



wwPDB EM Validation Summary Report ⓘ

Aug 17, 2026 – 09:34 PM EDT

PDB ID : 9PGF / pdb_00009pgf
EMDB ID : EMD-71630
Title : In situ structure of the human mitoribosome in the P state
Authors : Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on : 2025-07-07
Resolution : 2.93 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:

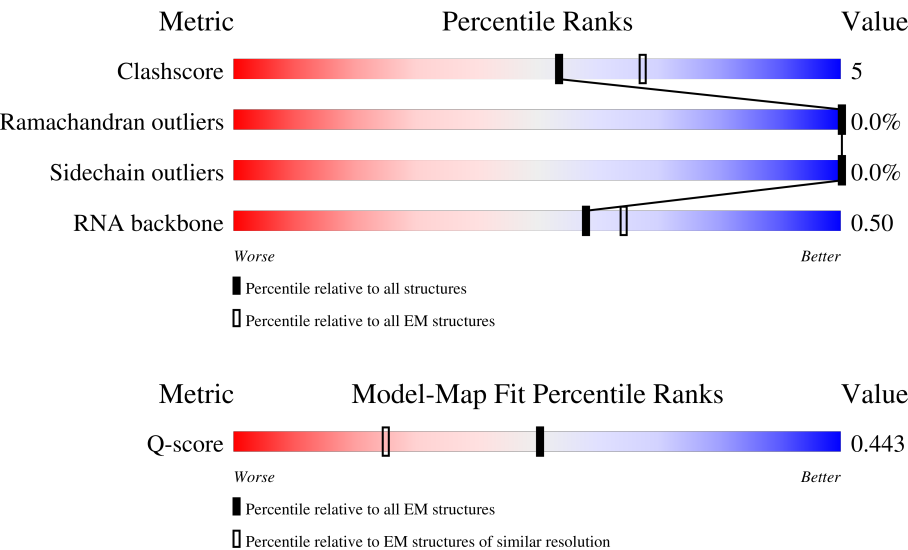
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.93 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.



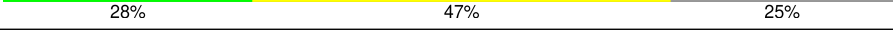
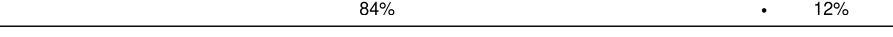
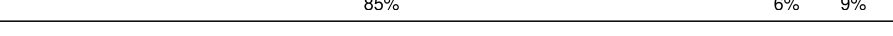
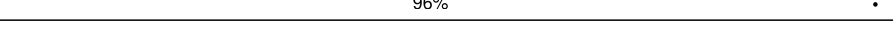
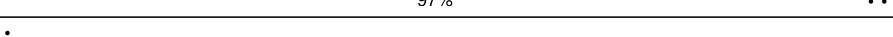
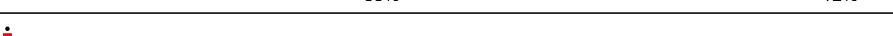
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13037 (2.43 - 3.43)

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	57% 41%
2	1	65	5% 80% 6% 14%
3	2	92	50% 50%

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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	G	198	
33	t	198	
33	u	198	
34	I	261	
35	V	216	
36	b	215	
37	d	306	
38	e	279	
39	g	166	
40	h	158	
41	i	128	
42	j	123	
43	l	138	
44	m	128	
45	n	43	
46	o	102	
47	q	222	
48	r	196	
49	c	332	
50	f	212	
51	p	206	

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Mol	Chain	Length	Quality of chain
52	s	439	
53	AB	296	
54	AC	167	
55	AD	430	
56	AE	125	
57	AF	242	
58	AG	396	
59	AH	201	
60	AJ	138	
61	AK	128	
62	AL	257	
63	AM	137	
64	AN	130	
65	AO	258	
66	AP	142	
67	AR	360	
68	AS	190	
69	AT	173	
70	AU	205	
71	AV	414	
72	AW	187	
73	AZ	106	
74	A0	217	
75	A1	323	
76	A3	199	

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Mol	Chain	Length	Quality of chain
77	Az	34	
78	AY	395	
79	AA	954	
80	AI	194	
81	OX	435	
82	a	142	
83	Ax	71	
84	A4	689	
85	B	72	
86	AX	398	
87	A2	118	
88	AQ	87	
89	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
92	SPD	AG	401	-	-	X	-
98	SPM	AA	1782	-	-	X	-
98	SPM	AA	1784	-	-	X	-

2 Entry composition

There are 100 unique types of molecules in this entry. The entry contains 315253 atoms, of which 136488 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 is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP Q9BYD1

- 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 39S ribosomal protein L12, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L46, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 45 is a protein called Nascent polypeptide.

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

- Molecule 46 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 50 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 51 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 53 is a protein called 28S ribosomal protein S2, mitochondrial.

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

- Molecule 54 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 55 is a protein called 28S ribosomal protein S5, mitochondrial.

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

- Molecule 56 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 57 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 58 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 59 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 60 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 61 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 62 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 63 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 64 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 65 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 66 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 67 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 68 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 69 is a protein called 28S ribosomal protein S25, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S26, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 72 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 73 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 74 is a protein called Small ribosomal subunit protein mS34.

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

- Molecule 75 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 76 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 77 is a RNA chain called mRNA.

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

- Molecule 78 is a protein called 28S ribosomal protein S31, mitochondrial.

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

- Molecule 79 is a RNA chain called 12S mitochondrial rRNA.

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

- Molecule 80 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 81 is a protein called Mitochondrial inner membrane protein OXA1L.

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

- Molecule 82 is a protein called 39S ribosomal protein L42, mitochondrial.

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

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

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

- Molecule 84 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 85 is a RNA chain called mitochondrial tRNA^{Val}.

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

- Molecule 86 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 87 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	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 88 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	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 89 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	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	1	ACE	-	acetylation	UNP Q96EL3

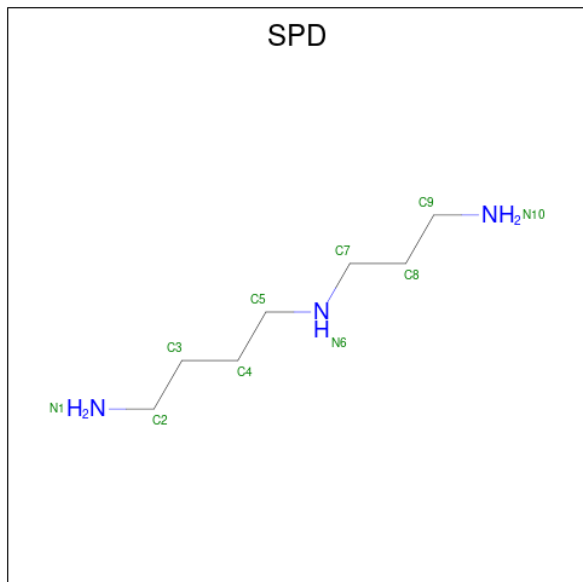
- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
90	0	1	Total	Zn	0
			1	1	
90	4	1	Total	Zn	0
			1	1	
90	AO	1	Total	Zn	0
			1	1	

- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K).

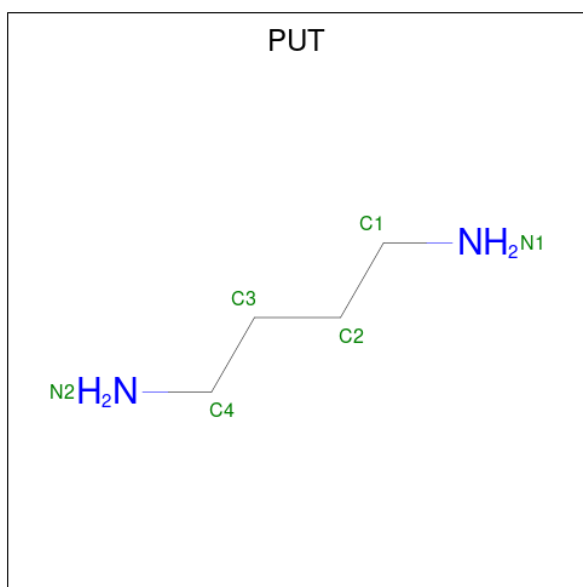
Mol	Chain	Residues	Atoms		AltConf
91	6	1	Total	K	0
			1	1	
91	A	29	Total	K	0
			29	29	
91	D	1	Total	K	0
			1	1	
91	M	2	Total	K	0
			2	2	
91	N	1	Total	K	0
			1	1	
91	W	1	Total	K	0
			1	1	
91	o	1	Total	K	0
			1	1	
91	AA	18	Total	K	0
			18	18	

- Molecule 92 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
92	A	1	Total	C	H	N	0
			32	7	22	3	
92	A	1	Total	C	H	N	0
			32	7	22	3	
92	A	1	Total	C	N		0
			10	7	3		
92	A	1	Total	C	N		0
			10	7	3		
92	A	1	Total	C	N		0
			10	7	3		
92	AG	1	Total	C	N		0
			10	7	3		
92	AA	1	Total	C	N		0
			10	7	3		
92	AA	1	Total	C	N		0
			10	7	3		

- Molecule 93 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).

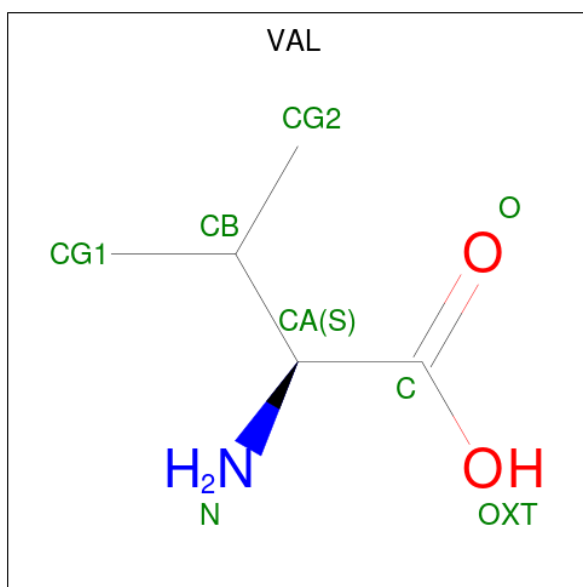


Mol	Chain	Residues	Atoms				AltConf
93	A	1	Total	C	H	N	0
			20	4	14	2	

- Molecule 94 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

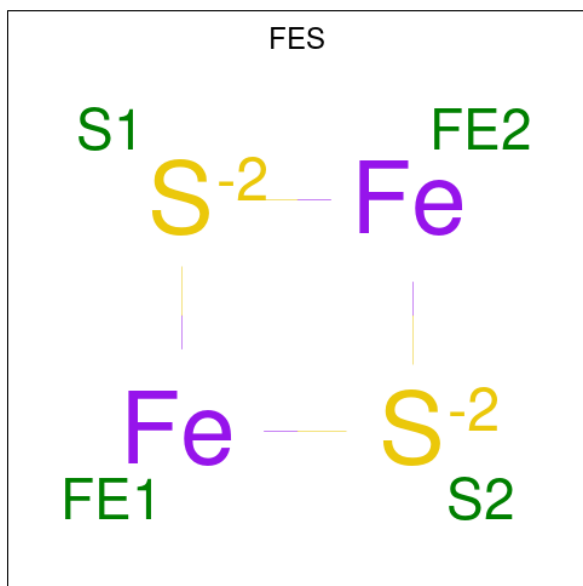
Mol	Chain	Residues	Atoms		AltConf
94	A	136	Total	Mg	0
			136	136	
94	D	2	Total	Mg	0
			2	2	
94	E	1	Total	Mg	0
			1	1	
94	I	1	Total	Mg	0
			1	1	
94	g	1	Total	Mg	0
			1	1	
94	AB	1	Total	Mg	0
			1	1	
94	A3	1	Total	Mg	0
			1	1	
94	AA	61	Total	Mg	0
			61	61	
94	AX	1	Total	Mg	0
			1	1	

- Molecule 95 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).



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

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



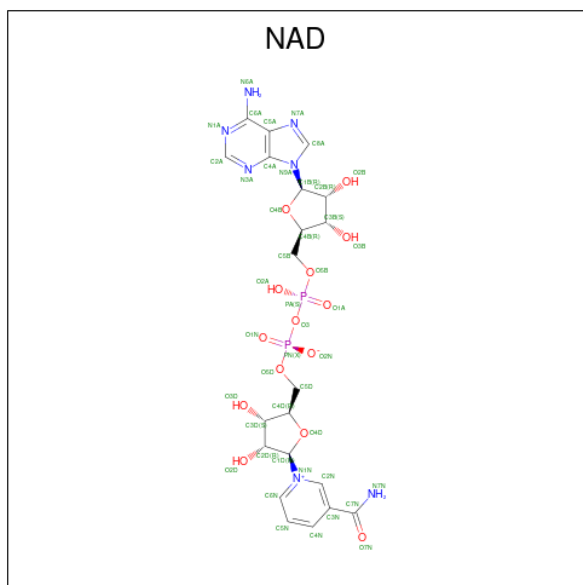
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
96	r	1	4	2	2	0
96	AP	1	4	2	2	0

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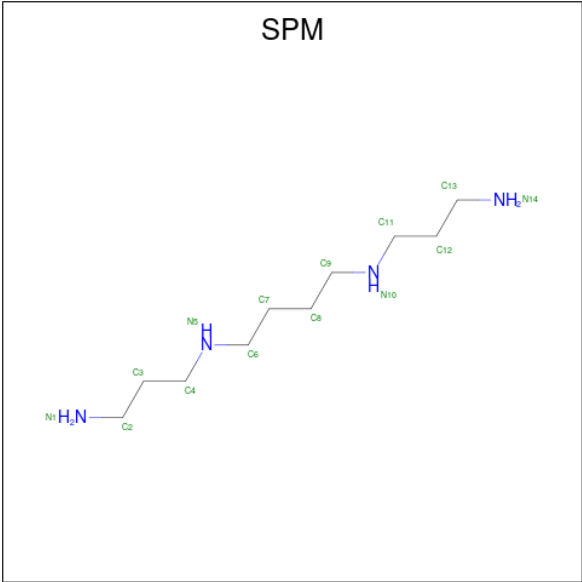
Mol	Chain	Residues	Atoms			AltConf
96	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 97 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



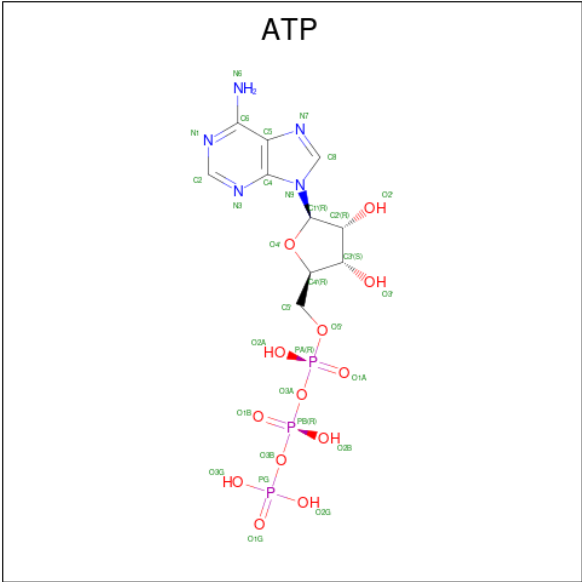
Mol	Chain	Residues	Atoms					AltConf
97	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 98 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



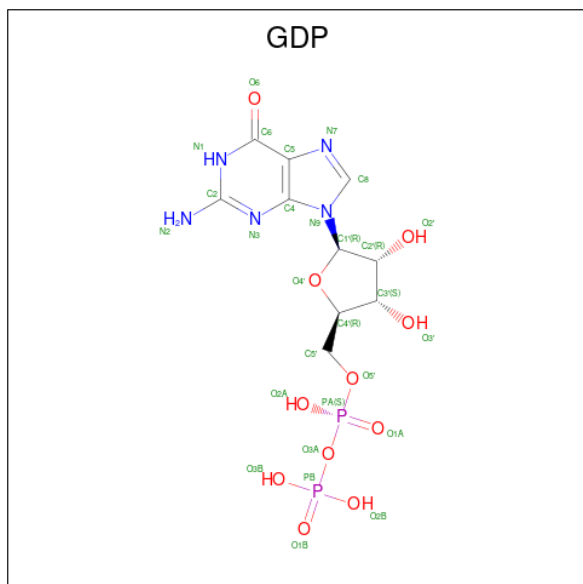
Mol	Chain	Residues	Atoms			AltConf
98	AA	1	Total	C	N	0
			14	10	4	
98	AA	1	Total	C	N	0
			14	10	4	
98	AA	1	Total	C	N	0
			14	10	4	

- Molecule 99 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

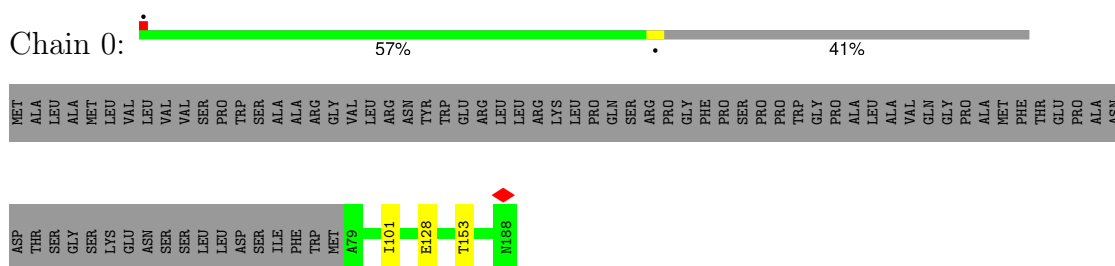
- Molecule 100 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



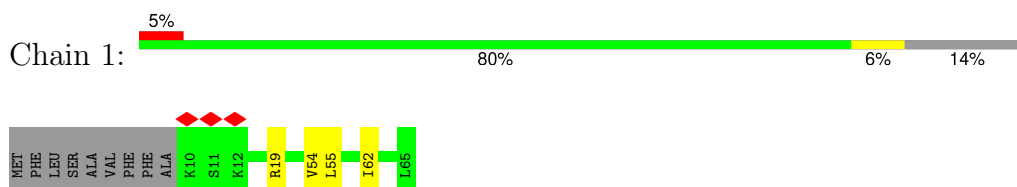
3 Residue-property plots [i](#)

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.

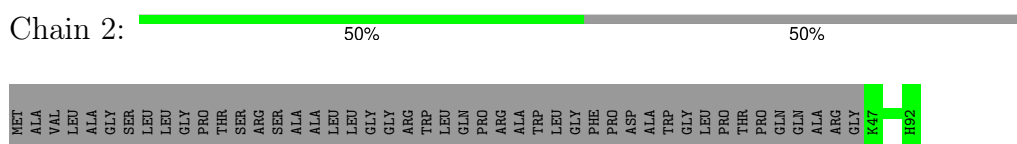
- Molecule 1: 39S ribosomal protein L32, mitochondrial



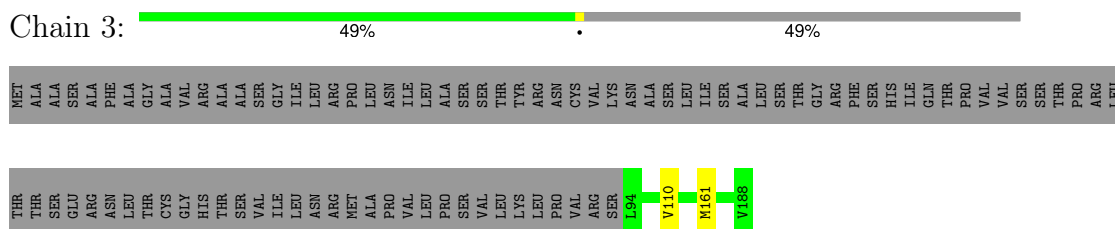
- Molecule 2: 39S ribosomal protein L33, mitochondrial



- Molecule 3: 39S ribosomal protein L34, mitochondrial

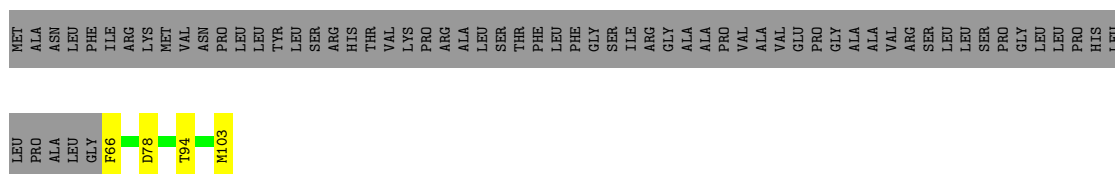


- Molecule 4: 39S ribosomal protein L35, mitochondrial



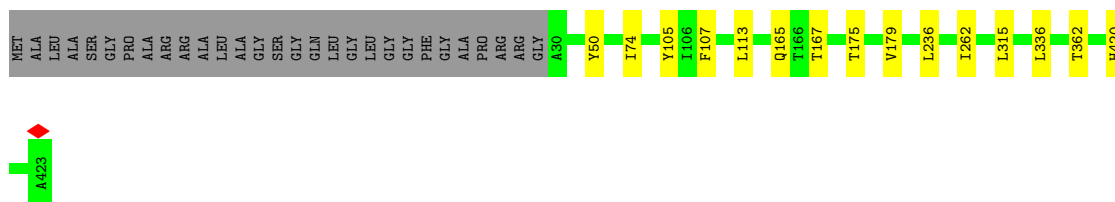
- Molecule 5: 39S ribosomal protein L36, mitochondrial





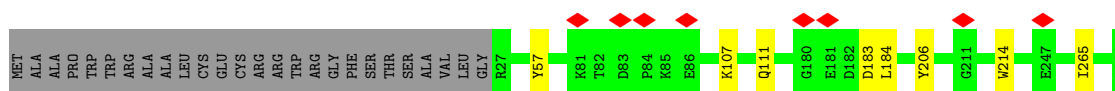
- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5: 90% 7%



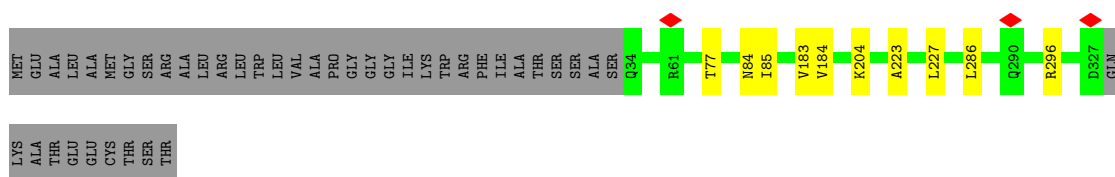
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 91% 7%



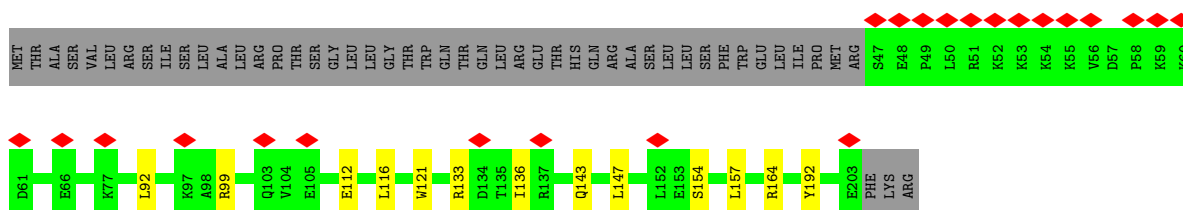
- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7: 84% 13%



