



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 04:43 PM JST

PDB ID : 5GUP / pdb_00005gup
EMDB ID : EMD-9539
Title : Cryo-EM structure of mammalian respiratory supercomplex I1III2IV1
Authors : Gu, J.; Wu, M.; Guo, R.; Yang, M.
Deposited on : 2016-08-30
Resolution : 4.00 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:

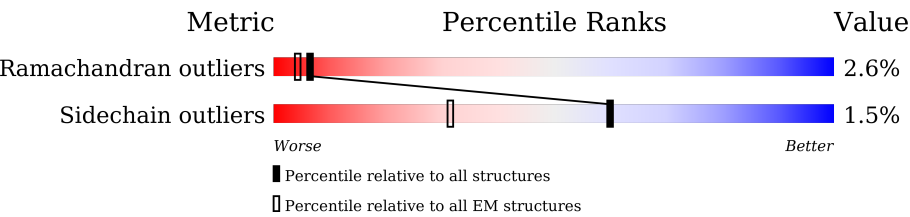
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	73	<div><div>100%</div><div><div></div><div></div><div></div><div></div></div><div>93%7%</div></div>
2	B	464	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>85%12%</div></div>
3	C	463	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>90%7%</div></div>
4	D	264	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>73%5%21%</div></div>
5	E	249	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>76%21%</div></div>
6	F	123	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>33%64%</div></div>
7	G	727	<div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>88%5%7%</div></div>
8	H	212	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>83%17%</div></div>
9	I	216	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>68%28%</div></div>

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Mol	Chain	Length	Quality of chain
10	J	175	
11	K	145	
11	R	145	
12	L	377	
13	M	113	
14	N	116	
15	O	156	
15	X	156	
16	P	99	
17	Q	128	
18	S	70	
19	T	84	
20	U	357	
21	V	141	
22	W	144	
23	Y	105	
24	Z	98	
25	a	189	
26	b	128	
27	c	186	
28	d	176	
29	e	154	
30	f	76	
31	g	122	
32	h	106	

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Mol	Chain	Length	Quality of chain
33	i	347	99% .
34	j	115	10% 97% ..
35	k	98	96% ..
36	l	606	97% .
37	m	175	9% 97% ..
38	n	58	81% 19%
39	o	129	94% 5% .
40	p	179	89% 6% . .
41	q	459	98% .
42	r	318	99% .
43	s	172	94% 5% .
44	t	137	7% 78% 6% 16%
45	5	480	45% 92% . 7%
45	u	480	11% 91% . 7%
46	6	453	56% 92% . 8%
46	v	453	22% 91% . 8%
47	7	379	39% 98% .
47	w	379	29% 98% .
48	8	326	26% 73% . 26%
48	x	326	25% 72% . 26%
49	9	111	34% 95% 5%
49	y	111	50% 95% 5%
50	Aa	82	40% 98% .
50	z	82	33% 95% . .
51	0	91	24% 70% 30%

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Mol	Chain	Length	Quality of chain
51	Ab	91	
52	1	64	
52	Ac	64	
53	2	274	
53	4	274	
54	3	56	
54	Ad	56	
55	Ae	78	
55	Af	78	
56	Ag	46	
57	Ah	59	
58	Ai	56	
59	Aj	47	
60	Ak	514	
61	Al	227	
62	Am	261	
63	An	147	
64	Ao	109	
65	Ap	98	
66	Aq	84	
67	Ar	85	

2 Entry composition

There are 81 unique types of molecules in this entry. The entry contains 109982 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	410	Total	C	N	O	S	0	0
			3128	1975	558	575	20		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	430	Total	C	N	O	S	0	0
			3391	2167	583	617	24		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1679	1088	290	299	2		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	197	Total	C	N	O	S	0	0
			1463	935	246	273	9		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	44	Total	C	N	O	S	0	0
			242	145	49	47	1		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	673	Total	C	N	O	S	0	0
			5005	3133	875	959	38		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	176	Total	C	N	O	S	0	0
			1408	884	242	269	13		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	156	Total	C	N	O	S	0	0
			1241	792	227	208	14		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	109	Total	C	N	O	S	0	0
			877	557	154	163	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O		0	0
			520	314	104	102			
11	R	18	Total	C	N	O		0	0
			90	54	18	18			

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	337	Total	C	N	O	S	0	0
			2665	1726	462	468	9		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	94	Total	C	N	O	S	0	0
			685	433	129	121	2		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	112	Total	C	N	O	S	0	0
			895	577	152	163	3		

- Molecule 15 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	85	Total	C	N	O	S	0	0
			647	417	97	128	5		
15	X	85	Total	C	N	O	S	0	0
			663	428	98	132	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			673	423	125	123	2		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	112	Total	C	N	O	S	0	0
			942	600	174	163	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	82	Total	C	N	O	S	0	0
			622	404	104	113	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	281	Total	C	N	O	S	0	0
			1941	1228	342	366	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	140	Total	C	N	O	S	0	0
			1009	644	172	187	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	138	Total	C	N	O	S	0	0
			1122	724	193	197	8		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	59	Total	C	N	O	S	0	0
			400	262	70	67	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	78	Total	C	N	O	0	0
			550	363	92	95		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	138	Total	C	N	O	S	0	0
			1124	736	190	195	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	b	113	Total	C	N	O	0	0
			741	478	137	126		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	148	Total	C	N	O	S	0	0
			1073	696	185	185	7		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	169	Total	C	N	O	S	0	0
			1233	763	233	229	8		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	97	Total	C	N	O	S	0	0
			757	490	127	136	4		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	f	36	Total	C	N	O	0	0
			300	201	51	48		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	121	Total	C	N	O	S	0	0
			996	648	173	169	6		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	104	Total	C	N	O	S	0	0
			798	501	150	141	6		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	347	Total	C	N	O	S	0	0
			2706	1779	419	462	46		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	114	Total	C	N	O	S	0	0
			893	601	130	155	7		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	97	Total	C	N	O	S	0	0
			718	473	109	123	13		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	606	Total	C	N	O	S	0	0
			4790	3177	742	821	50		

- Molecule 37 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	174	Total	C	N	O	S	0	0
			1280	855	187	226	12		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	47	Total	C	N	O	S	0	0
			359	233	66	59	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	128	Total	C	N	O	S	0	0
			1021	666	179	176			

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	171	Total	C	N	O	S	0	0
			1415	904	263	240	8		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	q	459	Total	C	N	O	S	0	0
			3627	2408	572	609	38		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	169	Total	C	N	O	S	0	0
			1350	858	247	235	10		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	115	Total	C	N	O	S	0	0
			749	463	151	130	5		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	446	Total	C	N	O	S	0	0
			3452	2157	603	673	19		
45	5	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	418	Total	C	N	O	S	0	0
			3127	1956	556	606	9		
46	6	418	Total	C	N	O	S	0	0
			3127	1956	556	606	9		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		
47	7	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	241	Total	C	N	O	S	0	0
			1918	1223	330	350	15		
48	8	241	Total	C	N	O	S	0	0
			1918	1223	330	350	15		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	9	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	79	Total	C	N	O	S	0	0
			666	434	122	108	2		
50	Aa	80	Total	C	N	O	S	0	0
			679	442	124	111	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
51	Ab	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	62	Total	C	N	O	S	0	0
			507	331	90	86			
52	Ac	62	Total	C	N	O	S	0	0
			507	331	90	86			

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		
53	4	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	51	Total	C	N	O	S	0	0
			414	277	74	63			
54	Ad	49	Total	C	N	O	S	0	0
			395	262	71	61	1		

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit Rieske transit peptide, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ae	57	Total	C	N	O	S	0	0
			394	243	74	75	2		
55	Af	57	Total	C	N	O	S	0	0
			389	240	71	76	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	Ag	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ah	56	Total	C	N	O	S	0	0
			431	277	73	78	3		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ai	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Aj	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Ak	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Al	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Am	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	An	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ao	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ap	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

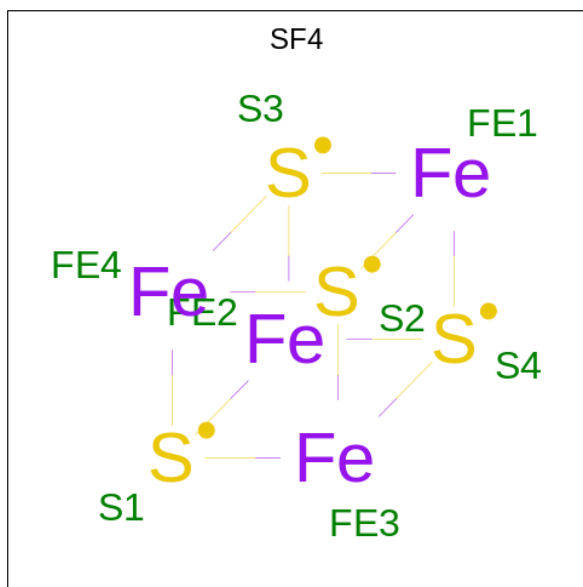
- Molecule 66 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Aq	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 67 is a protein called Cytochrome c oxidase subunit 6B1.

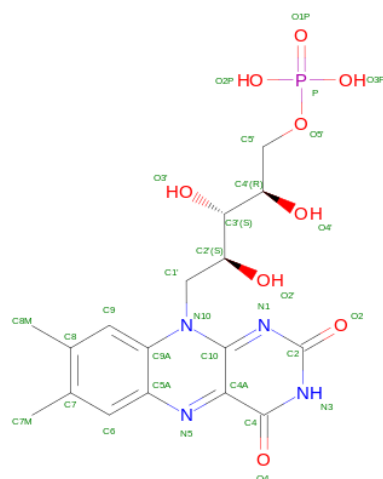
Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ar	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 68 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



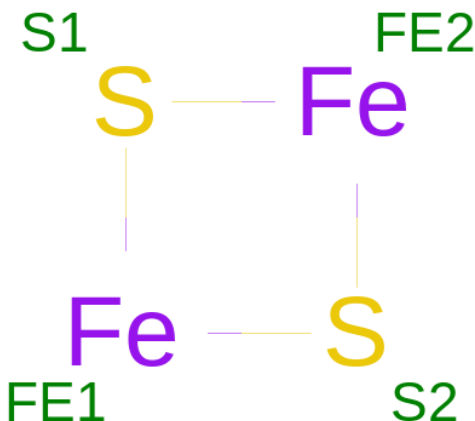
Mol	Chain	Residues	Atoms			AltConf
68	B	1	Total	Fe	S	0
			8	4	4	
68	G	1	Total	Fe	S	0
			8	4	4	
68	G	1	Total	Fe	S	0
			8	4	4	
68	H	1	Total	Fe	S	0
			8	4	4	
68	H	1	Total	Fe	S	0
			8	4	4	
68	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 69 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
69	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 70 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



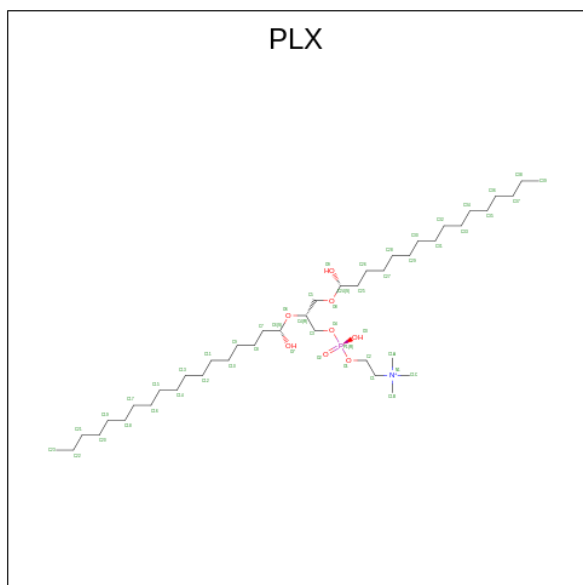
Mol	Chain	Residues	Atoms			AltConf
70	E	1	Total 4	Fe 2	S 2	0
70	G	1	Total 4	Fe 2	S 2	0
70	2	1	Total 4	Fe 2	S 2	0

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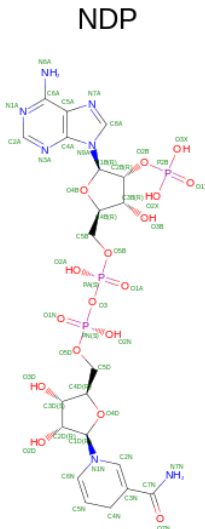
Mol	Chain	Residues	Atoms			AltConf
70	4	1	Total	Fe	S	0
			4	2	2	

- Molecule 71 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



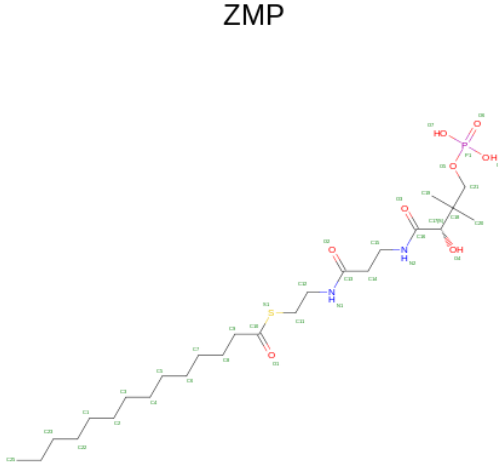
Mol	Chain	Residues	Atoms					AltConf
71	H	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	2	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	4	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 72 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



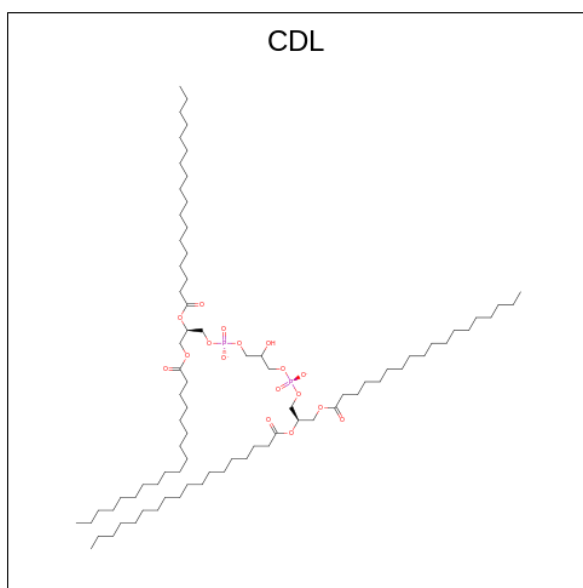
Mol	Chain	Residues	Atoms					AltConf
72	L	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 73 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl}]\text{-beta-alanyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



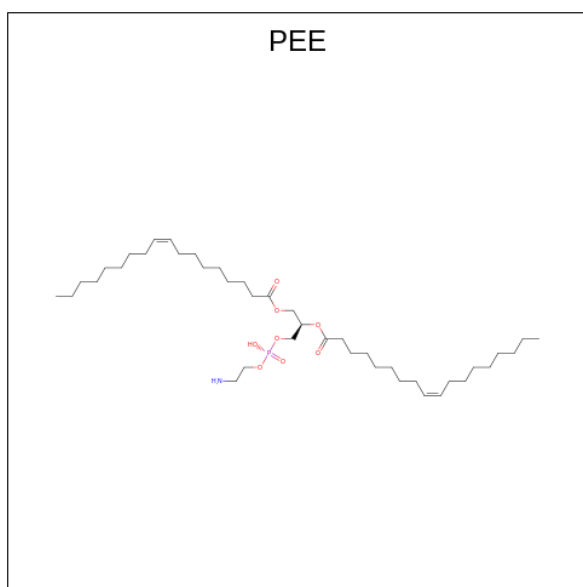
Mol	Chain	Residues	Atoms						AltConf
73	Q	1	Total 34	C 23	N 2	O 7	P 1	S 1	0
73	X	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 74 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



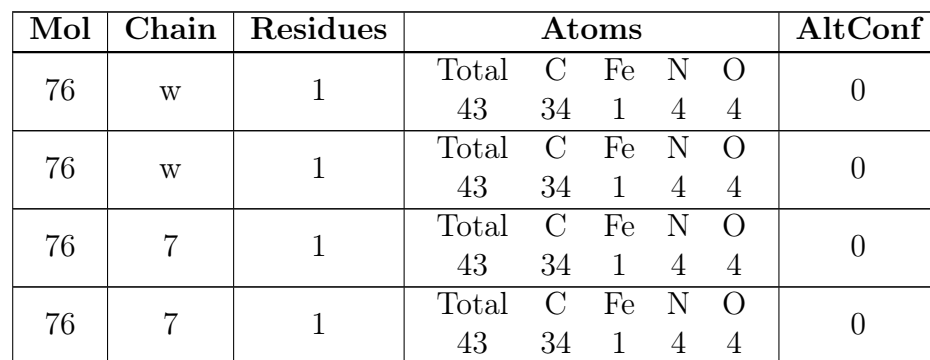
Mol	Chain	Residues	Atoms				AltConf
74	V	1	Total	C	O	P	0
			63	44	17	2	
74	i	1	Total	C	O	P	0
			64	45	17	2	
74	l	1	Total	C	O	P	0
			64	45	17	2	
74	s	1	Total	C	O	P	0
			64	45	17	2	
74	u	1	Total	C	O	P	0
			64	45	17	2	
74	x	1	Total	C	O	P	0
			64	45	17	2	
74	z	1	Total	C	O	P	0
			64	45	17	2	
74	5	1	Total	C	O	P	0
			64	45	17	2	
74	8	1	Total	C	O	P	0
			64	45	17	2	
74	Aa	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 75 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).

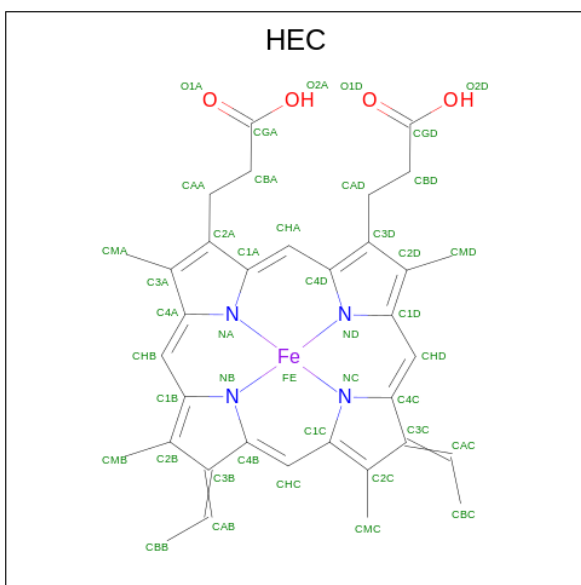


Mol	Chain	Residues	Atoms					AltConf
75	W	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	i	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	l	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	q	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	u	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	w	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	2	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	5	1	Total	C	N	O	P	0
			49	39	1	8	1	
75	7	1	Total	C	N	O	P	0
			41	31	1	8	1	
75	7	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 76 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

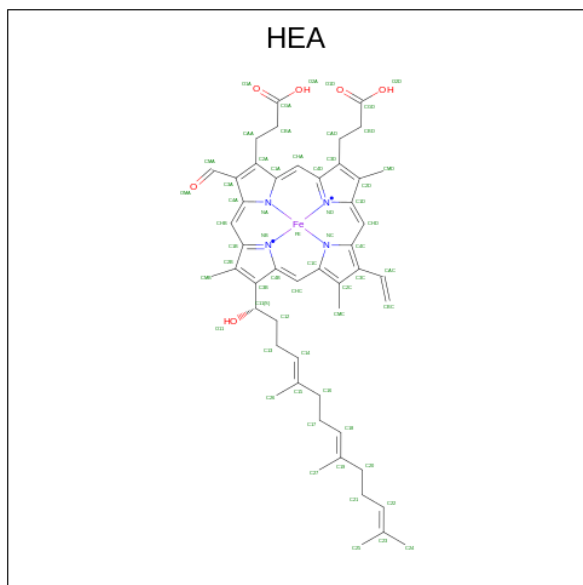


- Molecule 77 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					AltConf
77	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
77	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 78 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
78	Ak	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
78	Ak	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 79 is COPPER (II) ION (CCD ID: CU) (formula: Cu).


Mol	Chain	Residues	Atoms		AltConf
79	Ak	1	Total	Cu	0
			1	1	
79	Al	2	Total	Cu	0
			2	2	

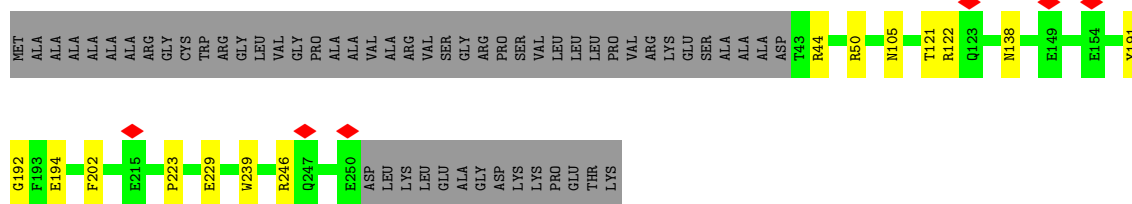
- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	Ak	1	Total	Mg	0
			1	1	


- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

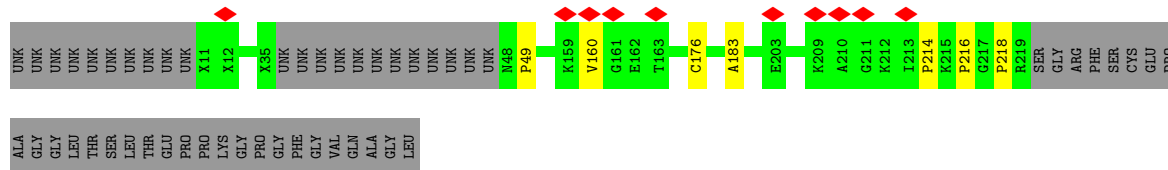
Mol	Chain	Residues	Atoms		AltConf
81	Ap	1	Total	Zn	0
			1	1	

Chain D:  73% 5% 21%



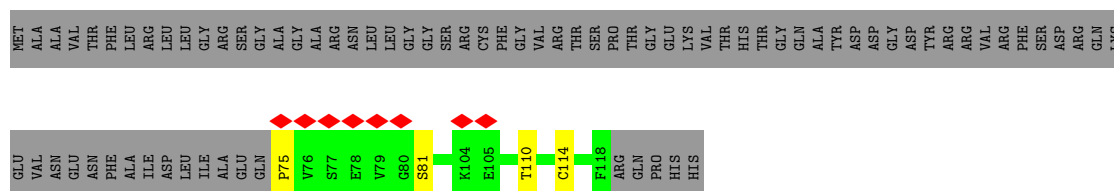
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  76% 21%




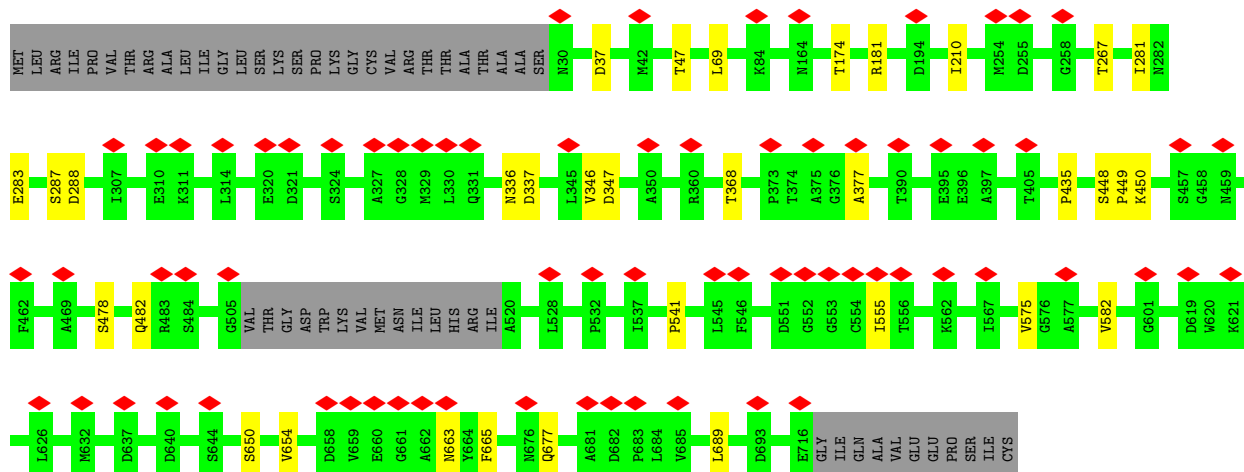
- Molecule 6: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain F:  7% 33% 64%



- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  10% 88% 5% 7%



- Molecule 8: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

MET	ARG	CYS	LEU	SER	THR	PRO	MET	LEU	LEU	ARG	ALA	ALA	GLN	GLN	GLN	ALA	ALA	ALA	HTS	GLY	HTS	PRO	SER	ALA	ALA	ARG	THR	LEU	HTS	SER	SER	ALA	VAL	ALA	ALA	ALA	T37	M43	R44	E45	M48	F175	R212
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- Chain I: 68% 28%

MET	ALA	ALA	ALA	LEU	ALA	ALA	SER	GLY	LEU	LEU	ARG	PRO	ILE	LEU	ALA	ALA	LEU	ARG	SER	SER	MET	GLY	ALA	ALA	ALA	VAL	GLN	VAL	ARG	PHE	VAL	HIS	PRO	SER	SER	ALA	ALA	THR	ASP	SER	PRO	SER	SER	SER	SER	GLN	PRO	ALA	VAL	VAL	GLN	ALA	GLY	ALA	VAL	VAL	VAL	SER	LYS	PRO	THR	THR	LEU	PRO
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Amino Acid	Number of Mutations
S61	1
V66	2
D71	2
L89	1
A90	2
C91	2
D105	1
S116	2
P147	1
C156	2
G159	2
G160	2
R171	1
R209	2
Y214	2
R215	2
R216	2

- Chain J:  61% 38%

MET	ALA	ALA	VAL	SER	MET	SER	VAL	VAL	ALA	ALA	LYS	GLN	ALA	ALA	LEU	TRP	GLY	ARG	ARG	ALA	ALA	ALA	ALA	VAL	VAL	GLY	ALA	VAL	SER	VAL	SER	LYS	LYS	VAL	PRO	THR	THR	ARG	LEU	LEU	SER	SER	THR	SER	THR	THR	TRP	LYS	LYS	LEU	ALA	GLN	ASP	GLN	GLN	THR	THR	GLN	ASP	VAL	VAL	ASP	GLU	K58	L59
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Diagram illustrating the protein structure of the C-terminal domain of the human protein. The structure is shown as a ribbon diagram with various residues highlighted. Red diamonds indicate specific residues: L64, T65, G66, K96, W97, K98, E139, G161, and W166. The residues are color-coded: L64, T65, G66, K96, W97, K98, E139, G161, and W166 are in green, while ASN, LYS, ARG, THR, ARG, VAL, SER, THR, and LYS are in grey.

