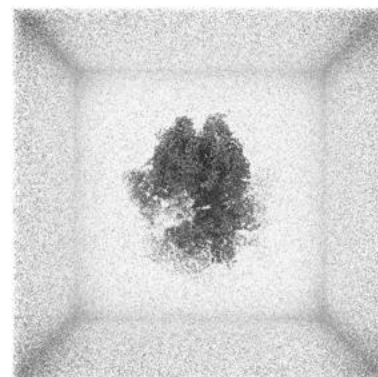
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

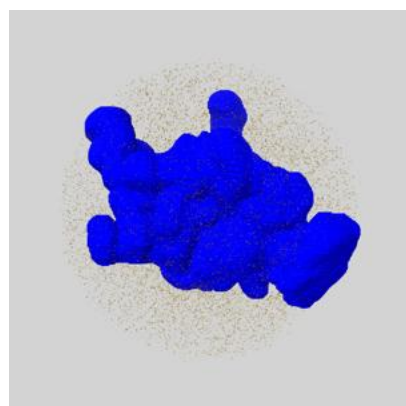
6.6 Mask visualisation [i](#)

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

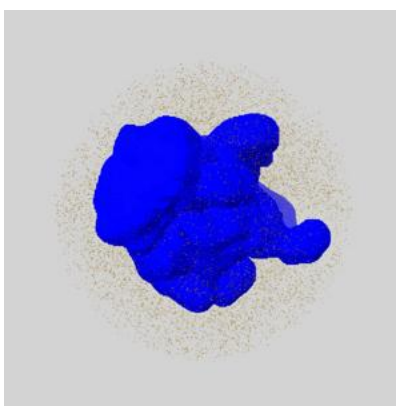
A mask typically either:

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

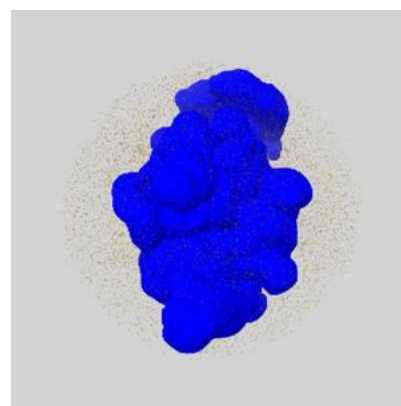
6.6.1 emd_71623_msk_1.map [i](#)



