



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:38 PM UTC

PDB ID : 8Q25 / pdb_00008q25
EMDB ID : EMD-18069
Title : Outward-facing, open1 proteoliposome complex I at 2.8 Å, after deactivation treatment. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-01
Resolution : 2.80 Å(reported)
Based on initial model : 7QSN

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:

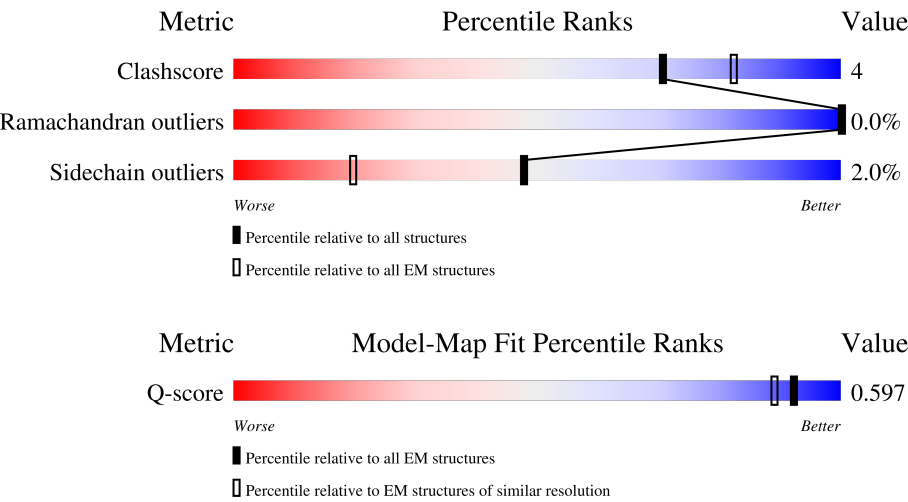
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	115	85%14%
2	B	216	65%6%28%
3	C	266	73%5%22%
4	D	463	84%6%10%

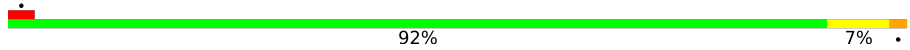
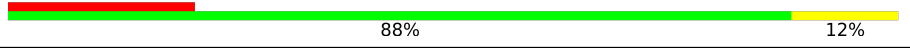
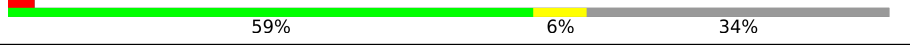
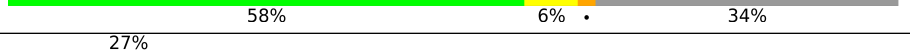
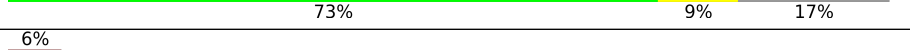
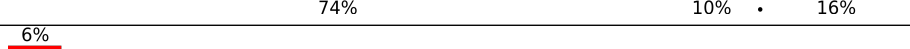
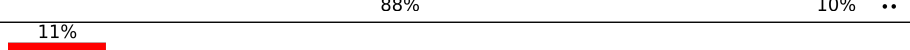
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 69693 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	622	133	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	207	Total	C	N	O	S	0	0
			1721	1111	296	311	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	419	Total	C	N	O	S	0	0
			3377	2159	580	613	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	0	0
			3326	2096	594	616	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	691	Total	C	N	O	S	0	0
			5298	3318	925	1016	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	339	Total	C	N	O	S	0	0
			2728	1765	484	474	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	N	O	S	0	0
			707	454	104	144	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	114	Total	C	N	O	S	0	0
			923	597	156	167	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	116	Total	C	N	O	S	0	0
			982	628	182	168	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	142	Total	C	N	O	S	0	0
			1157	743	202	203	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			654	427	109	116	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	98	Total	C	N	O	S	0	0
			825	521	157	141	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			846	544	140	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	127	Total	C	N	O	S	0	0
			1097	722	191	183	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	128	Total	C	N	O	S	0	0
			1070	686	188	196			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	174	Total	C	N	O	S	0	0
			1458	913	269	268	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1212	780	216	211	5		

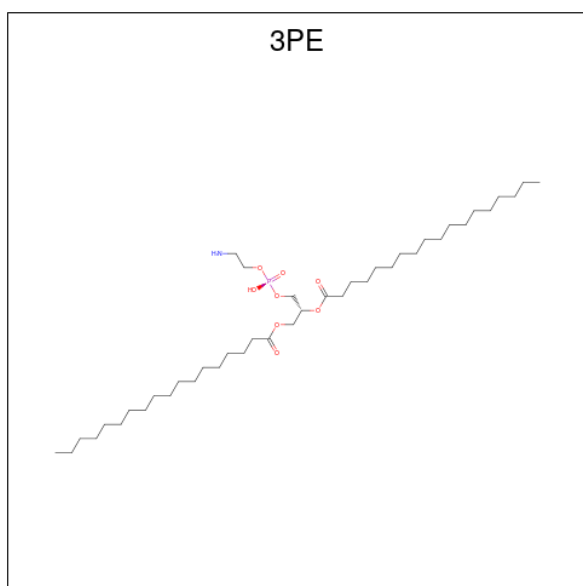
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			776	490	144	139	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	I	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	J	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	L	1	Total	C	N	O	P	0
			34	24	1	8	1	

Continued on next page...

Continued from previous page...

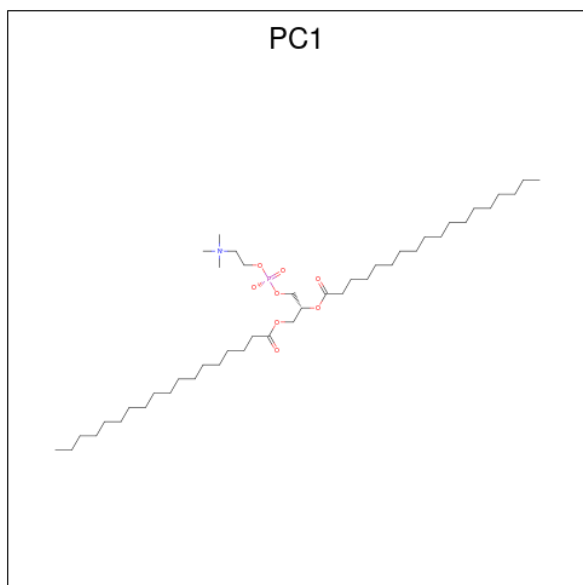
Mol	Chain	Residues	Atoms					AltConf
45	L	1	Total 41	C 31	N 1	O 8	P 1	0
45	M	1	Total 50	C 40	N 1	O 8	P 1	0
45	M	1	Total 45	C 35	N 1	O 8	P 1	0
45	N	1	Total 49	C 39	N 1	O 8	P 1	0
45	P	1	Total 38	C 28	N 1	O 8	P 1	0
45	Y	1	Total 41	C 31	N 1	O 8	P 1	0
45	Y	1	Total 27	C 17	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 45	C 35	N 1	O 8	P 1	0
45	Y	1	Total 36	C 26	N 1	O 8	P 1	0
45	Z	1	Total 42	C 32	N 1	O 8	P 1	0
45	a	1	Total 36	C 26	N 1	O 8	P 1	0
45	b	1	Total 36	C 26	N 1	O 8	P 1	0
45	b	1	Total 47	C 37	N 1	O 8	P 1	0
45	d	1	Total 49	C 39	N 1	O 8	P 1	0
45	f	1	Total 24	C 14	N 1	O 8	P 1	0
45	g	1	Total 29	C 19	N 1	O 8	P 1	0
45	m	1	Total 41	C 31	N 1	O 8	P 1	0
45	q	1	Total 51	C 41	N 1	O 8	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	r	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



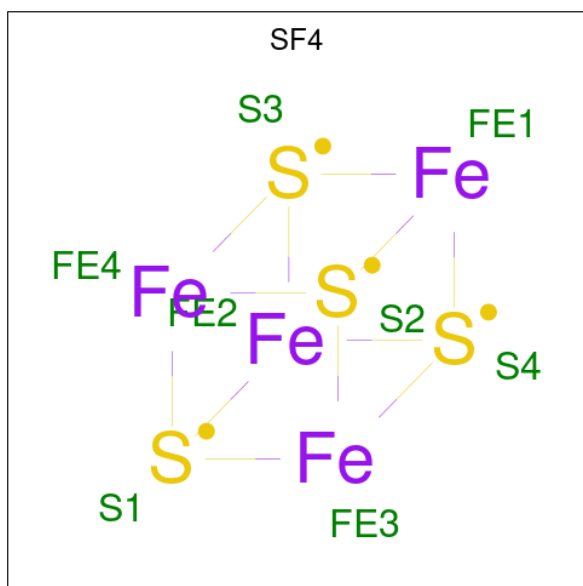
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	M	1	Total	C	N	O	P	0
			44	34	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
46	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	l	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



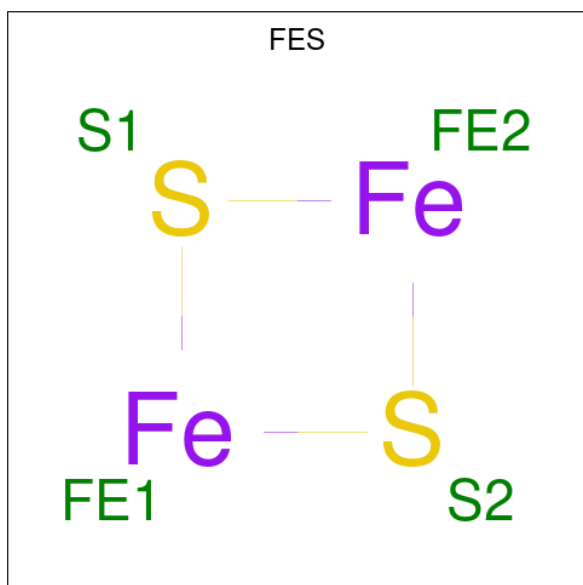
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

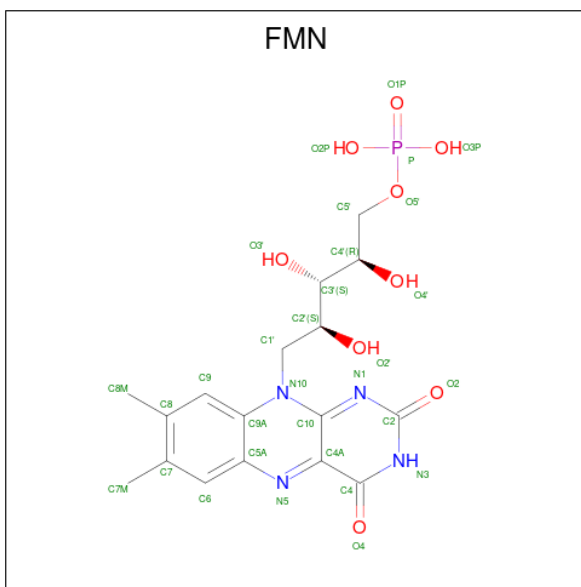
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

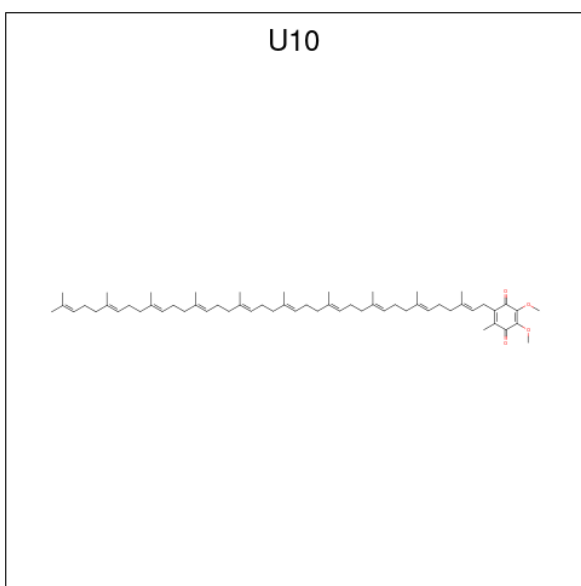


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

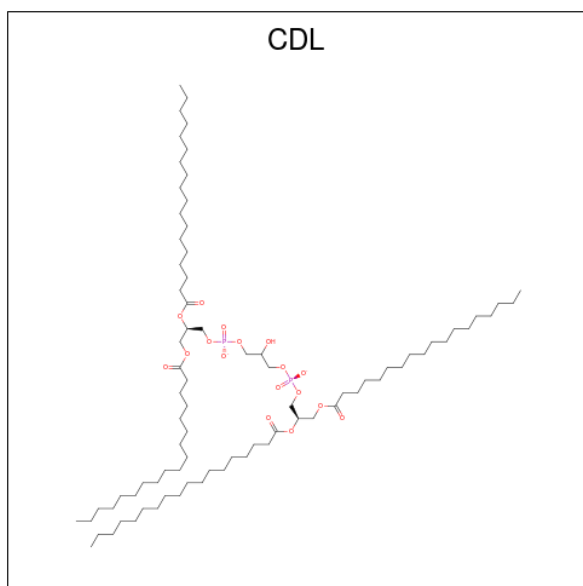
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



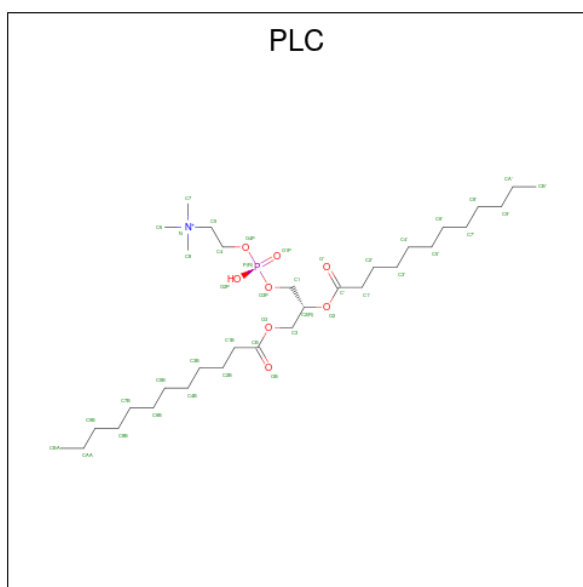
Mol	Chain	Residues	Atoms			AltConf
51	H	1	Total	C	O	0
			34	30	4	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
52	H	1	Total	C	O	P	0
			58	39	17	2	
52	L	1	Total	C	O	P	0
			100	81	17	2	
52	M	1	Total	C	O	P	0
			100	81	17	2	
52	N	1	Total	C	O	P	0
			94	75	17	2	
52	d	1	Total	C	O	P	0
			65	46	17	2	
52	d	1	Total	C	O	P	0
			87	68	17	2	
52	i	1	Total	C	O	P	0
			76	57	17	2	
52	r	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 53 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
53	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
53	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	M	1	Total	C	N	O	P	0
			34	24	1	8	1	
53	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
53	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
53	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
53	Z	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	b	1	Total	C	N	O	P	0
			38	28	1	8	1	
53	g	1	Total	C	N	O	P	0
			42	32	1	8	1	

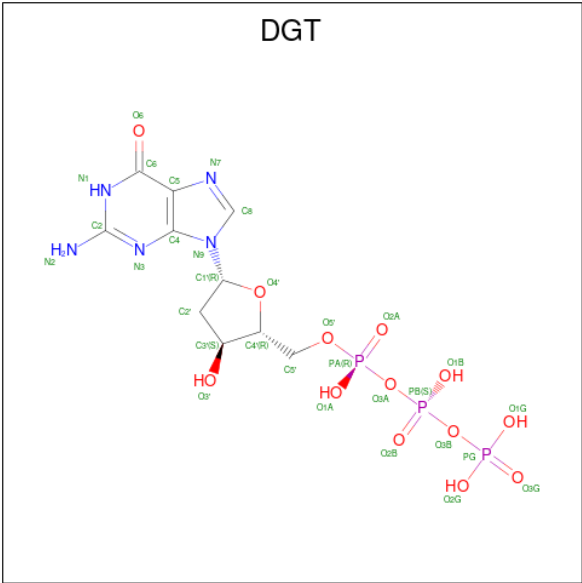
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	M	1	Total	Zn	0
			1	1	
54	R	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

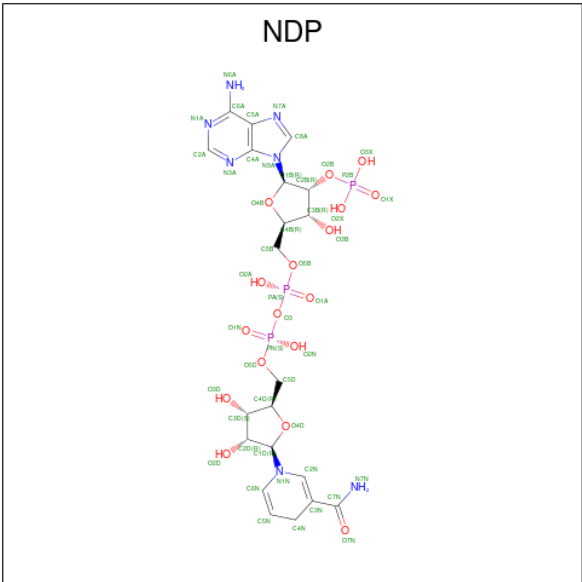
Mol	Chain	Residues	Atoms		AltConf
55	O	1	Total	Mg	0
			1	1	