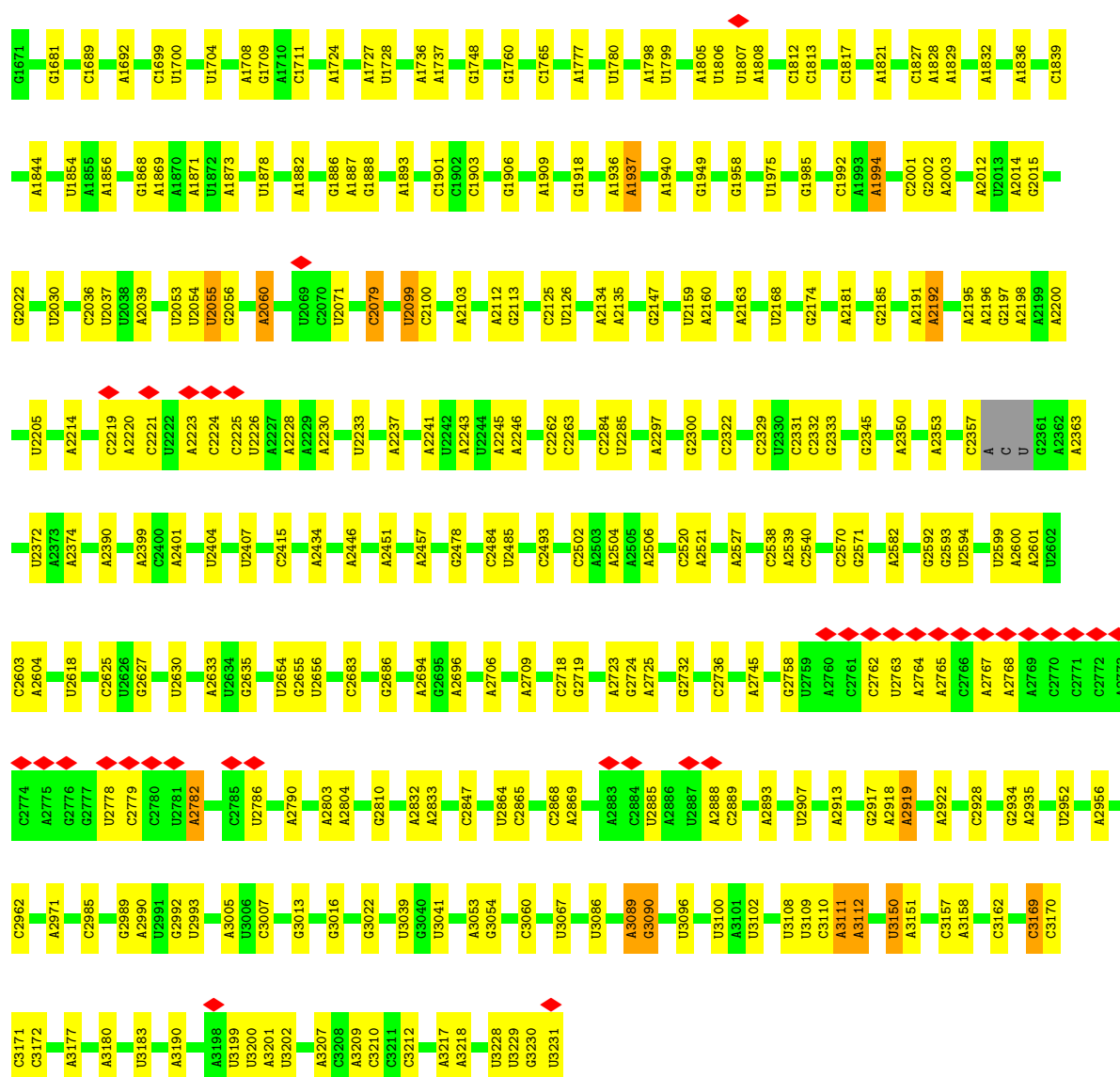
- Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8: 11% 70% 6% 24%

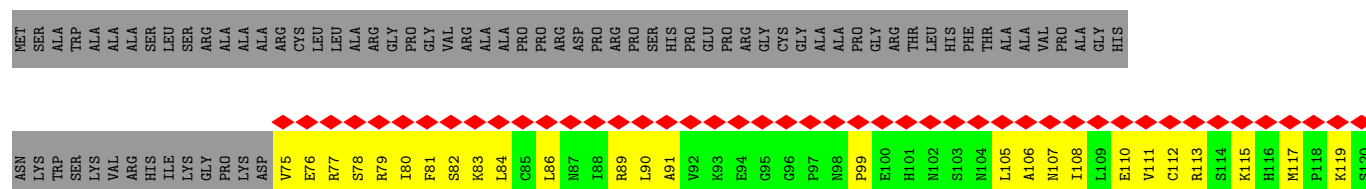


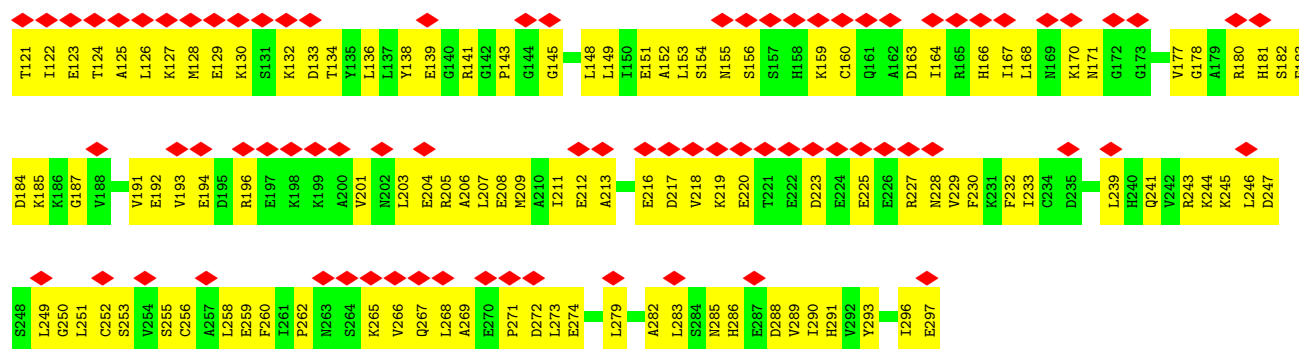
- Molecule 10: 39S ribosomal protein L41, mitochondrial

Chain 9: 91% 9%



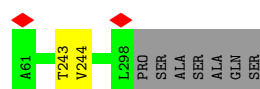
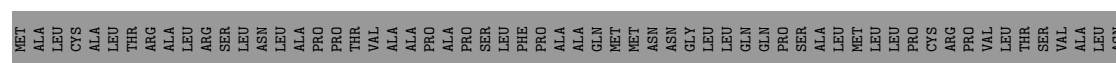
- Molecule 12: Translational activator of cytochrome c oxidase 1





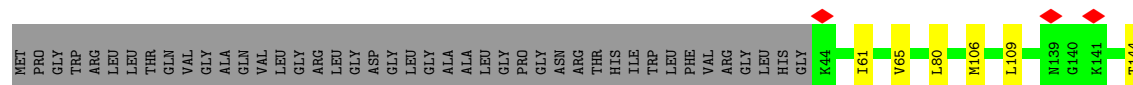
- Molecule 13: 39S ribosomal protein L2, mitochondrial

Chain D: 77% 22%



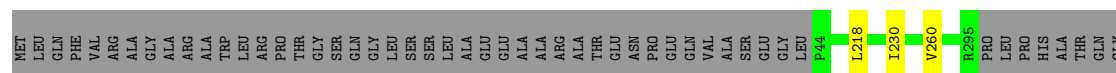
- Molecule 14: 39S ribosomal protein L3, mitochondrial

Chain E: 84% 12%



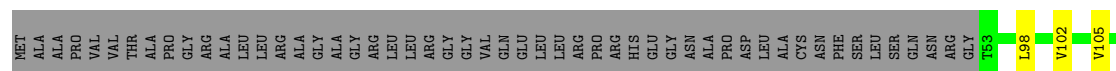
- Molecule 15: 39S ribosomal protein L4, mitochondrial

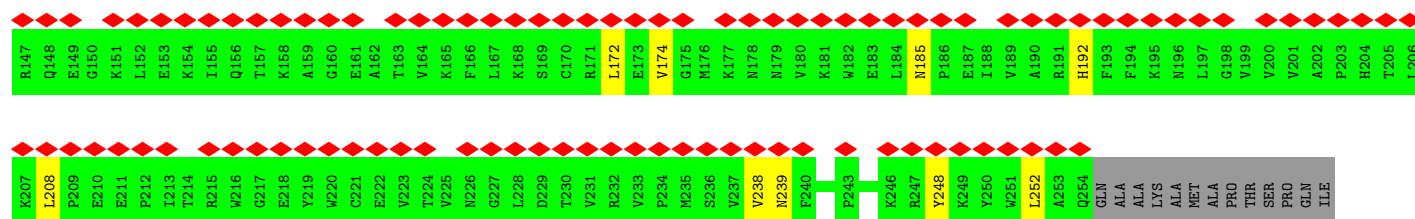
Chain F: 80% 19%



- Molecule 16: 39S ribosomal protein L9, mitochondrial

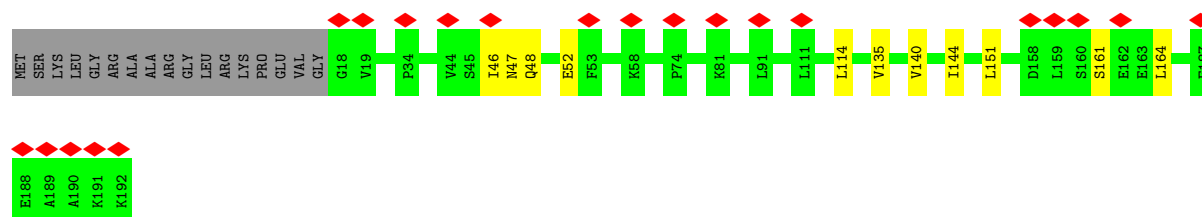
Chain H: 36% 71% 24%





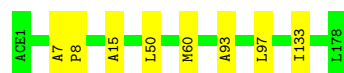
- Molecule 17: 39S ribosomal protein L11, mitochondrial

Chain J: 11% 85% 6% 9%



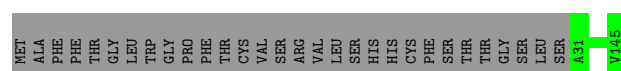
- Molecule 18: Large ribosomal subunit protein uL13m

Chain K: 96% 4%



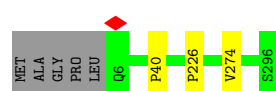
- Molecule 19: 39S ribosomal protein L14, mitochondrial

Chain L: 79% 21%



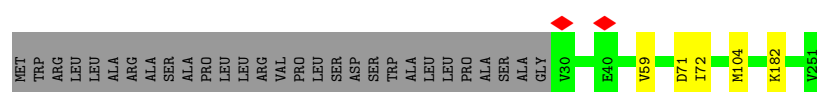
- Molecule 20: 39S ribosomal protein L15, mitochondrial

Chain M: 97% 3%



- Molecule 21: 39S ribosomal protein L16, mitochondrial

Chain N: 86% 12% 2%



- Molecule 22: 39S ribosomal protein L17, mitochondrial

MET ARG LEU SER VAL ALA ALA I9 R13 A44 P45 A94 P95 Q160 E161 A162 SER ASN HIS SER SER HIS THR ALA GLN THR PRO GLY ILE

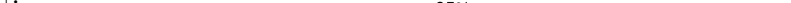
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 SER
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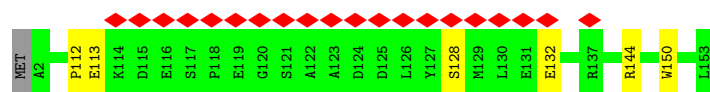
-
- Sequence logo for the 100th position. The y-axis shows amino acid frequencies: V63, D64, K65, H66, R67, P68, V69, E70, R73, L100, I240, I243, I286, R291, S292. The x-axis shows amino acid frequencies: MET, ALA, ALA, CYS, ILE, ALA, GLY, HIS, TRP, ALA, ALA, MET, GLY, LEU, GLY, ARG, SER, PHE, GLN, ALA, ALA, ARG, THR, LEU, LEU, PRO, PRO, PRO, ALA, SER, SER, ILE, ALA, CYS, ARG, VAL, HIS, ALA, GLY, PRO, VAL, ARG, GLN, GLN, SER, THR, GLY, PRO, SER, GLU, PRO, GLY, ALA. The logo shows a strong preference for V63, D64, K65, H66, R67, P68, V69, E70, R73, L100, I240, I243, I286, R291, S292 at the 100th position.

-
- Diagram illustrating the schematic representation of the protein structure of the C-terminal domain of the human histone H4. The residues shown are MET, VAL, PHE, LEU, THR, ALA, GLN, LEU, TRP, L10, M64, D134, G135, K136, and H149. The residues are color-coded: MET, VAL, PHE, LEU, THR, ALA, GLN, LEU, TRP are in grey; L10 is in green; M64 is in yellow; D134, G135, K136 are in green; and H149 is in green. Red diamonds are placed above the D134 and K136 residues.

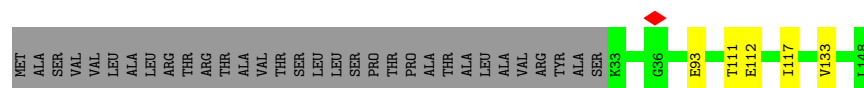
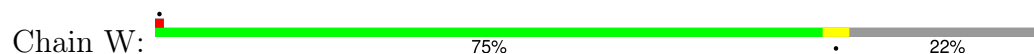
- | | | |
|------|------|------|
| MET | ALA | ALA | SER | SER | LEU | THR | VAL | THR | LEU | GLY | ARG | LEU | ALA | SER | ALA | CYS | HIS | SER | ILE | LEU | ARG | PRO | SER | GLY | PRO | GLY | ALA | ALA | SER | SER | LEU | TRP | SER | ALA | SER | ARG | ARG | PHE | ASN | SER | GLN | SER | THR | S45 | Y46 | L47 | P48 | G49 | L135 | L144 | L205 |
|------|------|------|

- | | | | | |
|------|------|------|------|------|
| MET | ALA | ALA | ALA | VAL | LEU | GLY | GLN | LEU | GLY | ALA | LEU | TRP | ILE | HIS | ASN | LEU | ARG | SER | ARG | GLY | LYS | LEU | ALA | LEU | GLY | VAL | LEU | PRO | GLN | SER | TYR | ILE | HIS | THR | SER | ALA | SER | LEU | ASP | 141 | R62 | R63 | H69 | L87 | M121 | H126 | H204 | T205 | L206 |
|------|------|------|------|------|

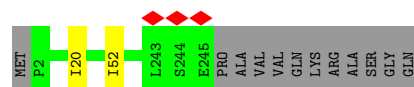
- Chain U:  13% 95%



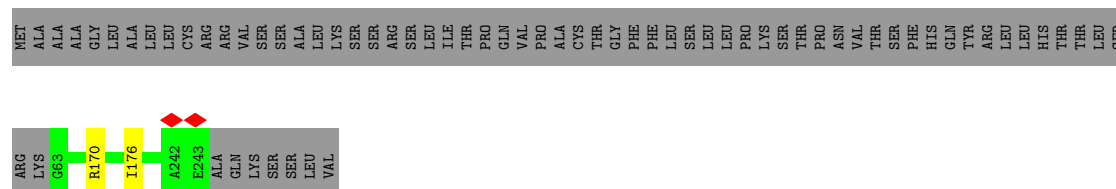
- Molecule 29: 39S ribosomal protein L27, mitochondrial



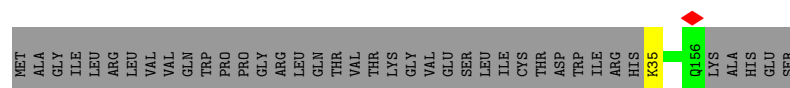
- Molecule 30: 39S ribosomal protein L28, mitochondrial



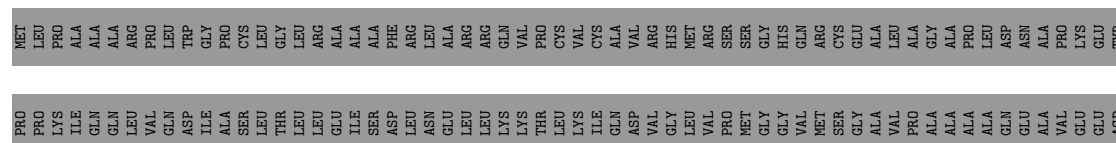
- Molecule 31: 39S ribosomal protein L47, mitochondrial



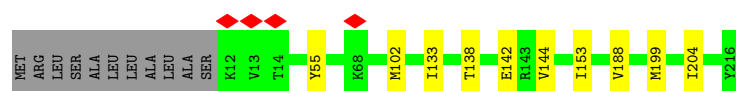
- Molecule 32: 39S ribosomal protein L30, mitochondrial



- Molecule 33: 39S ribosomal protein L12, mitochondrial

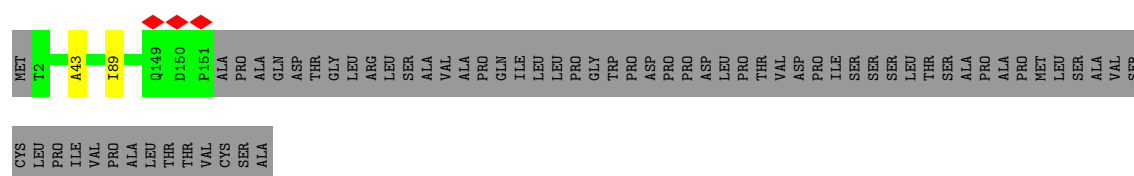


Chain V: 



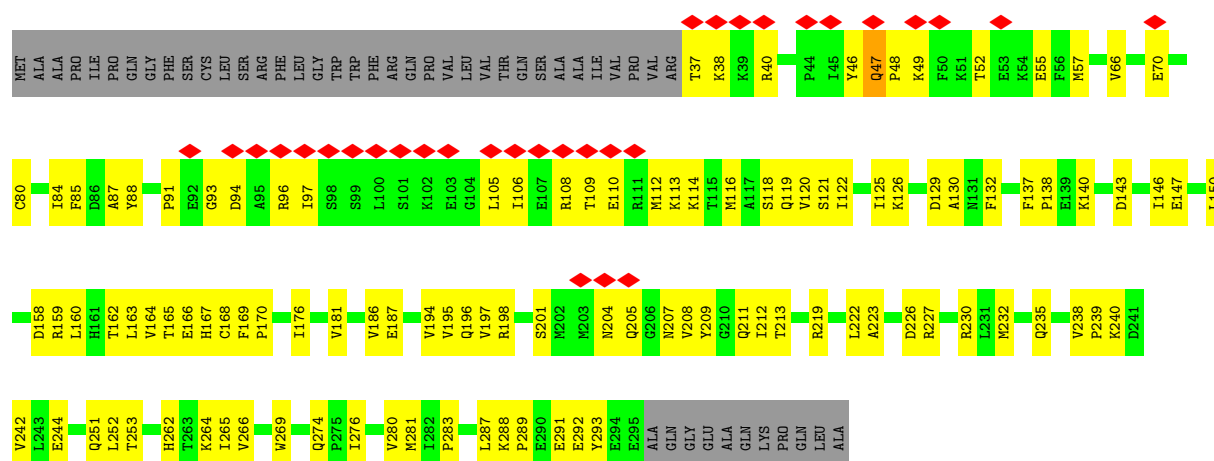
- Molecule 36: 39S ribosomal protein L43, mitochondrial

Chain b: 



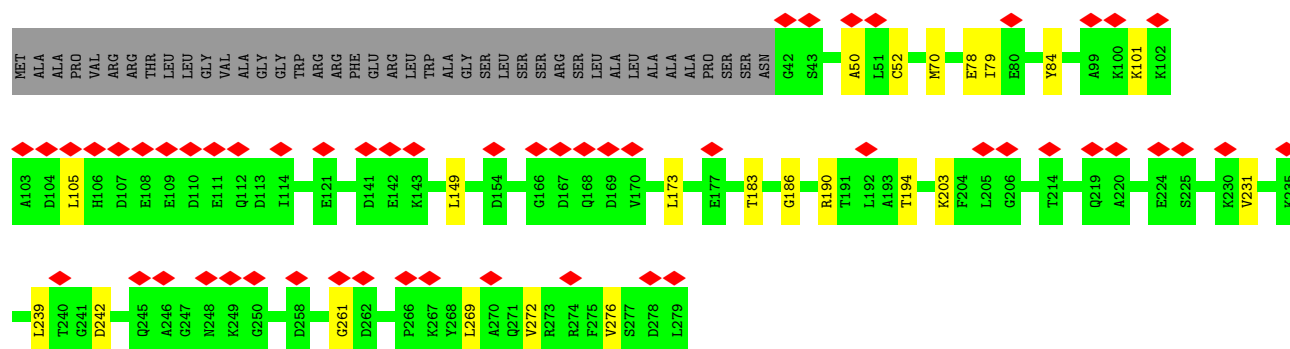
- Molecule 37: 39S ribosomal protein L45, mitochondrial

Chain d: 

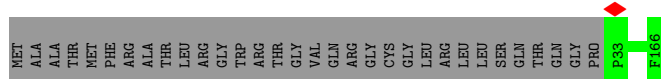
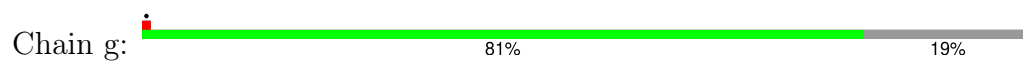


- Molecule 38: 39S ribosomal protein L46, mitochondrial

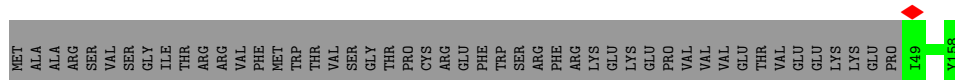
Chain e: 



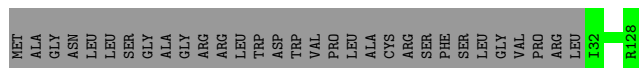
- Molecule 39: 39S ribosomal protein L49, mitochondrial



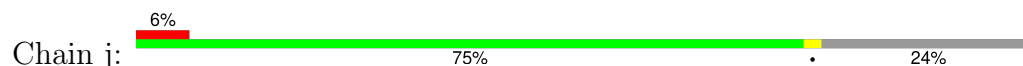
- Molecule 40: 39S ribosomal protein L50, mitochondrial