X



Y

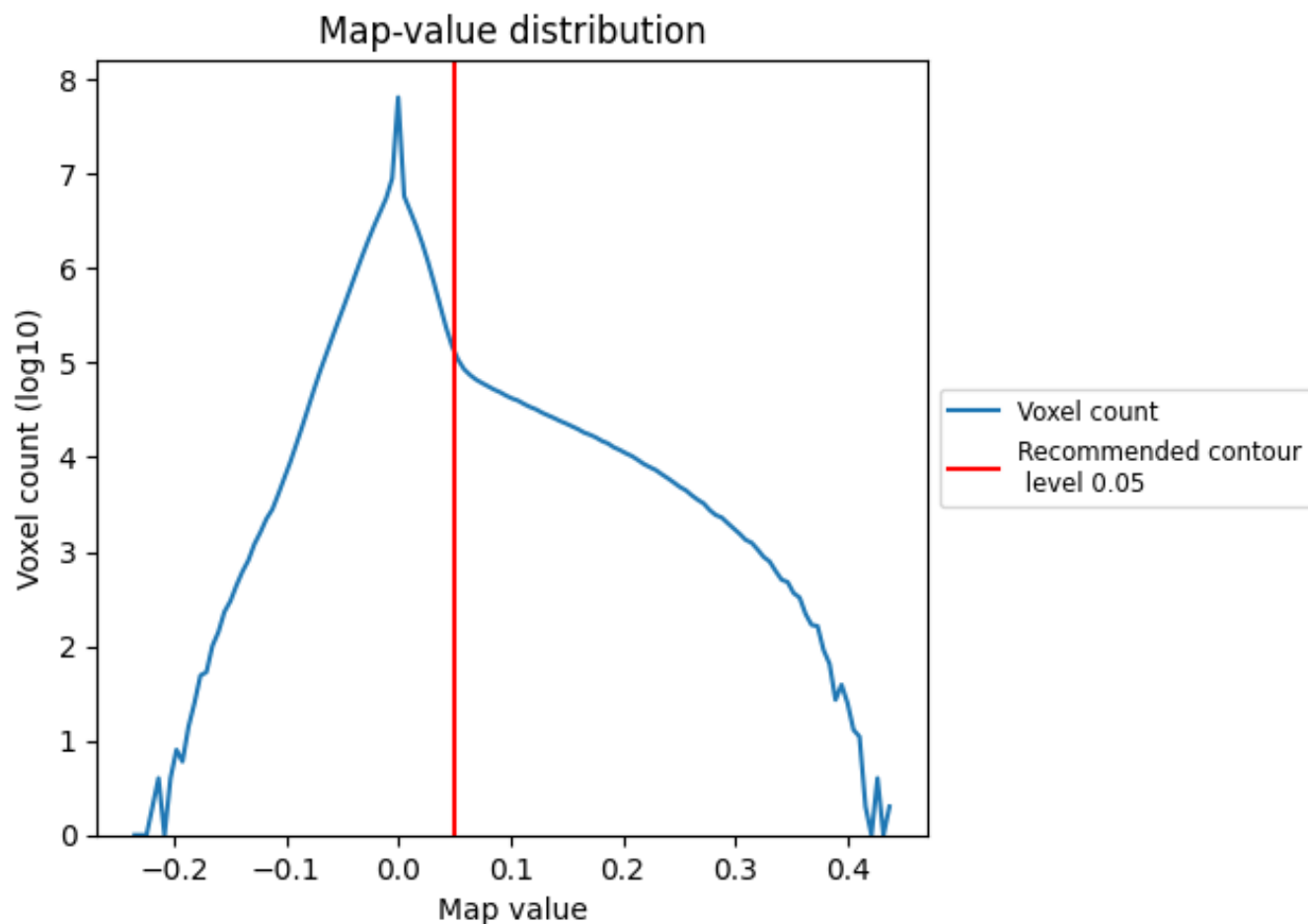


Z

7 Map analysis [i](#)