- Molecule 56 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



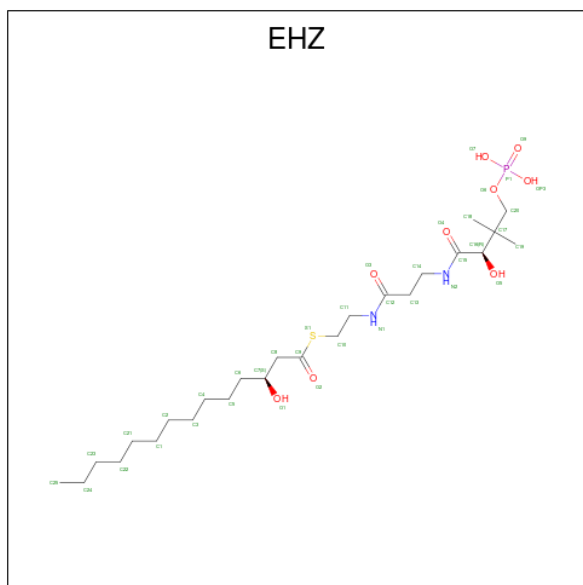
Mol	Chain	Residues	Atoms					AltConf
56	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



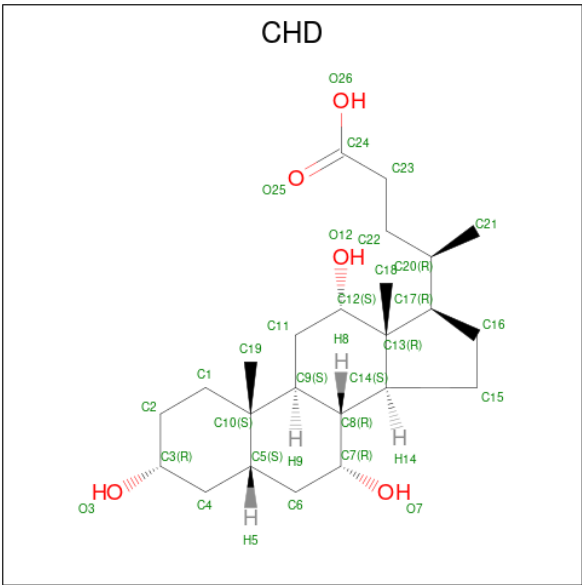
Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 58 is {S}-[2-[3-[[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



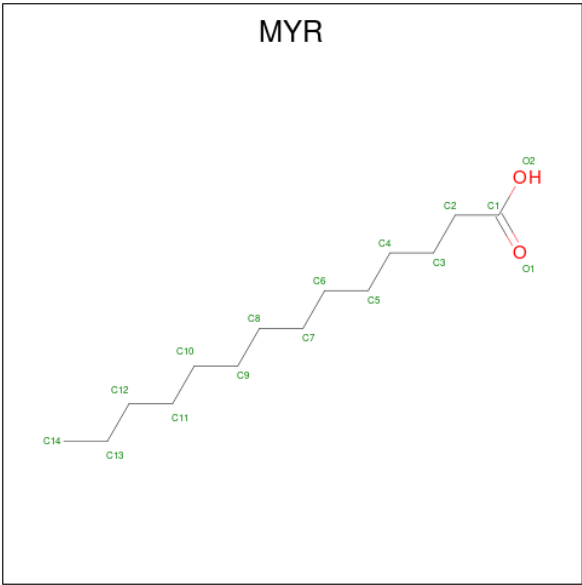
Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 59 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			AltConf
59	i	1	Total	C	O	0
			29	24	5	

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

3 Residue-property plots [i](#)

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

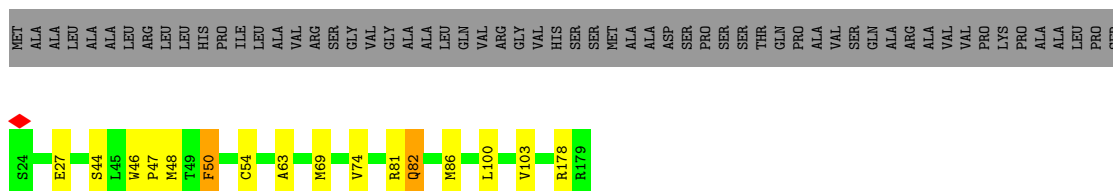
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



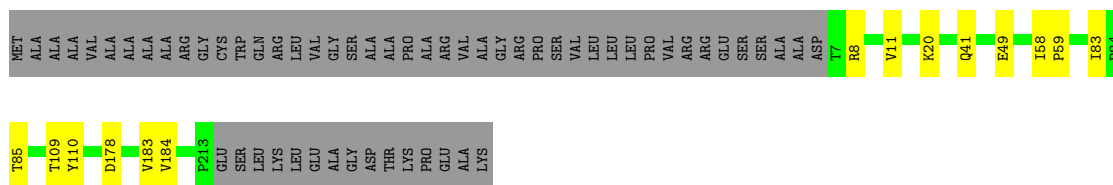
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



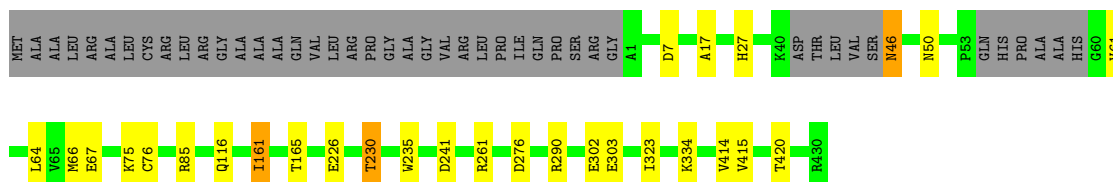
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



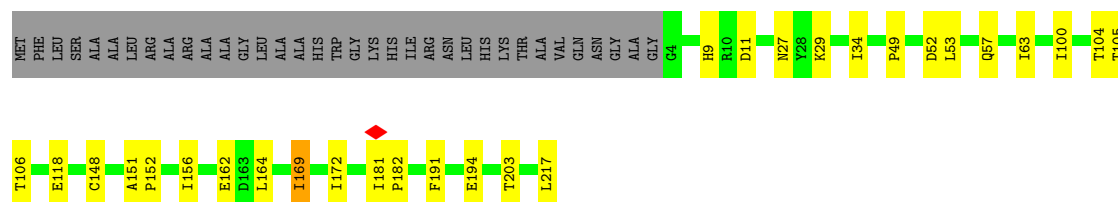
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 



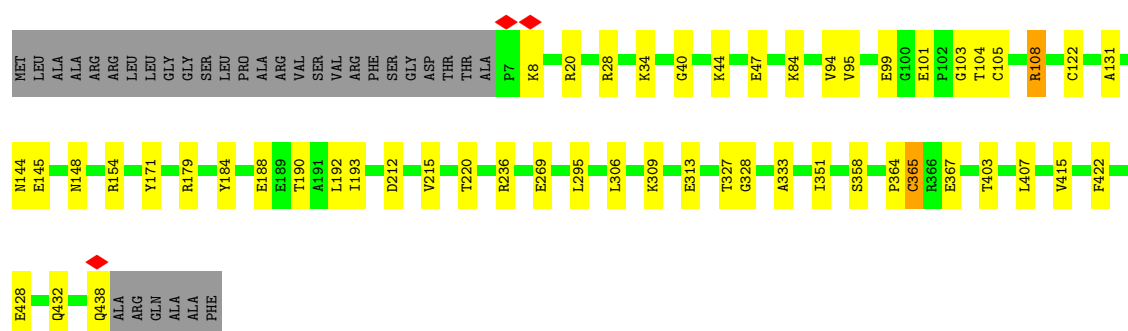
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  74% 11% 14%



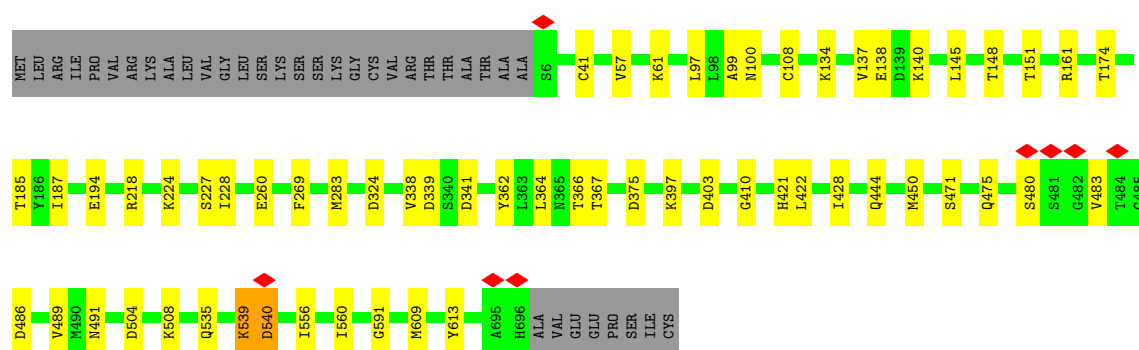
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  82% 11% 7%



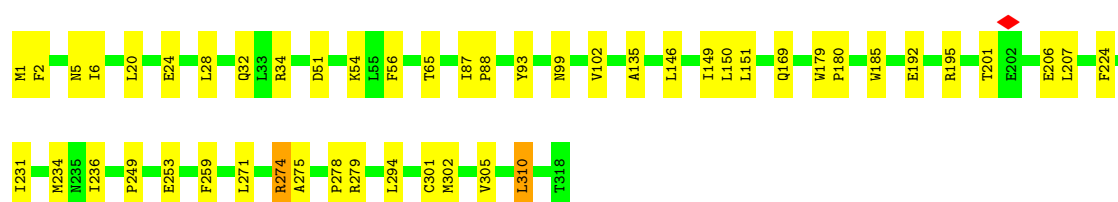
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  87% 8% 5%



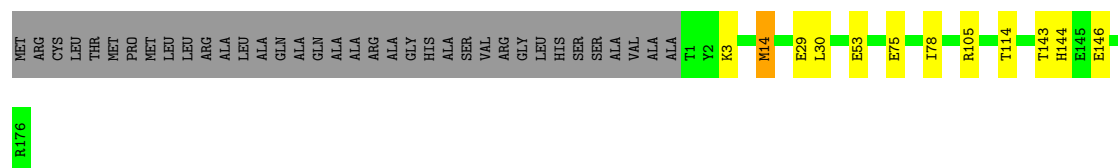
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  85% 15%



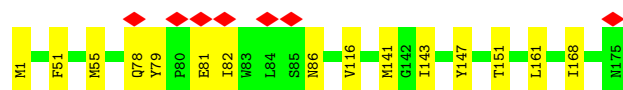
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  77% 5% 17%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  91% 9%



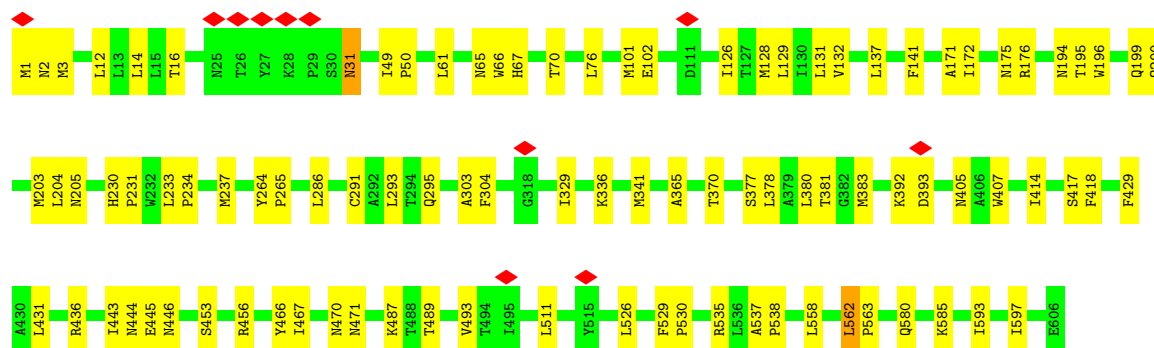
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  93% 7%

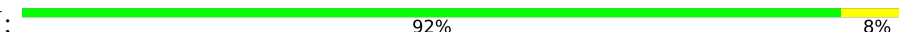


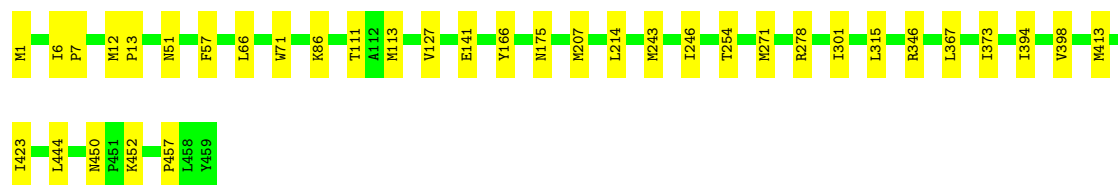
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  84% 16%



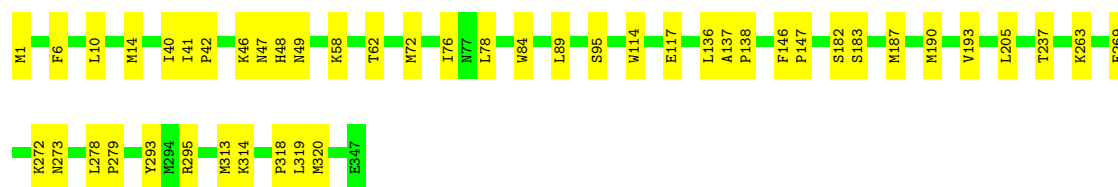
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  92% 8%



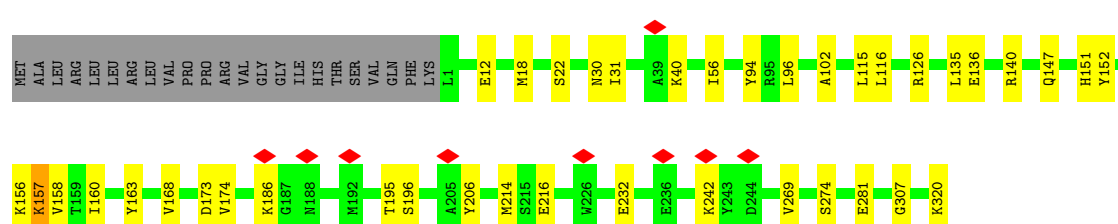
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  87% 13%



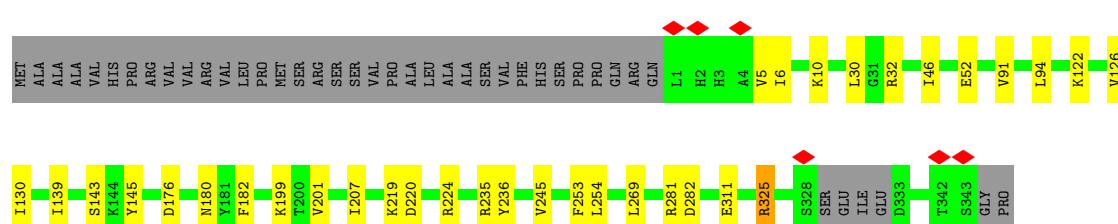
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  82% 11% 7%



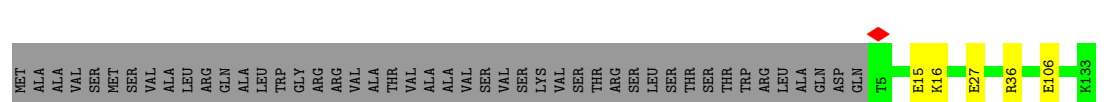
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  80% 9% 11%



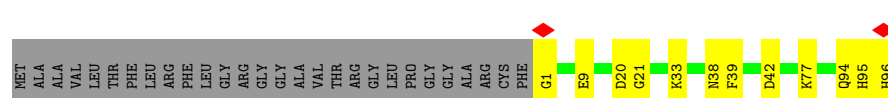
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  71% 26%

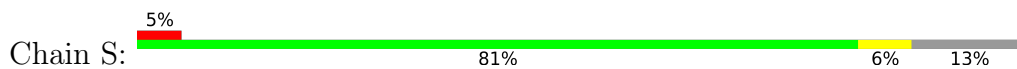


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

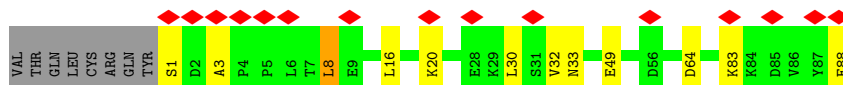
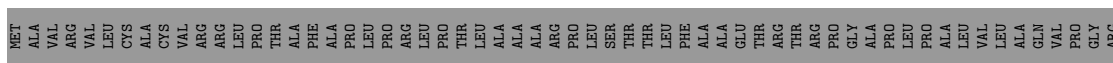
Chain R:  68% 10% 23%



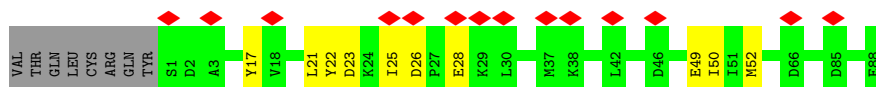
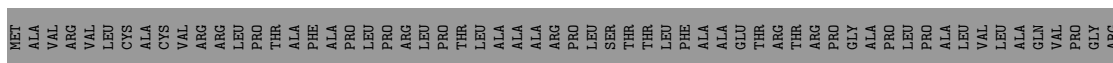
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 20: Acyl carrier protein, mitochondrial