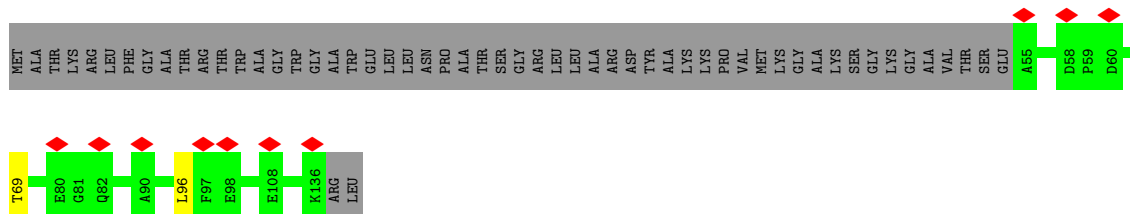
- Molecule 41: 39S ribosomal protein L51, mitochondrial



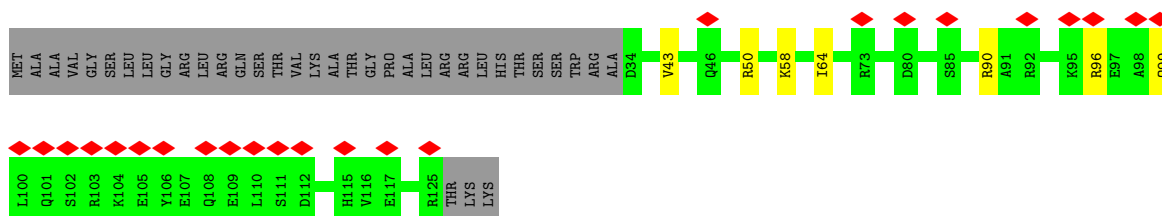
- Molecule 42: 39S ribosomal protein L52, mitochondrial



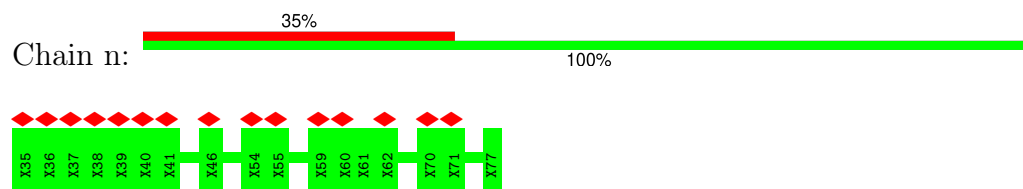
- Molecule 43: 39S ribosomal protein L54, mitochondrial



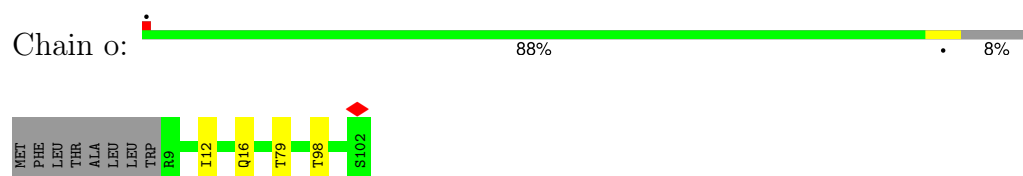
- Molecule 44: 39S ribosomal protein L55, mitochondrial



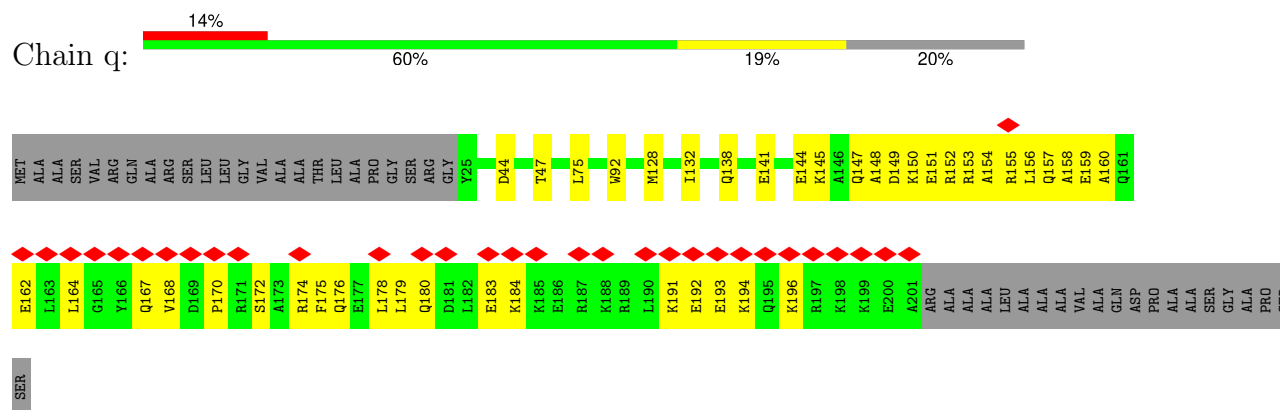
- Molecule 45: Nascent polypeptide



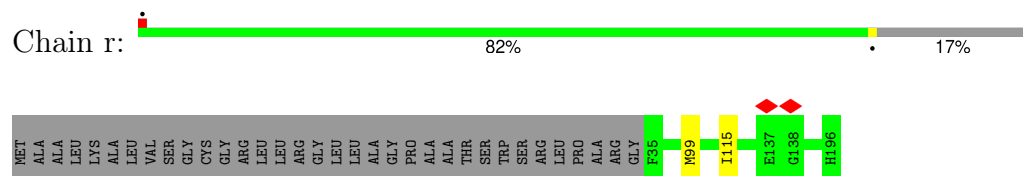
- Molecule 46: Ribosomal protein 63, mitochondrial



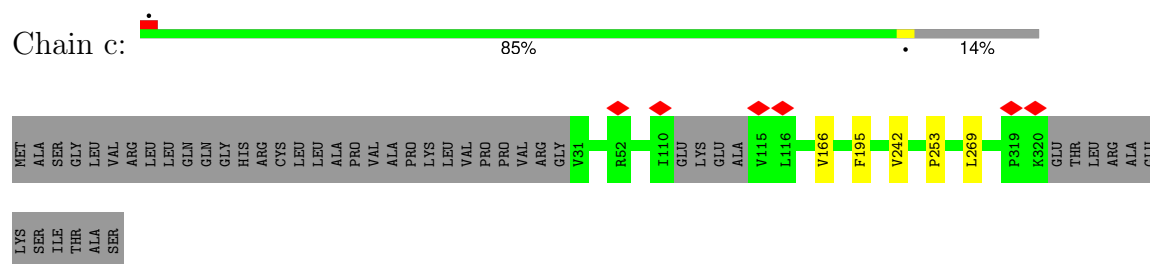
- Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 48: 39S ribosomal protein S18a, mitochondrial

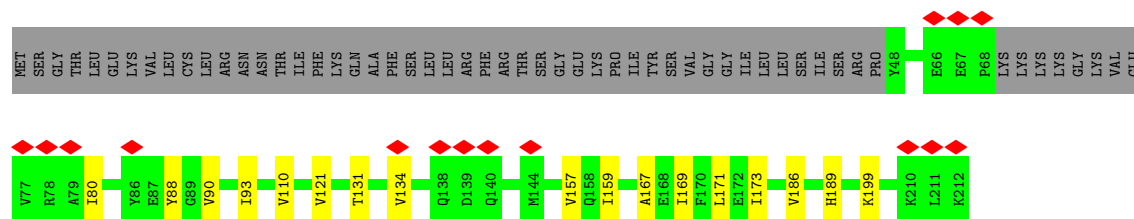


- Molecule 49: 39S ribosomal protein L44, mitochondrial

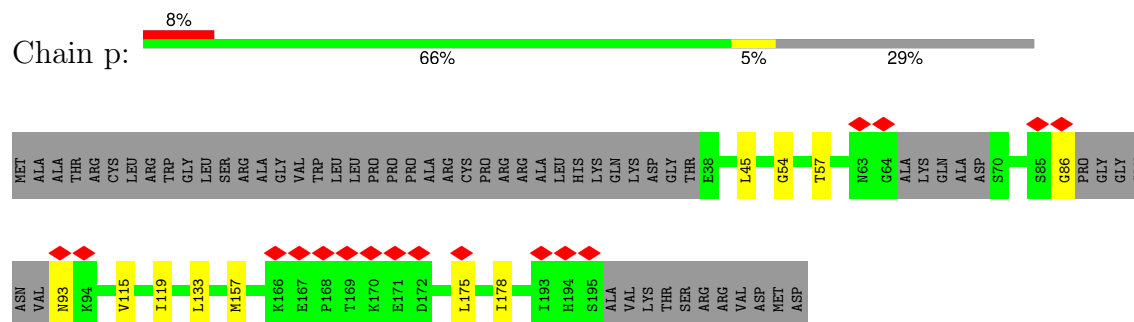


- Molecule 50: 39S ribosomal protein L48, mitochondrial

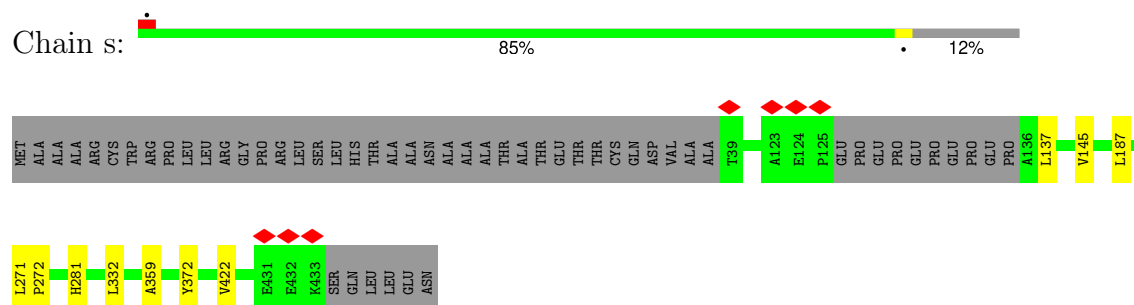




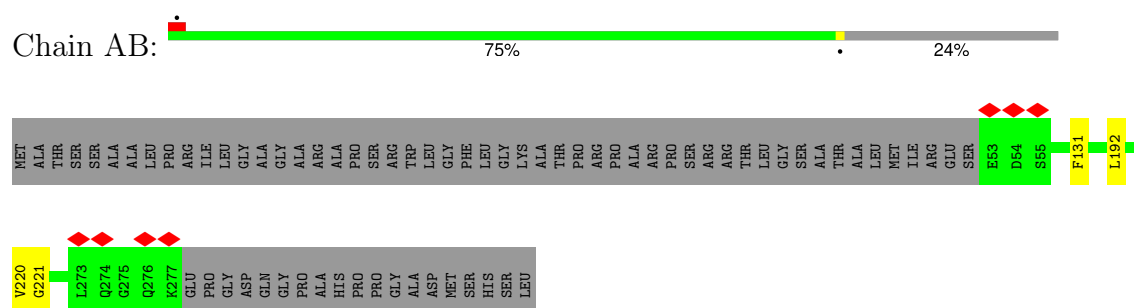
- Molecule 51: Peptidyl-tRNA hydrolase ICT1, mitochondrial



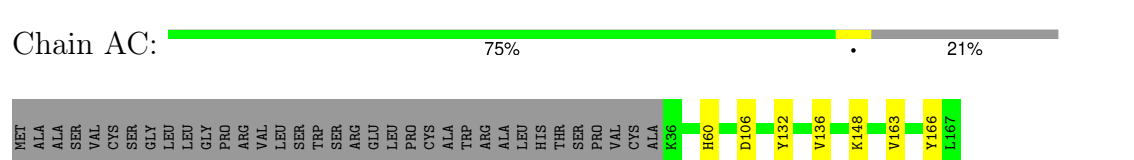
- Molecule 52: 39S ribosomal protein S30, mitochondrial



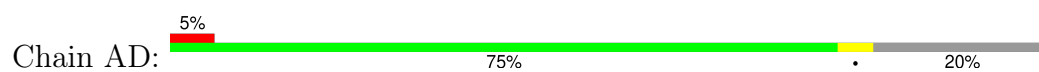
- Molecule 53: 28S ribosomal protein S2, mitochondrial



- Molecule 54: 28S ribosomal protein S24, mitochondrial



- Molecule 55: 28S ribosomal protein S5, mitochondrial



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

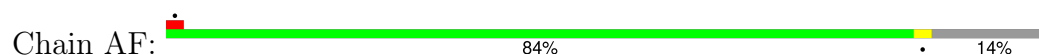
ALA SER LEU SER ARG ALA LEU GLN THR CYS LEU CYS ILE SER SER PRO SER GLY HIS LEU MET SER GLN TYR PRO S88 K100 R117 T118 K119 K120 M149 K150 N151 G152 A153 I157 E164 V168 D180 M185 K186 V187 K188 G212 V228 L244

- Molecule 56: 28S ribosomal protein S6, mitochondrial



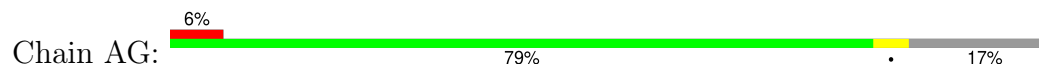
MET P2 L8 I9 L10 L22 I26 E101 R123 LYS

- Molecule 57: 28S ribosomal protein S7, mitochondrial



MET ALA ALA PRO VAL LYS VAL ALA ARG GLY TRP SER LEU ALA LEU VAL ARG ARG VAL LEU LEU PRO GLY THR GLN VAL ARG TRP S35 E56 E57 E60 F86 E132 I161 R166 V170 R234 W242

- Molecule 58: 28S ribosomal protein S9, mitochondrial



MET ALA ALA PRO CYS VAL SER TYR GLY ALA VAL THR ARG LEU LEU TRP GLY ARG ALA SER LEU ALA ARG GLN GLY LEU TRP LYS THR ALA ALA PRO GLU LEU GLN THR ASN VAL ARG SER GLN ILE LEU ARG LEU HIS THR A53 I56 P57 K58 K59 N60 V61

P62 T63 S64 K65 R66 E67 K85 H92 I104 P123 R136 K174 H175 Q176 SER HIS LEU GLN LYS SER LEU LEU PRO GLU THR VAL ARG ASP V194 I195 V210 E226 L229 T230 A235 V241 L250 E251 F315 V356 V361

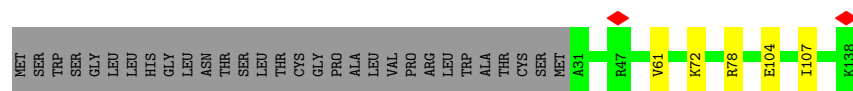
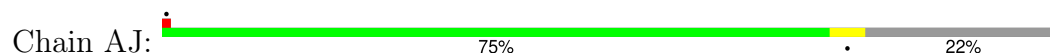
- Molecule 59: 28S ribosomal protein S10, mitochondrial



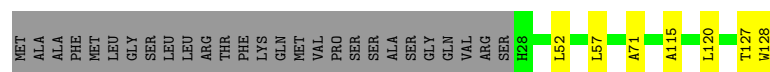
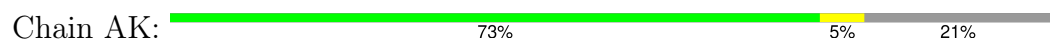
MET ALA ARG THR PHE GLY VAL CYS ARG ARG LEU TRP GLY LEU ASN PHE SER VAL ASN THR SER LYS GLY ASN THR LYS ALA ASN GLY LEU LEU SER THR ASN MET LYS TRP VAL GLN PHE SER ASN L50 H51 P55 K56 D57 L58 T59 D67 E68



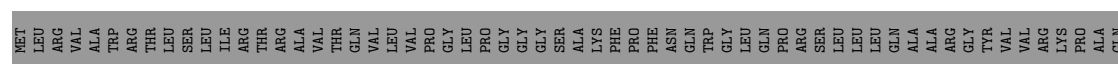
- Molecule 60: 28S ribosomal protein S12, mitochondrial



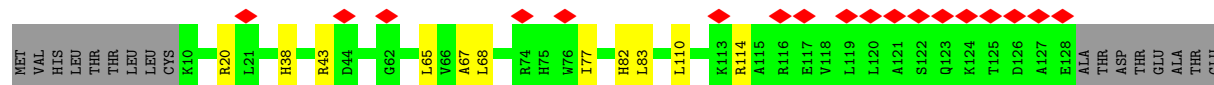
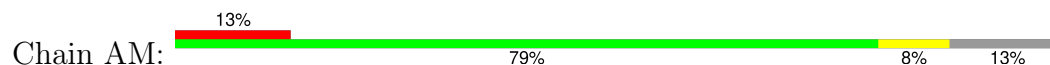
- Molecule 61: 28S ribosomal protein S14, mitochondrial



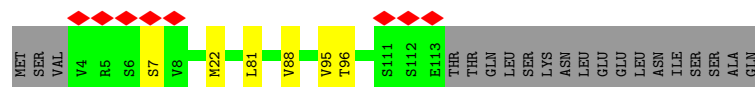
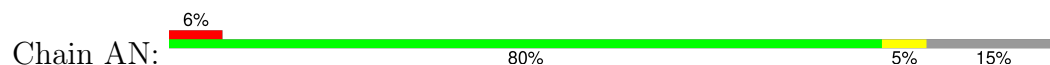
- Molecule 62: 28S ribosomal protein S15, mitochondrial



- Molecule 63: 28S ribosomal protein S16, mitochondrial

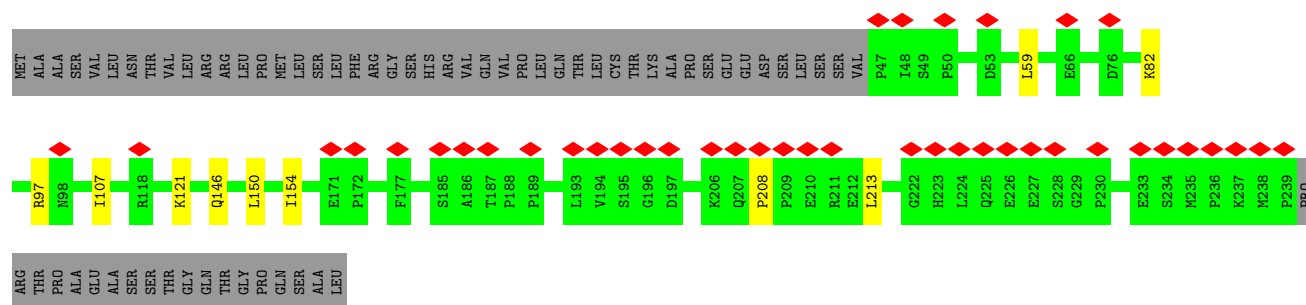


- Molecule 64: 28S ribosomal protein S17, mitochondrial

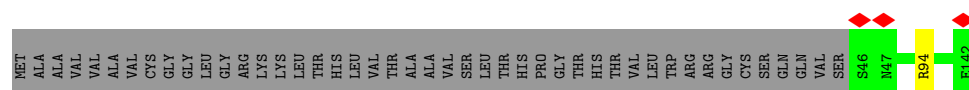


- Molecule 65: 28S ribosomal protein S18b, mitochondrial

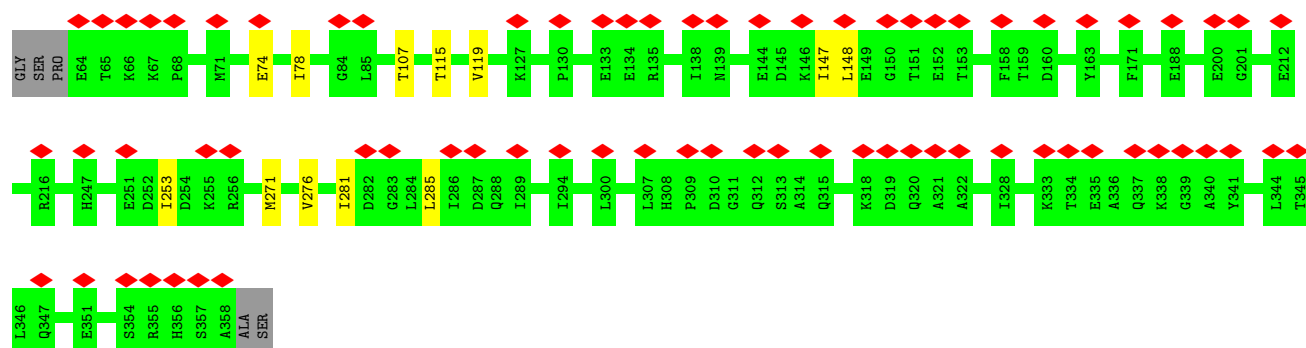
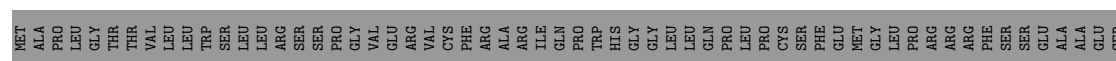
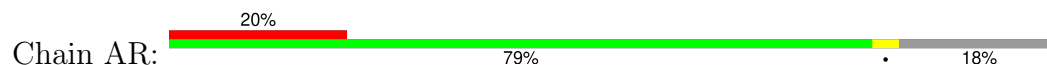




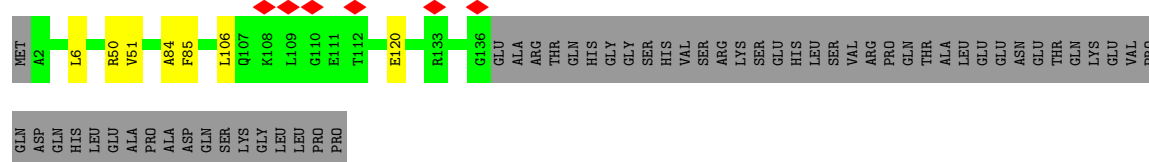
- Molecule 66: 28S ribosomal protein S18c, mitochondrial



- Molecule 67: 28S ribosomal protein S22, mitochondrial



- Molecule 68: 28S ribosomal protein S23, mitochondrial



- Molecule 69: 28S ribosomal protein S25, mitochondrial

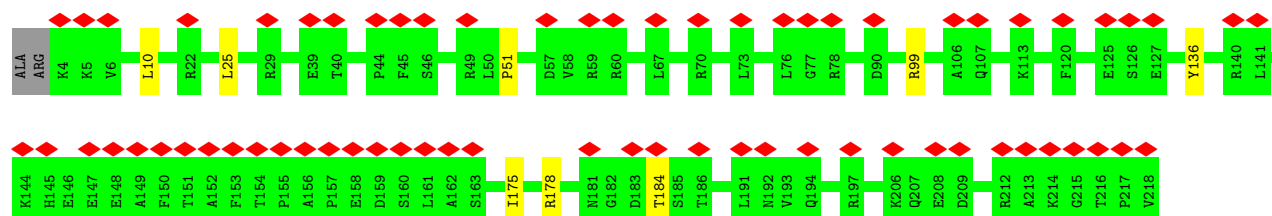




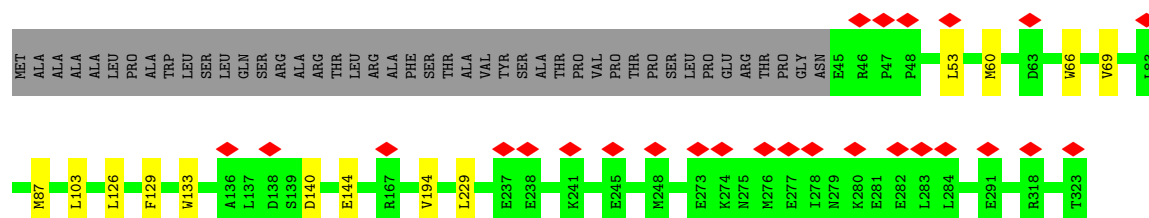
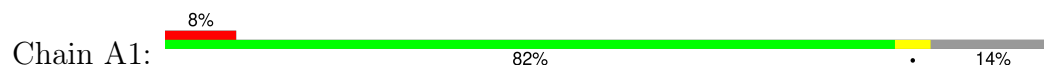
- Molecule 73: 28S ribosomal protein S33, mitochondrial



