



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2025 – 07:56 PM JST

PDB ID : 8ZO8 / pdb_00008zo8
EMDB ID : EMD-60284
Title : Respirasome open state 3 in presence of metformin (SC-MetO3)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-05-28
Resolution : 3.24 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

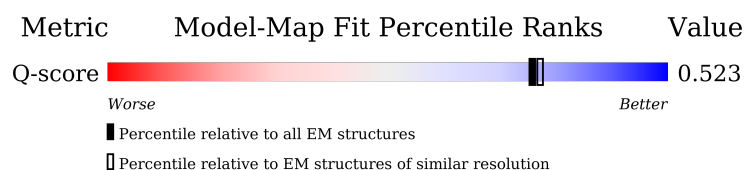
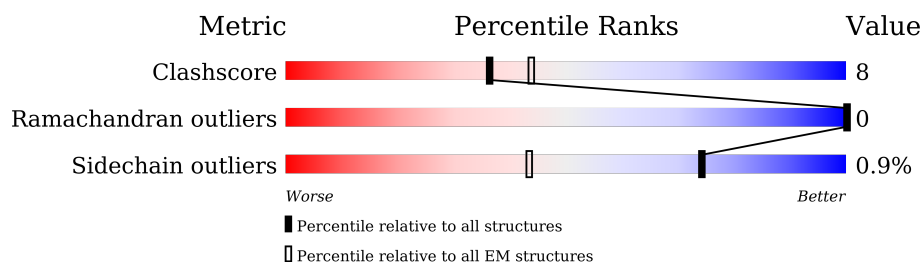
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 3.24 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.












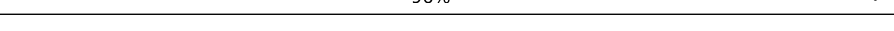
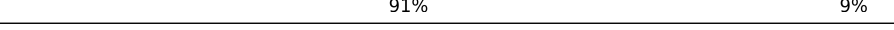





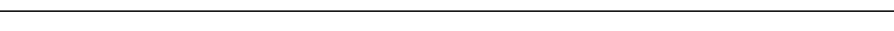
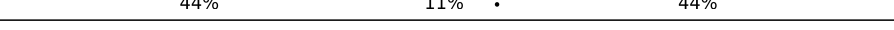







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14594 (2.74 - 3.74)

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	4L	98	 82% 18%
2	5A	102	 71% 29%
3	5B	95	 71% 29%
4	6A	75	 75% 25%







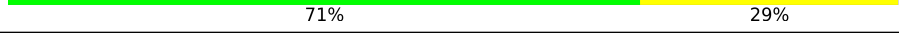
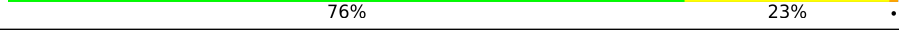
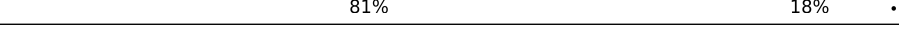
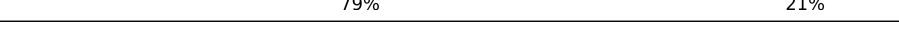
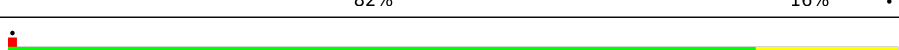

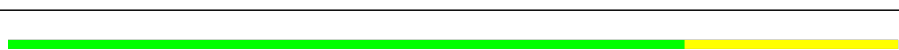

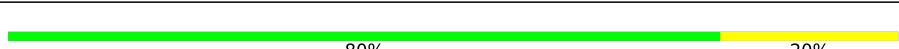





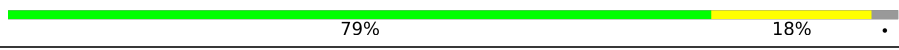
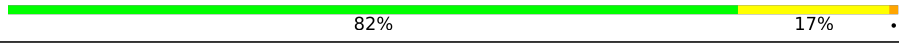



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Mol	Chain	Length	Quality of chain
5	6B	82	 73% 27%
6	6C	70	 79% 21%
7	7A	57	 74% 25%
8	7B	50	 86% 14%
9	7C	47	 89% 11%
10	8B	43	 72% 28%
11	A1	70	 91% 9%
12	A2	85	 88% 12%
13	A3	83	 96%
14	A5	112	 91% 9%
15	A6	114	 85% 15%
16	A7	112	 79% 7% 13%
17	A8	171	 85% 15%
18	A9	341	 82% 17%
19	AB	156	 40% 9% 51%
19	AC	156	 44% 11% 44%
20	AK	320	 79% 20%
21	AL	140	 88% 12%
22	AM	143	 88% 12%
23	AN	142	 82% 18%
24	B1	56	 91% 9%
25	B2	67	 90% 10%
26	B3	79	 85% 15%
27	B4	128	 88% 12%
28	B5	138	 86% 14%




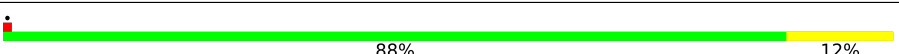
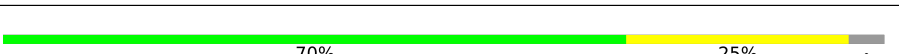
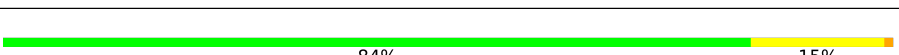
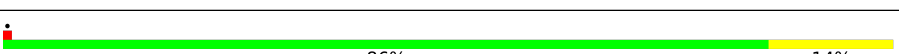
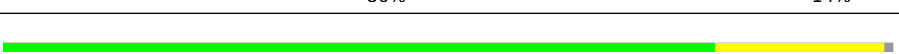

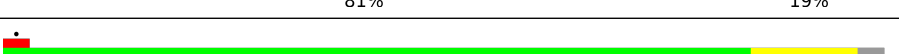
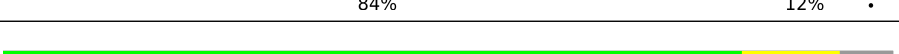
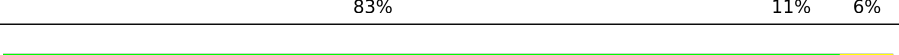
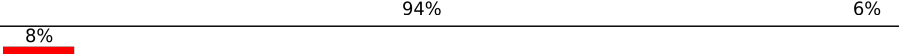
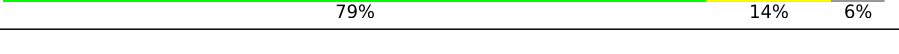





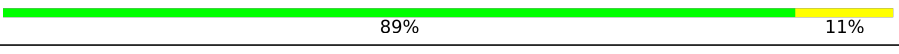

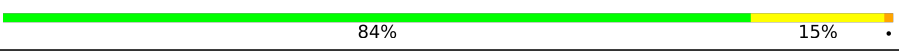



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Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	176	
34	BL	102	
35	C1	514	
36	C2	228	
37	C3	260	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	115	
44	N4	459	
45	N5	603	
46	N6	173	
47	QA	419	
47	Qa	419	
48	QB	446	
48	Qb	446	
49	QC	379	
49	Qc	379	
50	QD	241	

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Mol	Chain	Length	Quality of chain
50	Qd	241	
51	QE	196	
51	Qe	196	
52	QF	67	
52	Qf	67	
53	QG	101	
53	Qg	101	
54	QH	79	
54	Qh	79	
55	QI	64	
55	Qi	64	
56	QJ	49	
57	QK	78	
58	Qj	51	
59	S1	689	
60	S2	430	
61	S3	207	
62	S4	124	
63	S5	100	
64	S6	96	
65	S7	156	
66	S8	176	
67	V1	431	
68	V2	217	
69	V3	42	

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
85	FES	QE	304	-	-	X	-
86	SF4	S8	302	-	-	X	-

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 116743 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 NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4L	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	102	Total	C	N	O	S	0	0
			825	528	139	156	2		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	95	Total	C	N	O	S	0	0
			724	449	128	141	6		

- Molecule 4 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6A	75	Total	C	N	O	S	0	0
			620	401	118	100	1		

- Molecule 5 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6B	82	Total	C	N	O	S	0	0
			684	431	125	123	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6C	70	Total	C	N	O	S	0	0
			574	375	101	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7A	57	Total	C	N	O	S	0	0
			447	287	76	81	3		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7B	50	Total	C	N	O	S	0	0
			392	254	66	71	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7C	47	Total	C	N	O	S	0	0
			387	257	65	63	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8B	43	Total	C	N	O	0	0
			338	222	57	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A1	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	85	Total	C	N	O	S	0	0
			686	431	128	125	2		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A3	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A5	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A6	114	Total	C	N	O	S	0	0
			967	617	178	167	5		

- Molecule 16 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A7	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A8	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A9	337	Total	C	N	O	S	0	0
			2703	1750	472	472	9		

- Molecule 19 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	77	Total	C	N	O	S	0	0
			624	402	93	124	5		
19	AC	87	Total	C	N	O	S	0	0
			702	452	103	142	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AK	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AL	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AM	143	Total	C	N	O	S	0	0
			1195	764	216	211	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AN	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B1	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B2	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B3	79	Total	C	N	O	S	0	0
			632	413	106	112	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B4	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	101	Total	C	N	O	S	0	0
			861	562	153	145	1		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B7	125	Total	C	N	O	S	0	0
			1068	663	204	190	11		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B8	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B9	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	174	Total	C	N	O	S	0	0
			1456	913	264	271	8		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	99	Total	C	N	O	S	0	0
			828	531	137	156	4		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C1	514	Total	C	N	O	S	0	0
			4024	2692	625	675	32		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C2	228	Total	C	N	O	S	0	0
			1833	1193	282	340	18		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C3	260	Total	C	N	O	S	0	0
			2103	1403	337	353	10		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C4	138	Total	C	N	O	S	0	0
			1153	751	188	210	4		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	CA	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	CB	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	N1	311	Total	C	N	O	S	0	0
			2457	1644	377	415	21		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N2	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	N3	98	Total	C	N	O	S	0	0
			786	535	114	132	5		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N4	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	N5	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N6	163	Total	C	N	O	S	0	0
			1236	831	177	217	11		

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	QA	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		
47	Qa	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	QB	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
48	Qb	433	Total	C	N	O	S	0	0
			3367	2103	592	653	19		

- Molecule 49 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	QC	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
49	Qc	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 50 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	QD	241	Total	C	N	O	S	0	0
			1921	1225	330	350	16		
50	Qd	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 51 is a protein called Rieske domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	QE	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		
51	Qe	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	QF	67	Total	C	N	O	S	0	0
			552	336	100	111	5		
52	Qf	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	QG	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
53	Qg	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	QH	78	Total	C	N	O	S	0	0
			662	432	121	107	2		
54	Qh	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 55 is a protein called Ubiquinol-cytochrome c reductase complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	QI	62	Total	C	N	O	0	0
			507	331	90	86		
55	Qi	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	QJ	49	Total	C	N	O	S	0	0
			405	269	71	63	2		

- Molecule 57 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	QK	73	Total	C	N	O	S	0	0
			520	328	98	92	2		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Qj	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 59 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	S1	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	S2	421	Total	C	N	O	S	0	0
			3391	2169	580	618	24		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	S3	207	Total	C	N	O	S	0	0
			1729	1119	297	311	2		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	S4	124	Total	C	N	O	S	0	0
			1007	637	179	188	3		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	S5	100	Total	C	N	O	S	0	0
			825	525	153	141	6		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	S6	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	S7	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	S8	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	V1	431	Total	C	N	O	S	0	0
			3316	2092	592	612	20		

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	V2	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 69 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn).

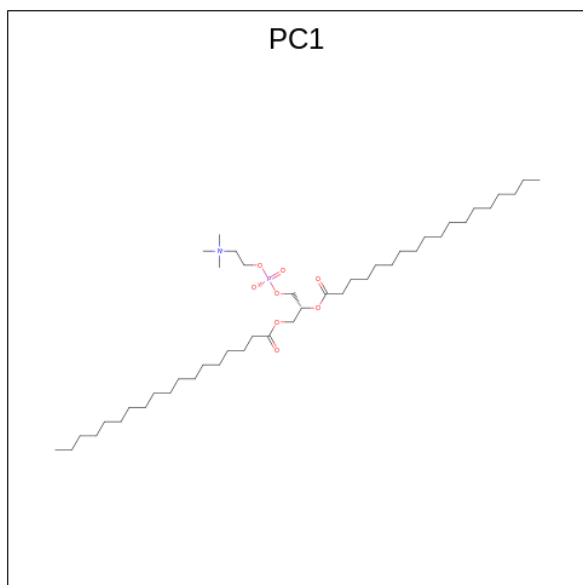
Mol	Chain	Residues	Atoms		AltConf
70	5B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
70	S6	1	Total	Zn	0
			1	1	

- Molecule 71 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



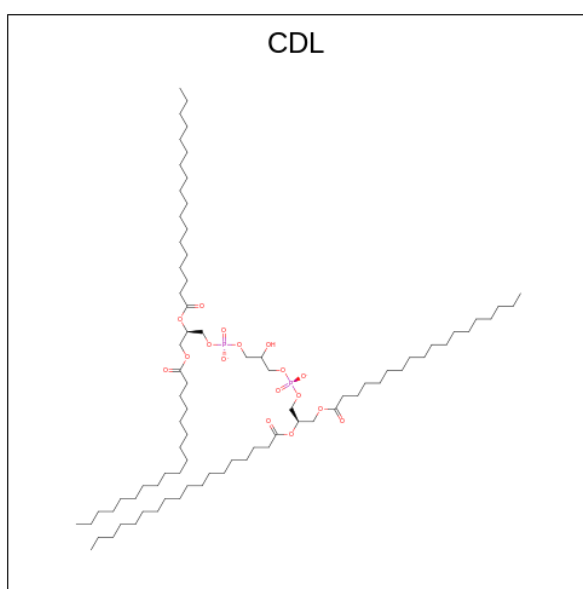
Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
71	7B	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	AL	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	C1	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
71	C3	1	Total	C	N	O	P	0
			43	33	1	8	1	
71	N5	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	N6	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	QC	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
71	QC	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	QH	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qb	1	Total	C	N	O	P	0
			29	19	1	8	1	
71	Qj	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 72 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
72	6A	1	Total	C	O	P	0
			69	50	17	2	
72	A8	1	Total	C	O	P	0
			83	64	17	2	
72	AL	1	Total	C	O	P	0
			84	65	17	2	
72	AL	1	Total	C	O	P	0
			93	74	17	2	
72	AL	1	Total	C	O	P	0
			80	61	17	2	
72	AM	1	Total	C	O	P	0
			51	32	17	2	
72	B5	1	Total	C	O	P	0
			100	81	17	2	

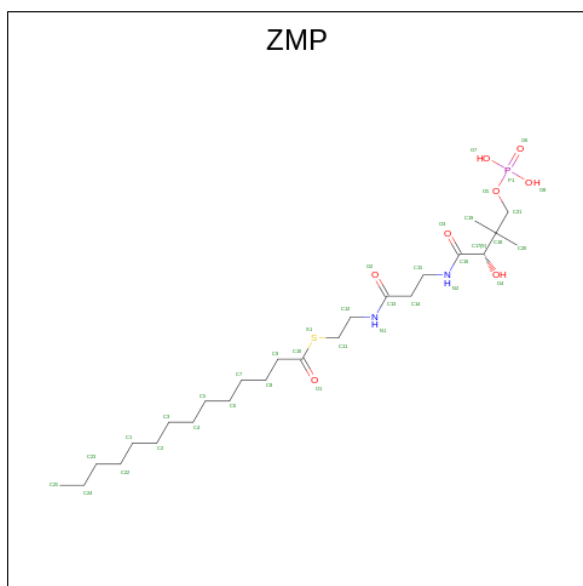
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Mol	Chain	Residues	Atoms				AltConf
72	CB	1	Total 100	C 81	O 17	P 2	0
72	N2	1	Total 68	C 49	O 17	P 2	0
72	N5	1	Total 89	C 70	O 17	P 2	0
72	N5	1	Total 100	C 81	O 17	P 2	0
72	QB	1	Total 64	C 45	O 17	P 2	0
72	QC	1	Total 94	C 75	O 17	P 2	0
72	QC	1	Total 55	C 36	O 17	P 2	0
72	QH	1	Total 61	C 42	O 17	P 2	0
72	Qb	1	Total 64	C 45	O 17	P 2	0
72	Qd	1	Total 64	C 45	O 17	P 2	0
72	Qh	1	Total 64	C 45	O 17	P 2	0

- # NDP

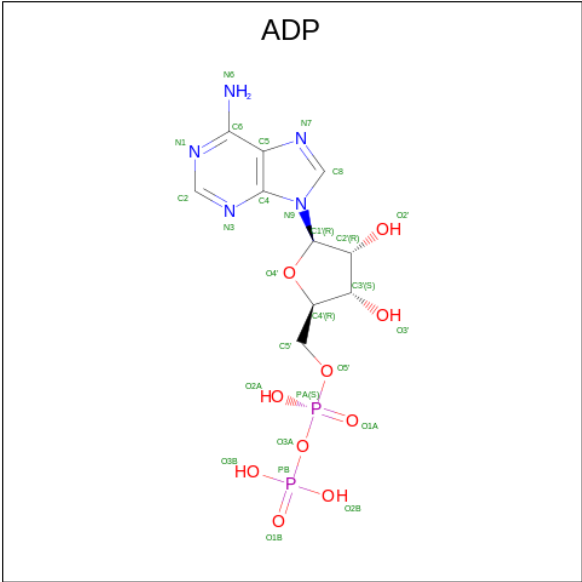
Mol	Chain	Residues	Atoms					AltConf
73	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 74 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



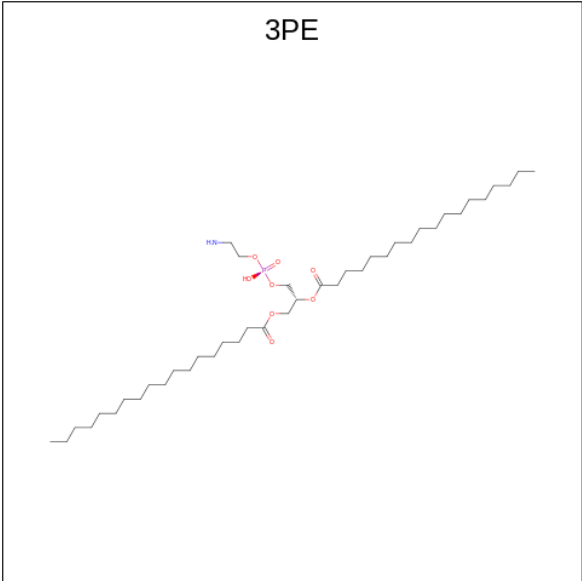
Mol	Chain	Residues	Atoms						AltConf
74	AB	1	Total 36	C 25	N 2	O 7	P 1	S 1	0
74	AC	1	Total 36	C 25	N 2	O 7	P 1	S 1	0

- Molecule 75 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
75	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 76 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



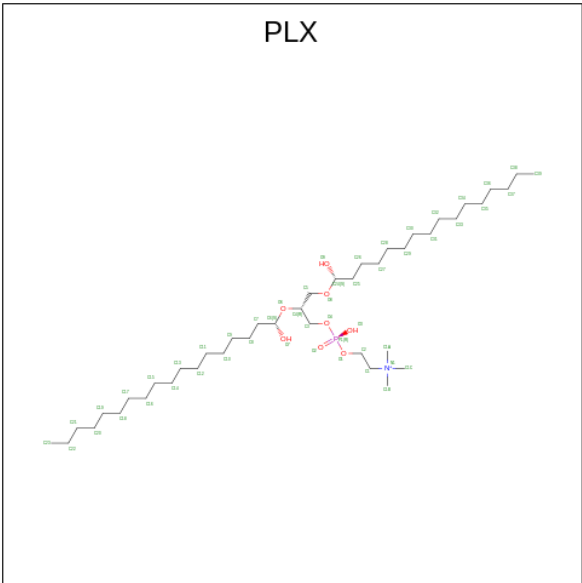
Mol	Chain	Residues	Atoms					AltConf
76	AL	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
76	C1	1	Total	C	N	O	P	0
			44	34	1	8	1	
76	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
76	N4	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	QE	1	Total	C	N	O	P	0
			44	34	1	8	1	
76	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 77 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).



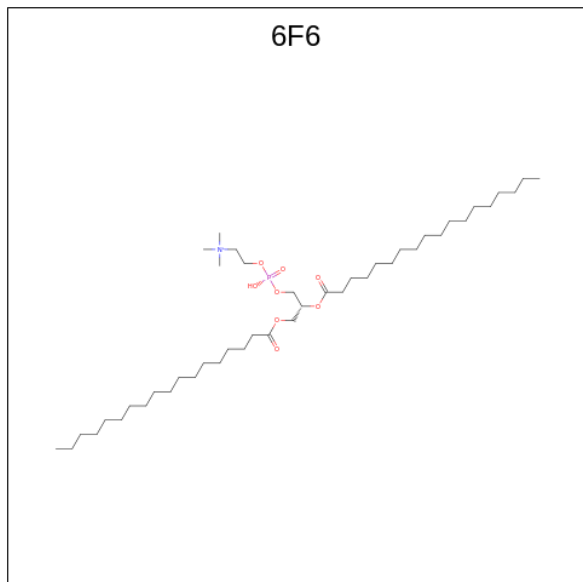
Mol	Chain	Residues	Atoms					AltConf
77	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	
77	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
77	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
77	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	

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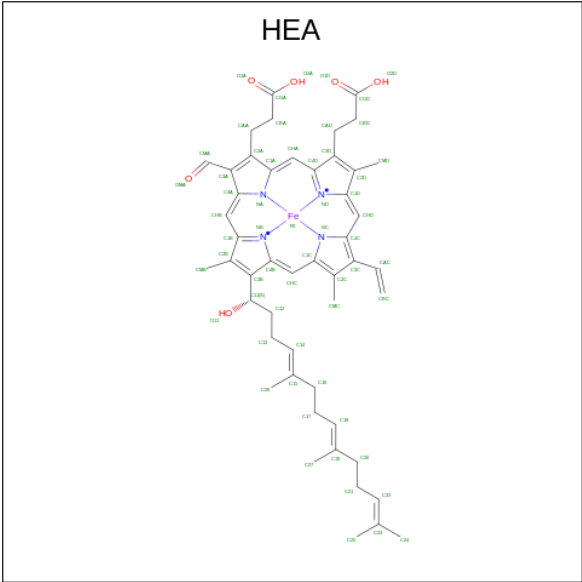
Mol	Chain	Residues	Atoms					AltConf
77	C2	1	Total	C	N	O	P	0
			43	33	1	8	1	
77	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
77	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
77	QE	1	Total	C	N	O	P	0
			46	36	1	8	1	
77	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 78 is (4S,7R)-4-hydroxy-N,N,N-trimethyl-7-(octadecanoyloxy)-4,10-dioxo-3,5,9-tri-oxa-4lambda 5 -phosphaheptacosan-1-aminium (CCD ID: 6F6) (formula: C₄₄H₈₉NO₈P).



Mol	Chain	Residues	Atoms					AltConf
78	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
78	QJ	1	Total	C	N	O	P	0
			54	44	1	8	1	
78	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
79	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0
79	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0

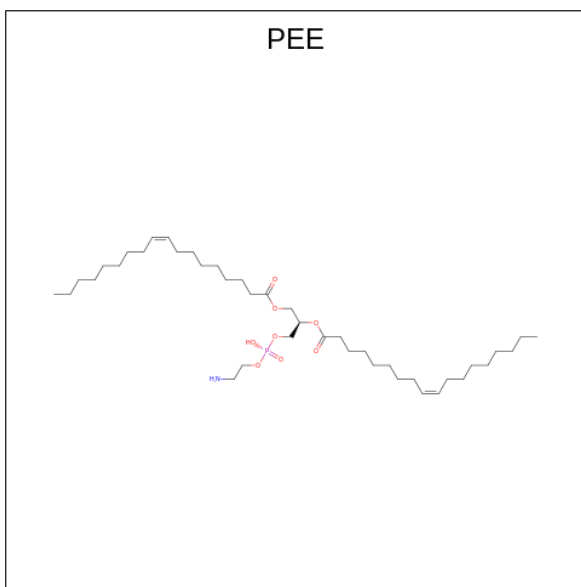
- Molecule 80 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
80	C1	1	Total	Cu	0
			1	1	
80	C2	2	Total	Cu	0
			2	2	

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	C1	1	Total	Mg	0
			1	1	
81	S1	1	Total	Mg	0
			1	1	

- Molecule 82 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



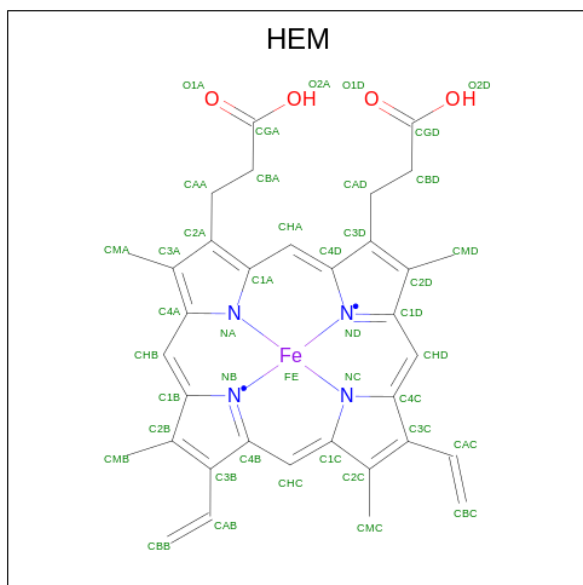
Mol	Chain	Residues	Atoms					AltConf
82	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
82	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
82	QB	1	Total	C	N	O	P	0
			27	17	1	8	1	
82	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	QC	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	QC	1	Total	C	N	O	P	0
			38	28	1	8	1	
82	QE	1	Total	C	N	O	P	0
			47	37	1	8	1	
82	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
82	Qd	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	Qh	1	Total	C	N	O	P	0
			41	31	1	8	1	
82	Qh	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	

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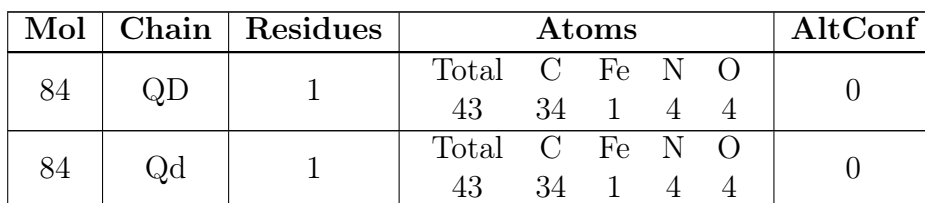
Mol	Chain	Residues	Atoms					AltConf
82	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 83 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
83	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 84 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



-
- Diagram illustrating the structure of a ferredoxin (FES) molecule, showing a square arrangement of two iron (Fe) and two sulfur (S) atoms. The atoms are labeled S1, FE2, FE1, and S2 in green text. The bonds between the atoms are colored: yellow for S-Fe bonds and purple for Fe-S bonds.

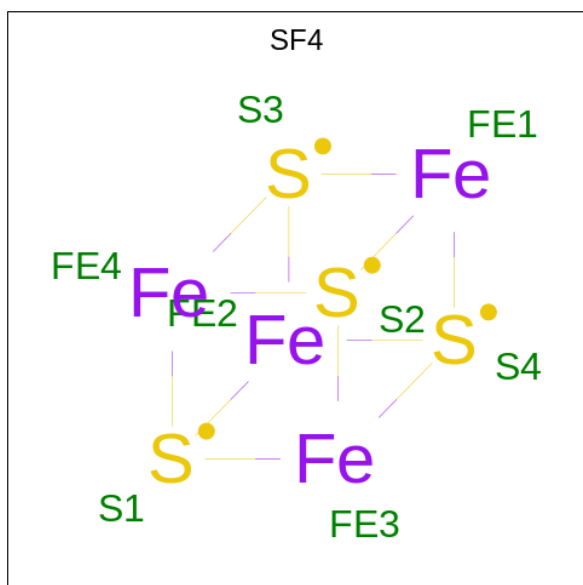
Mol	Chain	Residues	Atoms			AltConf
85	QE	1	Total 4	Fe 2	S 2	0
85	Qe	1	Total 4	Fe 2	S 2	0



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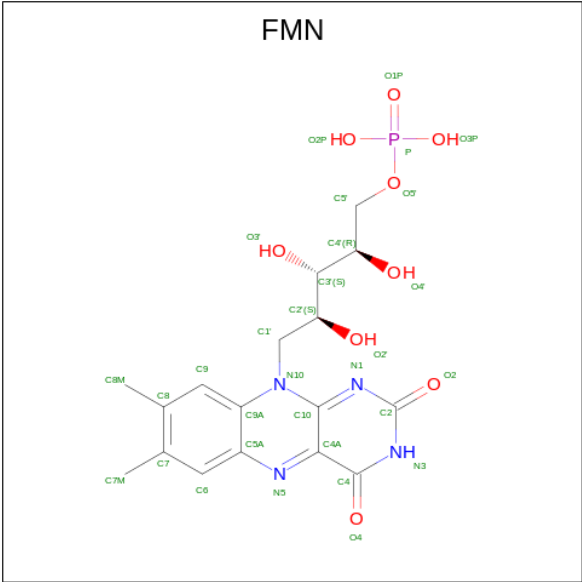
Mol	Chain	Residues	Atoms			AltConf
85	S1	1	Total	Fe	S	0
			4	2	2	
85	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 86 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
86	S1	1	Total	Fe	S	0
			8	4	4	
86	S1	1	Total	Fe	S	0
			8	4	4	
86	S7	1	Total	Fe	S	0
			8	4	4	
86	S8	1	Total	Fe	S	0
			8	4	4	
86	S8	1	Total	Fe	S	0
			8	4	4	
86	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 87 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).




Mol	Chain	Residues	Atoms					AltConf
87	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots

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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:  82% 18%



- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 5A:  71% 29%




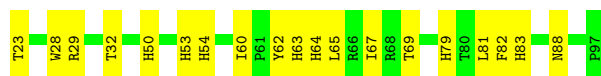
- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 5B:  71% 29%




- Molecule 4: Cytochrome c oxidase subunit

Chain 6A:  75% 25%

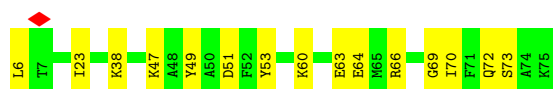
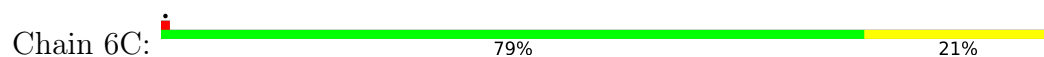


- Molecule 5: Cytochrome c oxidase subunit

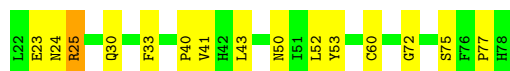
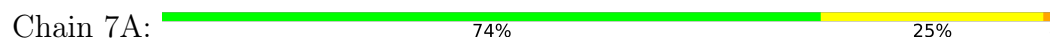
Chain 6B:  73% 27%



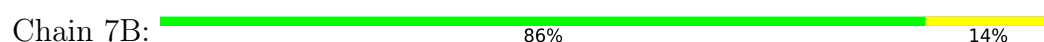
- Molecule 6: Cytochrome c oxidase subunit 6C



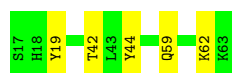
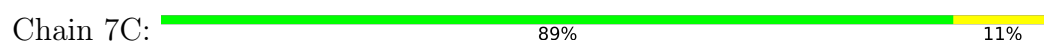
- Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



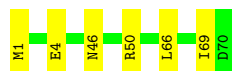
- Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



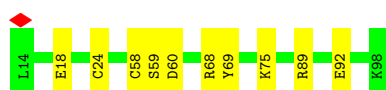
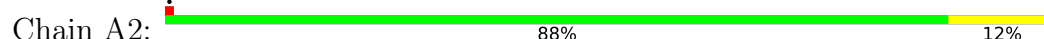
- Molecule 10: Cytochrome c oxidase subunit 8



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



- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



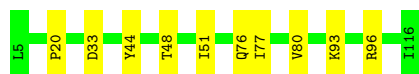
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain A3:  96% .




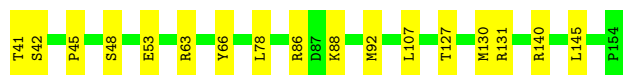
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5:  91% 9%




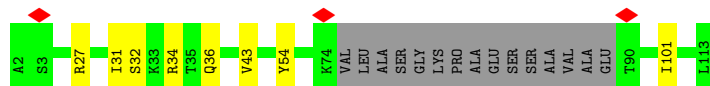
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:  85% 15%




- Molecule 16: Complex I-B14.5a

Chain A7:  79% 7% 13%




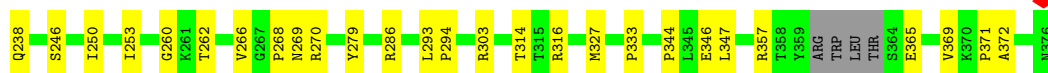
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:  85% 15%



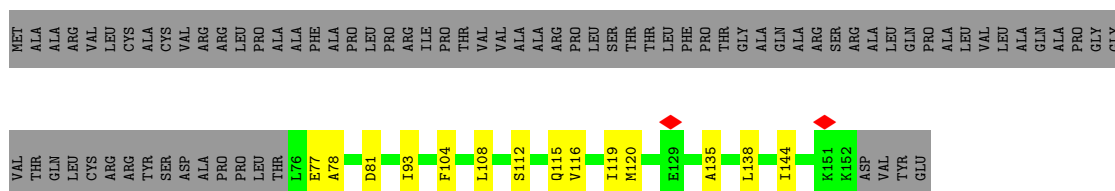
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain A9:  82% 17% .