- Chain K:  26% 61% 6% 33%


M1	L7	R8	Q12	Q13	V14	S15	G16	H17	L24	R25	V26	L27	F28	N31	D32	G36	T37	L38	V39	G40	E41	Y49	F55	M61	V62	I63	Y64	T65	T66	E67	M68	M69	G70	R71	D72	T73	F74	W75	D76	V77	M81	C92	M93	T94	P97	PRO	THR
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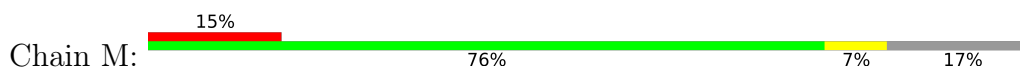
LYS	PRO	PRO	THR	ALA	ARG	LYS	TYR	ILE	TRP	THR	ASN	ASN	HIS	LYS	PHE	ASN	VAL	SER	GLY	THR	PRO	GLN	GLN	TYR	VAL	PRO	TYR	SER	THR	THR	ARG	LYS	LYS	ILE	GLN	GLU	TRP	VAL	PRO	PRO	SER	THR	PRO	TYR	LYS
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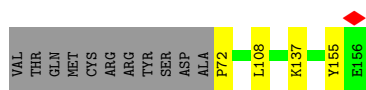
- Chain B:  8% 12% 88%

MET	GLU	LEU	VAL	GLN	VAL	LEU	ARG	ARG	GLY	GLN	GLN	VAL	SER	GLY	HIS	GLY	LEU	ARG	GLY	TYR	LEU	ARG	VAL	VAL	PHE	ALA	ASN	ASP	VAL	VAL	ARG	VAL	GLY	GLY	THR	LEU	LEU	VAL	GLY	GLU	ASP	LYS	TYR	GLY	ASN	LYS	TYR	GLU	ASP	ASN	GLN	PHE	PHI	GLY	ARG	HIS
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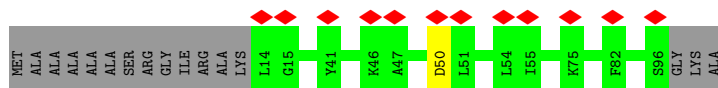
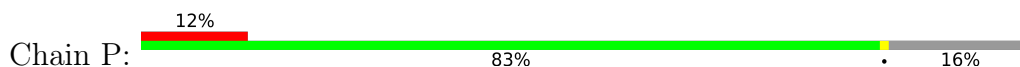
TRP	VAL	ILE	TYR	THR	THR	GLU	MET	ASN	GLY	ARG	ASP	THR	PHE	TRP	TRP	VAL	VAL	PRO	PRO	GLU	SER	MET	MET	VAL	THR	HIS	TRP	ARG	TRP	LEU	HIS	CYS	MET	THR	ASP	ASP	PRO	PRO	PRO	THR	THR	THR	THR	LYS	PRO	PRO	THR	THR	ALA	ARG	LYS	LYS	ILE	THR	THR	THR	ASN	HIS	LYS	PHE	ASN	VAL	SER	GLY
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- Chain L:  18% 85% 11%

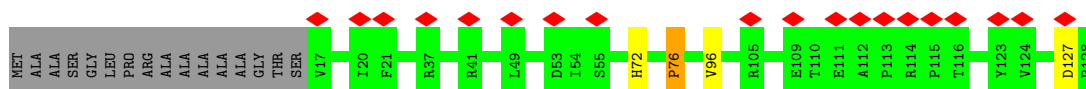
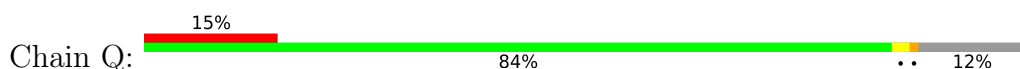




- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



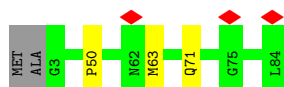
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



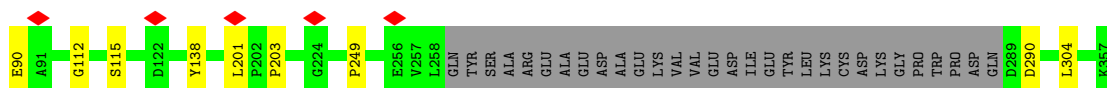
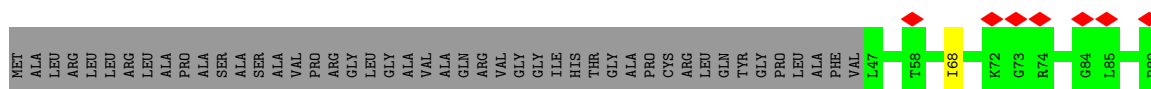
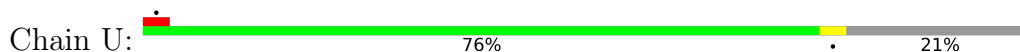
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

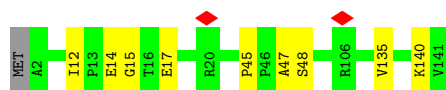


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

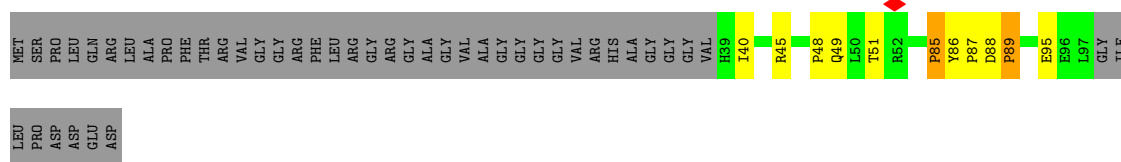




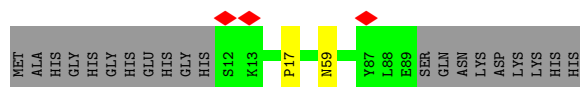
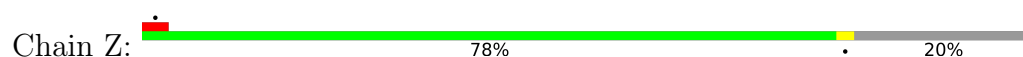
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



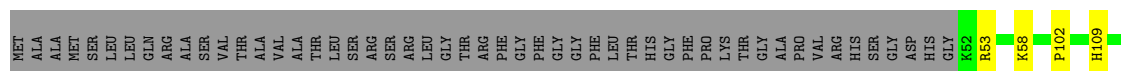
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



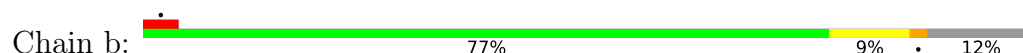
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



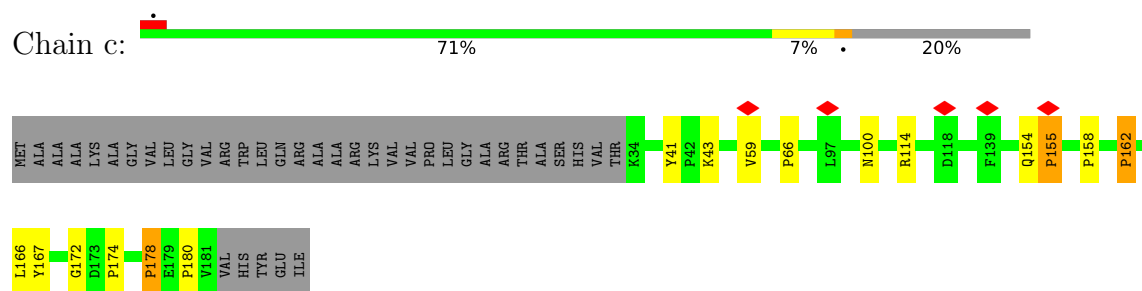
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



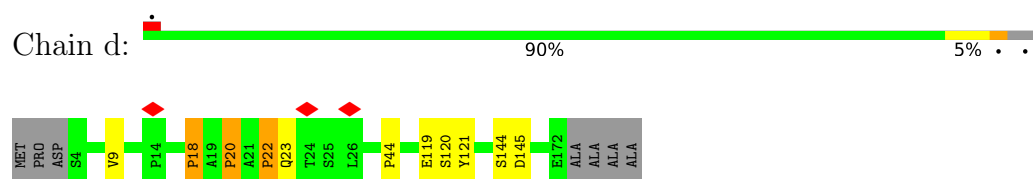
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



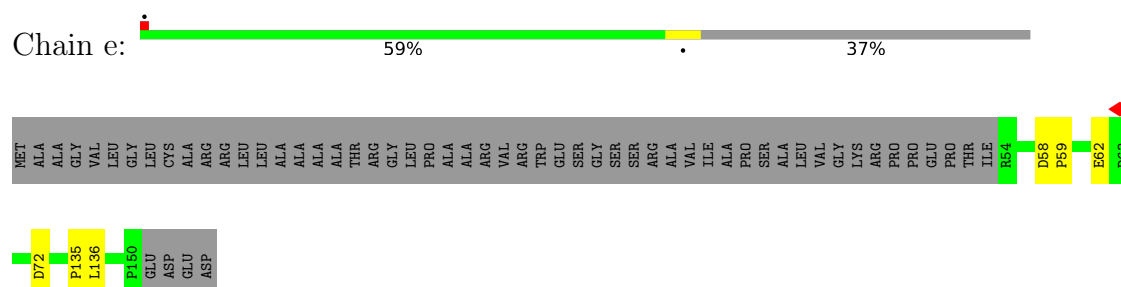
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



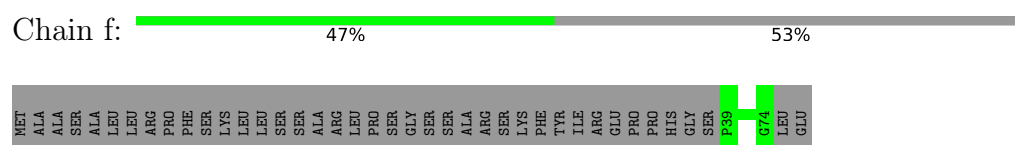
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



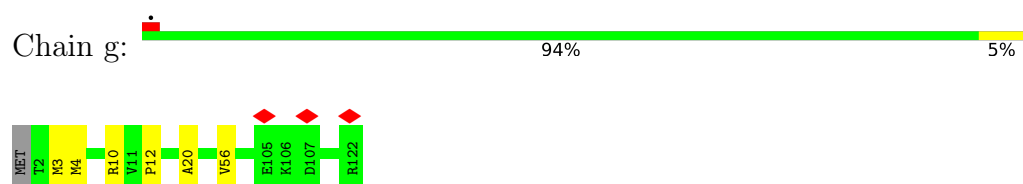
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

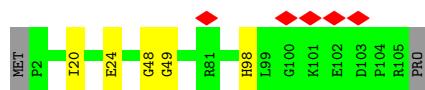


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5





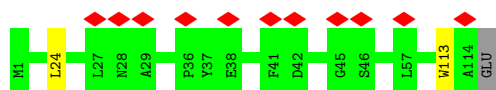
- Molecule 33: NADH-ubiquinone oxidoreductase chain 2

Chain i: 99%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 3

Chain j: 10% 97%



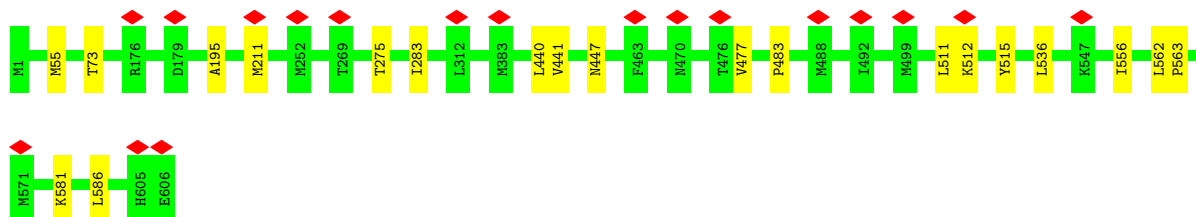
- Molecule 35: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 96%



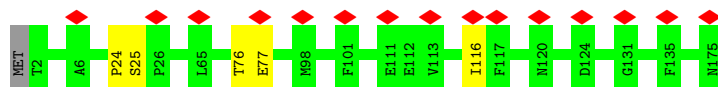
- Molecule 36: NADH-ubiquinone oxidoreductase chain 5

Chain l: 97%



- Molecule 37: NADH-ubiquinone oxidoreductase chain 6

Chain m: 9% 97%



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

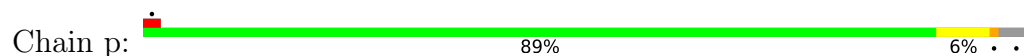
Chain n: 81% 19%



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



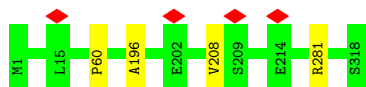
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 41: NADH-ubiquinone oxidoreductase chain 4



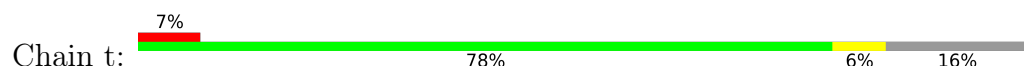
- Molecule 42: NADH-ubiquinone oxidoreductase chain 1



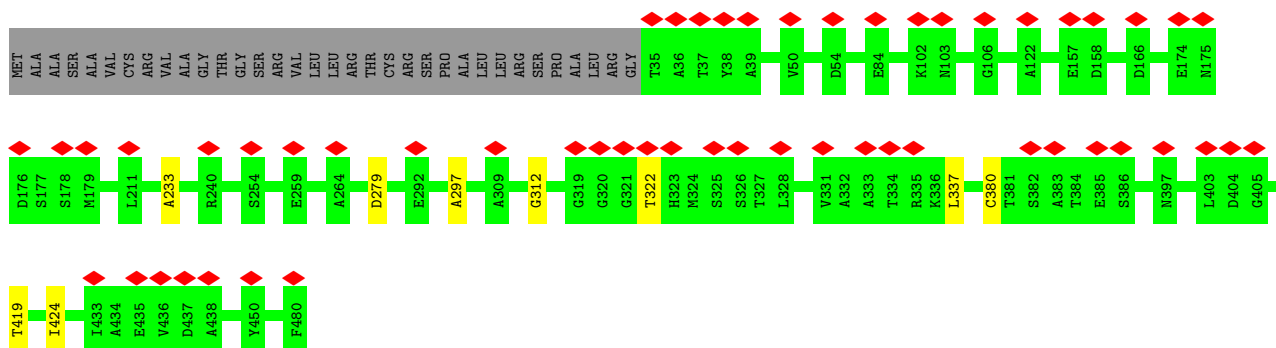
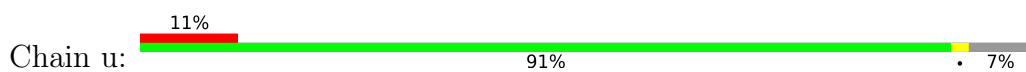
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



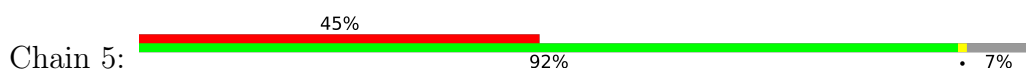
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



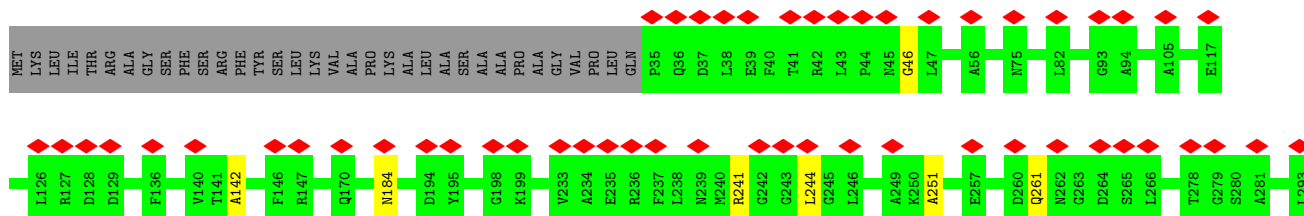
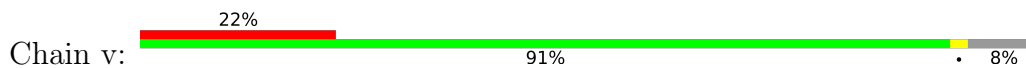
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

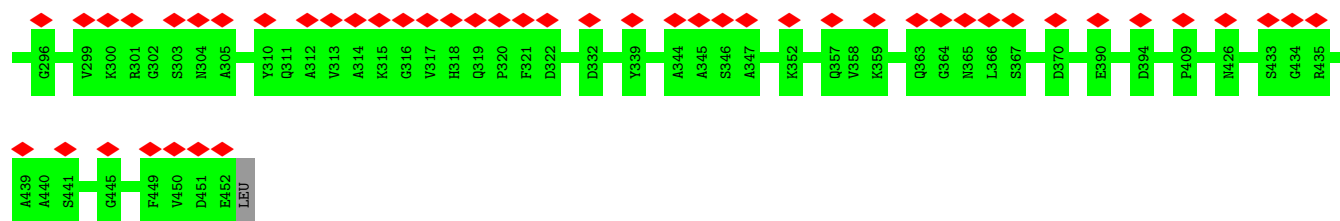


- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



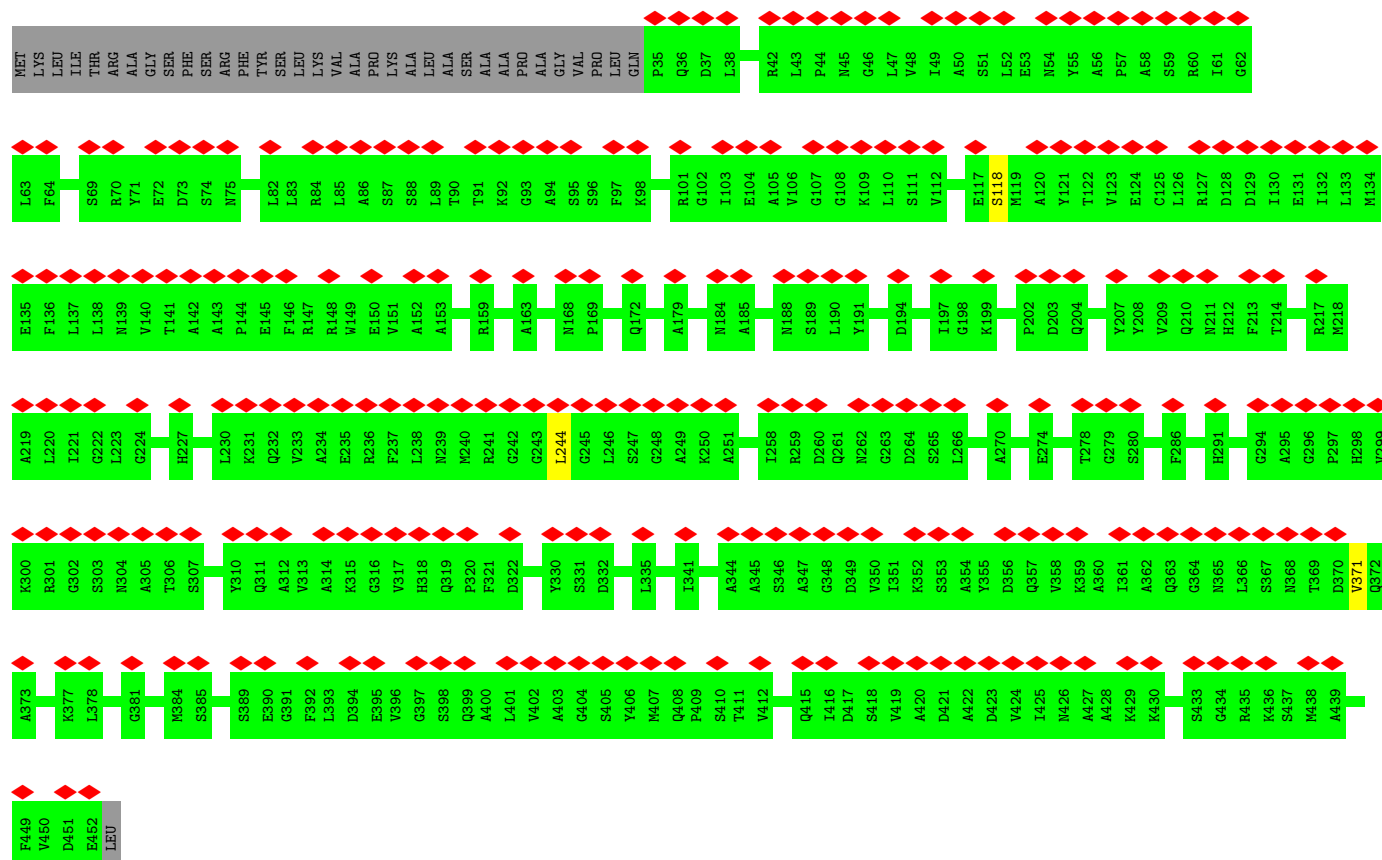
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial





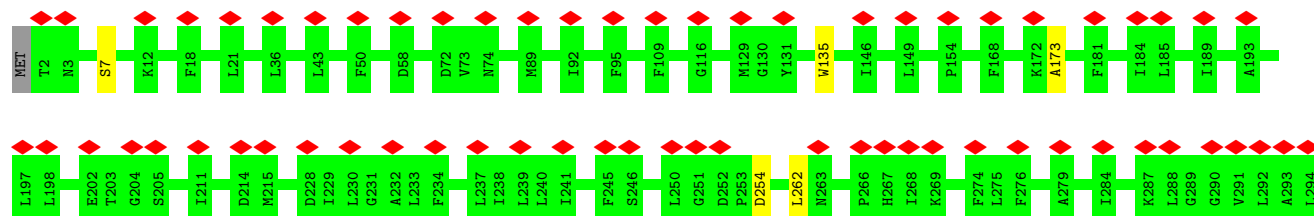
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