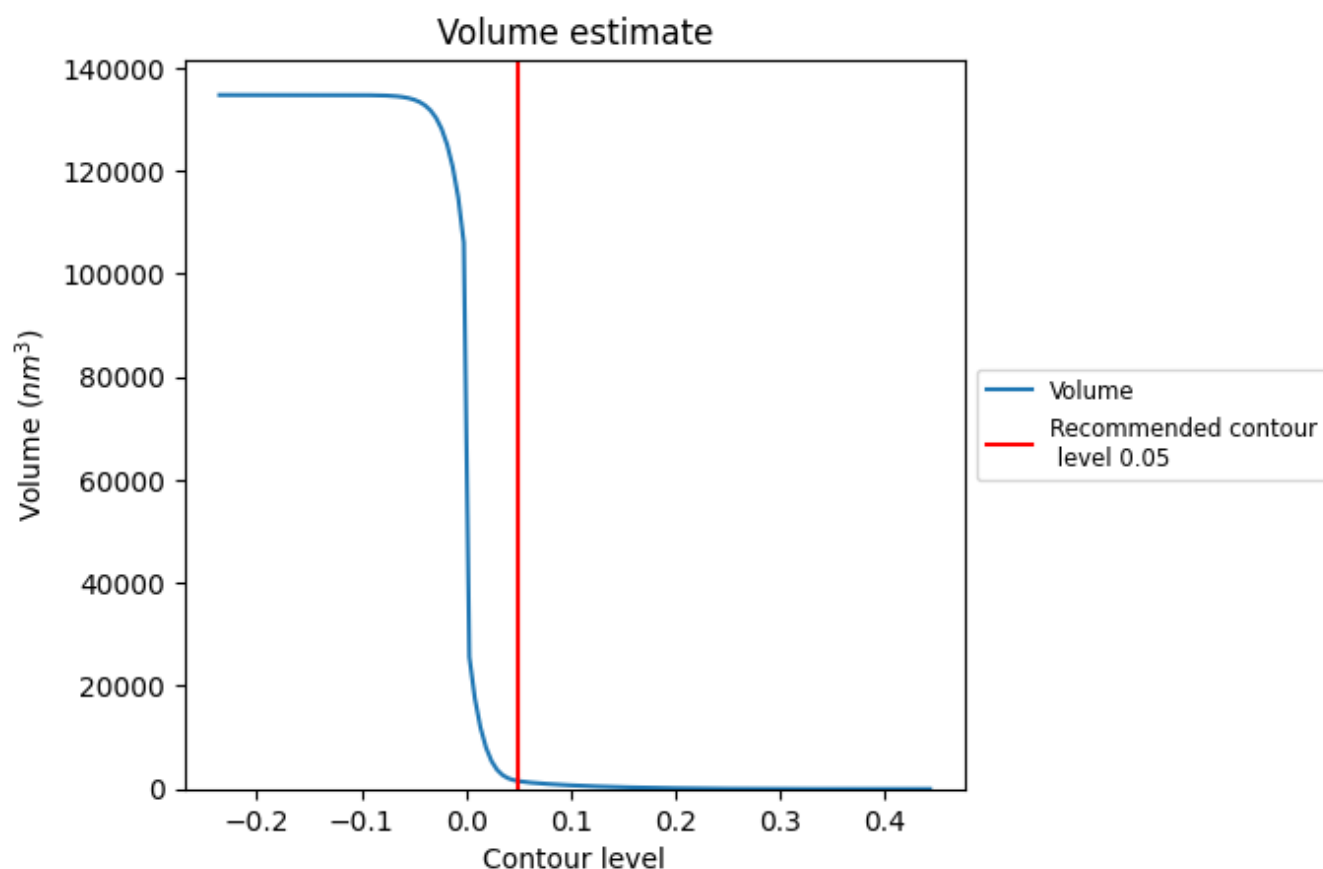
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