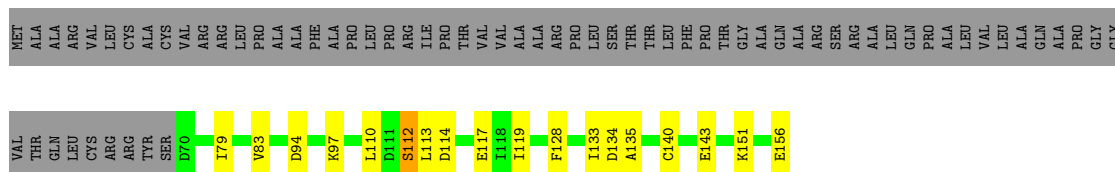
- Molecule 19: Acyl carrier protein

Chain AB:  40% 9% 51%



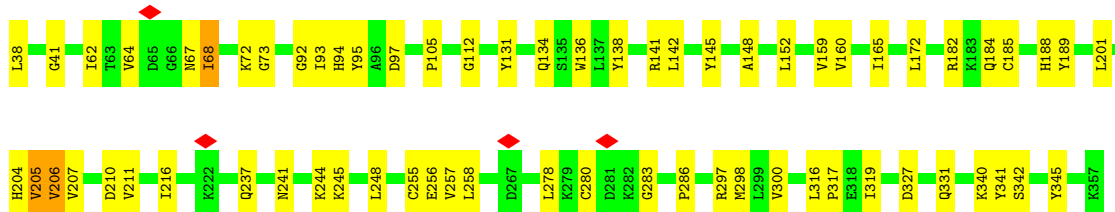
• Molecule 19: Acyl carrier protein

Chain AC: 44% 11% 44%



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

Chain AK: 79% 20%



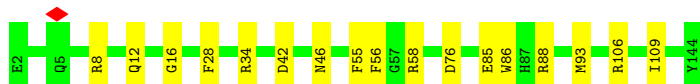
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AL: 88% 12%



• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AM: 88% 12%



• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AN: 82% 18%



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

Chain B1:  91% 9%




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain B2:  90% 10%




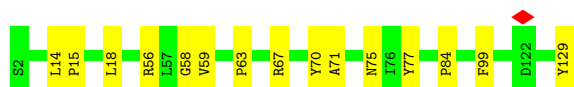
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain B3:  85% 15%




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:  88% 12%



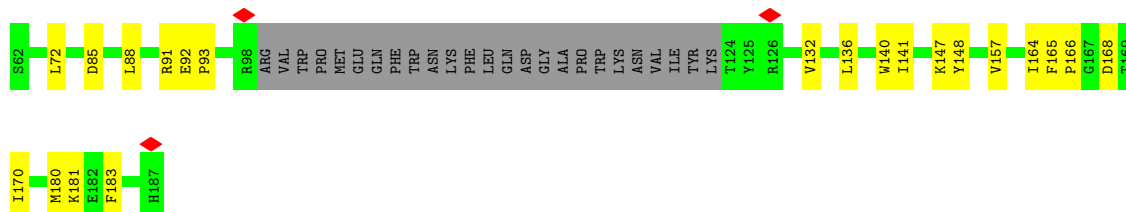
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:  86% 14%




- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:  63% 17% 20%




- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:  84% 16%




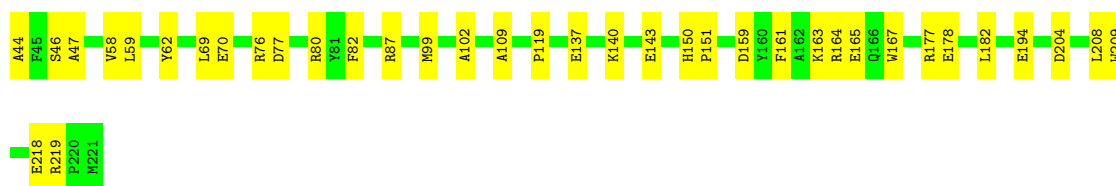
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:  89% 11%



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:  79% 21%




- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BK:  89% 10%



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BL:  83% 14%



- Molecule 35: Cytochrome c oxidase subunit 1

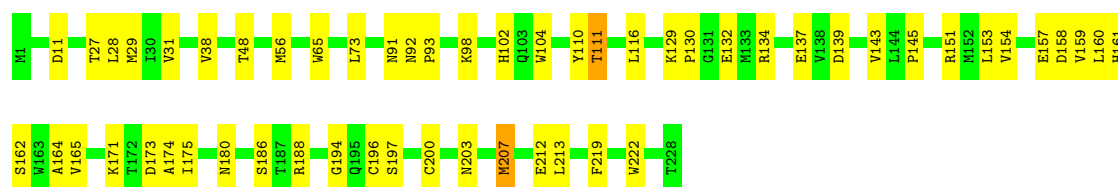
Chain C1:  71% 29%





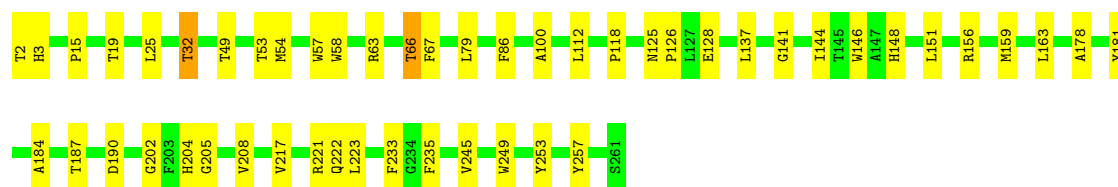
• Molecule 36: Cytochrome c oxidase subunit 2

Chain C2: 76% 23%



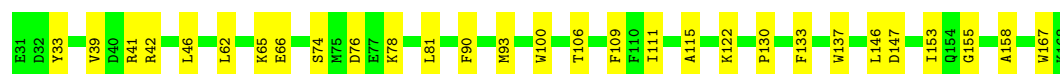
• Molecule 37: Cytochrome c oxidase subunit 3

Chain C3: 81% 18%



• Molecule 38: Cytochrome c oxidase subunit 4

Chain C4: 79% 21%



• Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain CA: 82% 16%



• Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB: 84% 16%



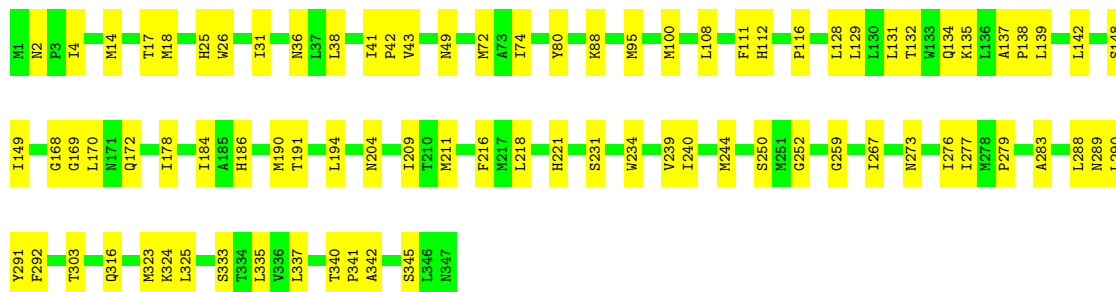
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain N1: 77% 21%



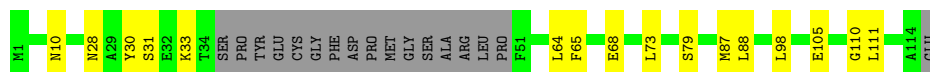
- Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2: 76% 24%



- Molecule 43: NADH-ubiquinone oxidoreductase chain 3

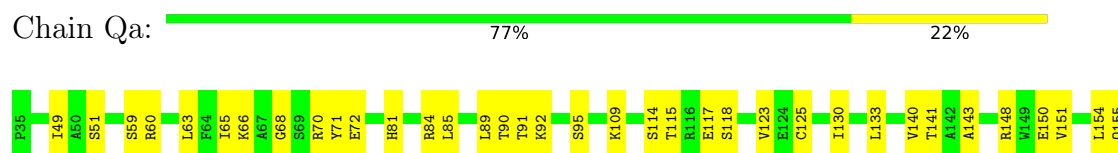
Chain N3: 71% 14% 15%

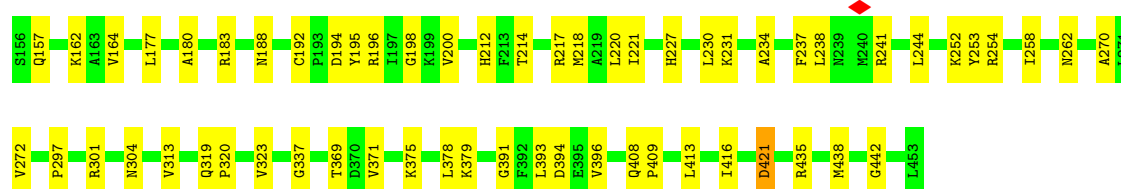


- Molecule 44: NADH-ubiquinone oxidoreductase chain 4

Chain N4: 80% 20%

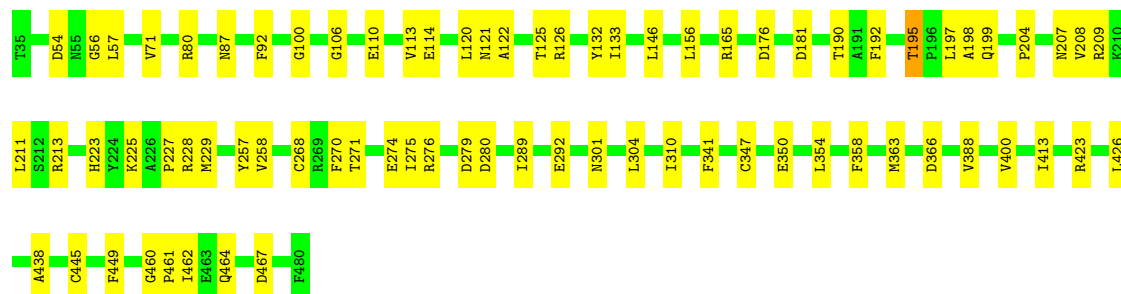






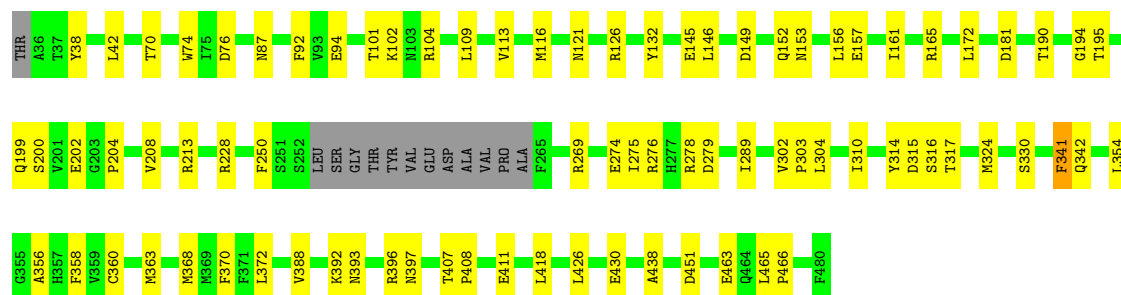
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain QB: 83% 17%



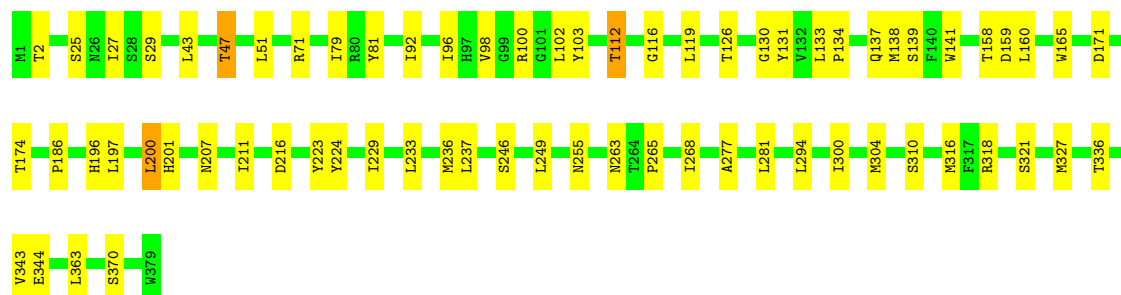
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Qb: 79% 18% .



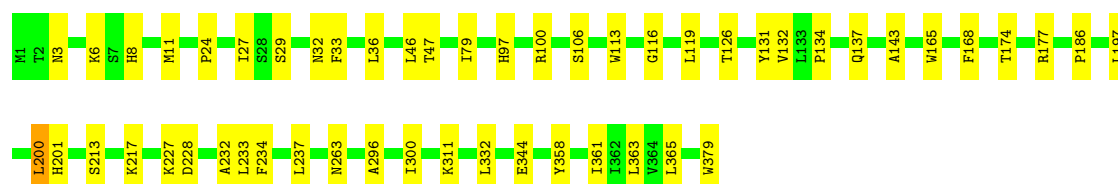
- Molecule 49: Cytochrome b

Chain QC: 82% 17% .

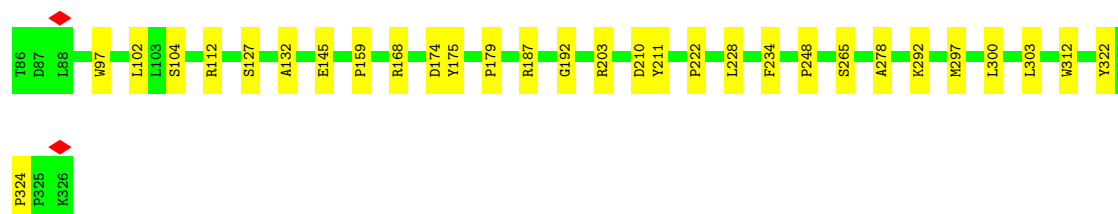


- Molecule 49: Cytochrome b

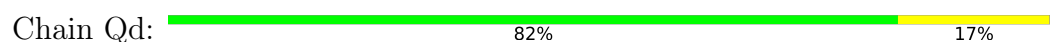
Chain Qc: 86% 13%



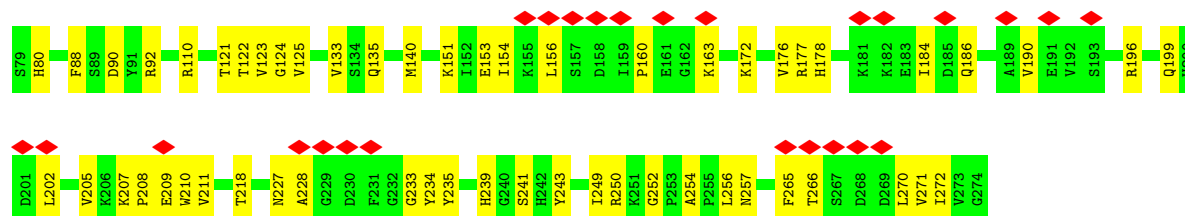
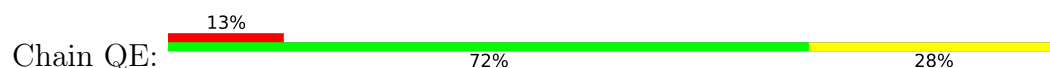
- Molecule 50: Cytochrome c domain-containing protein



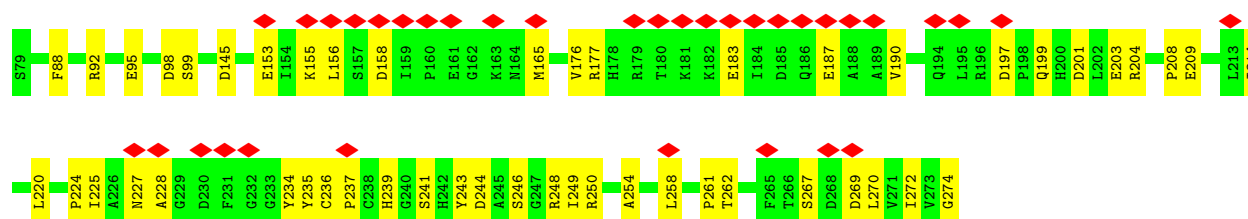
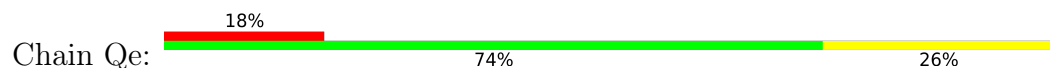
- Molecule 50: Cytochrome c domain-containing protein




- Molecule 51: Rieske domain-containing protein



- Molecule 51: Rieske domain-containing protein



- Molecule 52: Cytochrome b-c1 complex subunit 6

Chain QF:  88% 12%




- Molecule 52: Cytochrome b-c1 complex subunit 6

Chain Qf:  70% 25%




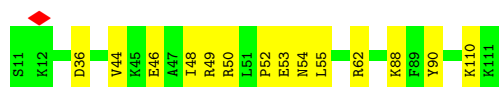
- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain QG:  84% 15%




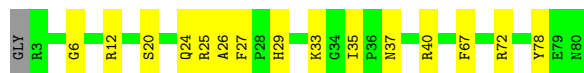
- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain Qg:  86% 14%




- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain QH:  80% 19%




- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain Qh:  81% 19%



- Molecule 55: Ubiquinol-cytochrome c reductase complex

Chain QI:  84% 12%



- Molecule 55: Ubiquinol-cytochrome c reductase complex

Chain Qi: 83% 11% 6%



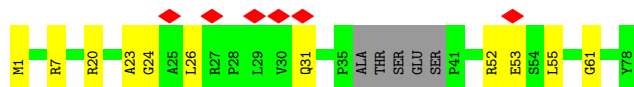
- Molecule 56: Cytochrome b-c1 complex subunit 10

Chain QJ: 94% 6%



- Molecule 57: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain QK: 8% 79% 14% 6%



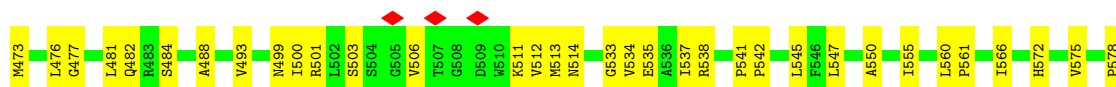
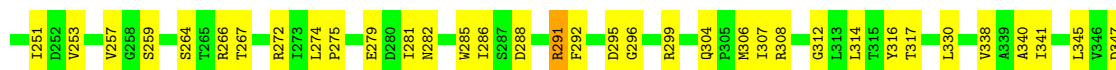
- Molecule 58: Cytochrome b-c1 complex subunit 10

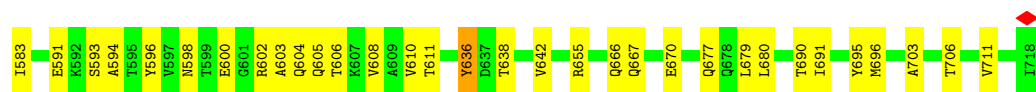
Chain Qj: 86% 14%



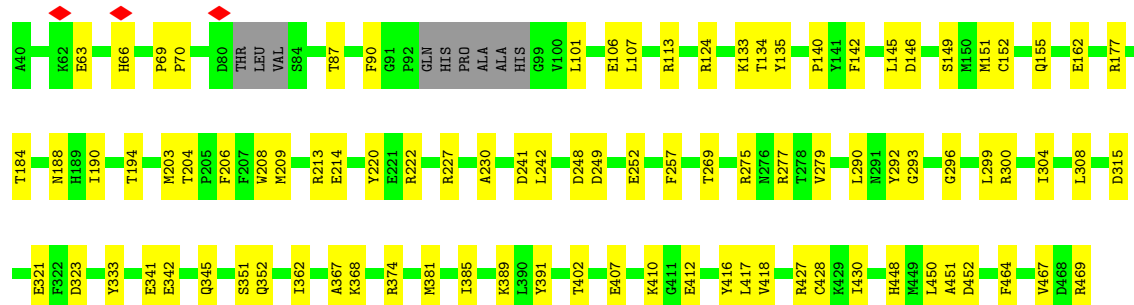
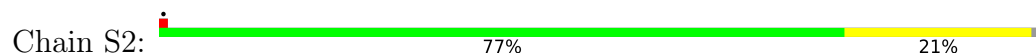
- Molecule 59: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain S1: 76% 24%

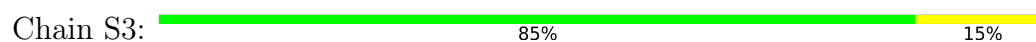




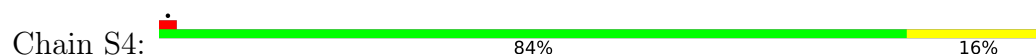
- Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



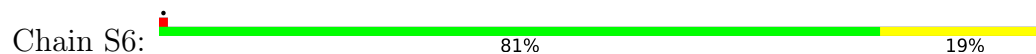
- Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



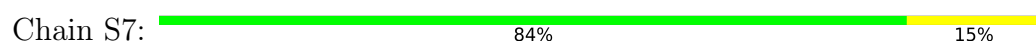
- Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

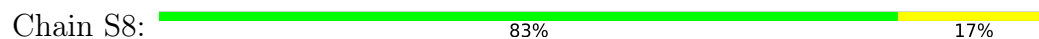


- Molecule 65: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

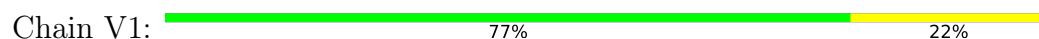




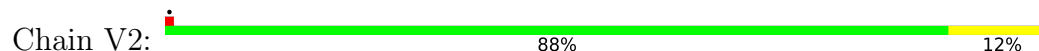
- Molecule 66: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



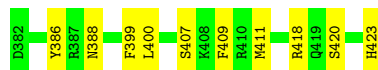
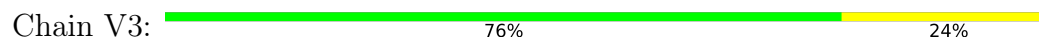
- Molecule 67: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 68: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 69: NADH:ubiquinone oxidoreductase subunit V3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181922	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	47.701	Depositor
Minimum map value	-16.089	Depositor
Average map value	-0.009	Depositor
Map value standard deviation	1.062	Depositor
Recommended contour level	4	Depositor
Map size (Å)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, HEA, PC1, HEC, SF4, MG, ZN, PEE, ZMP, CU, 2MR, FES, 3PE, PLX, FMN, HEM, 6F6, ADP, CDL

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	4L	0.20	0/759	0.28	0/1029
2	5A	0.16	0/843	0.28	0/1145
3	5B	0.18	0/739	0.33	0/1002
4	6A	0.13	0/648	0.25	0/888
5	6B	0.19	0/704	0.39	0/951
6	6C	0.16	0/587	0.25	0/781
7	7A	0.15	0/457	0.28	0/620
8	7B	0.12	0/405	0.22	0/555
9	7C	0.17	0/400	0.24	0/536
10	8B	0.15	0/349	0.32	0/477
11	A1	0.17	0/577	0.27	0/777
12	A2	0.15	0/697	0.27	0/938
13	A3	0.15	0/664	0.24	0/912
14	A5	0.16	0/929	0.24	0/1258
15	A6	0.17	0/991	0.28	0/1335
16	A7	0.16	0/798	0.25	0/1079
17	A8	0.17	0/1436	0.26	0/1938
18	A9	0.17	0/2777	0.31	2/3762 (0.1%)
19	AB	0.10	0/633	0.22	0/851
19	AC	0.18	0/714	0.25	0/965
20	AK	0.16	0/2650	0.34	2/3588 (0.1%)
21	AL	0.14	0/1042	0.23	0/1411
22	AM	0.15	0/1236	0.24	0/1683
23	AN	0.18	0/1204	0.27	0/1624
24	B1	0.16	0/491	0.26	0/663
25	B2	0.18	0/610	0.28	0/836
26	B3	0.16	0/651	0.27	0/880
27	B4	0.18	0/1092	0.26	0/1481
28	B5	0.19	0/1184	0.27	0/1603
29	B6	0.19	0/888	0.32	0/1208
30	B7	0.17	0/1092	0.26	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B8	0.17	0/1371	0.25	0/1875
32	B9	0.19	0/1590	0.30	0/2155
33	BK	0.18	0/1489	0.26	0/2008
34	BL	0.19	0/851	0.30	0/1155
35	C1	0.21	0/4164	0.34	0/5689
36	C2	0.18	0/1880	0.32	0/2564
37	C3	0.19	0/2186	0.30	0/2991
38	C4	0.16	0/1187	0.26	0/1606
39	CA	0.15	0/430	0.24	0/581
40	CB	0.19	0/1031	0.28	0/1394
41	N1	0.20	0/2528	0.33	0/3455
42	N2	0.22	0/2773	0.34	0/3768
43	N3	0.18	0/804	0.27	0/1097
44	N4	0.23	0/3723	0.34	0/5078
45	N5	0.21	0/4914	0.35	0/6683
46	N6	0.18	0/1266	0.32	0/1712
47	QA	0.18	0/3200	0.29	0/4333
47	Qa	0.17	0/3200	0.28	0/4333
48	QB	0.19	0/3531	0.30	0/4793
48	Qb	0.18	0/3436	0.28	0/4659
49	QC	0.20	0/3123	0.32	0/4269
49	Qc	0.21	0/3123	0.31	0/4269
50	QD	0.18	0/1979	0.27	0/2684
50	Qd	0.18	0/1962	0.28	0/2663
51	QE	0.13	0/1550	0.25	0/2098
51	Qe	0.13	0/1550	0.27	0/2098
52	QF	0.14	0/558	0.22	0/747
52	Qf	0.16	0/534	0.25	0/714
53	QG	0.17	0/913	0.27	0/1223
53	Qg	0.18	0/913	0.26	0/1223
54	QH	0.17	0/684	0.30	0/926
54	Qh	0.17	0/688	0.29	0/931
55	QI	0.15	0/520	0.19	0/701
55	Qi	0.18	0/506	0.24	0/683
56	QJ	0.13	0/420	0.21	0/576
57	QK	0.12	0/528	0.26	0/716
58	Qj	0.16	0/437	0.29	0/598
59	S1	0.21	0/5378	0.32	0/7287
60	S2	0.23	0/3465	0.31	0/4691
61	S3	0.22	0/1780	0.29	0/2424
62	S4	0.20	0/1030	0.29	0/1391
63	S5	0.18	0/845	0.25	0/1129
64	S6	0.17	0/755	0.27	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
65	S7	0.22	0/1279	0.29	0/1730
66	S8	0.22	0/1443	0.28	0/1952
67	V1	0.20	0/3391	0.31	0/4583
68	V2	0.17	0/1711	0.30	0/2328
69	V3	0.15	0/365	0.29	0/493
All	All	0.19	0/115231	0.30	4/156309 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A9	369	VAL	CA-C-N	7.40	135.01	120.94
18	A9	369	VAL	C-N-CA	7.40	135.01	120.94
20	AK	204	HIS	CA-C-N	-5.49	116.29	122.93
20	AK	204	HIS	C-N-CA	-5.49	116.29	122.93

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	4L	748	0	799	19	0
2	5A	825	0	823	19	0
3	5B	724	0	705	17	0
4	6A	620	0	589	19	0
5	6B	684	0	649	20	0
6	6C	574	0	590	14	0
7	7A	447	0	443	10	0
8	7B	392	0	372	7	0
9	7C	387	0	385	6	0
10	8B	338	0	342	9	0
11	A1	562	0	557	6	0
12	A2	686	0	699	6	0
13	A3	643	0	642	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A5	910	0	950	5	0
15	A6	967	0	972	13	0
16	A7	780	0	808	6	0
17	A8	1398	0	1372	22	0
18	A9	2703	0	2720	33	0
19	AB	624	0	625	10	0
19	AC	702	0	694	14	0
20	AK	2590	0	2551	43	0
21	AL	1021	0	1025	9	0
22	AM	1195	0	1149	12	0
23	AN	1173	0	1166	21	0
24	B1	479	0	486	4	0
25	B2	584	0	529	7	0
26	B3	632	0	612	8	0
27	B4	1062	0	1072	13	0
28	B5	1151	0	1164	17	0
29	B6	861	0	877	20	0
30	B7	1068	0	1041	15	0
31	B8	1315	0	1208	14	0
32	B9	1534	0	1470	29	0
33	BK	1456	0	1424	15	0
34	BL	828	0	788	11	0
35	C1	4024	0	4005	114	0
36	C2	1833	0	1843	44	0
37	C3	2103	0	2034	48	0
38	C4	1153	0	1130	25	0
39	CA	417	0	422	6	0
40	CB	1000	0	994	19	0
41	N1	2457	0	2554	52	0
42	N2	2710	0	2874	59	0
43	N3	786	0	836	14	0
44	N4	3631	0	3839	74	0
45	N5	4785	0	4933	96	0
46	N6	1236	0	1241	30	0
47	QA	3147	0	3129	48	0
47	Qa	3147	0	3129	62	0
48	QB	3459	0	3350	46	0
48	Qb	3367	0	3262	52	0
49	QC	3025	0	3090	50	0
49	Qc	3025	0	3090	37	0
50	QD	1921	0	1867	24	0
50	Qd	1904	0	1849	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	QE	1517	0	1500	45	0
51	Qe	1517	0	1500	33	0
52	QF	552	0	536	7	0
52	Qf	528	0	510	11	0
53	QG	893	0	888	10	0
53	Qg	893	0	888	10	0
54	QH	662	0	660	13	0
54	Qh	666	0	663	14	0
55	QI	507	0	509	6	0
55	Qi	493	0	491	6	0
56	QJ	405	0	405	2	0
57	QK	520	0	554	10	0
58	Qj	421	0	418	5	0
59	S1	5290	0	5321	105	0
60	S2	3391	0	3328	67	0
61	S3	1729	0	1687	18	0
62	S4	1007	0	1008	15	0
63	S5	825	0	834	13	0
64	S6	741	0	701	13	0
65	S7	1248	0	1254	17	0
66	S8	1412	0	1363	25	0
67	V1	3316	0	3272	68	0
68	V2	1671	0	1673	17	0
69	V3	355	0	329	10	0
70	5B	1	0	0	0	0
70	S6	1	0	0	0	0
71	6A	45	0	64	16	0
71	7B	54	0	88	4	0
71	AL	54	0	88	2	0
71	C1	100	0	157	4	0
71	C3	92	0	138	8	0
71	N5	54	0	88	1	0
71	N6	54	0	88	0	0
71	QC	108	0	176	6	0
71	QH	54	0	88	5	0
71	Qb	29	0	32	1	0
71	Qj	54	0	88	0	0
72	6A	69	0	85	4	0
72	A8	83	0	113	4	0
72	AL	257	0	361	7	0
72	AM	51	0	46	1	0
72	B5	100	0	156	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	CB	100	0	156	11	0
72	N2	68	0	80	2	0
72	N5	189	0	284	15	0
72	QB	64	0	72	0	0
72	QC	149	0	192	10	0
72	QH	61	0	66	3	0
72	Qb	64	0	72	2	0
72	Qd	64	0	72	6	0
72	Qh	64	0	72	3	0
73	A9	48	0	26	2	0
74	AB	36	0	47	1	0
74	AC	36	0	47	4	0
75	AK	27	0	12	4	0
76	AL	51	0	82	2	0
76	C1	95	0	147	2	0
76	CA	51	0	82	2	0
76	CB	46	0	69	2	0
76	N4	51	0	82	4	0
76	QE	44	0	65	3	0
76	S7	51	0	82	4	0
77	AL	47	0	75	5	0
77	AM	104	0	176	9	0
77	B5	52	0	88	5	0
77	C2	43	0	67	1	0
77	CB	52	0	88	4	0
77	N4	52	0	88	1	0
77	QE	46	0	73	6	0
77	QI	52	0	88	5	0
78	B5	54	0	0	0	0
78	QJ	54	0	0	0	0
78	Qc	54	0	0	1	0
79	C1	120	0	108	23	0
80	C1	1	0	0	0	0
80	C2	2	0	0	0	0
81	C1	1	0	0	0	0
81	S1	1	0	0	0	0
82	C1	51	0	82	3	0
82	N1	38	0	50	1	0
82	N3	51	0	82	2	0
82	N5	46	0	69	5	0
82	QB	78	0	110	2	0
82	QC	89	0	132	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	QE	47	0	71	5	0
82	Qc	42	0	61	0	0
82	Qd	51	0	82	4	0
82	Qh	92	0	138	8	0
82	S2	48	0	73	3	0
82	S8	51	0	82	1	0
83	QC	86	0	60	10	0
83	Qc	86	0	60	7	0
84	QD	43	0	30	2	0
84	Qd	43	0	32	3	0
85	QE	4	0	0	2	0
85	Qe	4	0	0	1	0
85	S1	4	0	0	0	0
85	V2	4	0	0	0	0
86	S1	16	0	0	0	0
86	S7	8	0	0	1	0
86	S8	16	0	0	2	0
86	V1	8	0	0	1	0
87	V1	31	0	19	1	0
All	All	116743	0	117808	1761	0

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

The worst 5 of 1761 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)
33:BK:140:GLN:O	33:BK:144:SER:HB2	1.72	0.89
71:7B:101:PC1:H2D1	71:7B:101:PC1:H3E1	1.57	0.84
36:C2:196:CYS:HB3	36:C2:207:MET:SD	2.18	0.82
66:S8:205:ILE:O	66:S8:209:TYR:HB3	1.80	0.81
36:C2:196:CYS:CB	36:C2:207:MET:SD	2.69	0.80

There are no symmetry-related clashes.

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	4L	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
2	5A	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
3	5B	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
4	6A	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
5	6B	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
6	6C	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
7	7A	55/57 (96%)	55 (100%)	0	0	100	100
8	7B	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
9	7C	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
10	8B	41/43 (95%)	41 (100%)	0	0	100	100
11	A1	68/70 (97%)	68 (100%)	0	0	100	100
12	A2	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
13	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
14	A5	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
15	A6	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
16	A7	93/112 (83%)	89 (96%)	4 (4%)	0	100	100
17	A8	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
18	A9	333/341 (98%)	322 (97%)	11 (3%)	0	100	100
19	AB	75/156 (48%)	74 (99%)	1 (1%)	0	100	100
19	AC	85/156 (54%)	85 (100%)	0	0	100	100
20	AK	318/320 (99%)	306 (96%)	12 (4%)	0	100	100
21	AL	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
22	AM	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
23	AN	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
24	B1	54/56 (96%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	B2	65/67 (97%)	65 (100%)	0	0	100	100
26	B3	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
27	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
28	B5	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
29	B6	97/126 (77%)	93 (96%)	4 (4%)	0	100	100
30	B7	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
31	B8	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
32	B9	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
33	BK	172/176 (98%)	171 (99%)	1 (1%)	0	100	100
34	BL	97/102 (95%)	90 (93%)	7 (7%)	0	100	100
35	C1	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
36	C2	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
37	C3	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
38	C4	136/138 (99%)	127 (93%)	9 (7%)	0	100	100
39	CA	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
40	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
41	N1	307/318 (96%)	295 (96%)	12 (4%)	0	100	100
42	N2	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
43	N3	94/115 (82%)	91 (97%)	3 (3%)	0	100	100
44	N4	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
45	N5	601/603 (100%)	568 (94%)	33 (6%)	0	100	100
46	N6	159/173 (92%)	146 (92%)	13 (8%)	0	100	100
47	QA	417/419 (100%)	404 (97%)	13 (3%)	0	100	100
47	Qa	417/419 (100%)	403 (97%)	14 (3%)	0	100	100
48	QB	444/446 (100%)	430 (97%)	14 (3%)	0	100	100
48	Qb	429/446 (96%)	421 (98%)	8 (2%)	0	100	100
49	QC	377/379 (100%)	368 (98%)	9 (2%)	0	100	100
49	Qc	377/379 (100%)	368 (98%)	9 (2%)	0	100	100
50	QD	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
50	Qd	237/241 (98%)	234 (99%)	3 (1%)	0	100	100
51	QE	194/196 (99%)	188 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	Qe	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
52	QF	65/67 (97%)	65 (100%)	0	0	100	100
52	Qf	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
53	QG	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
53	Qg	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
54	QH	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
54	Qh	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
55	QI	60/64 (94%)	59 (98%)	1 (2%)	0	100	100
55	Qi	58/64 (91%)	58 (100%)	0	0	100	100
56	QJ	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
57	QK	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
58	Qj	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
59	S1	687/689 (100%)	653 (95%)	34 (5%)	0	100	100
60	S2	414/430 (96%)	392 (95%)	22 (5%)	0	100	100
61	S3	205/207 (99%)	192 (94%)	13 (6%)	0	100	100
62	S4	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
63	S5	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
64	S6	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
65	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
66	S8	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
67	V1	429/431 (100%)	404 (94%)	25 (6%)	0	100	100
68	V2	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
69	V3	40/42 (95%)	36 (90%)	4 (10%)	0	100	100
All	All	13901/14350 (97%)	13434 (97%)	467 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	4L	85/85 (100%)	85 (100%)	0	100	100
2	5A	89/89 (100%)	88 (99%)	1 (1%)	70	84
3	5B	80/80 (100%)	80 (100%)	0	100	100
4	6A	66/66 (100%)	64 (97%)	2 (3%)	36	63
5	6B	73/73 (100%)	73 (100%)	0	100	100
6	6C	57/57 (100%)	56 (98%)	1 (2%)	54	75
7	7A	48/48 (100%)	44 (92%)	4 (8%)	9	33
8	7B	39/39 (100%)	39 (100%)	0	100	100
9	7C	40/40 (100%)	40 (100%)	0	100	100
10	8B	37/37 (100%)	37 (100%)	0	100	100
11	A1	58/58 (100%)	58 (100%)	0	100	100
12	A2	76/76 (100%)	76 (100%)	0	100	100
13	A3	69/69 (100%)	69 (100%)	0	100	100
14	A5	99/99 (100%)	98 (99%)	1 (1%)	73	85
15	A6	107/107 (100%)	106 (99%)	1 (1%)	75	87
16	A7	87/97 (90%)	86 (99%)	1 (1%)	70	84
17	A8	153/153 (100%)	152 (99%)	1 (1%)	81	90
18	A9	291/295 (99%)	290 (100%)	1 (0%)	91	95
19	AB	71/132 (54%)	71 (100%)	0	100	100
19	AC	80/132 (61%)	79 (99%)	1 (1%)	65	81
20	AK	283/283 (100%)	278 (98%)	5 (2%)	54	75
21	AL	101/101 (100%)	99 (98%)	2 (2%)	50	73
22	AM	129/129 (100%)	129 (100%)	0	100	100
23	AN	123/123 (100%)	121 (98%)	2 (2%)	58	77
24	B1	53/53 (100%)	53 (100%)	0	100	100
25	B2	62/62 (100%)	62 (100%)	0	100	100
26	B3	61/61 (100%)	61 (100%)	0	100	100
27	B4	113/113 (100%)	113 (100%)	0	100	100
28	B5	121/121 (100%)	121 (100%)	0	100	100
29	B6	96/119 (81%)	96 (100%)	0	100	100
30	B7	112/112 (100%)	112 (100%)	0	100	100
31	B8	141/141 (100%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	B9	159/159 (100%)	159 (100%)	0	100	100
33	BK	155/156 (99%)	155 (100%)	0	100	100
34	BL	91/94 (97%)	91 (100%)	0	100	100
35	C1	425/425 (100%)	415 (98%)	10 (2%)	44	68
36	C2	212/212 (100%)	209 (99%)	3 (1%)	62	80
37	C3	224/224 (100%)	222 (99%)	2 (1%)	75	87
38	C4	123/123 (100%)	122 (99%)	1 (1%)	79	88
39	CA	45/45 (100%)	43 (96%)	2 (4%)	24	54
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	269/275 (98%)	268 (100%)	1 (0%)	89	93
42	N2	311/311 (100%)	310 (100%)	1 (0%)	91	95
43	N3	86/100 (86%)	86 (100%)	0	100	100
44	N4	410/410 (100%)	409 (100%)	1 (0%)	92	96
45	N5	537/537 (100%)	533 (99%)	4 (1%)	81	90
46	N6	129/139 (93%)	127 (98%)	2 (2%)	58	77
47	QA	330/330 (100%)	329 (100%)	1 (0%)	91	95
47	Qa	330/330 (100%)	324 (98%)	6 (2%)	54	75
48	QB	372/372 (100%)	367 (99%)	5 (1%)	65	81
48	Qb	362/372 (97%)	357 (99%)	5 (1%)	62	80
49	QC	332/332 (100%)	325 (98%)	7 (2%)	48	72
49	Qc	332/332 (100%)	331 (100%)	1 (0%)	91	95
50	QD	206/206 (100%)	206 (100%)	0	100	100
50	Qd	204/206 (99%)	202 (99%)	2 (1%)	73	85
51	QE	166/166 (100%)	166 (100%)	0	100	100
51	Qe	166/166 (100%)	166 (100%)	0	100	100
52	QF	64/64 (100%)	64 (100%)	0	100	100
52	Qf	61/64 (95%)	61 (100%)	0	100	100
53	QG	93/93 (100%)	92 (99%)	1 (1%)	70	84
53	Qg	93/93 (100%)	93 (100%)	0	100	100
54	QH	70/70 (100%)	70 (100%)	0	100	100
54	Qh	70/70 (100%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	QI	50/52 (96%)	49 (98%)	1 (2%)	50	73
55	Qi	49/52 (94%)	49 (100%)	0	100	100
56	QJ	40/40 (100%)	40 (100%)	0	100	100
57	QK	55/59 (93%)	55 (100%)	0	100	100
58	Qj	41/41 (100%)	41 (100%)	0	100	100
59	S1	579/579 (100%)	574 (99%)	5 (1%)	75	87
60	S2	363/370 (98%)	362 (100%)	1 (0%)	91	95
61	S3	189/189 (100%)	186 (98%)	3 (2%)	58	77
62	S4	112/112 (100%)	109 (97%)	3 (3%)	40	66
63	S5	88/88 (100%)	88 (100%)	0	100	100
64	S6	79/79 (100%)	79 (100%)	0	100	100
65	S7	132/132 (100%)	130 (98%)	2 (2%)	60	78
66	S8	151/151 (100%)	149 (99%)	2 (1%)	65	81
67	V1	344/344 (100%)	337 (98%)	7 (2%)	50	73
68	V2	183/183 (100%)	181 (99%)	2 (1%)	70	84
69	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	12131/12346 (98%)	12027 (99%)	104 (1%)	74	87