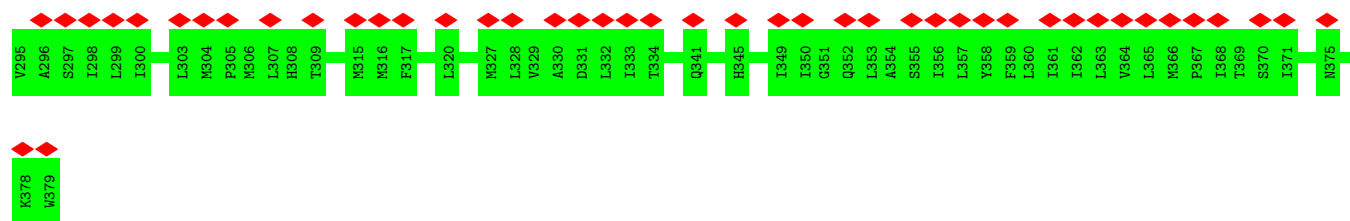
Chain 6: 56% 92% 8%



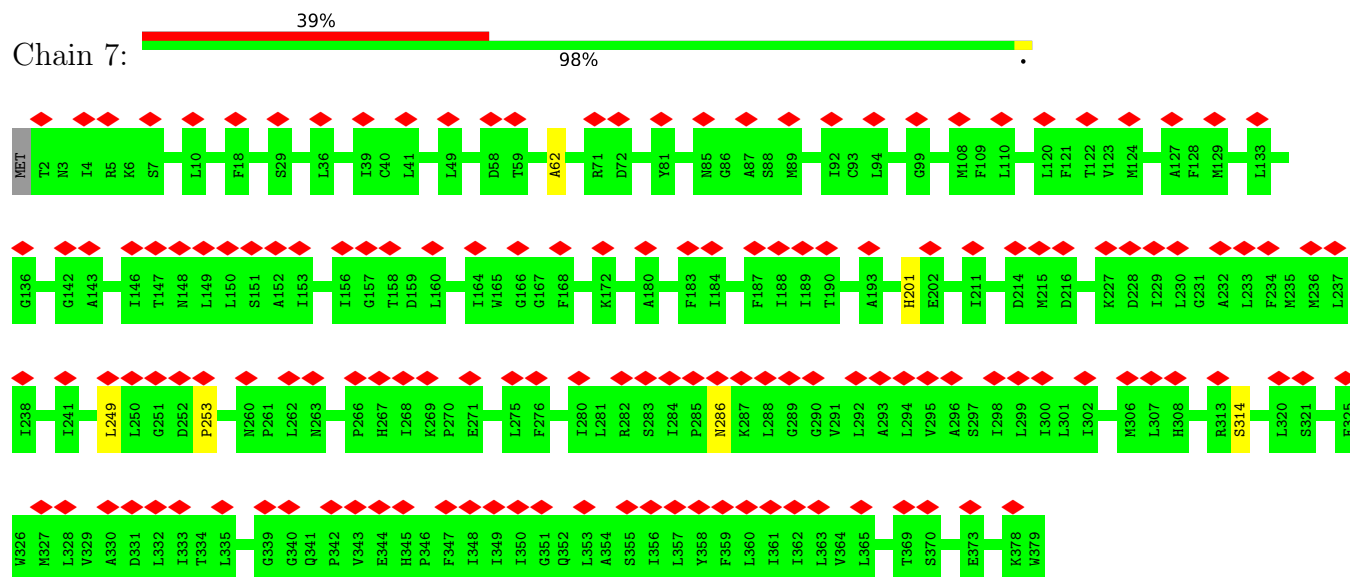
- Molecule 47: Cytochrome b

Chain w: 29% 98%

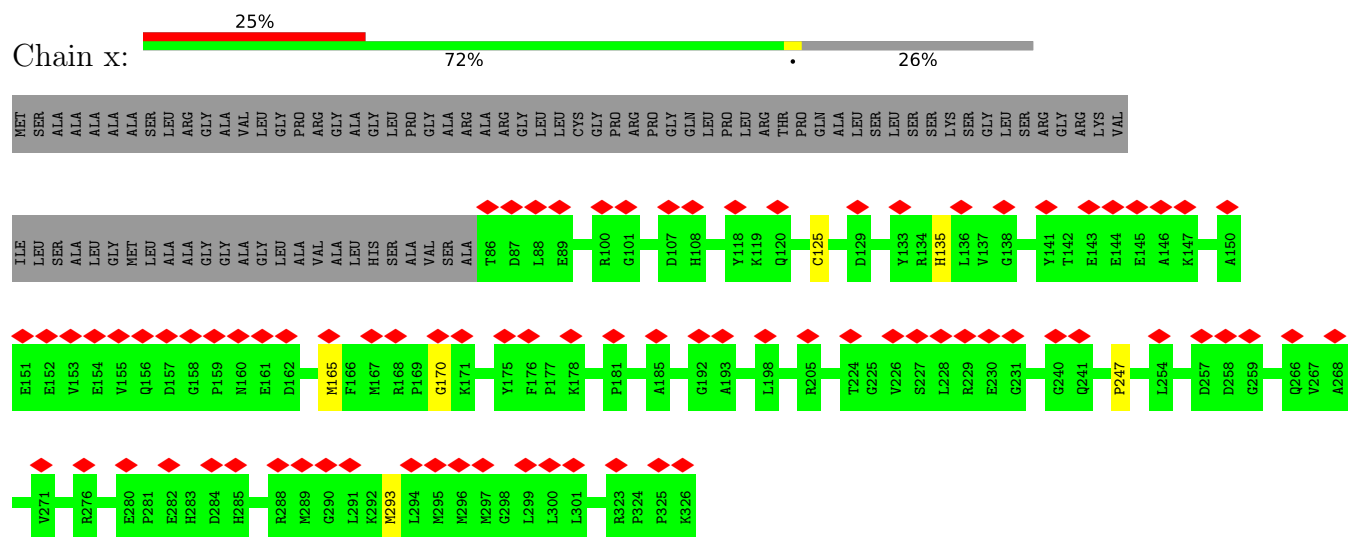




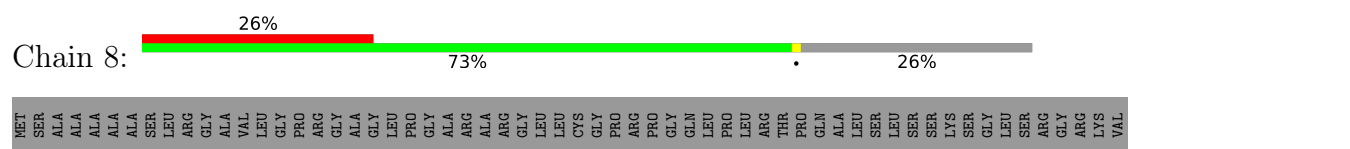
• Molecule 47: Cytochrome b

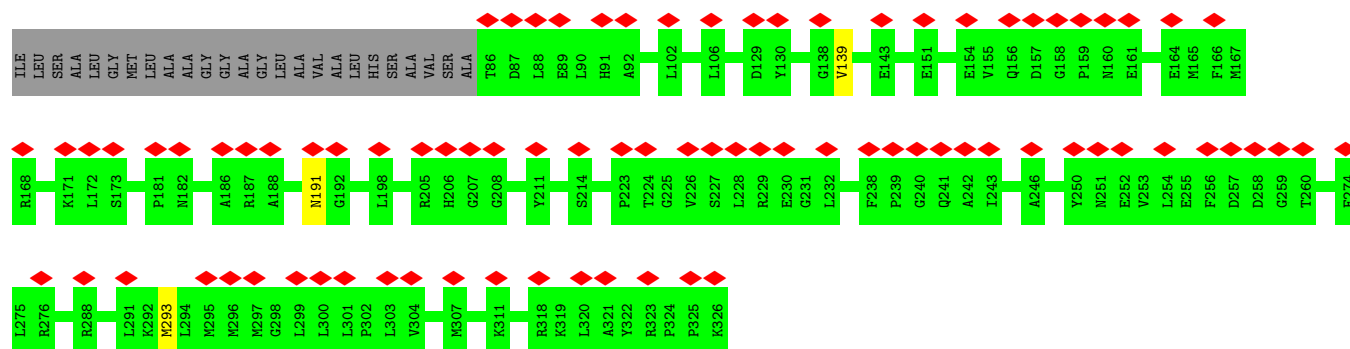


• Molecule 48: Cytochrome c1, heme protein, mitochondrial

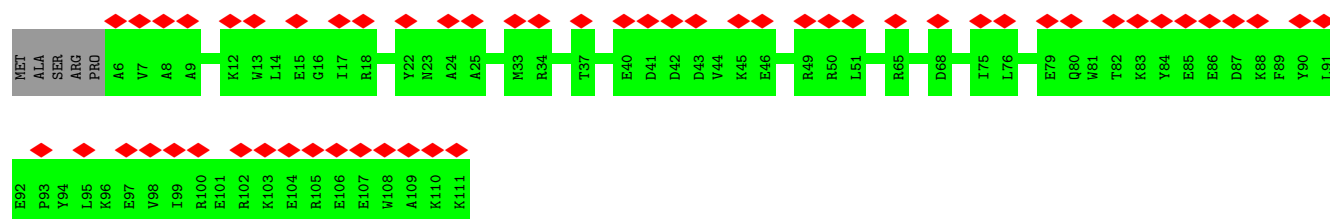


• Molecule 48: Cytochrome c1, heme protein, mitochondrial

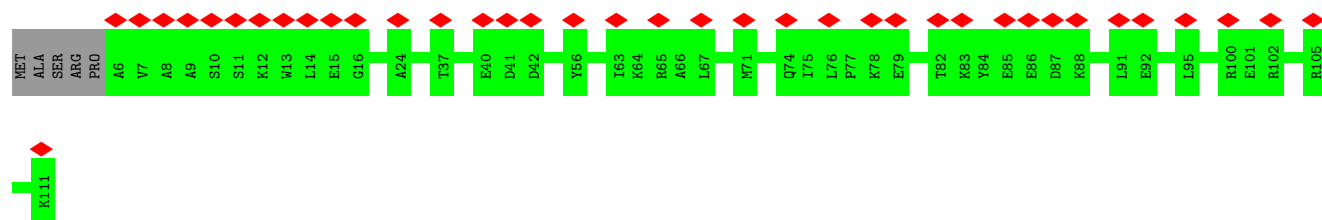




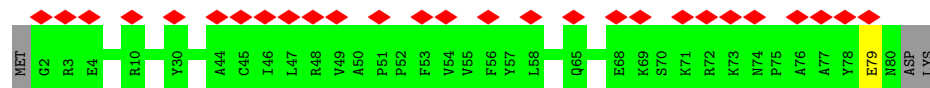
• Molecule 49: Cytochrome b-c1 complex subunit 7



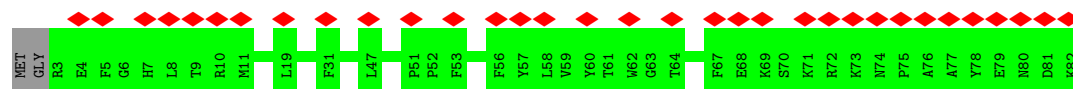
• Molecule 49: Cytochrome b-c1 complex subunit 7



• Molecule 50: Cytochrome b-c1 complex subunit 8



• Molecule 50: Cytochrome b-c1 complex subunit 8

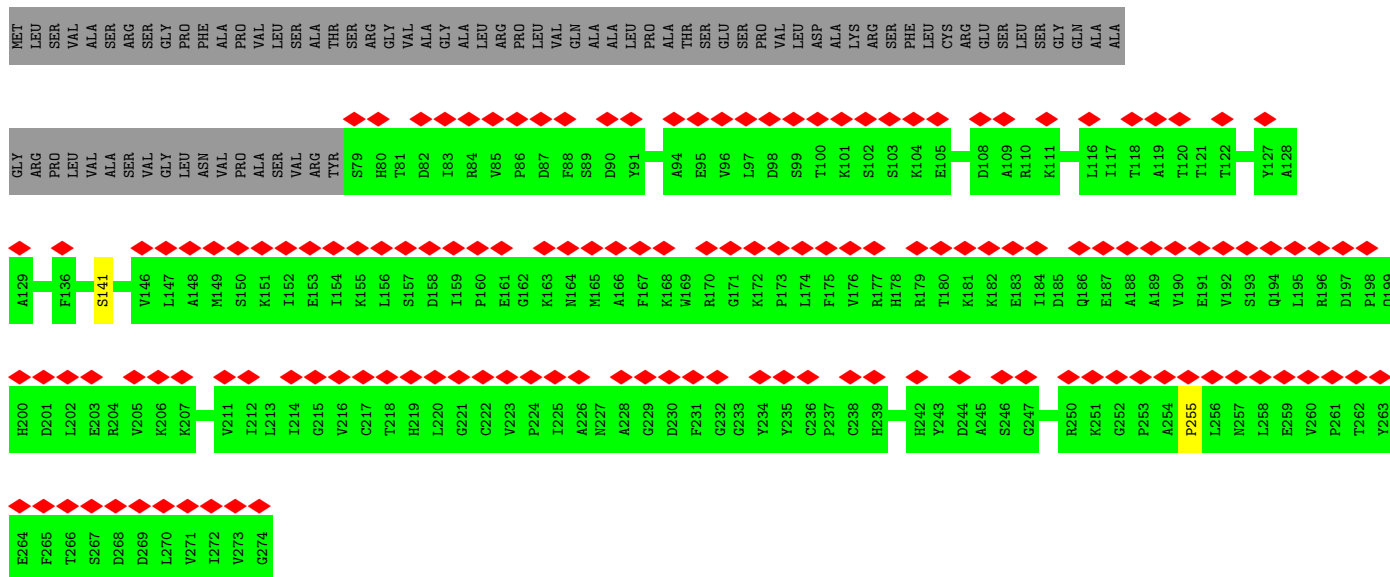


• Molecule 51: Cytochrome b-c1 complex subunit 6, mitochondrial



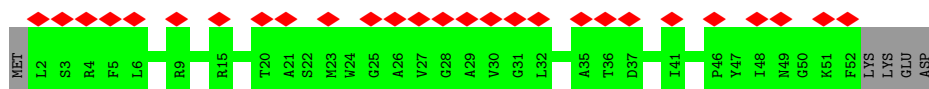
- Molecule 53: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 4: 53% 71% 28%



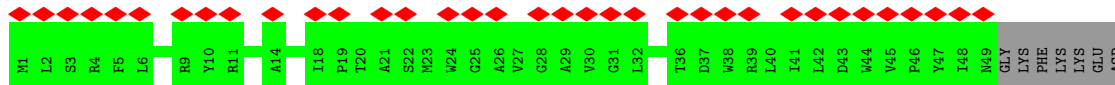
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3: 48% 91% 9%



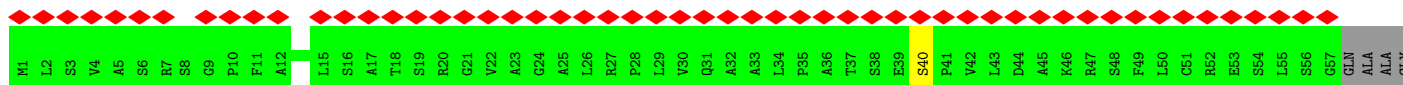
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain Ad: 62% 88% 12%



- Molecule 55: Cytochrome b-c1 complex subunit Rieske transit peptide, mitochondrial

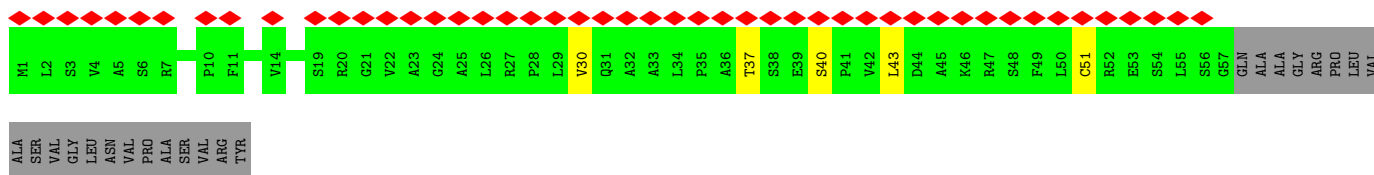
Chain Ae: 69% 72% 27%



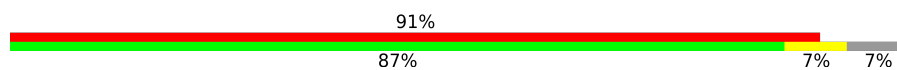
ARG PRO LEU VAL ALA SER VAL GLY LEU ASN VAL PRO ALA SER VAL ARG TYR

- Molecule 55: Cytochrome b-c1 complex subunit Rieske transit peptide, mitochondrial

Chain Af: 

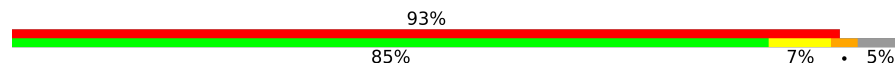


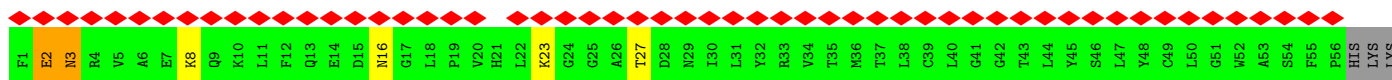
- Molecule 56: Cytochrome c oxidase subunit 8B, mitochondrial

Chain Ag: 




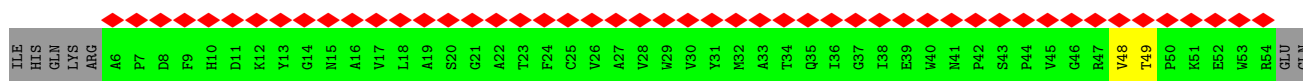
- Molecule 57: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain Ah: 

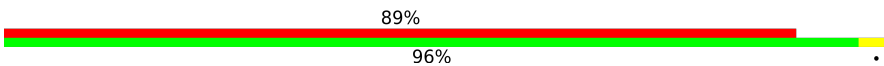



- Molecule 58: Cytochrome c oxidase subunit 7B, mitochondrial

Chain Ai: 



- Molecule 59: Cytochrome c oxidase subunit 7C, mitochondrial

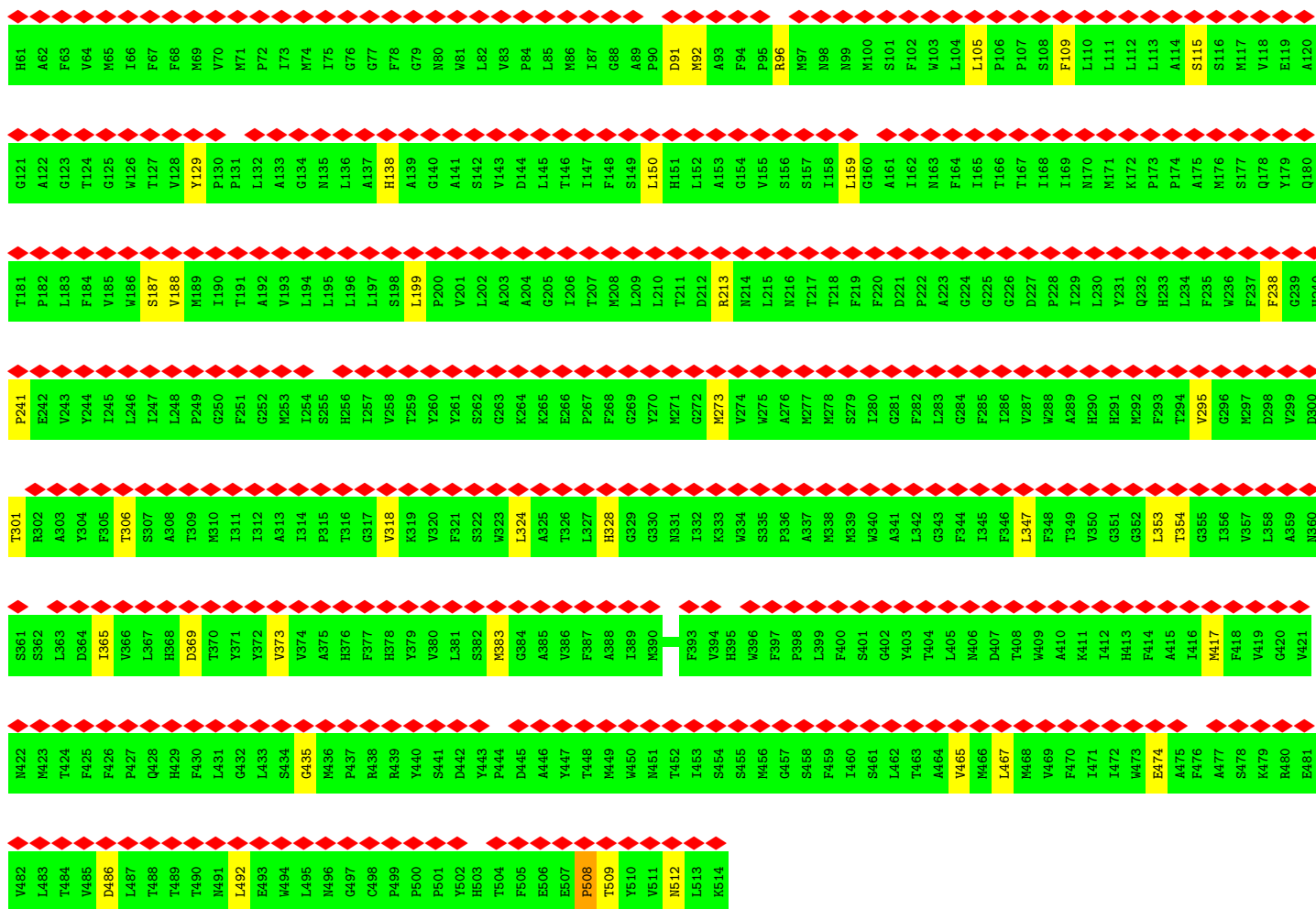
Chain Aj: 



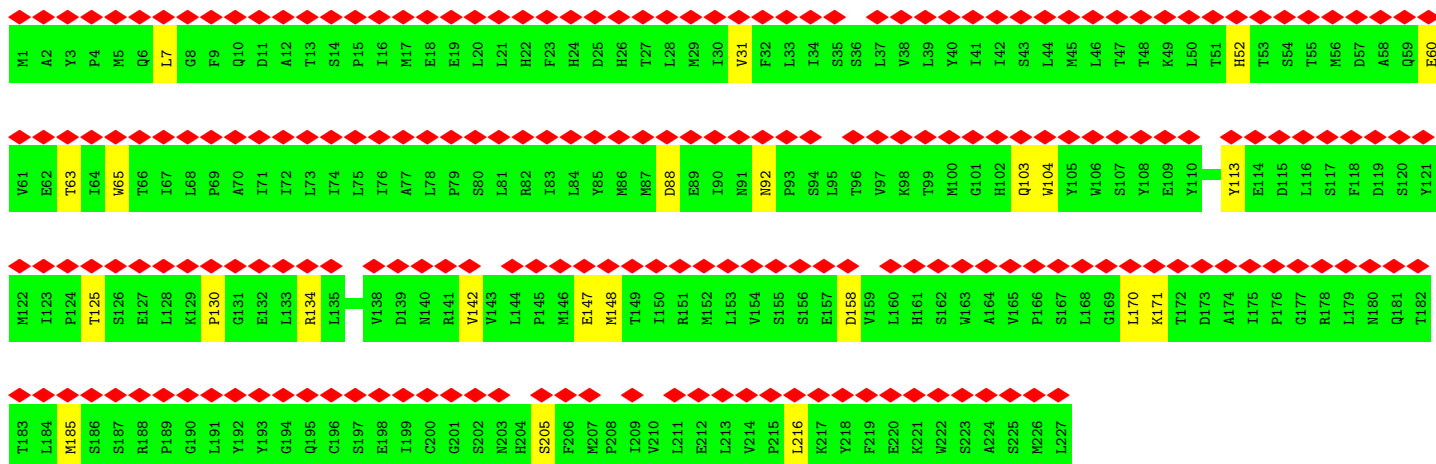
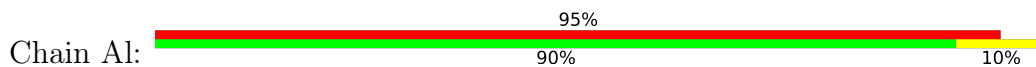
- Molecule 60: Cytochrome c oxidase subunit 1

Chain Ak: 



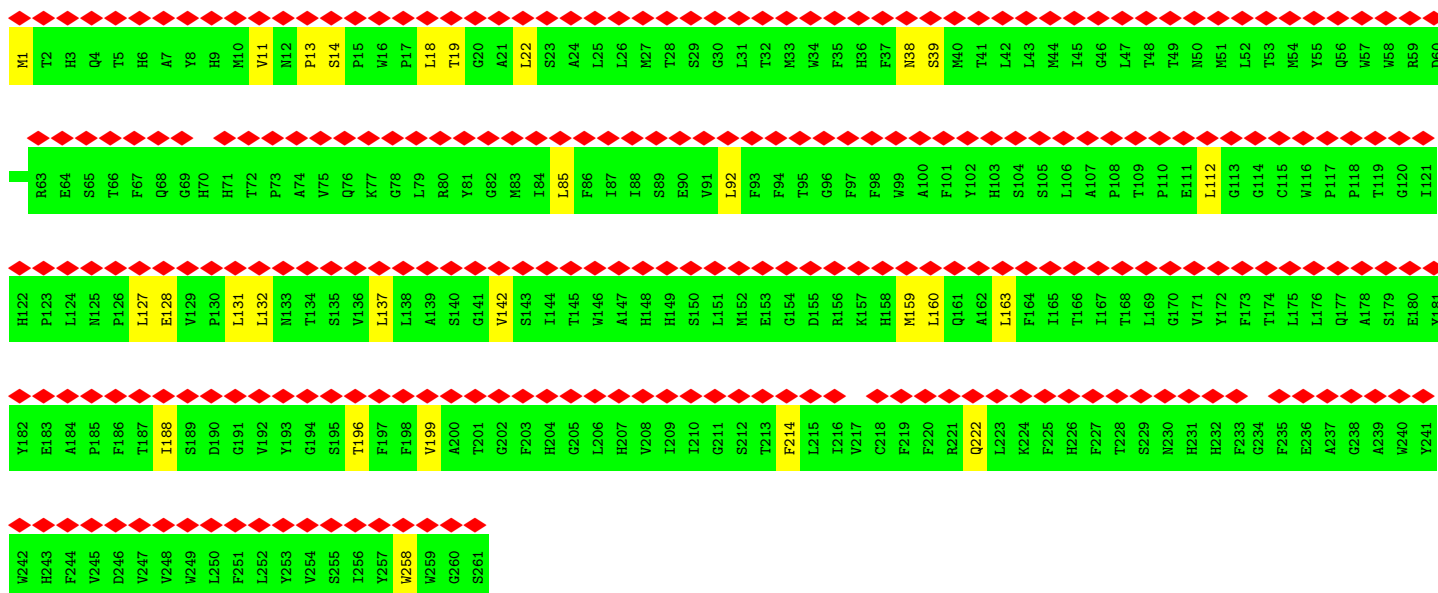


• Molecule 61: Cytochrome c oxidase subunit 2

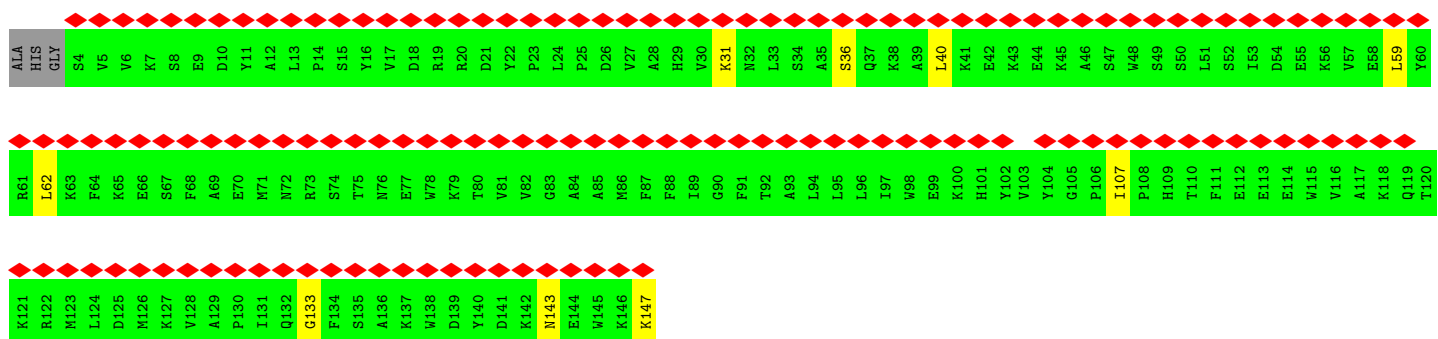
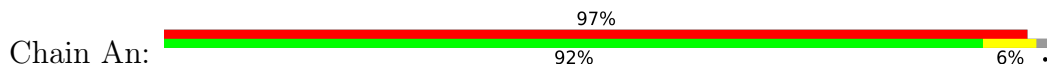


• Molecule 62: Cytochrome c oxidase subunit 3

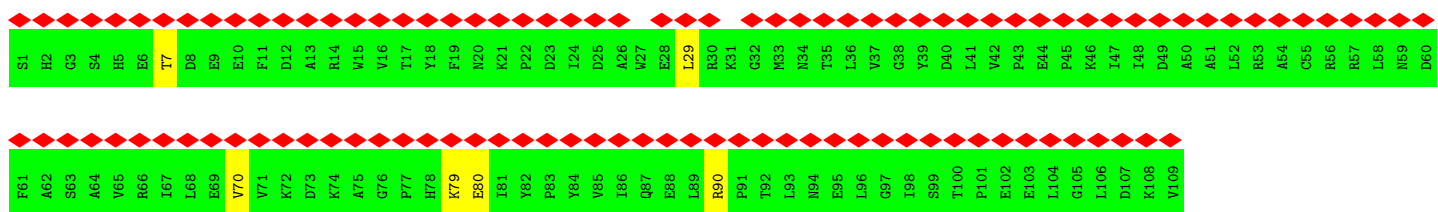




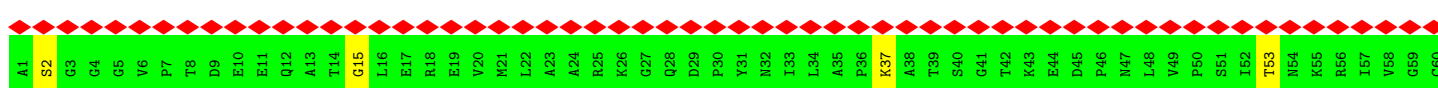
- Molecule 63: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