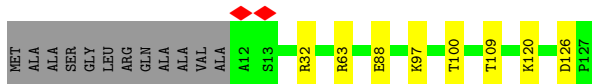
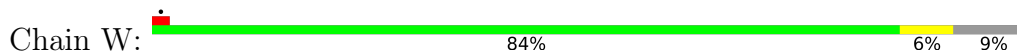
- Molecule 20: Acyl carrier protein, mitochondrial



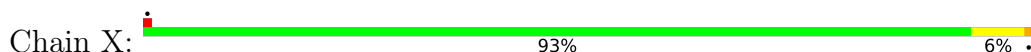
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  89% 11%



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  89% 10%

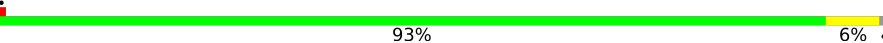


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  89% 11%



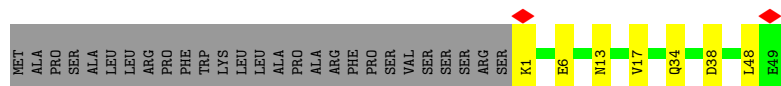
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  93% 6%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  55% 9% 36%



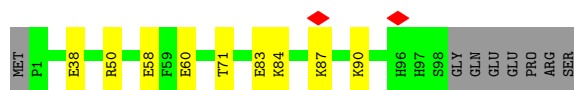
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  92% 7%

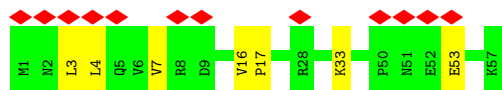
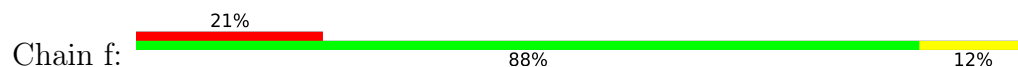


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

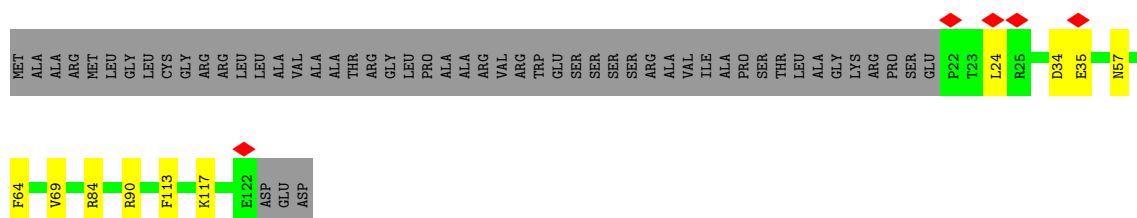
Chain e:  84% 8% 8%



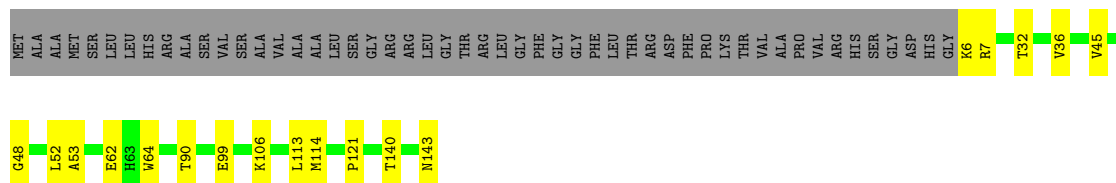
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



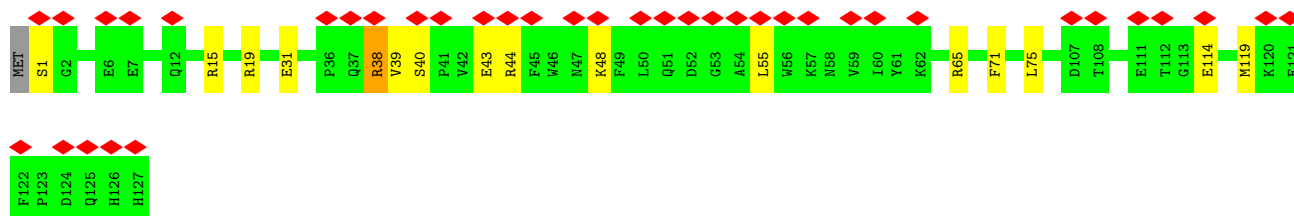
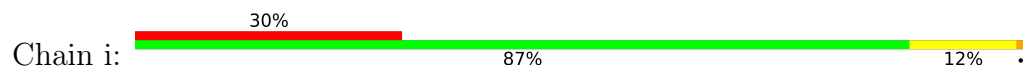
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



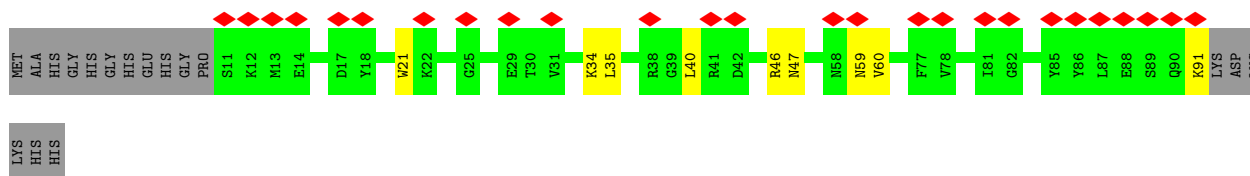
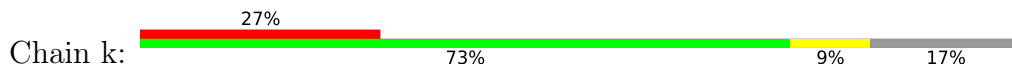
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



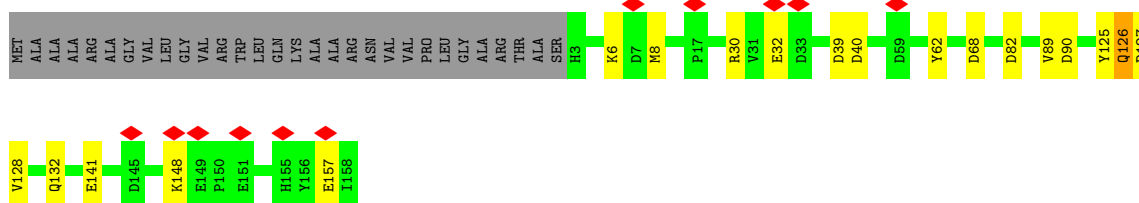
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



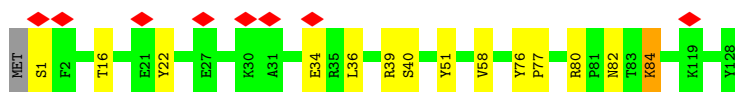
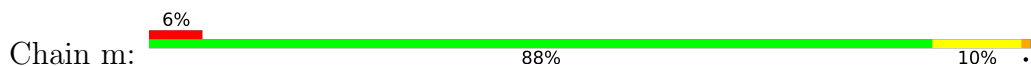
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



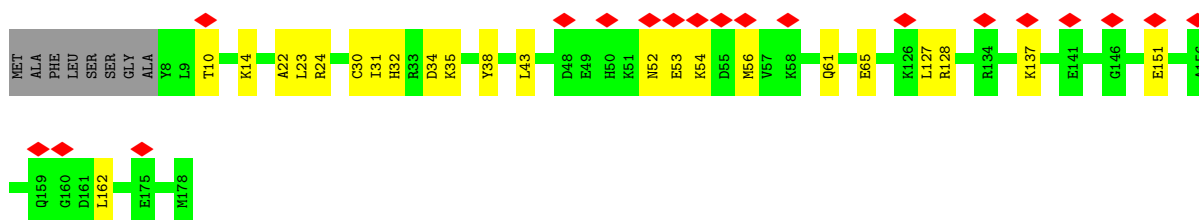
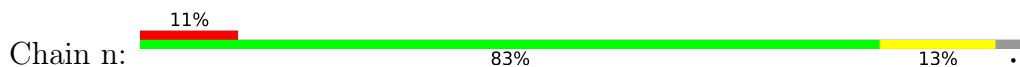
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



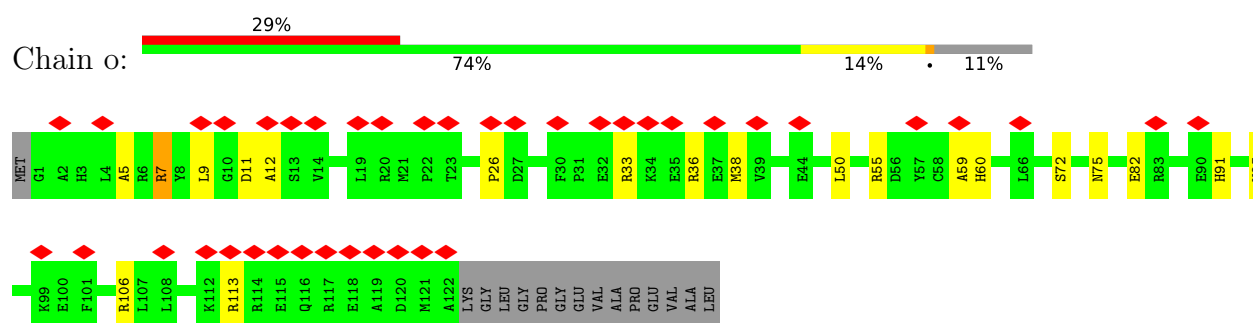
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



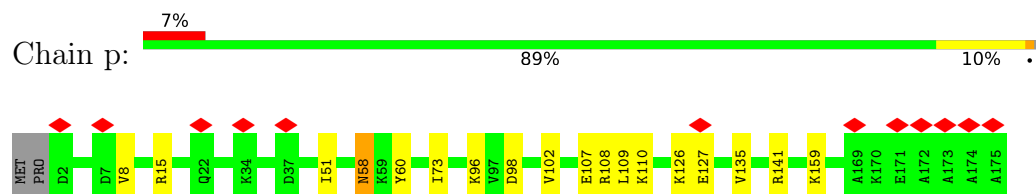
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



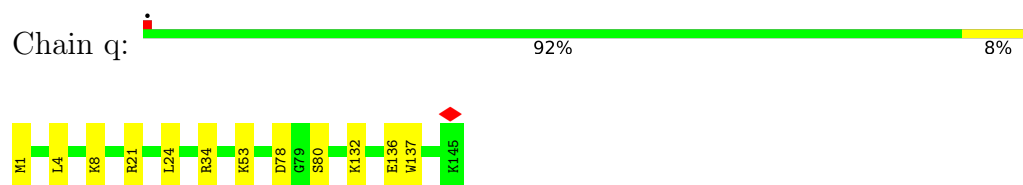
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



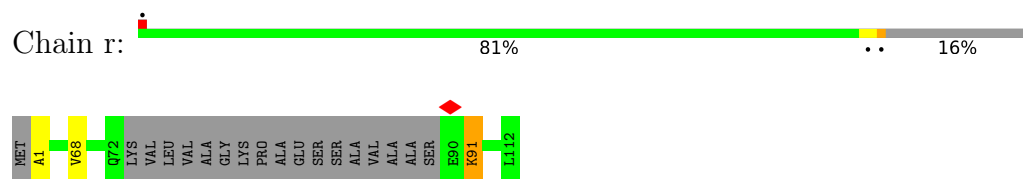
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



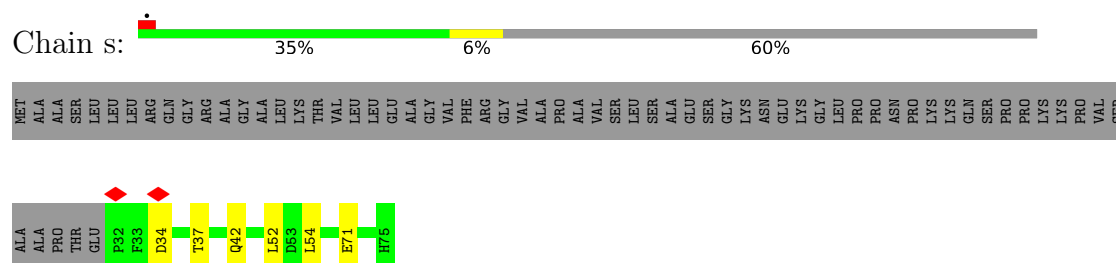
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45912	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 ($e^-/\text{\AA}^2$)	40, 40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.382	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, FES, K, U10, PLC, MYR, ZN, CHD, SF4, NDP, FME, PC1, FMN, CDL, 3PE, MG, EHZ, 2MR, SAC, DGT, AME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/936	0.23	0/1281
2	B	0.19	0/1278	0.27	0/1728
3	C	0.17	0/1772	0.27	0/2413
4	D	0.18	0/3450	0.25	0/4670
5	E	0.12	0/1699	0.29	0/2312
6	F	0.13	0/3401	0.25	0/4595
7	G	0.15	0/5387	0.26	0/7301
8	H	0.16	0/2571	0.28	0/3513
9	I	0.19	0/1445	0.28	0/1956
10	J	0.14	0/1370	0.24	0/1859
11	K	0.14	0/745	0.24	0/1008
12	L	0.11	0/4920	0.24	0/6694
13	M	0.14	0/3738	0.23	0/5097
14	N	0.15	0/2792	0.26	0/3800
15	O	0.11	0/2651	0.22	0/3587
16	P	0.14	0/2804	0.25	0/3803
17	Q	0.15	0/1072	0.24	0/1449
18	R	0.16	0/753	0.23	0/1014
19	S	0.09	0/702	0.23	0/945
20	T	0.11	0/719	0.22	0/971
20	U	0.10	0/719	0.21	0/971
21	V	0.12	0/943	0.22	0/1277
22	W	0.13	0/1006	0.24	0/1352
23	X	0.12	0/1439	0.22	0/1942
24	Y	0.11	0/1042	0.20	0/1414
25	Z	0.13	0/1186	0.22	0/1599
26	a	0.16	0/584	0.24	0/786
27	b	0.11	0/667	0.22	0/916
28	c	0.13	0/427	0.18	0/579
29	d	0.13	0/1018	0.22	0/1375
30	e	0.13	0/846	0.24	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.12	0/505	0.22	0/681
32	g	0.11	0/873	0.25	0/1186
33	h	0.12	0/1188	0.23	0/1607
34	i	0.09	0/1127	0.24	0/1534
35	j	0.11	0/624	0.20	0/855
36	k	0.07	0/672	0.19	0/906
37	l	0.10	0/1369	0.24	0/1873
38	m	0.10	0/1088	0.22	0/1472
39	n	0.09	0/1540	0.22	0/2085
40	o	0.12	0/1073	0.22	0/1437
41	p	0.09	0/1491	0.20	0/2011
42	q	0.14	0/1242	0.24	0/1688
43	r	0.15	0/789	0.28	0/1068
44	s	0.10	0/383	0.21	0/518
All	All	0.14	0/68046	0.24	0/92259

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	14	0
2	B	1247	0	1256	10	0
3	C	1721	0	1675	8	0
4	D	3377	0	3327	18	0
5	E	1659	0	1664	19	0
6	F	3326	0	3282	35	0
7	G	5298	0	5316	34	0
8	H	2509	0	2621	36	0
9	I	1414	0	1370	9	0
10	J	1345	0	1352	12	0
11	K	745	0	785	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	59	0
13	M	3654	0	3852	22	0
14	N	2733	0	2912	25	0
15	O	2589	0	2566	21	0
16	P	2728	0	2749	19	0
17	Q	1049	0	1045	3	0
18	R	740	0	714	6	0
19	S	691	0	706	3	0
20	T	707	0	700	7	0
20	U	707	0	700	10	0
21	V	923	0	964	3	0
22	W	982	0	999	6	0
23	X	1402	0	1383	10	0
24	Y	1030	0	1039	10	0
25	Z	1157	0	1156	12	0
26	a	569	0	568	6	0
27	b	654	0	663	1	0
28	c	414	0	415	3	0
29	d	999	0	988	8	0
30	e	825	0	826	5	0
31	f	492	0	501	5	0
32	g	846	0	798	8	0
33	h	1154	0	1168	11	0
34	i	1097	0	1108	10	0
35	j	597	0	536	6	0
36	k	653	0	639	7	0
37	l	1314	0	1210	14	0
38	m	1070	0	1068	9	0
39	n	1487	0	1433	17	0
40	o	1048	0	1016	12	0
41	p	1458	0	1430	15	0
42	q	1212	0	1183	7	0
43	r	776	0	782	1	0
44	s	371	0	344	6	0
45	A	82	0	115	0	0
45	I	37	0	51	2	0
45	J	81	0	113	2	0
45	L	120	0	168	0	0
45	M	95	0	141	1	0
45	N	49	0	75	0	0
45	P	38	0	50	0	0
45	Y	302	0	449	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	42	0	58	0	0
45	a	36	0	49	0	0
45	b	83	0	117	0	0
45	d	49	0	75	0	0
45	f	24	0	22	0	0
45	g	29	0	32	0	0
45	m	41	0	59	0	0
45	q	51	0	82	1	0
45	r	30	0	34	0	0
46	A	68	0	84	1	0
46	B	94	0	136	1	0
46	H	136	0	203	3	0
46	I	54	0	88	2	0
46	J	35	0	44	0	0
46	M	79	0	109	2	0
46	Z	44	0	62	0	0
46	d	39	0	52	2	0
46	h	38	0	53	0	0
46	l	47	0	71	0	0
46	m	41	0	56	0	0
46	q	49	0	75	2	0
47	B	8	0	0	0	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	0	0
50	G	1	0	0	0	0
51	H	34	0	41	14	0
52	H	58	0	63	1	0
52	L	100	0	156	0	0
52	M	100	0	156	1	0
52	N	94	0	141	1	0
52	d	152	0	204	2	0
52	i	76	0	96	0	0
52	r	61	0	66	0	0
53	J	35	0	47	0	0
53	L	36	0	49	0	0
53	M	34	0	45	0	0
53	O	62	0	77	0	0
53	Y	42	0	64	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	Z	36	0	49	0	0
53	b	38	0	53	0	0
53	g	42	0	64	0	0
54	M	1	0	0	0	0
54	R	1	0	0	0	0
55	O	1	0	0	0	0
56	O	31	0	12	0	0
57	P	48	0	26	2	0
58	T	37	0	0	1	0
58	U	37	0	0	1	0
59	i	29	0	38	6	0
60	o	15	0	27	0	0
All	All	69693	0	70937	493	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 4.