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	QC	112	THR
48	Qb	92	PHE
67	V1	347	THR
49	QC	171	ASP
47	Qa	231	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 268 such sidechains are listed below:

Mol	Chain	Res	Type
60	S2	66	HIS
61	S3	123	GLN
68	V2	41	HIS
37	C3	231	HIS
37	C3	125	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
60	2MR	S2	124	60	10,12,13	2.41	3 (30%)	5,13,15	0.90	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
60	2MR	S2	124	60	-	3/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	S2	124	2MR	CZ-NE	5.08	1.45	1.34
60	S2	124	2MR	CZ-NH2	4.94	1.44	1.33
60	S2	124	2MR	CQ1-NH1	-2.06	1.42	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	S2	124	2MR	NE-CD-CG-CB
60	S2	124	2MR	CA-CB-CG-CD
60	S2	124	2MR	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 97 ligands modelled in this entry, 7 are monoatomic - leaving 90 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	$\# Z > 2$
86	SF4	S8	301	66	0,12,12	-	-	-		
72	CDL	Qh	102	-	63,63,99	0.37	0	69,75,111	0.37	0
82	PEE	Qc	401	-	41,41,50	1.27	4 (9%)	44,46,55	1.21	4 (9%)
82	PEE	QB	502	-	26,26,50	1.36	3 (11%)	29,31,55	1.22	2 (6%)
82	PEE	C1	609	-	50,50,50	1.32	5 (10%)	53,55,55	1.16	3 (5%)
77	PLX	C2	301	-	42,42,51	1.17	4 (9%)	46,50,59	0.85	1 (2%)
77	PLX	AM	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.88	1 (1%)
71	PC1	C3	301	-	48,48,53	0.31	0	54,56,61	0.38	0
72	CDL	Qb	501	-	63,63,99	0.37	0	69,75,111	0.38	0
75	ADP	AK	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
72	CDL	QC	408	-	54,54,99	0.39	0	60,66,111	0.38	0
86	SF4	S8	302	66	0,12,12	-	-	-		
73	NDP	A9	401	-	45,52,52	0.55	0	53,80,80	0.53	1 (1%)
71	PC1	Qj	101	-	53,53,53	0.30	0	59,61,61	0.34	0
78	6F6	B5	203	-	53,53,53	0.29	0	59,61,61	0.33	0
76	3PE	S7	302	-	50,50,50	0.31	0	53,55,55	0.34	0
72	CDL	6A	102	-	68,68,99	0.35	0	74,80,111	0.35	0
76	3PE	C1	601	-	50,50,50	0.30	0	53,55,55	0.30	0
71	PC1	QC	405	-	53,53,53	0.30	0	59,61,61	0.30	0
71	PC1	N5	704	-	53,53,53	0.29	0	59,61,61	0.28	0
76	3PE	N4	502	-	50,50,50	0.31	0	53,55,55	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
77	PLX	AM	203	-	51,51,51	1.10	3 (5%)	55,59,59	0.89	1 (1%)
72	CDL	N5	702	-	88,88,99	0.31	0	94,100,111	0.32	0
86	SF4	S1	802	59	0,12,12	-	-	-	-	-
71	PC1	C1	607	-	45,45,53	0.31	0	51,53,61	0.35	0
76	3PE	QE	303	-	43,43,50	0.32	0	46,48,55	0.31	0
82	PEE	QB	503	-	50,50,50	1.31	5 (10%)	53,55,55	1.16	3 (5%)
72	CDL	QB	501	-	63,63,99	0.37	0	69,75,111	0.41	0
84	HEC	Qd	402	50	32,50,50	2.07	4 (12%)	24,82,82	2.23	12 (50%)
76	3PE	CB	202	-	45,45,50	0.31	0	48,50,55	0.29	0
77	PLX	AL	205	-	46,46,51	1.13	4 (8%)	50,54,59	0.93	2 (4%)
72	CDL	AM	202	-	50,50,99	0.40	0	56,62,111	0.34	0
72	CDL	AL	203	-	92,92,99	0.31	0	98,104,111	0.29	0
77	PLX	CB	201	-	51,51,51	1.11	3 (5%)	55,59,59	0.92	1 (1%)
82	PEE	S2	501	-	47,47,50	1.35	5 (10%)	50,52,55	1.18	3 (6%)
71	PC1	AL	206	-	53,53,53	0.29	0	59,61,61	0.31	0
74	ZMP	AC	201	19	29,35,36	0.73	1 (3%)	34,42,45	0.76	0
83	HEM	QC	403	49	41,50,50	1.27	3 (7%)	45,82,82	1.69	7 (15%)
82	PEE	Qd	403	-	50,50,50	1.31	5 (10%)	53,55,55	1.20	4 (7%)
71	PC1	N6	201	-	53,53,53	0.30	0	59,61,61	0.26	0
72	CDL	B5	202	-	99,99,99	0.31	0	105,111,111	0.29	0
82	PEE	N3	201	-	50,50,50	1.30	5 (10%)	53,55,55	1.19	5 (9%)
83	HEM	QC	402	49	41,50,50	1.24	4 (9%)	45,82,82	1.72	9 (20%)
72	CDL	CB	203	-	99,99,99	0.30	0	105,111,111	0.29	0
71	PC1	QH	102	-	53,53,53	0.29	0	59,61,61	0.32	0
87	FMN	V1	502	-	33,33,33	0.31	0	48,50,50	0.44	0
85	FES	Qe	301	51	0,4,4	-	-	-	-	-
72	CDL	AL	204	-	79,79,99	0.33	0	85,91,111	0.42	0
82	PEE	N1	401	-	37,37,50	1.47	5 (13%)	39,42,55	1.27	4 (10%)
77	PLX	N4	501	-	51,51,51	1.11	3 (5%)	55,59,59	0.92	2 (3%)
76	3PE	C1	608	-	43,43,50	0.33	0	46,48,55	0.41	0
82	PEE	Qh	103	-	50,50,50	1.32	5 (10%)	53,55,55	1.18	4 (7%)
78	6F6	QJ	101	-	53,53,53	0.29	0	59,61,61	0.30	0
78	6F6	Qc	404	-	53,53,53	0.29	0	59,61,61	0.38	0
86	SF4	S1	801	59	0,12,12	-	-	-	-	-
77	PLX	B5	201	-	51,51,51	1.11	3 (5%)	55,59,59	0.91	1 (1%)
72	CDL	AL	201	-	83,83,99	0.32	0	89,95,111	0.34	0
82	PEE	QC	401	-	50,50,50	1.32	5 (10%)	53,55,55	1.22	3 (5%)
74	ZMP	AB	201	19	29,35,36	0.70	1 (3%)	34,42,45	0.90	2 (5%)
72	CDL	QC	406	-	93,93,99	0.31	0	99,105,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
77	PLX	QE	301	-	45,45,51	1.18	3 (6%)	49,53,59	0.92	1 (2%)
72	CDL	N2	401	-	67,67,99	0.35	0	73,79,111	0.30	0
77	PLX	QI	301	-	51,51,51	1.12	3 (5%)	55,59,59	0.89	1 (1%)
86	SF4	V1	501	67	0,12,12	-	-	-	-	-
84	HEC	QD	401	50	32,50,50	2.06	4 (12%)	24,82,82	2.37	13 (54%)
71	PC1	C1	606	-	53,53,53	0.28	0	59,61,61	0.27	0
71	PC1	6A	101	-	44,44,53	0.32	0	50,52,61	0.33	0
76	3PE	CA	101	-	50,50,50	0.30	0	53,55,55	0.33	0
82	PEE	QC	404	-	37,37,50	1.34	4 (10%)	40,42,55	1.15	2 (5%)
85	FES	QE	304	51	0,4,4	-	-	-	-	-
82	PEE	S8	303	-	50,50,50	1.30	5 (10%)	53,55,55	1.20	4 (7%)
76	3PE	AL	202	-	50,50,50	0.31	0	53,55,55	0.32	0
82	PEE	QE	302	-	46,46,50	1.35	5 (10%)	49,51,55	1.28	4 (8%)
71	PC1	QC	407	-	53,53,53	0.29	0	59,61,61	0.32	0
72	CDL	N5	703	-	99,99,99	0.30	0	105,111,111	0.30	0
71	PC1	Qb	502	-	28,28,53	0.39	0	34,36,61	0.40	0
85	FES	S1	803	59	0,4,4	-	-	-	-	-
72	CDL	A8	301	-	82,82,99	0.33	0	88,94,111	0.33	0
85	FES	V2	301	68	0,4,4	-	-	-	-	-
83	HEM	Qc	402	49	41,50,50	1.24	3 (7%)	45,82,82	1.72	8 (17%)
72	CDL	QH	101	-	60,60,99	0.38	0	66,72,111	0.37	0
79	HEA	C1	603	35	57,67,67	2.01	16 (28%)	61,103,103	2.70	26 (42%)
86	SF4	S7	301	65	0,12,12	-	-	-	-	-
82	PEE	N5	701	-	45,45,50	1.38	5 (11%)	48,50,55	1.18	2 (4%)
71	PC1	C3	302	-	42,42,53	0.33	0	48,50,61	0.31	0
82	PEE	Qh	101	-	40,40,50	1.47	5 (12%)	42,45,55	1.14	3 (7%)
79	HEA	C1	602	35	57,67,67	2.02	15 (26%)	61,103,103	2.70	28 (45%)
83	HEM	Qc	403	49	41,50,50	1.25	3 (7%)	45,82,82	1.71	8 (17%)
72	CDL	Qd	401	-	63,63,99	0.37	0	69,75,111	0.36	0
71	PC1	7B	101	-	53,53,53	0.29	0	59,61,61	0.27	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
86	SF4	S8	301	66	-	-	0/6/5/5
72	CDL	Qh	102	-	-	27/74/74/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEE	Qc	401	-	-	26/45/45/54	-
82	PEE	QB	502	-	-	13/30/30/54	-
82	PEE	C1	609	-	-	25/54/54/54	-
77	PLX	C2	301	-	-	21/46/46/55	-
77	PLX	AM	201	-	-	19/55/55/55	-
71	PC1	C3	301	-	-	17/52/52/57	-
72	CDL	Qb	501	-	-	18/74/74/110	-
75	ADP	AK	401	-	-	2/12/32/32	0/3/3/3
72	CDL	QC	408	-	-	18/65/65/110	-
86	SF4	S8	302	66	-	-	0/6/5/5
73	NDP	A9	401	-	-	6/30/77/77	0/5/5/5
71	PC1	Qj	101	-	-	18/57/57/57	-
78	6F6	B5	203	-	-	11/57/57/57	-
76	3PE	S7	302	-	-	15/54/54/54	-
72	CDL	6A	102	-	-	28/79/79/110	-
76	3PE	C1	601	-	-	11/54/54/54	-
71	PC1	QC	405	-	-	16/57/57/57	-
71	PC1	N5	704	-	-	11/57/57/57	-
76	3PE	N4	502	-	-	12/54/54/54	-
77	PLX	AM	203	-	-	24/55/55/55	-
72	CDL	N5	702	-	-	22/99/99/110	-
86	SF4	S1	802	59	-	-	0/6/5/5
71	PC1	C1	607	-	-	10/49/49/57	-
76	3PE	QE	303	-	-	7/47/47/54	-
82	PEE	QB	503	-	-	23/54/54/54	-
72	CDL	QB	501	-	-	21/74/74/110	-
84	HEC	Qd	402	50	-	1/10/54/54	-
76	3PE	CB	202	-	-	8/49/49/54	-
77	PLX	AL	205	-	-	21/50/50/55	-
72	CDL	AM	202	-	-	9/61/61/110	-
72	CDL	AL	203	-	-	22/103/103/110	-
77	PLX	CB	201	-	-	27/55/55/55	-
82	PEE	S2	501	-	-	30/51/51/54	-
71	PC1	AL	206	-	-	15/57/57/57	-
74	ZMP	AC	201	19	-	18/40/42/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	HEM	QC	403	49	-	4/12/54/54	-
82	PEE	Qd	403	-	-	24/54/54/54	-
71	PC1	N6	201	-	-	6/57/57/57	-
72	CDL	B5	202	-	-	17/110/110/110	-
82	PEE	N3	201	-	-	24/54/54/54	-
83	HEM	QC	402	49	-	7/12/54/54	-
72	CDL	CB	203	-	-	31/110/110/110	-
71	PC1	QH	102	-	-	9/57/57/57	-
87	FMN	V1	502	-	-	6/18/18/18	0/3/3/3
85	FES	Qe	301	51	-	-	0/1/1/1
72	CDL	AL	204	-	-	25/90/90/110	-
82	PEE	N1	401	-	-	19/41/41/54	-
77	PLX	N4	501	-	-	17/55/55/55	-
76	3PE	C1	608	-	-	12/47/47/54	-
82	PEE	Qh	103	-	-	17/54/54/54	-
78	6F6	QJ	101	-	-	18/57/57/57	-
78	6F6	Qc	404	-	-	13/57/57/57	-
86	SF4	S1	801	59	-	-	0/6/5/5
77	PLX	B5	201	-	-	23/55/55/55	-
72	CDL	AL	201	-	-	28/94/94/110	-
82	PEE	QC	401	-	-	26/54/54/54	-
74	ZMP	AB	201	19	-	16/40/42/43	-
72	CDL	QC	406	-	-	23/104/104/110	-
77	PLX	QE	301	-	-	19/49/49/55	-
72	CDL	N2	401	-	-	25/78/78/110	-
77	PLX	QI	301	-	-	19/55/55/55	-
86	SF4	V1	501	67	-	-	0/6/5/5
84	HEC	QD	401	50	-	2/10/54/54	-
71	PC1	C1	606	-	-	11/57/57/57	-
71	PC1	6A	101	-	-	15/48/48/57	-
76	3PE	CA	101	-	-	11/54/54/54	-
82	PEE	QC	404	-	-	12/41/41/54	-
85	FES	QE	304	51	-	-	0/1/1/1
82	PEE	S8	303	-	-	22/54/54/54	-
76	3PE	AL	202	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PEE	QE	302	-	-	20/50/50/54	-
71	PC1	QC	407	-	-	10/57/57/57	-
72	CDL	N5	703	-	-	21/110/110/110	-
71	PC1	Qb	502	-	-	11/32/32/57	-
85	FES	S1	803	59	-	-	0/1/1/1
72	CDL	A8	301	-	-	24/93/93/110	-
85	FES	V2	301	68	-	-	0/1/1/1
83	HEM	Qc	402	49	-	7/12/54/54	-
72	CDL	QH	101	-	-	12/71/71/110	-
79	HEA	C1	603	35	-	10/32/76/76	-
86	SF4	S7	301	65	-	-	0/6/5/5
82	PEE	N5	701	-	-	15/49/49/54	-
71	PC1	C3	302	-	-	9/46/46/57	-
82	PEE	Qh	101	-	-	25/44/44/54	-
79	HEA	C1	602	35	-	11/32/76/76	-
83	HEM	Qc	403	49	-	7/12/54/54	-
72	CDL	Qd	401	-	-	17/74/74/110	-
71	PC1	7B	101	-	-	16/57/57/57	-

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Qd	402	HEC	C3C-C2C	-6.77	1.33	1.40
84	QD	401	HEC	C3C-C2C	-6.67	1.33	1.40
84	Qd	402	HEC	C2B-C3B	-6.46	1.34	1.40
84	QD	401	HEC	C2B-C3B	-6.31	1.34	1.40
79	C1	602	HEA	C3B-C2B	5.25	1.46	1.34

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	C1	603	HEA	CAD-CBD-CGD	-8.30	95.74	113.60
79	C1	602	HEA	CAD-CBD-CGD	-7.80	96.81	113.60
79	C1	603	HEA	C3D-C4D-ND	6.02	116.18	110.36
79	C1	602	HEA	C3D-C4D-ND	5.65	115.83	110.36
79	C1	602	HEA	C13-C12-C11	-5.51	106.07	114.35

There are no chirality outliers.

5 of 1298 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
71	6A	101	PC1	C11-O13-P-O14
71	7B	101	PC1	C1-O11-P-O12
71	7B	101	PC1	C1-O11-P-O14
71	7B	101	PC1	O13-C11-C12-N
71	AL	206	PC1	C11-O13-P-O14

There are no ring outliers.

78 monomers are involved in 256 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	Qh	102	CDL	3	0
82	QB	502	PEE	1	0
82	C1	609	PEE	3	0
77	C2	301	PLX	1	0
77	AM	201	PLX	5	0
71	C3	301	PC1	6	0
72	Qb	501	CDL	2	0
75	AK	401	ADP	4	0
72	QC	408	CDL	4	0
86	S8	302	SF4	2	0
73	A9	401	NDP	2	0
76	S7	302	3PE	4	0
72	6A	102	CDL	4	0
76	C1	601	3PE	2	0
71	QC	405	PC1	3	0
71	N5	704	PC1	1	0
76	N4	502	3PE	4	0
77	AM	203	PLX	5	0
72	N5	702	CDL	12	0
71	C1	607	PC1	1	0
76	QE	303	3PE	3	0
82	QB	503	PEE	1	0
84	Qd	402	HEC	3	0
76	CB	202	3PE	2	0
77	AL	205	PLX	5	0
72	AM	202	CDL	1	0
72	AL	203	CDL	1	0
77	CB	201	PLX	4	0
82	S2	501	PEE	3	0
71	AL	206	PC1	2	0
74	AC	201	ZMP	4	0

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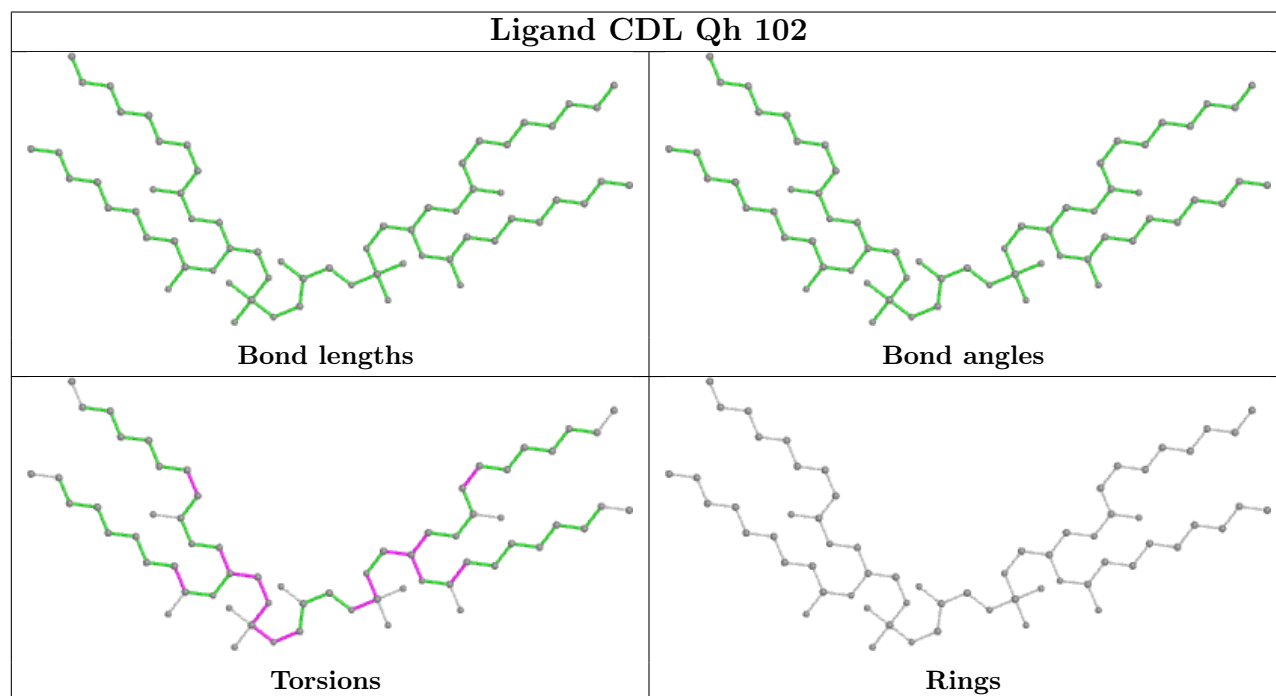
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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82	Qd	403	PEE	4	0
72	B5	202	CDL	3	0
82	N3	201	PEE	2	0
83	QC	402	HEM	4	0
72	CB	203	CDL	11	0
71	QH	102	PC1	5	0
87	V1	502	FMN	1	0
85	Qe	301	FES	1	0
72	AL	204	CDL	4	0
82	N1	401	PEE	1	0
77	N4	501	PLX	1	0
82	Qh	103	PEE	3	0
78	Qc	404	6F6	1	0
77	B5	201	PLX	5	0
72	AL	201	CDL	2	0
82	QC	401	PEE	1	0
74	AB	201	ZMP	1	0
72	QC	406	CDL	6	0
77	QE	301	PLX	6	0
72	N2	401	CDL	2	0
77	QI	301	PLX	5	0
86	V1	501	SF4	1	0
84	QD	401	HEC	2	0
71	C1	606	PC1	3	0
71	6A	101	PC1	16	0
76	CA	101	3PE	2	0
82	QC	404	PEE	2	0
85	QE	304	FES	2	0
82	S8	303	PEE	1	0
76	AL	202	3PE	2	0
82	QE	302	PEE	5	0
71	QC	407	PC1	3	0
72	N5	703	CDL	3	0
71	Qb	502	PC1	1	0
72	A8	301	CDL	4	0
83	Qc	402	HEM	2	0
72	QH	101	CDL	3	0
79	C1	603	HEA	16	0
86	S7	301	SF4	1	0
82	N5	701	PEE	5	0
71	C3	302	PC1	2	0

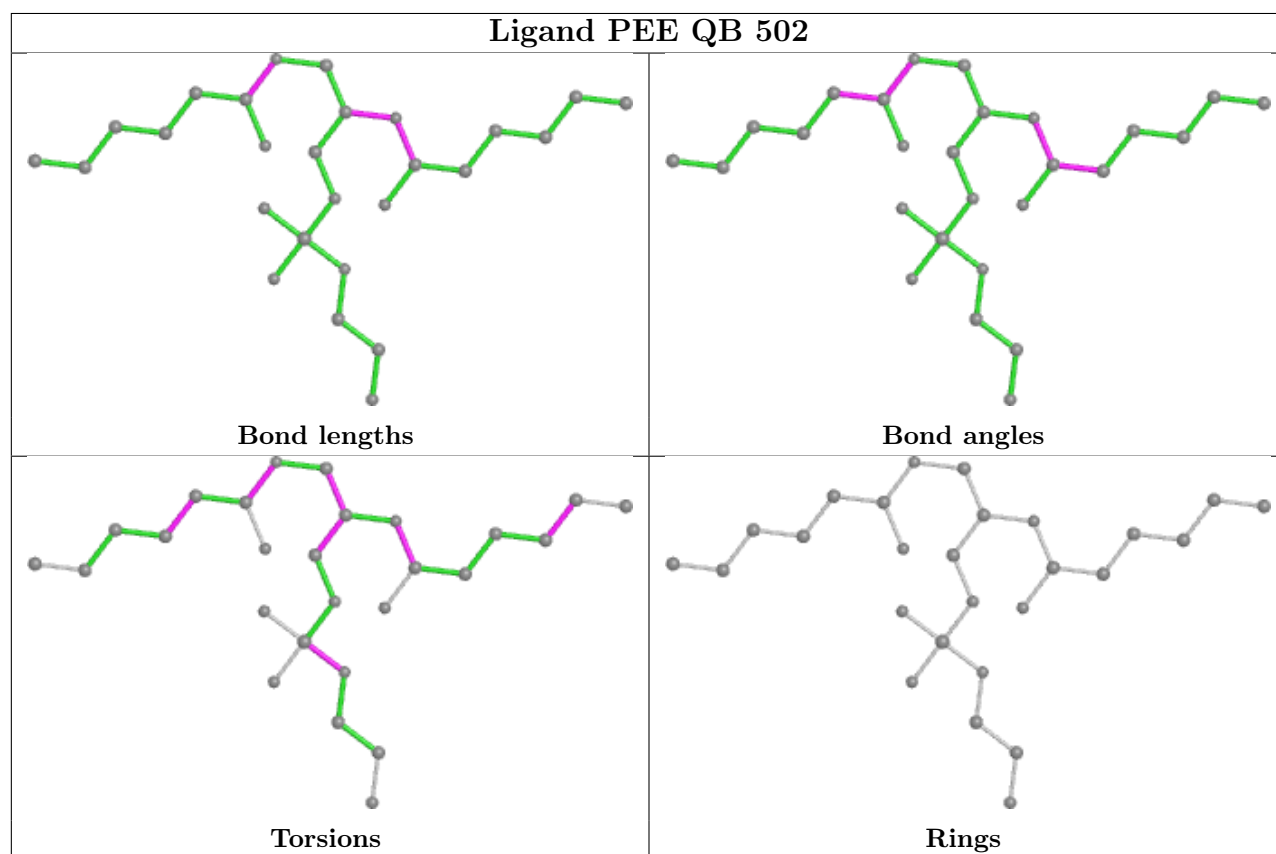
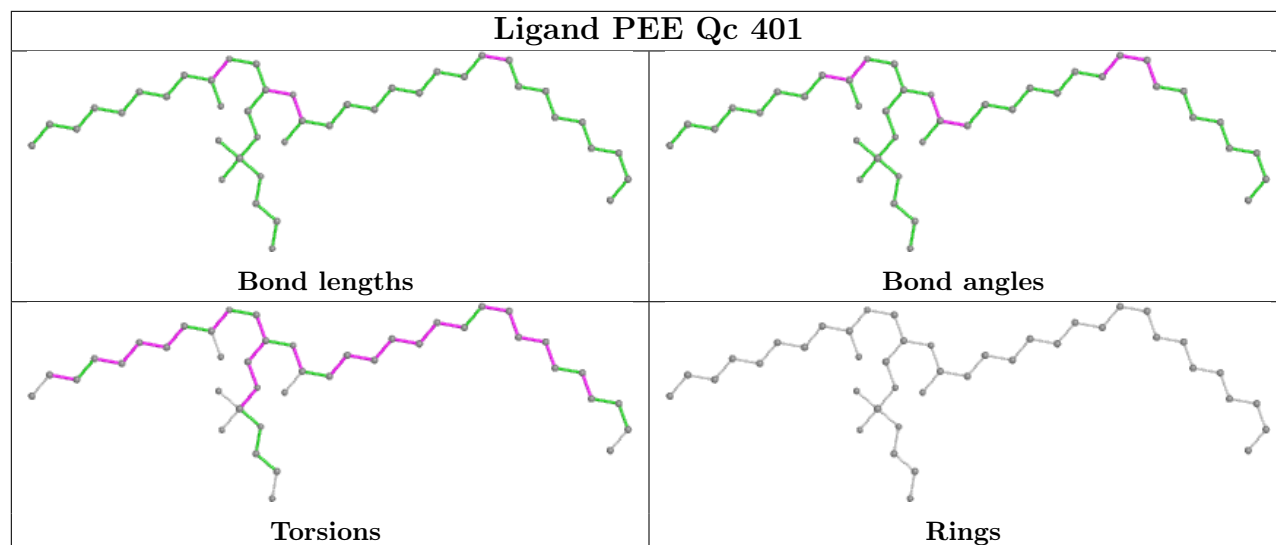
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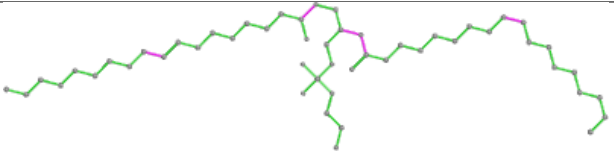
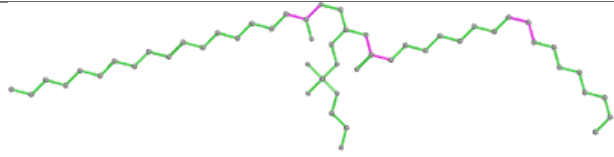
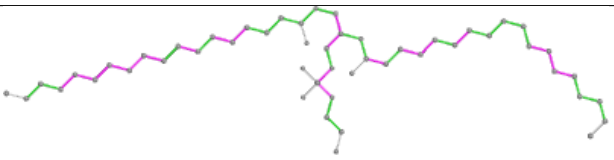
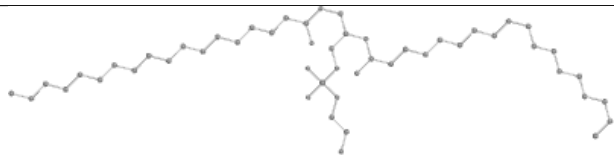
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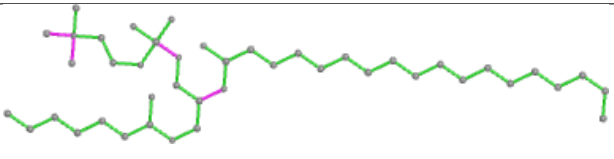
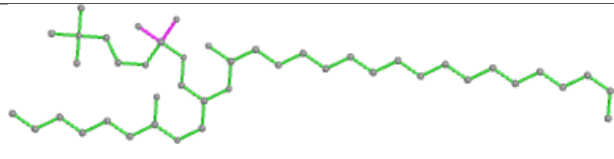
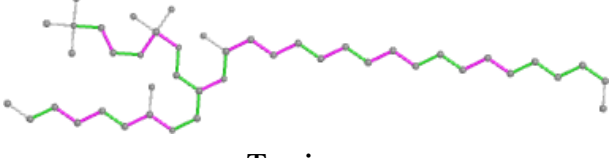
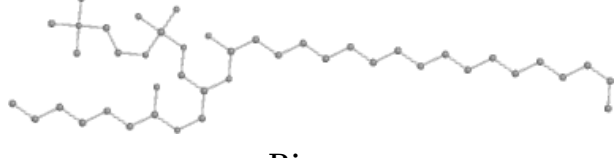
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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79	C1	602	HEA	7	0
83	Qc	403	HEM	5	0
72	Qd	401	CDL	6	0
71	7B	101	PC1	4	0

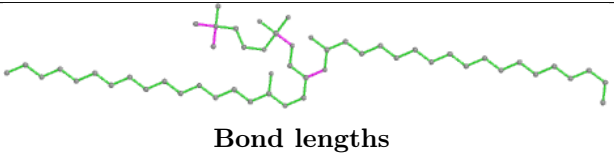
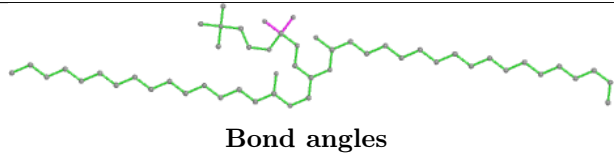
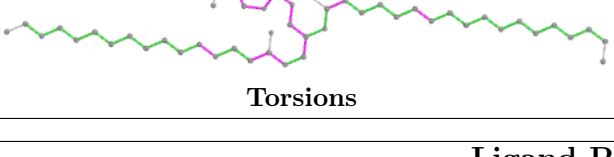

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

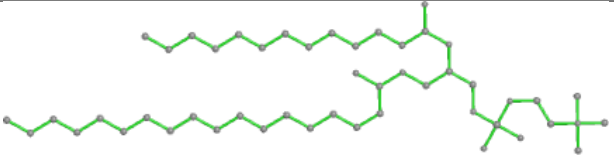
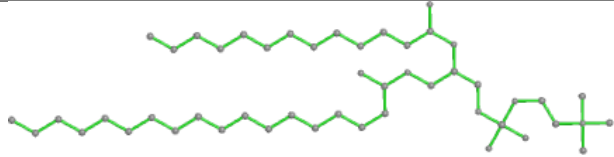
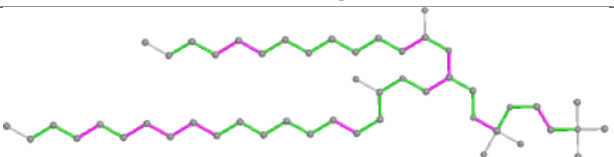
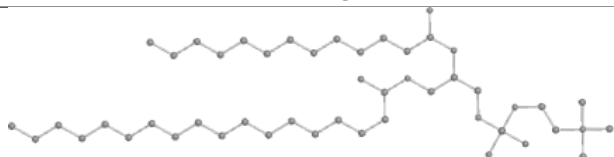


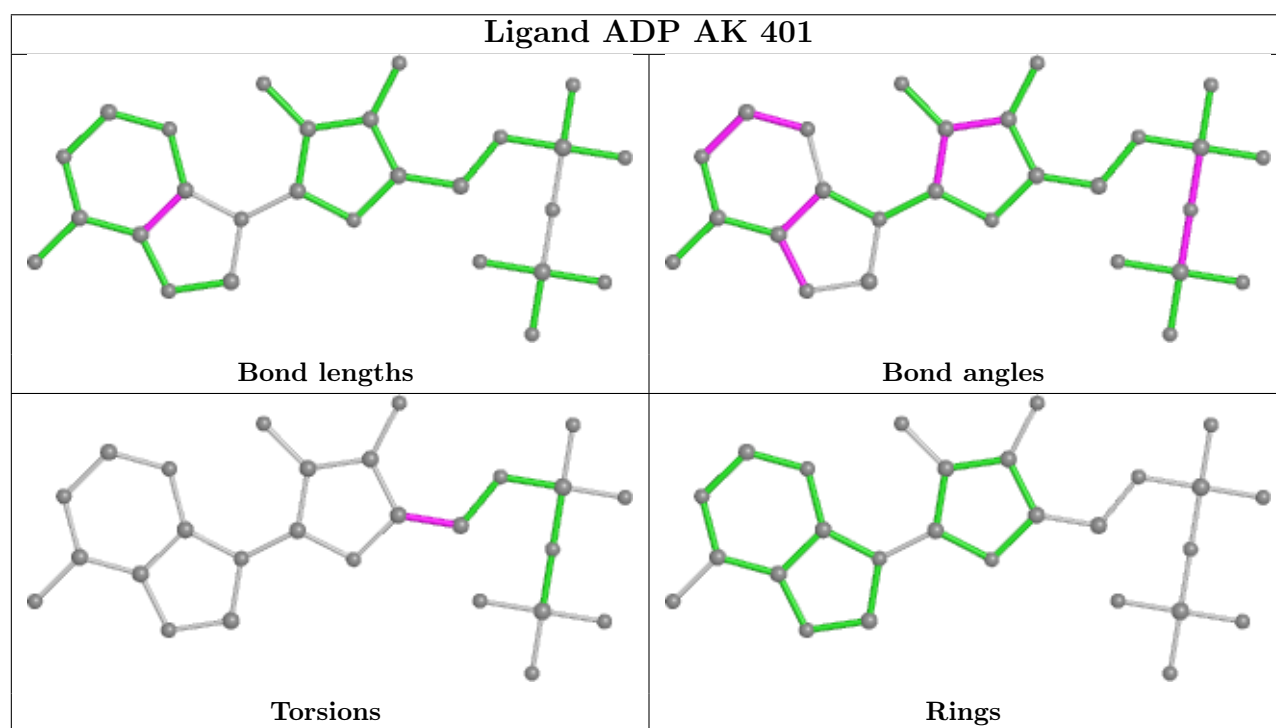
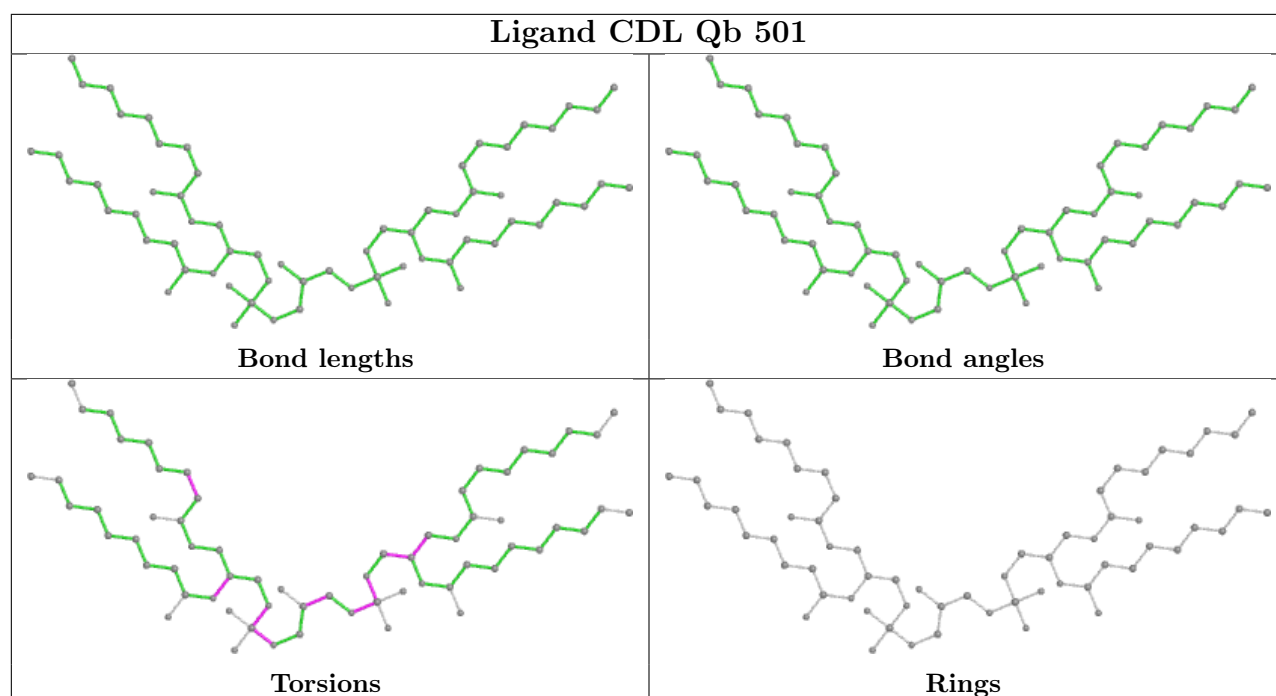