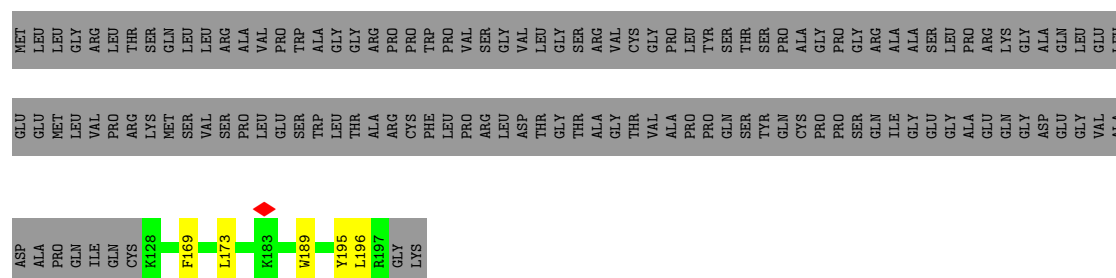
- Molecule 74: Small ribosomal subunit protein mS34



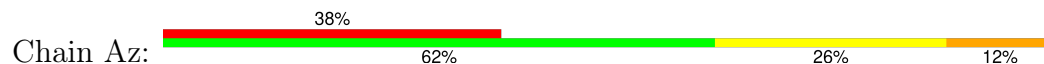
- Molecule 75: 28S ribosomal protein S35, mitochondrial

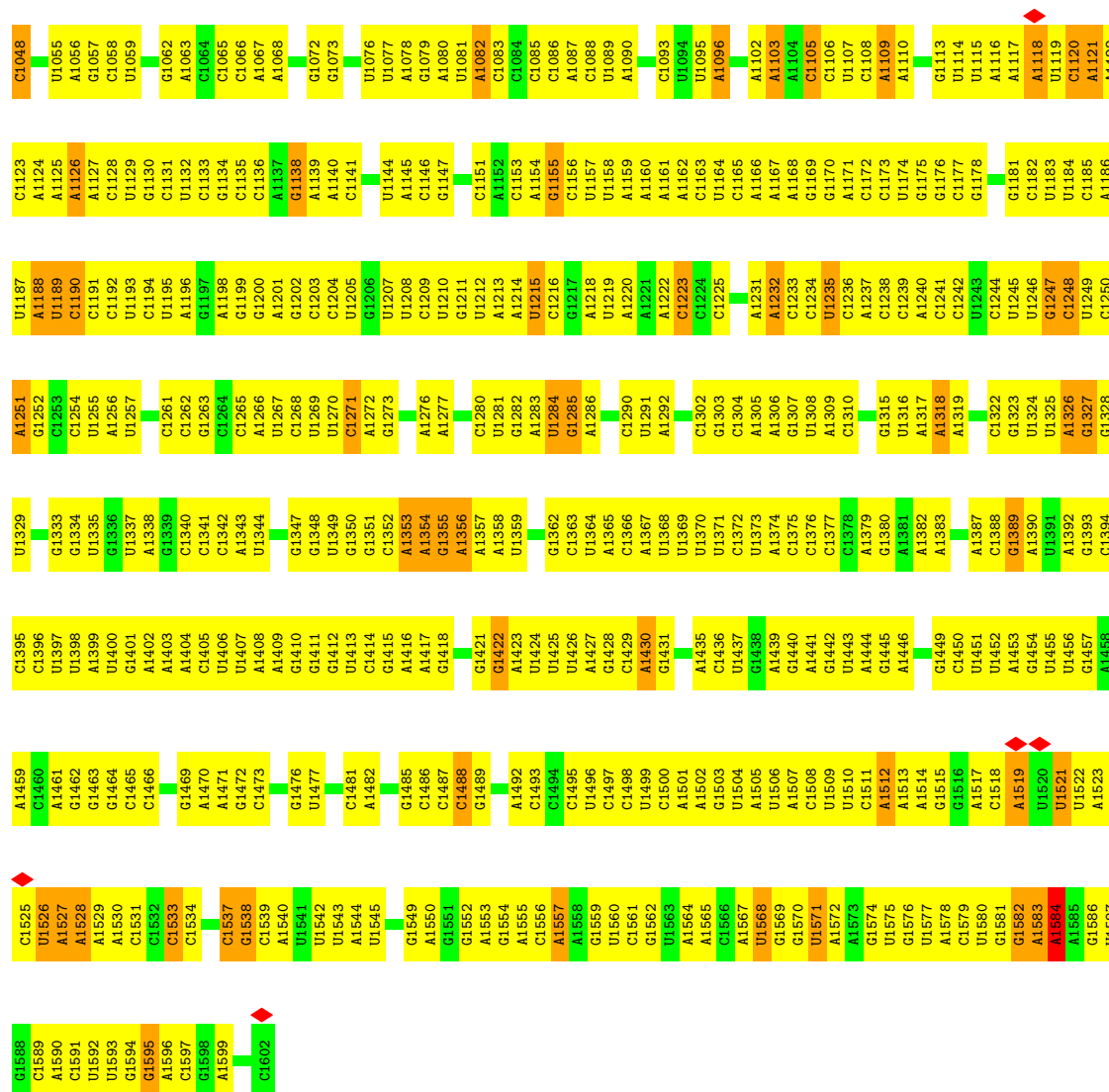


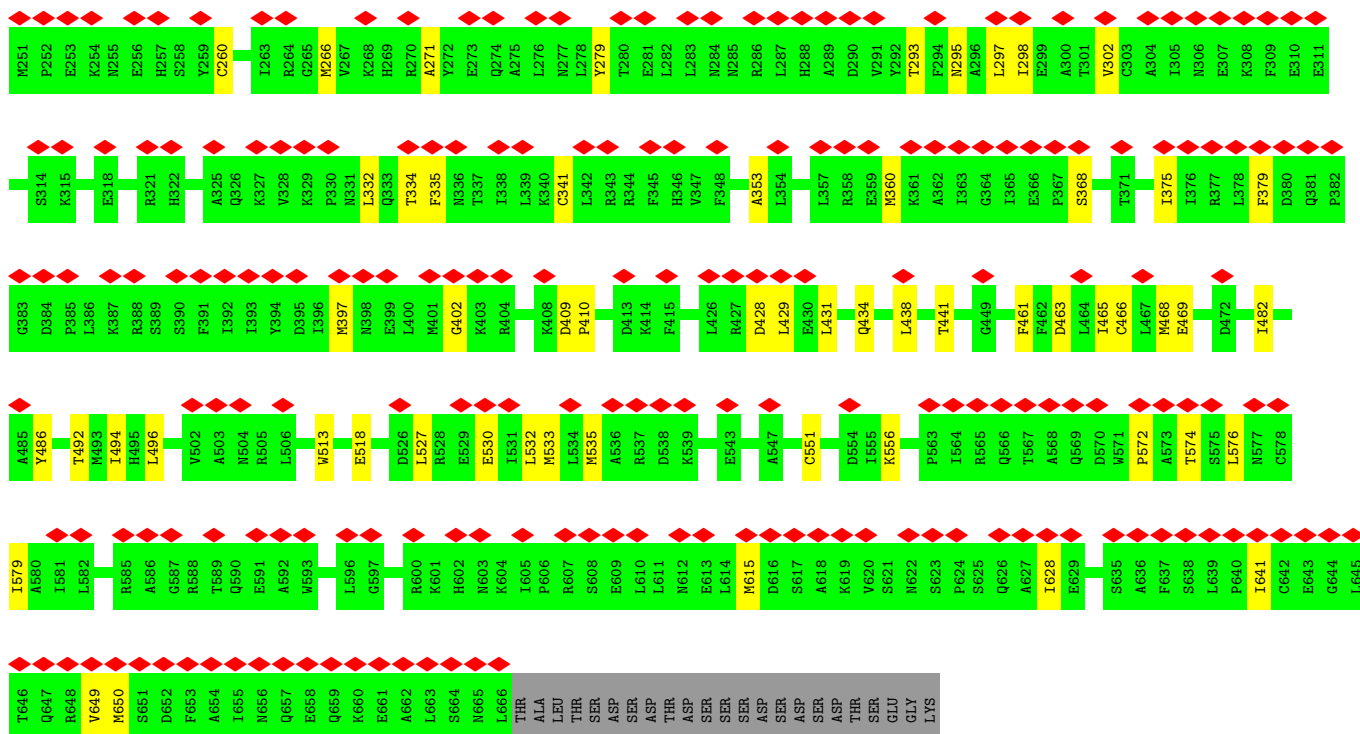
- Molecule 76: Aurora kinase A-interacting protein



- Molecule 77: mRNA



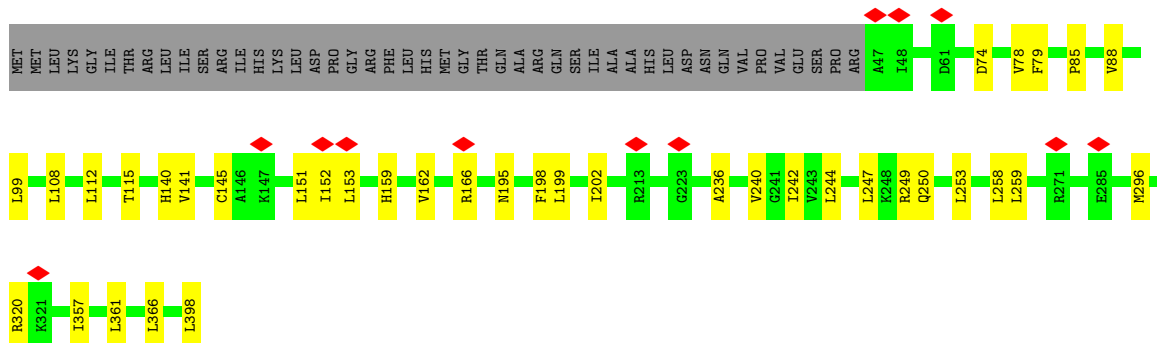
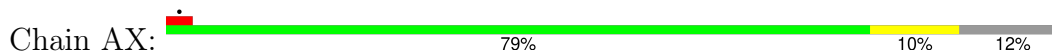




• Molecule 85: mitochondrial tRNA^{Val}



• Molecule 86: 28S ribosomal protein S29, mitochondrial



• Molecule 87: Small ribosomal subunit protein mS37



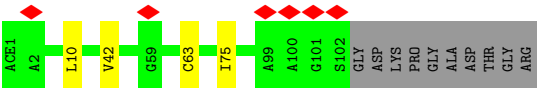
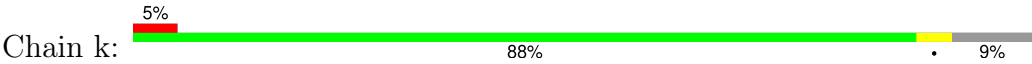


- Molecule 88: Small ribosomal subunit protein bS21m



There are no outlier residues recorded for this chain.

- Molecule 89: 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	133433	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)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.531	Depositor
Minimum map value	-0.242	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/913	0.28	0/1224
2	1	0.21	0/469	0.29	0/621
3	2	0.31	0/383	0.29	0/507
4	3	0.30	0/853	0.29	0/1136
5	4	0.27	0/350	0.27	0/461
6	5	0.23	0/3305	0.29	0/4502
7	6	0.21	0/3043	0.29	0/4140
8	7	0.20	0/2447	0.27	0/3310
9	8	0.15	0/1354	0.31	0/1819
10	9	0.23	0/1025	0.28	0/1379
11	A	0.30	0/36876	0.29	0/57402
12	C	0.10	0/1754	0.24	0/2357
13	D	0.25	0/1896	0.29	0/2549
14	E	0.25	0/2475	0.30	0/3355
15	F	0.27	0/2090	0.30	0/2842
16	H	0.15	0/1698	0.25	0/2292
17	J	0.13	0/1348	0.27	0/1813
18	K	0.27	0/1497	0.29	0/2031
19	L	0.24	0/905	0.30	0/1218
20	M	0.26	0/2381	0.29	0/3212
21	N	0.25	0/1833	0.29	0/2468
22	O	0.26	0/1283	0.30	0/1727
23	P	0.22	0/1199	0.28	0/1623
24	Q	0.23	0/2039	0.27	0/2750
25	R	0.29	0/1175	0.28	0/1572
26	S	0.27	0/1320	0.30	0/1789
27	T	0.28	0/1403	0.30	0/1886
28	U	0.25	0/1279	0.32	0/1730
29	W	0.27	0/926	0.31	0/1244
30	X	0.23	0/2099	0.25	0/2837
31	Y	0.26	0/1593	0.26	0/2136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.27	0/1021	0.29	0/1378
33	G	0.10	0/562	0.32	0/754
33	t	0.12	0/358	0.29	0/486
33	u	0.15	0/259	0.32	0/350
34	I	0.18	0/1478	0.31	0/1999
35	V	0.20	0/1721	0.28	0/2333
36	b	0.26	0/1218	0.28	0/1649
37	d	0.18	0/2181	0.27	0/2949
38	e	0.12	0/1970	0.26	0/2658
39	g	0.26	0/1151	0.28	0/1569
40	h	0.19	0/918	0.24	0/1249
41	i	0.29	0/850	0.27	0/1135
42	j	0.25	0/760	0.27	0/1023
43	l	0.14	0/707	0.27	0/960
44	m	0.13	0/805	0.27	0/1081
46	o	0.27	0/819	0.29	0/1097
47	q	0.18	0/1529	0.26	0/2055
48	r	0.23	0/1362	0.28	0/1846
49	c	0.23	0/2347	0.26	0/3171
50	f	0.17	0/1273	0.30	0/1716
51	p	0.19	0/1223	0.28	0/1641
52	s	0.25	0/3231	0.29	0/4389
53	AB	0.18	0/1871	0.25	0/2531
54	AC	0.17	0/1113	0.27	0/1505
55	AD	0.17	0/2783	0.26	0/3724
56	AE	0.19	0/989	0.29	0/1335
57	AF	0.15	0/1767	0.24	0/2373
58	AG	0.16	0/2746	0.25	0/3681
59	AH	0.16	0/1178	0.28	0/1598
60	AJ	0.15	0/855	0.28	0/1148
61	AK	0.16	0/880	0.25	0/1182
62	AL	0.17	0/1477	0.24	0/1974
63	AM	0.13	0/963	0.29	0/1295
64	AN	0.17	0/886	0.25	0/1199
65	AO	0.13	0/1648	0.26	0/2243
66	AP	0.19	0/798	0.26	0/1070
67	AR	0.12	0/2456	0.24	0/3317
68	AS	0.15	0/1138	0.23	0/1533
69	AT	0.15	0/1402	0.27	0/1883
70	AU	0.14	0/1510	0.26	0/2025
71	AV	0.13	0/3030	0.30	0/4093
72	AW	0.16	0/801	0.25	0/1079
73	AZ	0.14	0/857	0.26	0/1141

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	A0	0.11	0/1834	0.26	0/2484
75	A1	0.14	0/2313	0.28	0/3129
76	A3	0.22	0/636	0.28	0/839
77	Az	0.15	0/804	0.29	0/1248
78	AY	0.14	0/1040	0.24	0/1402
79	AA	0.21	0/22537	0.24	0/35085
80	AI	0.19	0/1039	0.26	0/1400
81	OX	0.19	0/478	0.39	0/639
82	a	0.23	0/891	0.30	0/1208
83	Ax	0.18	0/1673	0.30	0/2602
84	A4	0.13	0/4877	0.29	0/6598
85	B	0.14	0/1627	0.24	0/2527
86	AX	0.14	0/2921	0.29	0/3954
87	A2	0.17	0/947	0.25	0/1266
88	AQ	0.21	0/754	0.23	0/1003
89	k	0.15	0/783	0.24	0/1057
All	All	0.23	0/187256	0.27	0/265790

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 ⓘ

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	4	0
3	2	377	407	406	0	0
4	3	832	884	883	2	0
5	4	342	362	361	5	0
6	5	3210	3209	3206	10	0
7	6	2948	2844	2841	6	0
8	7	2390	2399	2397	9	0
9	8	1327	1369	1368	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	9	997	988	987	0	0
11	A	33070	16801	16793	40	0
12	C	1732	0	1740	186	0
13	D	1859	1921	1920	1	0
14	E	2406	2416	2415	7	0
15	F	2031	2066	2065	2	0
16	H	1661	1736	1734	9	0
17	J	1330	1408	1407	9	0
18	K	1455	1452	1452	6	0
19	L	890	942	941	0	0
20	M	2327	2396	2395	3	0
21	N	1786	1818	1817	3	0
22	O	1259	1295	1294	4	0
23	P	1173	1166	1165	2	0
24	Q	1990	2031	2031	4	0
25	R	1154	1215	1214	1	0
26	S	1293	1366	1365	1	0
27	T	1369	1412	1410	6	0
28	U	1248	1228	1228	4	0
29	W	904	936	935	3	0
30	X	2044	2061	2060	2	0
31	Y	1556	1598	1597	2	0
32	Z	996	1045	1044	1	0
33	G	558	0	612	122	0
33	t	354	378	377	4	0
33	u	257	284	283	12	0
34	I	1446	1533	1532	8	0
35	V	1676	1689	1687	7	0
36	b	1193	1186	1191	1	0
37	d	2124	0	2125	99	0
38	e	1931	1917	1916	14	0
39	g	1113	1097	1097	0	0
40	h	895	883	881	0	0
41	i	828	859	857	0	0
42	j	745	747	746	1	0
43	l	688	675	674	4	0
44	m	791	760	796	6	0
45	n	215	0	52	0	0
46	o	798	806	804	4	0
47	q	1495	942	1492	57	0
48	r	1322	1349	1348	1	0
49	c	2299	2322	2320	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	f	1252	1271	1269	12	0
51	p	1205	1225	1223	6	0
52	s	3148	3137	3131	8	0
53	AB	1828	1816	1815	2	0
54	AC	1083	1089	1088	5	0
55	AD	2731	2805	2804	14	0
56	AE	972	1000	1000	2	0
57	AF	1725	1771	1769	5	0
58	AG	2688	2689	2687	10	0
59	AH	1152	1187	1183	16	0
60	AJ	839	888	887	5	0
61	AK	862	886	885	6	0
62	AL	1453	1541	1540	9	0
63	AM	942	966	965	10	0
64	AN	868	929	928	5	0
65	AO	1592	1557	1557	7	0
66	AP	781	806	806	1	0
67	AR	2409	2430	2428	10	0
68	AS	1111	1116	1115	8	0
69	AT	1371	1393	1393	2	0
70	AU	1488	1501	1499	6	0
71	AV	2969	2964	2961	41	0
72	AW	789	804	802	4	0
73	AZ	839	859	858	1	0
74	A0	1787	1797	1796	7	0
75	A1	2265	2296	2294	12	0
76	A3	625	701	699	6	0
77	Az	719	360	360	3	0
78	AY	1010	963	957	8	0
79	AA	20260	0	10285	833	0
80	AI	1019	1058	1059	4	0
81	OX	468	465	464	2	0
82	a	865	830	829	5	0
83	Ax	1498	766	766	3	0
84	A4	4768	4767	4766	53	0
85	B	1524	780	779	1	0
86	AX	2849	2844	2844	25	0
87	A2	935	971	971	6	0
88	AQ	744	758	758	0	0
89	k	774	785	784	3	0
90	0	1	0	0	0	0
90	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	AO	1	0	0	0	0
91	6	1	0	0	0	0
91	A	29	0	0	0	0
91	AA	18	0	0	0	0
91	D	1	0	0	0	0
91	M	2	0	0	0	0
91	N	1	0	0	0	0
91	W	1	0	0	0	0
91	o	1	0	0	0	0
92	A	50	44	95	5	0
92	AA	20	0	36	5	0
92	AG	10	0	17	6	0
93	A	6	14	12	0	0
94	A	136	0	0	0	0
94	A3	1	0	0	0	0
94	AA	61	0	0	0	0
94	AB	1	0	0	0	0
94	AX	1	0	0	0	0
94	D	2	0	0	0	0
94	E	1	0	0	0	0
94	I	1	0	0	0	0
94	g	1	0	0	0	0
95	e	7	8	8	0	0
96	AP	4	0	0	0	0
96	AT	4	0	0	0	0
96	r	4	0	0	0	0
97	AA	44	0	26	1	0
98	AA	42	0	75	18	0
99	AX	31	11	12	0	0
100	AX	28	12	12	1	0
All	All	178765	136488	151985	1718	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1718 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	33:G:143:VAL:HG12	1.23	1.11
47:q:164:LEU:HB3	47:q:168:VAL:HG21	1.38	1.04
12:C:90:LEU:HG	12:C:153:LEU:HD22	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:G:185:LYS:HD2	33:G:188:LEU:HD11	1.46	0.96
12:C:268:LEU:HD23	12:C:272:ASP:HB3	1.50	0.93