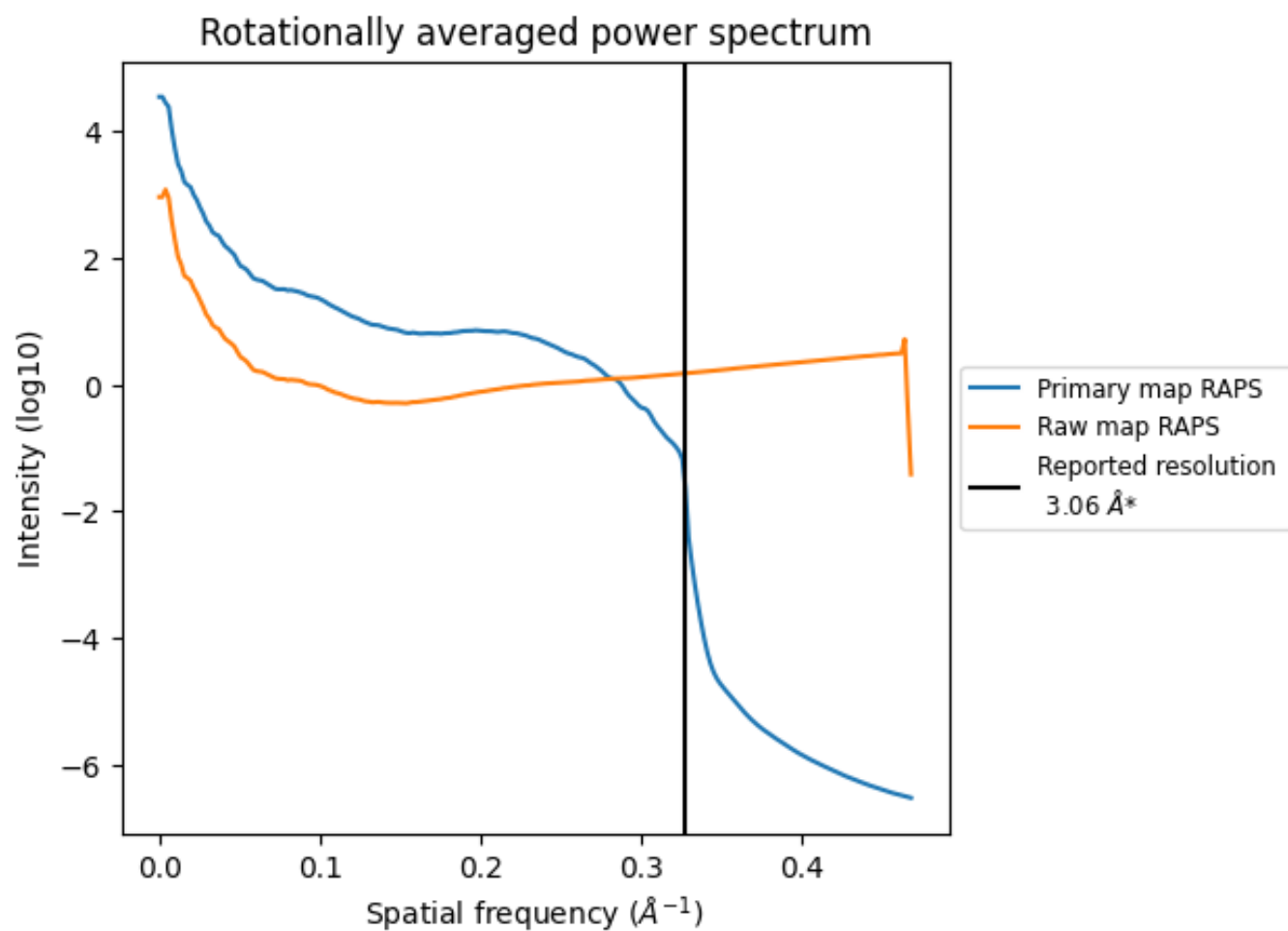
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1532 nm^3 ; this corresponds to an approximate mass of 1384 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 ⓘ