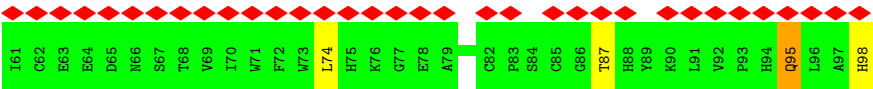


- Molecule 64: Cytochrome c oxidase subunit 5A, mitochondrial

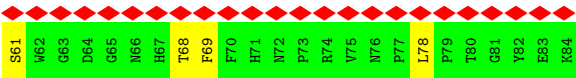
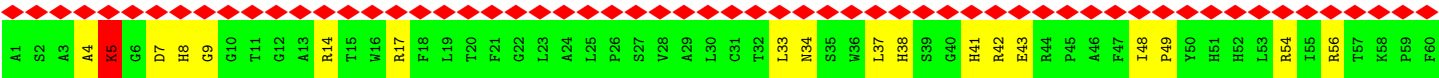
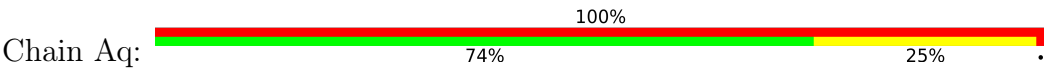


- Molecule 65: Cytochrome c oxidase subunit 5B, mitochondrial

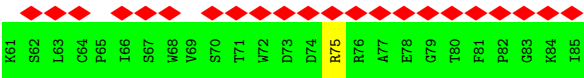
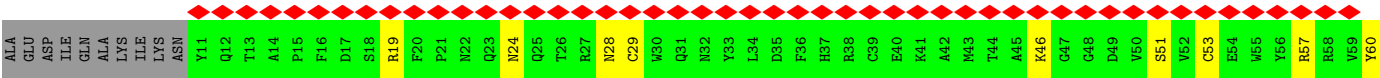
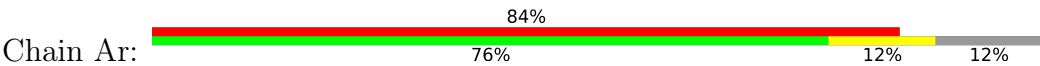




• Molecule 66: Cytochrome c oxidase subunit 6A, mitochondrial



• Molecule 67: Cytochrome c oxidase subunit 6B1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161912	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.519	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0504	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, CU, CDL, ZMP, HEC, ZN, MG, PLX, SF4, FES, HEM, NDP, PEE, FMN

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	A	0.60	0/611	0.65	0/810
2	B	0.37	0/3199	0.55	0/4327
3	C	0.59	0/3479	0.64	2/4718 (0.0%)
4	D	0.45	0/1727	0.65	0/2355
5	E	0.39	0/1367	0.60	2/1860 (0.1%)
6	F	0.49	0/244	0.63	1/332 (0.3%)
7	G	0.43	0/5084	0.61	3/6898 (0.0%)
8	H	0.62	0/1439	0.61	0/1948
9	I	0.68	0/1272	0.64	0/1721
10	J	0.42	0/900	0.56	0/1218
11	K	0.42	0/526	0.56	1/728 (0.1%)
11	R	0.24	0/89	0.69	0/123
12	L	0.38	0/2740	0.57	2/3721 (0.1%)
13	M	0.36	0/702	0.56	0/959
14	N	0.38	0/914	0.58	0/1241
15	O	0.36	0/656	0.56	1/890 (0.1%)
15	X	0.47	0/673	0.62	1/912 (0.1%)
16	P	0.33	0/684	0.56	0/922
17	Q	0.40	0/965	0.62	1/1301 (0.1%)
18	S	0.47	0/582	0.56	0/783
19	T	0.44	0/643	0.59	0/886
20	U	0.43	0/1981	0.59	2/2711 (0.1%)
21	V	0.49	0/1030	0.62	0/1397
22	W	0.48	0/1153	0.59	0/1561
23	Y	0.46	0/412	0.66	3/567 (0.5%)
24	Z	0.42	0/567	0.51	0/777
25	a	0.52	0/1157	0.59	0/1571
26	b	0.46	0/756	0.76	8/1042 (0.8%)
27	c	0.53	0/1115	0.71	6/1535 (0.4%)
28	d	0.50	0/1253	0.64	4/1697 (0.2%)
29	e	0.54	0/778	0.55	0/1059
30	f	0.49	0/308	0.51	0/415

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	g	0.51	0/1027	0.62	0/1389
32	h	0.48	0/812	0.58	0/1087
33	i	0.63	0/2769	0.70	0/3764
34	j	0.51	0/916	0.60	0/1253
35	k	0.61	0/728	0.72	0/988
36	l	0.50	0/4919	0.63	1/6693 (0.0%)
37	m	0.57	0/1312	0.62	0/1784
38	n	0.44	0/368	0.55	0/499
39	o	0.50	0/1050	0.58	0/1430
40	p	0.51	0/1463	0.63	3/1984 (0.2%)
41	q	0.59	0/3718	0.70	0/5070
42	r	0.57	0/2581	0.68	0/3529
43	s	0.44	0/1387	0.57	0/1876
44	t	0.41	0/758	0.61	4/1032 (0.4%)
45	5	0.30	0/3531	0.51	0/4793
45	u	0.39	0/3523	0.54	0/4782
46	6	0.29	0/3179	0.51	0/4303
46	v	0.32	0/3179	0.53	0/4303
47	7	0.36	0/3115	0.54	0/4259
47	w	0.40	0/3115	0.58	0/4259
48	8	0.32	0/1976	0.51	0/2681
48	x	0.35	0/1976	0.55	0/2681
49	9	0.32	0/941	0.52	0/1262
49	y	0.33	0/941	0.50	0/1262
50	Aa	0.31	0/701	0.51	0/948
50	z	0.37	0/688	0.57	0/931
51	0	0.31	0/534	0.52	0/714
51	Ab	0.30	0/534	0.49	0/714
52	1	0.31	0/520	0.51	0/701
52	Ac	0.29	0/520	0.51	0/701
53	2	0.30	0/1549	0.51	0/2095
53	4	0.29	0/1549	0.49	0/2095
54	3	0.29	0/430	0.50	0/590
54	Ad	0.28	0/410	0.51	0/564
55	Ae	0.25	0/399	0.53	0/542
55	Af	0.26	0/394	0.59	0/536
56	Ag	0.51	0/345	0.65	0/470
57	Ah	0.60	0/440	0.72	0/596
58	Ai	0.57	0/398	0.66	0/546
59	Aj	0.63	0/399	0.62	0/534
60	Ak	0.60	0/4164	0.76	2/5688 (0.0%)
61	Al	0.58	0/1868	0.80	0/2544
62	Am	0.56	0/2211	0.69	0/3023

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
63	An	0.57	0/1229	0.65	1/1658 (0.1%)
64	Ao	0.50	0/898	0.66	0/1218
65	Ap	0.56	0/765	0.81	0/1038
66	Aq	0.55	0/699	0.73	1/950 (0.1%)
67	Ar	0.55	0/648	0.73	0/877
All	All	0.47	0/110582	0.61	49/150221 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
4	D	0	1
10	J	0	1
21	V	0	1
25	a	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	An	133	GLY	N-CA-C	6.44	129.20	113.10
26	b	30	PRO	N-CA-CB	6.38	110.95	103.30
26	b	124	PRO	N-CA-CB	6.29	110.85	103.30
40	p	155	PRO	N-CA-CB	6.28	110.84	103.30
28	d	44	PRO	N-CA-CB	6.22	110.77	103.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	327	ILE	Peptide
4	D	223	PRO	Peptide
10	J	98	LYS	Peptide
21	V	12	ILE	Peptide
25	a	109	HIS	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
2	B	408/464 (88%)	365 (90%)	30 (7%)	13 (3%)	3	26
3	C	428/463 (92%)	388 (91%)	28 (6%)	12 (3%)	4	28
4	D	206/264 (78%)	164 (80%)	29 (14%)	13 (6%)	1	16
5	E	170/249 (68%)	154 (91%)	11 (6%)	5 (3%)	3	27
6	F	42/123 (34%)	29 (69%)	10 (24%)	3 (7%)	1	14
7	G	669/727 (92%)	574 (86%)	66 (10%)	29 (4%)	2	21
8	H	174/212 (82%)	166 (95%)	7 (4%)	1 (1%)	22	58
9	I	154/216 (71%)	134 (87%)	12 (8%)	8 (5%)	1	19
10	J	107/175 (61%)	94 (88%)	12 (11%)	1 (1%)	14	49
11	K	95/145 (66%)	74 (78%)	14 (15%)	7 (7%)	1	13
11	R	16/145 (11%)	13 (81%)	2 (12%)	1 (6%)	1	16
12	L	335/377 (89%)	308 (92%)	15 (4%)	12 (4%)	3	24
13	M	90/113 (80%)	76 (84%)	6 (7%)	8 (9%)	0	11
14	N	110/116 (95%)	99 (90%)	6 (6%)	5 (4%)	2	21
15	O	83/156 (53%)	77 (93%)	2 (2%)	4 (5%)	2	20
15	X	83/156 (53%)	76 (92%)	4 (5%)	3 (4%)	3	24
16	P	81/99 (82%)	74 (91%)	6 (7%)	1 (1%)	11	43
17	Q	110/128 (86%)	99 (90%)	7 (6%)	4 (4%)	3	24
18	S	68/70 (97%)	63 (93%)	2 (3%)	3 (4%)	2	21
19	T	80/84 (95%)	69 (86%)	8 (10%)	3 (4%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	U	277/357 (78%)	249 (90%)	22 (8%)	6 (2%)	5	32
21	V	138/141 (98%)	127 (92%)	3 (2%)	8 (6%)	1	17
22	W	136/144 (94%)	124 (91%)	9 (7%)	3 (2%)	5	32
23	Y	57/105 (54%)	42 (74%)	5 (9%)	10 (18%)	0	2
24	Z	76/98 (78%)	71 (93%)	3 (4%)	2 (3%)	4	30
25	a	136/189 (72%)	118 (87%)	14 (10%)	4 (3%)	3	27
26	b	109/128 (85%)	95 (87%)	4 (4%)	10 (9%)	0	10
27	c	146/186 (78%)	119 (82%)	14 (10%)	13 (9%)	0	11
28	d	167/176 (95%)	151 (90%)	6 (4%)	10 (6%)	1	16
29	e	95/154 (62%)	83 (87%)	6 (6%)	6 (6%)	1	16
30	f	34/76 (45%)	29 (85%)	5 (15%)	0	100	100
31	g	119/122 (98%)	106 (89%)	7 (6%)	6 (5%)	1	19
32	h	102/106 (96%)	89 (87%)	8 (8%)	5 (5%)	2	19
33	i	345/347 (99%)	325 (94%)	17 (5%)	3 (1%)	14	49
34	j	112/115 (97%)	101 (90%)	9 (8%)	2 (2%)	7	36
35	k	95/98 (97%)	88 (93%)	4 (4%)	3 (3%)	3	26
36	l	604/606 (100%)	545 (90%)	41 (7%)	18 (3%)	3	27
37	m	172/175 (98%)	156 (91%)	11 (6%)	5 (3%)	3	27
38	n	45/58 (78%)	41 (91%)	4 (9%)	0	100	100
39	o	126/129 (98%)	108 (86%)	11 (9%)	7 (6%)	1	18
40	p	167/179 (93%)	145 (87%)	13 (8%)	9 (5%)	1	19
41	q	457/459 (100%)	426 (93%)	21 (5%)	10 (2%)	5	32
42	r	316/318 (99%)	285 (90%)	27 (8%)	4 (1%)	10	42
43	s	167/172 (97%)	149 (89%)	14 (8%)	4 (2%)	5	31
44	t	111/137 (81%)	100 (90%)	8 (7%)	3 (3%)	4	29
45	5	444/480 (92%)	412 (93%)	29 (6%)	3 (1%)	19	55
45	u	444/480 (92%)	407 (92%)	28 (6%)	9 (2%)	6	34
46	6	416/453 (92%)	383 (92%)	30 (7%)	3 (1%)	19	55
46	v	416/453 (92%)	379 (91%)	30 (7%)	7 (2%)	7	37
47	7	376/379 (99%)	348 (93%)	22 (6%)	6 (2%)	8	38
47	w	376/379 (99%)	352 (94%)	19 (5%)	5 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	8	239/326 (73%)	221 (92%)	16 (7%)	2 (1%)	16	53
48	x	239/326 (73%)	219 (92%)	15 (6%)	5 (2%)	5	33
49	9	104/111 (94%)	102 (98%)	2 (2%)	0	100	100
49	y	104/111 (94%)	100 (96%)	4 (4%)	0	100	100
50	Aa	78/82 (95%)	70 (90%)	8 (10%)	0	100	100
50	z	77/82 (94%)	70 (91%)	6 (8%)	1 (1%)	10	42
51	0	62/91 (68%)	61 (98%)	1 (2%)	0	100	100
51	Ab	62/91 (68%)	60 (97%)	2 (3%)	0	100	100
52	1	60/64 (94%)	55 (92%)	2 (3%)	3 (5%)	1	19
52	Ac	60/64 (94%)	57 (95%)	2 (3%)	1 (2%)	7	37
53	2	194/274 (71%)	178 (92%)	14 (7%)	2 (1%)	13	47
53	4	194/274 (71%)	178 (92%)	14 (7%)	2 (1%)	13	47
54	3	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
54	Ad	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
55	Ae	55/78 (70%)	41 (74%)	13 (24%)	1 (2%)	7	36
55	Af	55/78 (70%)	40 (73%)	10 (18%)	5 (9%)	0	11
56	Ag	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
57	Ah	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2	23
58	Ai	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
59	Aj	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
60	Ak	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	53
61	Al	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	10	42
62	Am	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
63	An	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
64	Ao	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
65	Ap	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	22
66	Aq	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	16
67	Ar	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	40
All	All	13723/15851 (87%)	12412 (90%)	950 (7%)	361 (3%)	6	30

5 of 361 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	73	PRO
2	B	105	PRO
2	B	121	GLU
2	B	379	CYS
3	C	84	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	58/58 (100%)	53 (91%)	5 (9%)	8	30
2	B	322/368 (88%)	321 (100%)	1 (0%)	91	92
3	C	351/393 (89%)	350 (100%)	1 (0%)	91	92
4	D	176/228 (77%)	176 (100%)	0	100	100
5	E	145/173 (84%)	145 (100%)	0	100	100
6	F	9/97 (9%)	9 (100%)	0	100	100
7	G	518/610 (85%)	517 (100%)	1 (0%)	92	93
8	H	150/176 (85%)	150 (100%)	0	100	100
9	I	129/177 (73%)	128 (99%)	1 (1%)	79	84
10	J	95/152 (62%)	95 (100%)	0	100	100
11	K	11/131 (8%)	11 (100%)	0	100	100
12	L	280/323 (87%)	277 (99%)	3 (1%)	70	80
13	M	65/98 (66%)	65 (100%)	0	100	100
14	N	95/101 (94%)	95 (100%)	0	100	100
15	O	66/132 (50%)	66 (100%)	0	100	100
15	X	71/132 (54%)	71 (100%)	0	100	100
16	P	75/82 (92%)	75 (100%)	0	100	100
17	Q	101/112 (90%)	101 (100%)	0	100	100
18	S	58/58 (100%)	58 (100%)	0	100	100
19	T	65/70 (93%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	U	151/307 (49%)	149 (99%)	2 (1%)	65	77
21	V	98/102 (96%)	98 (100%)	0	100	100
22	W	114/124 (92%)	114 (100%)	0	100	100
23	Y	24/84 (29%)	24 (100%)	0	100	100
24	Z	41/76 (54%)	41 (100%)	0	100	100
25	a	114/158 (72%)	113 (99%)	1 (1%)	75	83
26	b	46/121 (38%)	46 (100%)	0	100	100
27	c	87/160 (54%)	87 (100%)	0	100	100
28	d	99/156 (64%)	99 (100%)	0	100	100
29	e	74/129 (57%)	74 (100%)	0	100	100
30	f	31/66 (47%)	31 (100%)	0	100	100
31	g	107/109 (98%)	107 (100%)	0	100	100
32	h	75/94 (80%)	75 (100%)	0	100	100
33	i	310/311 (100%)	310 (100%)	0	100	100
34	j	97/100 (97%)	97 (100%)	0	100	100
35	k	78/85 (92%)	78 (100%)	0	100	100
36	l	534/540 (99%)	533 (100%)	1 (0%)	92	93
37	m	129/141 (92%)	129 (100%)	0	100	100
38	n	33/55 (60%)	33 (100%)	0	100	100
39	o	101/114 (89%)	101 (100%)	0	100	100
40	p	134/160 (84%)	133 (99%)	1 (1%)	81	86
41	q	408/409 (100%)	407 (100%)	1 (0%)	92	93
42	r	275/275 (100%)	275 (100%)	0	100	100
43	s	142/154 (92%)	138 (97%)	4 (3%)	38	59
44	t	41/120 (34%)	40 (98%)	1 (2%)	44	63
45	5	372/397 (94%)	372 (100%)	0	100	100
45	u	370/397 (93%)	370 (100%)	0	100	100
46	6	326/354 (92%)	326 (100%)	0	100	100
46	v	326/354 (92%)	326 (100%)	0	100	100
47	7	331/332 (100%)	331 (100%)	0	100	100
47	w	331/332 (100%)	331 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	8	205/259 (79%)	204 (100%)	1 (0%)	86	89
48	x	205/259 (79%)	204 (100%)	1 (0%)	86	89
49	9	95/99 (96%)	95 (100%)	0	100	100
49	y	95/99 (96%)	95 (100%)	0	100	100
50	Aa	72/73 (99%)	72 (100%)	0	100	100
50	z	70/73 (96%)	70 (100%)	0	100	100
51	0	61/85 (72%)	61 (100%)	0	100	100
51	Ab	61/85 (72%)	61 (100%)	0	100	100
52	1	50/52 (96%)	50 (100%)	0	100	100
52	Ac	50/52 (96%)	50 (100%)	0	100	100
53	2	165/225 (73%)	165 (100%)	0	100	100
53	4	165/225 (73%)	165 (100%)	0	100	100
54	3	39/46 (85%)	39 (100%)	0	100	100
54	Ad	37/46 (80%)	37 (100%)	0	100	100
55	Ae	41/59 (70%)	41 (100%)	0	100	100
55	Af	41/59 (70%)	41 (100%)	0	100	100
56	Ag	37/38 (97%)	34 (92%)	3 (8%)	9	32
57	Ah	45/50 (90%)	39 (87%)	6 (13%)	3	17
58	Ai	39/46 (85%)	37 (95%)	2 (5%)	20	43
59	Aj	40/40 (100%)	38 (95%)	2 (5%)	20	44
60	Ak	427/427 (100%)	389 (91%)	38 (9%)	8	28
61	Al	211/211 (100%)	191 (90%)	20 (10%)	7	24
62	Am	226/226 (100%)	199 (88%)	27 (12%)	4	19
63	An	128/129 (99%)	120 (94%)	8 (6%)	15	38
64	Ao	95/95 (100%)	89 (94%)	6 (6%)	15	38
65	Ap	81/81 (100%)	76 (94%)	5 (6%)	15	38
66	Aq	68/68 (100%)	50 (74%)	18 (26%)	0	3
67	Ar	67/75 (89%)	58 (87%)	9 (13%)	3	17
All	All	11155/13269 (84%)	10986 (98%)	169 (2%)	60	75

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
62	Am	160	LEU
66	Aq	7	ASP
62	Am	199	VAL
63	An	147	LYS
66	Aq	38	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 214 such sidechains are listed below:

Mol	Chain	Res	Type
46	v	45	ASN
45	5	193	GLN
62	Am	12	ASN
46	v	291	HIS
48	x	285	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 5 are monoatomic - leaving 47 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
77	HEC	8	402	48	32,50,50	2.23	3 (9%)	24,82,82	1.49	4 (16%)
71	PLX	V	202	-	51,51,51	0.77	1 (1%)	55,59,59	0.58	1 (1%)
71	PLX	i	502	-	51,51,51	0.75	1 (1%)	55,59,59	0.65	1 (1%)
75	PEE	W	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.98	2 (3%)
74	CDL	z	101	-	63,63,99	1.22	5 (7%)	69,75,111	1.08	6 (8%)
76	HEM	7	403	47	41,50,50	4.58	12 (29%)	45,82,82	3.73	26 (57%)
72	NDP	L	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.32	4 (7%)
74	CDL	u	501	-	63,63,99	1.25	5 (7%)	69,75,111	1.00	4 (5%)
71	PLX	4	301	-	51,51,51	0.79	1 (1%)	55,59,59	0.61	1 (1%)
69	FMN	B	502	-	33,33,33	1.42	6 (18%)	48,50,50	1.30	8 (16%)
73	ZMP	X	201	-	27,33,36	1.96	6 (22%)	32,40,45	1.98	7 (21%)
73	ZMP	Q	201	-	27,33,36	1.94	5 (18%)	32,40,45	1.89	6 (18%)
75	PEE	i	501	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
74	CDL	Aa	101	-	63,63,99	1.27	5 (7%)	69,75,111	1.13	5 (7%)
70	FES	2	303	-	0,4,4	-	-	-	-	-
75	PEE	7	402	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
68	SF4	H	301	8	0,12,12	-	-	-	-	-
74	CDL	l	702	-	63,63,99	1.22	5 (7%)	69,75,111	1.06	4 (5%)
74	CDL	5	501	-	63,63,99	1.24	5 (7%)	69,75,111	0.99	4 (5%)
68	SF4	B	501	2	0,12,12	-	-	-	-	-
68	SF4	G	802	7	0,12,12	-	-	-	-	-
74	CDL	x	402	-	63,63,99	1.26	5 (7%)	69,75,111	1.08	5 (7%)
68	SF4	G	801	7	0,12,12	-	-	-	-	-
74	CDL	8	401	-	63,63,99	1.24	6 (9%)	69,75,111	0.99	4 (5%)
74	CDL	s	201	-	63,63,99	1.23	5 (7%)	69,75,111	1.04	4 (5%)
75	PEE	2	302	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
68	SF4	H	302	8	0,12,12	-	-	-	-	-
78	HEA	Ak	601	60	57,67,67	1.24	6 (10%)	61,103,103	1.47	11 (18%)
75	PEE	w	403	-	48,48,50	1.33	4 (8%)	51,53,55	0.98	2 (3%)
75	PEE	7	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
76	HEM	w	402	47	41,50,50	4.55	13 (31%)	45,82,82	3.39	22 (48%)
76	HEM	7	404	-	41,50,50	4.58	12 (29%)	45,82,82	3.46	18 (40%)
70	FES	4	302	53	0,4,4	-	-	-	-	-
68	SF4	I	301	9	0,12,12	-	-	-	-	-
70	FES	G	803	7	0,4,4	-	-	-	-	-
71	PLX	H	303	-	51,51,51	0.78	1 (1%)	55,59,59	0.63	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PEE	5	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
74	CDL	V	201	-	61,61,99	1.18	5 (8%)	64,71,111	1.11	4 (6%)
75	PEE	q	501	-	48,48,50	1.35	4 (8%)	51,53,55	0.92	2 (3%)
77	HEC	x	401	48	32,50,50	2.37	3 (9%)	24,82,82	1.64	5 (20%)
70	FES	E	301	-	0,4,4	-	-	-	-	-
75	PEE	l	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.94	2 (3%)
71	PLX	2	301	-	51,51,51	0.77	1 (1%)	55,59,59	0.58	1 (1%)
76	HEM	w	401	47	41,50,50	4.55	12 (29%)	45,82,82	3.37	22 (48%)
78	HEA	Ak	602	60	57,67,67	1.48	6 (10%)	61,103,103	1.46	12 (19%)
74	CDL	i	503	-	63,63,99	1.22	5 (7%)	69,75,111	1.07	4 (5%)
75	PEE	u	502	-	48,48,50	1.38	4 (8%)	51,53,55	0.91	2 (3%)

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
77	HEC	8	402	48	-	4/10/54/54	-
71	PLX	V	202	-	-	32/55/55/55	-
71	PLX	i	502	-	-	25/55/55/55	-
75	PEE	W	401	-	-	21/52/52/54	-
74	CDL	z	101	-	-	44/74/74/110	-
76	HEM	7	403	47	-	8/12/54/54	-
72	NDP	L	401	-	-	15/30/77/77	0/5/5/5
74	CDL	u	501	-	-	38/74/74/110	-
71	PLX	4	301	-	-	26/55/55/55	-
69	FMN	B	502	-	-	4/18/18/18	0/3/3/3
73	ZMP	X	201	-	-	7/38/40/43	-
73	ZMP	Q	201	-	-	11/38/40/43	-
75	PEE	i	501	-	-	32/52/52/54	-
74	CDL	Aa	101	-	-	32/74/74/110	-
70	FES	2	303	-	-	-	0/1/1/1
75	PEE	7	402	-	-	30/52/52/54	-
68	SF4	H	301	8	-	-	0/6/5/5
74	CDL	5	501	-	-	40/74/74/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	CDL	8	401	-	-	37/74/74/110	-
74	CDL	x	402	-	-	44/74/74/110	-
74	CDL	l	702	-	-	25/74/74/110	-
75	PEE	2	302	-	-	27/52/52/54	-
78	HEA	Ak	601	60	-	7/32/76/76	-
68	SF4	B	501	2	-	-	0/6/5/5
74	CDL	s	201	-	-	40/74/74/110	-
68	SF4	G	801	7	-	-	0/6/5/5
68	SF4	G	802	7	-	-	0/6/5/5
68	SF4	H	302	8	-	-	0/6/5/5
75	PEE	w	403	-	-	20/52/52/54	-
75	PEE	7	401	-	-	17/44/44/54	-
76	HEM	w	402	47	-	5/12/54/54	-
76	HEM	7	404	-	-	5/12/54/54	-
70	FES	4	302	53	-	-	0/1/1/1
68	SF4	I	301	9	-	-	0/6/5/5
71	PLX	H	303	-	-	33/55/55/55	-
75	PEE	5	502	-	-	20/52/52/54	-
70	FES	G	803	7	-	-	0/1/1/1
74	CDL	V	201	-	-	28/69/69/110	-
75	PEE	q	501	-	-	22/52/52/54	-
77	HEC	x	401	48	-	6/10/54/54	-
70	FES	E	301	-	-	-	0/1/1/1
75	PEE	l	701	-	-	30/52/52/54	-
71	PLX	2	301	-	-	27/55/55/55	-
76	HEM	w	401	47	-	5/12/54/54	-
78	HEA	Ak	602	60	-	5/32/76/76	-
74	CDL	i	503	-	-	41/74/74/110	-
75	PEE	u	502	-	-	22/52/52/54	-

The worst 5 of 182 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7	403	HEM	C4A-CHB	13.21	1.77	1.41
76	7	404	HEM	C4A-CHB	12.89	1.76	1.41
76	w	401	HEM	C4A-CHB	12.72	1.76	1.41
76	w	402	HEM	C4A-CHB	12.54	1.75	1.41
76	w	401	HEM	C1A-CHA	12.36	1.75	1.41

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	7	403	HEM	C4A-C3A-C2A	-12.30	98.44	107.00
76	7	403	HEM	C4B-CHC-C1C	-10.37	108.87	122.56
76	w	402	HEM	C4C-CHD-C1D	-9.52	109.99	122.56
76	7	404	HEM	C4A-C3A-C2A	-9.50	100.39	107.00
76	7	404	HEM	C4B-CHC-C1C	-9.41	110.14	122.56

There are no chirality outliers.