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%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	40 (91%)	4 (9%)	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	380 (97%)	12 (3%)	0	100	100
7	6	352/380 (93%)	338 (96%)	14 (4%)	0	100	100
8	7	292/338 (86%)	281 (96%)	11 (4%)	0	100	100
9	8	155/206 (75%)	151 (97%)	4 (3%)	0	100	100
10	9	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
12	C	221/297 (74%)	216 (98%)	5 (2%)	0	100	100
13	D	236/305 (77%)	226 (96%)	10 (4%)	0	100	100
14	E	303/348 (87%)	291 (96%)	12 (4%)	0	100	100
15	F	250/311 (80%)	244 (98%)	6 (2%)	0	100	100
16	H	200/267 (75%)	193 (96%)	7 (4%)	0	100	100
17	J	173/192 (90%)	171 (99%)	2 (1%)	0	100	100
18	K	176/178 (99%)	171 (97%)	5 (3%)	0	100	100
19	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	M	289/296 (98%)	280 (97%)	9 (3%)	0	100	100
21	N	220/251 (88%)	216 (98%)	4 (2%)	0	100	100
22	O	152/175 (87%)	145 (95%)	7 (5%)	0	100	100
23	P	142/180 (79%)	136 (96%)	6 (4%)	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%)	153 (96%)	6 (4%)	0	100	100
27	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
28	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
29	W	114/148 (77%)	109 (96%)	5 (4%)	0	100	100
30	X	242/256 (94%)	238 (98%)	4 (2%)	0	100	100
31	Y	179/250 (72%)	174 (97%)	5 (3%)	0	100	100
32	Z	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
33	G	70/198 (35%)	68 (97%)	2 (3%)	0	100	100
33	t	44/198 (22%)	42 (96%)	2 (4%)	0	100	100
33	u	30/198 (15%)	30 (100%)	0	0	100	100
34	I	179/261 (69%)	173 (97%)	6 (3%)	0	100	100
35	V	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
36	b	148/215 (69%)	143 (97%)	5 (3%)	0	100	100
37	d	257/306 (84%)	237 (92%)	19 (7%)	1 (0%)	30	54
38	e	236/279 (85%)	224 (95%)	12 (5%)	0	100	100
39	g	132/166 (80%)	125 (95%)	7 (5%)	0	100	100
40	h	108/158 (68%)	103 (95%)	5 (5%)	0	100	100
41	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
42	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
43	l	80/138 (58%)	77 (96%)	3 (4%)	0	100	100
44	m	90/128 (70%)	86 (96%)	4 (4%)	0	100	100
46	o	92/102 (90%)	91 (99%)	1 (1%)	0	100	100
47	q	175/222 (79%)	174 (99%)	1 (1%)	0	100	100
48	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
49	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	f	153/212 (72%)	147 (96%)	6 (4%)	0	100	100
51	p	141/206 (68%)	136 (96%)	5 (4%)	0	100	100
52	s	381/439 (87%)	371 (97%)	10 (3%)	0	100	100
53	AB	223/296 (75%)	216 (97%)	7 (3%)	0	100	100
54	AC	130/167 (78%)	124 (95%)	6 (5%)	0	100	100
55	AD	341/430 (79%)	329 (96%)	12 (4%)	0	100	100
56	AE	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
57	AF	206/242 (85%)	203 (98%)	3 (2%)	0	100	100
58	AG	323/396 (82%)	313 (97%)	10 (3%)	0	100	100
59	AH	138/201 (69%)	131 (95%)	6 (4%)	1 (1%)	18	40
60	AJ	106/138 (77%)	103 (97%)	3 (3%)	0	100	100
61	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
62	AL	172/257 (67%)	169 (98%)	3 (2%)	0	100	100
63	AM	117/137 (85%)	111 (95%)	6 (5%)	0	100	100
64	AN	108/130 (83%)	103 (95%)	5 (5%)	0	100	100
65	AO	191/258 (74%)	183 (96%)	8 (4%)	0	100	100
66	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
67	AR	293/360 (81%)	282 (96%)	11 (4%)	0	100	100
68	AS	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
69	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
70	AU	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
71	AV	358/414 (86%)	344 (96%)	14 (4%)	0	100	100
72	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
73	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
74	A0	213/217 (98%)	207 (97%)	6 (3%)	0	100	100
75	A1	277/323 (86%)	267 (96%)	10 (4%)	0	100	100
76	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
78	AY	117/395 (30%)	117 (100%)	0	0	100	100
80	AI	135/194 (70%)	127 (94%)	8 (6%)	0	100	100
81	OX	51/435 (12%)	47 (92%)	4 (8%)	0	100	100
82	a	99/142 (70%)	93 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	A4	584/689 (85%)	563 (96%)	21 (4%)	0	100	100
86	AX	350/398 (88%)	332 (95%)	18 (5%)	0	100	100
87	A2	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
88	AQ	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
89	k	100/112 (89%)	99 (99%)	1 (1%)	0	100	100
All	All	14658/19297 (76%)	14209 (97%)	447 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	AH	126	ILE
37	d	47	GLN

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	137 (99%)	1 (1%)	76	86
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	G	60/158 (38%)	60 (100%)	0	100	100
33	t	40/158 (25%)	40 (100%)	0	100	100
33	u	31/158 (20%)	31 (100%)	0	100	100
34	I	165/232 (71%)	165 (100%)	0	100	100
35	V	183/191 (96%)	183 (100%)	0	100	100
36	b	132/186 (71%)	132 (100%)	0	100	100
37	d	237/274 (86%)	237 (100%)	0	100	100
38	e	207/236 (88%)	207 (100%)	0	100	100
39	g	124/148 (84%)	124 (100%)	0	100	100
40	h	104/148 (70%)	104 (100%)	0	100	100
41	i	86/110 (78%)	86 (100%)	0	100	100
42	j	74/97 (76%)	74 (100%)	0	100	100
43	l	76/116 (66%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	m	85/113 (75%)	85 (100%)	0	100	100
46	o	80/87 (92%)	80 (100%)	0	100	100
47	q	153/178 (86%)	153 (100%)	0	100	100
48	r	147/169 (87%)	147 (100%)	0	100	100
49	c	251/288 (87%)	251 (100%)	0	100	100
50	f	139/188 (74%)	139 (100%)	0	100	100
51	p	135/181 (75%)	135 (100%)	0	100	100
52	s	339/381 (89%)	339 (100%)	0	100	100
53	AB	198/249 (80%)	198 (100%)	0	100	100
54	AC	115/143 (80%)	115 (100%)	0	100	100
55	AD	286/357 (80%)	286 (100%)	0	100	100
56	AE	104/107 (97%)	104 (100%)	0	100	100
57	AF	185/209 (88%)	185 (100%)	0	100	100
58	AG	285/342 (83%)	285 (100%)	0	100	100
59	AH	130/180 (72%)	130 (100%)	0	100	100
60	AJ	93/118 (79%)	93 (100%)	0	100	100
61	AK	91/113 (80%)	91 (100%)	0	100	100
62	AL	158/226 (70%)	158 (100%)	0	100	100
63	AM	97/113 (86%)	97 (100%)	0	100	100
64	AN	96/115 (84%)	96 (100%)	0	100	100
65	AO	174/230 (76%)	174 (100%)	0	100	100
66	AP	88/123 (72%)	88 (100%)	0	100	100
67	AR	264/318 (83%)	264 (100%)	0	100	100
68	AS	116/164 (71%)	116 (100%)	0	100	100
69	AT	153/157 (98%)	153 (100%)	0	100	100
70	AU	152/174 (87%)	152 (100%)	0	100	100
71	AV	325/364 (89%)	325 (100%)	0	100	100
72	AW	87/158 (55%)	87 (100%)	0	100	100
73	AZ	90/95 (95%)	90 (100%)	0	100	100
74	A0	188/189 (100%)	188 (100%)	0	100	100
75	A1	257/291 (88%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	A3	65/166 (39%)	65 (100%)	0	100	100
78	AY	110/357 (31%)	110 (100%)	0	100	100
80	AI	105/147 (71%)	105 (100%)	0	100	100
81	OX	49/372 (13%)	49 (100%)	0	100	100
82	a	99/133 (74%)	99 (100%)	0	100	100
84	A4	526/609 (86%)	526 (100%)	0	100	100
86	AX	311/351 (89%)	311 (100%)	0	100	100
87	A2	100/100 (100%)	100 (100%)	0	100	100
88	AQ	78/78 (100%)	78 (100%)	0	100	100
89	k	83/89 (93%)	83 (100%)	0	100	100
All	All	13096/16645 (79%)	13095 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	J	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
65	AO	147	HIS
81	OX	399	GLN
67	AR	326	ASN
74	A0	24	GLN
86	AX	148	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1561 (99%)	250 (16%)	3 (0%)
77	Az	33/34 (97%)	13 (39%)	0
79	AA	953/954 (99%)	139 (14%)	1 (0%)
83	Ax	70/71 (98%)	15 (21%)	0
85	B	71/72 (98%)	18 (25%)	0
All	All	2683/2692 (99%)	435 (16%)	4 (0%)

5 of 435 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 (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2112	A
11	A	2245	A
11	A	2484	C
79	AA	1234	C

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	$\# Z > 2$
79	B8T	AA	1486	94,79	19,22,23	0.41	0	25,31,34	0.38	0
85	2MG	B	10	85	23,26,27	0.36	0	33,38,41	0.42	0
79	MA6	AA	1583	79	23,26,27	0.32	0	33,38,41	0.66	1 (3%)
85	1MA	B	9	85	21,25,26	0.39	0	30,37,40	0.59	0
11	OMG	A	2815	83,91,11	23,26,27	0.36	0	32,38,41	0.38	0
79	MA6	AA	1584	79	23,26,27	0.32	0	33,38,41	0.67	1 (3%)
11	OMG	A	3040	11	23,26,27	0.34	0	32,38,41	0.37	0
11	OMU	A	3039	91,11	19,22,23	0.30	0	25,31,34	0.66	1 (4%)
11	1MA	A	2617	11	21,25,26	0.42	0	30,37,40	0.61	0
11	PSU	A	3067	11	18,21,22	1.18	2 (11%)	21,30,33	0.77	1 (4%)
79	5MC	AA	1488	79	19,22,23	0.84	1 (5%)	26,32,35	0.50	0
85	PSU	B	39	85	18,21,22	1.06	1 (5%)	21,30,33	0.66	0
79	5MU	AA	1076	79	19,22,23	0.35	0	27,32,35	0.41	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
79	B8T	AA	1486	94,79	-	0/7/27/28	0/2/2/2
85	2MG	B	10	85	-	0/9/27/28	0/3/3/3
79	MA6	AA	1583	79	-	0/11/29/30	0/3/3/3
85	1MA	B	9	85	-	0/7/25/26	0/3/3/3
11	OMG	A	2815	83,91,11	-	0/9/27/28	0/3/3/3
79	MA6	AA	1584	79	-	1/11/29/30	0/3/3/3
11	OMG	A	3040	11	-	2/9/27/28	0/3/3/3
11	OMU	A	3039	91,11	-	0/9/27/28	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2
79	5MC	AA	1488	79	-	0/7/25/26	0/2/2/2
85	PSU	B	39	85	-	0/7/25/26	0/2/2/2
79	5MU	AA	1076	79	-	5/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	3067	PSU	C6-C5	3.64	1.39	1.35
85	B	39	PSU	C6-C5	3.61	1.39	1.35
79	AA	1488	5MC	C5-C4	-3.31	1.41	1.44
11	A	3067	PSU	O4'-C1'	-2.64	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	AA	1583	MA6	C2-N1-C6	2.77	118.60	111.83
79	AA	1584	MA6	C2-N1-C6	2.70	118.43	111.83
11	A	3039	OMU	C2'-C1'-N1	-2.47	109.56	114.24
11	A	3067	PSU	O4'-C1'-C2'	2.33	108.37	105.15

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
79	AA	1076	5MU	O4'-C4'-C5'-O5'
79	AA	1076	5MU	C3'-C4'-C5'-O5'
79	AA	1584	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
11	A	3040	OMG	O4'-C4'-C5'-O5'
11	A	3040	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
79	AA	1486	B8T	1	0
79	AA	1583	MA6	5	0
79	AA	1584	MA6	2	0
79	AA	1488	5MC	3	0
79	AA	1076	5MU	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	$\# Z > 2$
97	NAD	AA	1701	94	46,48,48	2.64	18 (39%)	64,73,73	1.60	7 (10%)
96	FES	AT	201	69,63	0,4,4	-	-	-		
96	FES	AP	201	66,56	0,4,4	-	-	-		
92	SPD	AG	401	92	9,9,9	0.32	0	8,8,8	0.83	0
95	VAL	e	301	-	4,6,7	0.55	0	6,7,9	0.86	0
92	SPD	A	3470	-	9,9,9	0.32	0	8,8,8	0.91	0
92	SPD	A	3471	-	9,9,9	0.32	0	8,8,8	0.92	0
93	PUT	A	3303	-	5,5,5	0.19	0	4,4,4	0.55	0
92	SPD	AA	1785	92	9,9,9	0.33	0	8,8,8	0.78	0
96	FES	r	201	34,48	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
99	ATP	AX	501	94	32,33,33	0.52	0	48,52,52	0.59	0
92	SPD	A	3469	-	9,9,9	0.32	0	8,8,8	0.83	0
92	SPD	A	3302	-	9,9,9	0.33	0	8,8,8	0.92	0
92	SPD	AA	1703	-	9,9,9	0.32	0	8,8,8	0.89	0
98	SPM	AA	1784	98	13,13,13	0.35	0	12,12,12	0.91	0
92	SPD	A	3301	94	9,9,9	0.36	0	8,8,8	0.72	0
98	SPM	AA	1782	98	13,13,13	0.35	0	12,12,12	0.95	0
100	GDP	AX	503	-	29,30,30	2.86	13 (44%)	45,47,47	1.53	9 (20%)
98	SPM	AA	1702	-	13,13,13	0.36	0	12,12,12	1.02	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
97	NAD	AA	1701	94	-	11/30/62/62	0/5/5/5
96	FES	AT	201	69,63	-	-	0/1/1/1
96	FES	AP	201	66,56	-	-	0/1/1/1
92	SPD	AG	401	92	-	3/7/7/7	-
95	VAL	e	301	-	-	1/5/6/8	-
92	SPD	A	3470	-	-	3/7/7/7	-
92	SPD	A	3471	-	-	4/7/7/7	-
93	PUT	A	3303	-	-	0/3/3/3	-
92	SPD	AA	1785	92	-	2/7/7/7	-
96	FES	r	201	34,48	-	-	0/1/1/1
99	ATP	AX	501	94	-	0/22/38/38	0/3/3/3
92	SPD	A	3469	-	-	3/7/7/7	-
92	SPD	A	3302	-	-	3/7/7/7	-
92	SPD	AA	1703	-	-	1/7/7/7	-
98	SPM	AA	1784	98	-	3/11/11/11	-
92	SPD	A	3301	94	-	2/7/7/7	-
98	SPM	AA	1782	98	-	6/11/11/11	-
100	GDP	AX	503	-	-	5/16/32/32	0/3/3/3
98	SPM	AA	1702	-	-	1/11/11/11	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
100	AX	503	GDP	O6-C6	8.80	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AA	1701	NAD	C7N-N7N	7.03	1.45	1.33
97	AA	1701	NAD	O4D-C1D	6.41	1.49	1.40
97	AA	1701	NAD	PN-O3	5.81	1.65	1.59
97	AA	1701	NAD	C6A-N6A	5.54	1.48	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	AA	1701	NAD	C4A-N9A-C8A	8.55	114.71	105.74
100	AX	503	GDP	C8-N9-C4	4.50	114.45	106.03
100	AX	503	GDP	C2-N1-C6	-3.03	119.62	125.11
100	AX	503	GDP	C3'-C2'-C1'	3.02	107.18	101.46
97	AA	1701	NAD	C4D-O4D-C1D	-3.01	107.17	109.92

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
95	e	301	VAL	O-C-CA-CB
100	AX	503	GDP	PA-O3A-PB-O3B
100	AX	503	GDP	C5'-O5'-PA-O1A
98	AA	1782	SPM	C6-C7-C8-C9
98	AA	1782	SPM	N5-C6-C7-C8

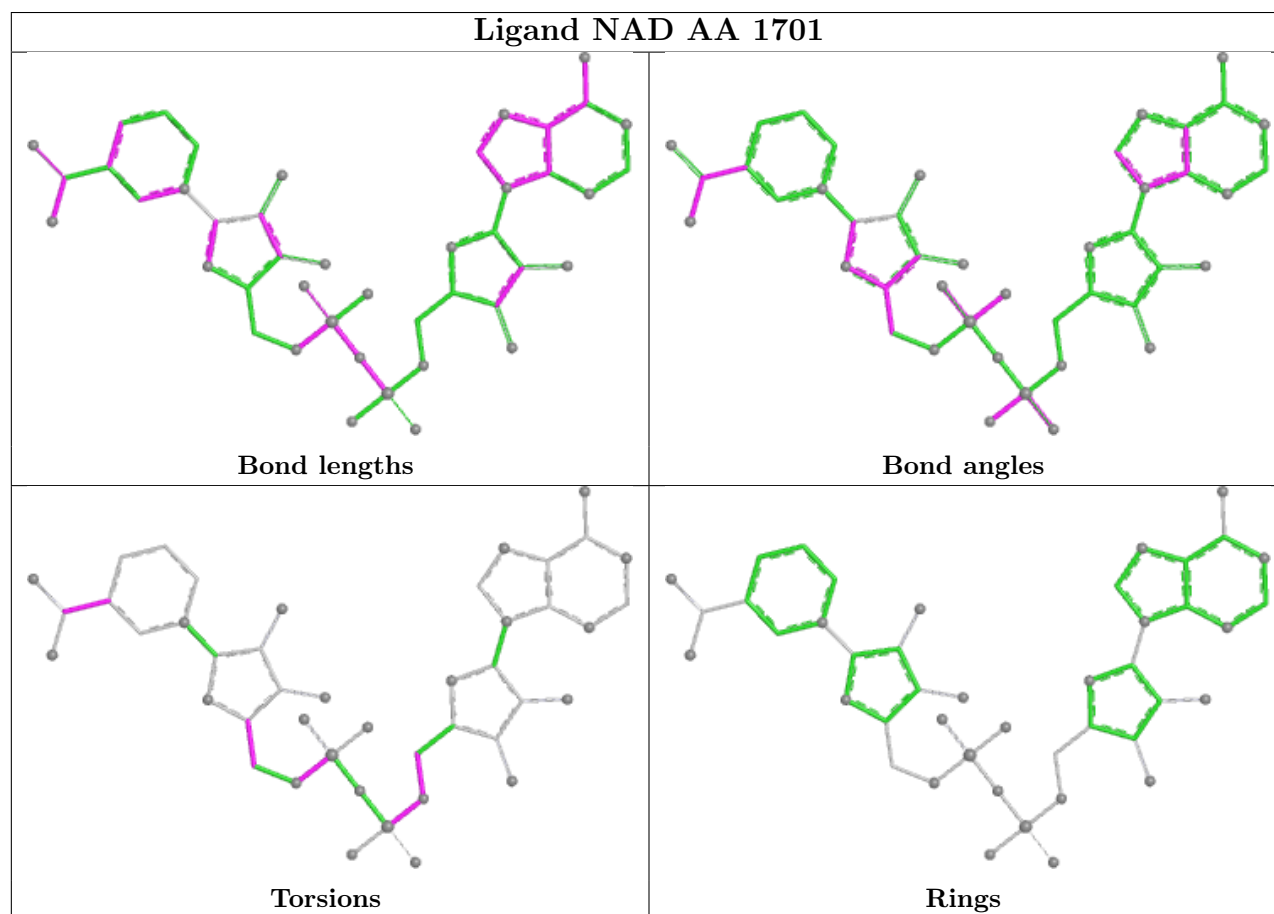
There are no ring outliers.

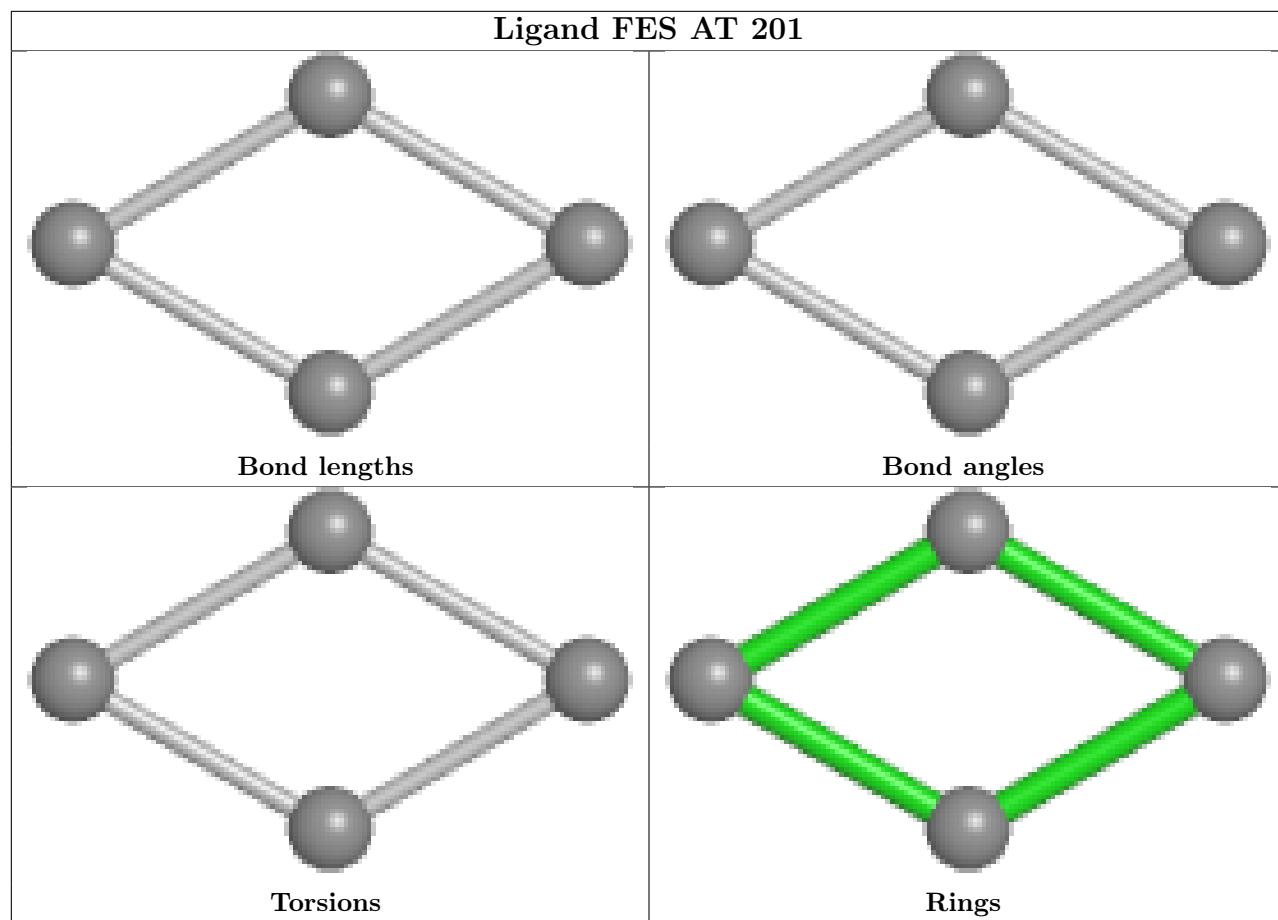
9 monomers are involved in 32 short contacts:

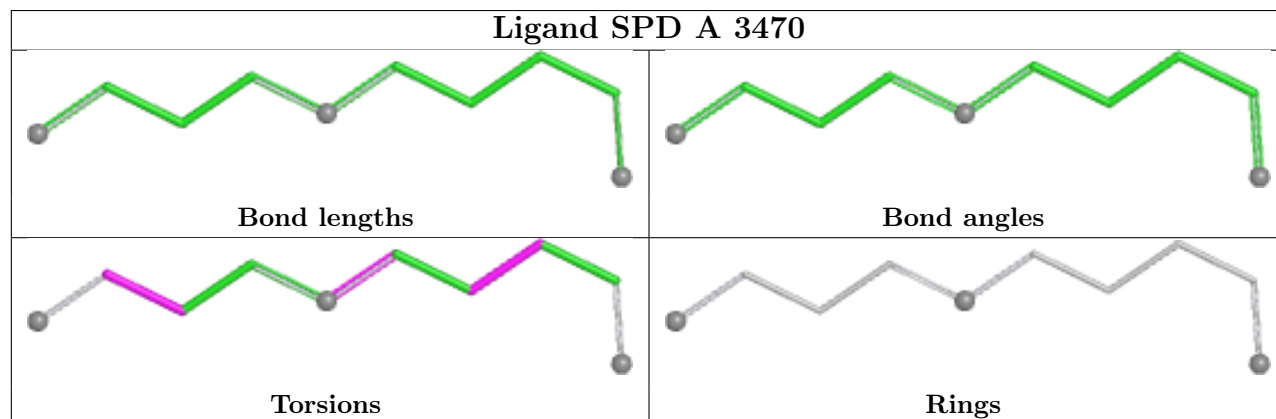
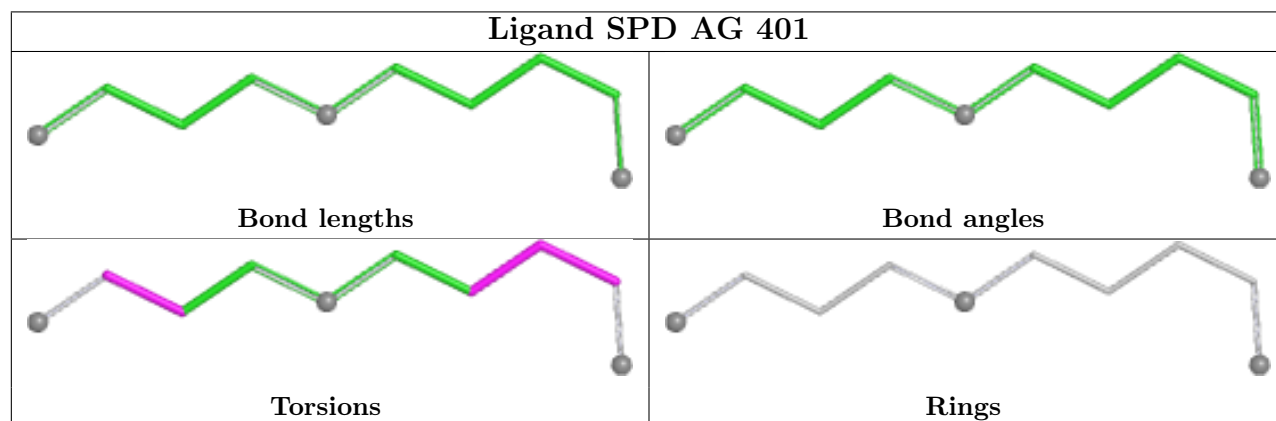
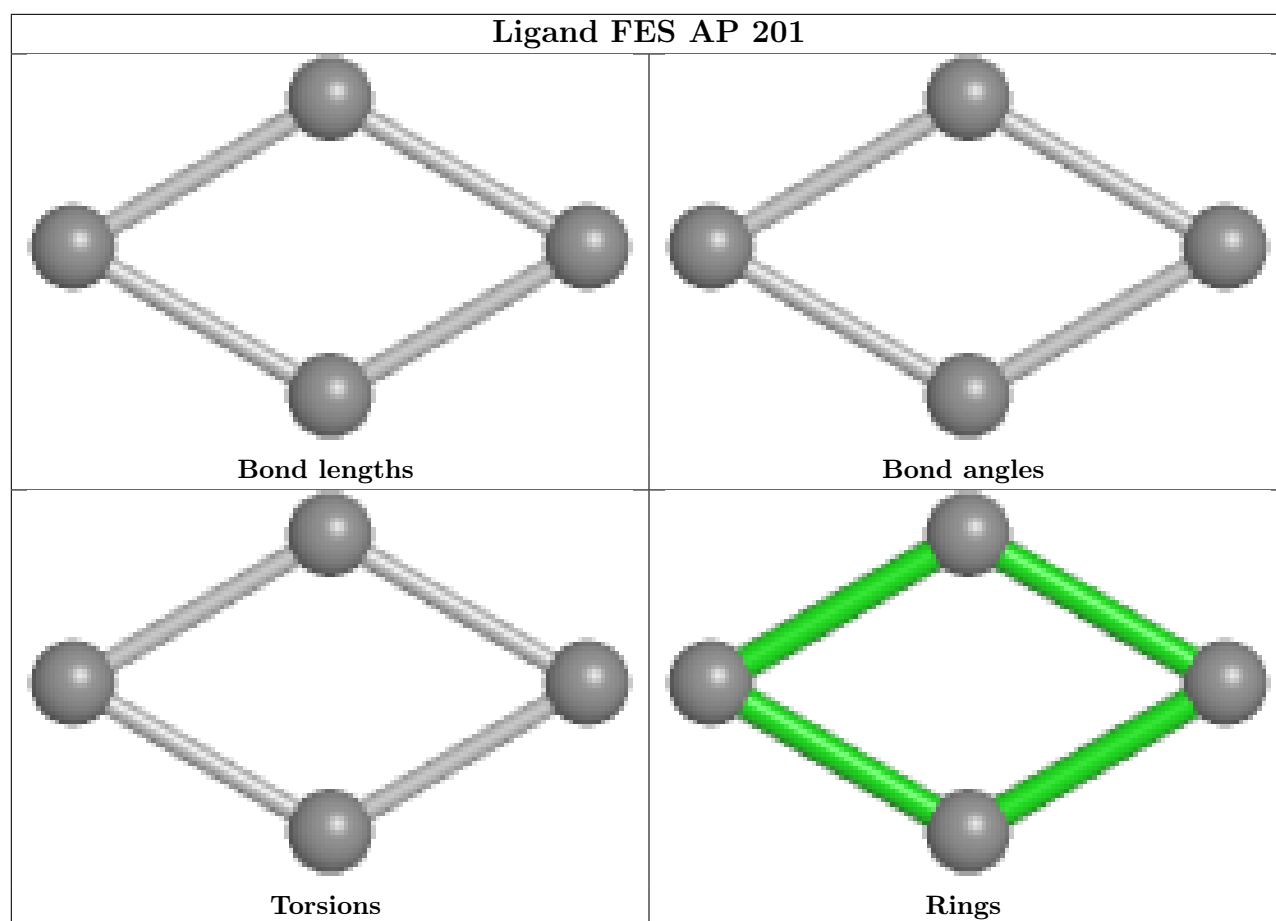
Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	AA	1701	NAD	1	0
92	AG	401	SPD	6	0
92	A	3470	SPD	1	0
92	A	3471	SPD	4	0
92	AA	1785	SPD	5	0
98	AA	1784	SPM	15	0
98	AA	1782	SPM	14	0
100	AX	503	GDP	1	0
98	AA	1702	SPM	3	0

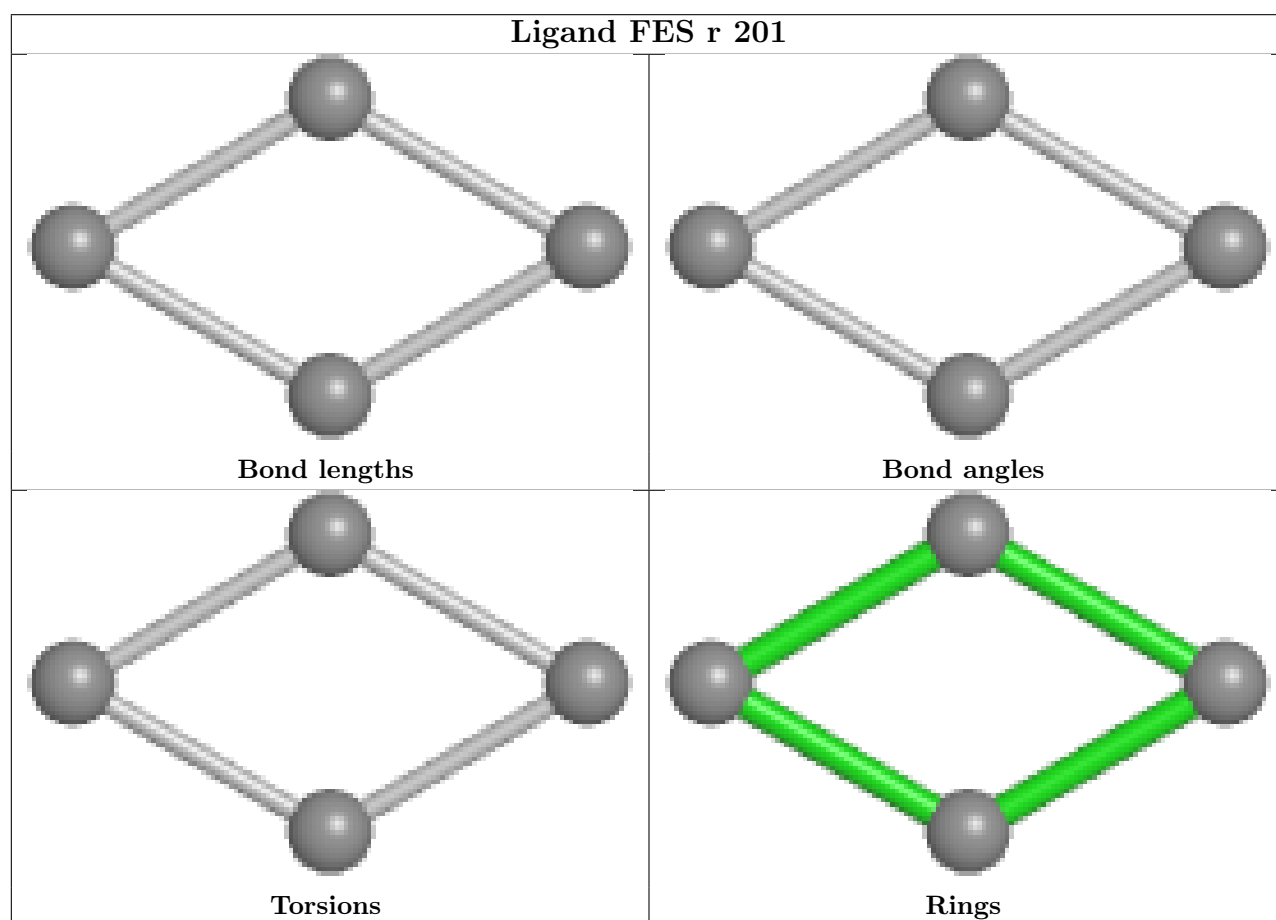
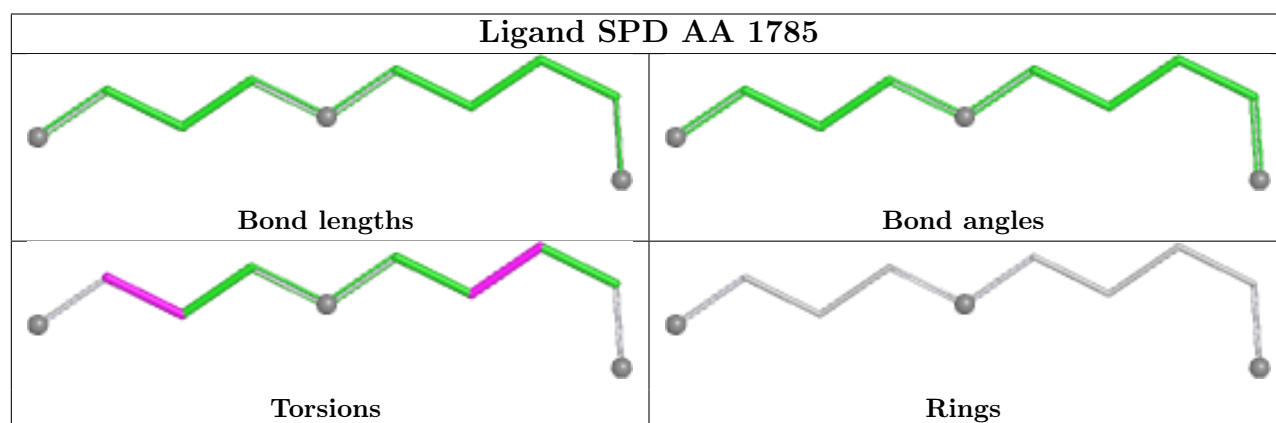
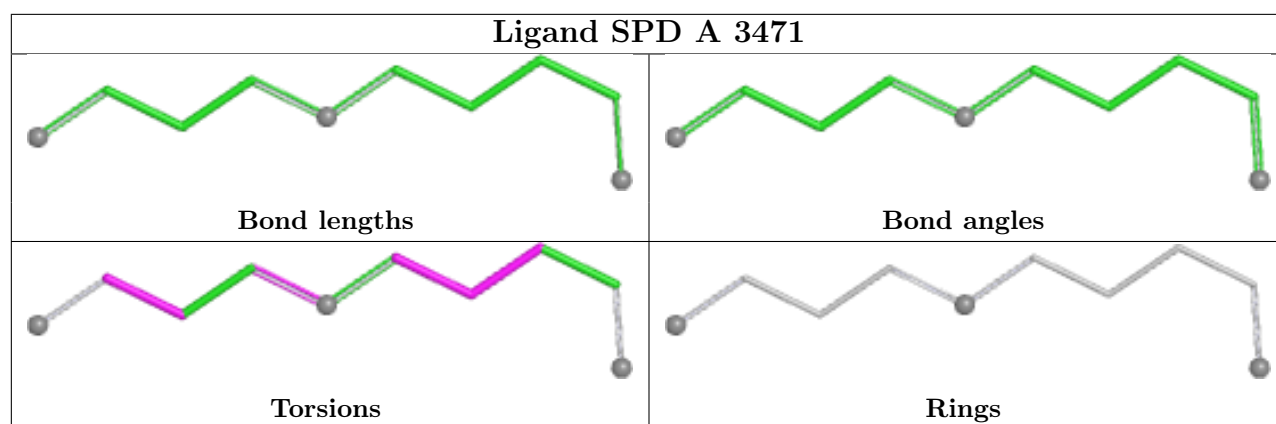
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

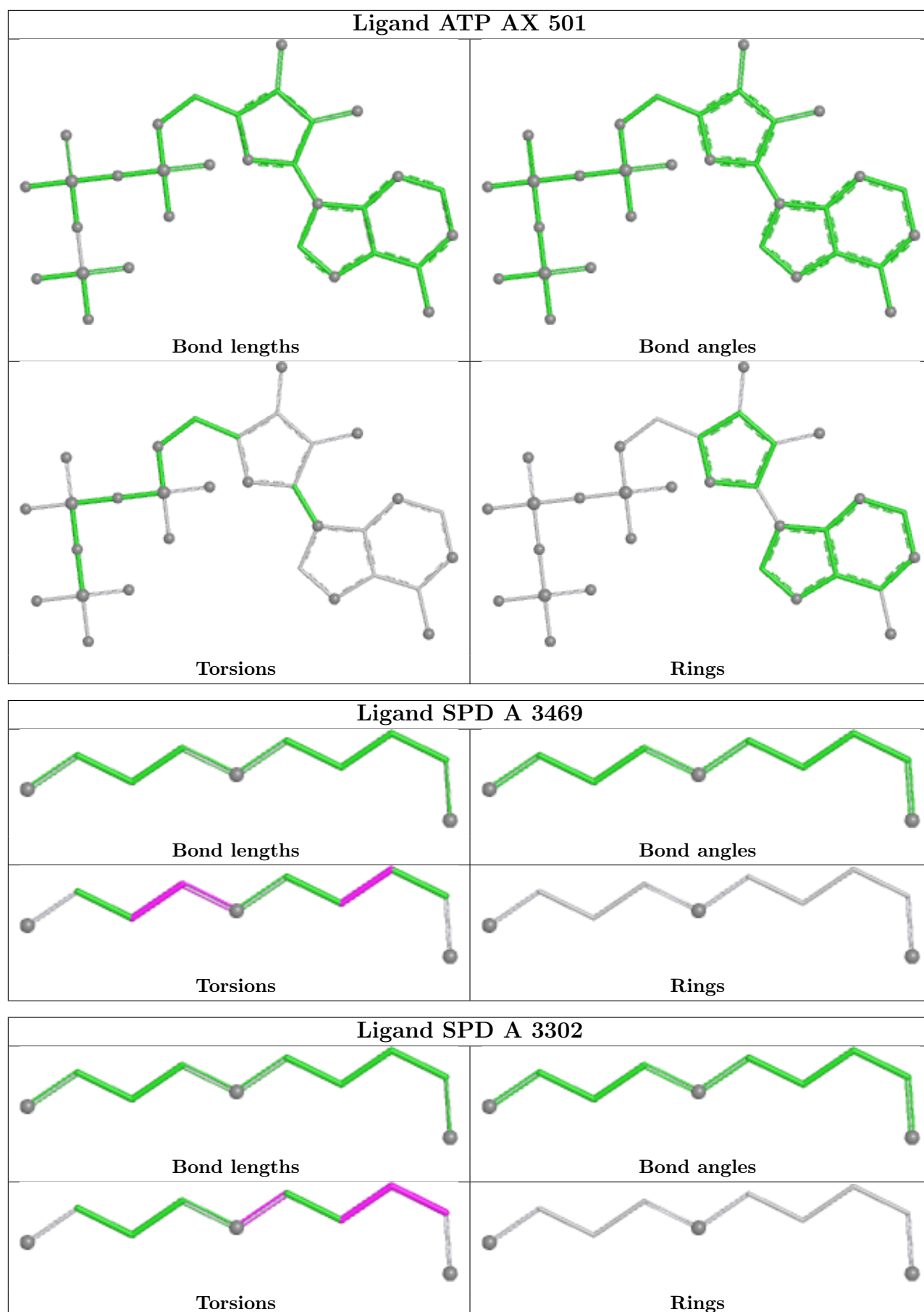
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

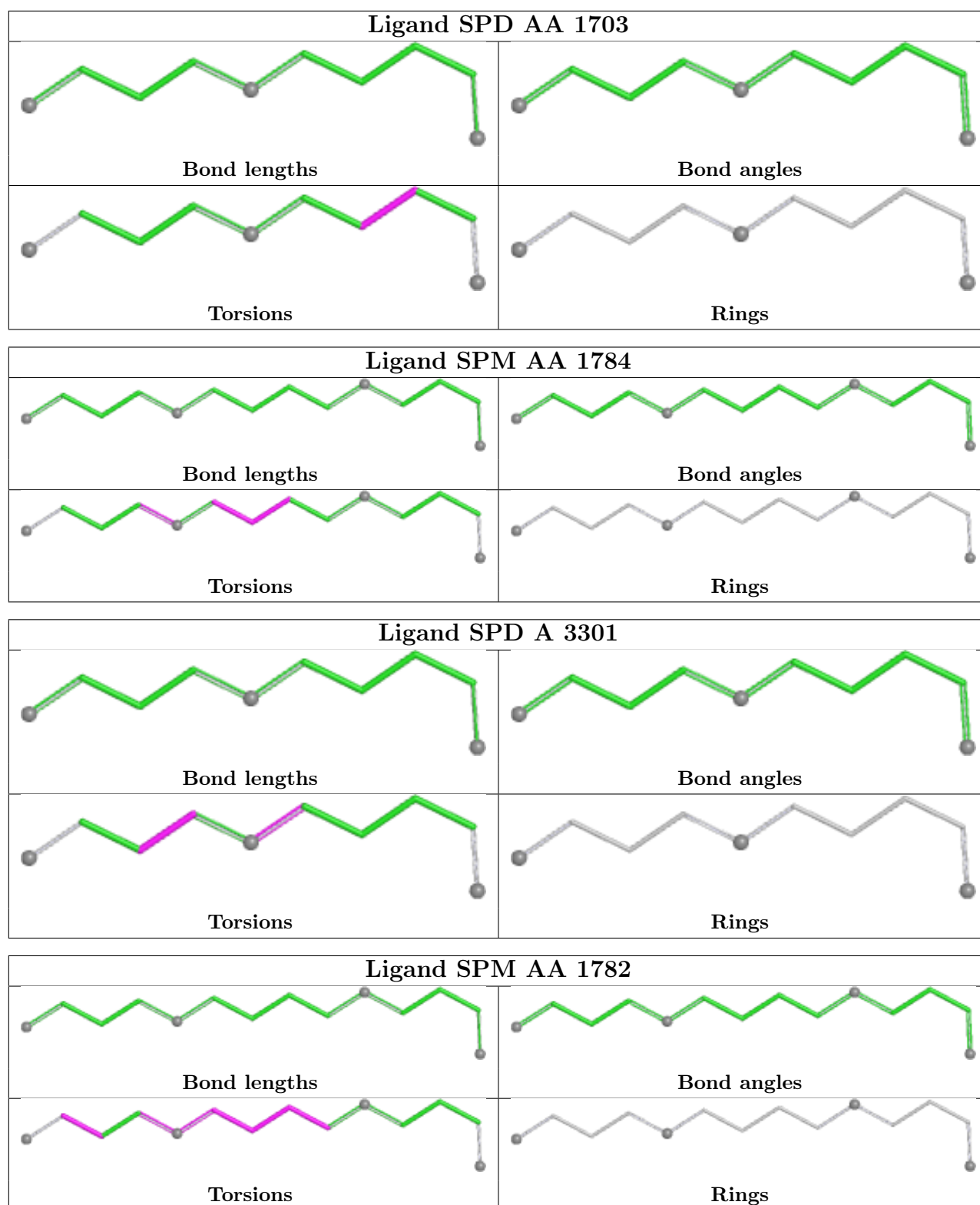


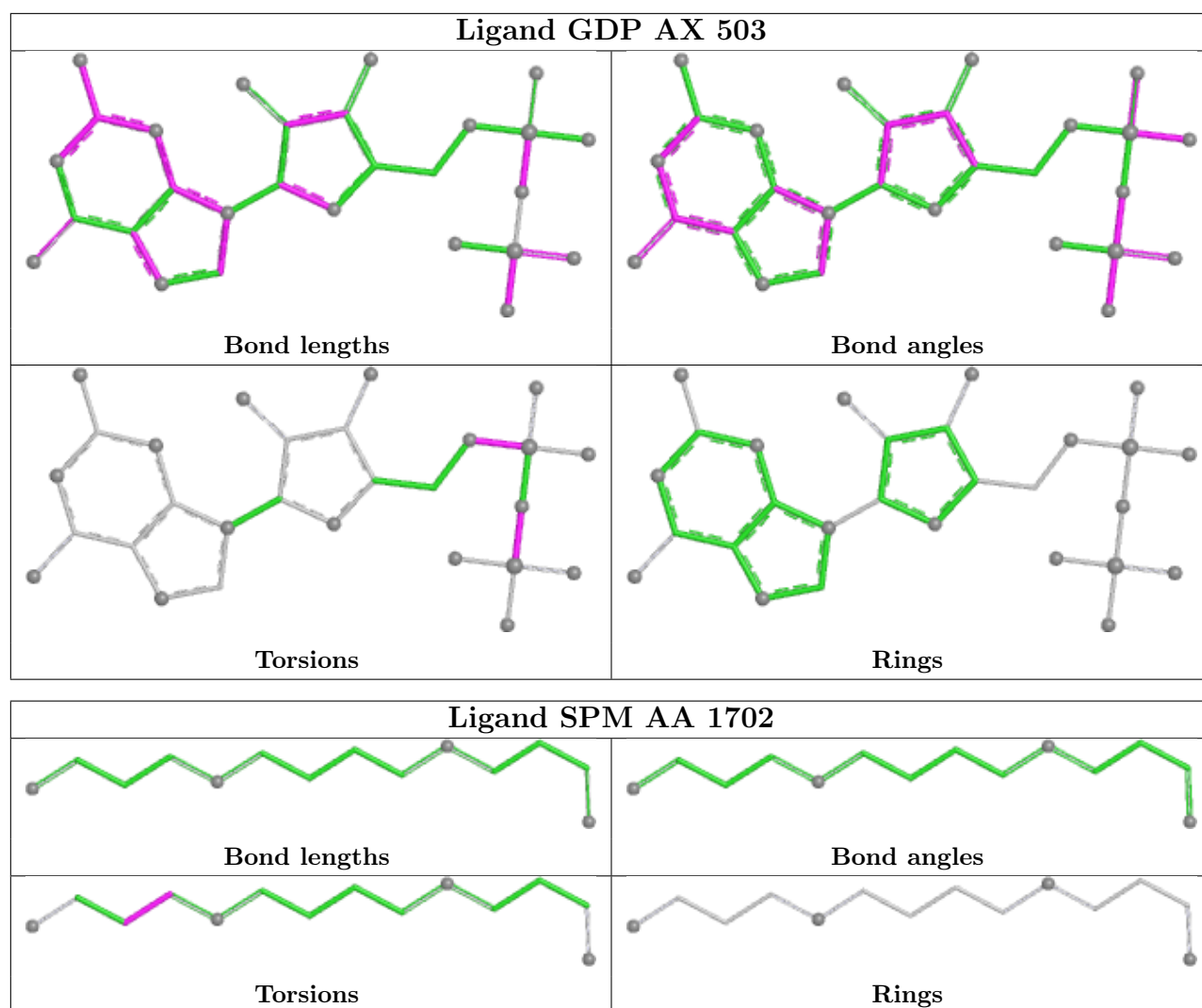












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

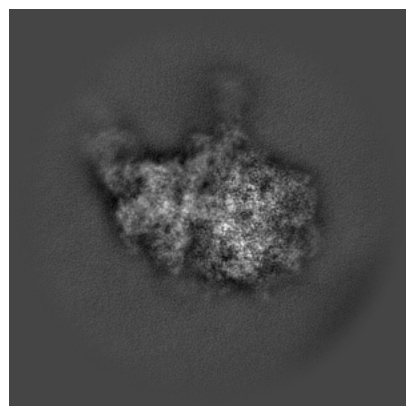
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71630. These allow visual inspection of the internal detail of the map and identification of artifacts.