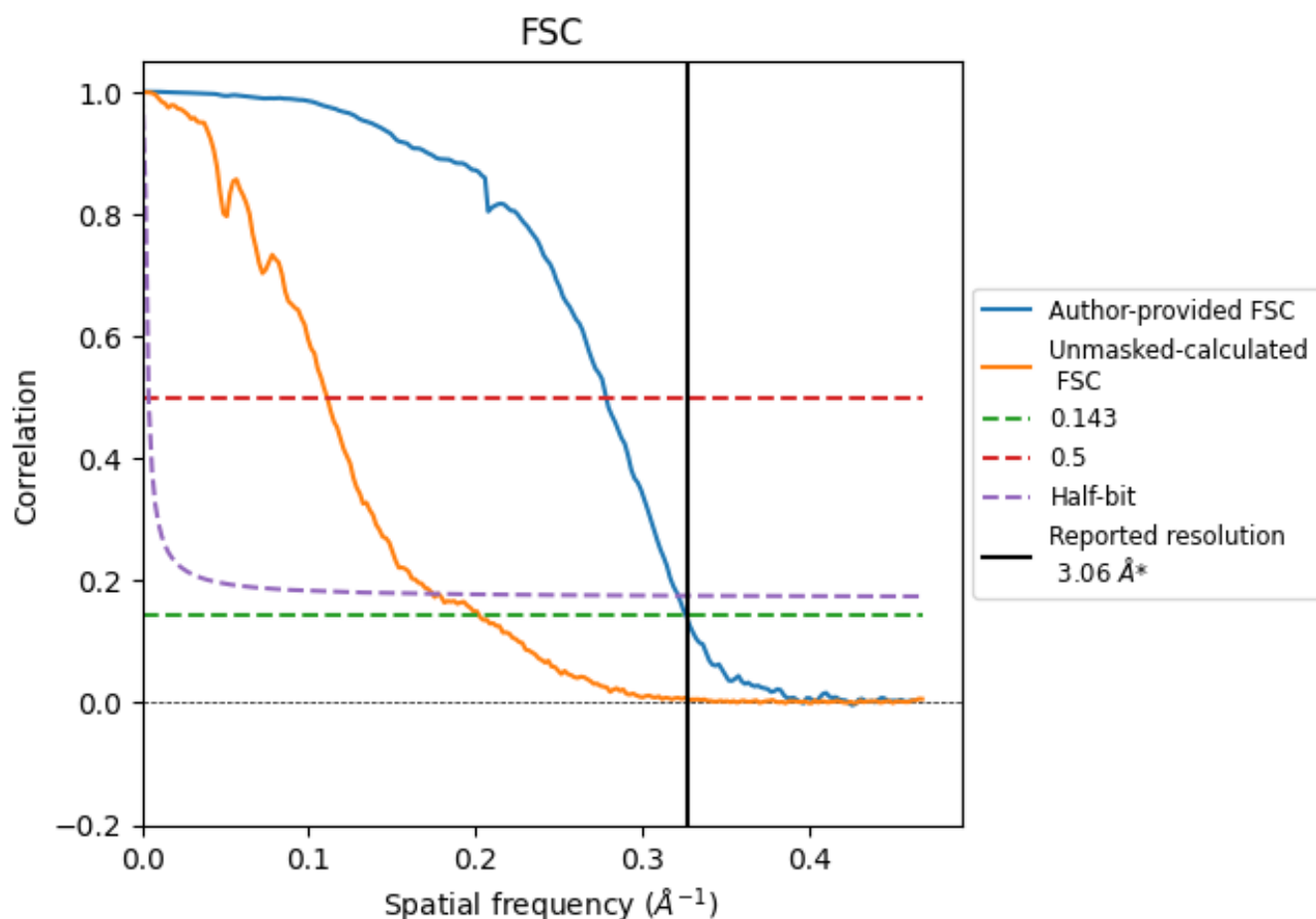


*Reported resolution corresponds to spatial frequency of 0.327 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

8.2 Resolution estimates [i](#)

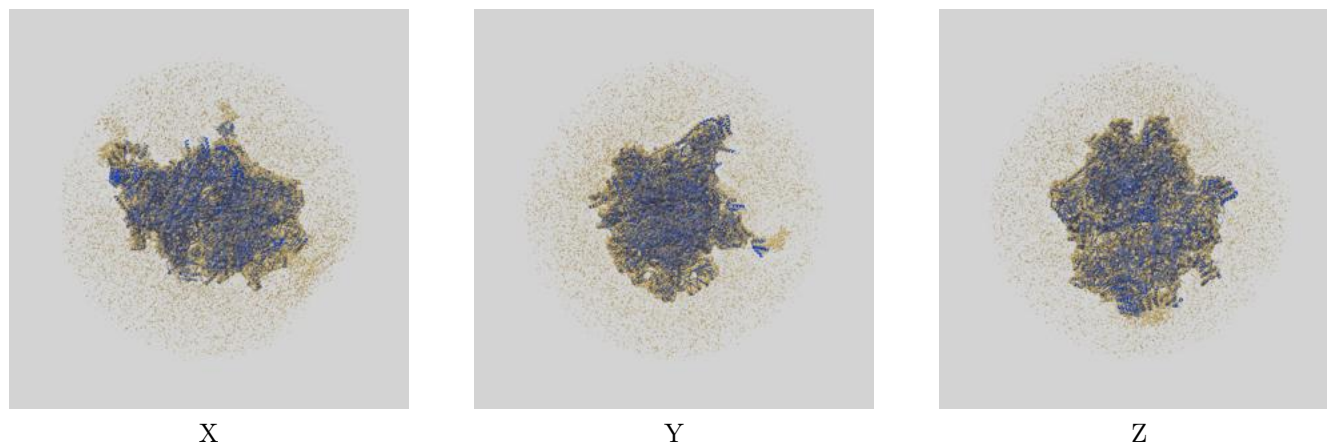
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.59	3.11
Unmasked-calculated*	4.95	9.01	5.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.95 differs from the reported value 3.06 by more than 10 %