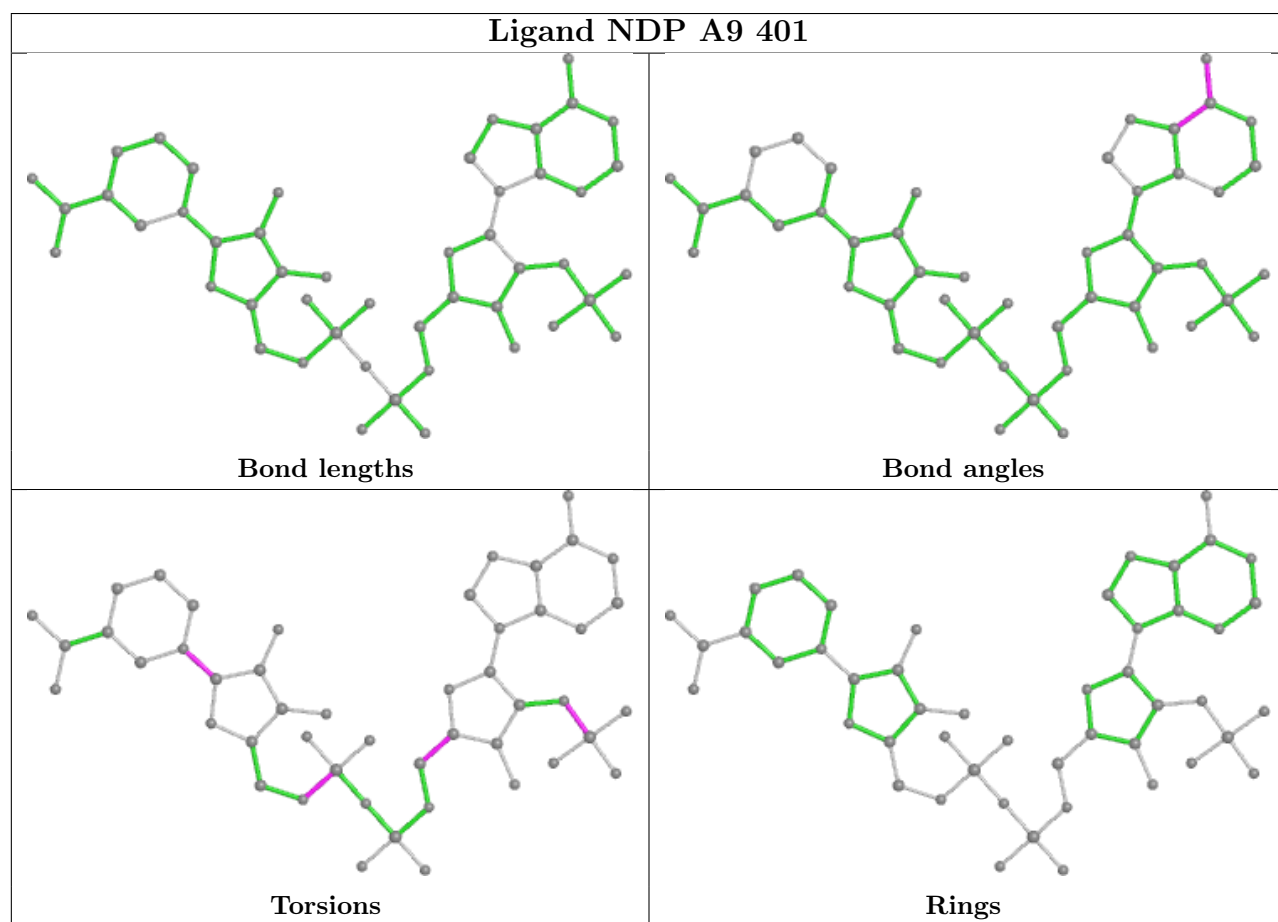
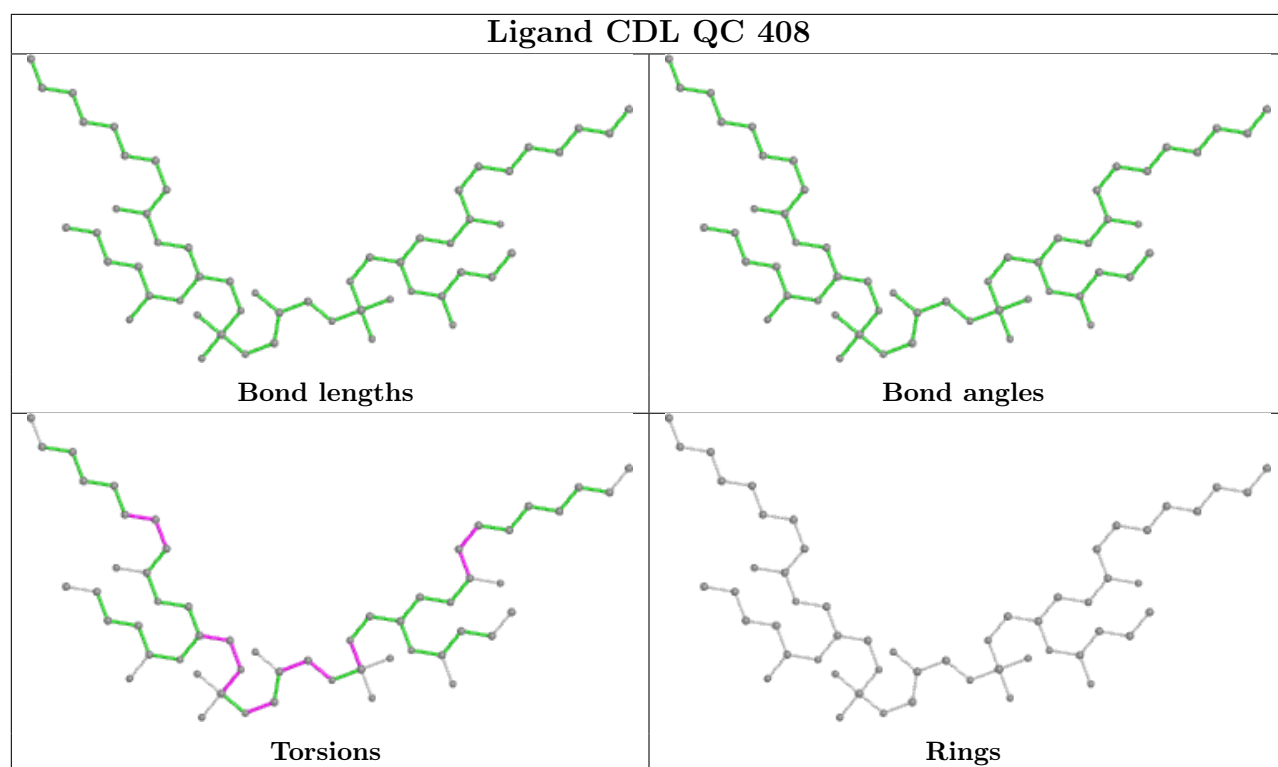
Ligand PEE C1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

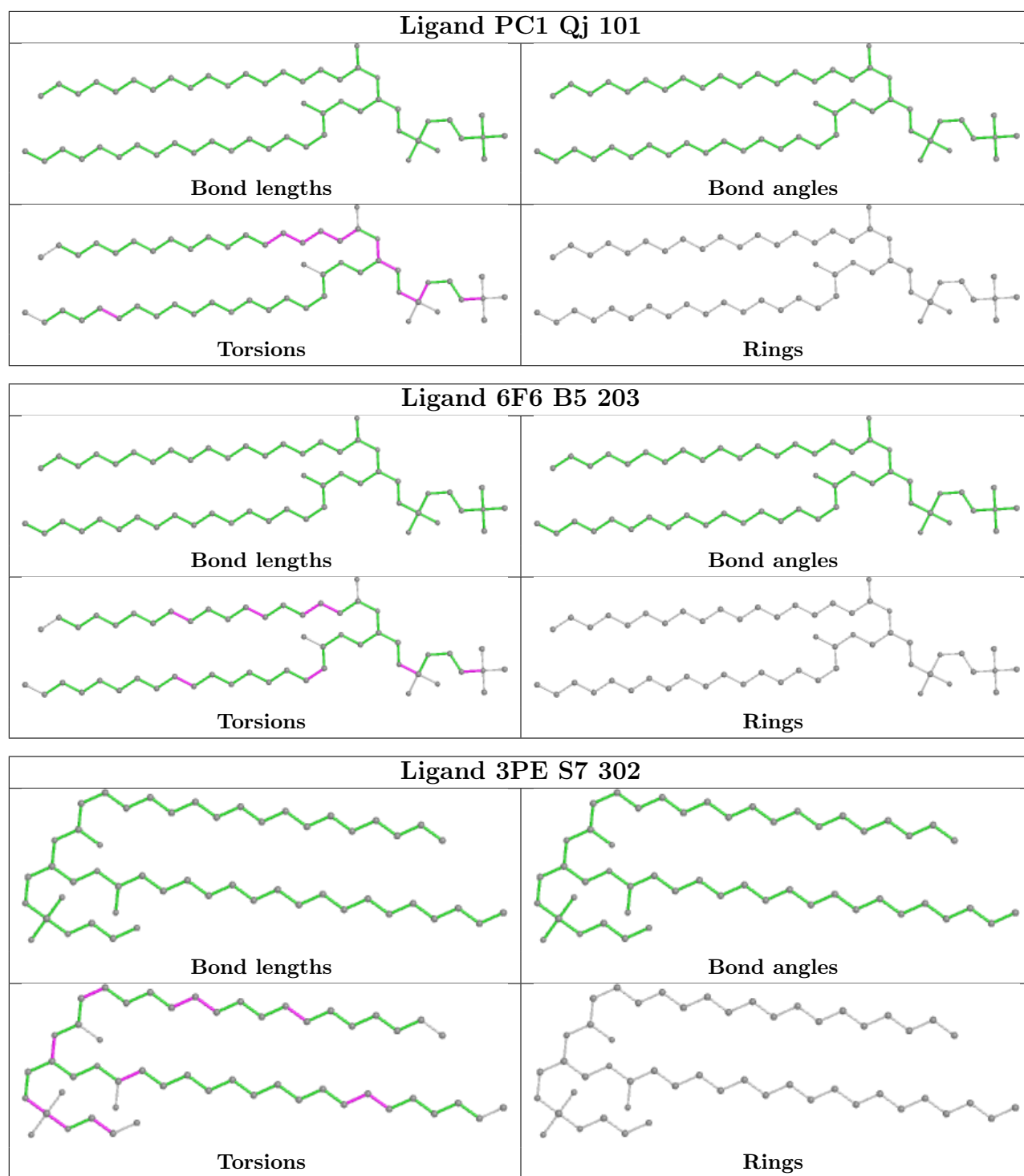
Ligand PLX C2 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

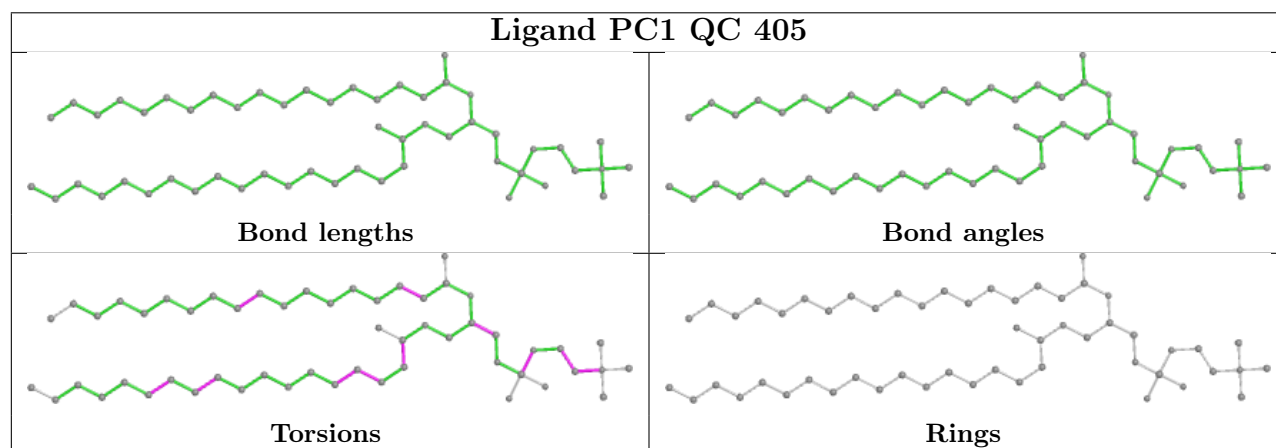
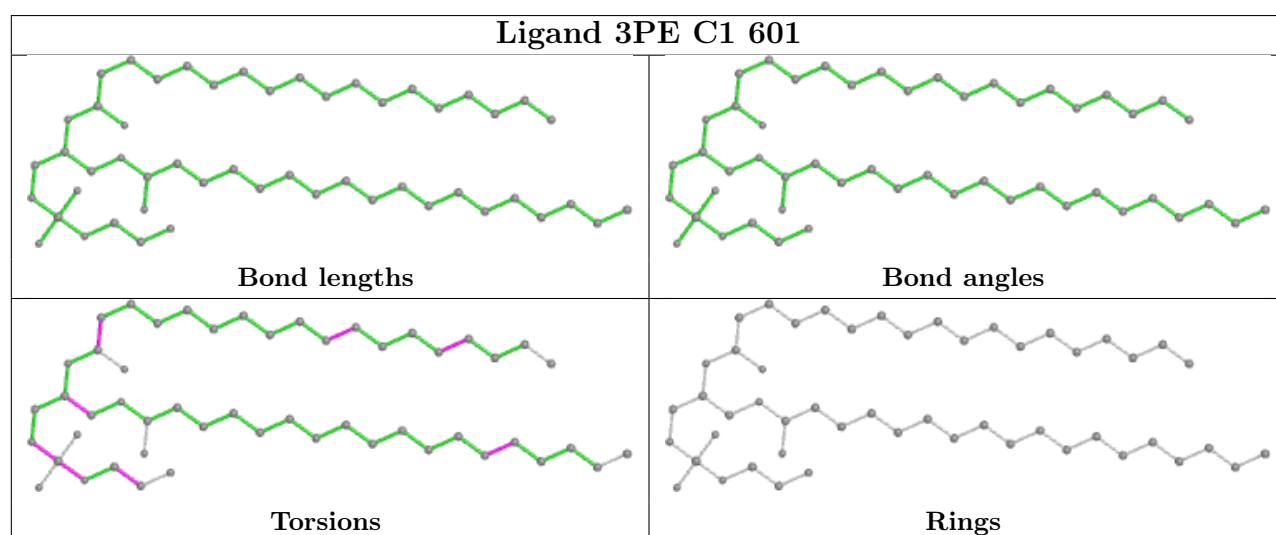
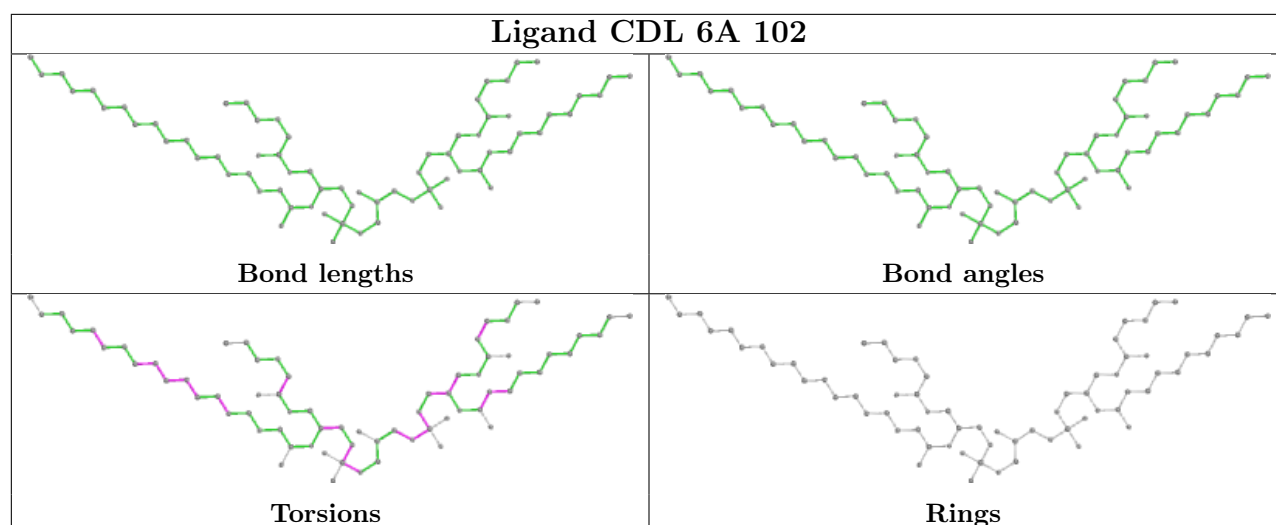
Ligand PLX AM 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

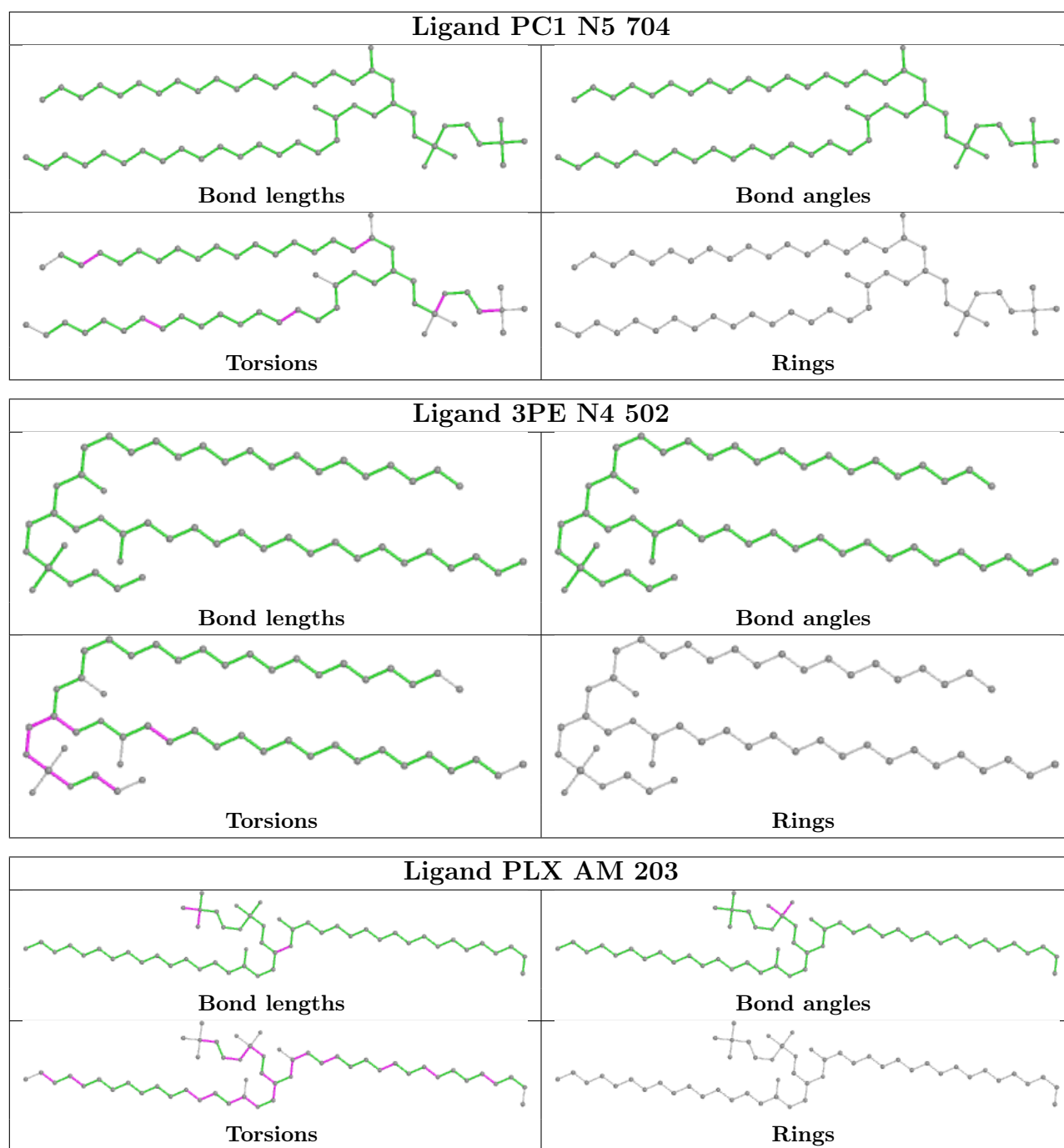
Ligand PC1 C3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

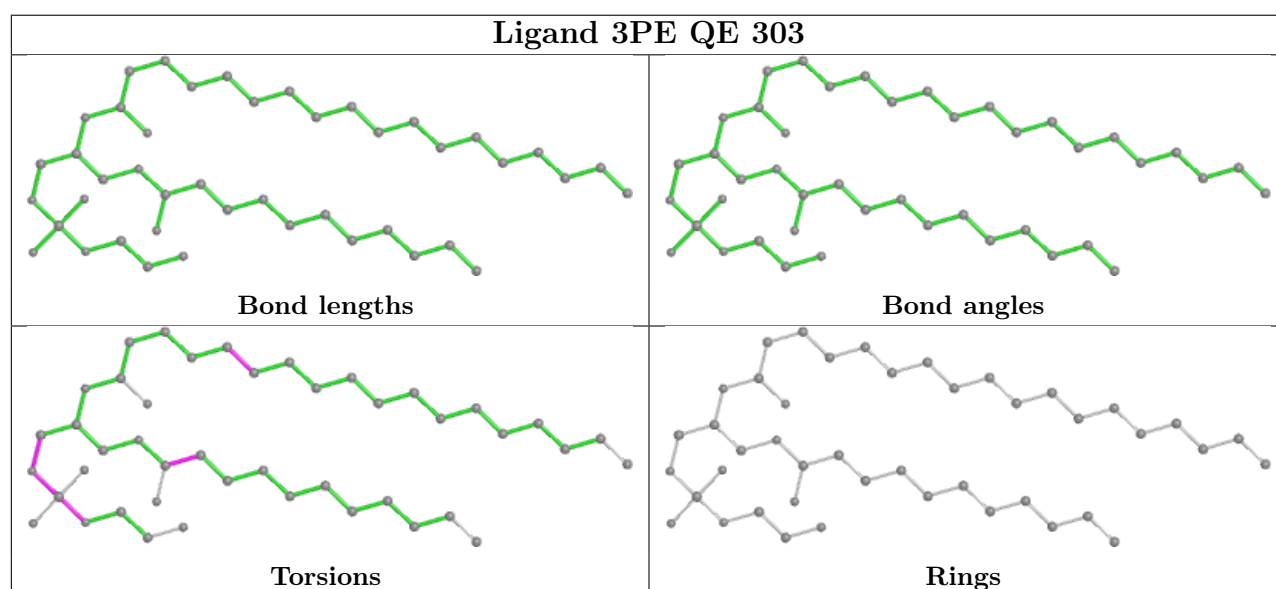
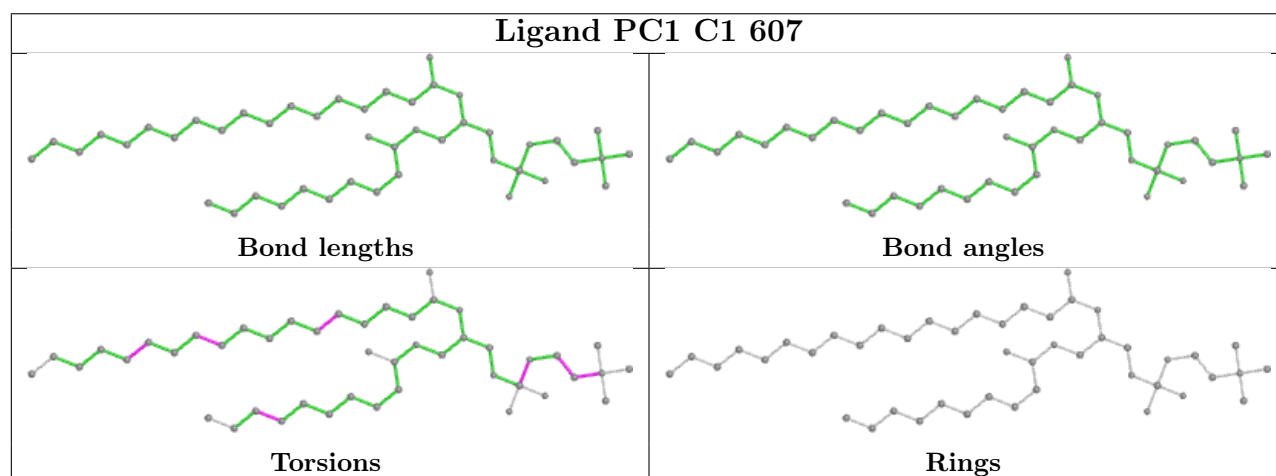
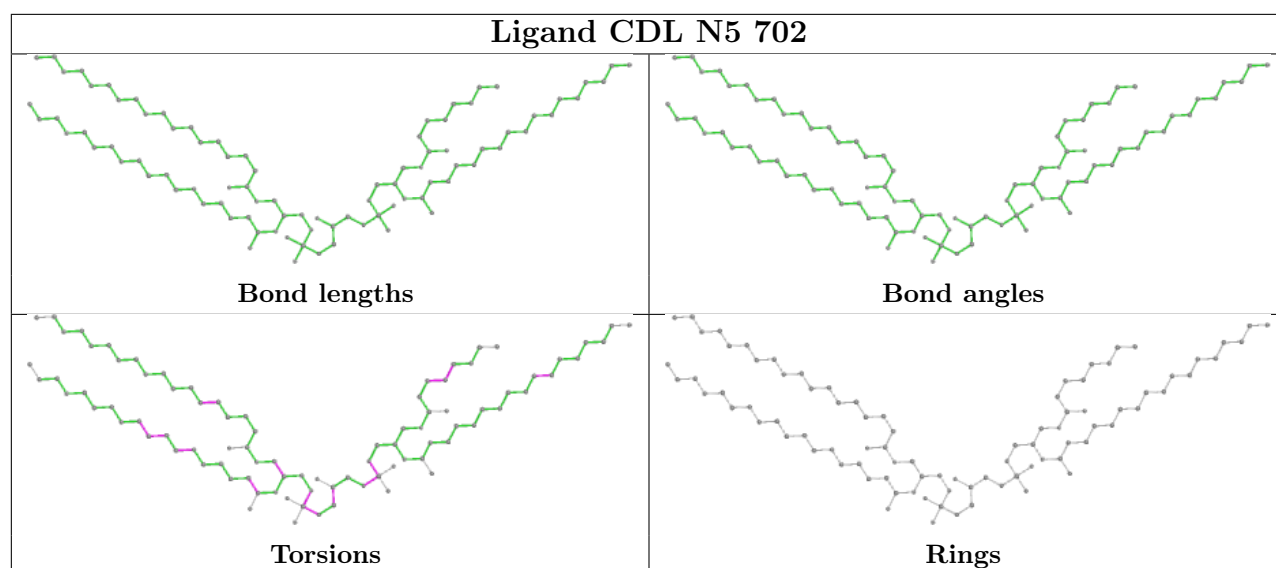


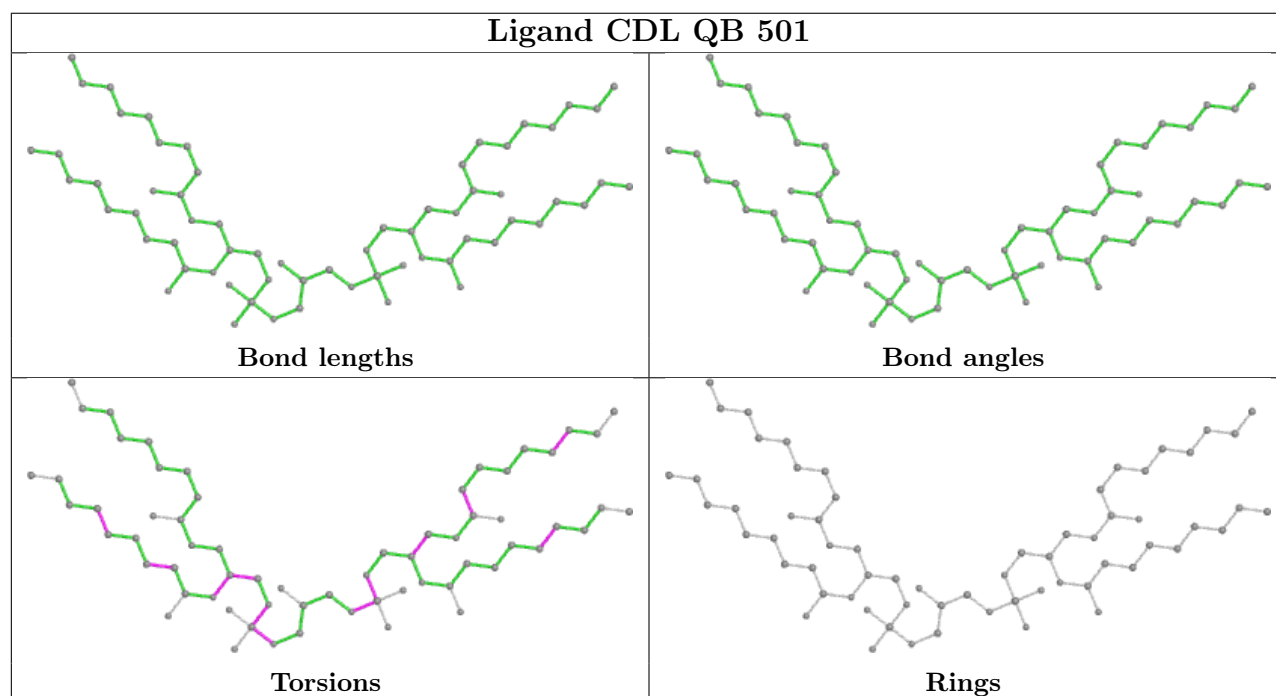
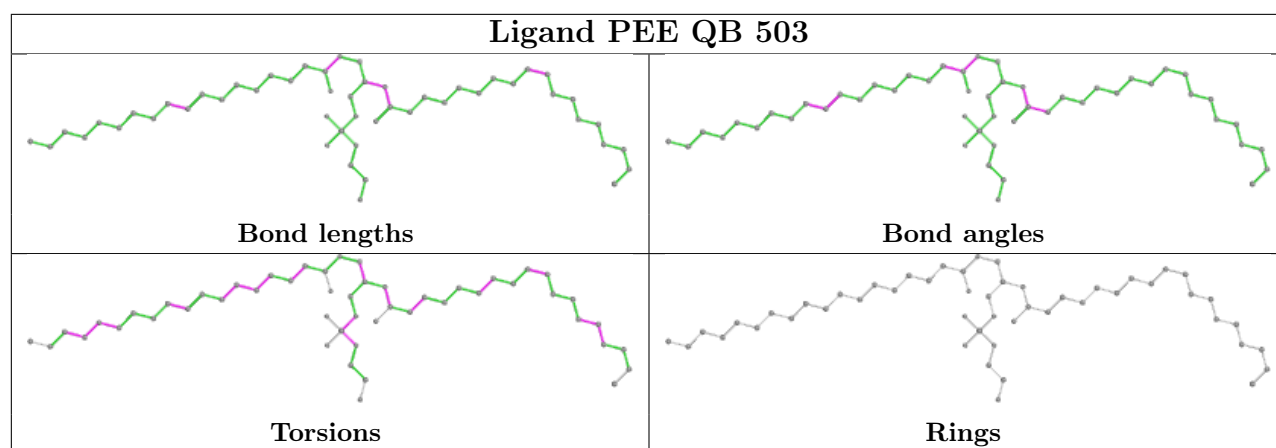