5 of 835 torsion outliers are listed below:

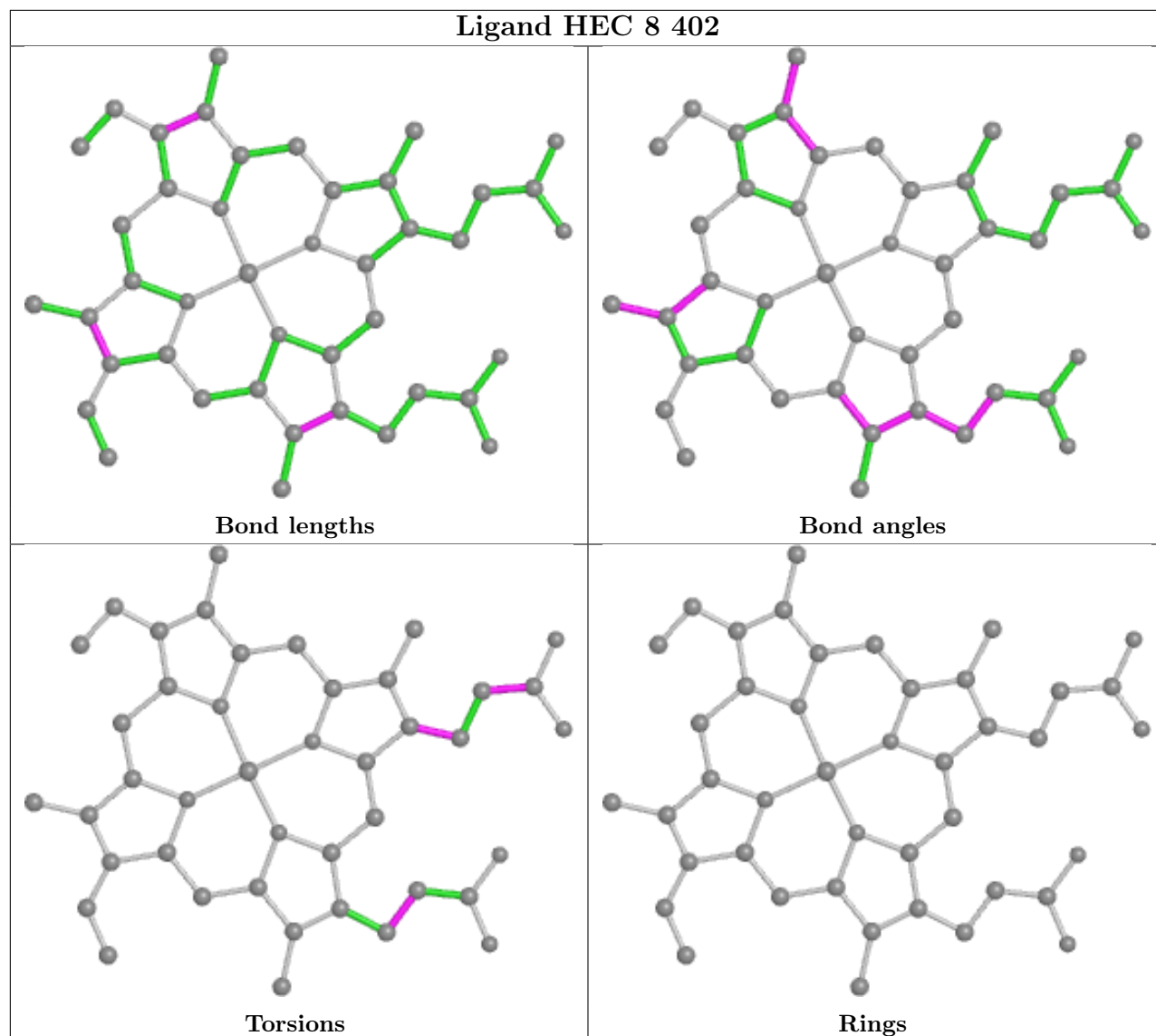
Mol	Chain	Res	Type	Atoms
69	B	502	FMN	C1'-C2'-C3'-C4'
69	B	502	FMN	C3'-C4'-C5'-O5'
69	B	502	FMN	O4'-C4'-C5'-O5'
71	H	303	PLX	O7-C6-O6-C4
71	H	303	PLX	O9-C24-O8-C5

There are no ring outliers.

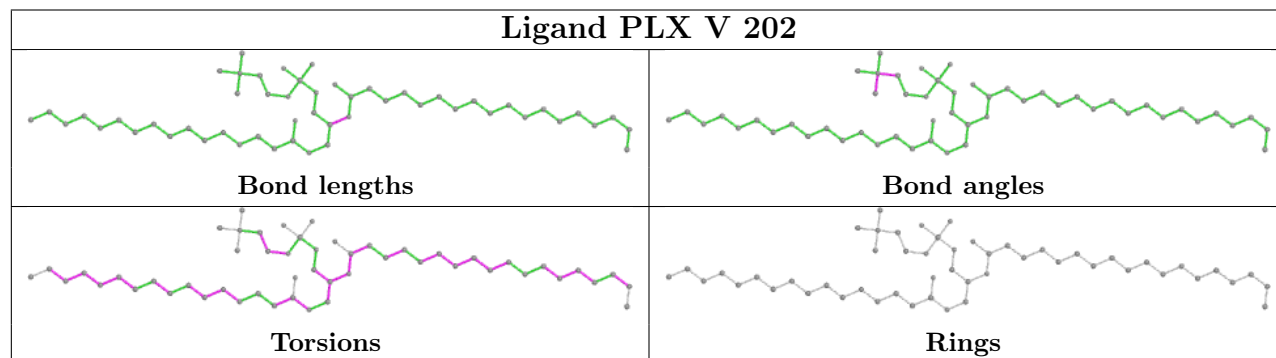
No monomer is involved in short contacts.

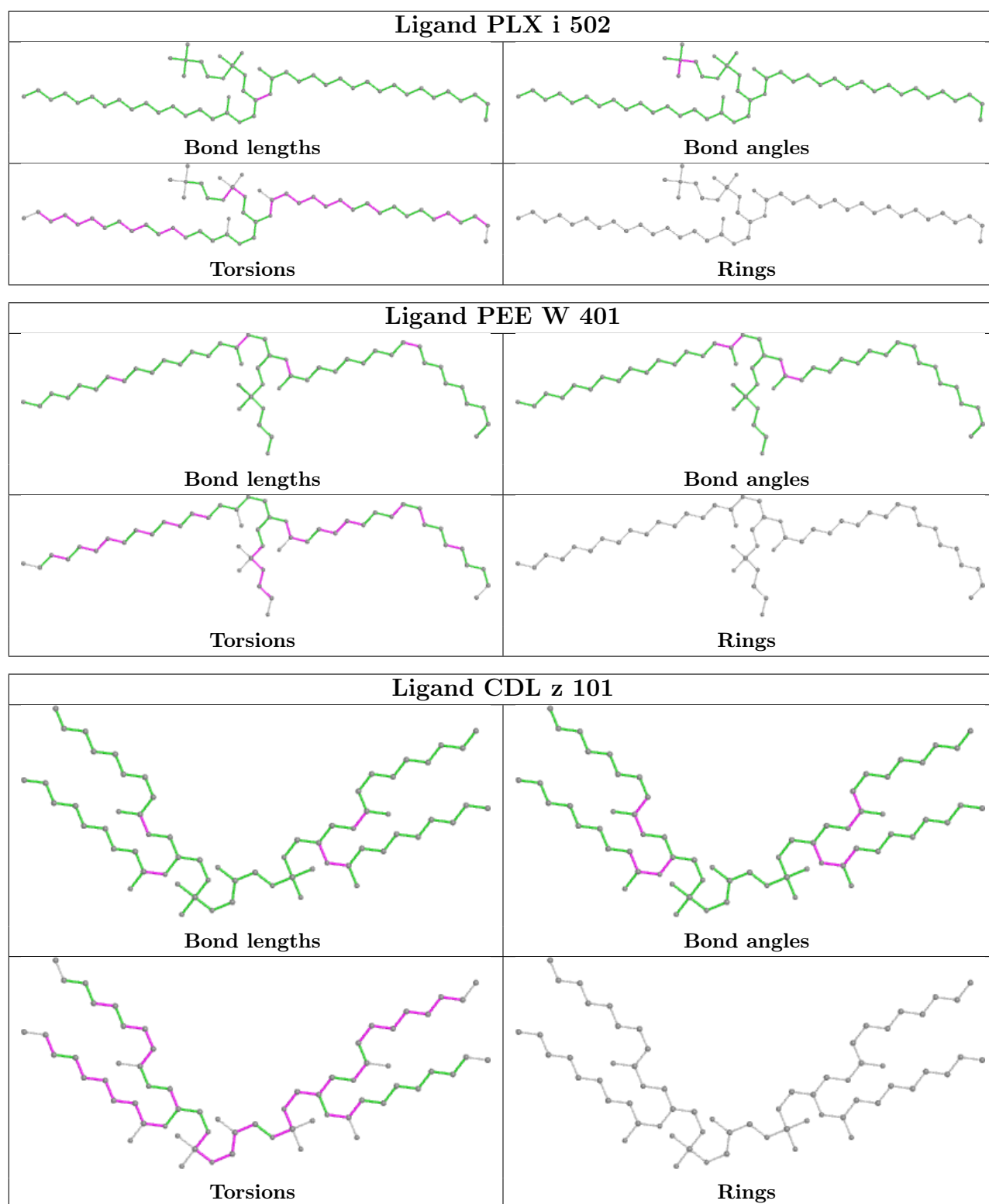
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

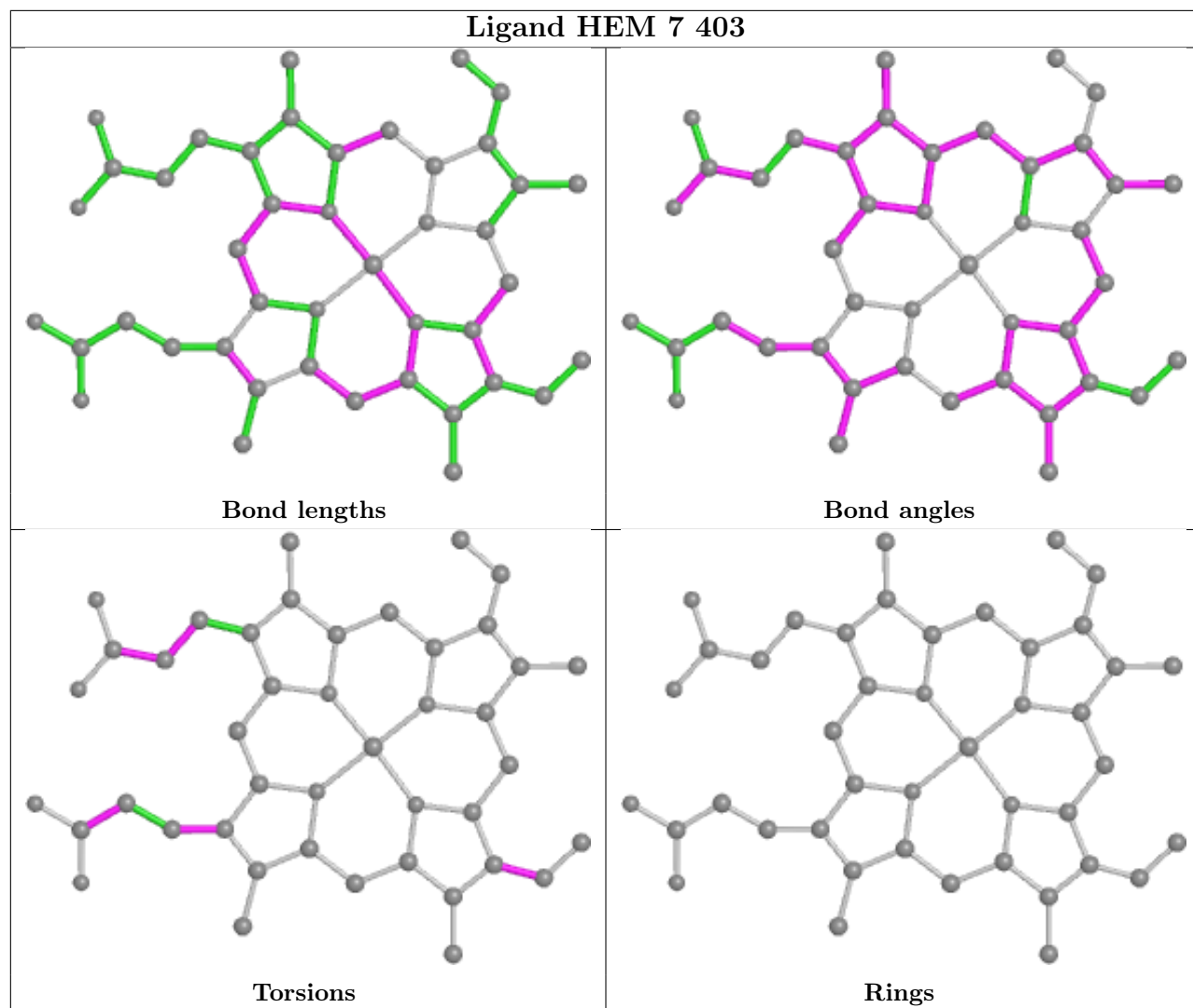
Ligand HEC 8 402

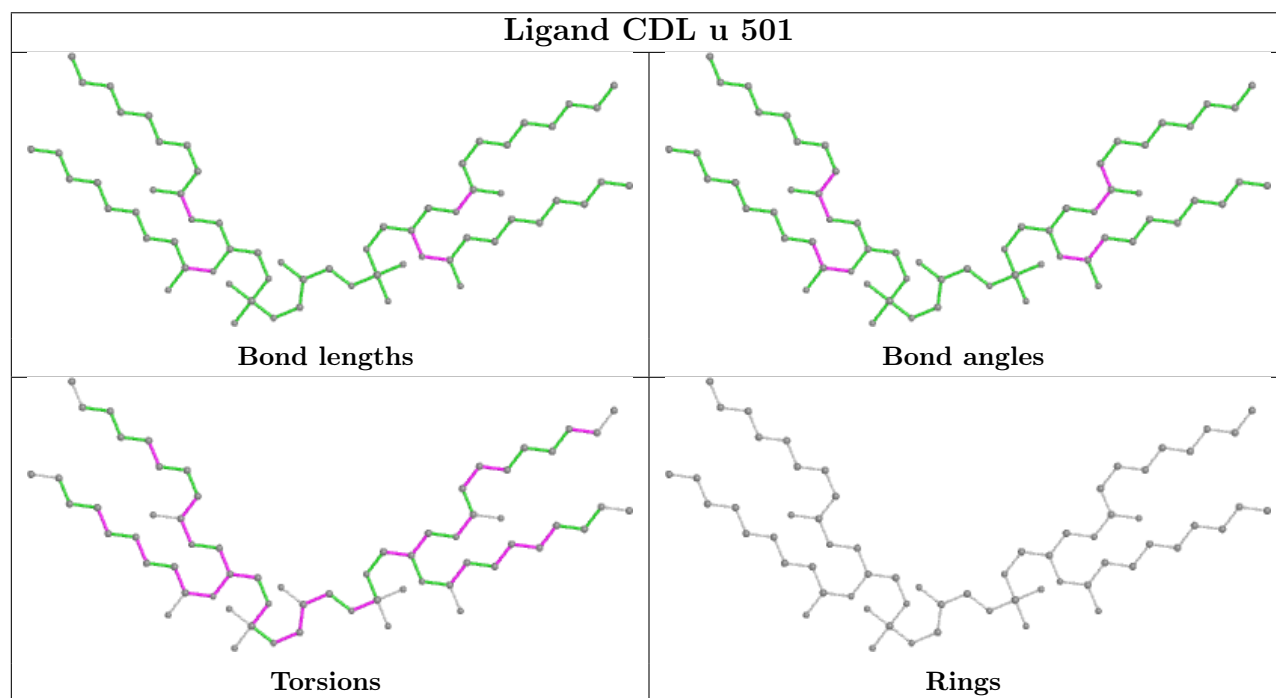
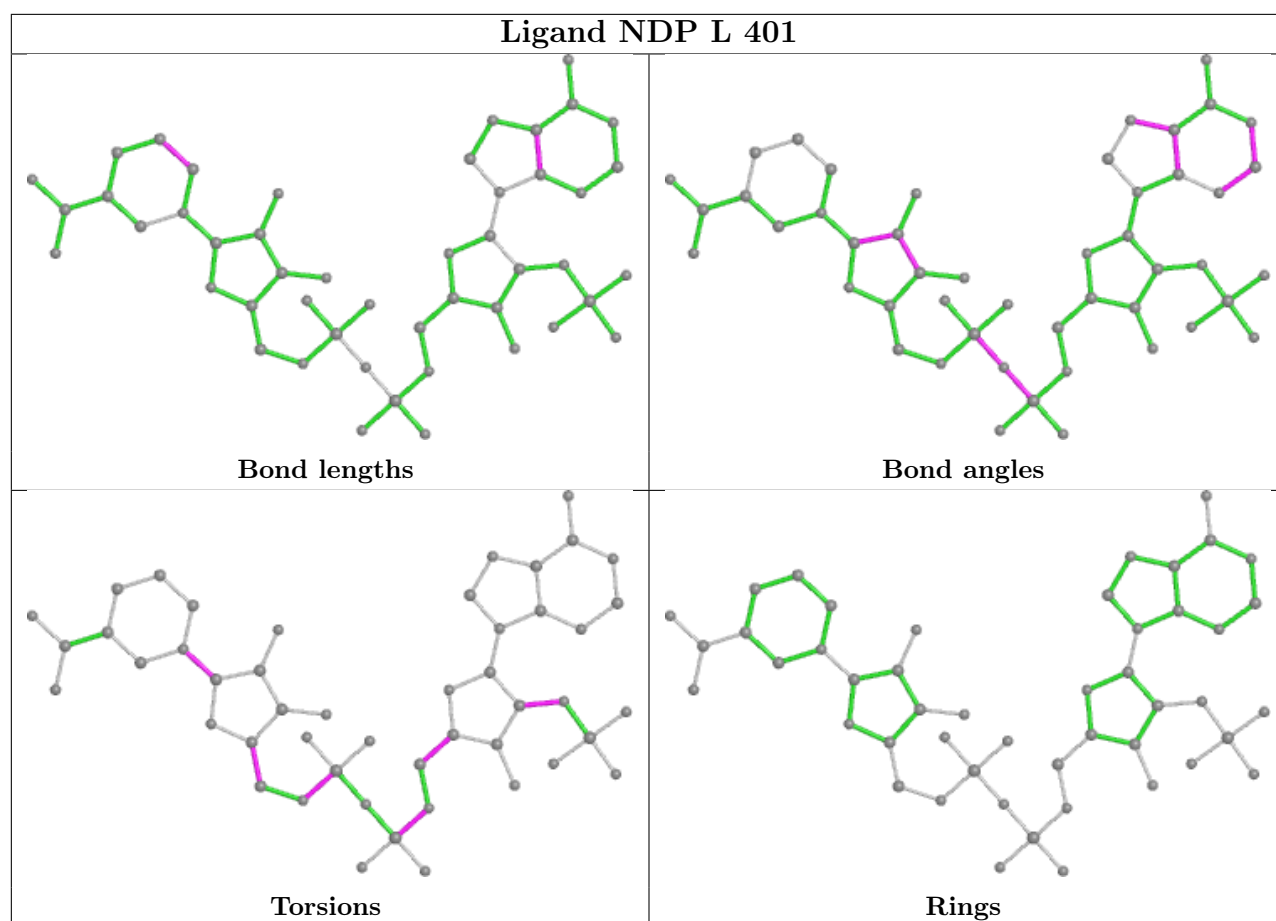


Ligand PLX V 202

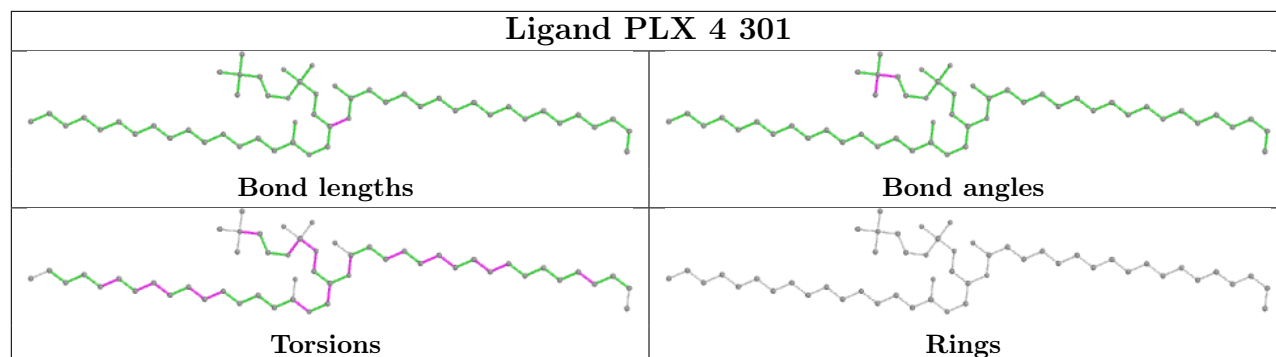




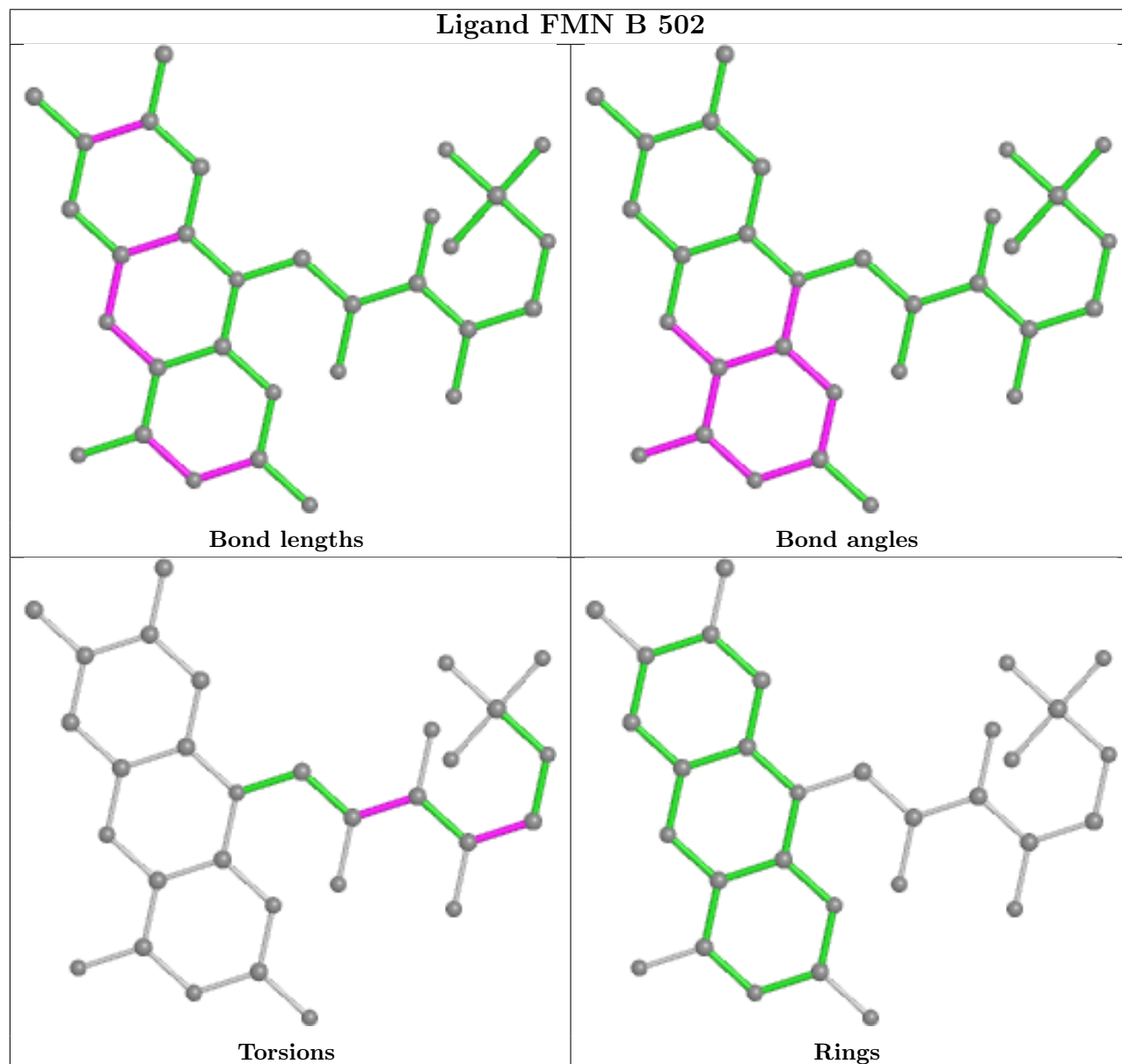


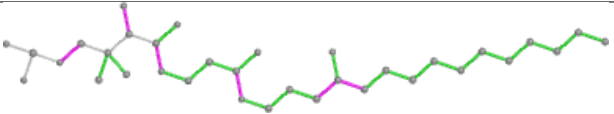
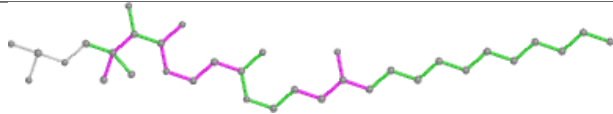
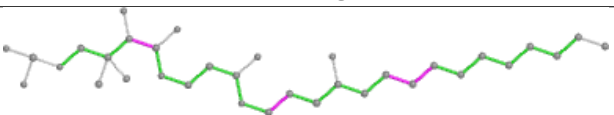
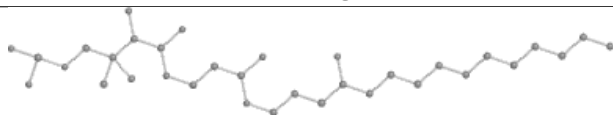
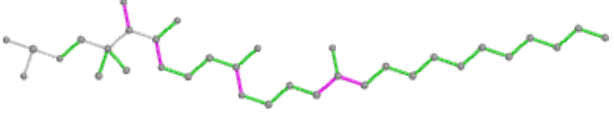
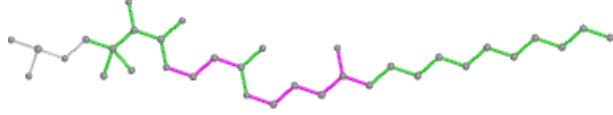
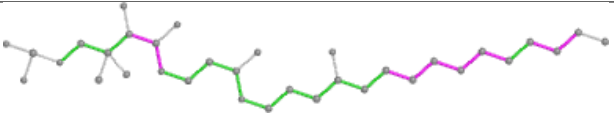
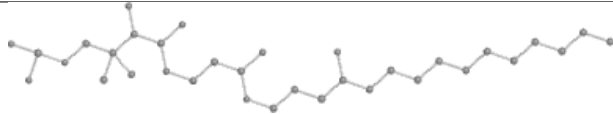
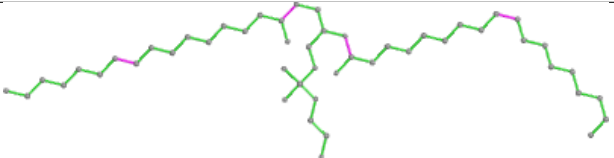
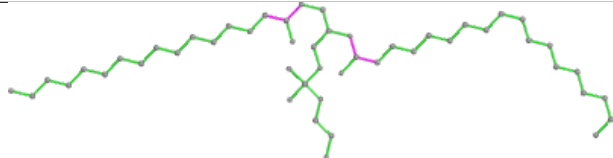
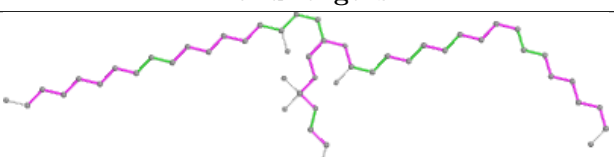
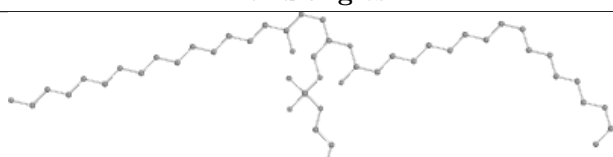