The worst 5 of 493 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)
51:H:401:U10:H101	51:H:401:U10:H13	1.54	0.89
13:M:457:PRO:O	32:g:84:ARG:NH2	2.05	0.89
5:E:194:GLU:OE1	6:F:28:ARG:NH1	2.08	0.86
40:o:59:ALA:O	40:o:60:HIS:ND1	2.09	0.85
8:H:224:PHE:CE1	51:H:401:U10:H72	2.14	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	154/216 (71%)	148 (96%)	6 (4%)	0	100	100
3	C	205/266 (77%)	200 (98%)	5 (2%)	0	100	100
4	D	412/463 (89%)	399 (97%)	13 (3%)	0	100	100
5	E	212/249 (85%)	202 (95%)	10 (5%)	0	100	100
6	F	430/464 (93%)	412 (96%)	18 (4%)	0	100	100
7	G	689/727 (95%)	668 (97%)	21 (3%)	0	100	100
8	H	316/318 (99%)	300 (95%)	16 (5%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
11	K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	12	38
12	L	604/606 (100%)	577 (96%)	26 (4%)	1 (0%)	43	72
13	M	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
14	N	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
15	O	318/343 (93%)	315 (99%)	3 (1%)	0	100	100
16	P	335/380 (88%)	327 (98%)	8 (2%)	0	100	100
17	Q	127/175 (73%)	127 (100%)	0	0	100	100
18	R	94/124 (76%)	89 (95%)	5 (5%)	0	100	100
19	S	84/99 (85%)	84 (100%)	0	0	100	100
20	T	86/156 (55%)	79 (92%)	7 (8%)	0	100	100
20	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
21	V	112/116 (97%)	108 (96%)	4 (4%)	0	100	100
22	W	114/128 (89%)	111 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
25	Z	140/144 (97%)	137 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	e	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
31	f	55/57 (96%)	54 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	i	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
35	j	69/108 (64%)	66 (96%)	3 (4%)	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	m	126/129 (98%)	123 (98%)	3 (2%)	0	100	100
39	n	169/179 (94%)	161 (95%)	8 (5%)	0	100	100
40	o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
41	p	172/176 (98%)	167 (97%)	5 (3%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	91/113 (80%)	89 (98%)	2 (2%)	0	100	100
44	s	42/109 (38%)	42 (100%)	0	0	100	100
All	All	8173/9213 (89%)	7927 (97%)	244 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
11	K	2	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	97 (97%)	3 (3%)	36	72
2	B	132/175 (75%)	128 (97%)	4 (3%)	36	72
3	C	188/228 (82%)	187 (100%)	1 (0%)	81	93
4	D	361/392 (92%)	353 (98%)	8 (2%)	45	78
5	E	183/205 (89%)	177 (97%)	6 (3%)	33	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	346/368 (94%)	341 (99%)	5 (1%)	59	85
7	G	579/608 (95%)	568 (98%)	11 (2%)	50	81
8	H	274/274 (100%)	269 (98%)	5 (2%)	51	82
9	I	151/175 (86%)	149 (99%)	2 (1%)	61	86
10	J	141/141 (100%)	140 (99%)	1 (1%)	76	91
11	K	85/85 (100%)	83 (98%)	2 (2%)	43	77
12	L	533/533 (100%)	523 (98%)	10 (2%)	50	81
13	M	412/412 (100%)	406 (98%)	6 (2%)	57	84
14	N	315/315 (100%)	311 (99%)	4 (1%)	61	86
15	O	283/303 (93%)	277 (98%)	6 (2%)	47	79
16	P	293/327 (90%)	285 (97%)	8 (3%)	39	74
17	Q	116/153 (76%)	115 (99%)	1 (1%)	70	89
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	86
19	S	76/82 (93%)	74 (97%)	2 (3%)	40	75
20	T	81/135 (60%)	76 (94%)	5 (6%)	16	45
20	U	81/135 (60%)	80 (99%)	1 (1%)	63	87
21	V	101/102 (99%)	99 (98%)	2 (2%)	48	80
22	W	108/114 (95%)	107 (99%)	1 (1%)	70	89
23	X	154/155 (99%)	153 (99%)	1 (1%)	78	92
24	Y	101/102 (99%)	97 (96%)	4 (4%)	28	63
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	90
26	a	59/59 (100%)	57 (97%)	2 (3%)	32	68
27	b	71/72 (99%)	69 (97%)	2 (3%)	38	73
28	c	45/68 (66%)	43 (96%)	2 (4%)	25	59
29	d	105/105 (100%)	102 (97%)	3 (3%)	37	73
30	e	89/96 (93%)	86 (97%)	3 (3%)	32	68
31	f	54/54 (100%)	53 (98%)	1 (2%)	50	81
32	g	92/131 (70%)	89 (97%)	3 (3%)	33	69
33	h	121/158 (77%)	119 (98%)	2 (2%)	53	83
34	i	120/121 (99%)	117 (98%)	3 (2%)	42	76
35	j	61/84 (73%)	58 (95%)	3 (5%)	22	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	63/76 (83%)	61 (97%)	2 (3%)	34	70
37	l	140/159 (88%)	135 (96%)	5 (4%)	31	66
38	m	113/114 (99%)	111 (98%)	2 (2%)	51	82
39	n	156/161 (97%)	154 (99%)	2 (1%)	61	86
40	o	110/120 (92%)	108 (98%)	2 (2%)	51	82
41	p	155/157 (99%)	152 (98%)	3 (2%)	50	81
42	q	130/130 (100%)	127 (98%)	3 (2%)	44	78
43	r	85/97 (88%)	83 (98%)	2 (2%)	43	77
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7205/7891 (91%)	7059 (98%)	146 (2%)	48	80

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	g	57	ASN
42	q	136	GLU
34	i	38	ARG
37	l	148	LYS
12	L	31	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
21	V	82	GLN
36	k	20	GLN
22	W	50	GLN
30	e	76	HIS
37	l	28	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2MR	D	85	4	10,12,13	2.44	2 (20%)	5,13,15	1.33	1 (20%)
11	FME	K	1	11	8,9,10	1.51	1 (12%)	8,9,11	1.41	2 (25%)
29	AME	d	1	29	9,10,11	1.52	1 (11%)	9,11,13	1.24	1 (11%)
27	AYA	b	1	27	6,7,8	1.88	1 (16%)	6,8,10	1.32	1 (16%)
34	SAC	i	1	34	7,8,9	1.73	1 (14%)	7,9,11	1.51	1 (14%)
12	FME	L	1	12	8,9,10	1.51	1 (12%)	8,9,11	1.39	1 (12%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	8,9,11	1.44	1 (12%)
42	AME	q	1	42	9,10,11	1.50	1 (11%)	9,11,13	1.33	1 (11%)
8	FME	H	1	8	8,9,10	1.49	1 (12%)	8,9,11	1.48	2 (25%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	8,9,11	1.38	1 (12%)
38	SAC	m	1	38	7,8,9	1.74	1 (14%)	7,9,11	1.29	1 (14%)
14	FME	N	1	14	8,9,10	1.50	1 (12%)	8,9,11	1.38	1 (12%)
43	AYA	r	1	43	6,7,8	1.87	2 (33%)	6,8,10	1.23	1 (16%)
24	AYA	Y	1	24	6,7,8	1.87	2 (33%)	6,8,10	1.42	1 (16%)
13	FME	M	1	13	8,9,10	1.51	1 (12%)	8,9,11	1.40	1 (12%)

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
4	2MR	D	85	4	-	0/10/13/15	-
11	FME	K	1	11	-	4/7/9/11	-
29	AME	d	1	29	-	5/9/10/12	-
27	AYA	b	1	27	-	0/5/6/8	-
34	SAC	i	1	34	-	2/7/8/10	-
12	FME	L	1	12	-	2/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-
42	AME	q	1	42	-	4/9/10/12	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	H	1	8	-	0/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
38	SAC	m	1	38	-	1/7/8/10	-
14	FME	N	1	14	-	3/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
24	AYA	Y	1	24	-	0/5/6/8	-
13	FME	M	1	13	-	2/7/9/11	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.42	1.44	1.33
4	D	85	2MR	CZ-NE	5.10	1.45	1.34
10	J	1	FME	CN-N	3.74	1.45	1.33
12	L	1	FME	CN-N	3.73	1.45	1.33
13	M	1	FME	CN-N	3.72	1.45	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	2.87	120.88	116.12
24	Y	1	AYA	CM-CT-N	2.50	120.27	116.12
42	q	1	AME	CT2-CT1-N	2.40	120.10	116.12
38	m	1	SAC	C2A-C1A-N	2.36	120.04	116.12
27	b	1	AYA	CM-CT-N	2.33	119.98	116.12

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
29	d	1	AME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	1	AME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 4 are monoatomic - leaving 79 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	$\# Z > 2$
45	3PE	L	704	-	40,40,50	0.97	4 (10%)	43,45,55	1.14	2 (4%)
53	PLC	O	403	-	30,30,41	0.55	0	34,37,49	0.59	0
60	MYR	o	201	40	13,14,15	0.43	0	12,13,15	0.84	0
45	3PE	Y	206	-	44,44,50	0.93	4 (9%)	47,49,55	1.09	2 (4%)
52	CDL	r	201	-	60,60,99	1.12	8 (13%)	66,72,111	1.13	4 (6%)
58	EHZ	U	101	20	31,36,37	1.56	5 (16%)	36,44,47	1.60	6 (16%)
53	PLC	Z	203	-	35,35,41	0.54	0	41,43,49	0.64	1 (2%)
46	PC1	B	203	-	47,47,53	1.01	4 (8%)	53,55,61	1.08	2 (3%)
57	NDP	P	501	-	51,52,52	4.01	28 (54%)	71,80,80	1.89	14 (19%)
52	CDL	L	701	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)
45	3PE	b	102	-	46,46,50	0.91	4 (8%)	49,51,55	1.05	2 (4%)
46	PC1	I	204	-	53,53,53	0.94	4 (7%)	59,61,61	1.03	2 (3%)
47	SF4	F	501	6	0,12,12	-	-	-	-	-
52	CDL	M	602	-	99,99,99	0.88	8 (8%)	105,111,111	1.11	4 (3%)
52	CDL	i	202	-	75,75,99	1.01	8 (10%)	81,87,111	1.13	4 (4%)
47	SF4	I	201	9	0,12,12	-	-	-	-	-
45	3PE	q	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.05	2 (3%)
45	3PE	d	203	-	48,48,50	0.89	4 (8%)	51,53,55	1.03	2 (3%)
46	PC1	H	404	-	40,40,53	1.09	4 (10%)	46,48,61	1.01	2 (4%)
53	PLC	L	705	-	35,35,41	0.54	0	41,43,49	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	B	202	-	45,45,53	1.03	4 (8%)	51,53,61	1.03	2 (3%)
46	PC1	h	201	-	37,37,53	1.07	3 (8%)	43,45,61	0.96	1 (2%)
59	CHD	i	201	-	32,32,32	3.26	11 (34%)	51,51,51	2.39	17 (33%)
45	3PE	Y	204	-	50,50,50	0.87	4 (8%)	53,55,55	1.07	2 (3%)
52	CDL	N	401	-	93,93,99	0.90	8 (8%)	99,105,111	1.09	4 (4%)
53	PLC	J	204	-	34,34,41	0.55	0	40,42,49	0.56	0
47	SF4	I	202	9	0,12,12	-	-	-		
47	SF4	G	802	7	0,12,12	-	-	-		
45	3PE	b	101	-	35,35,50	1.03	4 (11%)	38,40,55	1.13	2 (5%)
52	CDL	d	202	-	86,86,99	0.94	8 (9%)	92,98,111	1.12	4 (4%)
52	CDL	H	402	-	57,57,99	1.11	7 (12%)	63,69,111	1.17	3 (4%)
47	SF4	B	201	2	0,12,12	-	-	-		
46	PC1	Z	202	-	43,43,53	1.05	4 (9%)	49,51,61	1.01	2 (4%)
45	3PE	I	203	-	36,36,50	1.02	4 (11%)	39,41,55	1.09	2 (5%)
49	FMN	F	502	-	33,33,33	2.73	10 (30%)	48,50,50	1.76	13 (27%)
45	3PE	Y	207	-	35,35,50	1.03	4 (11%)	38,40,55	1.15	2 (5%)
45	3PE	P	502	-	37,37,50	1.00	4 (10%)	40,42,55	1.12	2 (5%)
53	PLC	Y	208	-	41,41,41	0.51	0	47,49,49	0.51	0
45	3PE	J	202	-	43,43,50	0.93	3 (6%)	46,48,55	1.12	2 (4%)
51	U10	H	401	-	34,34,63	1.99	17 (50%)	42,44,79	1.70	10 (23%)
46	PC1	A	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.06	2 (5%)
48	FES	E	301	5	0,4,4	-	-	-		
52	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.12	4 (5%)
46	PC1	A	204	-	32,32,53	1.22	4 (12%)	38,40,61	1.05	2 (5%)
46	PC1	d	204	-	38,38,53	1.12	3 (7%)	44,46,61	1.05	2 (4%)
48	FES	G	803	7	0,4,4	-	-	-		
53	PLC	O	404	-	30,30,41	0.59	0	36,38,49	0.58	0
45	3PE	Y	203	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
45	3PE	A	202	-	41,41,50	0.95	4 (9%)	44,46,55	1.10	2 (4%)
45	3PE	f	101	-	23,23,50	1.25	4 (17%)	26,28,55	1.39	2 (7%)
53	PLC	g	202	-	41,41,41	0.51	0	47,49,49	0.49	0
46	PC1	M	606	-	34,34,53	1.17	4 (11%)	40,42,61	1.09	2 (5%)
45	3PE	Y	205	-	50,50,50	0.87	4 (8%)	53,55,55	1.04	2 (3%)
45	3PE	m	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.15	2 (4%)
45	3PE	g	201	-	28,28,50	1.15	4 (14%)	31,33,55	1.35	3 (9%)
46	PC1	l	701	-	46,46,53	1.02	4 (8%)	52,54,61	0.97	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	H	405	-	46,46,53	1.02	4 (8%)	52,54,61	1.05	2 (3%)
45	3PE	Y	202	-	26,26,50	1.19	4 (15%)	29,31,55	1.16	2 (6%)
46	PC1	J	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.08	2 (5%)
46	PC1	q	202	-	48,48,53	1.01	4 (8%)	54,56,61	1.02	2 (3%)
53	PLC	b	103	-	37,37,41	0.55	0	43,45,49	0.52	0
45	3PE	L	702	-	44,44,50	0.92	4 (9%)	47,49,55	1.05	2 (4%)
46	PC1	m	202	-	40,40,53	1.08	4 (10%)	46,48,61	1.01	2 (4%)
56	DGT	O	402	55	32,33,33	3.32	14 (43%)	48,52,52	1.95	13 (27%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	L	703	-	33,33,50	1.06	4 (12%)	36,38,55	1.16	2 (5%)
45	3PE	J	201	-	36,36,50	1.02	4 (11%)	39,41,55	1.19	2 (5%)
46	PC1	H	403	-	47,47,53	1.02	4 (8%)	53,55,61	1.06	2 (3%)
45	3PE	a	101	-	35,35,50	1.02	4 (11%)	38,40,55	1.01	2 (5%)
45	3PE	Y	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.12	2 (4%)
45	3PE	Z	201	-	41,41,50	0.95	4 (9%)	44,46,55	1.05	2 (4%)
45	3PE	M	603	-	49,49,50	0.88	4 (8%)	52,54,55	1.09	2 (3%)
53	PLC	M	607	-	33,33,41	0.57	0	39,41,49	0.52	0
45	3PE	A	201	-	39,39,50	0.98	4 (10%)	42,44,55	1.04	2 (4%)
45	3PE	r	202	-	29,29,50	1.13	4 (13%)	32,34,55	1.21	2 (6%)
45	3PE	M	604	-	44,44,50	0.93	4 (9%)	47,49,55	1.10	2 (4%)
45	3PE	N	402	-	48,48,50	0.88	4 (8%)	51,53,55	1.07	2 (3%)
46	PC1	M	605	-	43,43,53	1.05	4 (9%)	49,51,61	1.00	2 (4%)
58	EHZ	T	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.72	8 (22%)