9 Map-model fit [i](#)

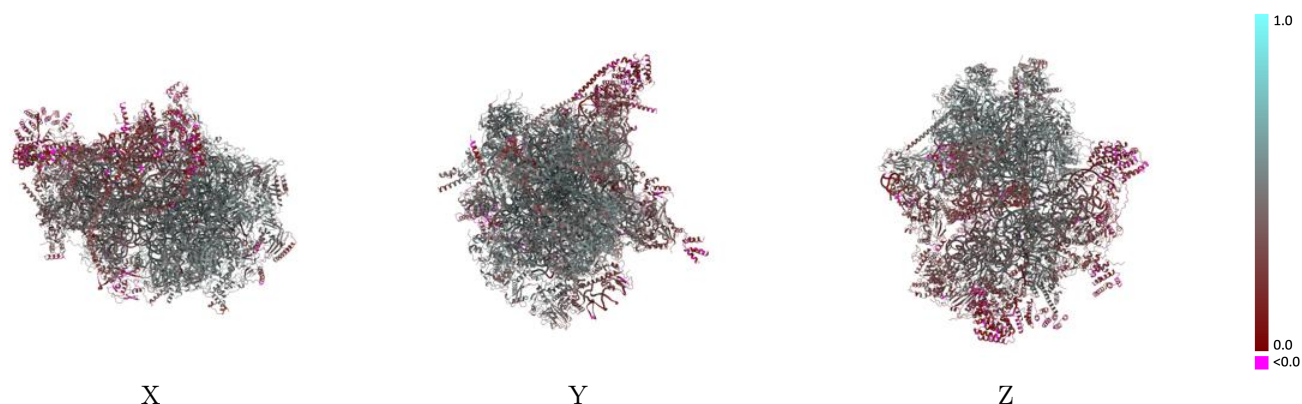
This section contains information regarding the fit between EMDB map EMD-71623 and PDB model 9PG8. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



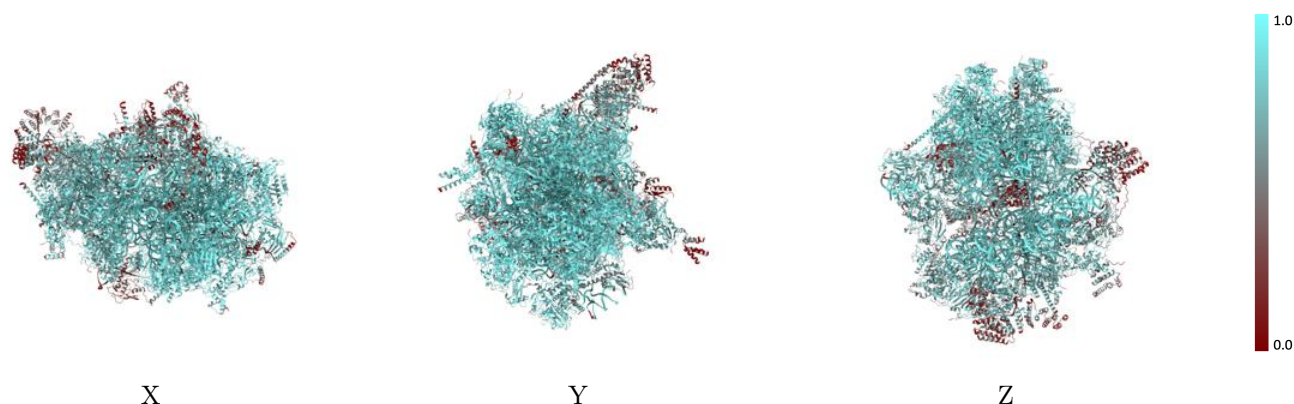
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