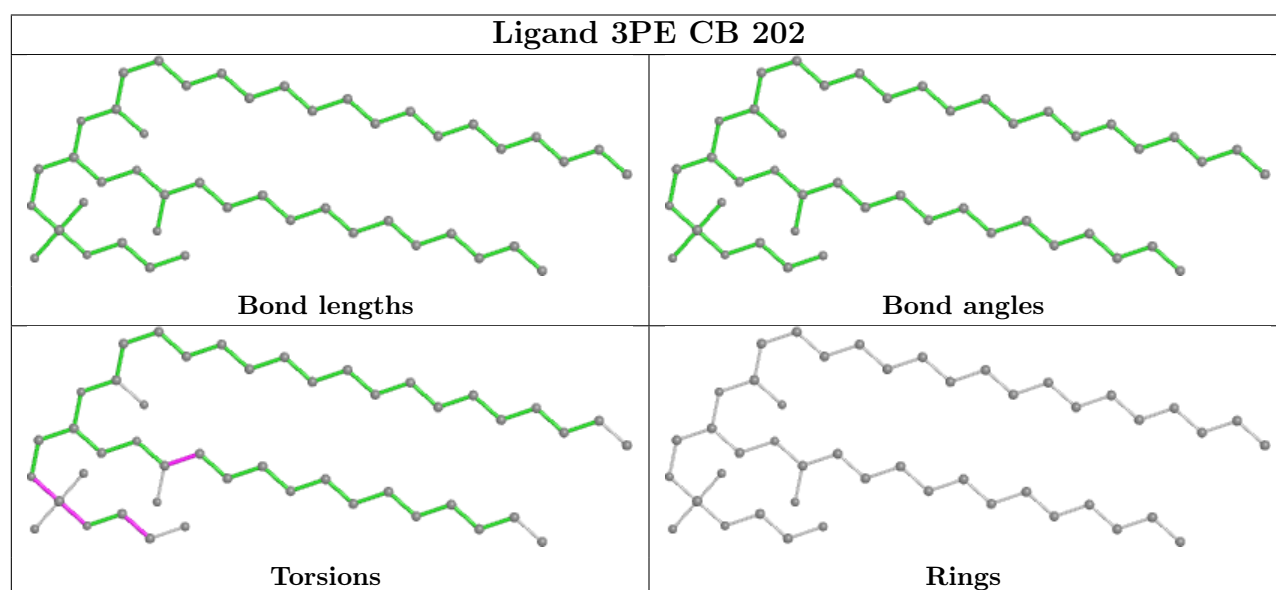
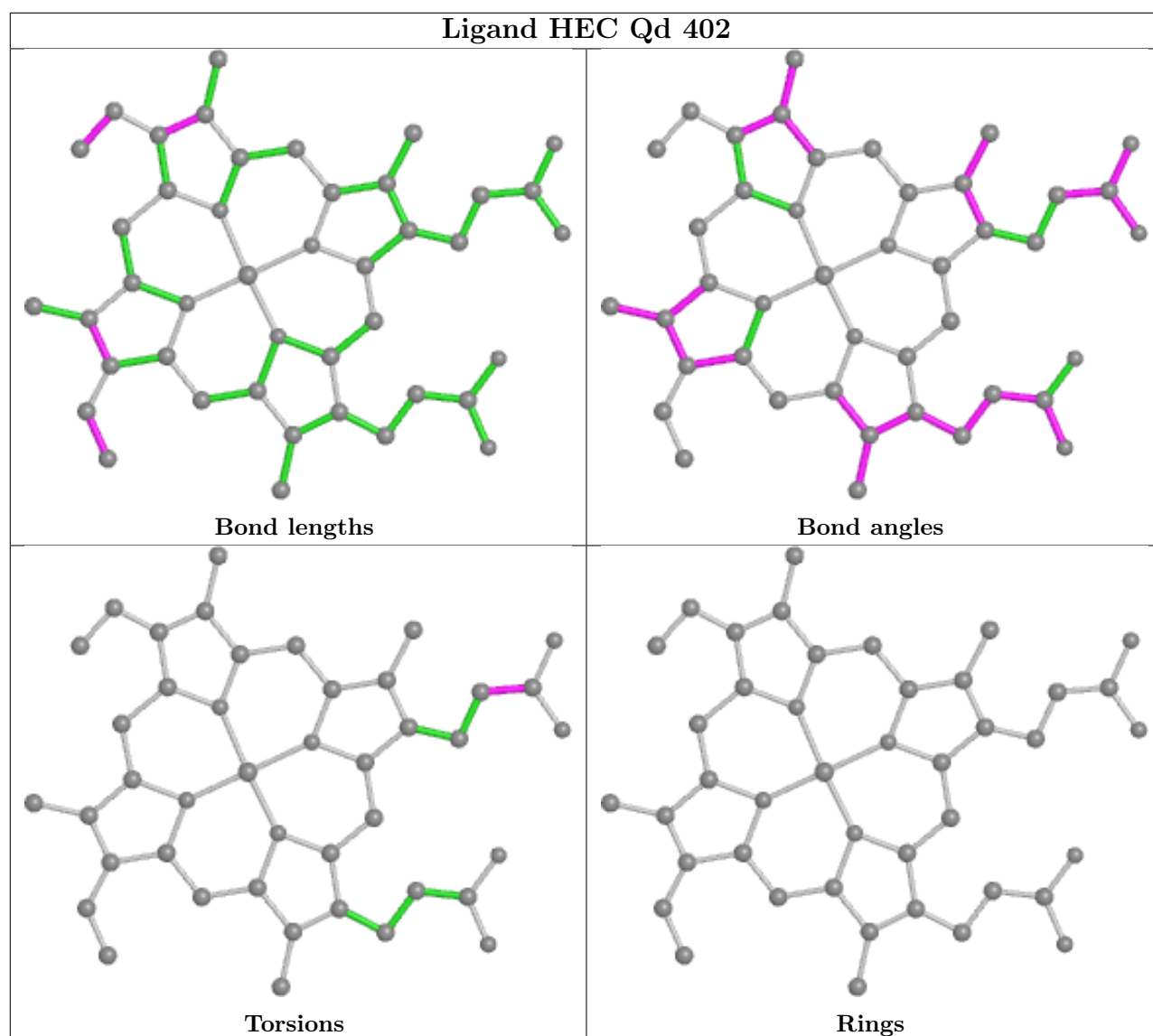


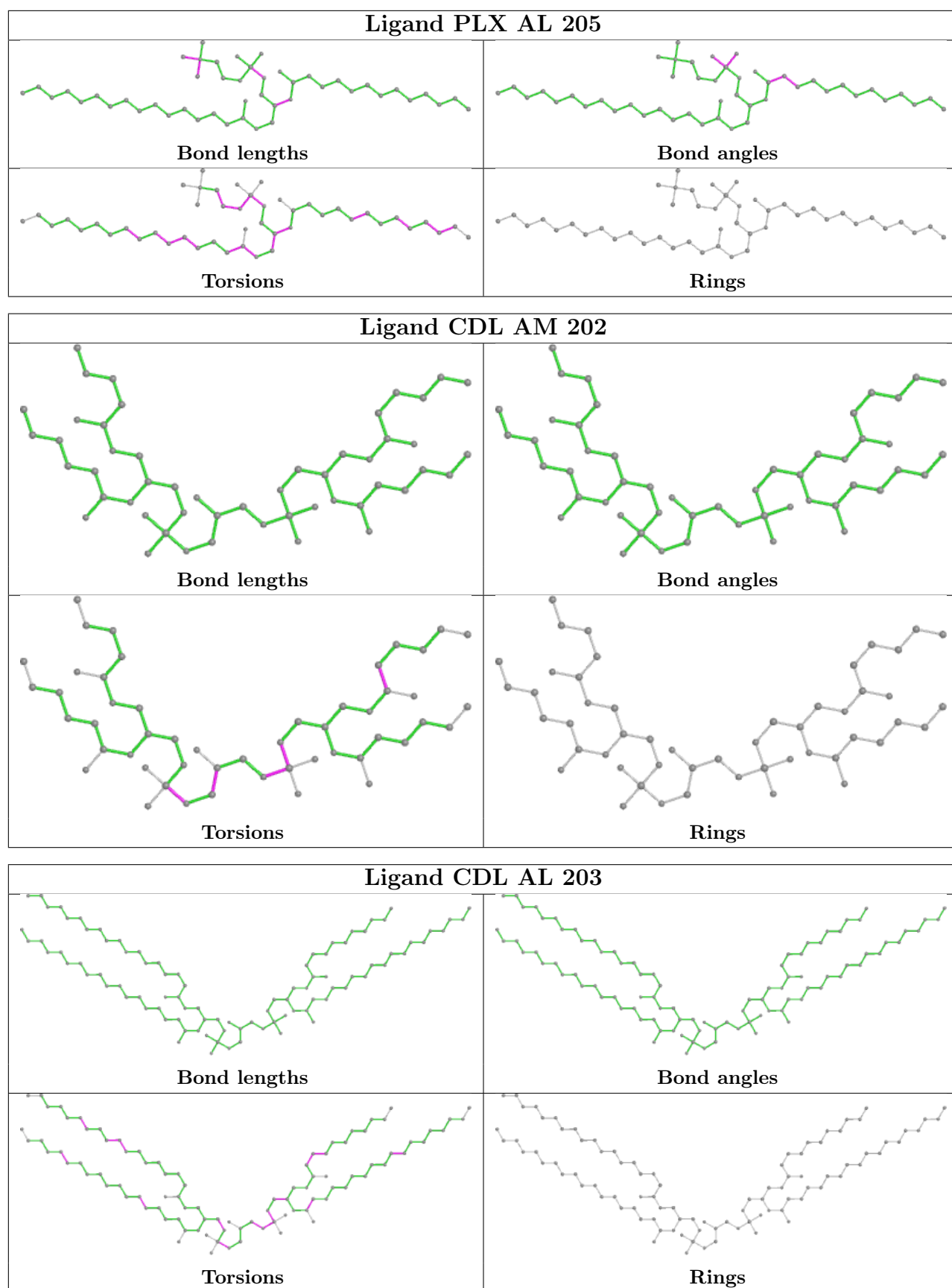


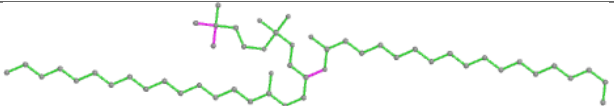
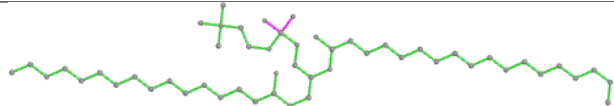
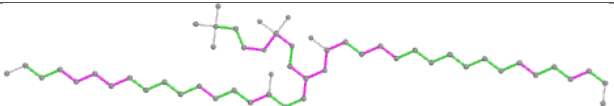
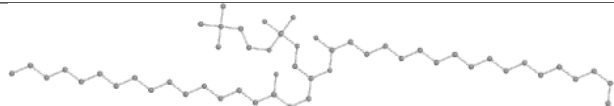


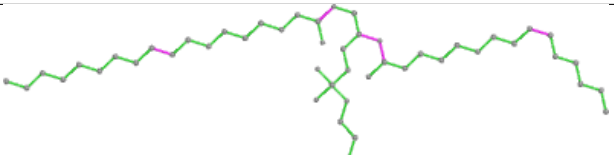
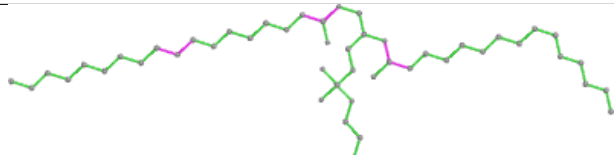
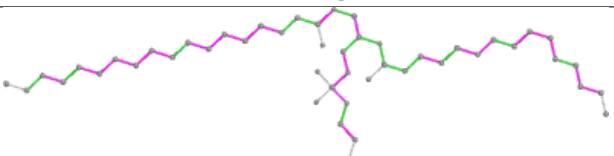
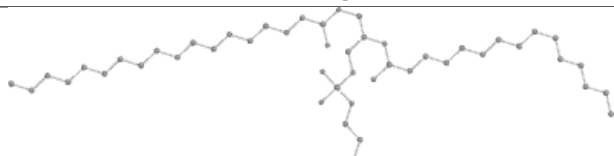


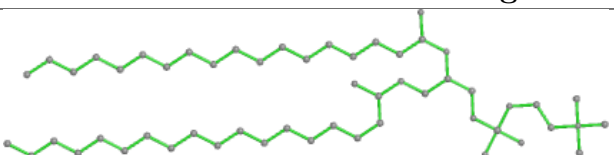
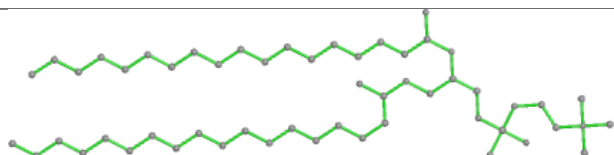
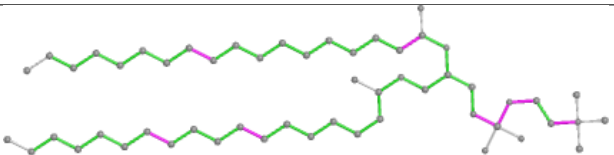
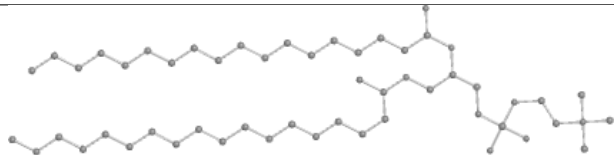


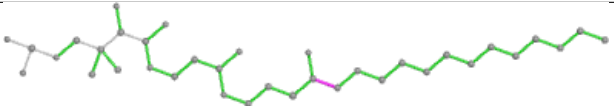
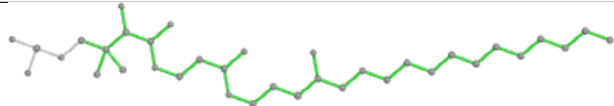
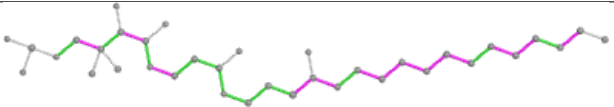
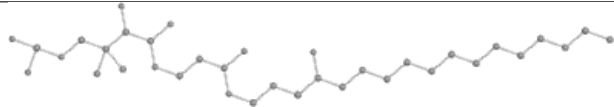


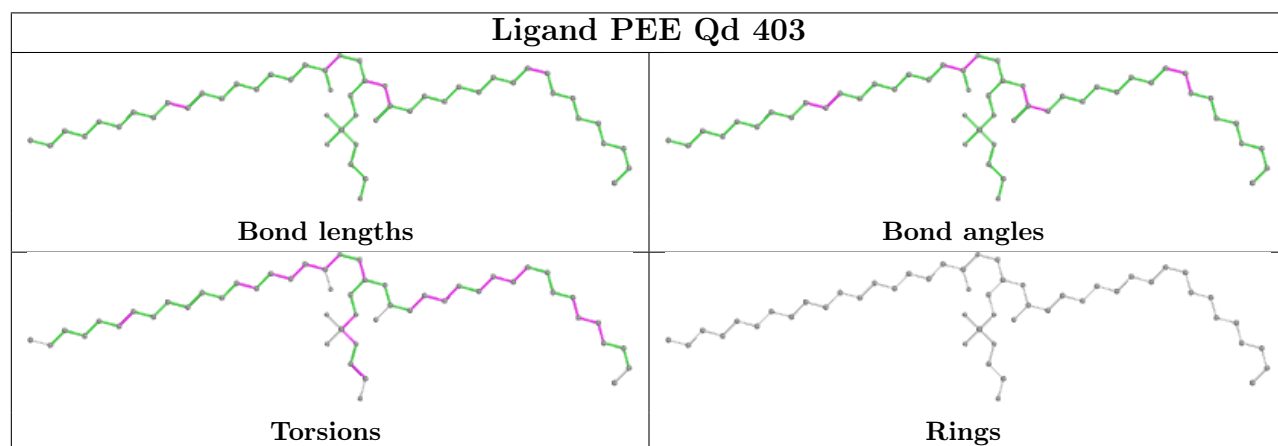
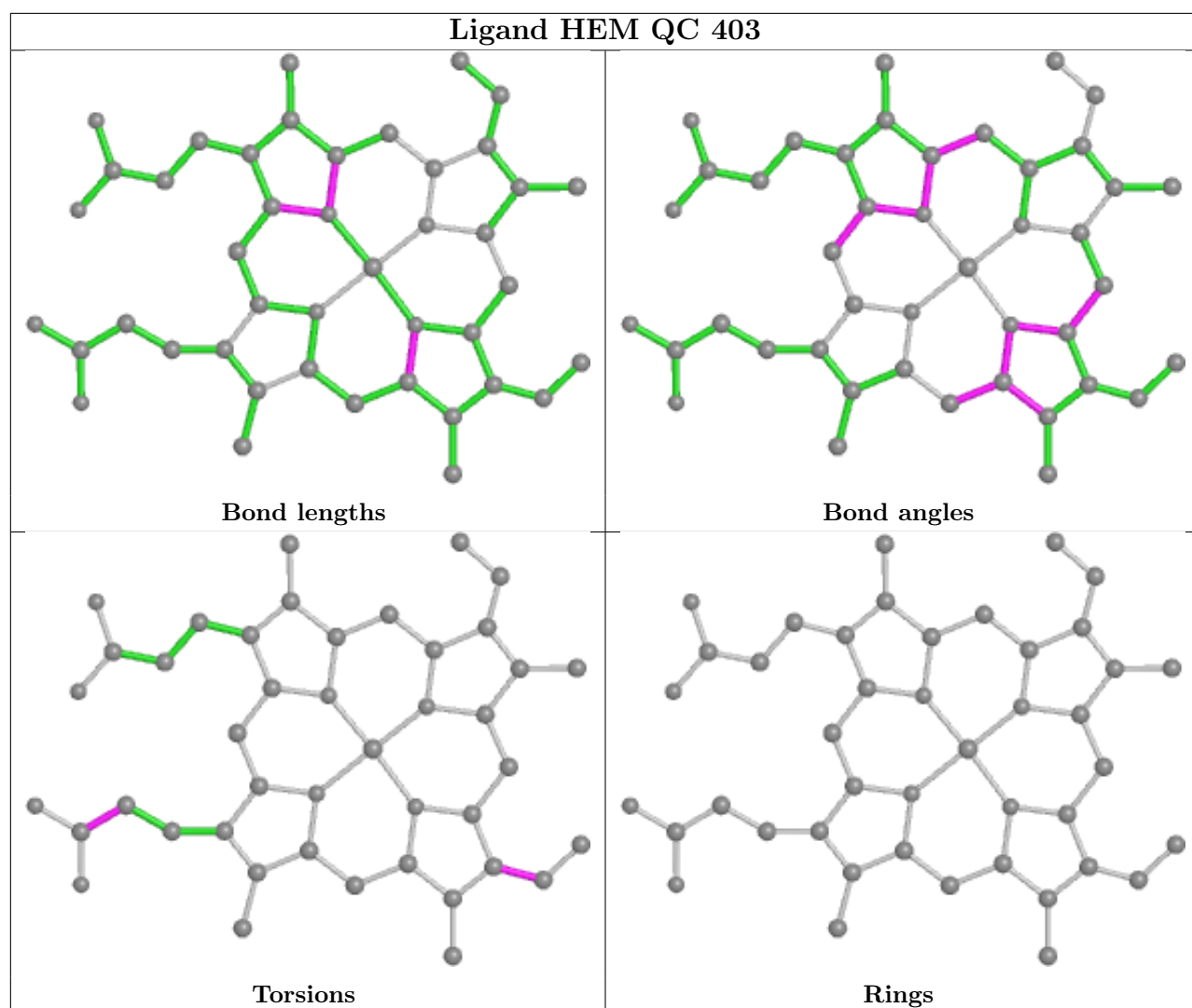


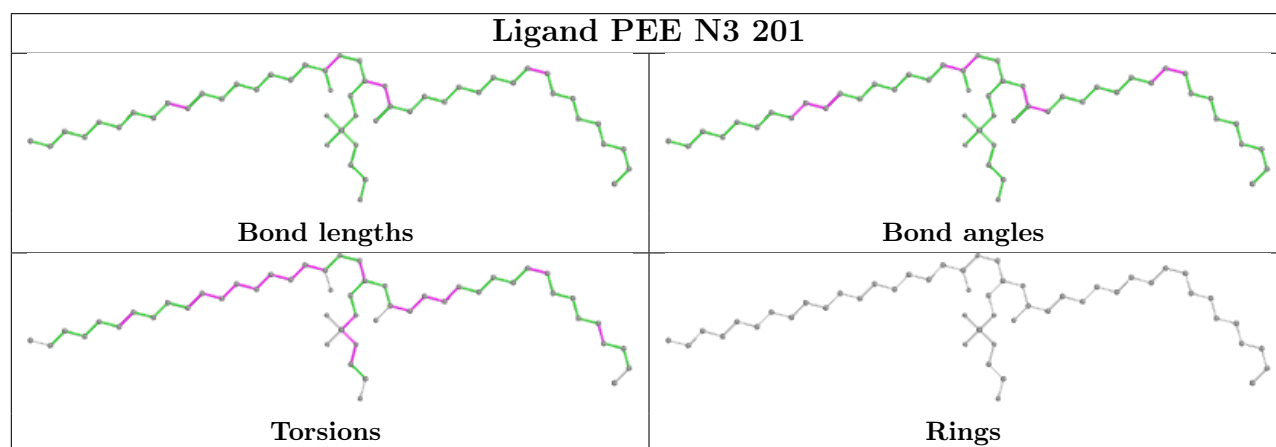
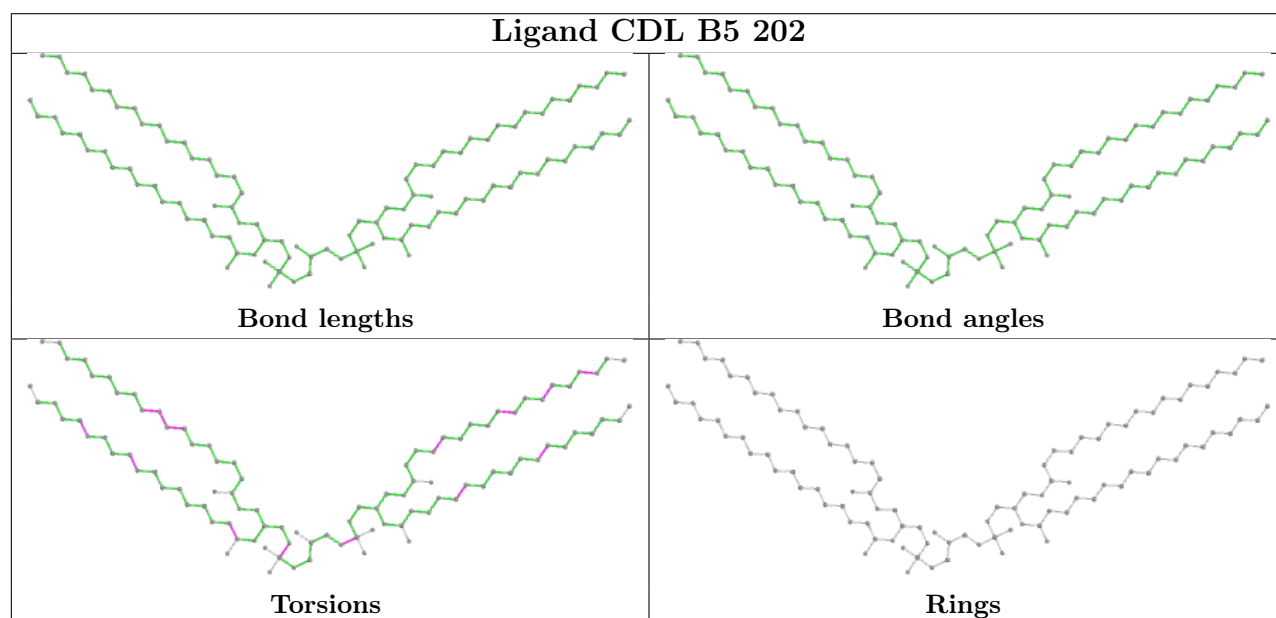
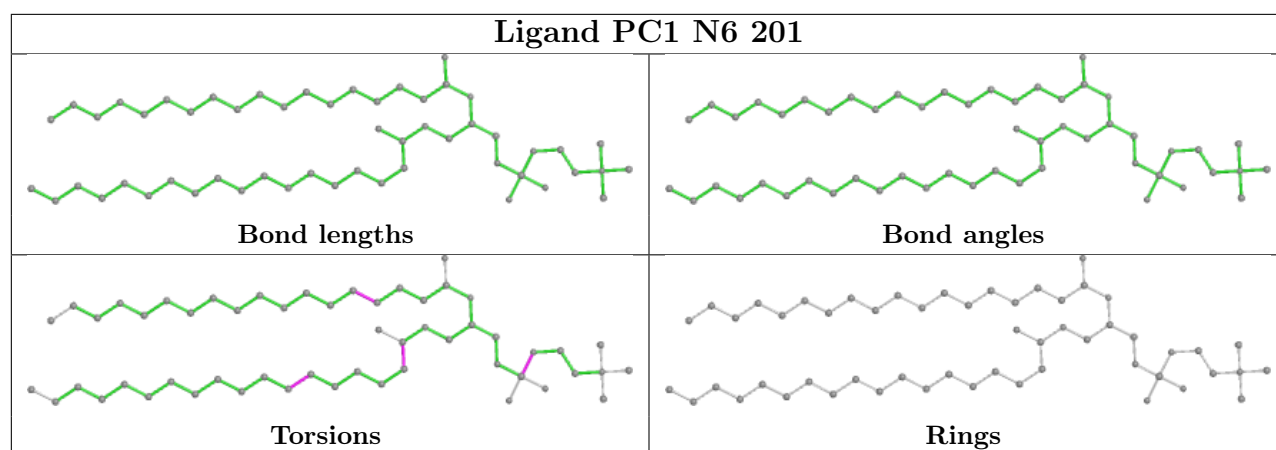
Ligand PLX CB 201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

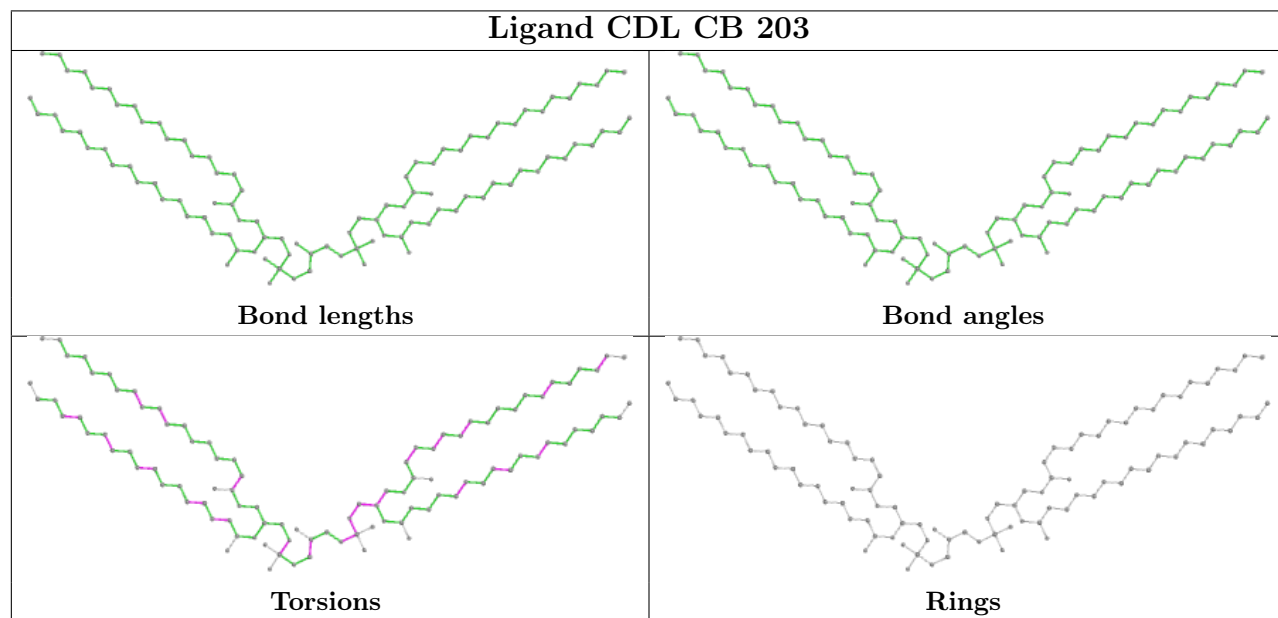
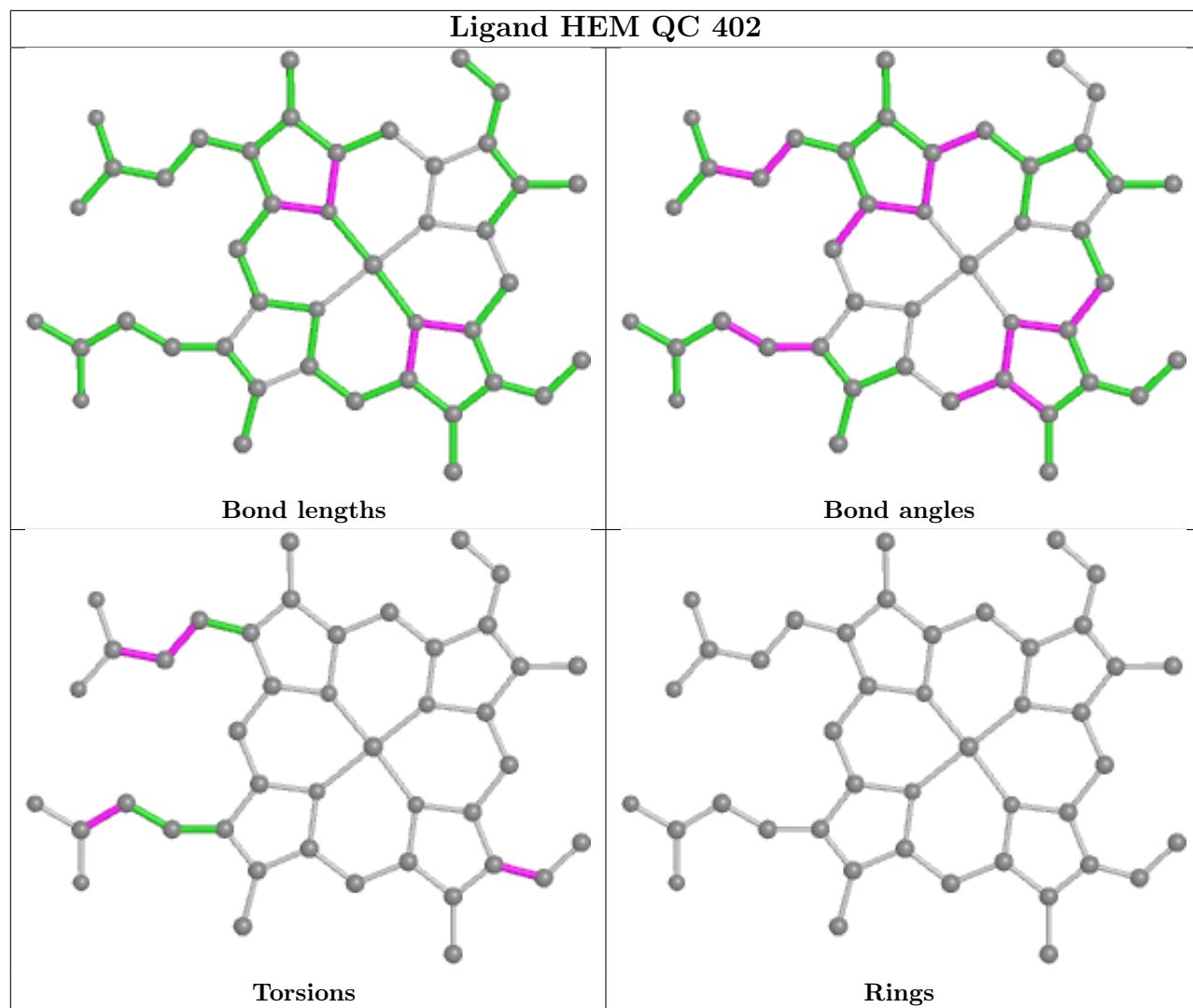
Ligand PEE S2 501	
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 <p>Torsions</p>	 <p>Rings</p>

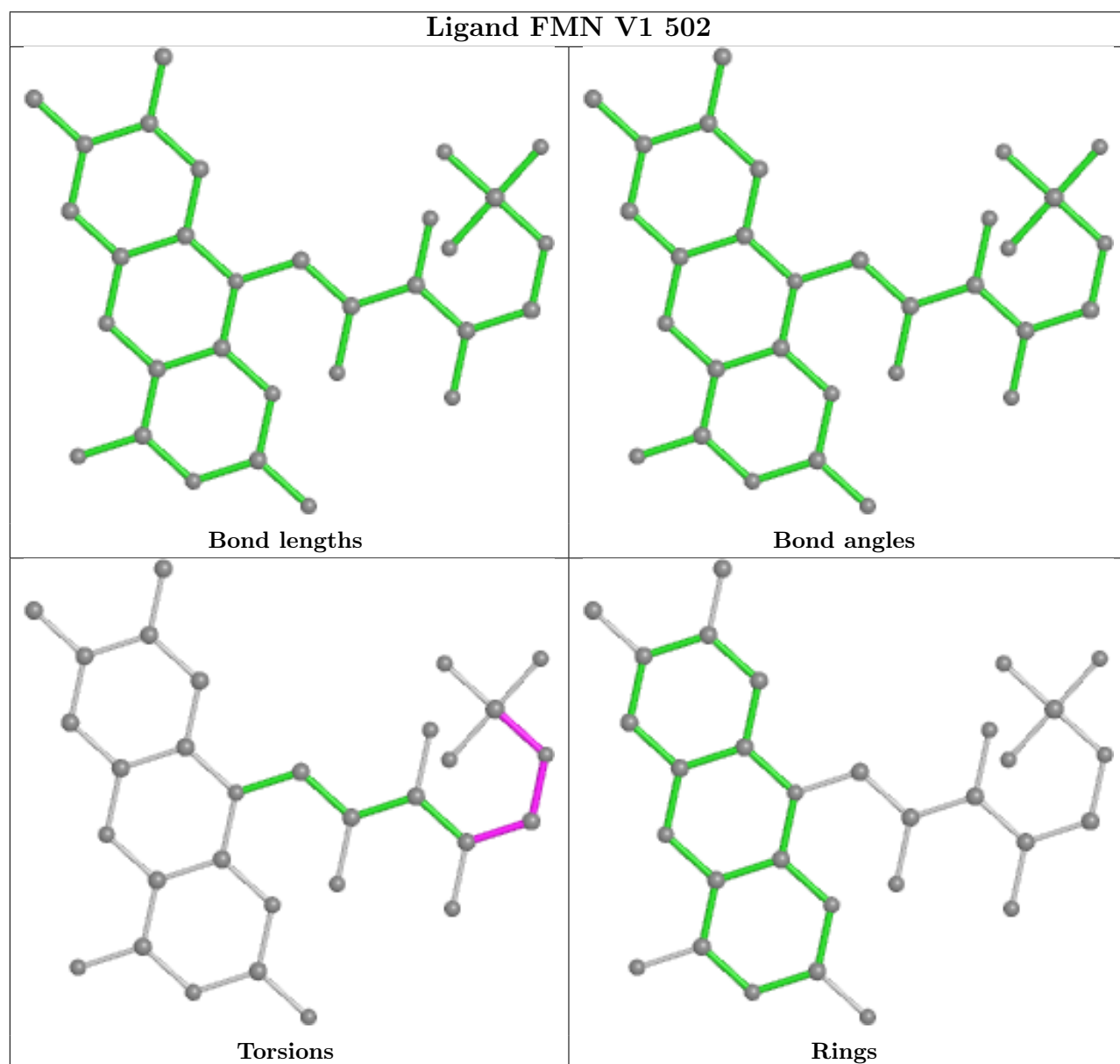
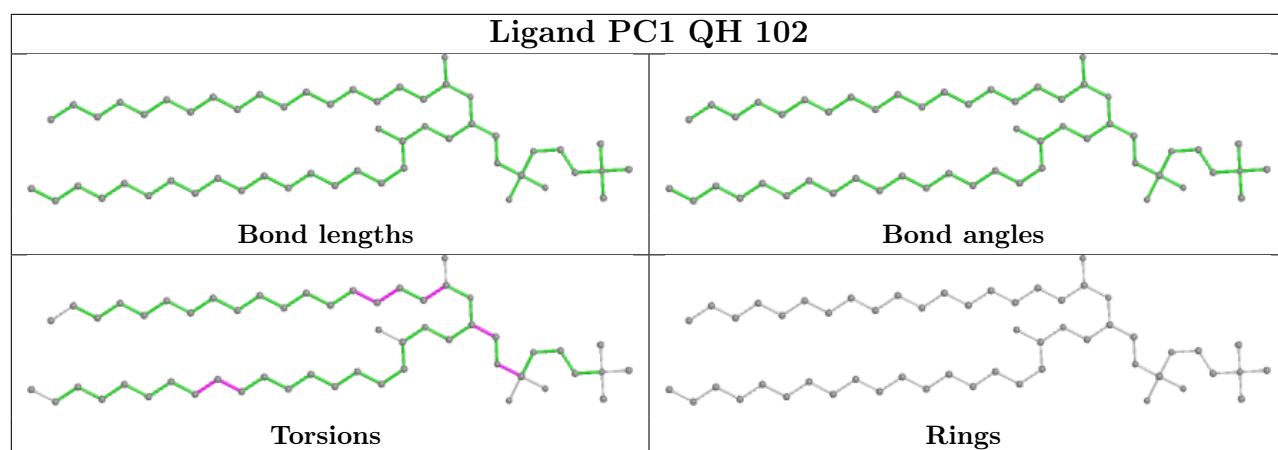
Ligand PC1 AL 206	
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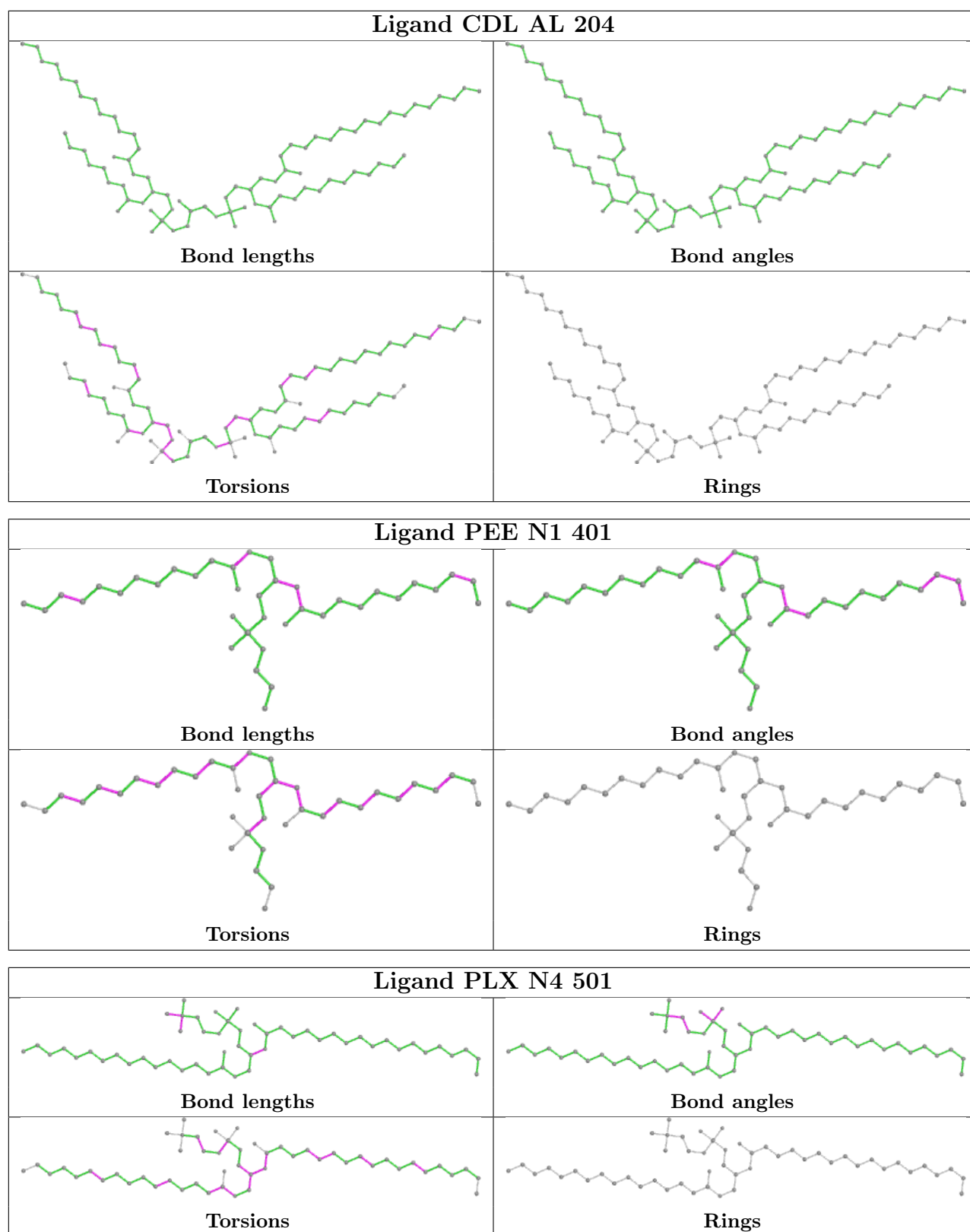
Ligand ZMP AC 201	
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 <p>Torsions</p>	 <p>Rings</p>