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
45	3PE	L	704	-	-	20/44/44/54	-
53	PLC	O	403	-	-	10/33/33/45	-
60	MYR	o	201	40	-	2/12/12/13	-
45	3PE	Y	206	-	-	18/48/48/54	-
52	CDL	r	201	-	-	28/71/71/110	-
58	EHZ	U	101	20	-	10/42/44/45	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	PLC	Z	203	-	-	14/39/39/45	-
46	PC1	B	203	-	-	19/51/51/57	-
57	NDP	P	501	-	-	9/34/77/77	0/5/5/5
52	CDL	L	701	-	-	40/110/110/110	-
45	3PE	b	102	-	-	21/50/50/54	-
46	PC1	I	204	-	-	16/57/57/57	-
47	SF4	F	501	6	-	-	0/6/5/5
52	CDL	M	602	-	-	49/110/110/110	-
52	CDL	i	202	-	-	38/86/86/110	-
47	SF4	I	201	9	-	-	0/6/5/5
45	3PE	q	201	-	-	24/54/54/54	-
45	3PE	d	203	-	-	25/52/52/54	-
46	PC1	H	404	-	-	14/44/44/57	-
53	PLC	L	705	-	-	13/39/39/45	-
46	PC1	B	202	-	-	20/49/49/57	-
46	PC1	h	201	-	-	10/40/40/57	-
59	CHD	i	201	-	-	3/9/74/74	0/4/4/4
45	3PE	Y	204	-	-	25/54/54/54	-
52	CDL	N	401	-	-	40/104/104/110	-
53	PLC	J	204	-	-	12/38/38/45	-
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5
45	3PE	b	101	-	-	20/39/39/54	-
52	CDL	d	202	-	-	48/97/97/110	-
52	CDL	H	402	-	-	32/67/67/110	-
47	SF4	B	201	2	-	-	0/6/5/5
46	PC1	Z	202	-	-	18/47/47/57	-
45	3PE	I	203	-	-	13/40/40/54	-
49	FMN	F	502	-	-	3/18/18/18	0/3/3/3
45	3PE	Y	207	-	-	15/39/39/54	-
45	3PE	P	502	-	-	17/41/41/54	-
53	PLC	Y	208	-	-	16/45/45/45	-
45	3PE	J	202	-	-	13/47/47/54	-
51	U10	H	401	-	-	10/29/53/87	0/1/1/1
46	PC1	A	203	-	-	17/38/38/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	FES	E	301	5	-	-	0/1/1/1
52	CDL	d	201	-	-	33/75/75/110	-
46	PC1	A	204	-	-	18/36/36/57	-
46	PC1	d	204	-	-	16/42/42/57	-
48	FES	G	803	7	-	-	0/1/1/1
53	PLC	O	404	-	-	9/34/34/45	-
45	3PE	Y	203	-	-	20/54/54/54	-
45	3PE	A	202	-	-	23/45/45/54	-
45	3PE	f	101	-	-	14/26/26/54	-
53	PLC	g	202	-	-	13/45/45/45	-
46	PC1	M	606	-	-	14/38/38/57	-
45	3PE	Y	205	-	-	22/54/54/54	-
45	3PE	m	201	-	-	15/44/44/54	-
45	3PE	g	201	-	-	16/31/31/54	-
46	PC1	l	701	-	-	17/50/50/57	-
46	PC1	H	405	-	-	24/50/50/57	-
45	3PE	Y	202	-	-	15/30/30/54	-
46	PC1	J	203	-	-	13/38/38/57	-
46	PC1	q	202	-	-	15/52/52/57	-
53	PLC	b	103	-	-	18/41/41/45	-
45	3PE	L	702	-	-	22/48/48/54	-
46	PC1	m	202	-	-	14/44/44/57	-
56	DGT	O	402	55	-	5/22/34/34	0/3/3/3
47	SF4	G	801	7	-	-	0/6/5/5
45	3PE	L	703	-	-	17/37/37/54	-
45	3PE	J	201	-	-	11/40/40/54	-
46	PC1	H	403	-	-	25/51/51/57	-
45	3PE	a	101	-	-	15/39/39/54	-
45	3PE	Y	201	-	-	17/44/44/54	-
45	3PE	Z	201	-	-	13/45/45/54	-
45	3PE	M	603	-	-	20/53/53/54	-
53	PLC	M	607	-	-	14/37/37/45	-
45	3PE	A	201	-	-	21/43/43/54	-
45	3PE	r	202	-	-	13/33/33/54	-
45	3PE	M	604	-	-	23/48/48/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	N	402	-	-	32/52/52/54	-
46	PC1	M	605	-	-	17/47/47/57	-
58	EHZ	T	101	20	-	8/42/44/45	-

The worst 5 of 334 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	PA-O3	10.42	1.70	1.59
57	P	501	NDP	C2B-C1B	-9.01	1.30	1.53
59	i	201	CHD	C11-C12	8.89	1.67	1.53
56	O	402	DGT	O6-C6	8.78	1.40	1.23
57	P	501	NDP	O4B-C1B	8.67	1.62	1.42

The worst 5 of 205 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	O	402	DGT	C8-N9-C4	7.41	119.91	106.03
59	i	201	CHD	C17-C13-C14	6.54	106.68	100.11
59	i	201	CHD	C13-C17-C20	-6.20	111.98	119.48
58	T	101	EHZ	C8-C9-S1	6.00	121.13	113.56
57	P	501	NDP	N6A-C6A-N1A	-5.63	105.84	118.38

There are no chirality outliers.

5 of 1304 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O13
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O12

There are no ring outliers.

23 monomers are involved in 48 short contacts:

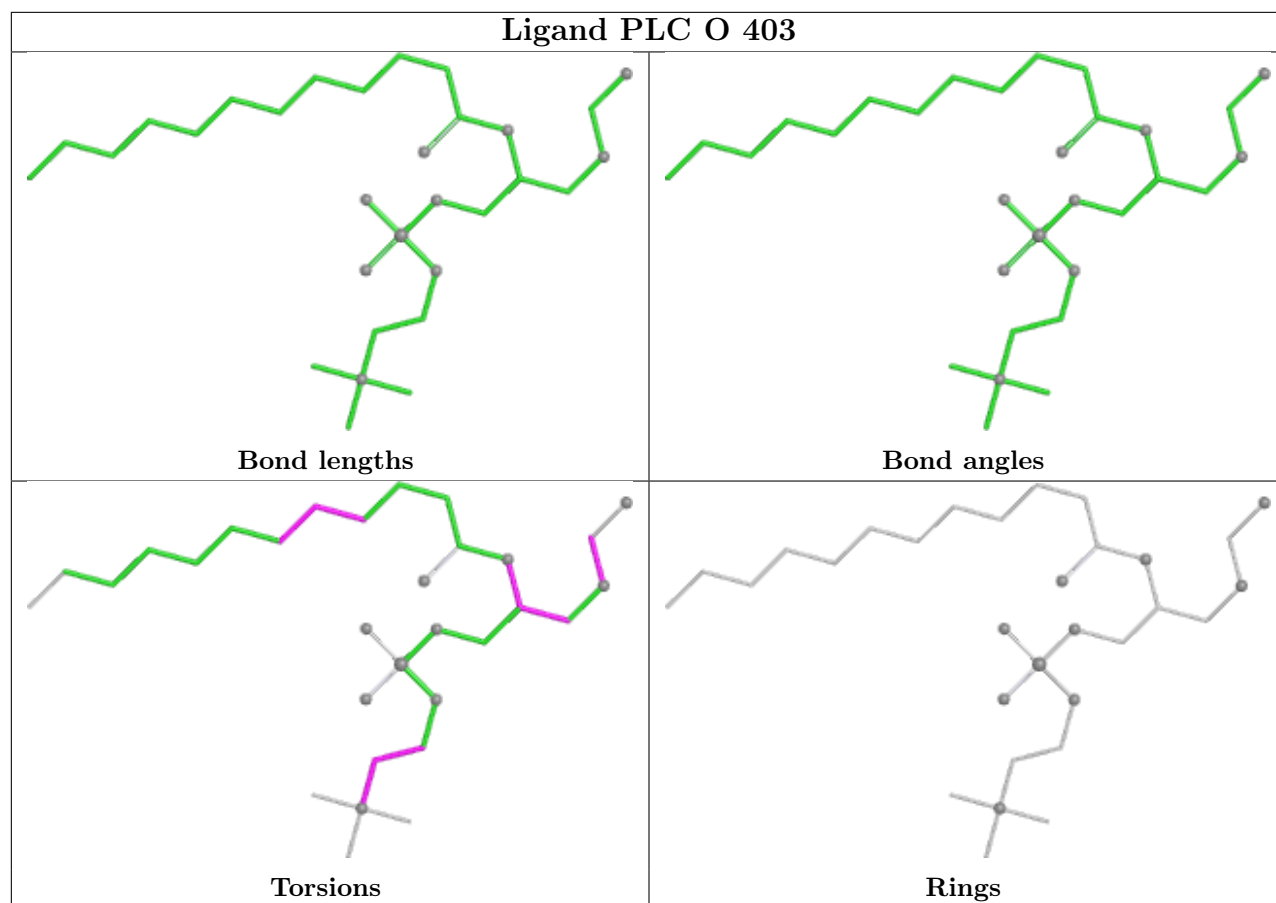
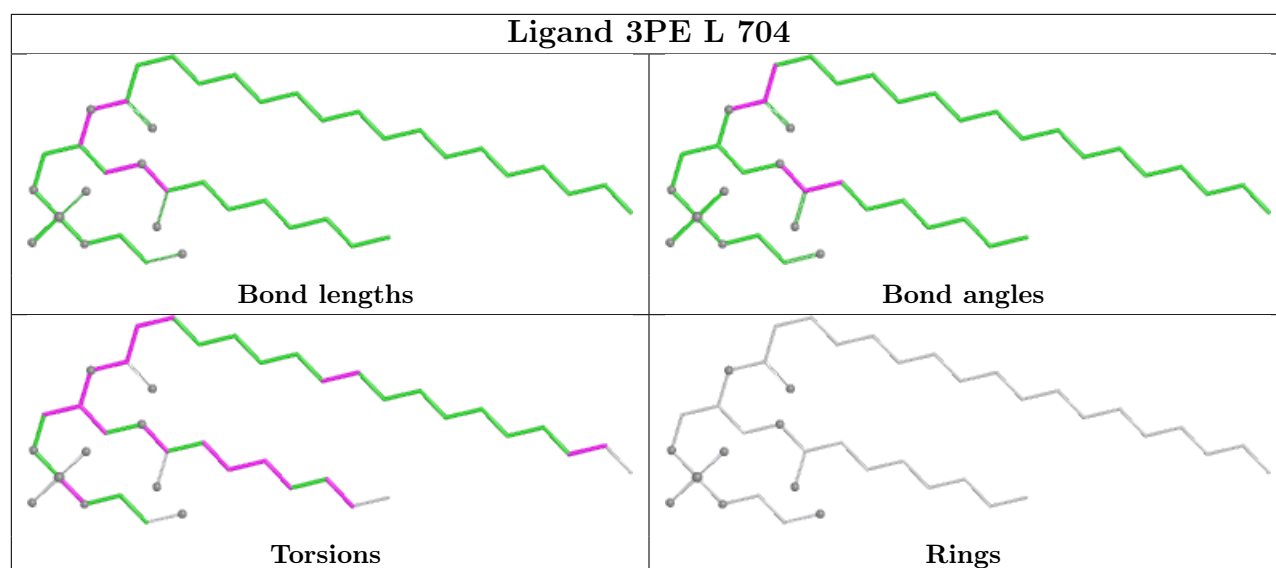
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	U	101	EHZ	1	0
57	P	501	NDP	2	0
46	I	204	PC1	2	0
52	M	602	CDL	1	0

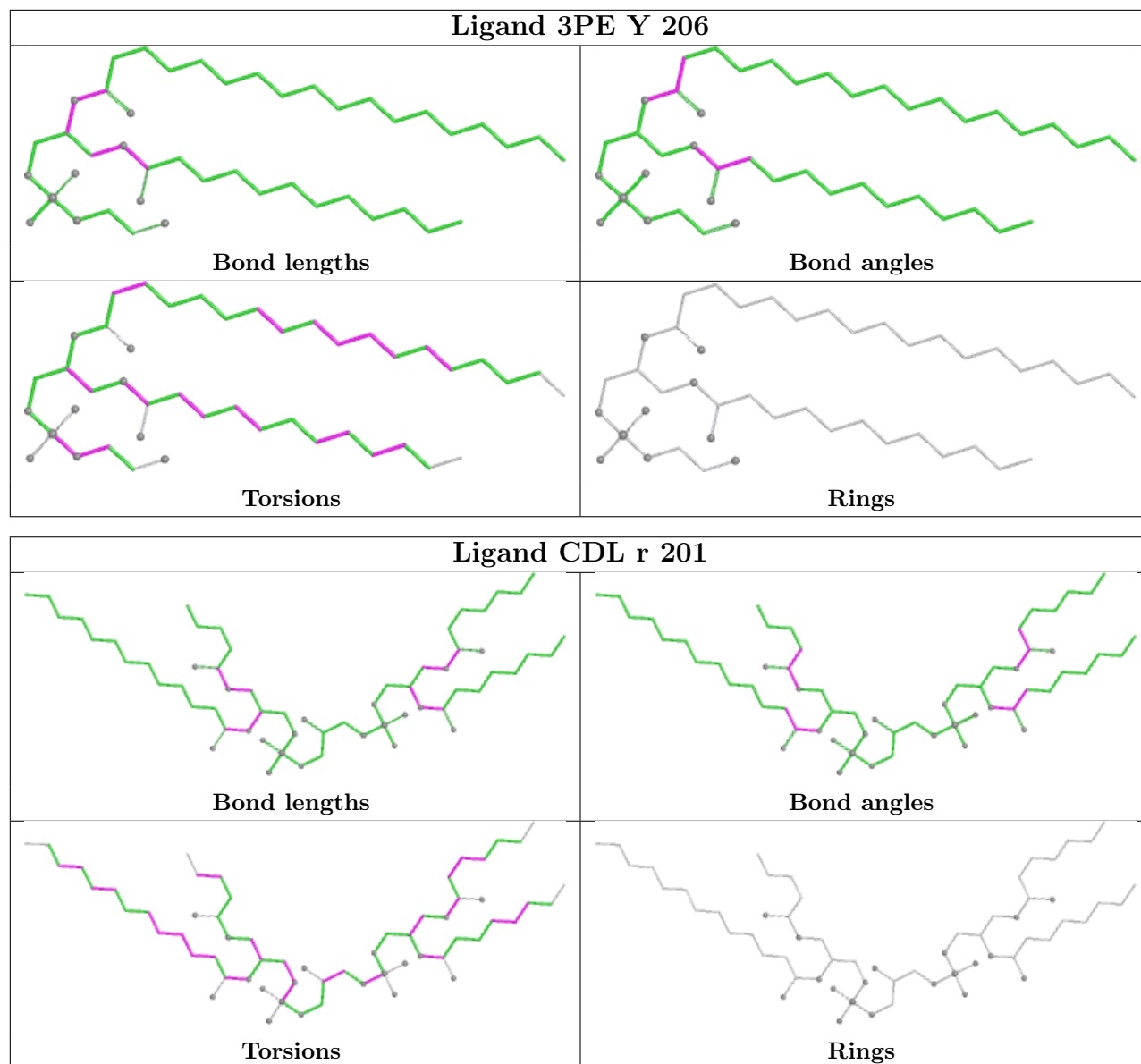
Continued on next page...