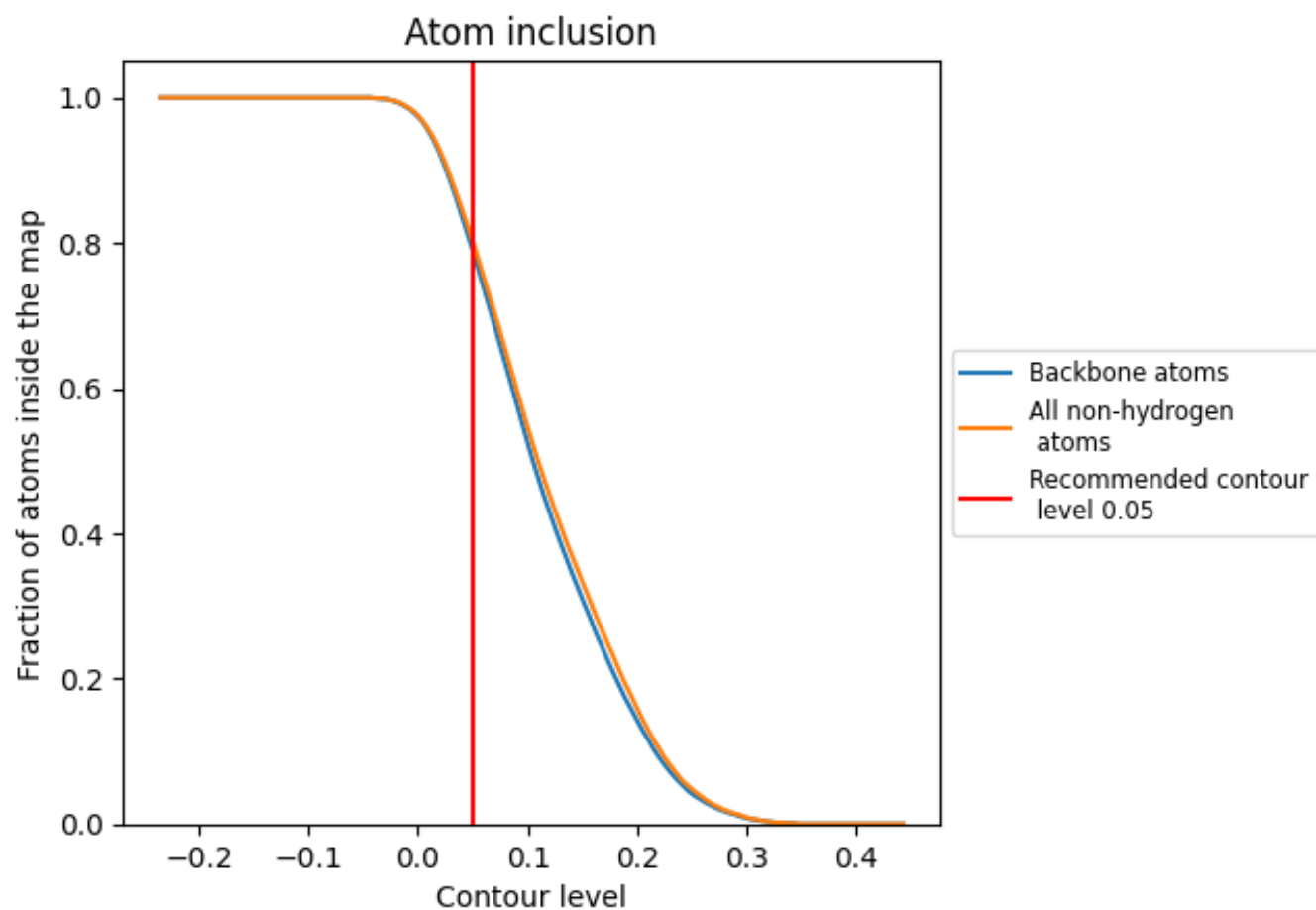
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 80% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.4170
0	 0.8920	 0.5130
1	 0.8140	 0.4890
2	 0.9420	 0.5480
3	 0.9240	 0.5420
4	 0.8930	 0.5260
5	 0.8690	 0.4930
6	 0.8240	 0.4390
7	 0.8280	 0.4470
8	 0.6240	 0.3020
9	 0.8570	 0.4810
A	 0.9550	 0.4900
A0	 0.5240	 0.2090
A1	 0.6730	 0.3210
A2	 0.7320	 0.4120
A3	 0.8140	 0.4660
A4	 0.4300	 0.1830
AA	 0.9570	 0.4360
AB	 0.8010	 0.4340
AC	 0.7340	 0.4170
AD	 0.7330	 0.4050
AE	 0.7900	 0.4590
AF	 0.7600	 0.3970
AG	 0.7260	 0.3820
AH	 0.6810	 0.3650
AI	 0.8120	 0.4520
AJ	 0.7450	 0.4400
AK	 0.8150	 0.4200
AL	 0.7590	 0.4030
AM	 0.6280	 0.2590
AN	 0.7610	 0.4240
AO	 0.6360	 0.2960
AP	 0.8090	 0.4610
AQ	 0.8350	 0.4650
AR	 0.5840	 0.2480