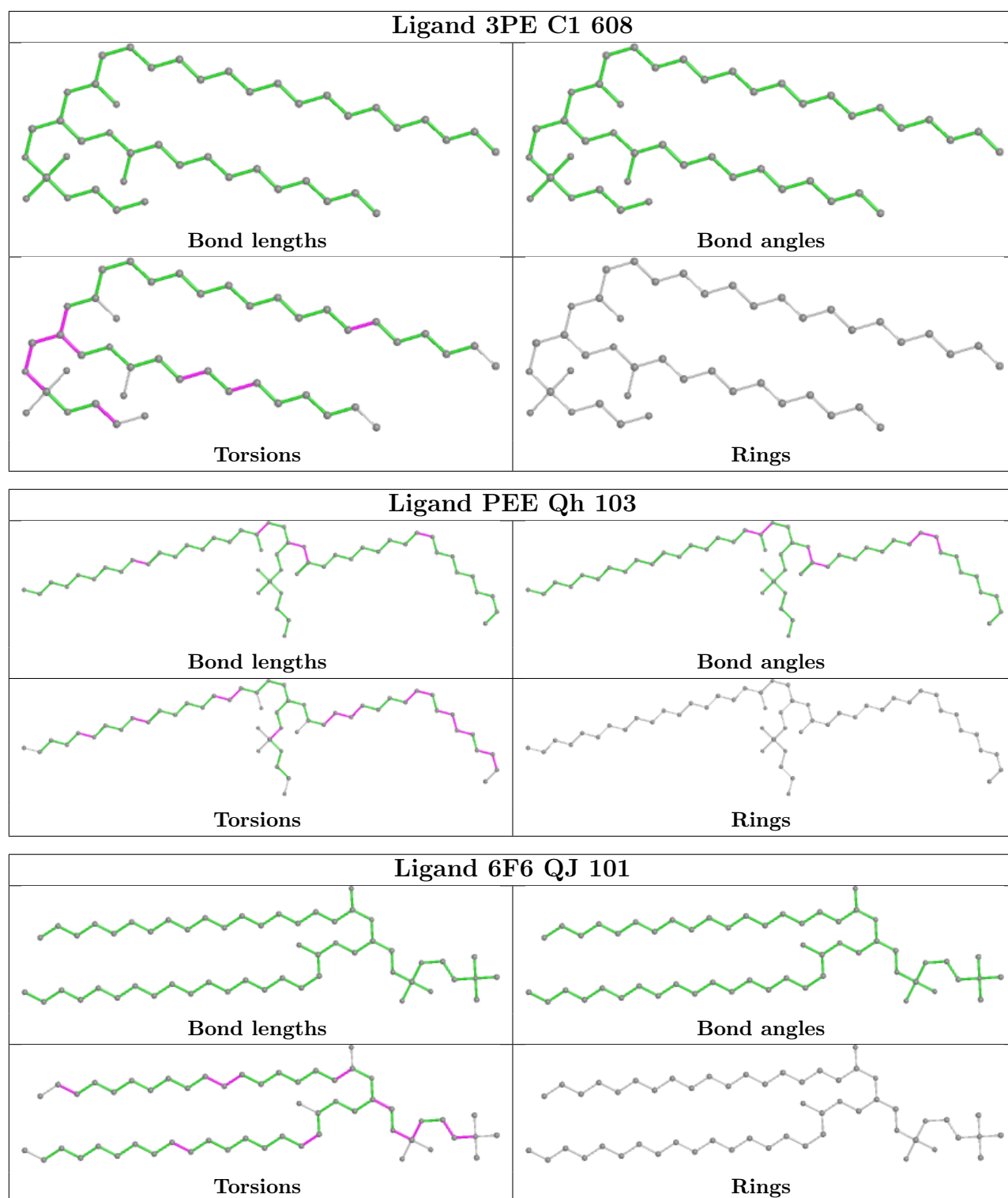


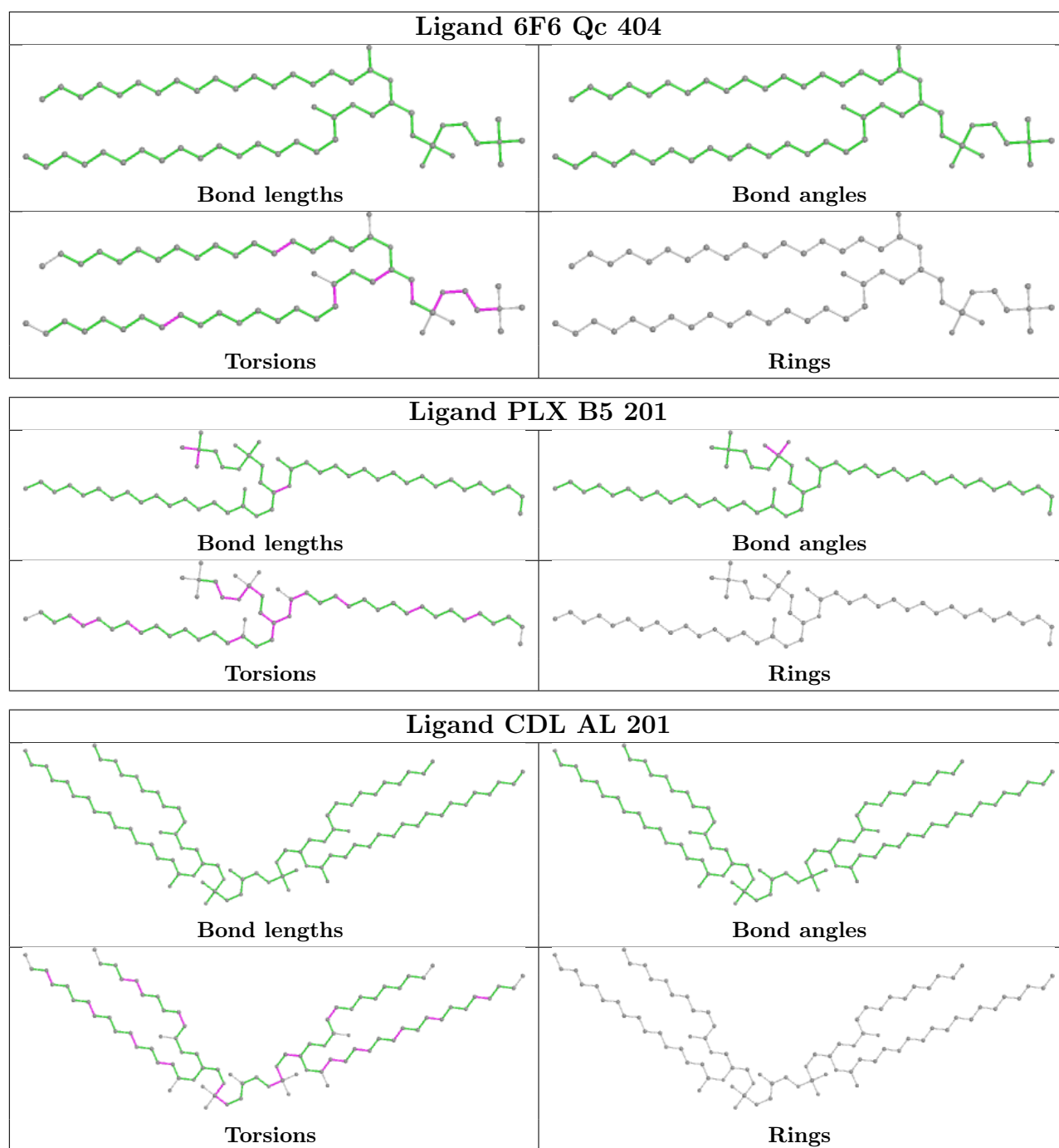


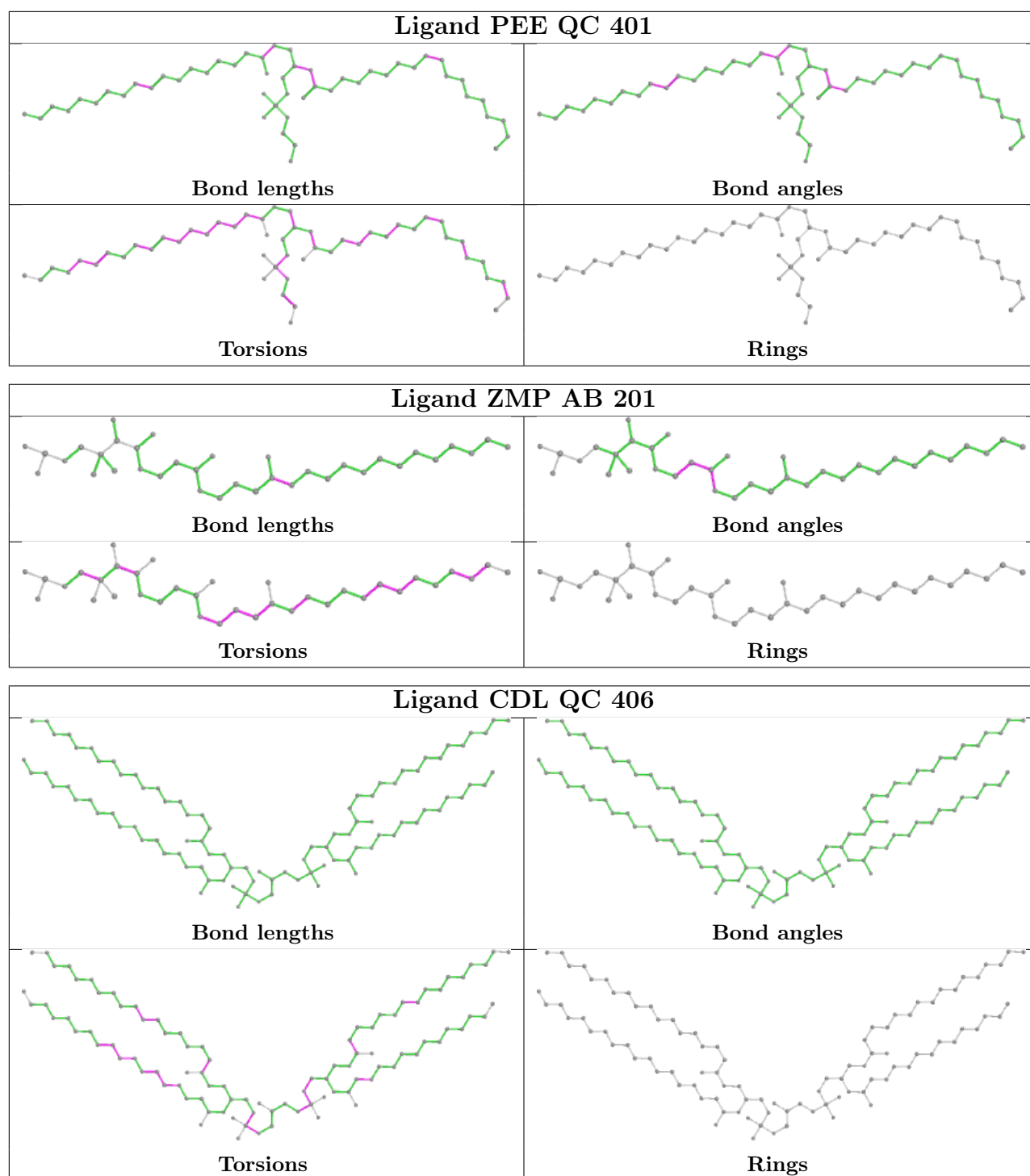


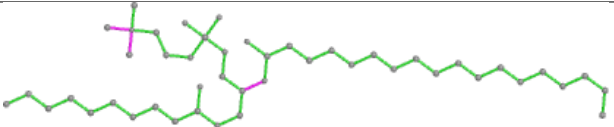
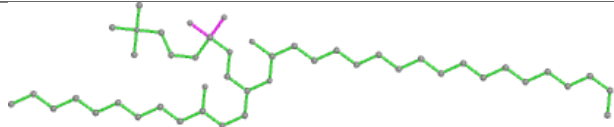
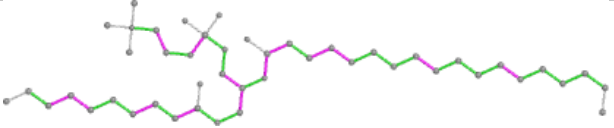
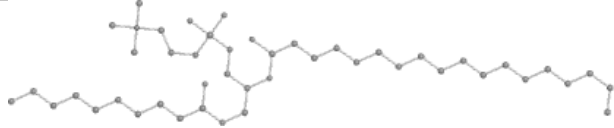


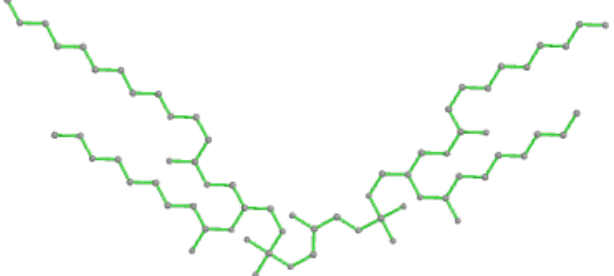
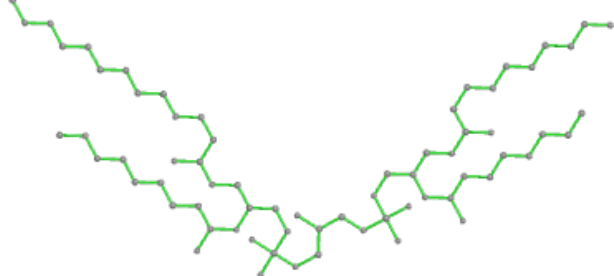
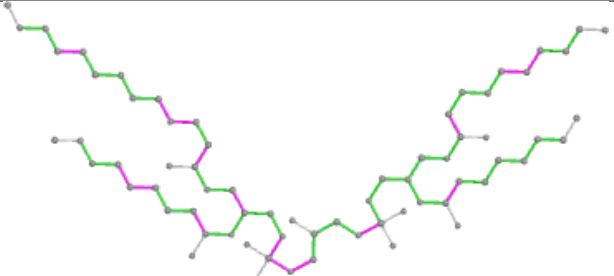
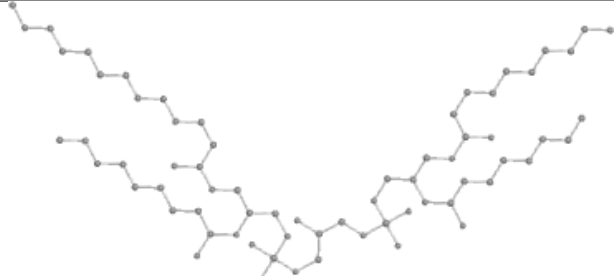


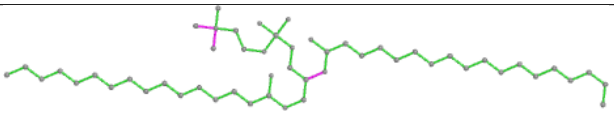
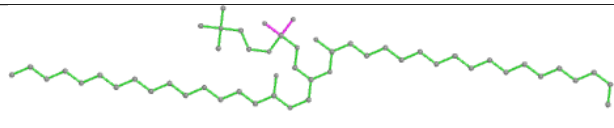
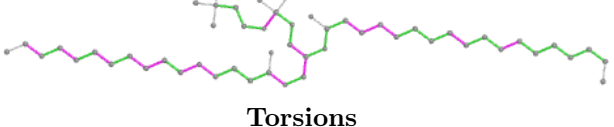





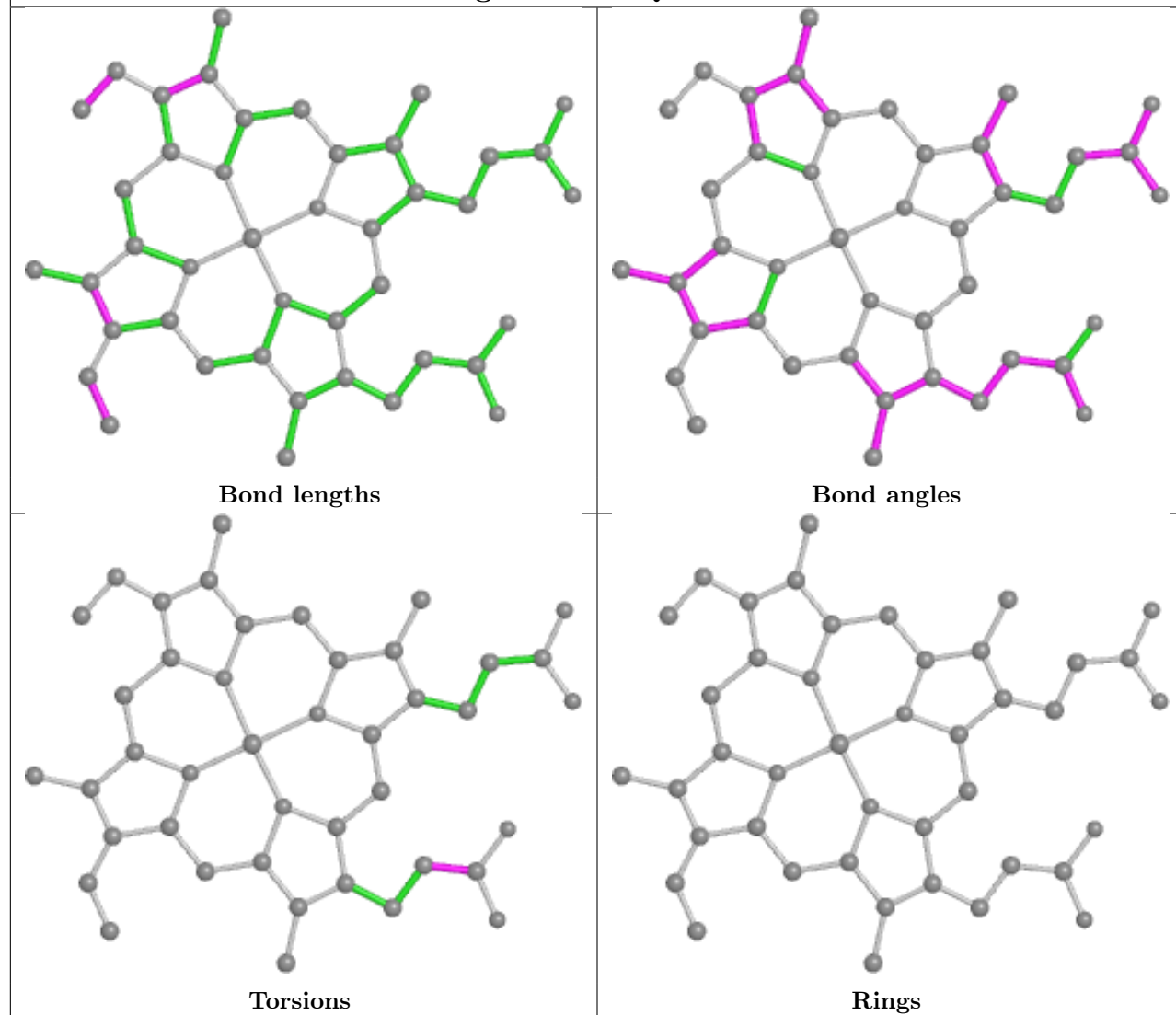


Ligand PLX QE 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

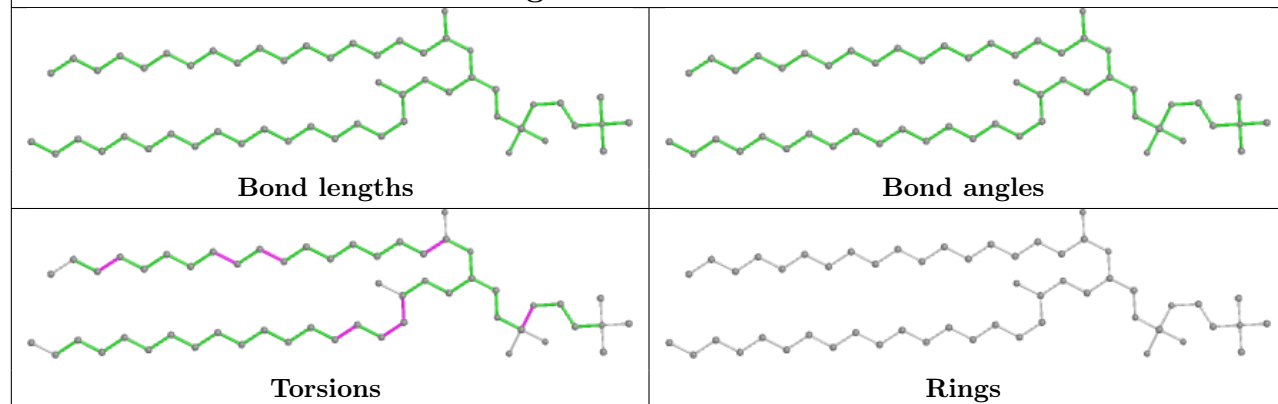
Ligand CDL N2 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

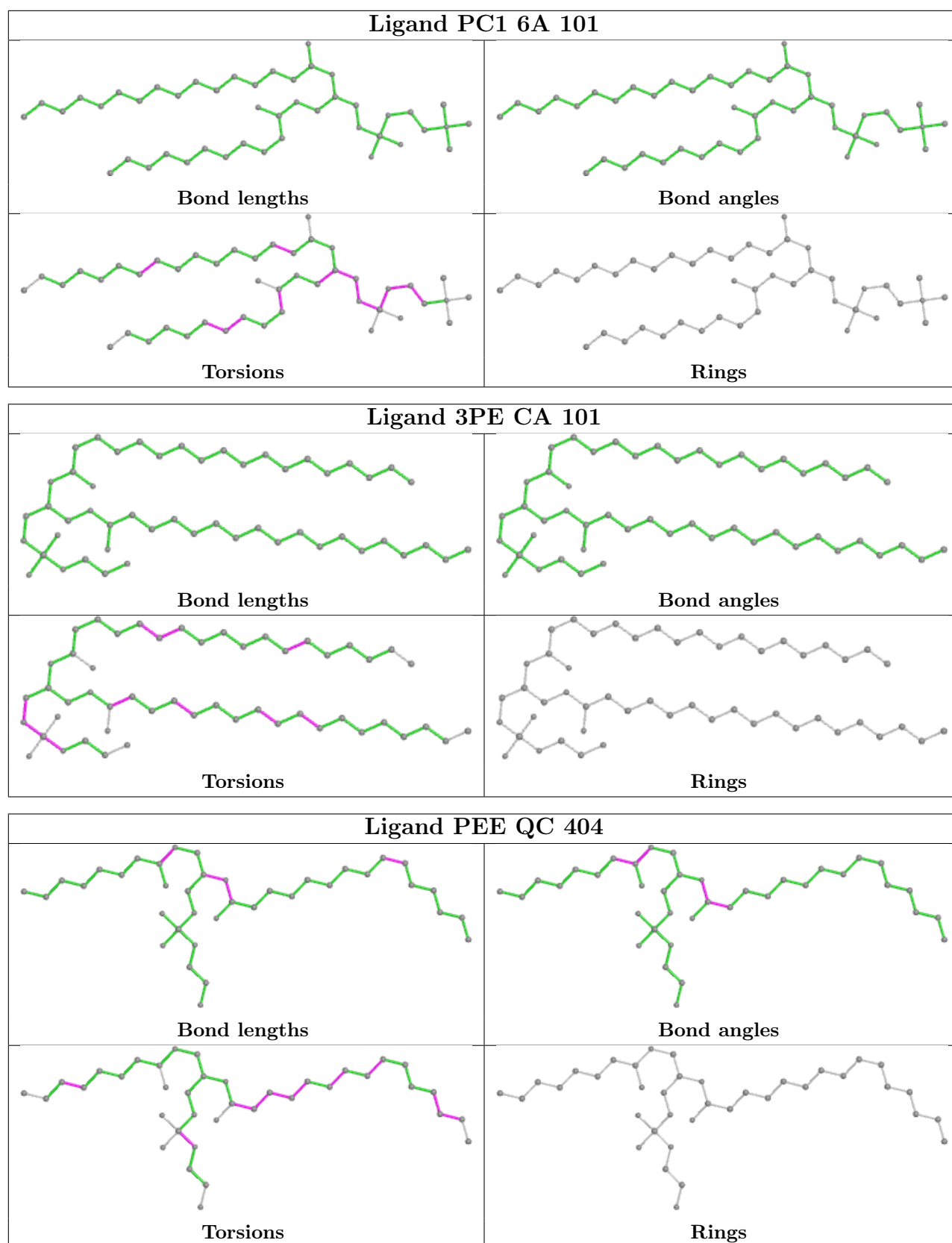
Ligand PLX QI 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

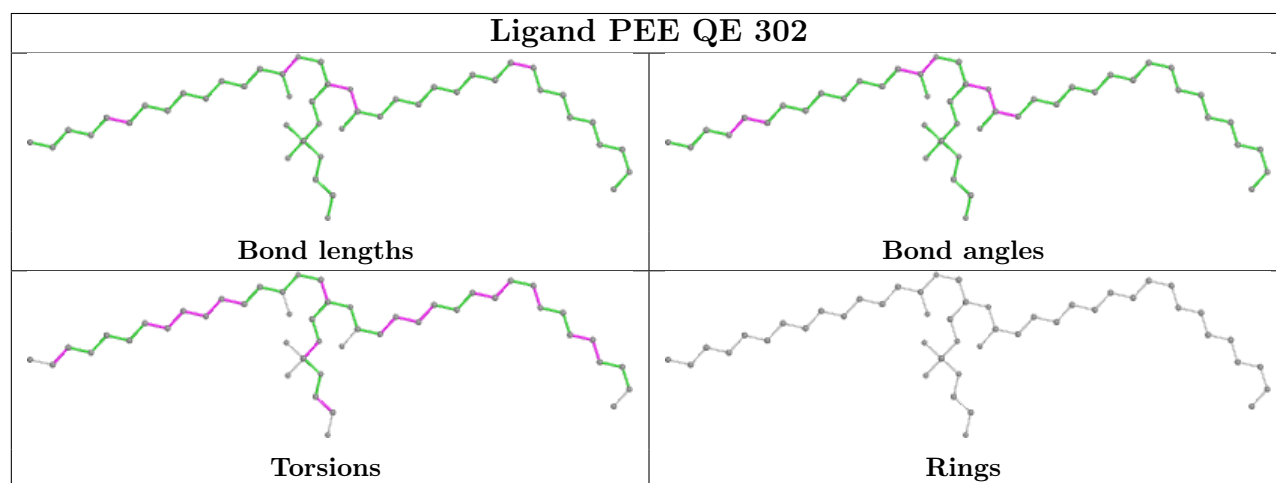
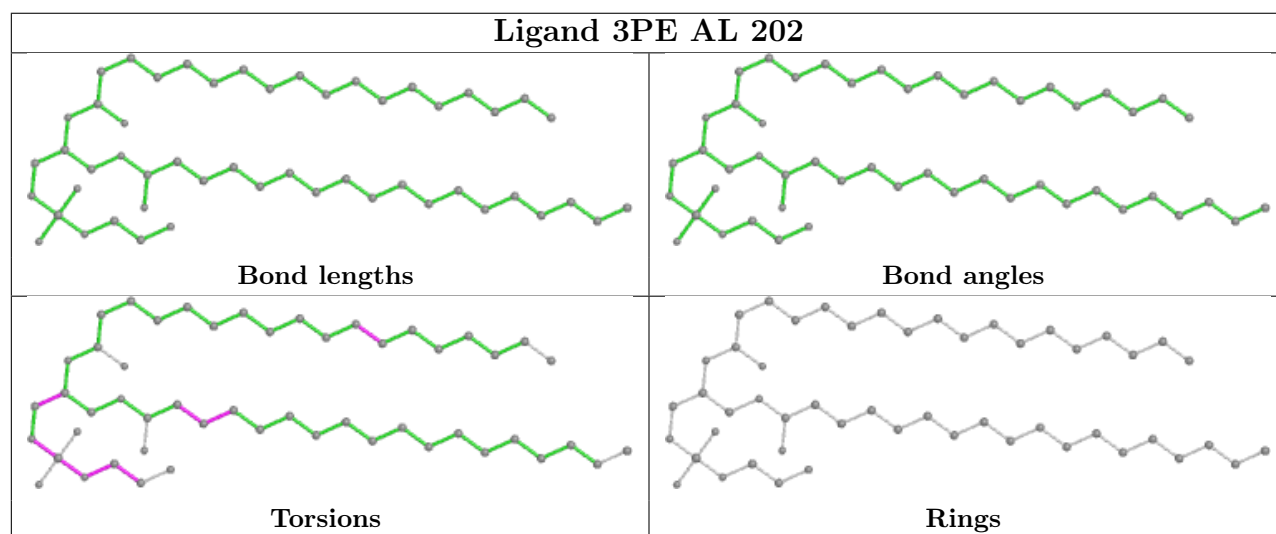
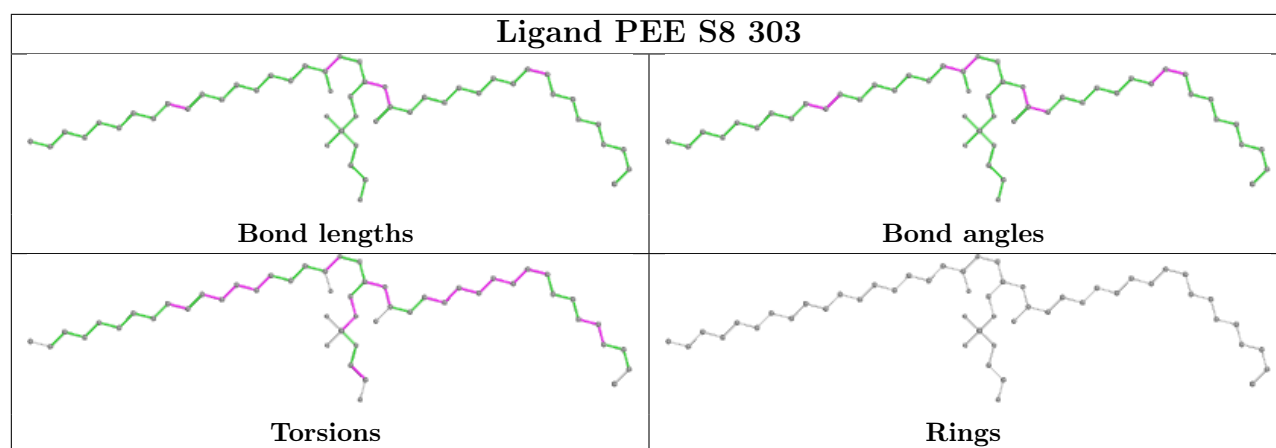
Ligand HEC QD 401

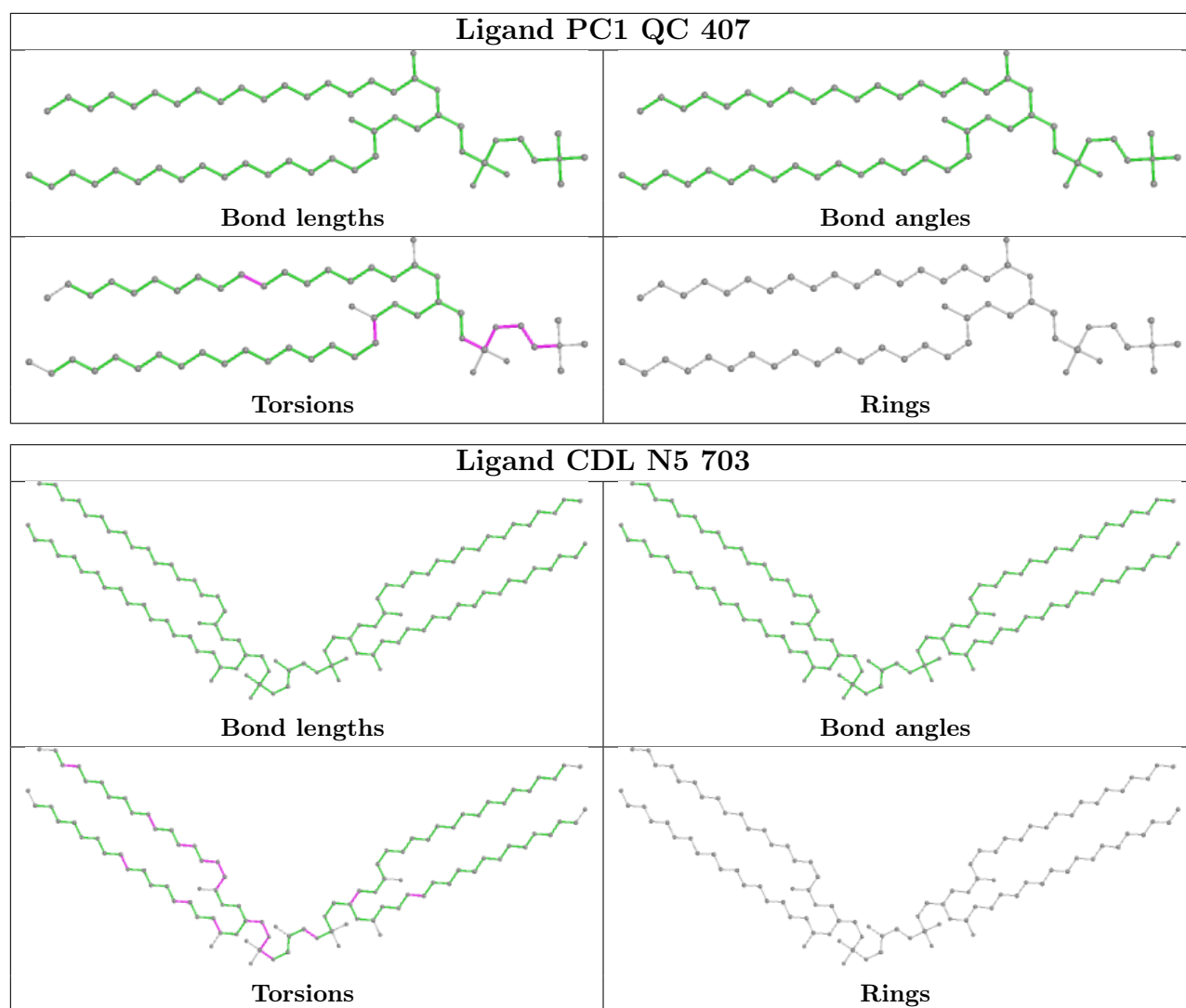


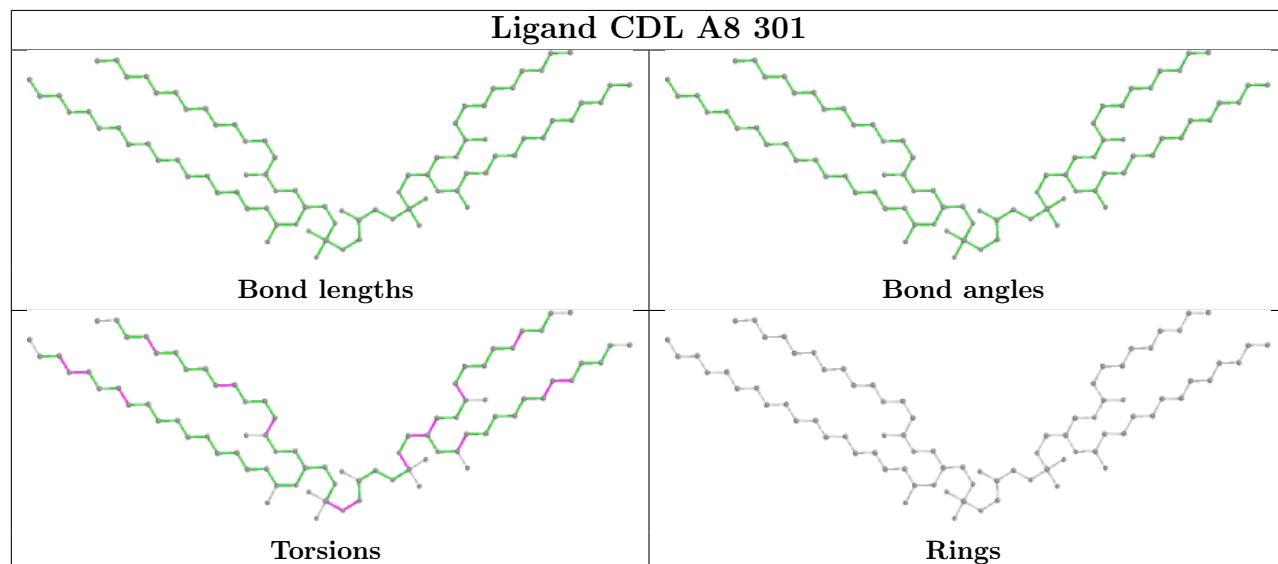
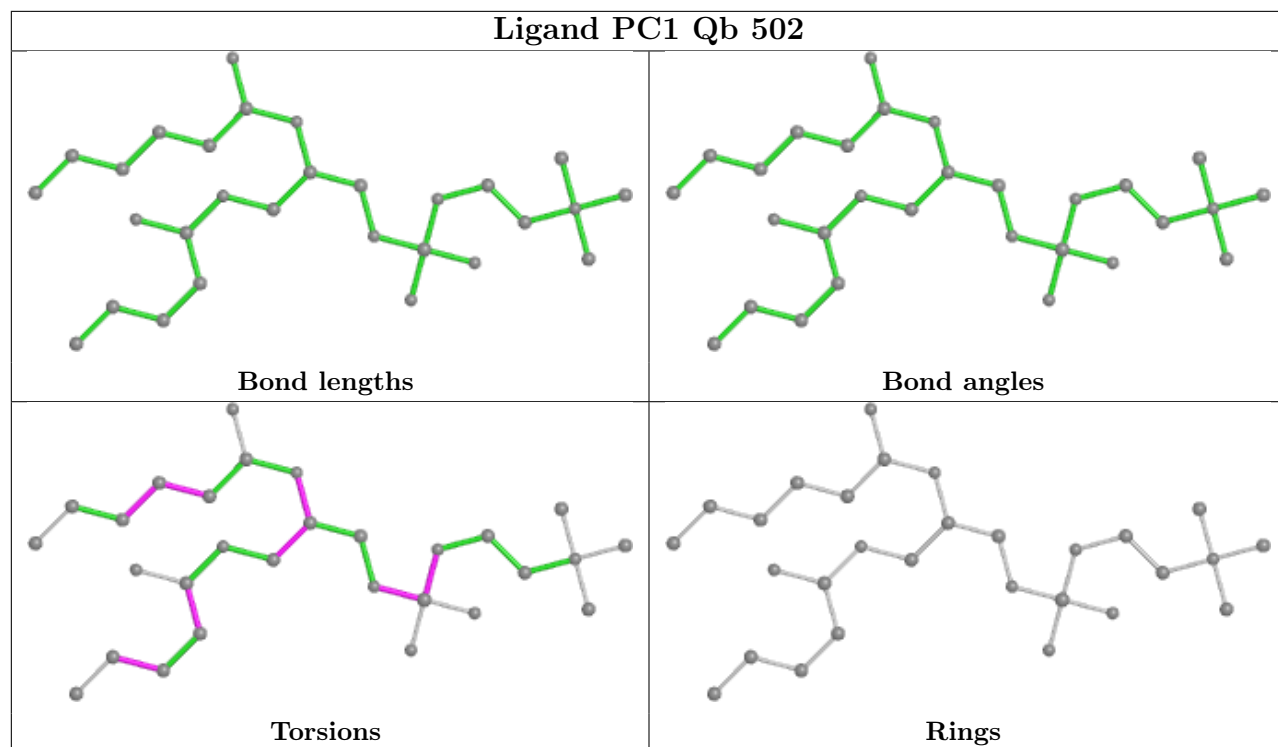
Ligand PC1 C1 606