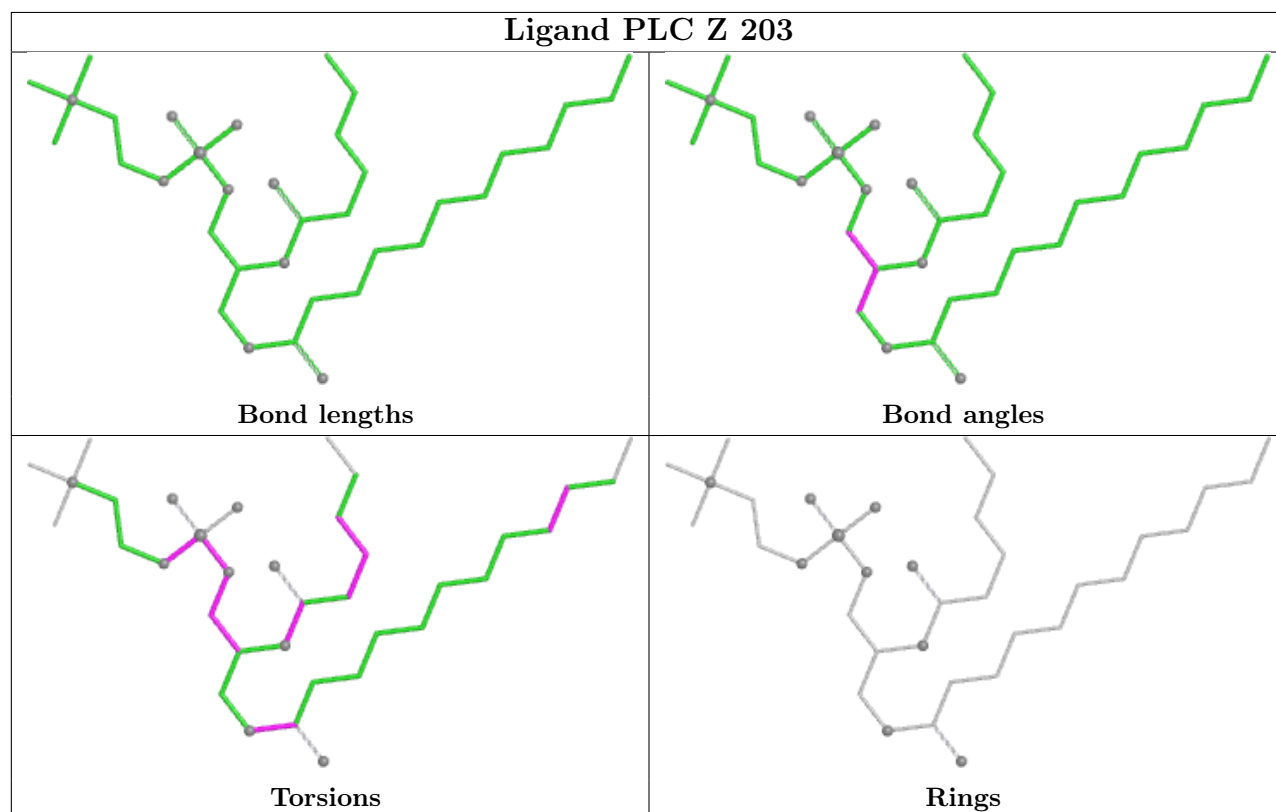
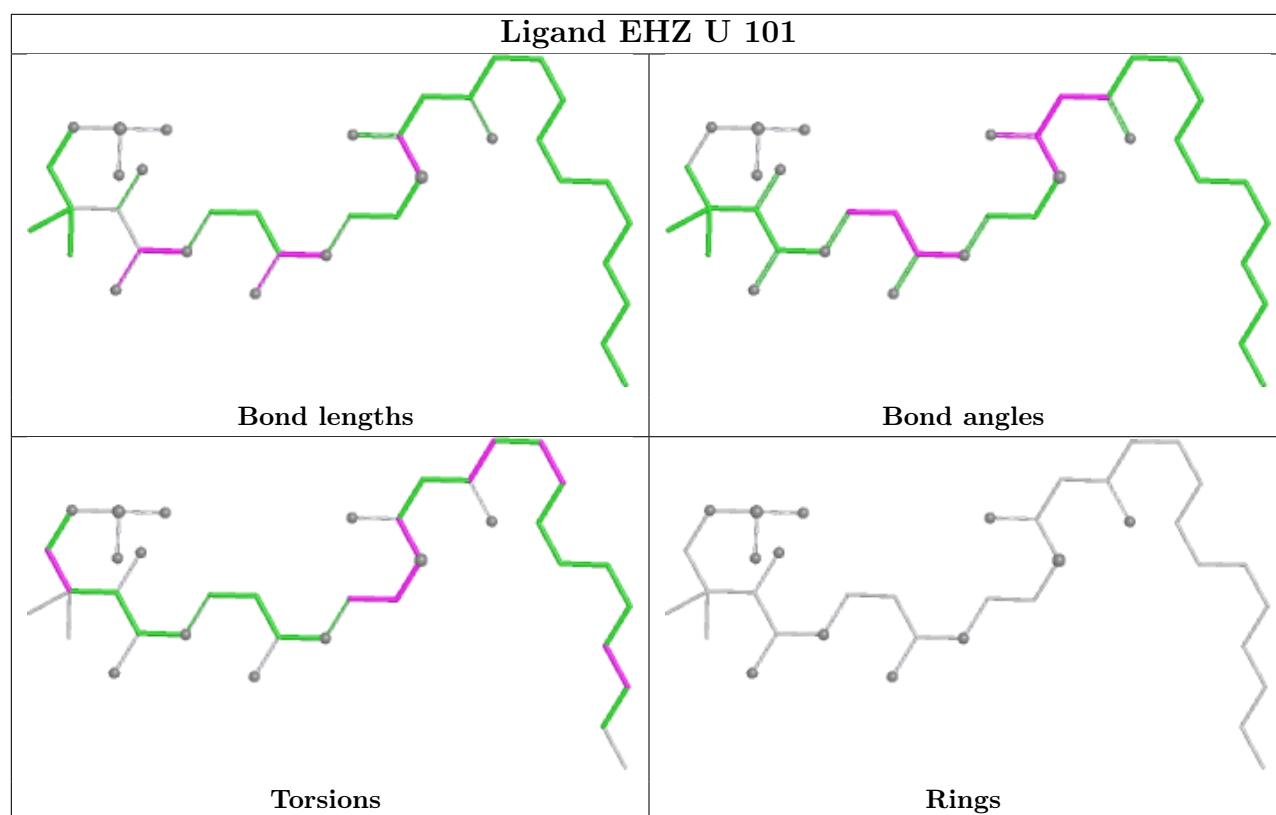
Continued from previous page...

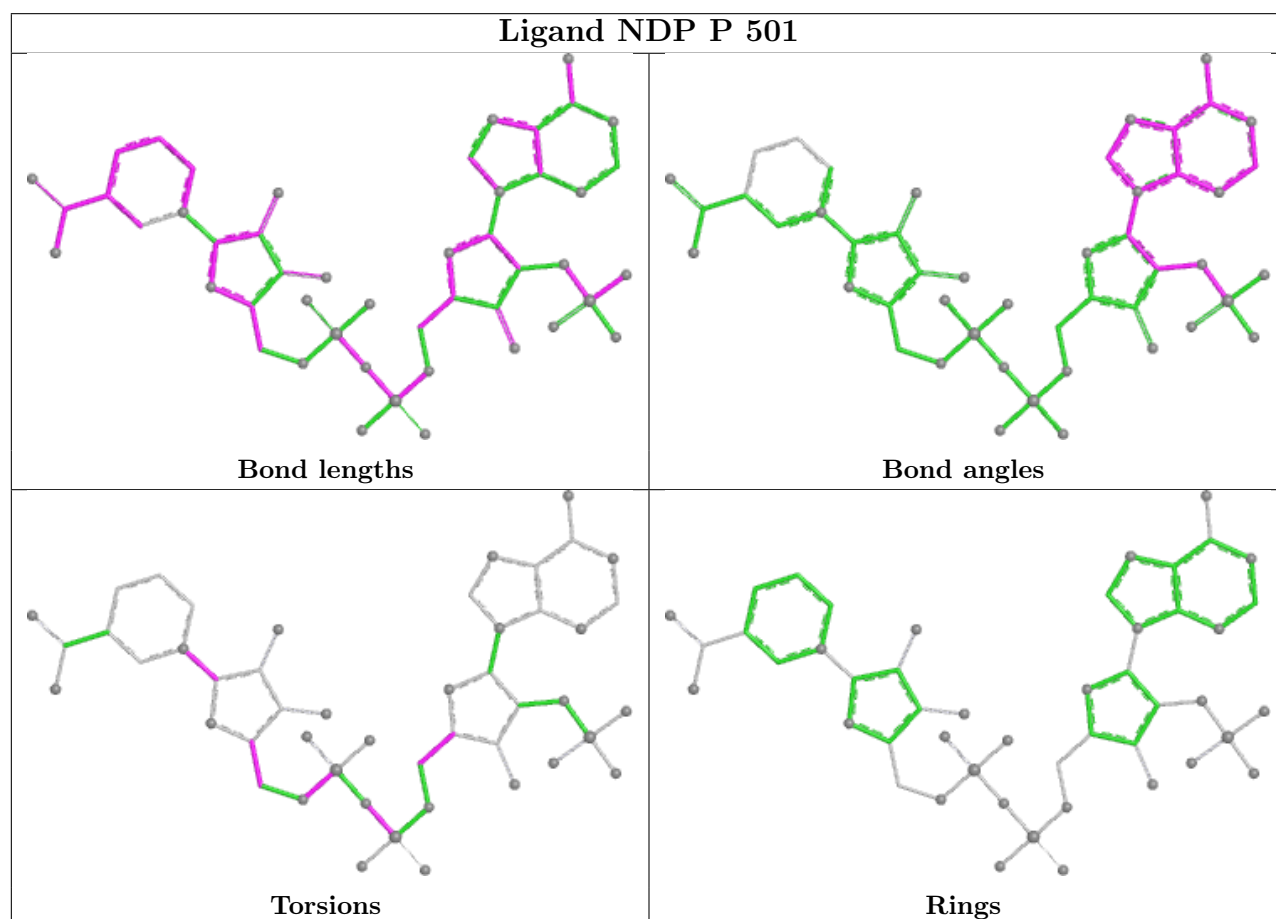
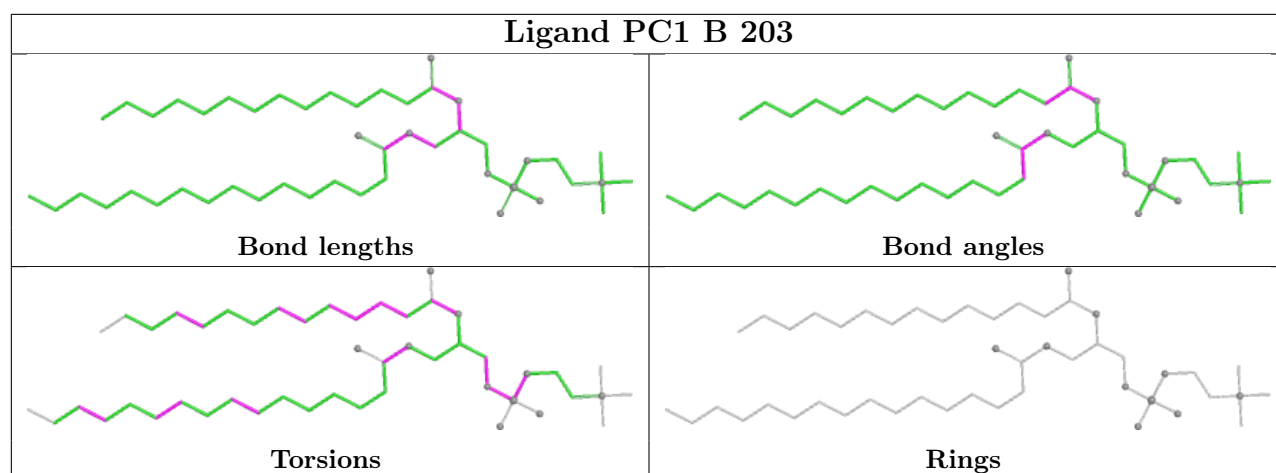
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	q	201	3PE	1	0
46	H	404	PC1	1	0
46	B	202	PC1	1	0
59	i	201	CHD	6	0
45	Y	204	3PE	1	0
52	N	401	CDL	1	0
52	H	402	CDL	1	0
45	I	203	3PE	2	0
45	J	202	3PE	1	0
51	H	401	U10	14	0
46	A	203	PC1	1	0
52	d	201	CDL	2	0
46	d	204	PC1	2	0
46	M	606	PC1	2	0
46	q	202	PC1	2	0
45	J	201	3PE	1	0
46	H	403	PC1	2	0
45	M	604	3PE	1	0
58	T	101	EHZ	1	0

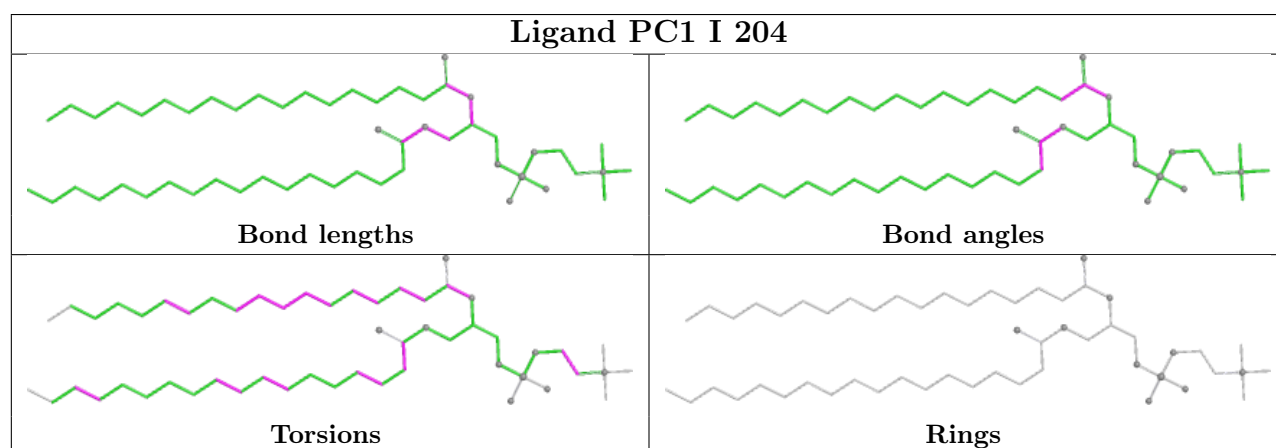
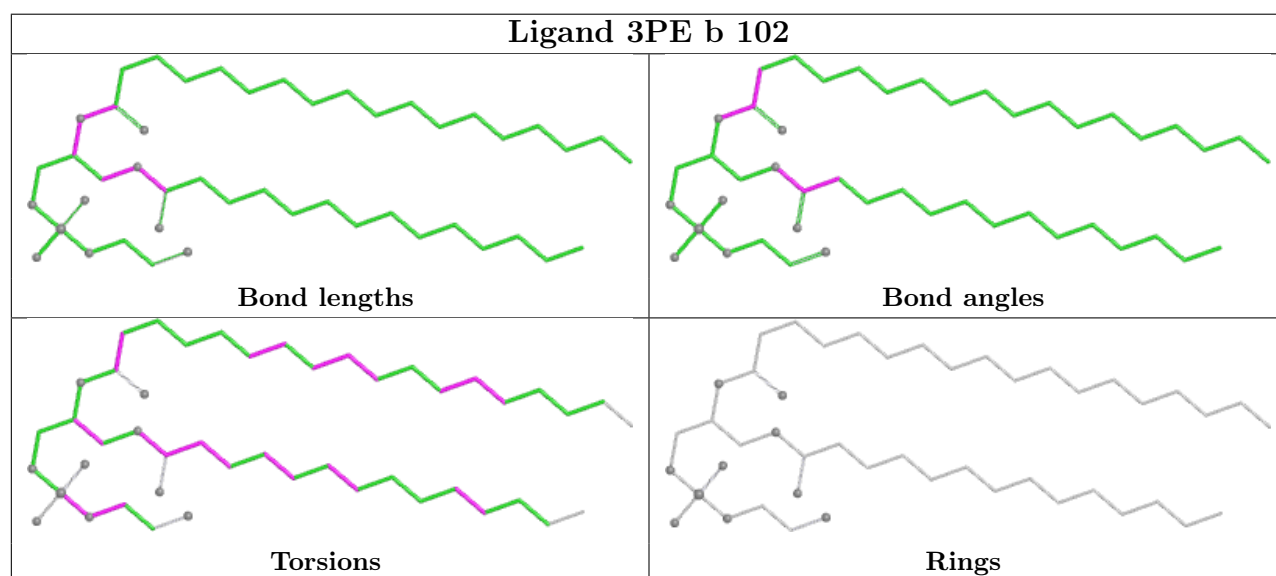
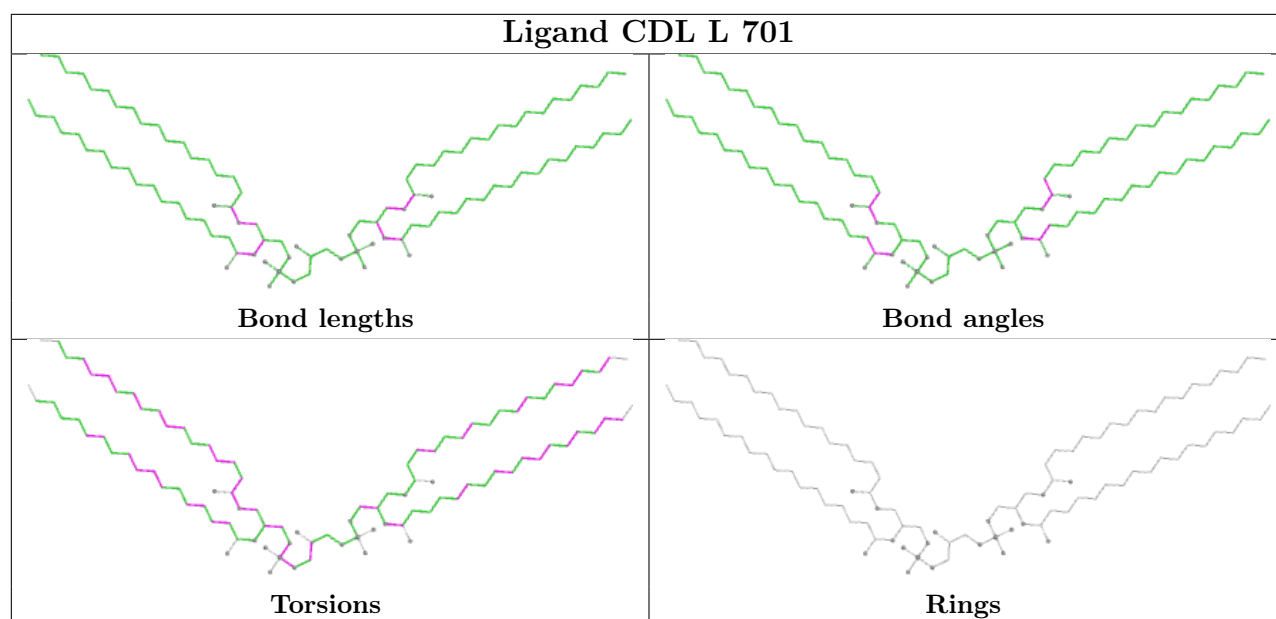
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