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Chain	Atom inclusion	Q-score
AS	 0.7040	 0.3630
AT	 0.7290	 0.3780
AU	 0.6640	 0.2930
AV	 0.3730	 0.1580
AW	 0.7450	 0.4260
AX	 0.7020	 0.3210
AY	 0.6150	 0.2980
AZ	 0.7240	 0.3580
Ax	 0.8840	 0.3720
Ay	 0.7310	 0.1900
Az	 0.5690	 0.2510
B	 0.8390	 0.3010
C	 0.3050	 0.2910
D	 0.8960	 0.5260
E	 0.8830	 0.5130
F	 0.9010	 0.5220
G	 0.1570	 0.1980
H	 0.4890	 0.2870
I	 0.7050	 0.3560
J	 0.6270	 0.2750
K	 0.9100	 0.5230
L	 0.8590	 0.5150
M	 0.8930	 0.5130
N	 0.8740	 0.5100
O	 0.8820	 0.5120
OX	 0.5610	 0.2920
P	 0.8600	 0.4800
Q	 0.7960	 0.4830
R	 0.9070	 0.5250
S	 0.8730	 0.5180
T	 0.9120	 0.5370
U	 0.7970	 0.4650
V	 0.8370	 0.4630
W	 0.8790	 0.5270
X	 0.8510	 0.4930
Y	 0.8850	 0.5030
Z	 0.8930	 0.5250
a	 0.7750	 0.4550
b	 0.8960	 0.5210
c	 0.8480	 0.4800
d	 0.7250	 0.4170
e	 0.6060	 0.2550

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Chain	Atom inclusion	Q-score
f	 0.6950	 0.3580
g	 0.8740	 0.5020
h	 0.8270	 0.4440
i	 0.9200	 0.5360
j	 0.8270	 0.4670
k	 0.7360	 0.3920
l	 0.6590	 0.3120
m	 0.5970	 0.2810
n	 0.5390	 0.3320
o	 0.9160	 0.5330
p	 0.7390	 0.4120
q	 0.6870	 0.3570
r	 0.8780	 0.5010
s	 0.8780	 0.5020
t	 0.2440	 0.1470
u	 0.2770	 0.1690
z	 0.1730	 0.1040