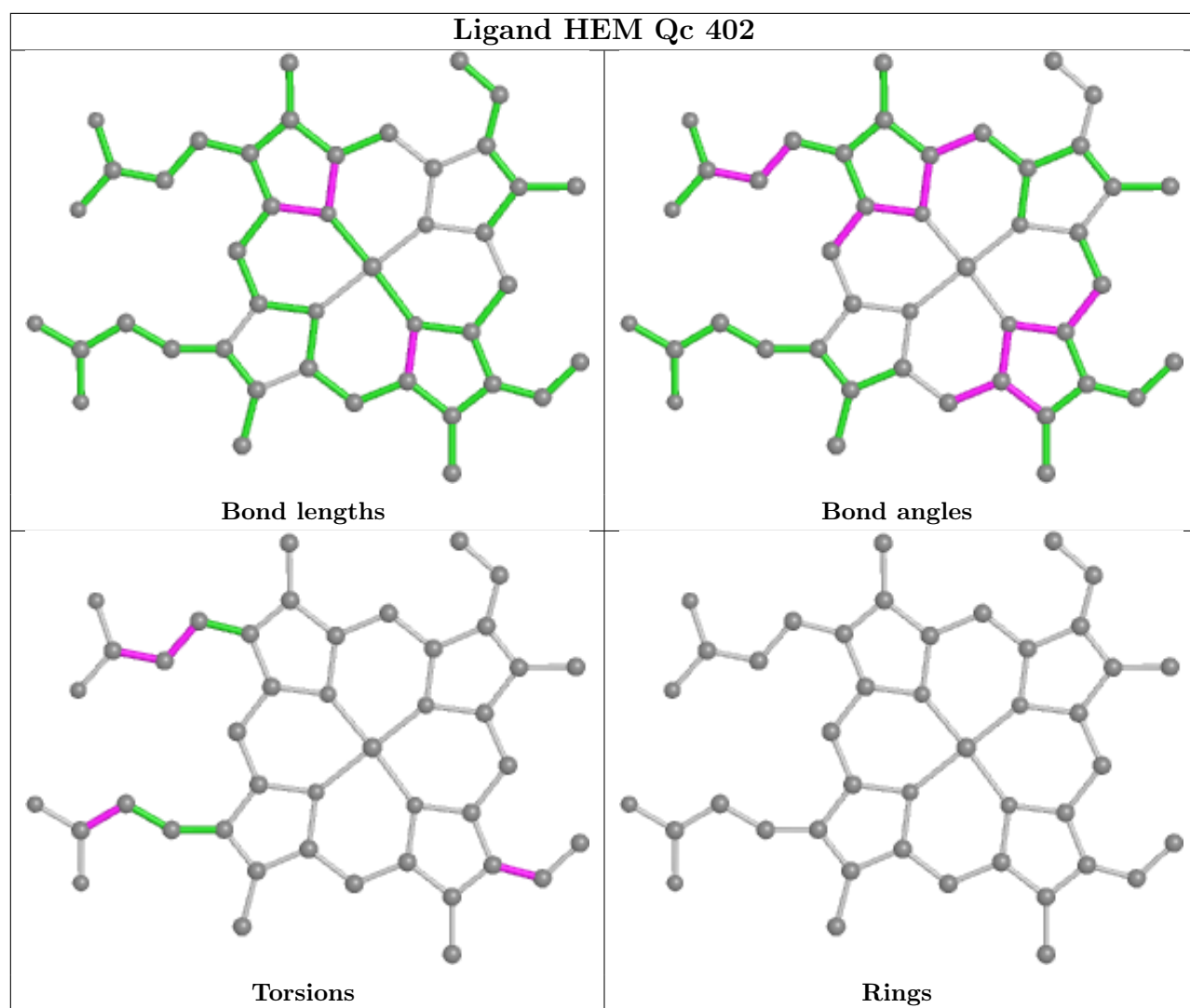


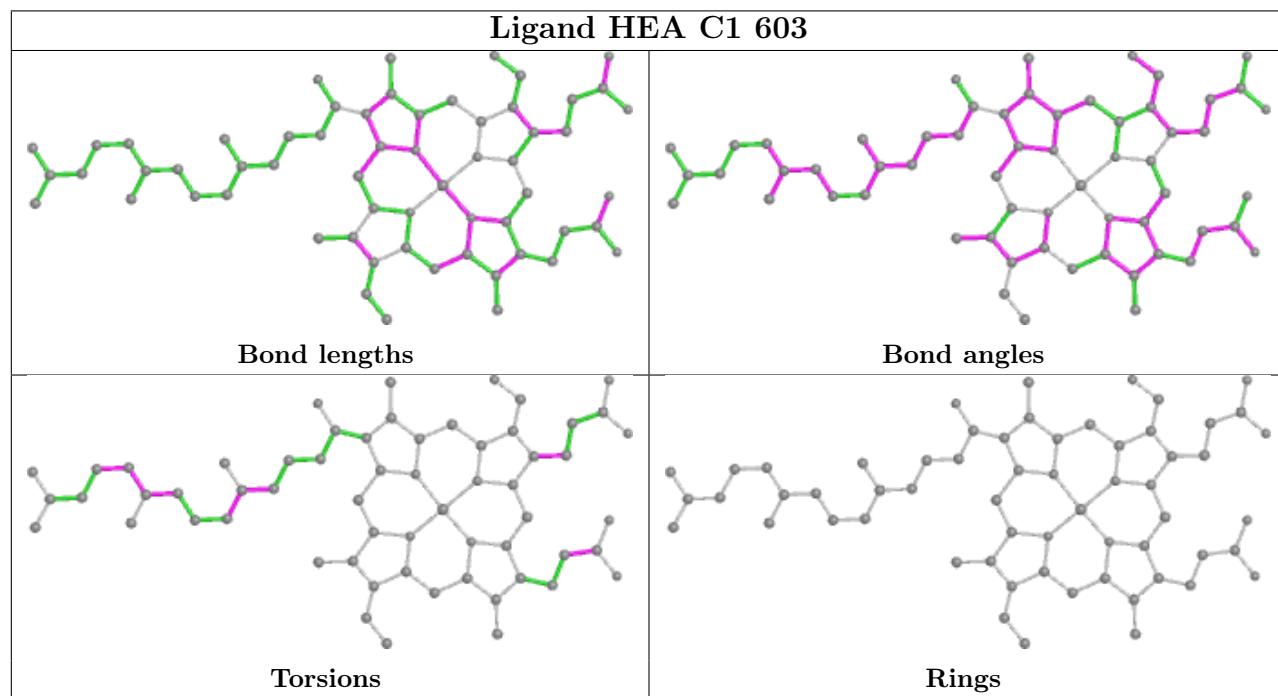
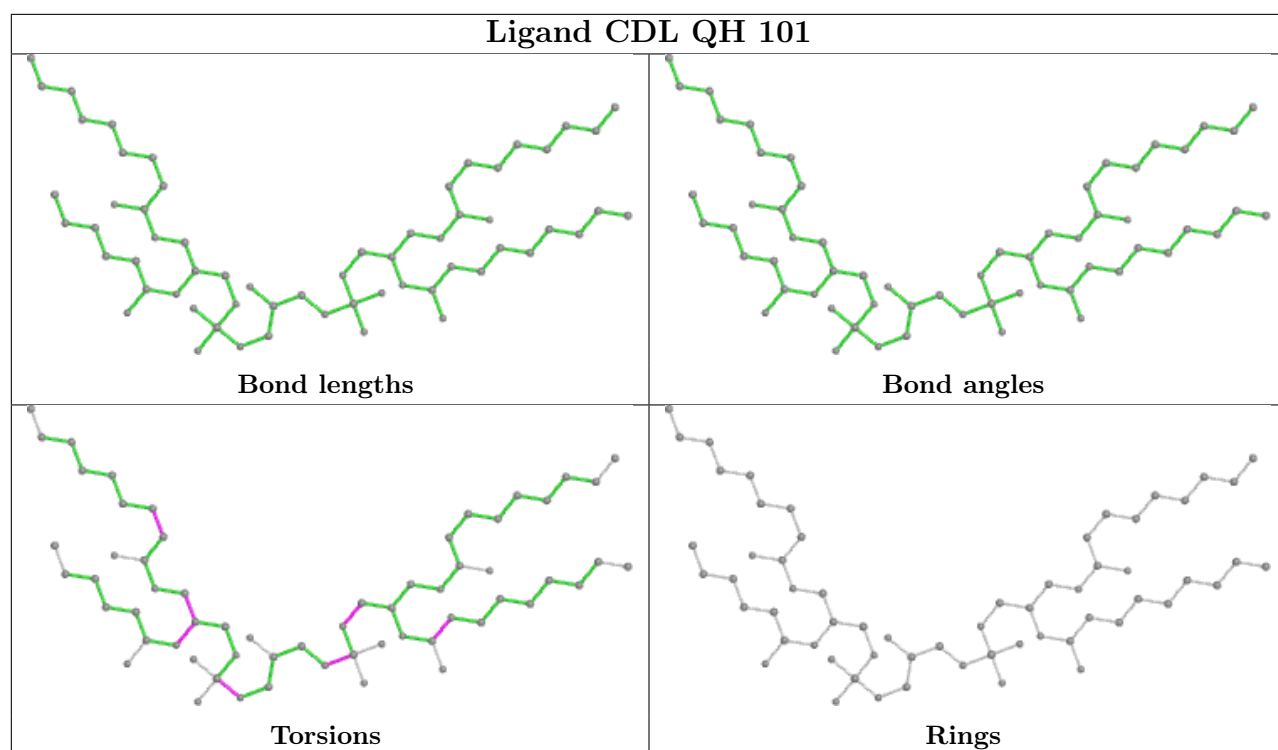


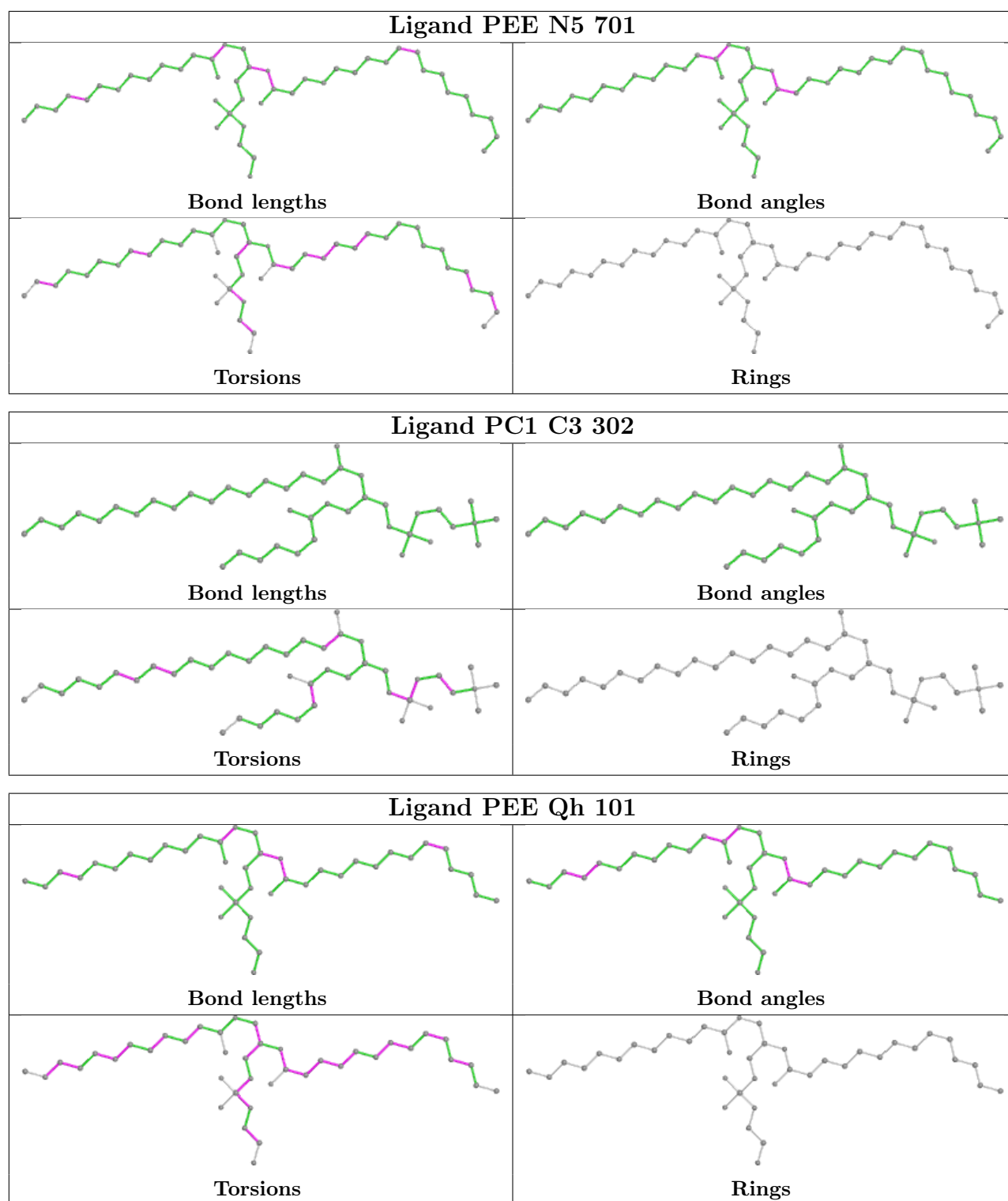




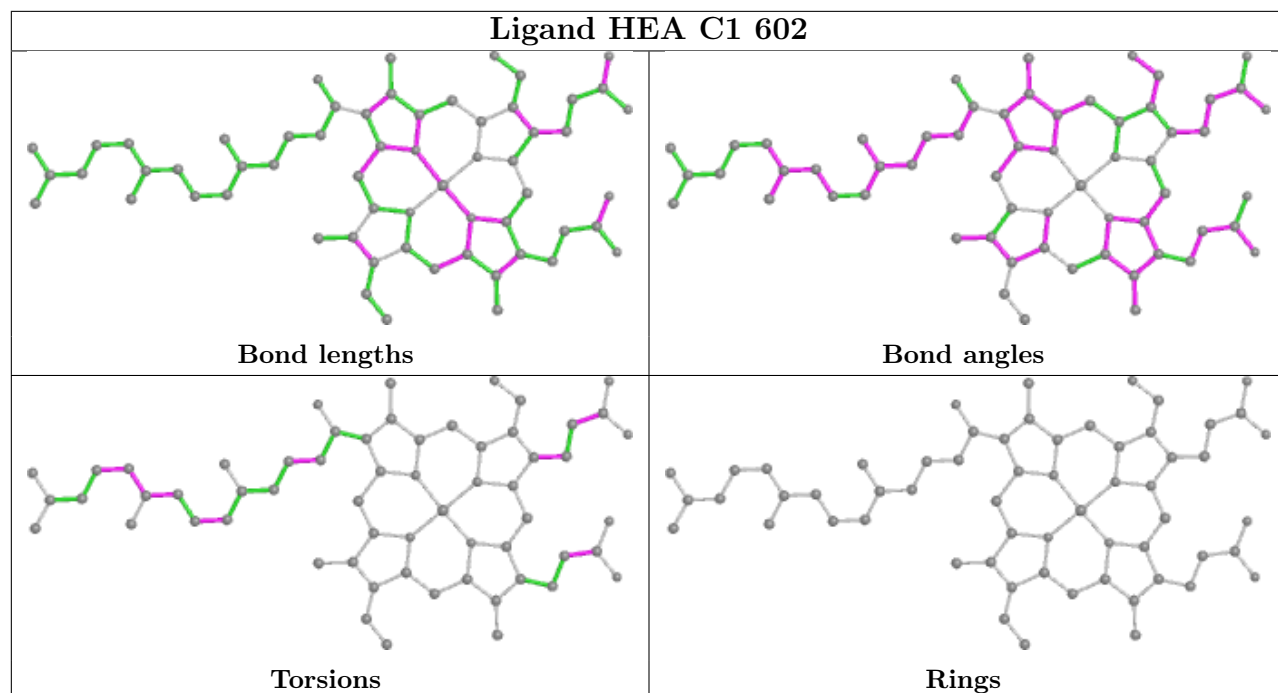




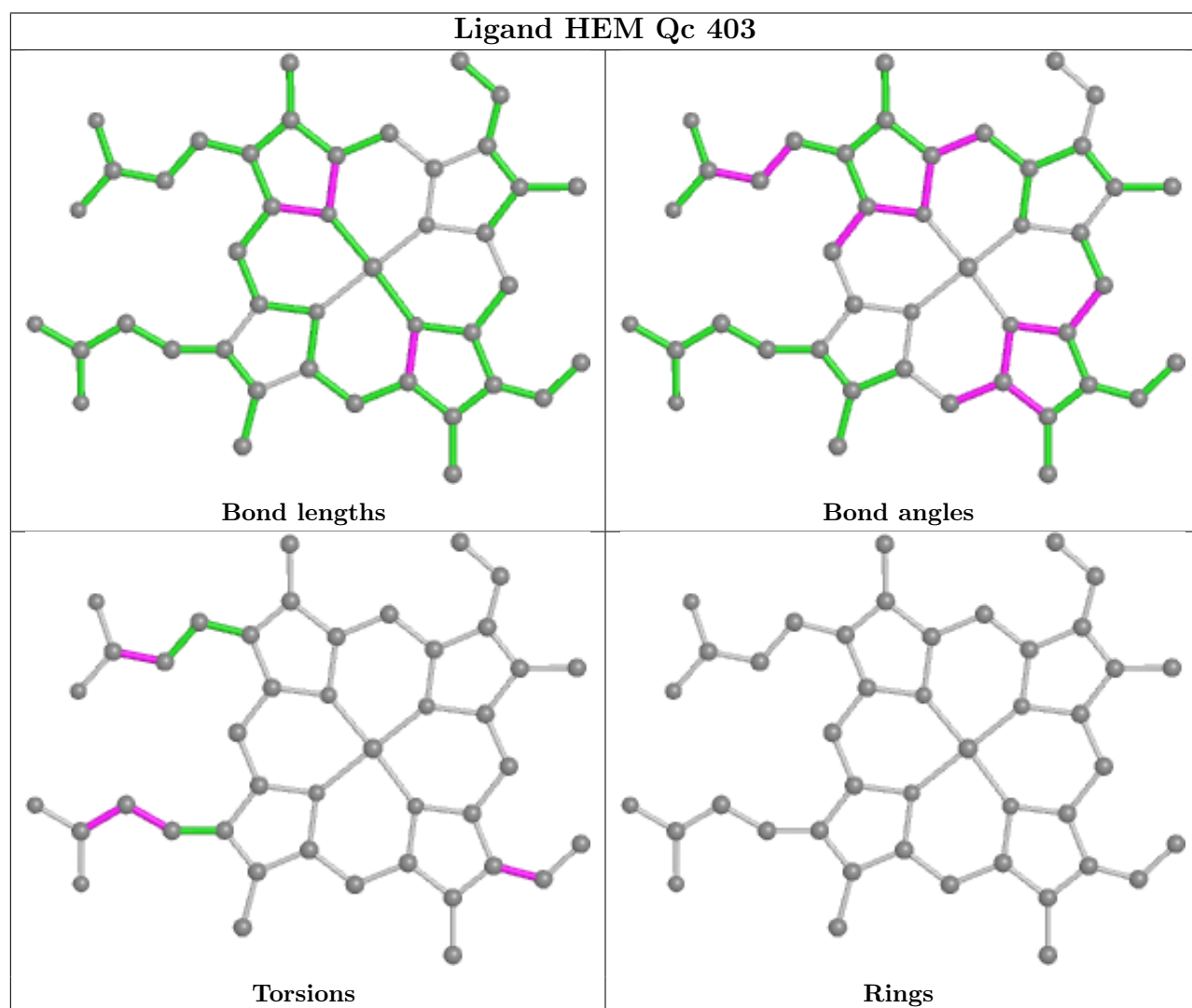


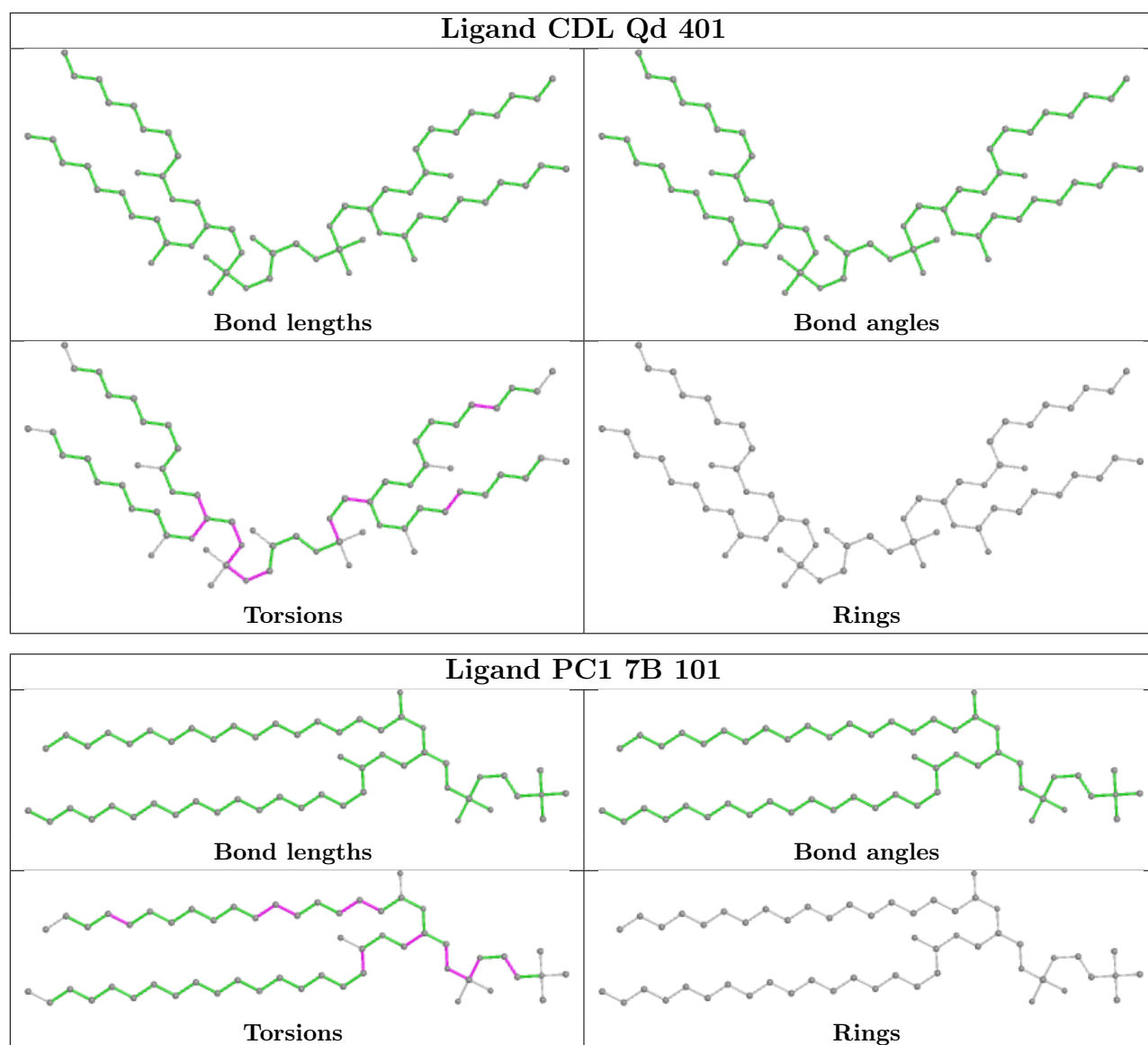


Ligand HEA C1 602



Ligand HEM Qc 403





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.

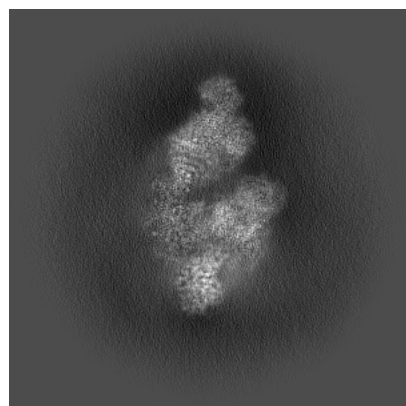
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60284. These allow visual inspection of the internal detail of the map and identification of artifacts.

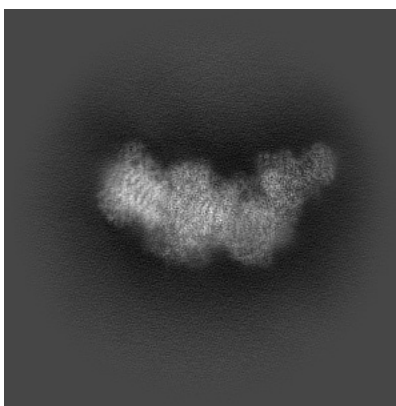
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

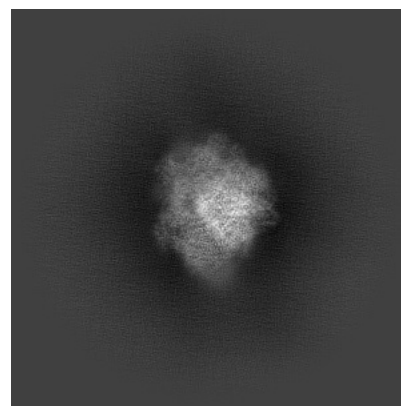
6.1.1 Primary map



X

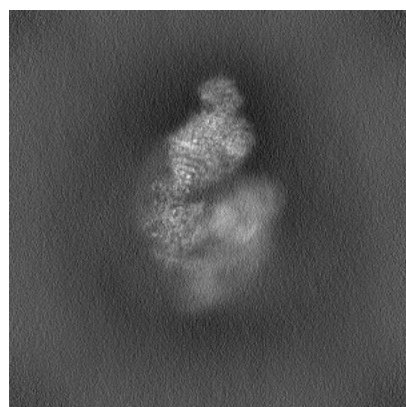


Y

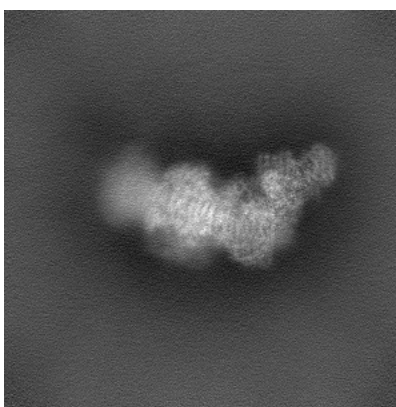


Z

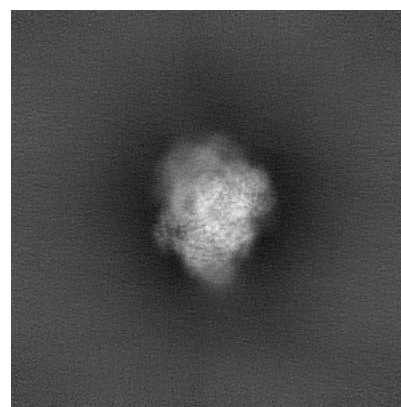
6.1.2 Raw map



X



Y

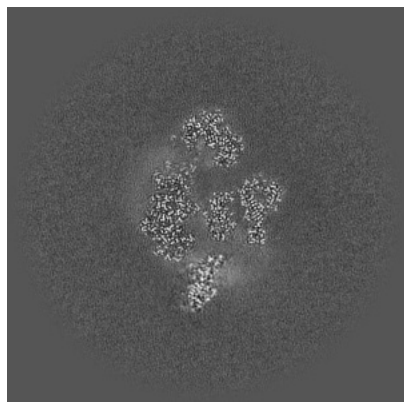


Z

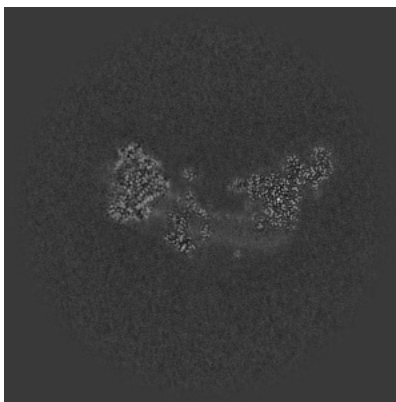
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

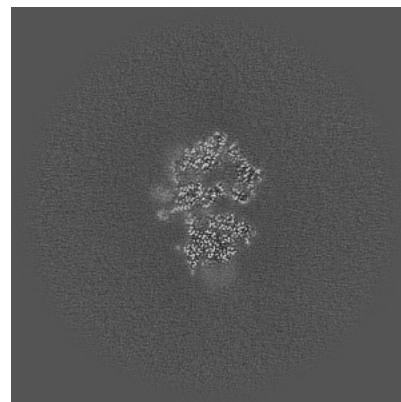
6.2.1 Primary map



X Index: 240

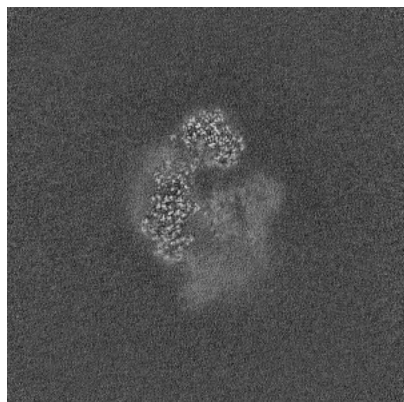


Y Index: 240

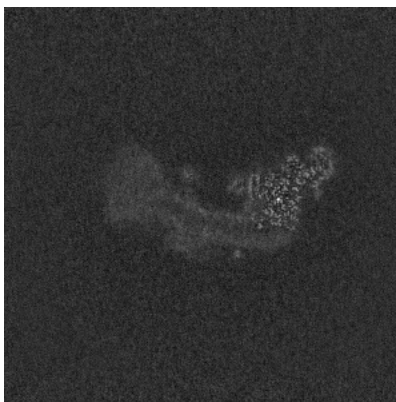


Z Index: 240

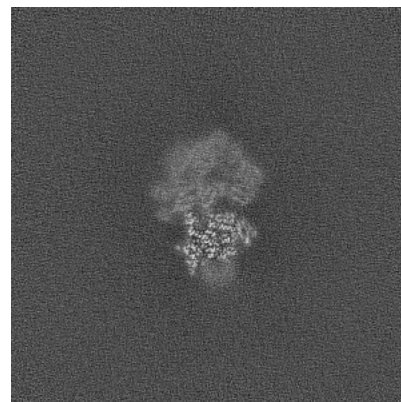
6.2.2 Raw map



X Index: 240



Y Index: 240

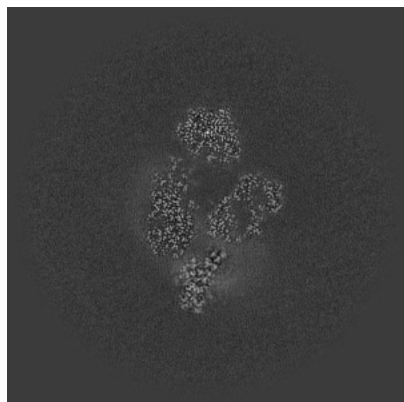


Z Index: 240

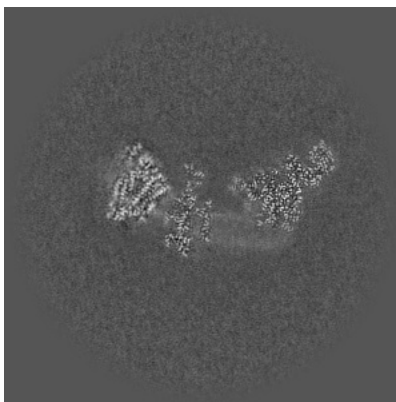
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

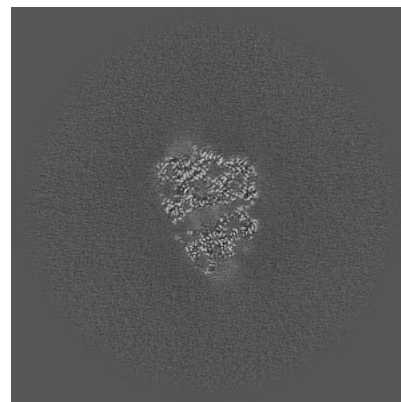
6.3.1 Primary map



X Index: 248

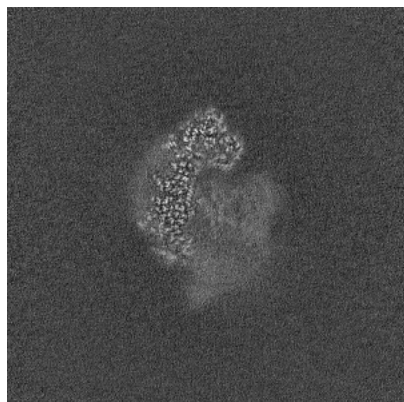


Y Index: 243

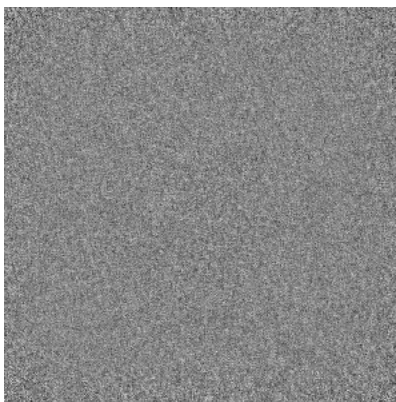


Z Index: 217

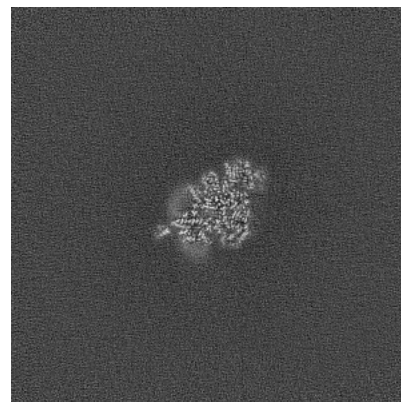
6.3.2 Raw map



X Index: 235



Y Index: 0

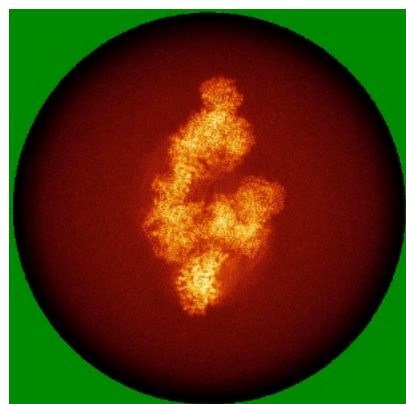


Z Index: 321

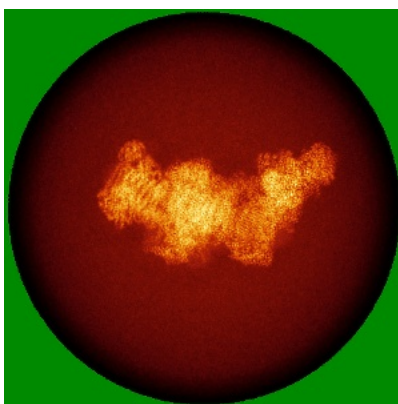
The images above show the largest variance slices of the map in three orthogonal directions.