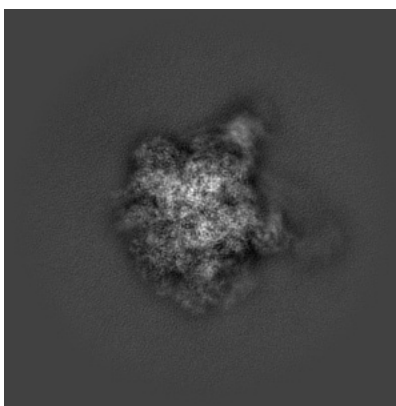
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

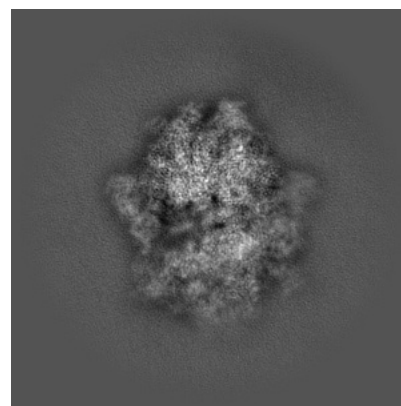
6.1.1 Primary map



X

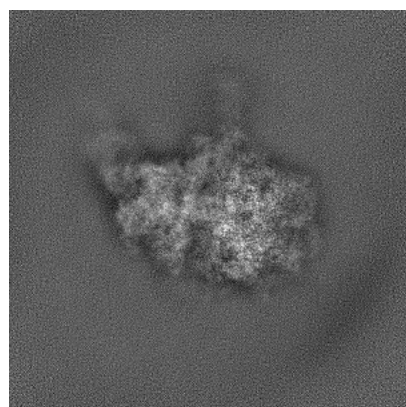


Y

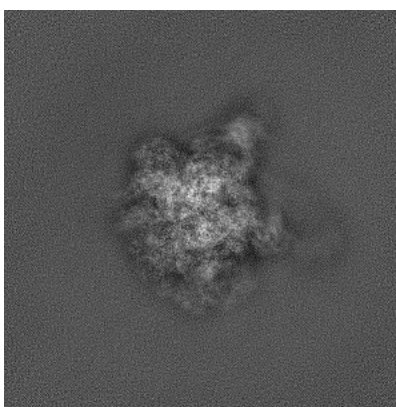


Z

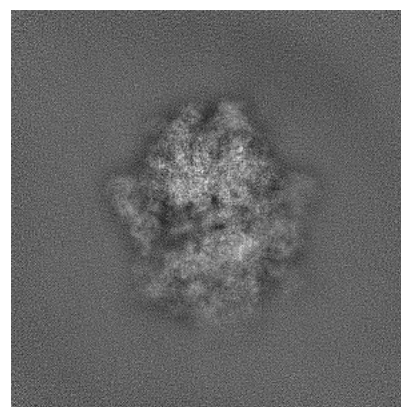
6.1.2 Raw map



X



Y

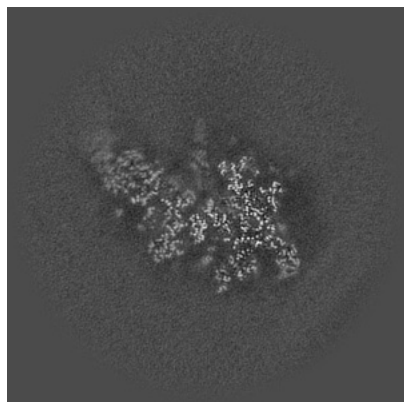


Z

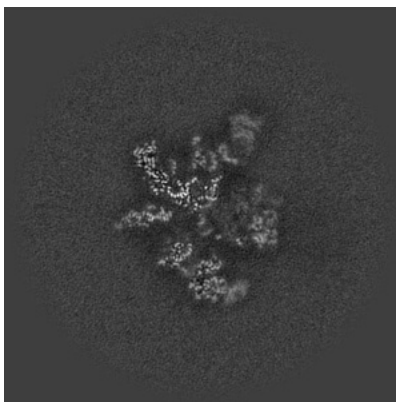
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

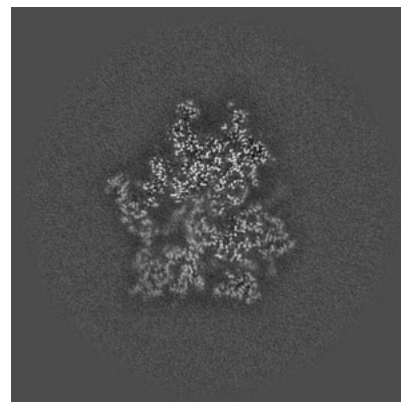
6.2.1 Primary map



X Index: 240

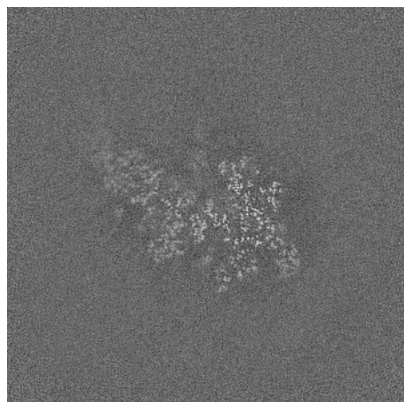


Y Index: 240

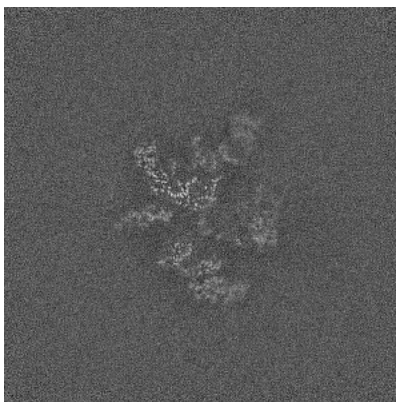


Z Index: 240

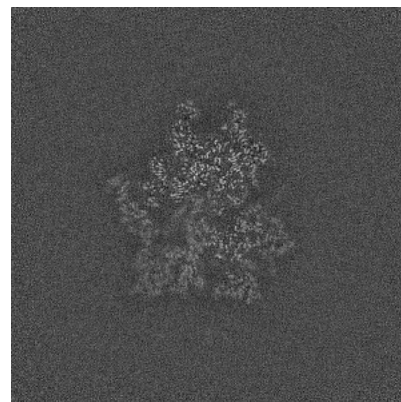
6.2.2 Raw map



X Index: 240



Y Index: 240

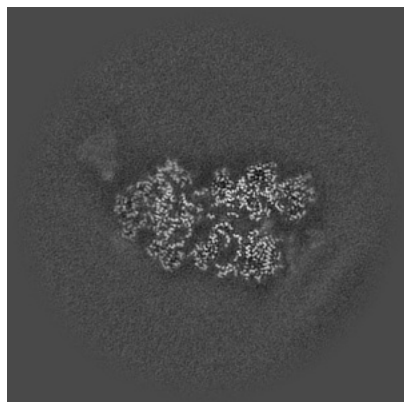


Z Index: 240

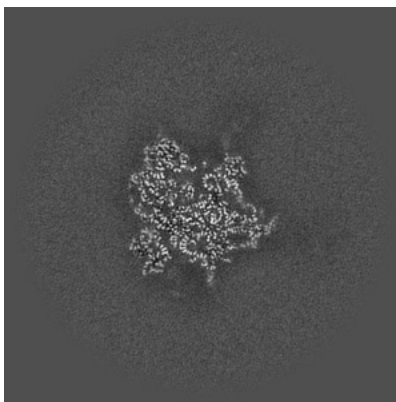
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

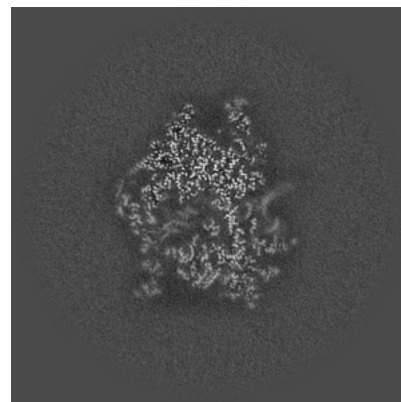
6.3.1 Primary map



X Index: 275

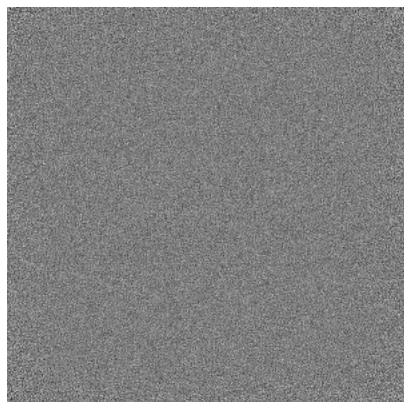


Y Index: 287

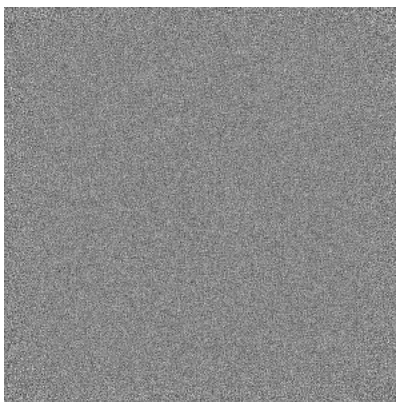


Z Index: 249

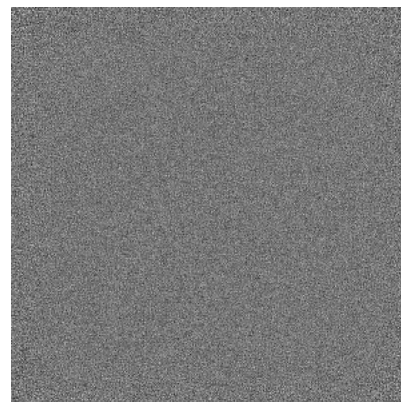
6.3.2 Raw map



X Index: 0



Y Index: 0

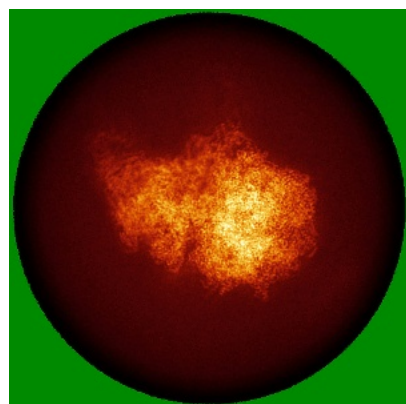


Z Index: 0

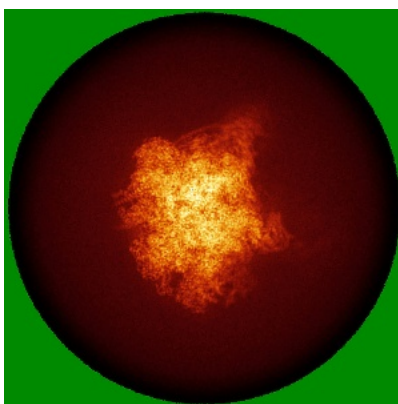
The images above show the largest variance slices of the map in three orthogonal directions.

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

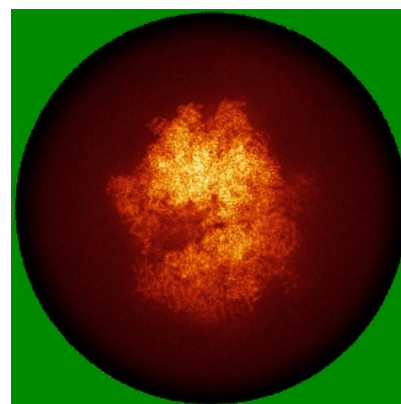
6.4.1 Primary map



X

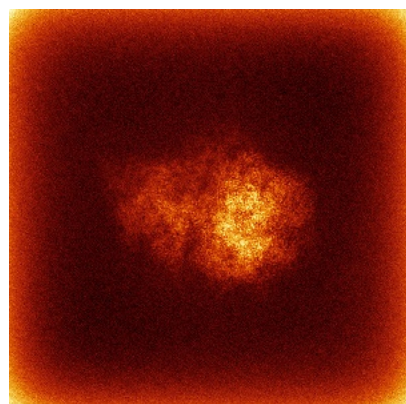


Y

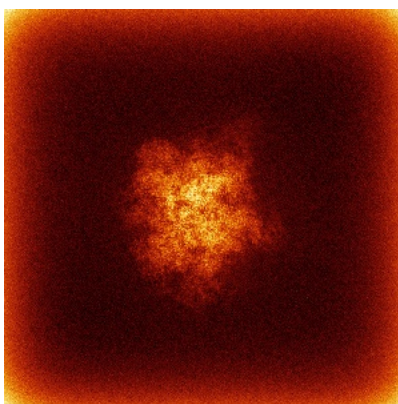


Z

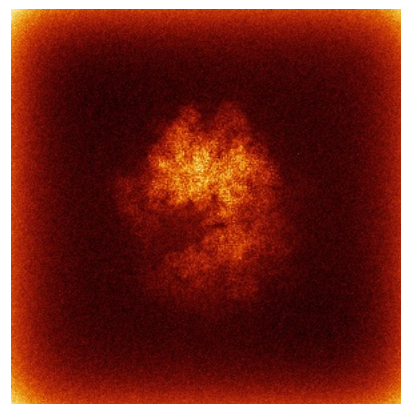
6.4.2 Raw map



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.

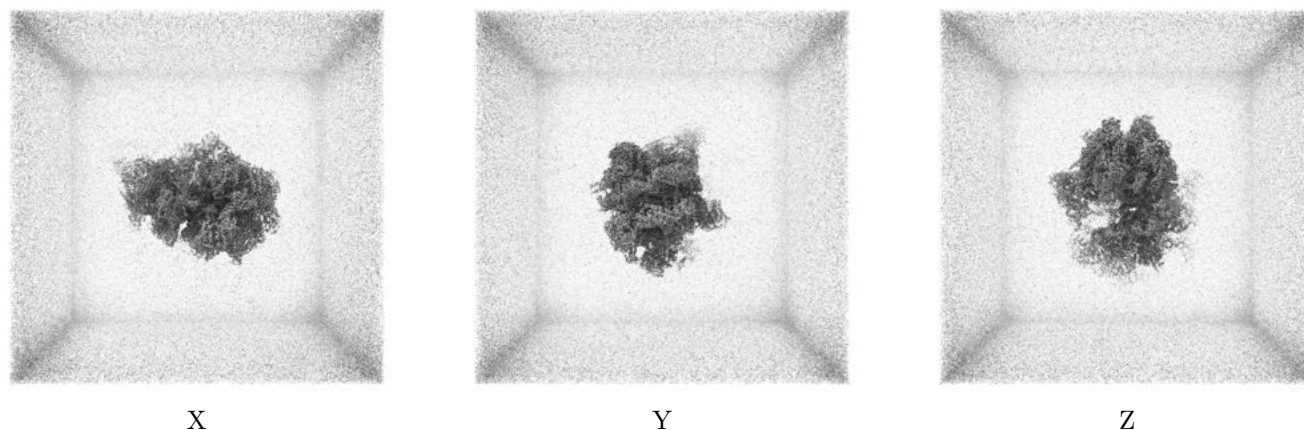
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

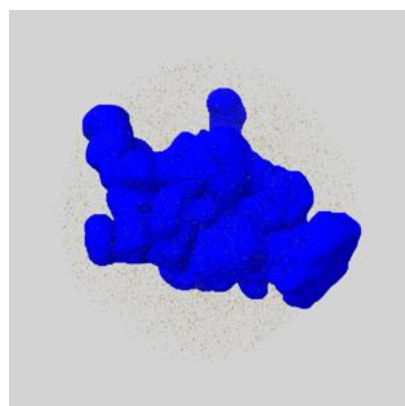
6.6 Mask visualisation [i](#)

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

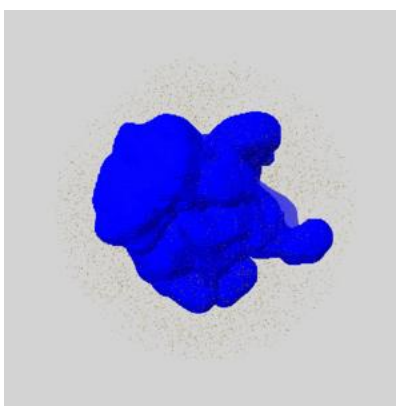
A mask typically either:

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

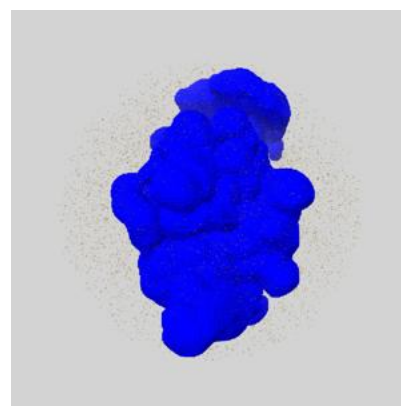
6.6.1 emd_71630_msk_1.map [i](#)



X



Y

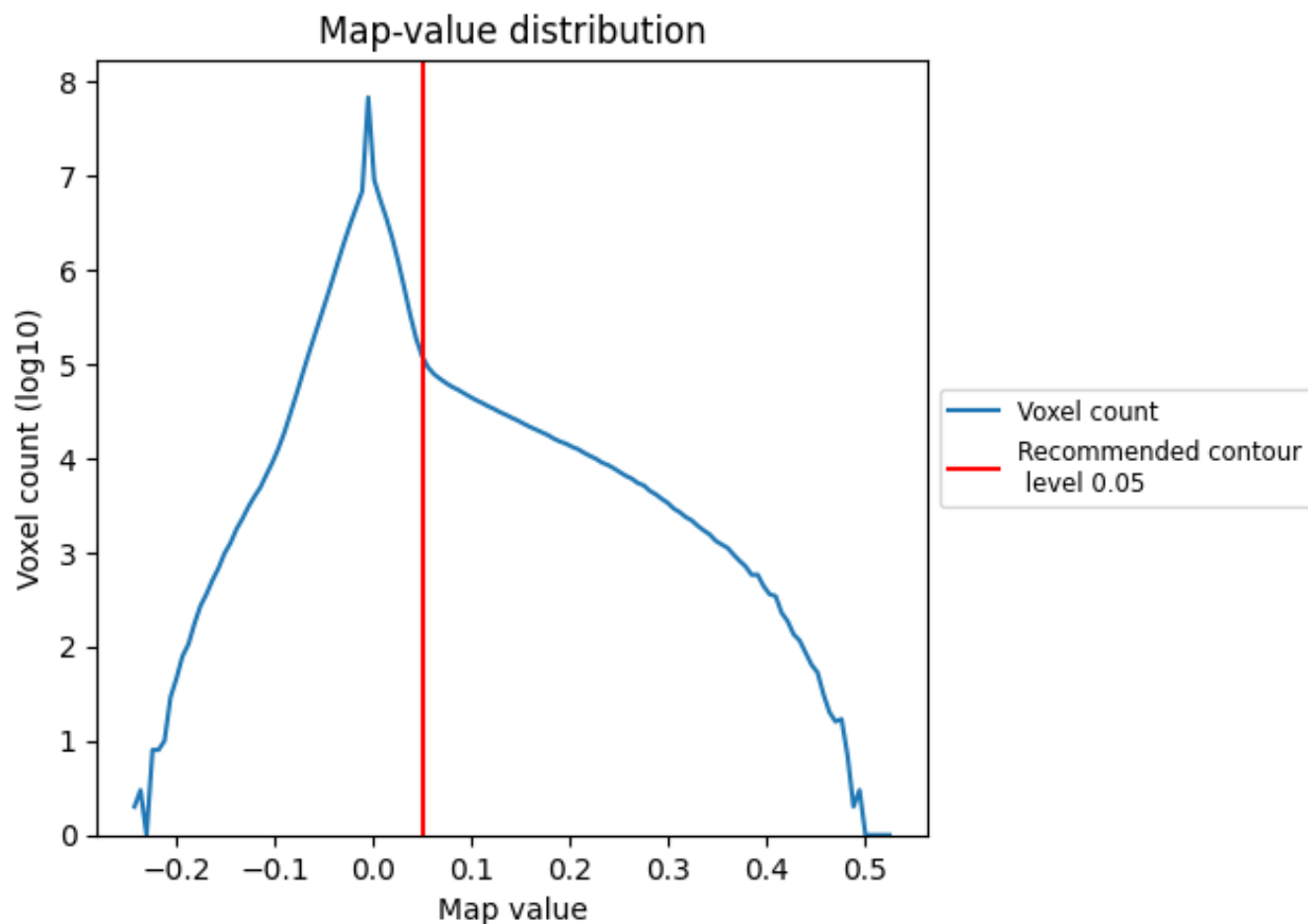


Z

7 Map analysis [i](#)

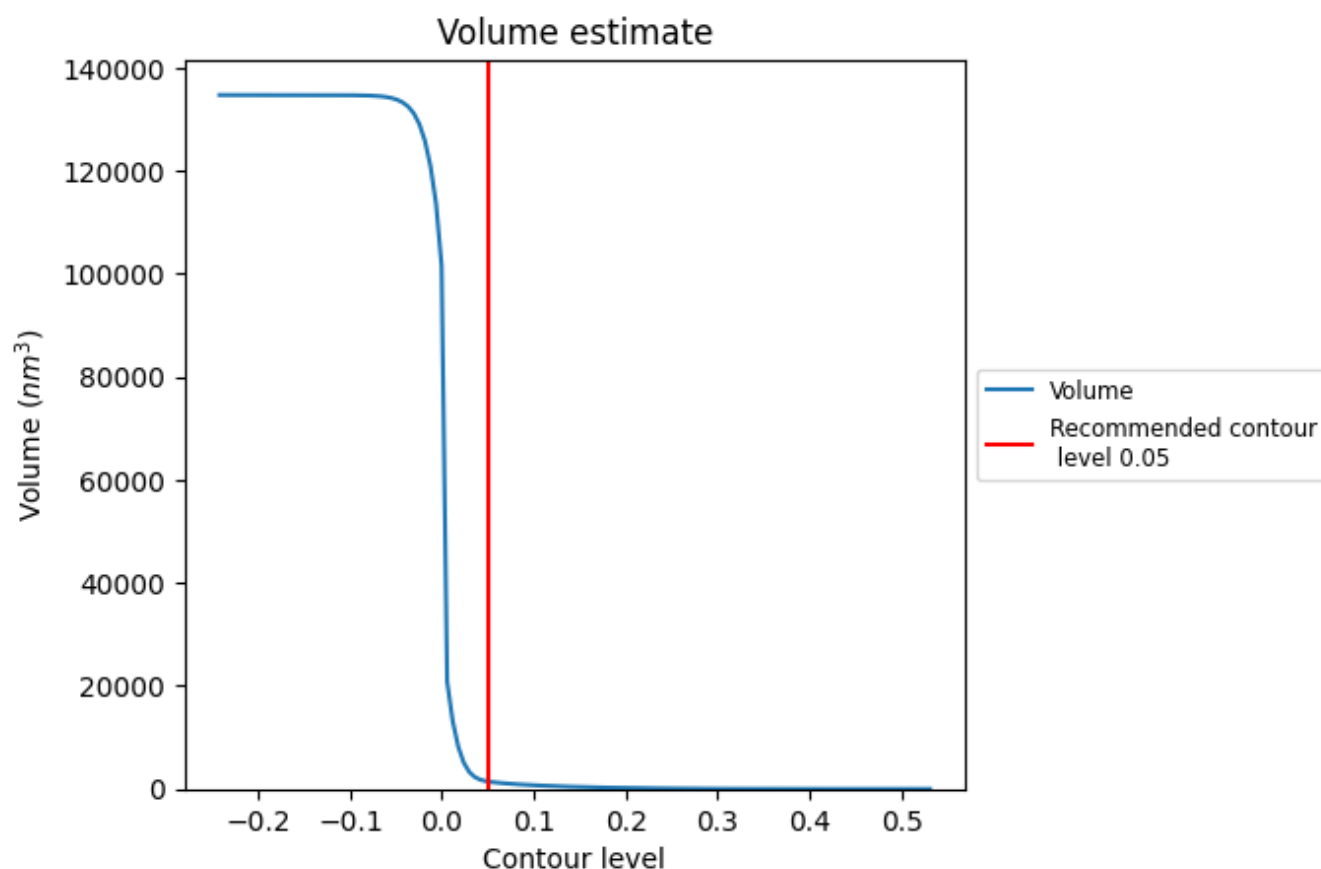
This section contains the results of statistical analysis of the map.