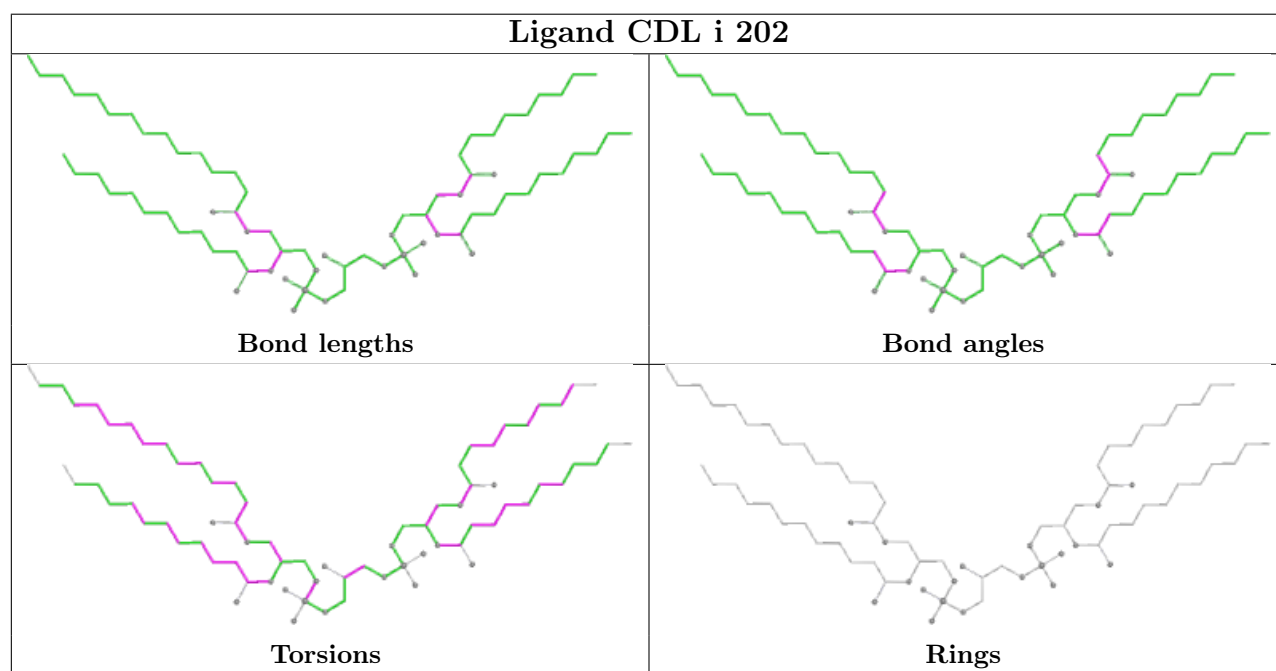
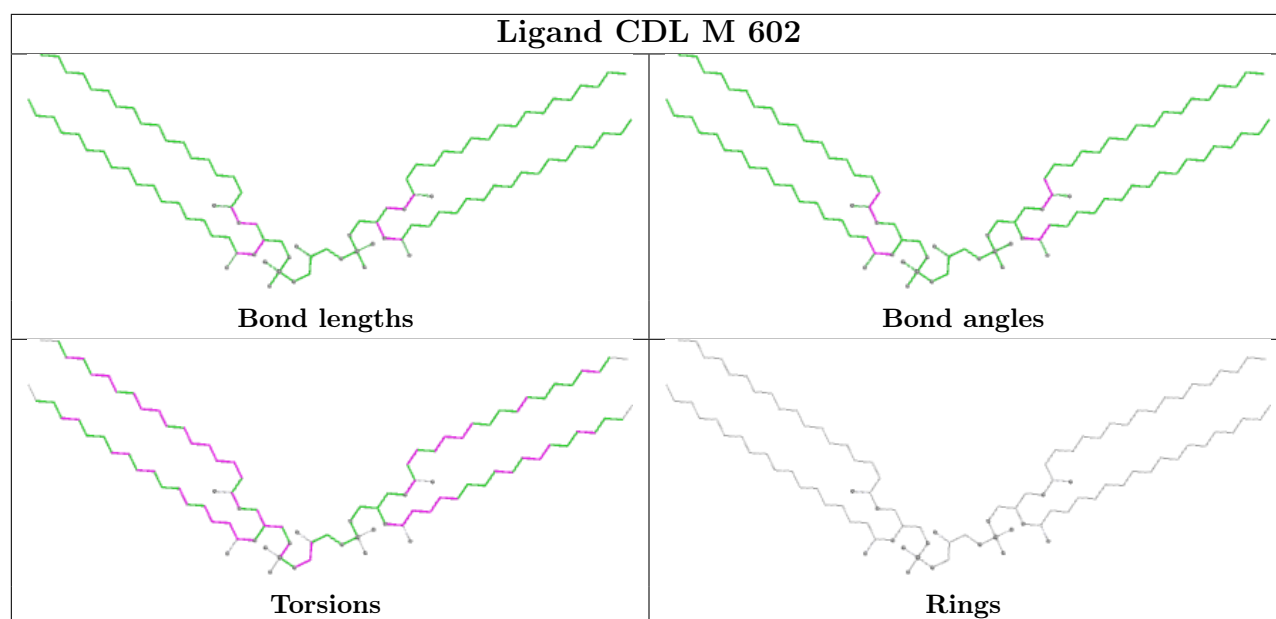


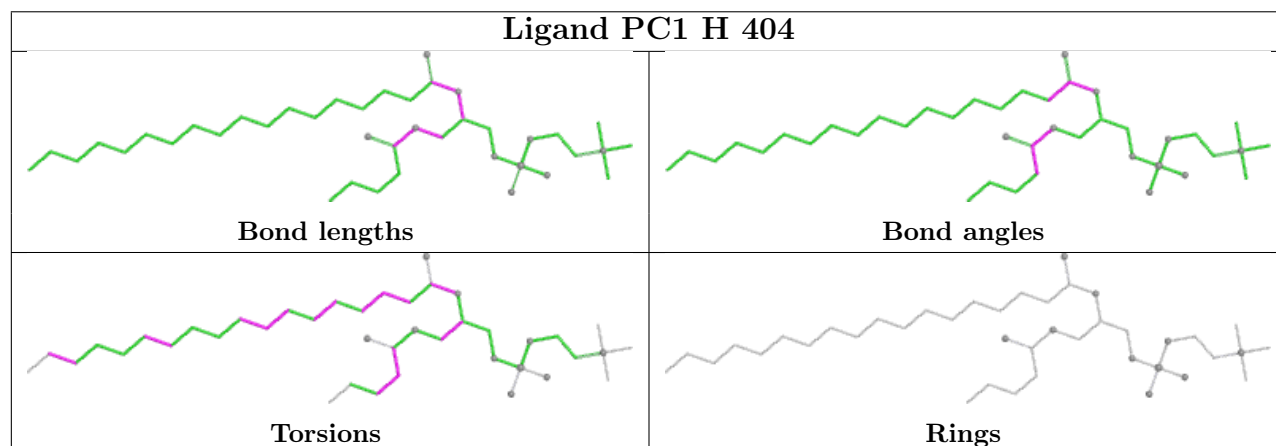
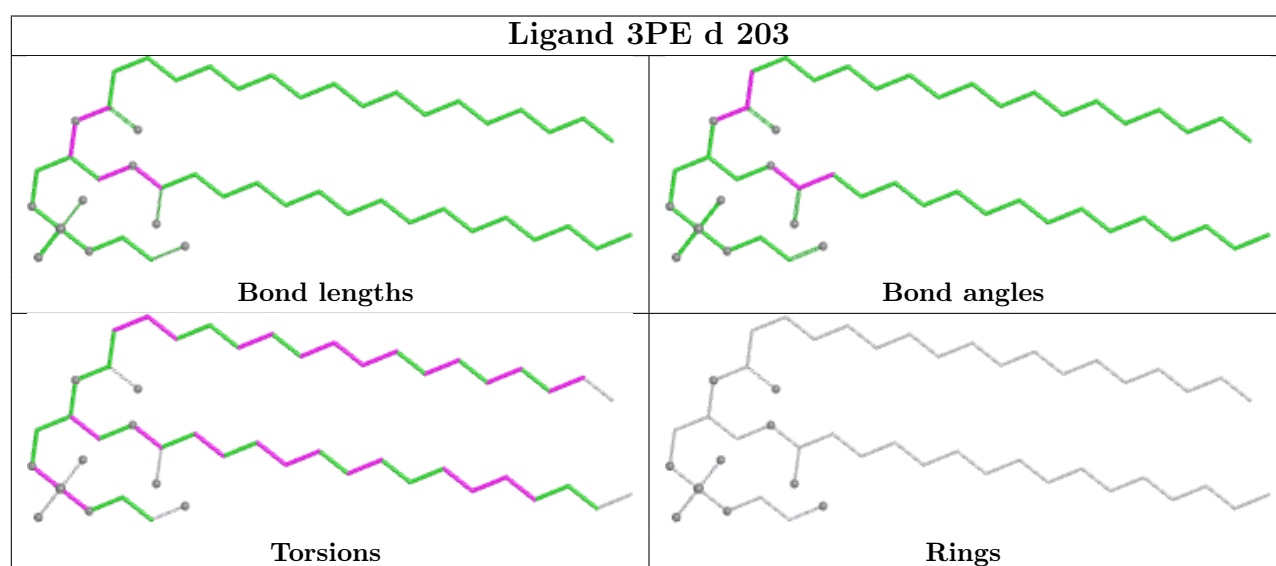
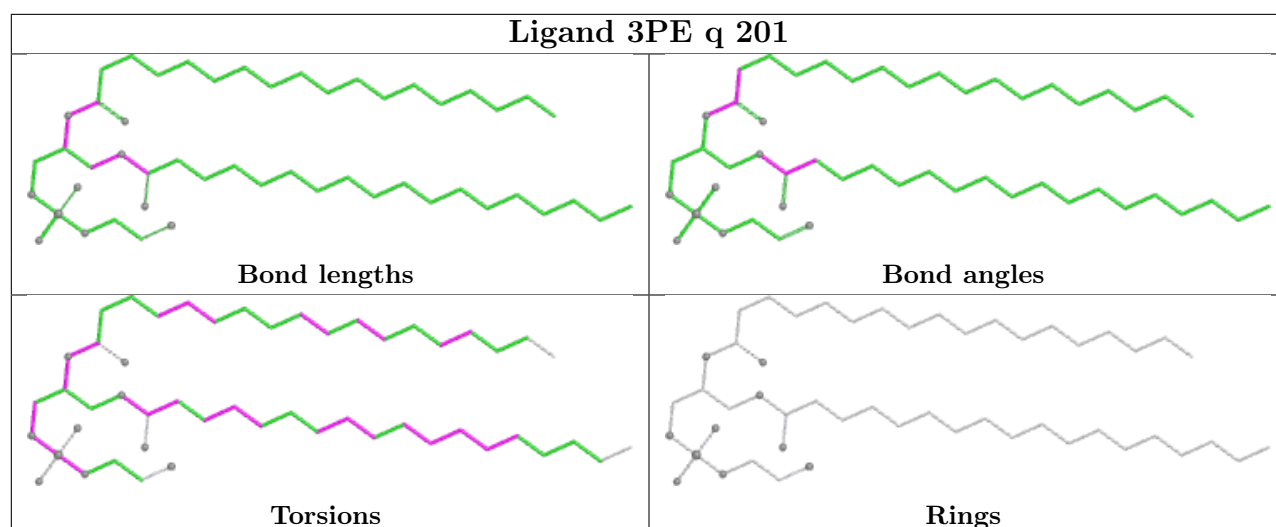


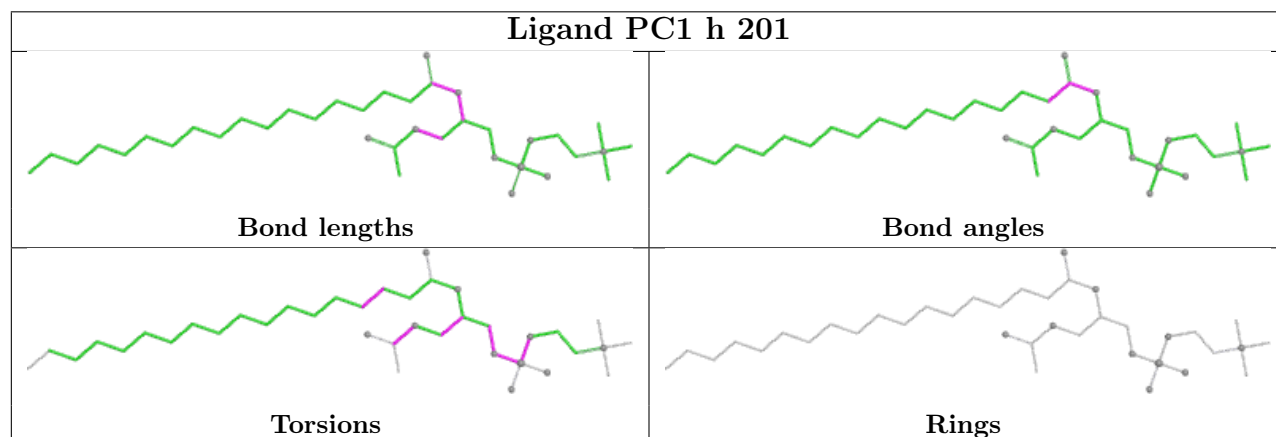
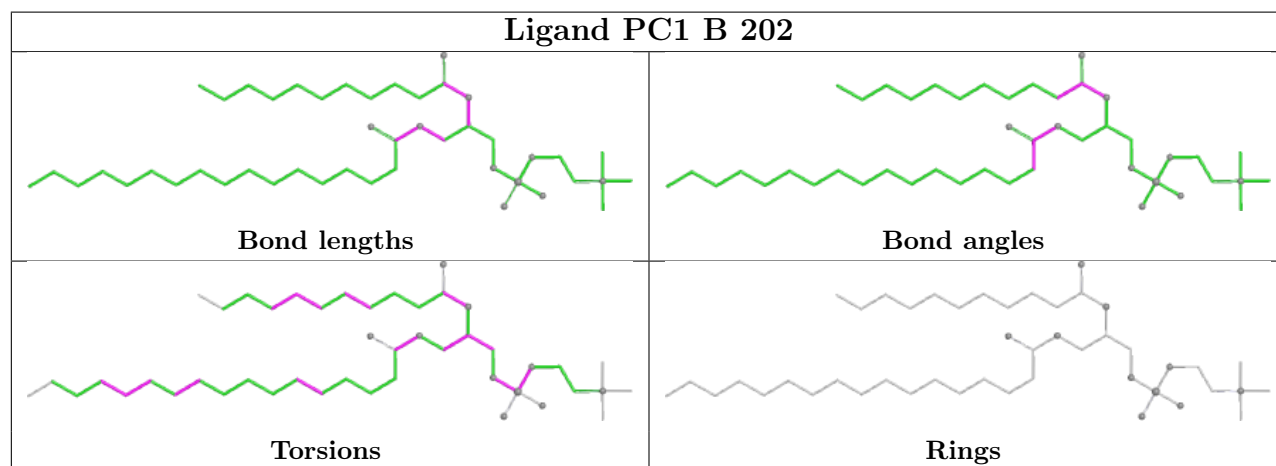
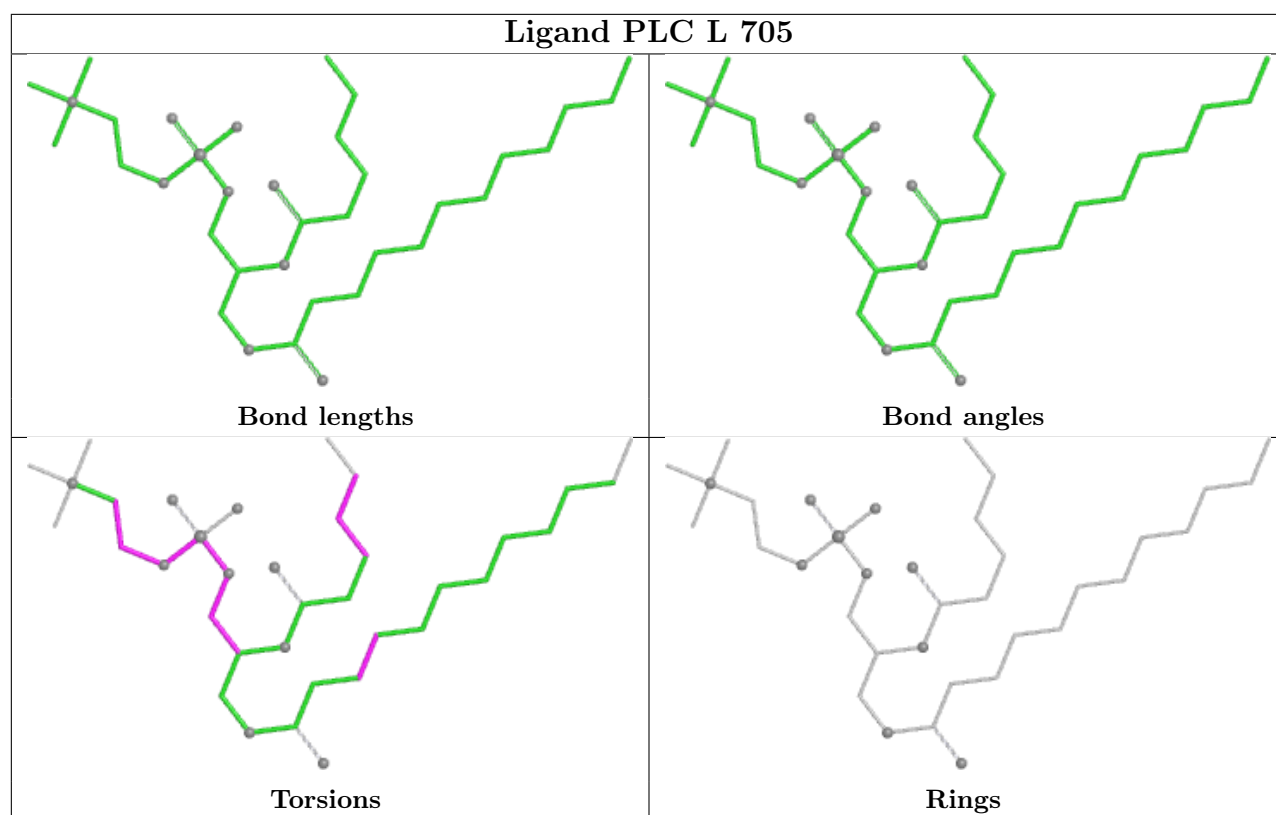