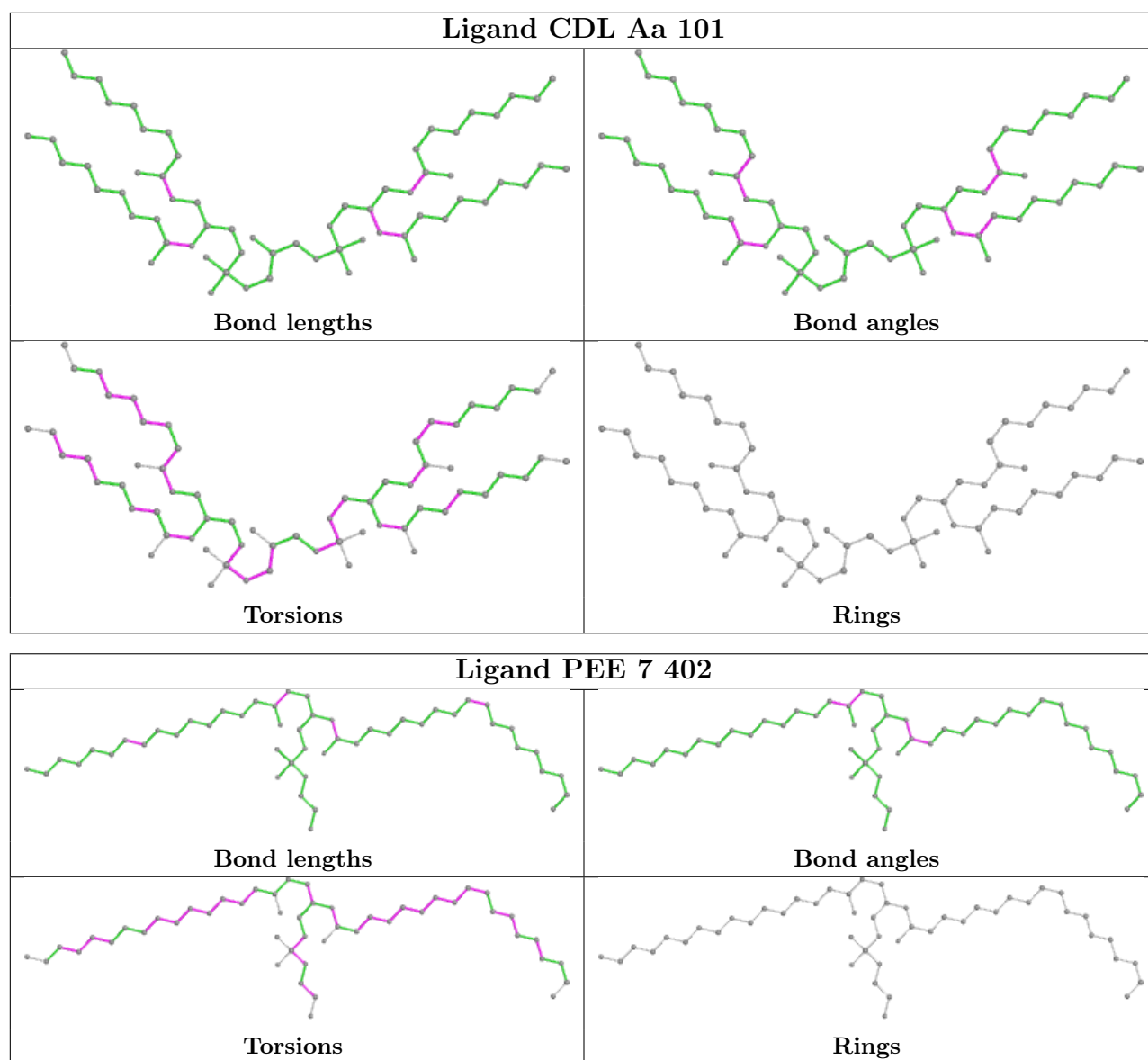
Ligand PLX 4 301

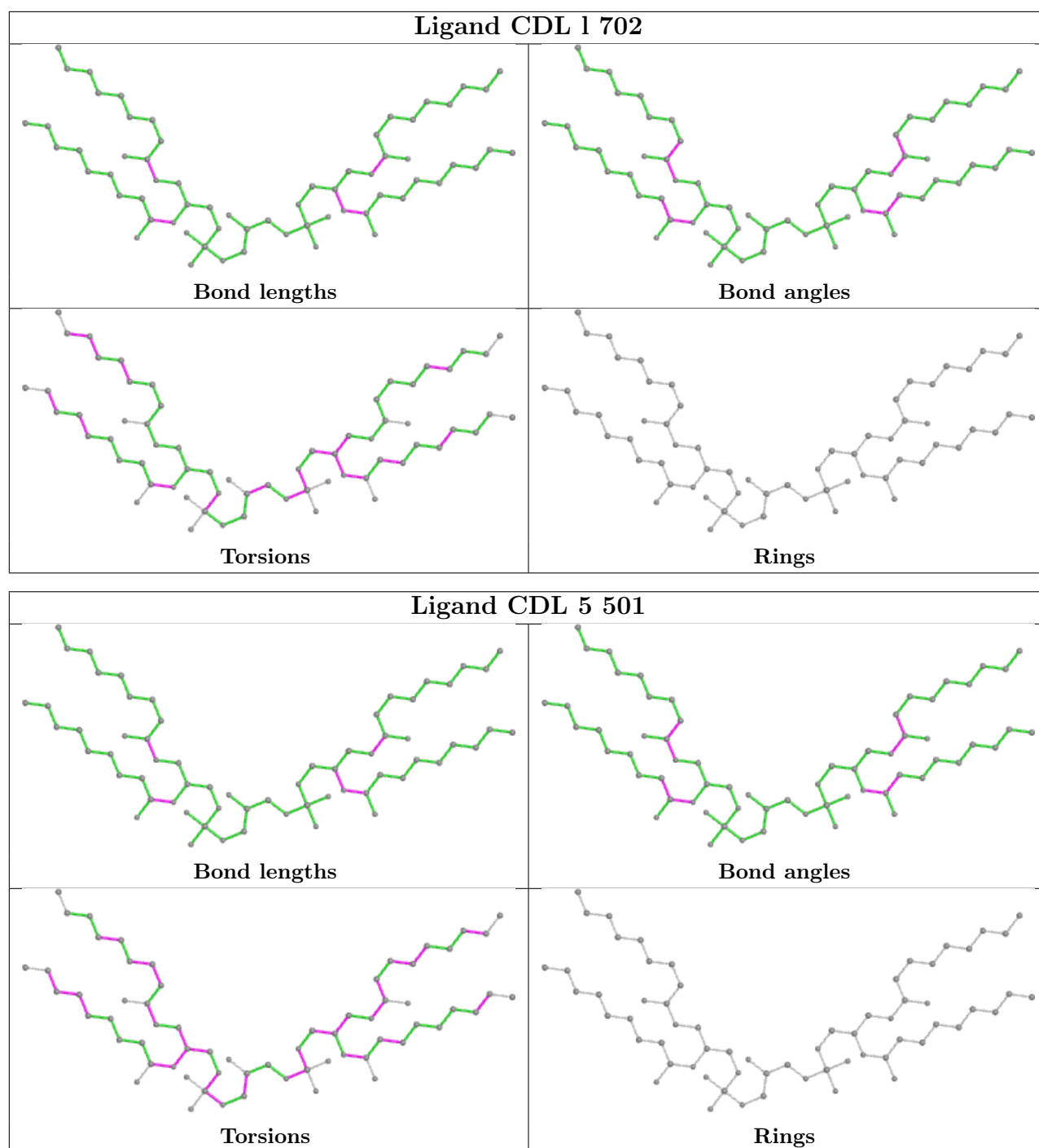


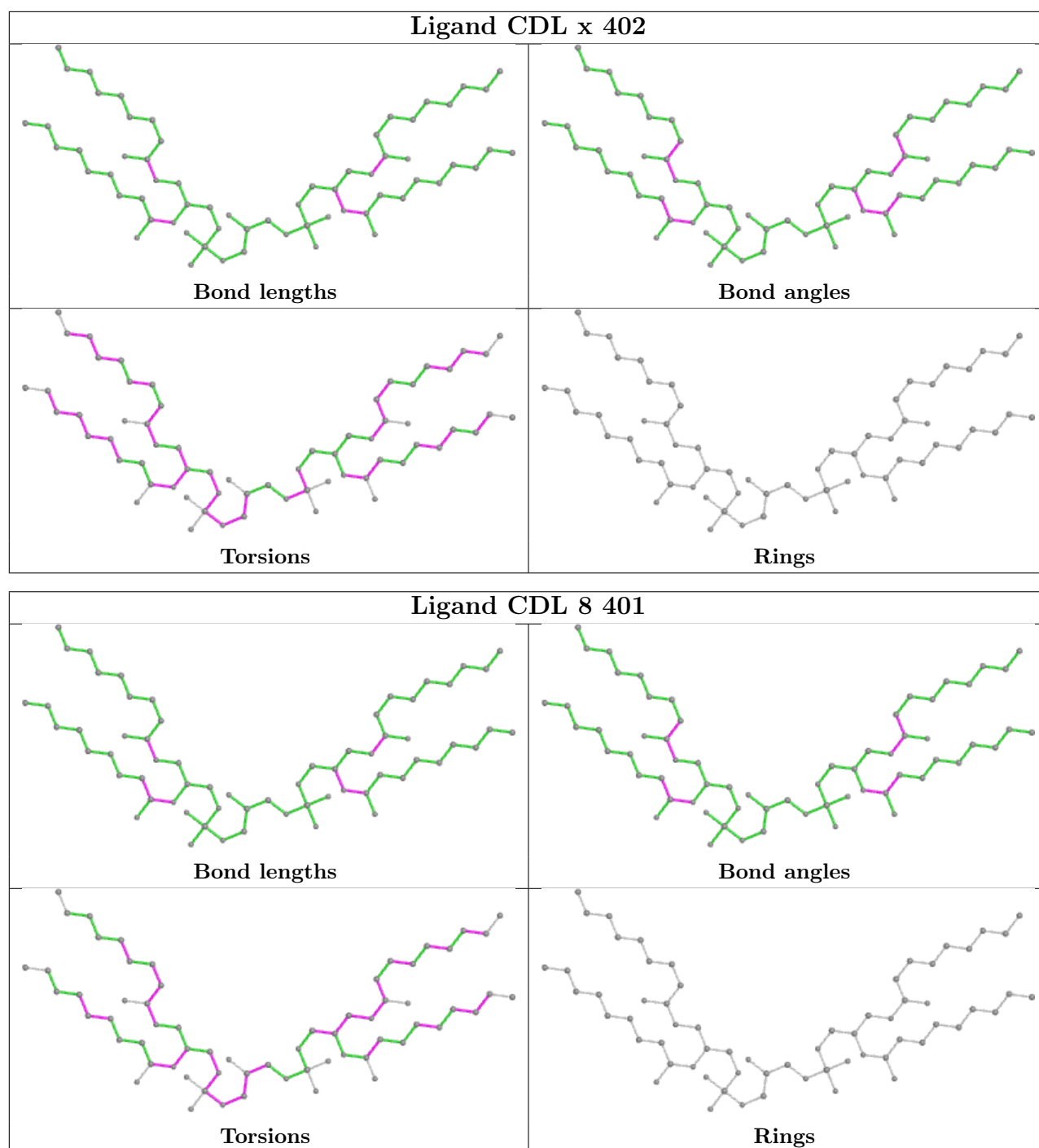
Ligand FMN B 502

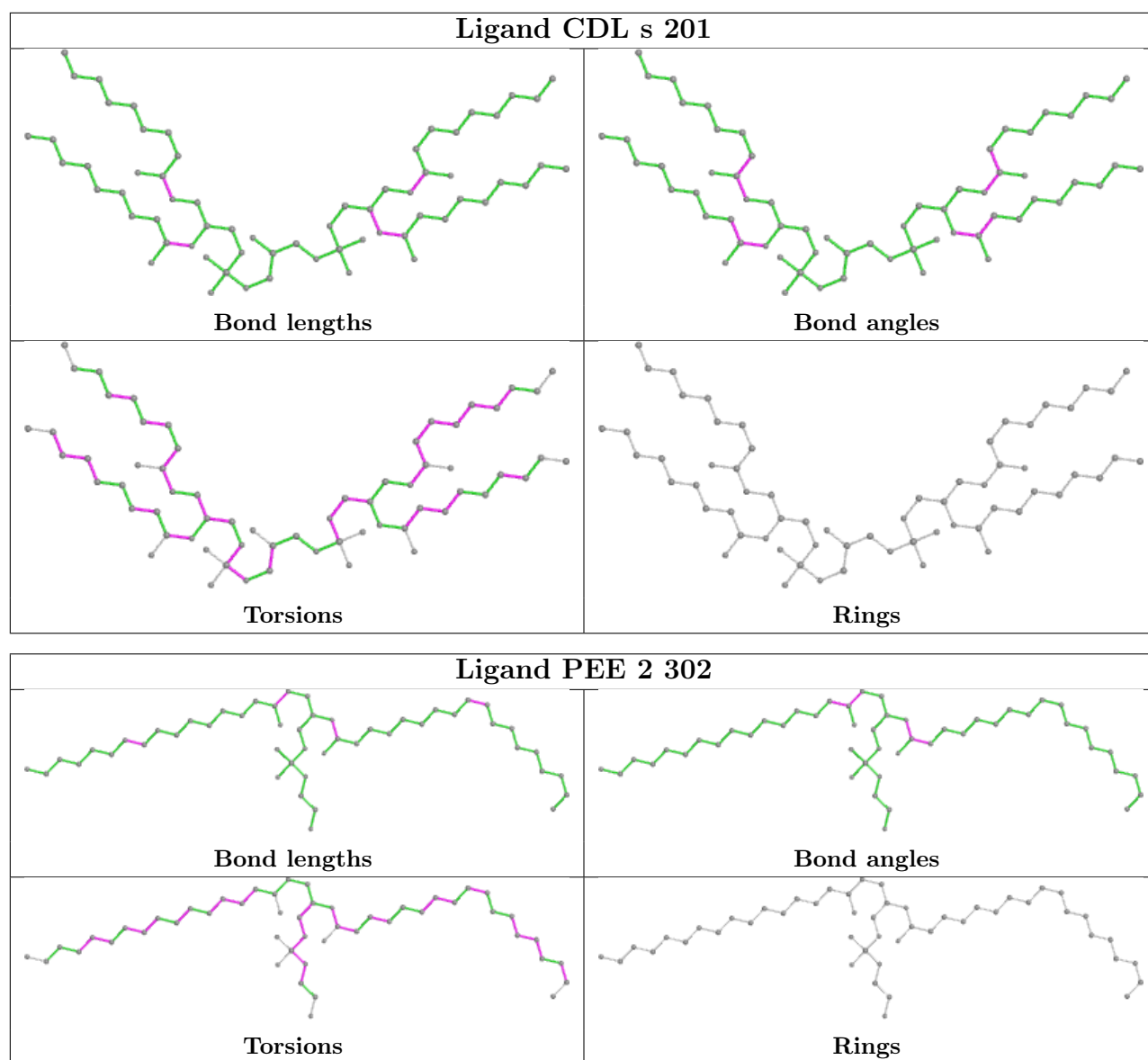


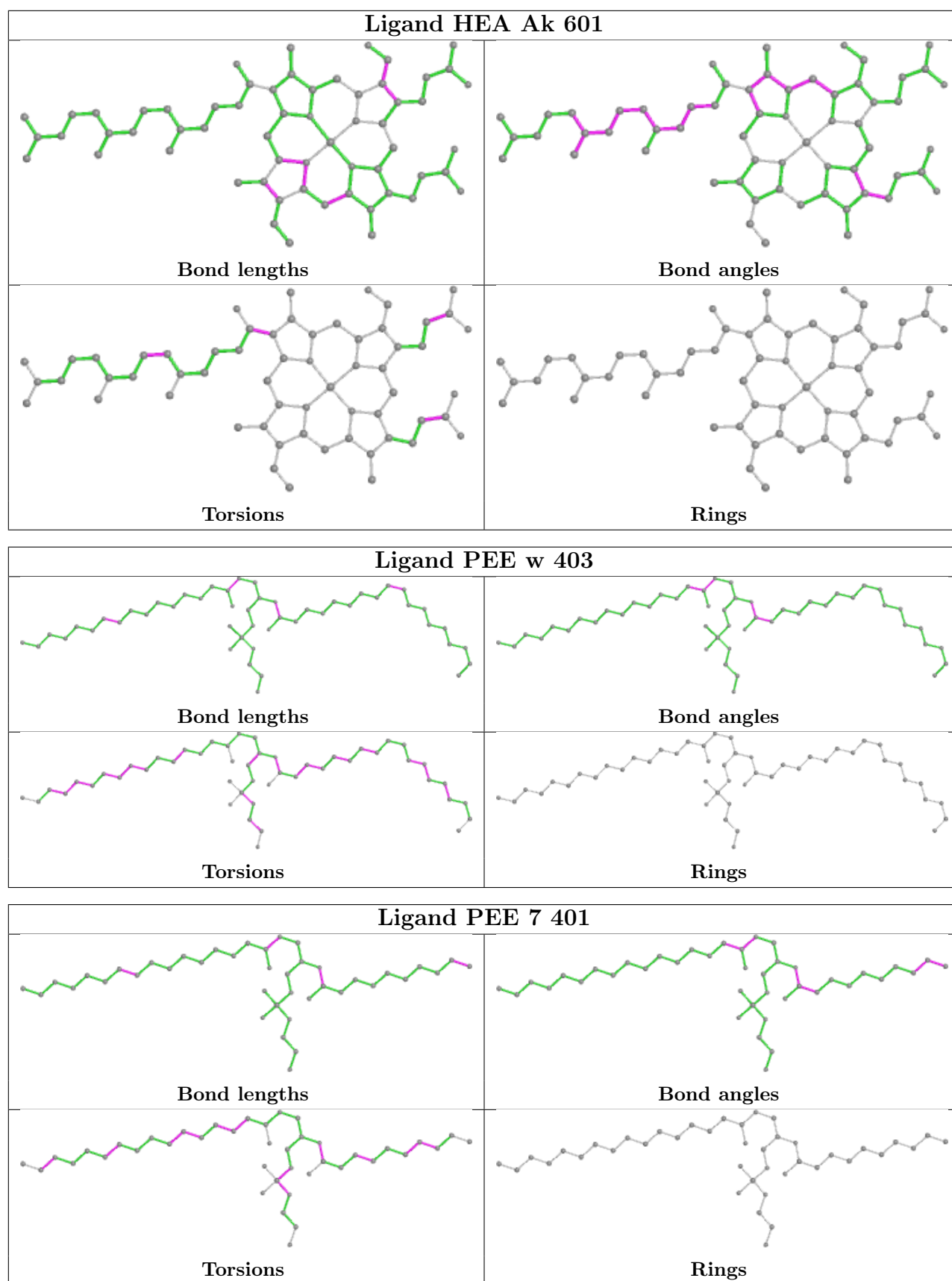
Ligand ZMP X 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand ZMP Q 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEE i 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

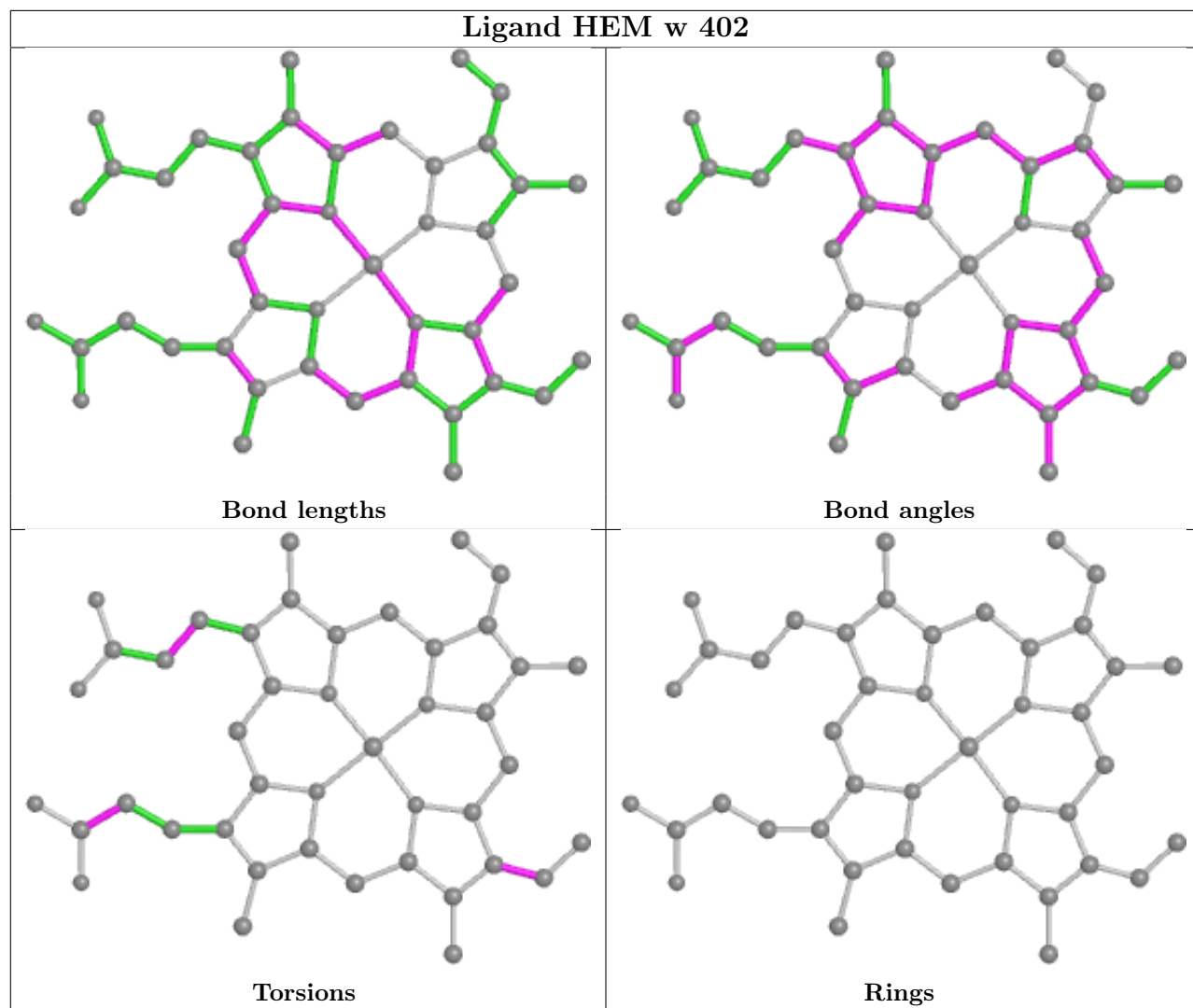


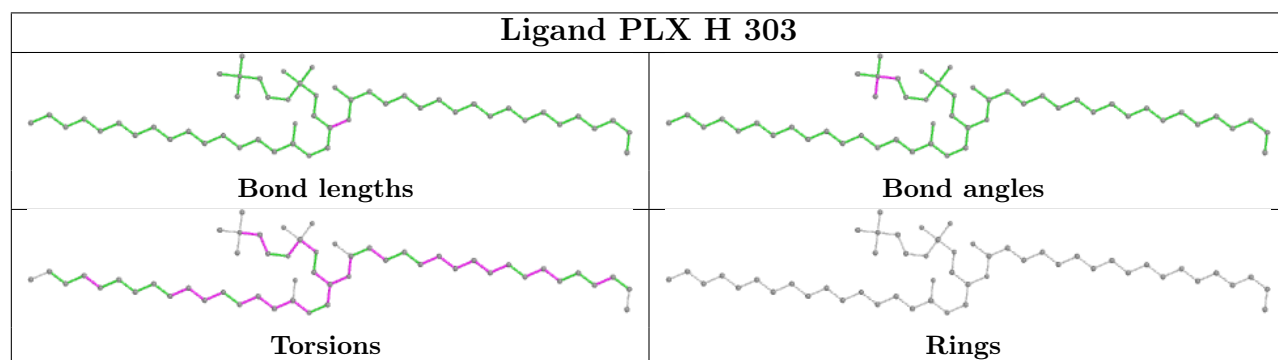
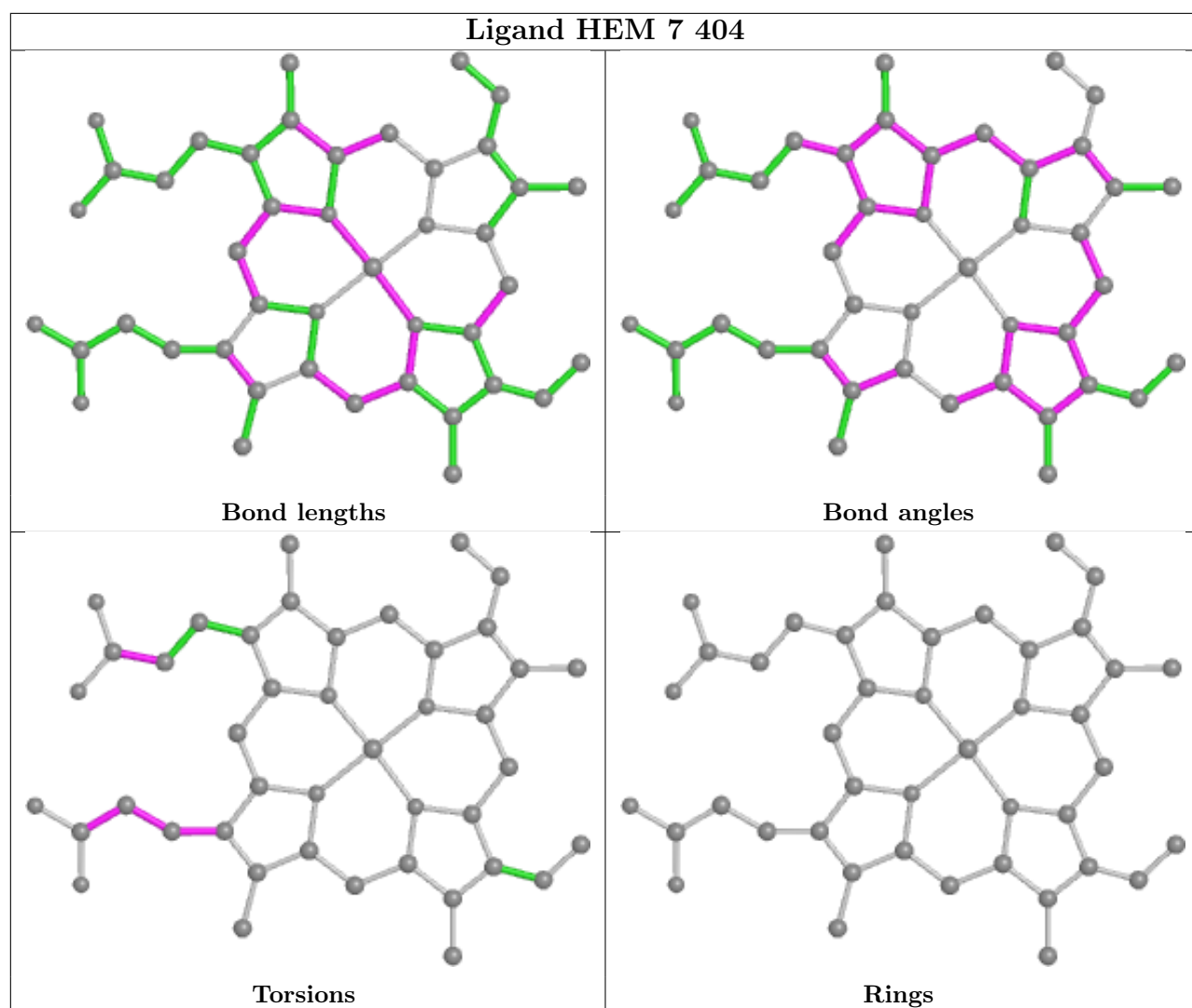