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

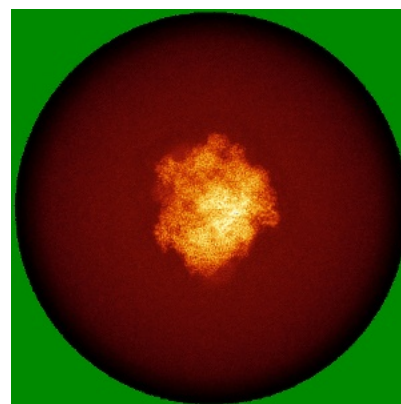
6.4.1 Primary map



X

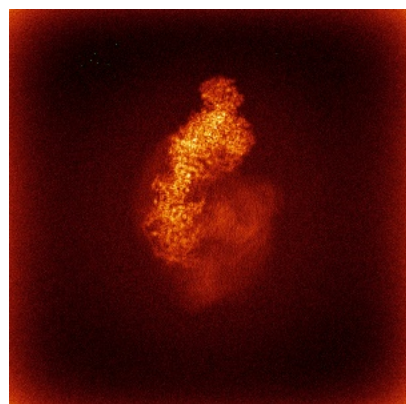


Y

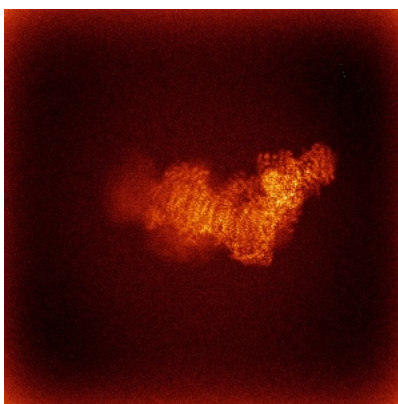


Z

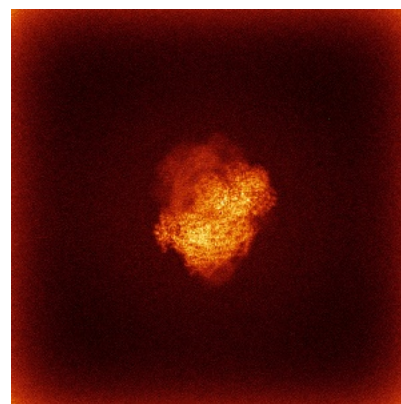
6.4.2 Raw map



X



Y

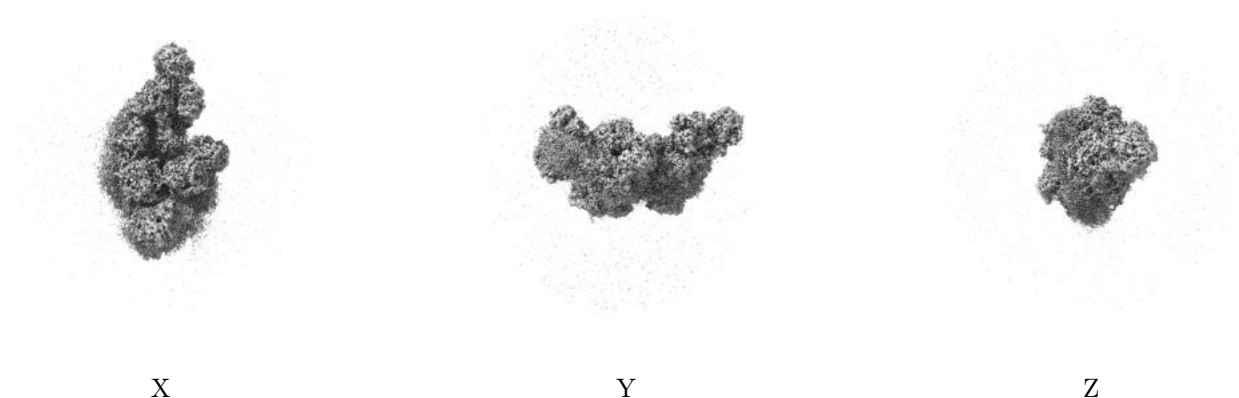


Z

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.

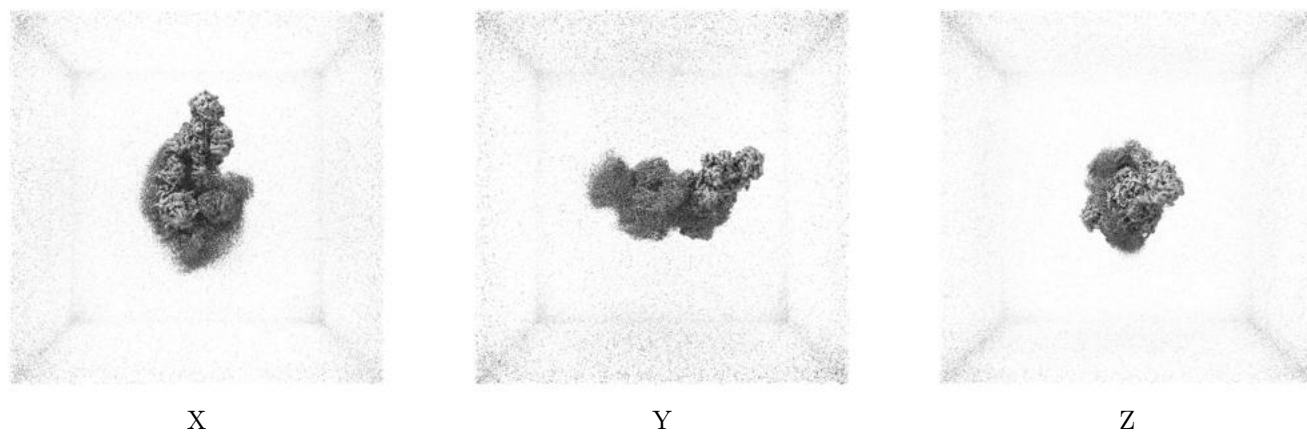
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

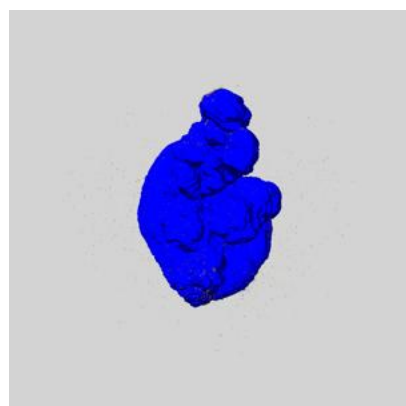
6.6 Mask visualisation [i](#)

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

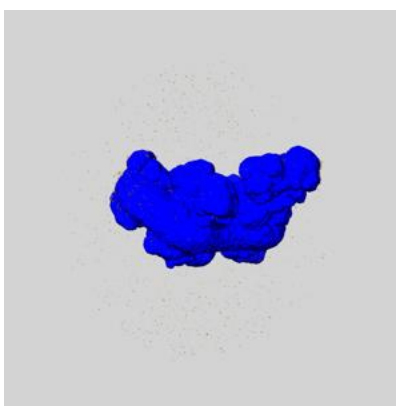
A mask typically either:

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

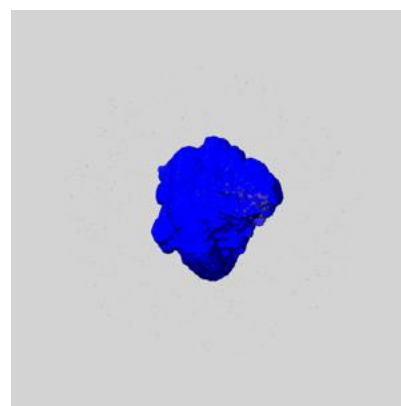
6.6.1 emd_60284_msk_1.map [i](#)



X



Y

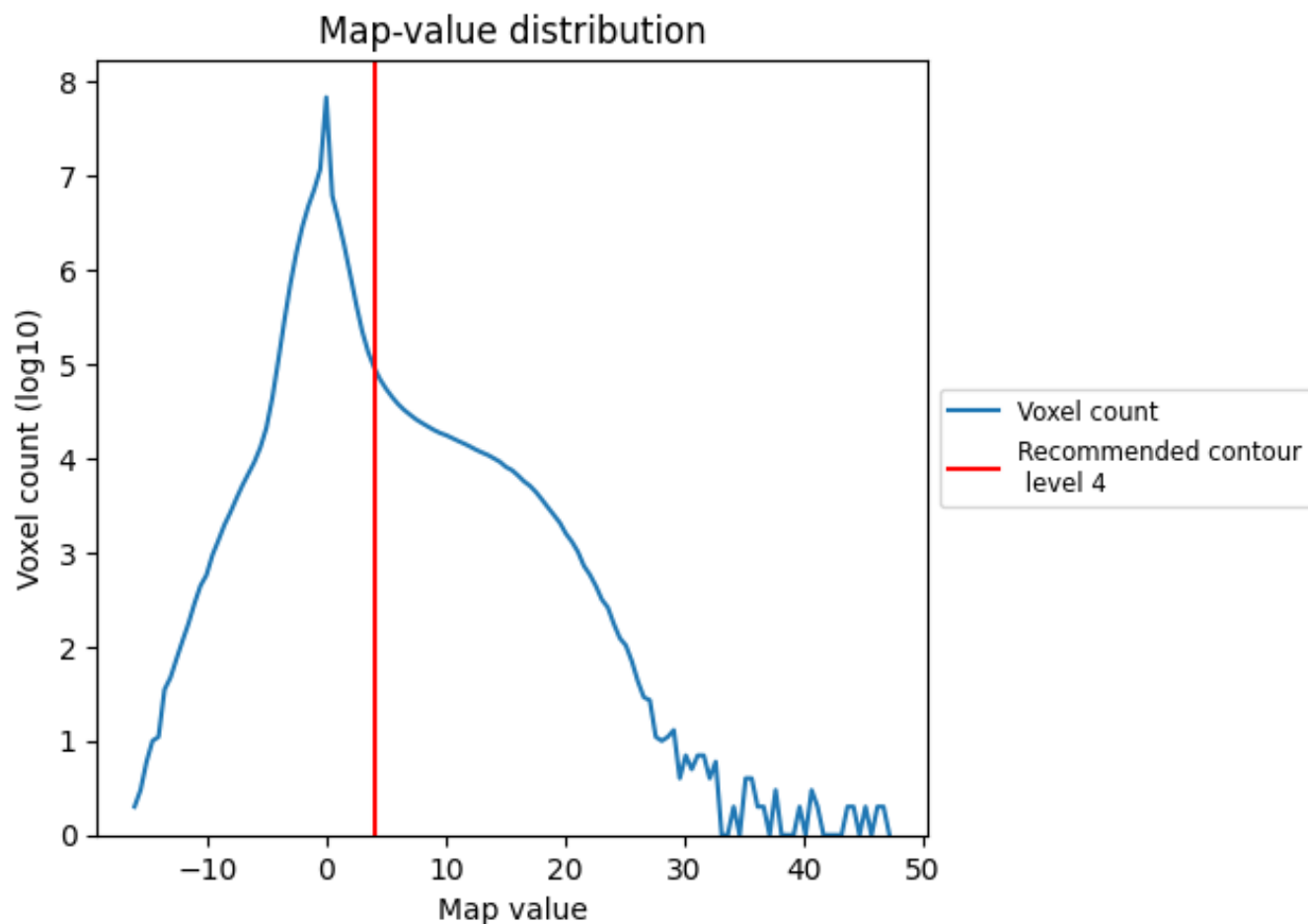


Z

7 Map analysis [i](#)

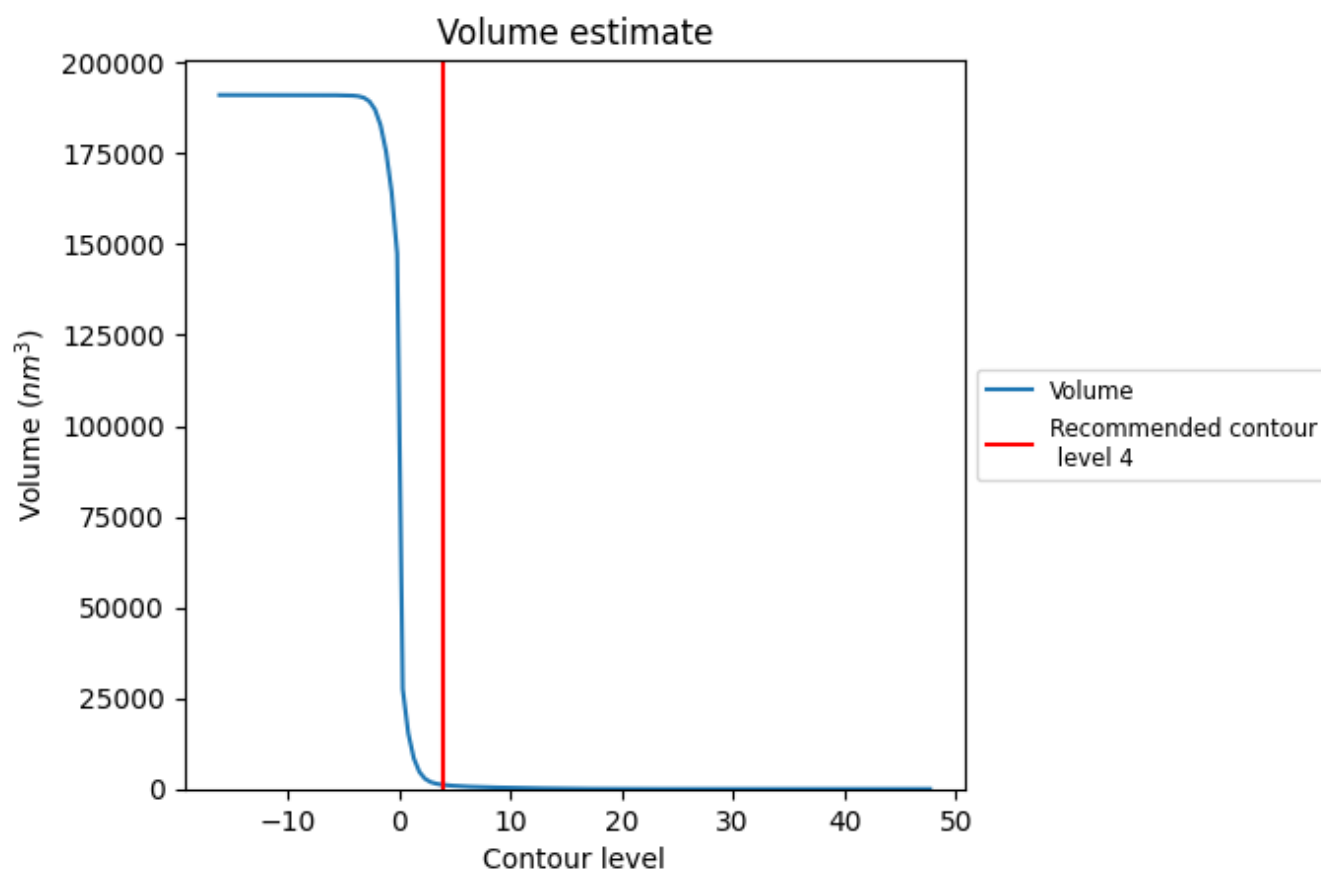
This section contains the results of statistical analysis of the map.

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.

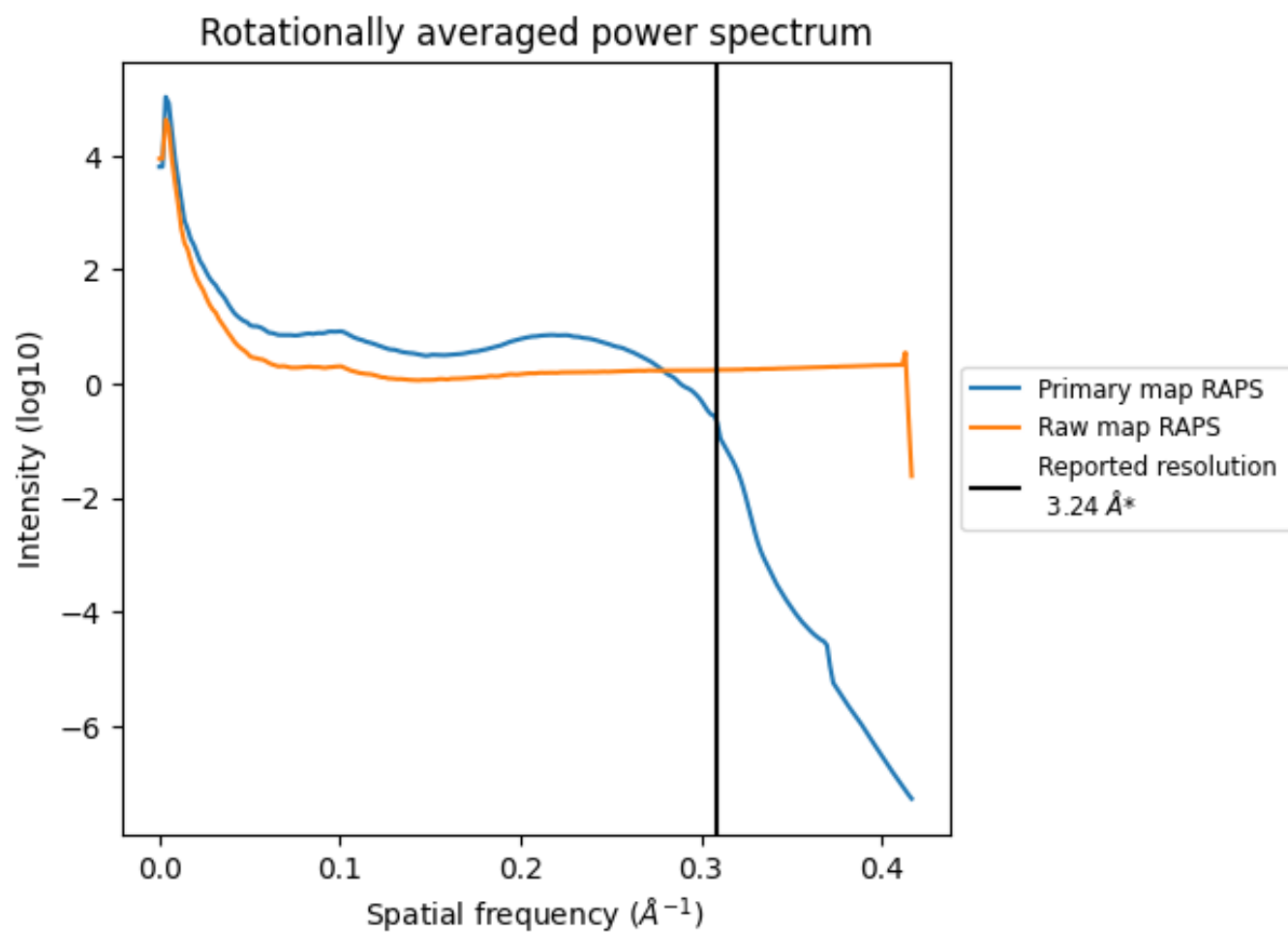
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1136 nm^3 ; this corresponds to an approximate mass of 1026 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 ⓘ

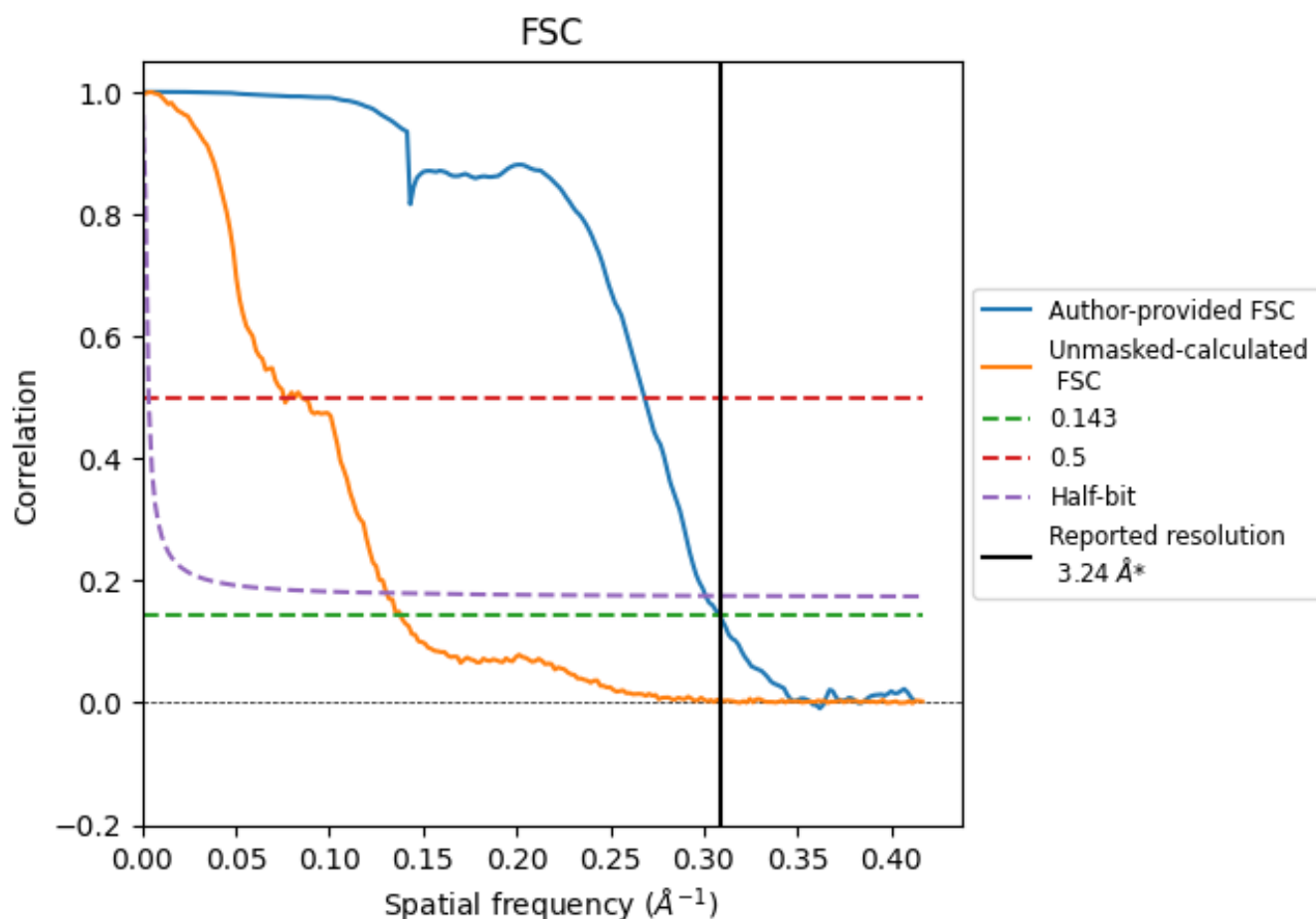


*Reported resolution corresponds to spatial frequency of 0.309 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.309 Å⁻¹

8.2 Resolution estimates [i](#)

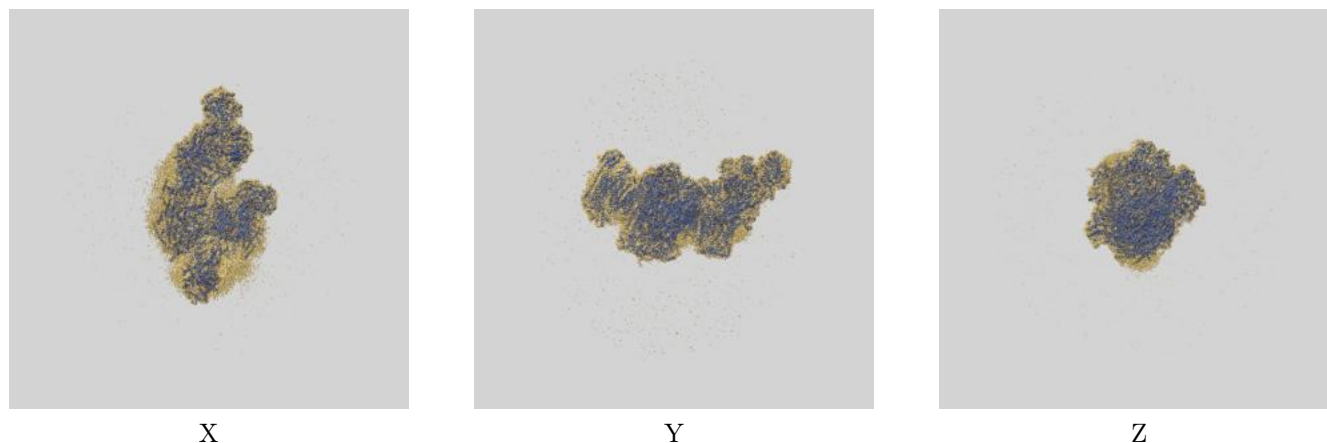
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.24	3.72	3.32
Unmasked-calculated*	7.25	13.21	7.66

*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 7.25 differs from the reported value 3.24 by more than 10 %

9 Map-model fit [i](#)

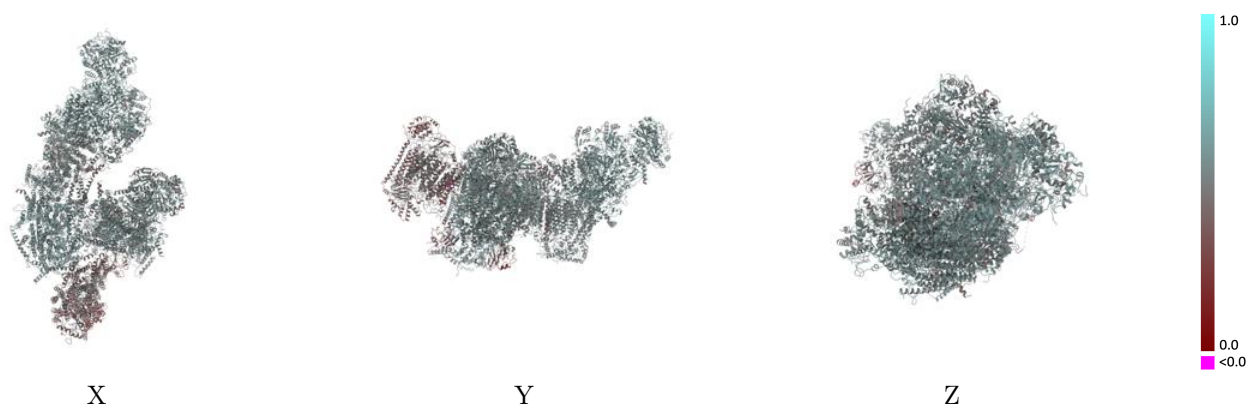
This section contains information regarding the fit between EMDB map EMD-60284 and PDB model 8ZO8. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



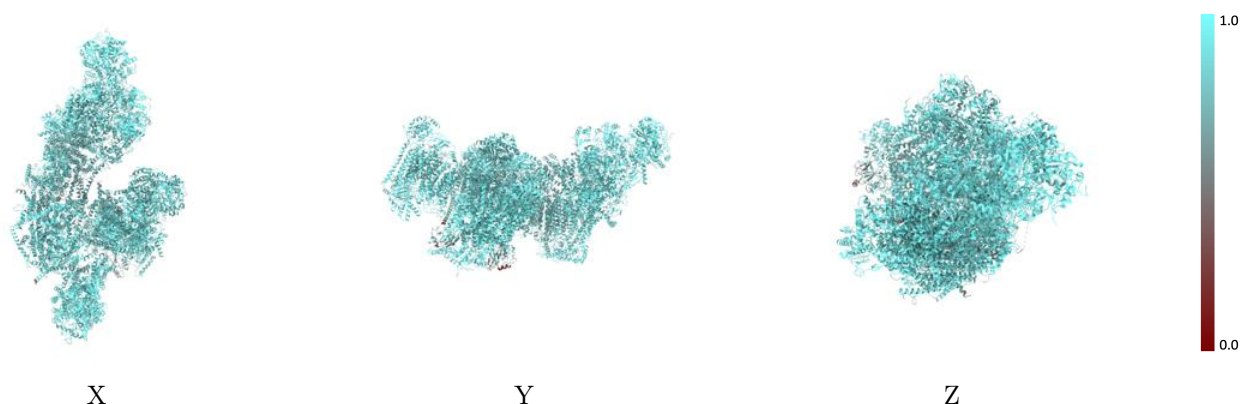
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



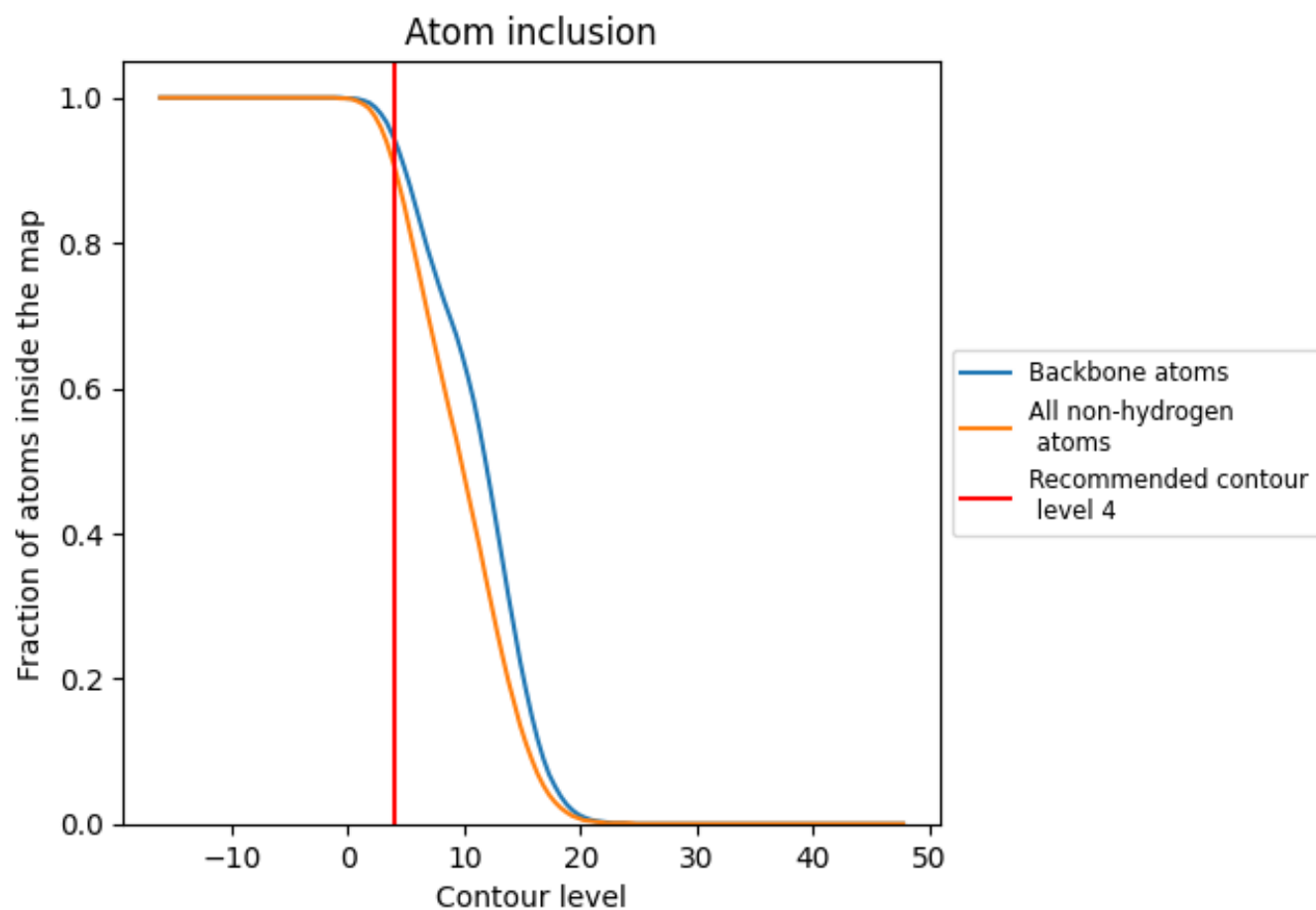
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9060	 0.5230
4L	 0.8920	 0.5330
5A	 0.8780	 0.3720
5B	 0.9470	 0.3950
6A	 0.9500	 0.3820
6B	 0.9550	 0.4030
6C	 0.8530	 0.3780
7A	 0.9200	 0.3970
7B	 0.8800	 0.4190
7C	 0.9610	 0.4060
8B	 0.9550	 0.4040
A1	 0.9560	 0.5430
A2	 0.9040	 0.5270
A3	 0.9520	 0.5390
A5	 0.9130	 0.5320
A6	 0.9060	 0.5390
A7	 0.8810	 0.5380
A8	 0.9350	 0.5470
A9	 0.9270	 0.5480
AB	 0.7680	 0.4310
AC	 0.9130	 0.5590
AK	 0.8350	 0.5000
AL	 0.8060	 0.5060
AM	 0.8860	 0.5400
AN	 0.9410	 0.5390
B1	 0.8600	 0.5310
B2	 0.9260	 0.5520
B3	 0.8940	 0.5380
B4	 0.8830	 0.5500
B5	 0.9220	 0.5710
B6	 0.8690	 0.5350
B7	 0.9020	 0.5510
B8	 0.9040	 0.5610
B9	 0.9120	 0.5620
BK	 0.8910	 0.5490







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Chain	Atom inclusion	Q-score
BL	 0.8770	 0.5430
C1	 0.9430	 0.4490
C2	 0.9360	 0.4280
C3	 0.9370	 0.4070
C4	 0.9020	 0.3950
CA	 0.8680	 0.5190
CB	 0.9090	 0.5530
N1	 0.9280	 0.5420
N2	 0.9340	 0.5510
N3	 0.9110	 0.5370
N4	 0.9220	 0.5690
N5	 0.9150	 0.5680
N6	 0.8620	 0.4940
QA	 0.9000	 0.5270
QB	 0.9030	 0.5350
QC	 0.9190	 0.5400
QD	 0.9090	 0.5310
QE	 0.7200	 0.4260
QF	 0.8220	 0.4780
QG	 0.9140	 0.5330
QH	 0.9090	 0.5250
QI	 0.9090	 0.5260
QJ	 0.8890	 0.4980
QK	 0.7450	 0.4870
Qa	 0.8870	 0.5260
Qb	 0.9010	 0.5300
Qc	 0.9390	 0.5360
Qd	 0.9110	 0.5390
Qe	 0.6850	 0.4040
Qf	 0.8160	 0.4670
Qg	 0.8860	 0.5230
Qh	 0.8910	 0.5260
Qi	 0.9290	 0.5290
Qj	 0.8840	 0.5140
S1	 0.9300	 0.5560
S2	 0.9260	 0.5650
S3	 0.9660	 0.5800
S4	 0.9240	 0.5630
S5	 0.9210	 0.5370
S6	 0.9210	 0.5560
S7	 0.9440	 0.5670
S8	 0.9650	 0.5740

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Chain	Atom inclusion	Q-score
V1	 0.9330	 0.5460
V2	 0.9140	 0.5410
V3	 0.9450	 0.5440