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.

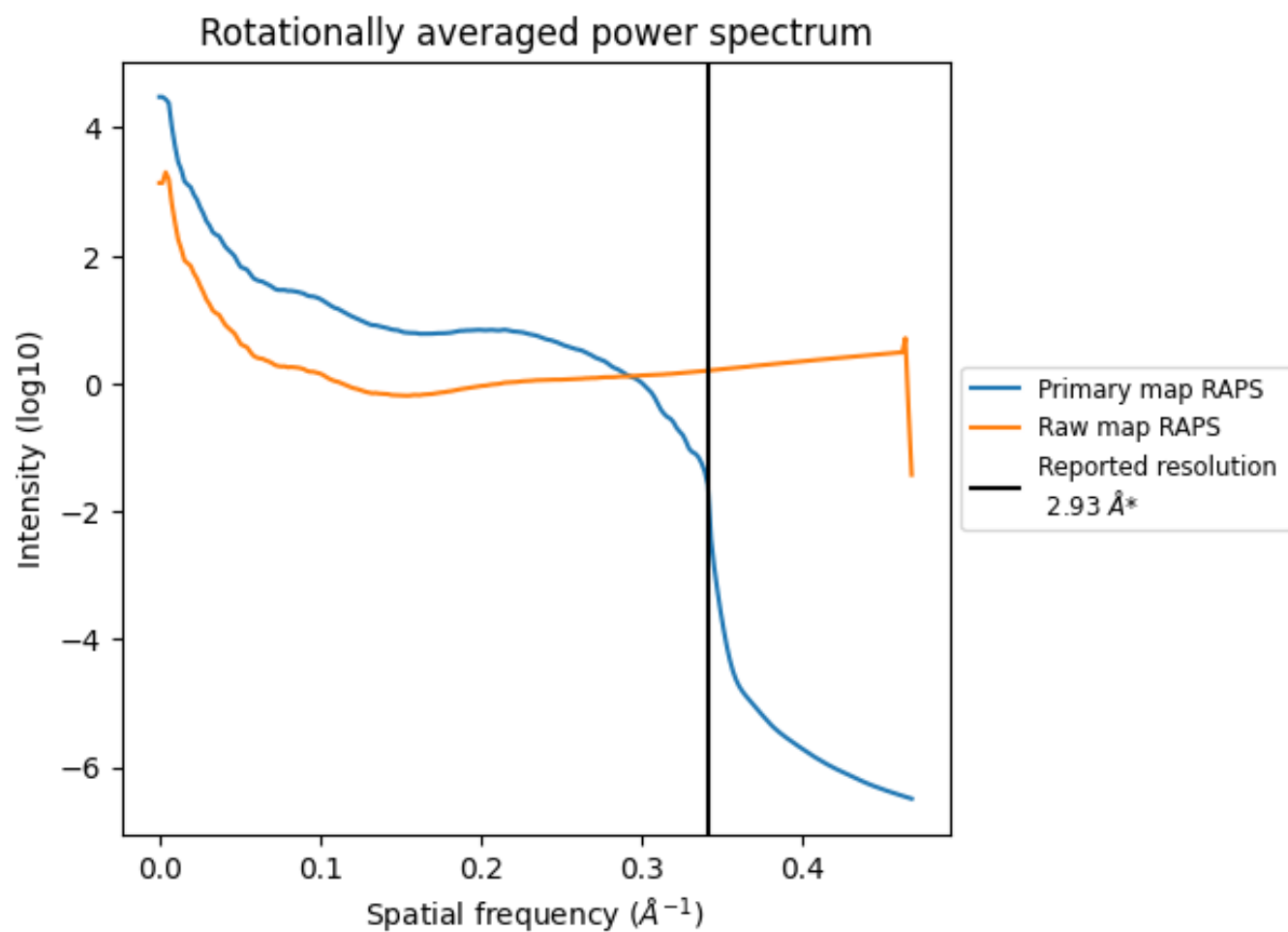
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1452 nm^3 ; this corresponds to an approximate mass of 1312 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 ⓘ

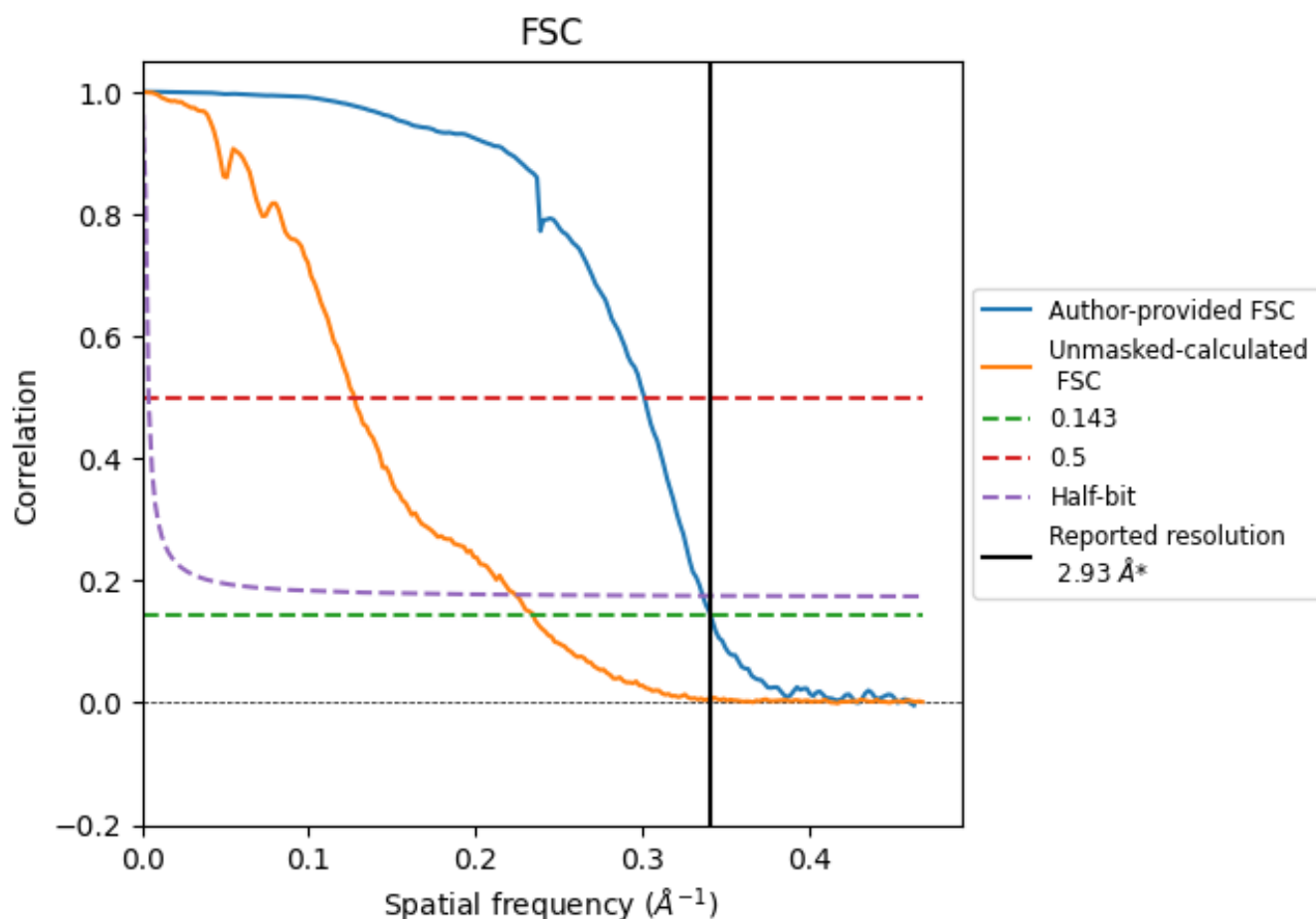


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

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 0.341 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

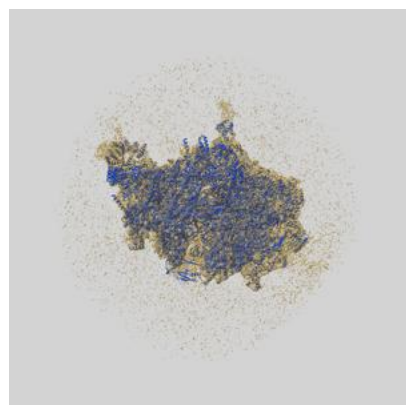
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.93	3.32	2.97
Unmasked-calculated*	4.26	7.86	4.47

*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 4.26 differs from the reported value 2.93 by more than 10 %

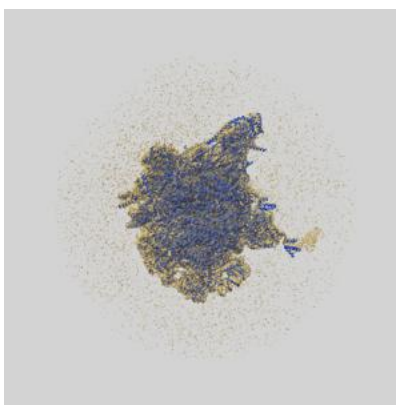
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71630 and PDB model 9PGF. Per-residue inclusion information can be found in section [3](#) on page [27](#).

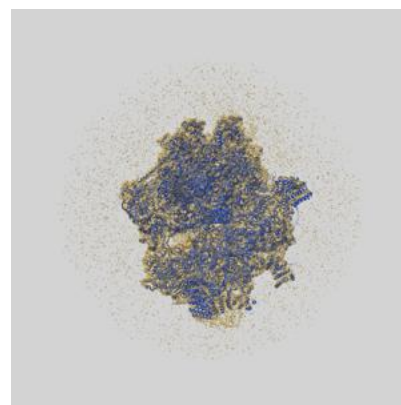
9.1 Map-model overlay [i](#)



X



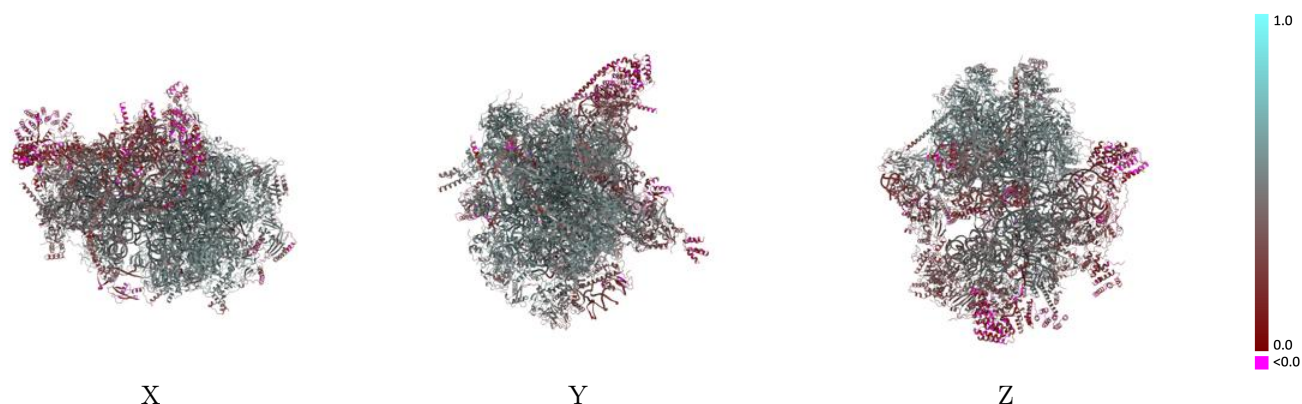
Y



Z

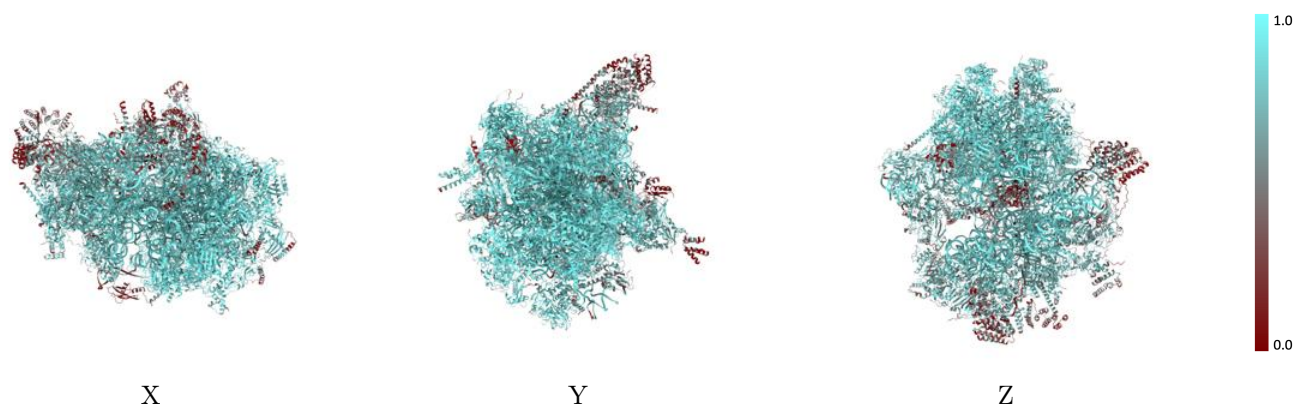
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



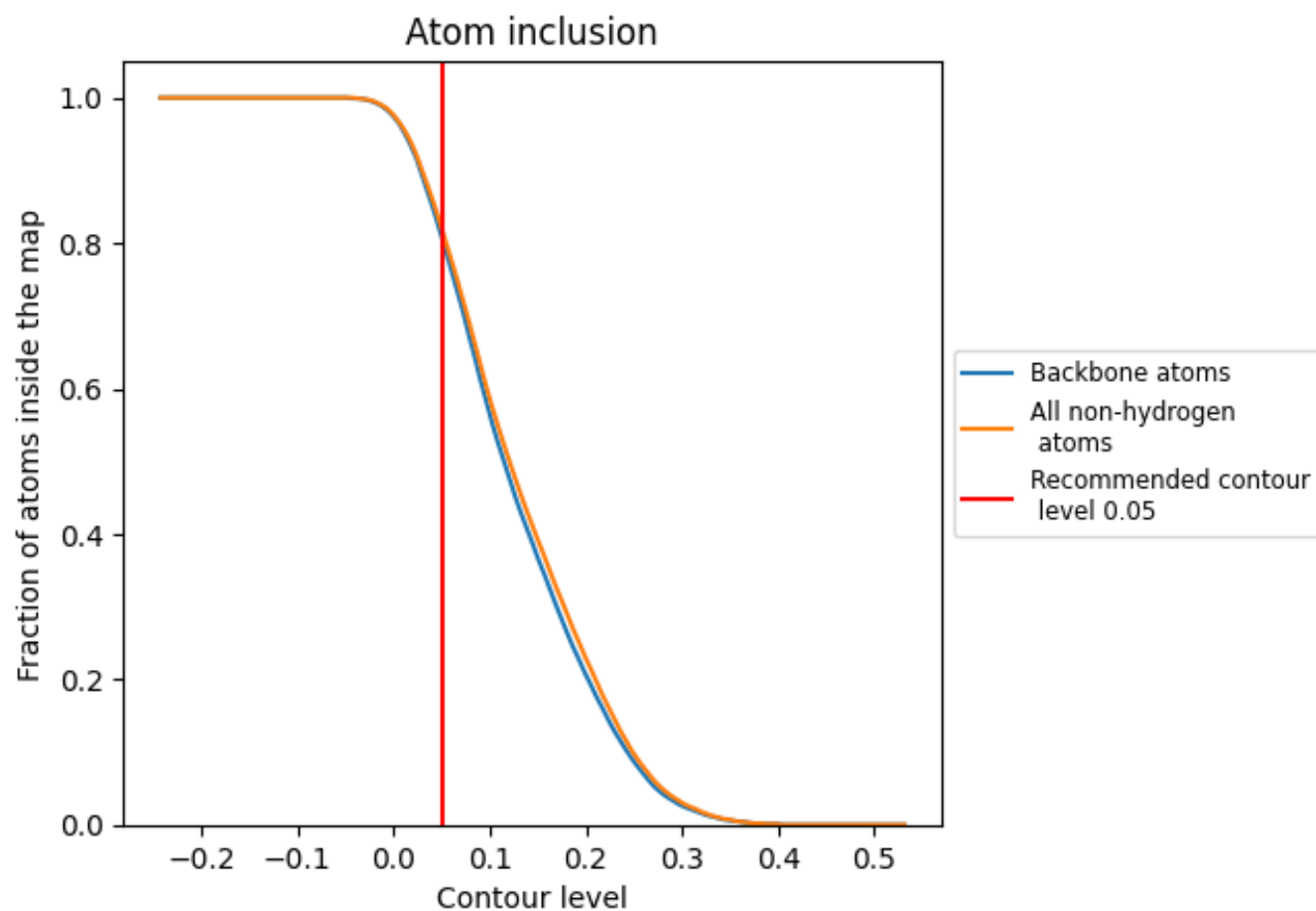
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 82% 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	 0.8210	 0.4430
0	 0.8900	 0.5360
1	 0.8360	 0.4930
2	 0.9750	 0.5730
3	 0.9500	 0.5710
4	 0.9170	 0.5480
5	 0.8830	 0.5210
6	 0.8370	 0.4560
7	 0.8410	 0.4770
8	 0.6380	 0.3120
9	 0.8710	 0.5040
A	 0.9590	 0.5200
A0	 0.5310	 0.2190
A1	 0.6840	 0.3420
A2	 0.7450	 0.4290
A3	 0.8510	 0.4970
A4	 0.4260	 0.1690
AA	 0.9590	 0.4590
AB	 0.8140	 0.4530
AC	 0.7800	 0.4480
AD	 0.7530	 0.4170
AE	 0.8000	 0.4770
AF	 0.7870	 0.4210
AG	 0.7280	 0.4000
AH	 0.7030	 0.3980
AI	 0.8330	 0.4760
AJ	 0.7790	 0.4660
AK	 0.8310	 0.4360
AL	 0.7700	 0.4330
AM	 0.6320	 0.2780
AN	 0.7620	 0.4440
AO	 0.6620	 0.3230
AP	 0.8350	 0.4800
AQ	 0.8770	 0.5010
AR	 0.5760	 0.2510



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Chain	Atom inclusion	Q-score
AS	 0.7580	 0.3950
AT	 0.7550	 0.3970
AU	 0.6620	 0.2950
AV	 0.3470	 0.1240
AW	 0.7700	 0.4470
AX	 0.7250	 0.3510
AY	 0.6280	 0.3000
AZ	 0.7330	 0.3740
Ax	 0.8710	 0.3880
Az	 0.5450	 0.2530
B	 0.8430	 0.3280
C	 0.3250	 0.2880
D	 0.9230	 0.5540
E	 0.9020	 0.5430
F	 0.9320	 0.5500
G	 0.1160	 0.1570
H	 0.4730	 0.2940
I	 0.7070	 0.3760
J	 0.6290	 0.2760
K	 0.9280	 0.5480
L	 0.9090	 0.5380
M	 0.9110	 0.5380
N	 0.8920	 0.5320
O	 0.9230	 0.5440
OX	 0.5500	 0.3040
P	 0.8700	 0.4940
Q	 0.8280	 0.5020
R	 0.9310	 0.5520
S	 0.9040	 0.5440
T	 0.9310	 0.5610
U	 0.8190	 0.4840
V	 0.8630	 0.4980
W	 0.9060	 0.5520
X	 0.8820	 0.5220
Y	 0.9030	 0.5350
Z	 0.9130	 0.5440
a	 0.7750	 0.4760
b	 0.9200	 0.5430
c	 0.8730	 0.5060
d	 0.7340	 0.4390
e	 0.5960	 0.2620
f	 0.6860	 0.3690

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Chain	Atom inclusion	Q-score
g	 0.8960	 0.5280
h	 0.8560	 0.4700
i	 0.9420	 0.5660
j	 0.8380	 0.4890
k	 0.7420	 0.3980
l	 0.6800	 0.3310
m	 0.5910	 0.2760
n	 0.5720	 0.3420
o	 0.9410	 0.5600
p	 0.7590	 0.4260
q	 0.6670	 0.3570
r	 0.8850	 0.5240
s	 0.8930	 0.5280
t	 0.2720	 0.1800
u	 0.2110	 0.1320