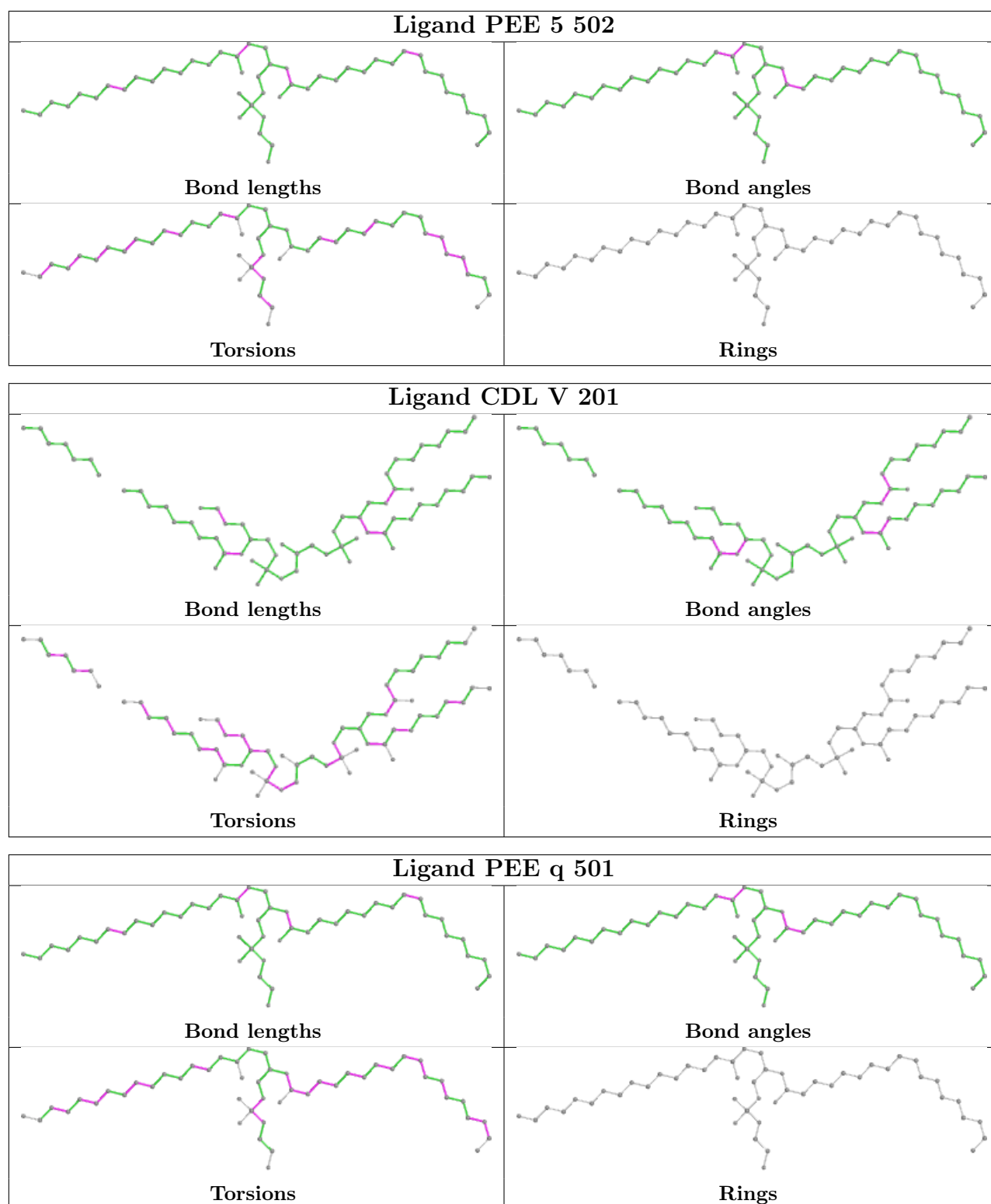


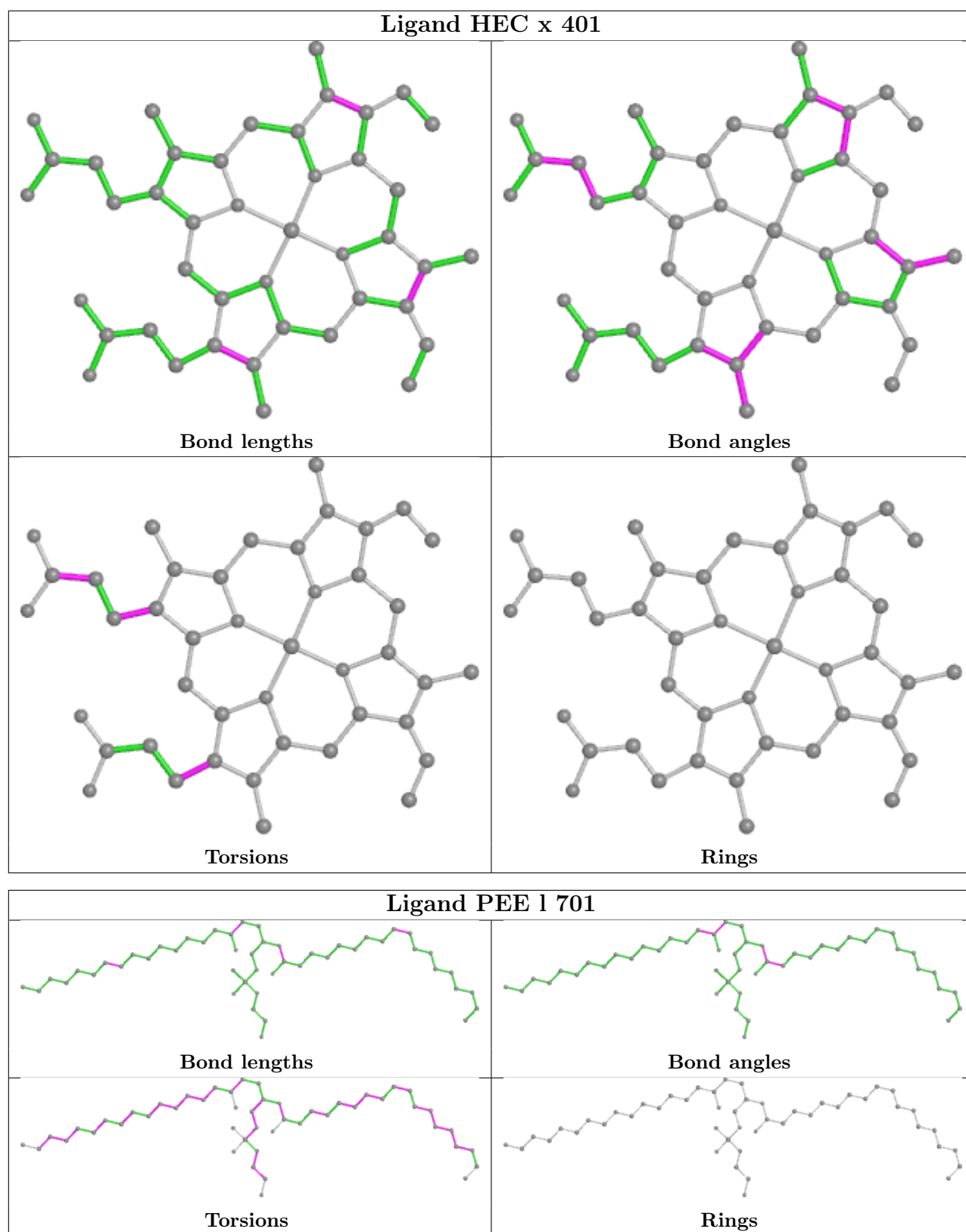


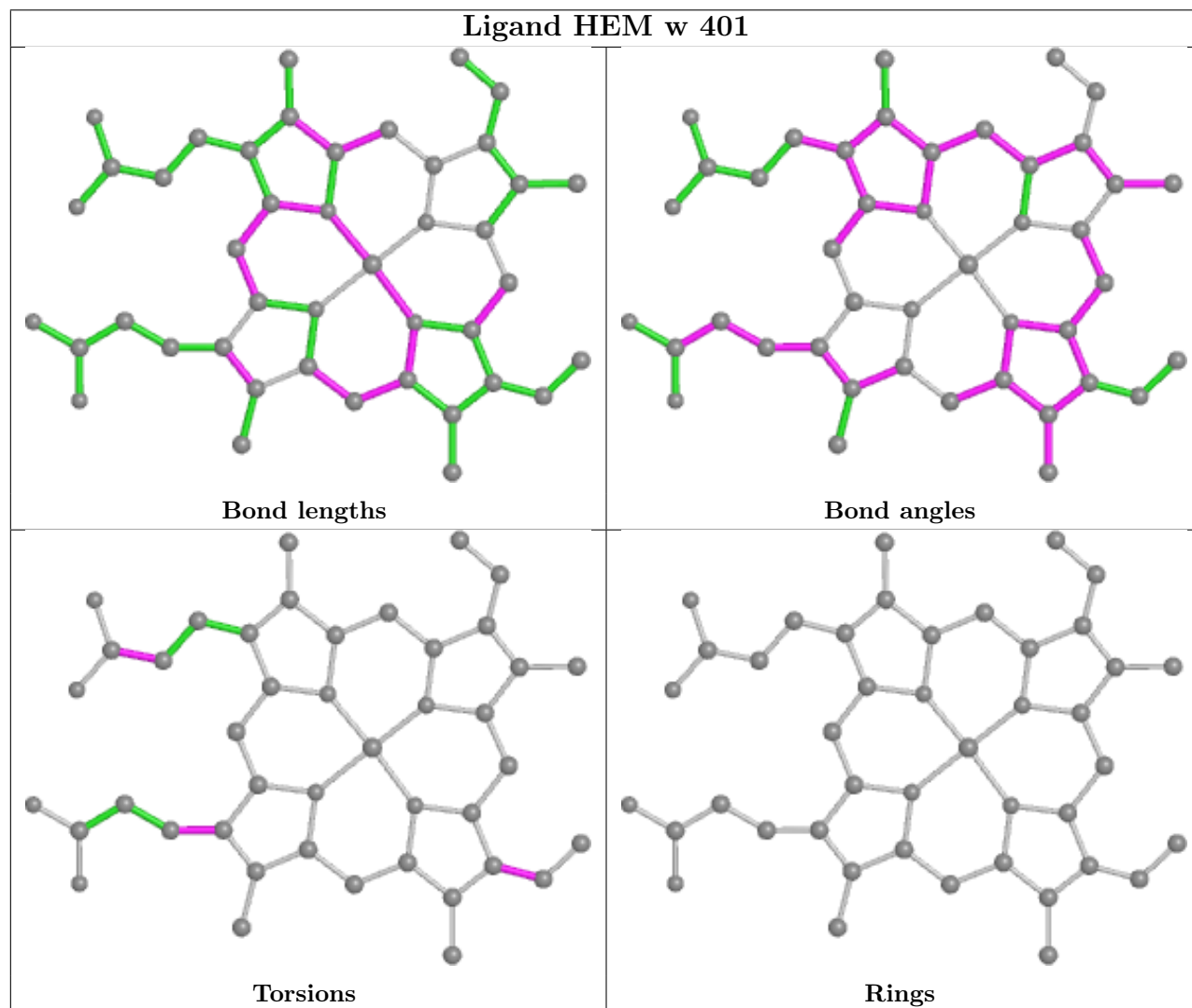
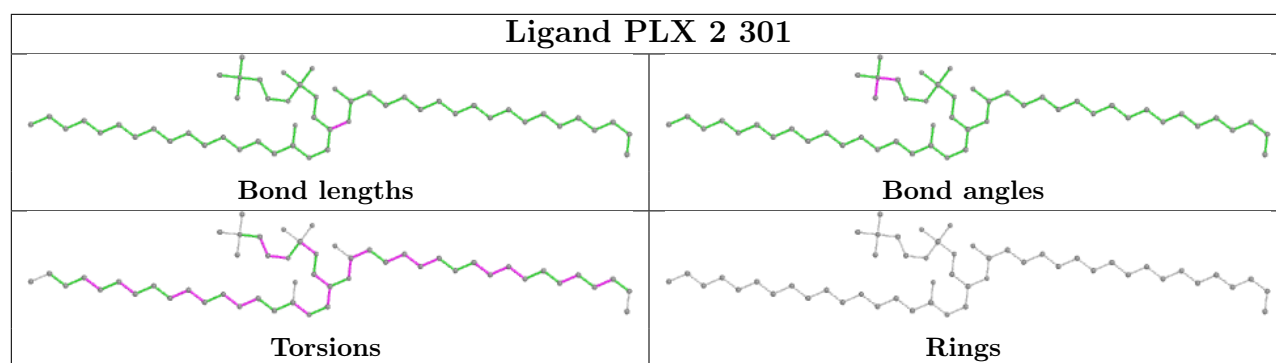


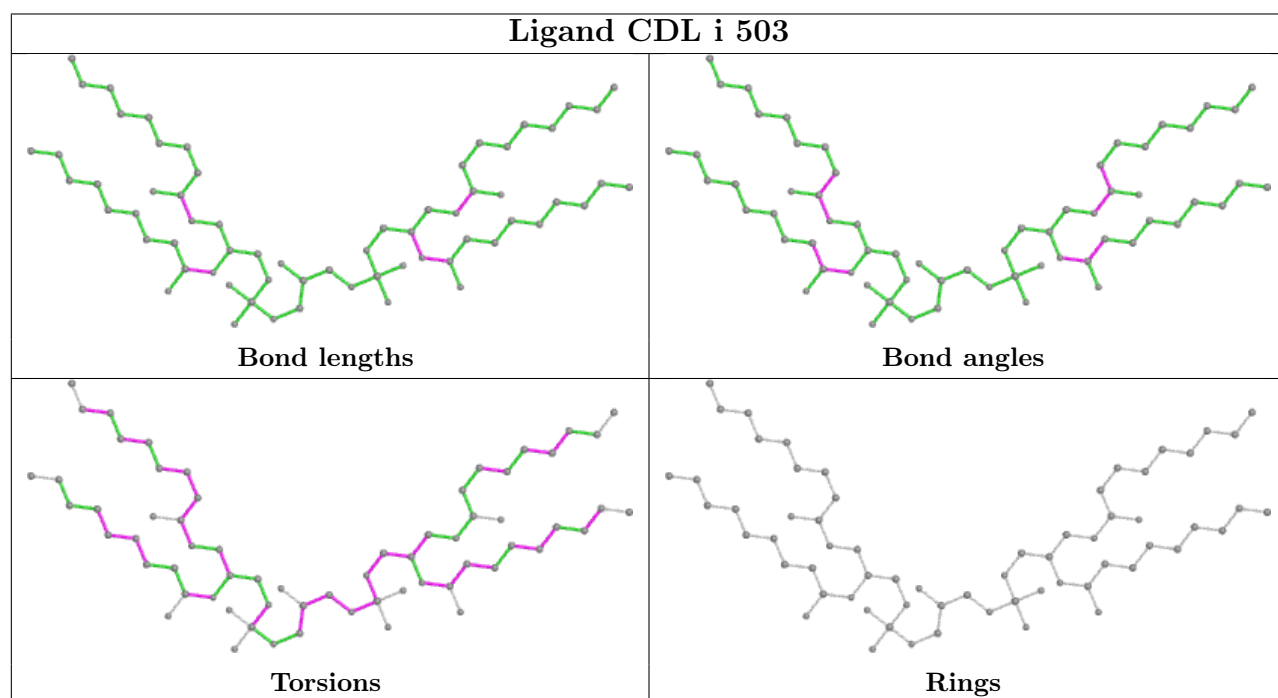
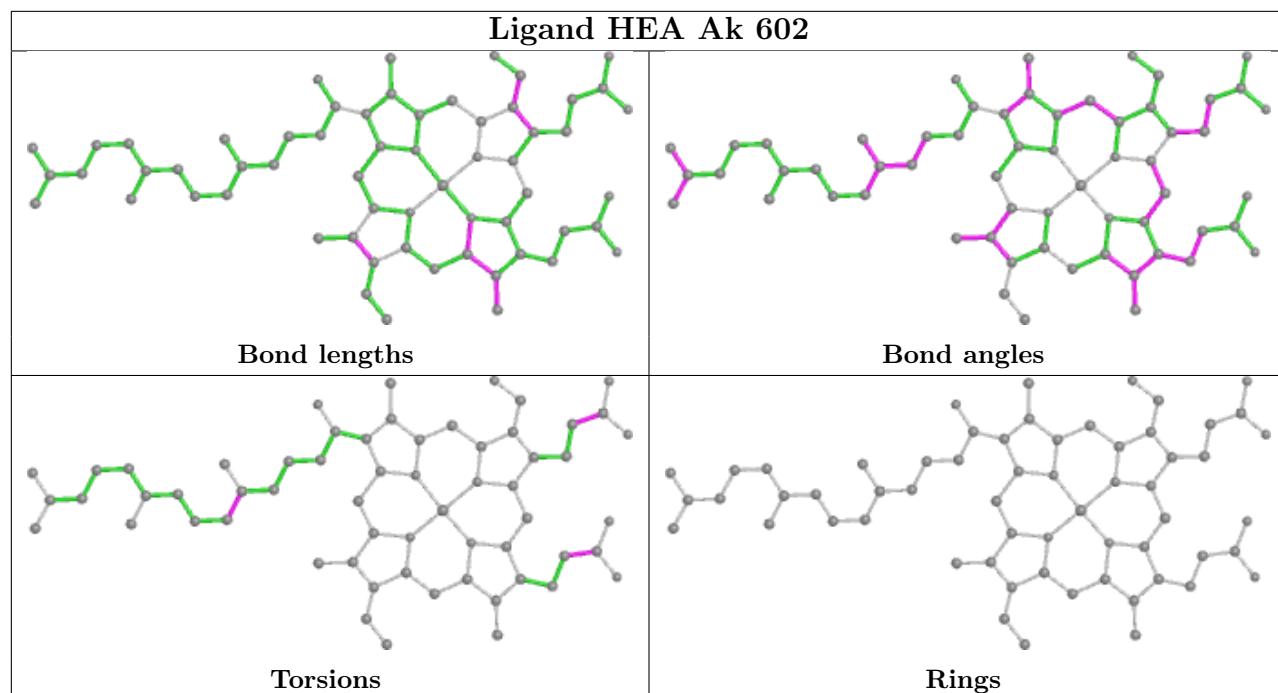


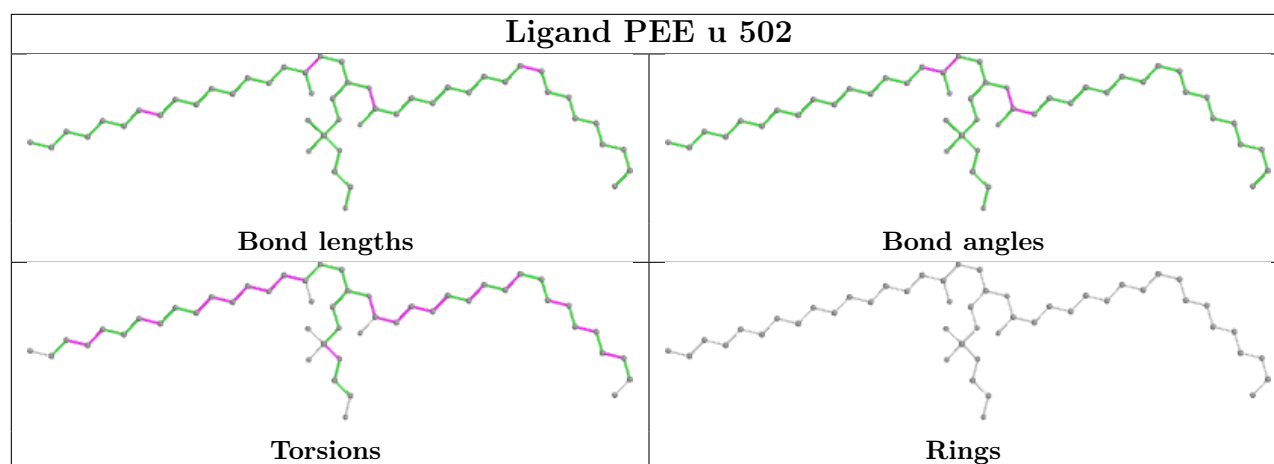












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

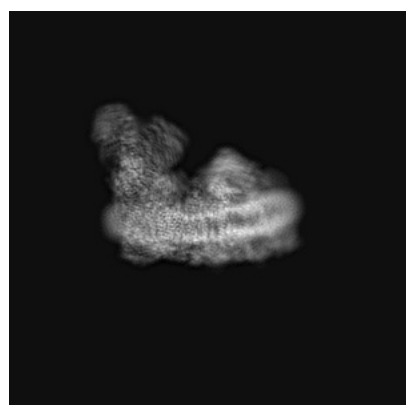
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9539. These allow visual inspection of the internal detail of the map and identification of artifacts.

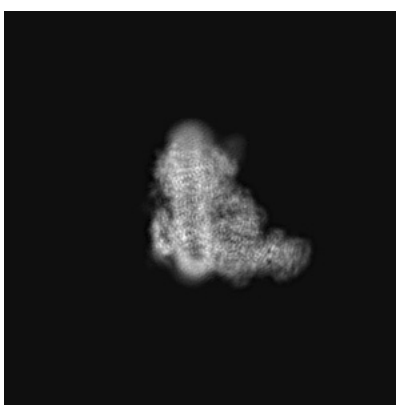
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

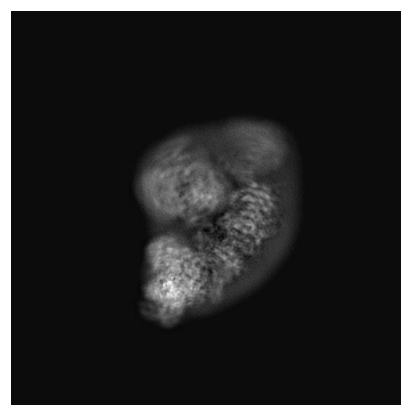
6.1.1 Primary map



X



Y



Z

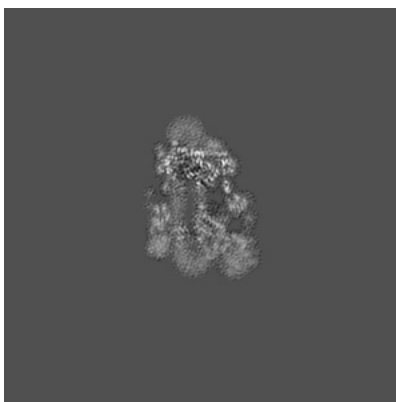
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

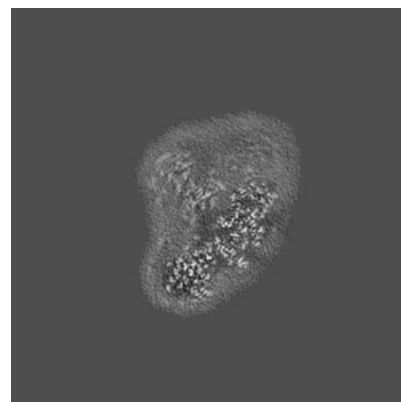
6.2.1 Primary map



X Index: 240



Y Index: 240

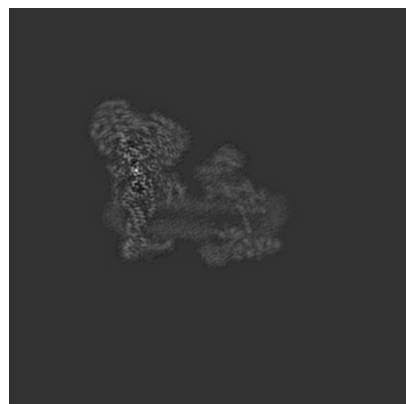


Z Index: 240

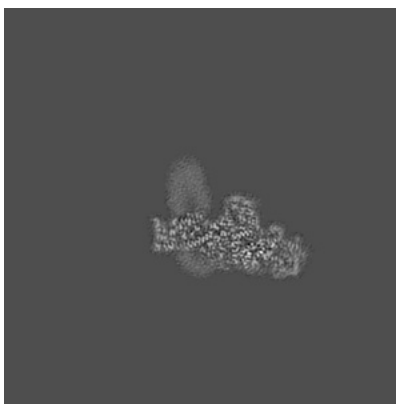
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

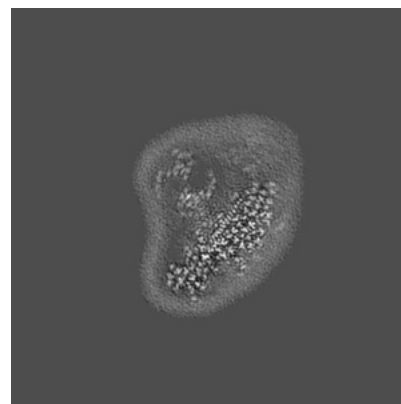
6.3.1 Primary map



X Index: 191



Y Index: 145

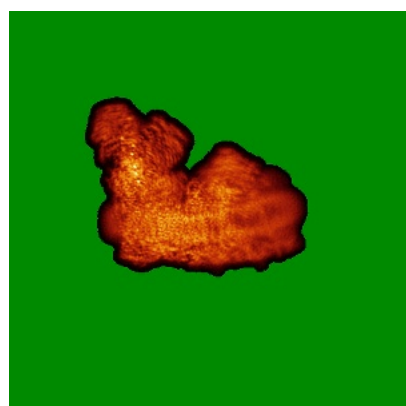


Z Index: 231

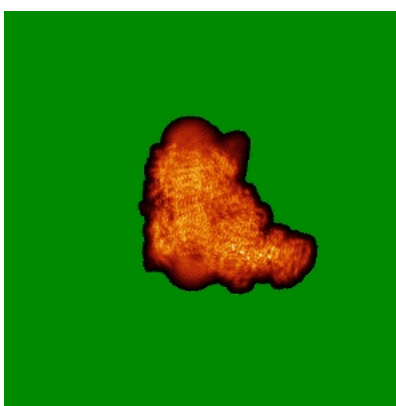
The images above show the largest variance slices of the map in three orthogonal directions.

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

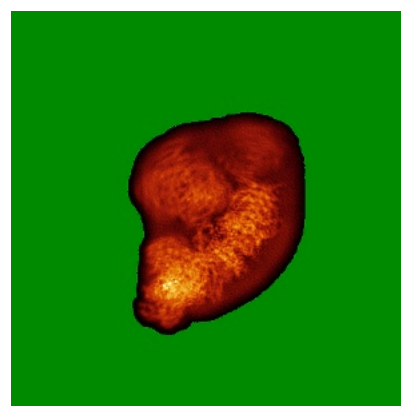
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0504. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

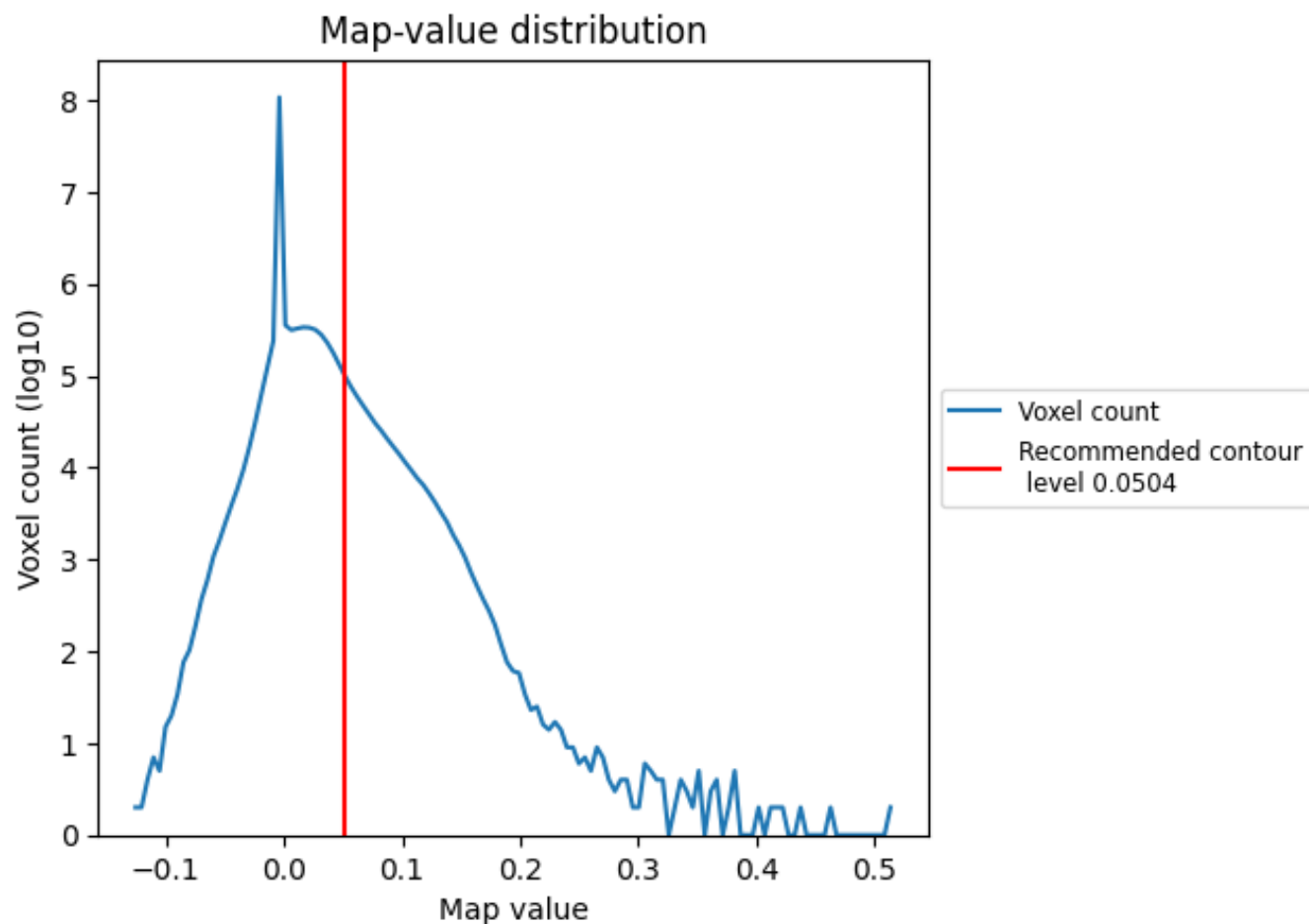
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

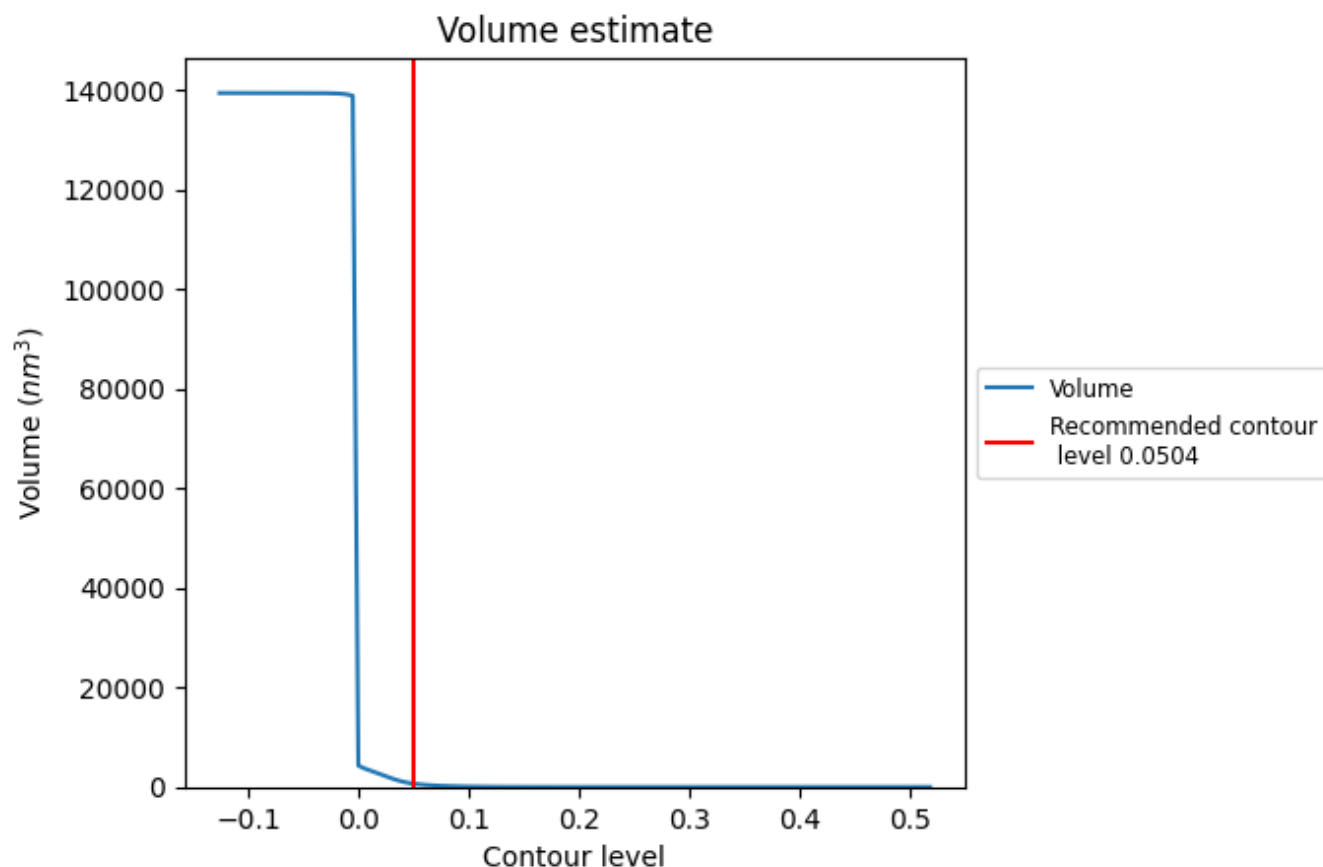
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

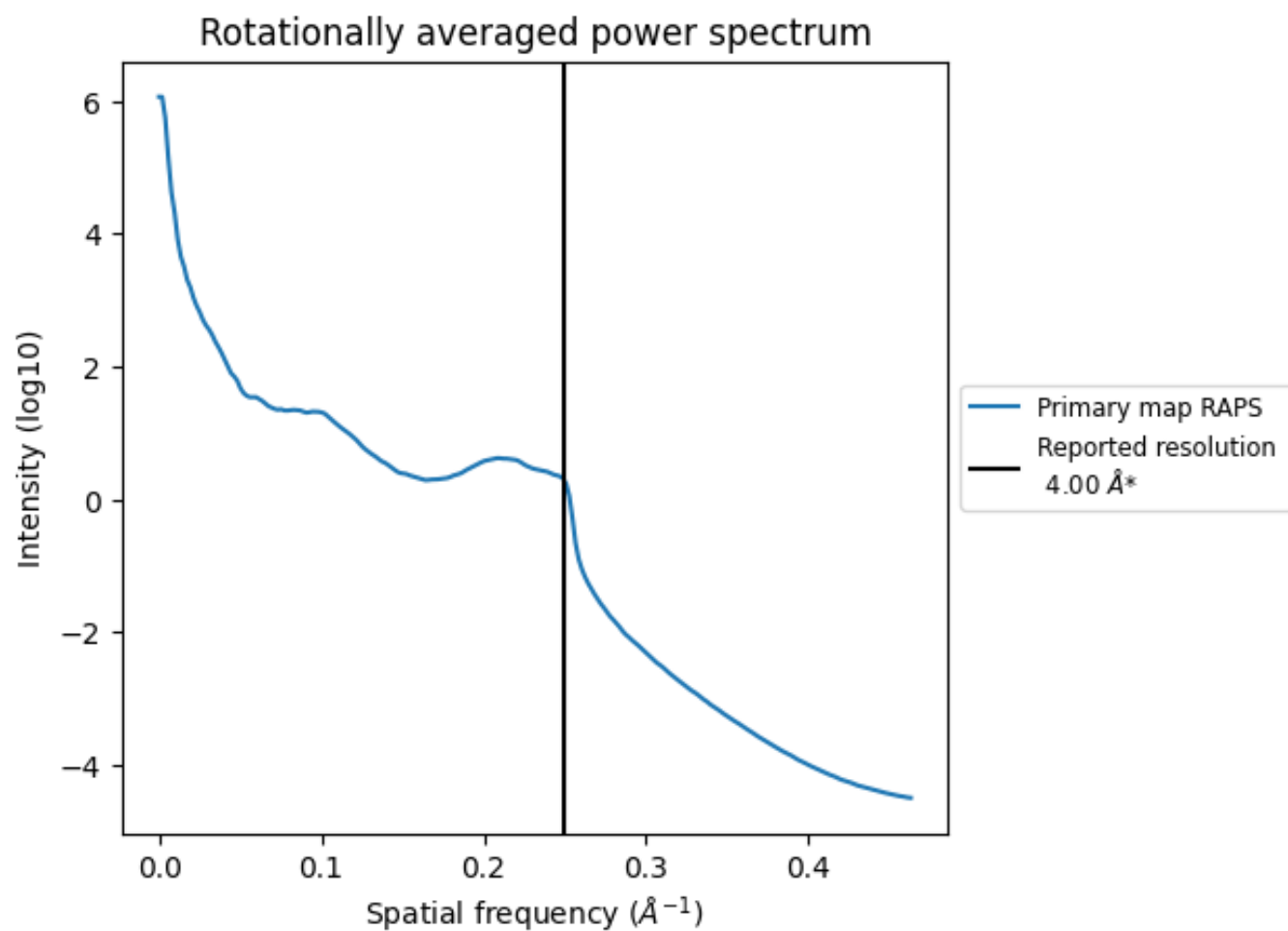
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 645 nm^3 ; this corresponds to an approximate mass of 583 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 0.250 Å⁻¹

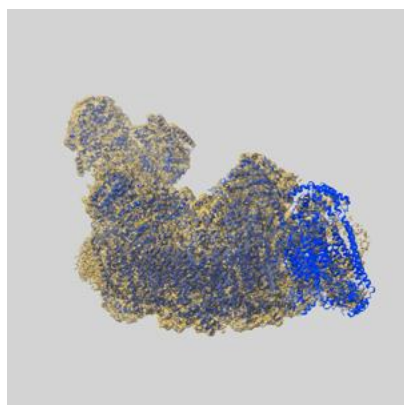
8 Fourier-Shell correlation

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

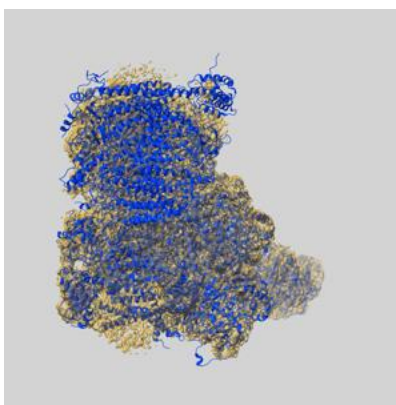
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9539 and PDB model 5GUP. Per-residue inclusion information can be found in section [3](#) on page [26](#).

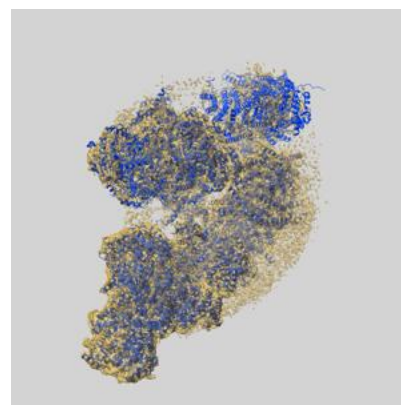
9.1 Map-model overlay [i](#)



X



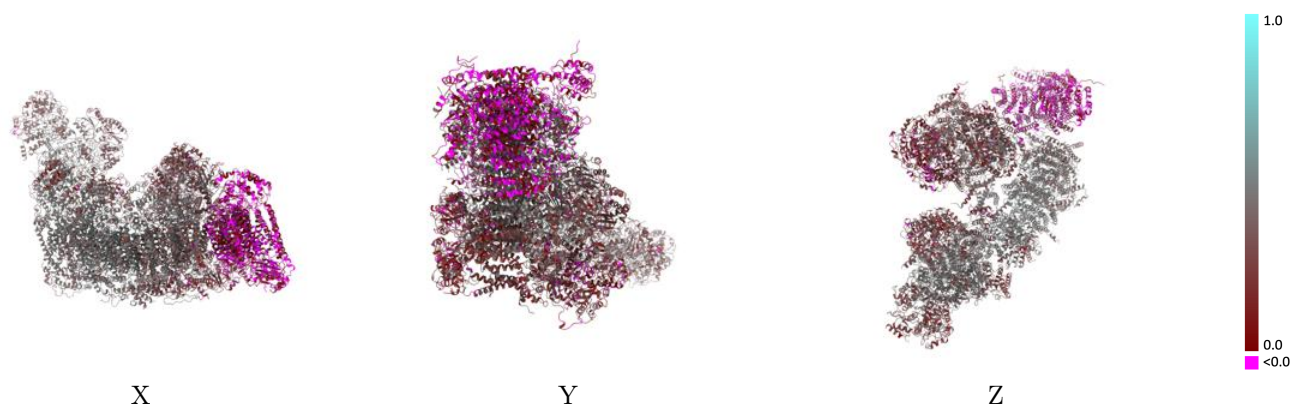
Y



Z

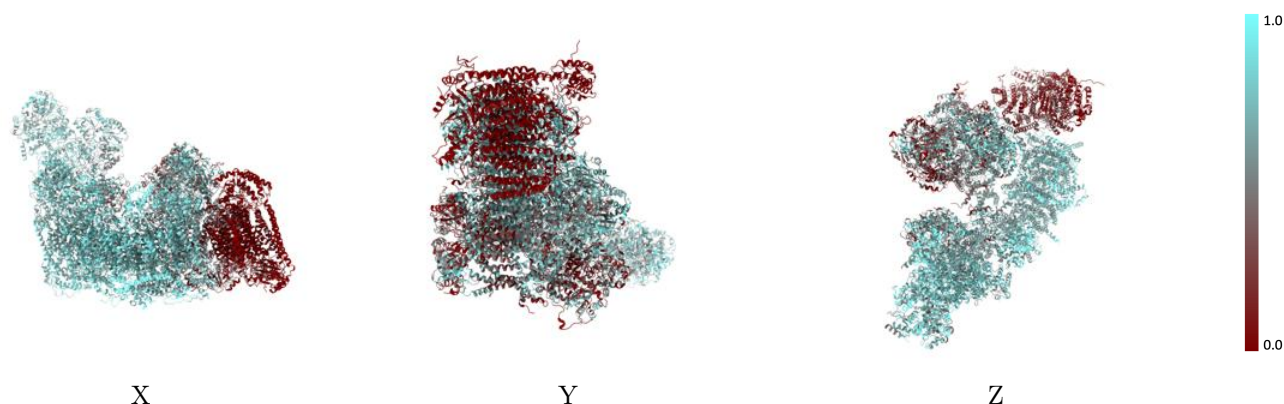
The images above show the 3D surface view of the map at the recommended contour level 0.0504 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



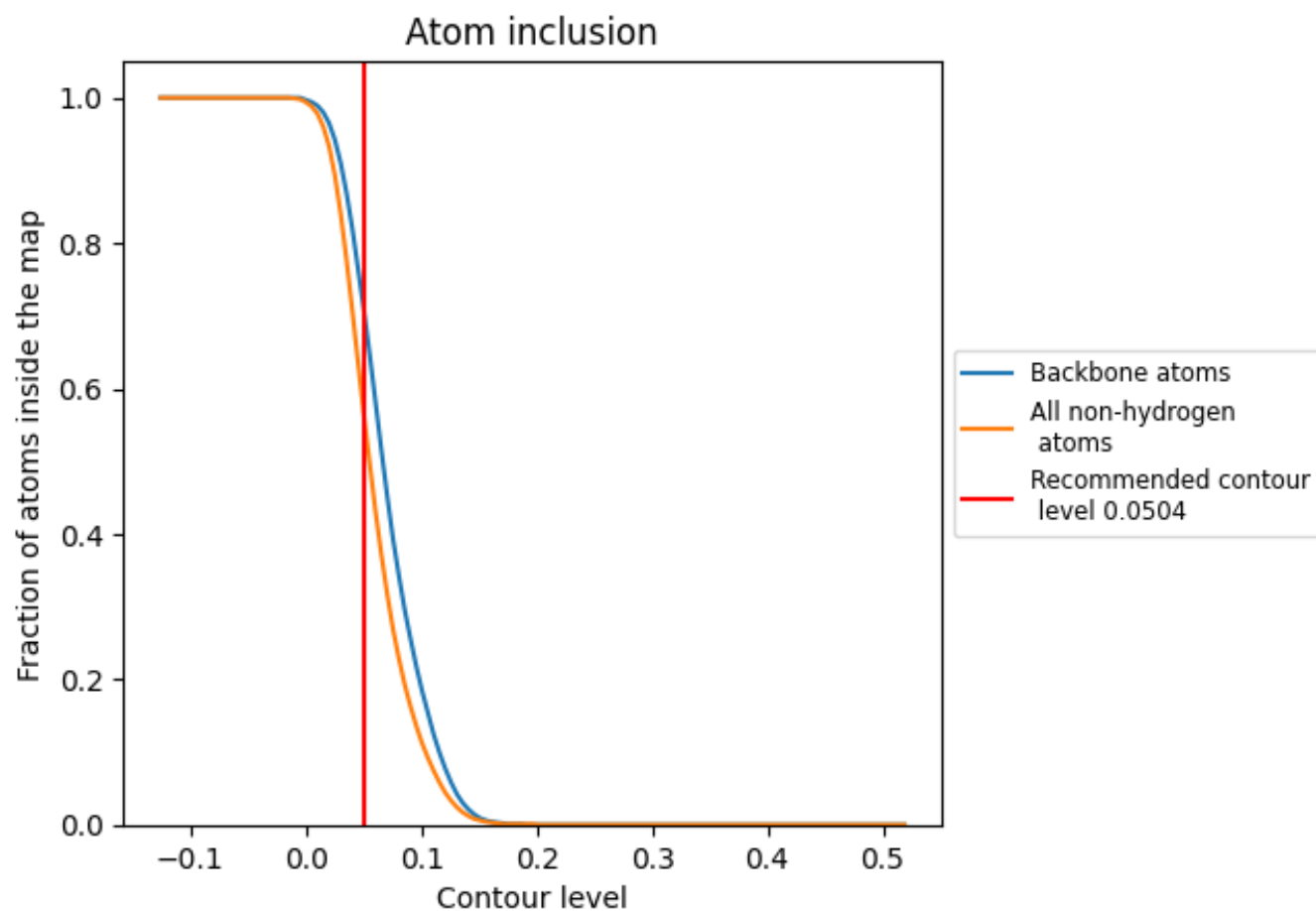
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0504).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 56% 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 (0.0504) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5630	 0.3210
0	 0.5190	 0.2820
1	 0.3490	 0.2500
2	 0.2290	 0.2380
3	 0.4180	 0.3100
4	 0.2310	 0.2150
5	 0.4020	 0.2360
6	 0.3350	 0.2240
7	 0.4720	 0.3060
8	 0.5010	 0.2670
9	 0.5120	 0.2880
A	 0.0090	 0.0280
Aa	 0.4200	 0.2560
Ab	 0.3860	 0.2050
Ac	 0.4020	 0.2340
Ad	 0.2830	 0.2220
Ae	 0.0550	 0.1380
Af	 0.1310	 0.2360
Ag	 0.0630	 0.0600
Ah	 0.0350	 -0.0050
Ai	 0.0080	 -0.0150
Aj	 0.1320	 0.0390
Ak	 0.0560	 0.0150
Al	 0.0760	 0.0170
Am	 0.0400	 0.0350
An	 0.0380	 0.0370
Ao	 0.0340	 0.0210
Ap	 0.0640	 0.0150
Aq	 0.0080	 -0.0050
Ar	 0.0480	 0.0160
B	 0.7030	 0.3330
C	 0.7990	 0.4620
D	 0.7920	 0.4200
E	 0.7200	 0.3530
F	 0.7660	 0.3820











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Chain	Atom inclusion	Q-score
G	 0.7160	 0.3650
H	 0.8140	 0.4740
I	 0.7820	 0.4530
J	 0.7020	 0.4110
K	 0.5310	 0.3890
L	 0.6070	 0.3330
M	 0.6570	 0.4030
N	 0.6690	 0.3080
O	 0.4760	 0.2630
P	 0.6540	 0.2970
Q	 0.6320	 0.3480
R	 0.4000	 0.3430
S	 0.7430	 0.4220
T	 0.7790	 0.4160
U	 0.8140	 0.4130
V	 0.6730	 0.4320
W	 0.7710	 0.4210
X	 0.7570	 0.4130
Y	 0.8420	 0.4200
Z	 0.7900	 0.3920
a	 0.8130	 0.4420
b	 0.8330	 0.4090
c	 0.8310	 0.4510
d	 0.8390	 0.4140
e	 0.7800	 0.4310
f	 0.7530	 0.3890
g	 0.8030	 0.4500
h	 0.7790	 0.4240
i	 0.7810	 0.4840
j	 0.6500	 0.4360
k	 0.7770	 0.4640
l	 0.7240	 0.4290
m	 0.6480	 0.4130
n	 0.7970	 0.4250
o	 0.7690	 0.4440
p	 0.8140	 0.4270
q	 0.7820	 0.4750
r	 0.7300	 0.4580
s	 0.8040	 0.4260
t	 0.7890	 0.3280
u	 0.6340	 0.3640
v	 0.5800	 0.3020

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Chain	Atom inclusion	Q-score
w	 0.5450	 0.3340
x	 0.5320	 0.2960
y	 0.4060	 0.2970
z	 0.5060	 0.3470