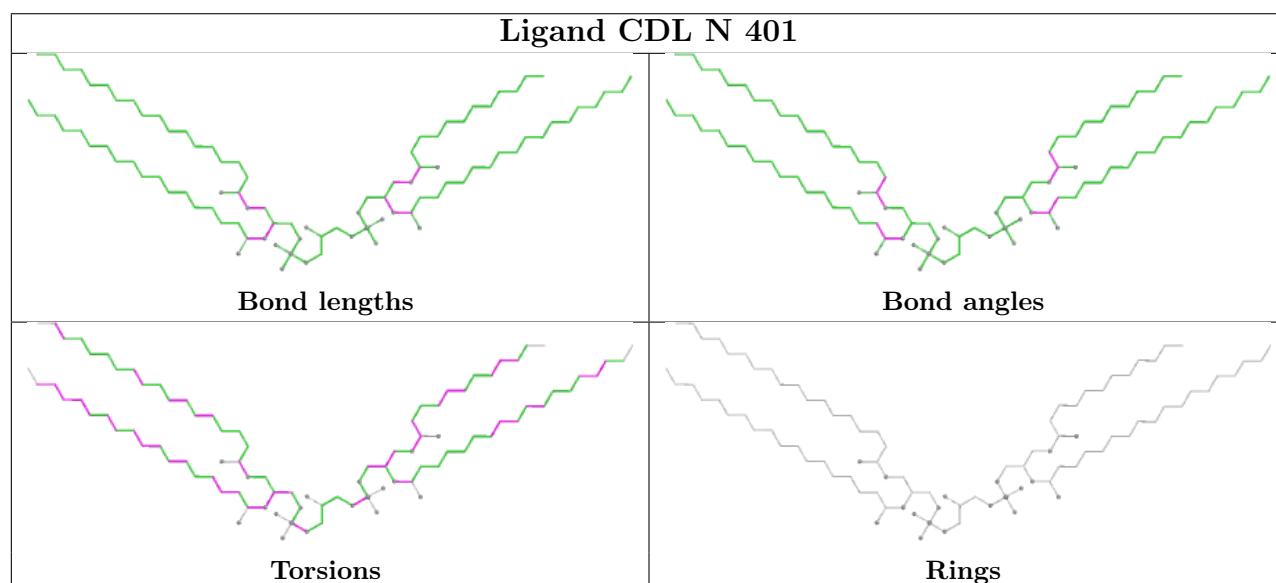
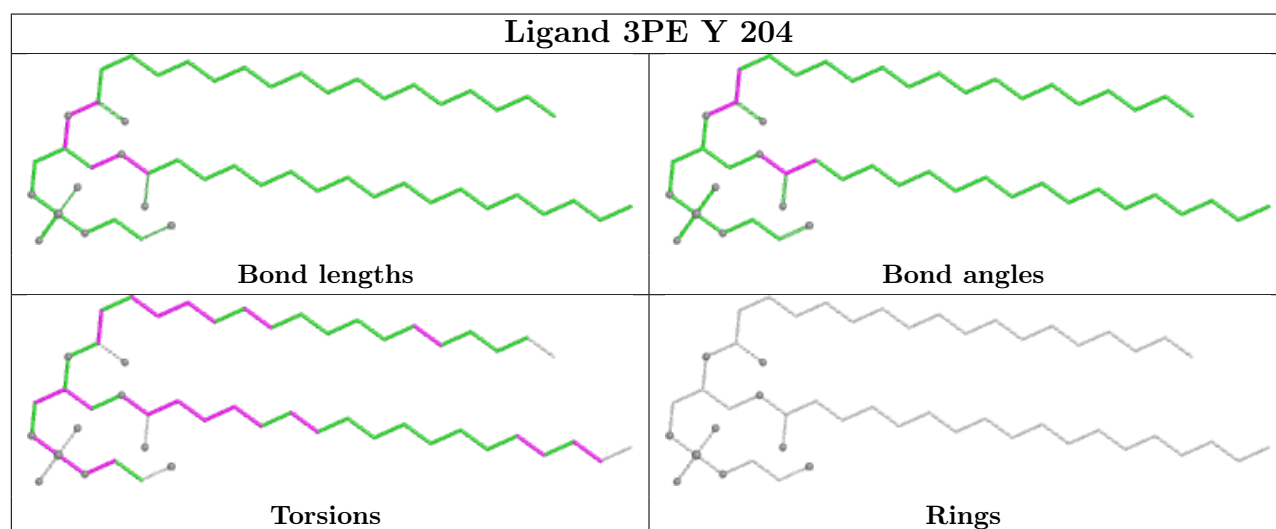
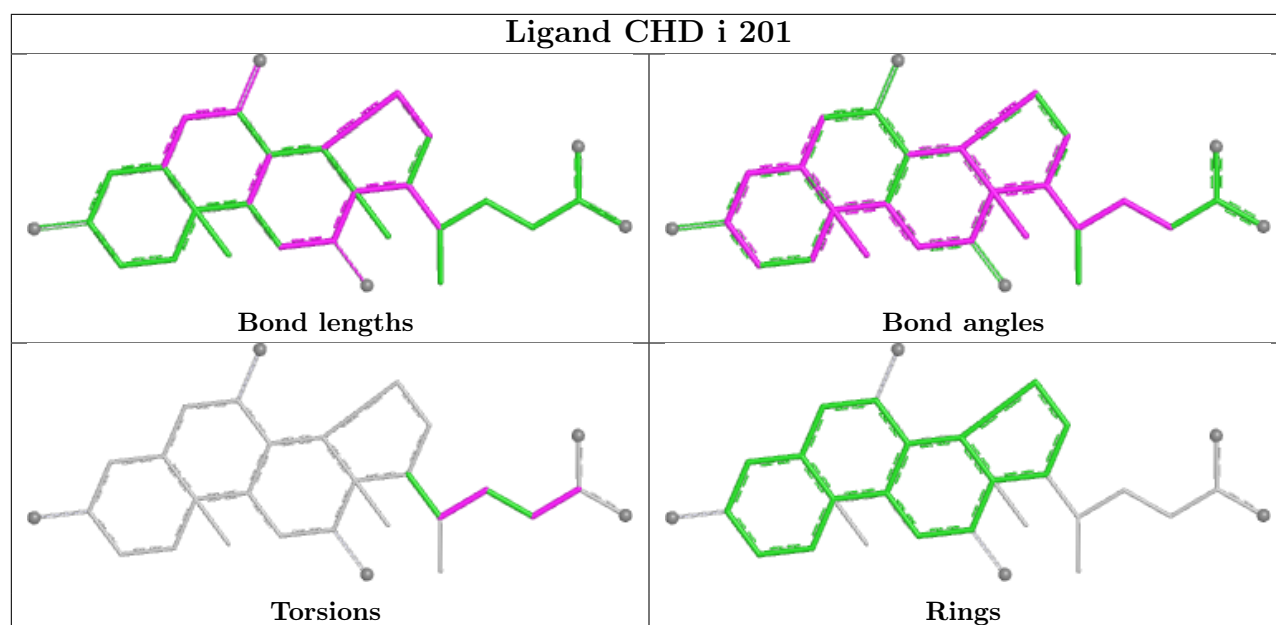


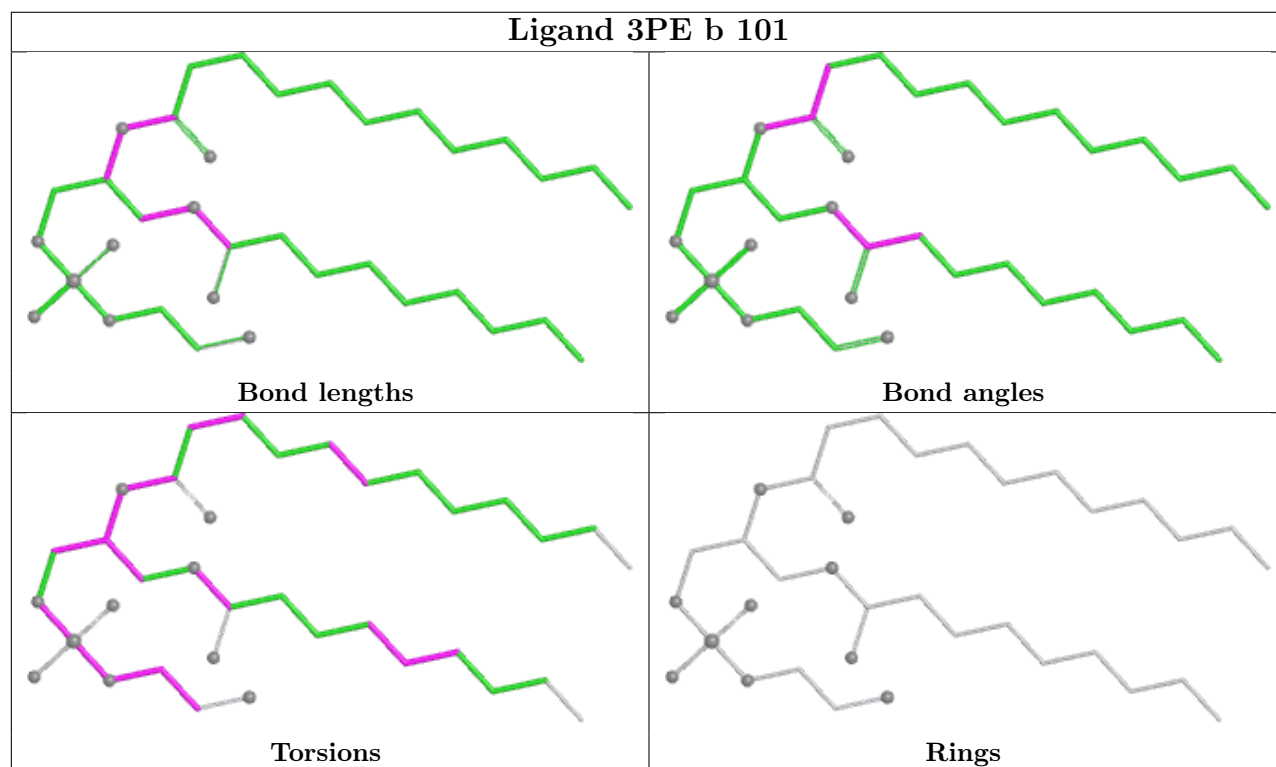
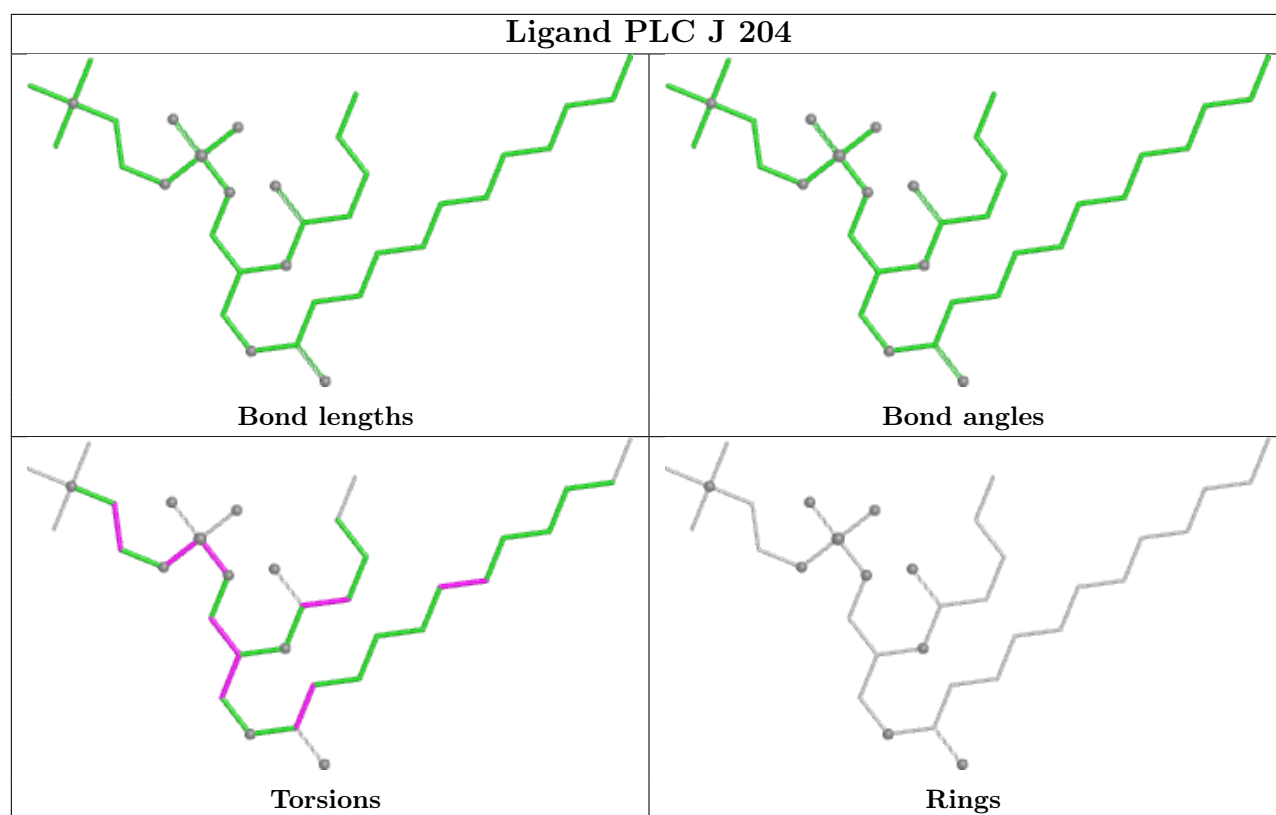


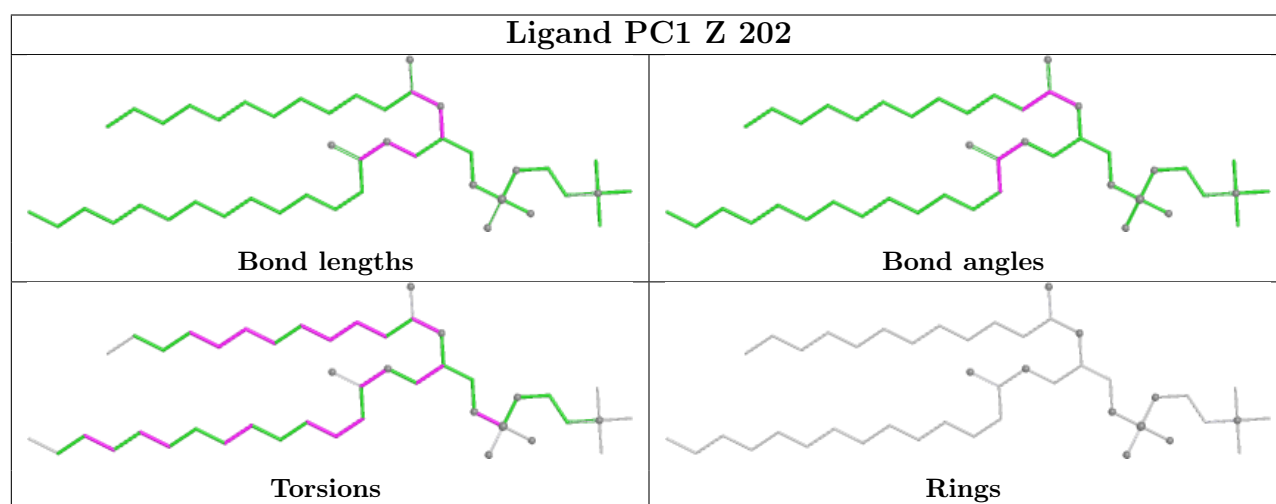
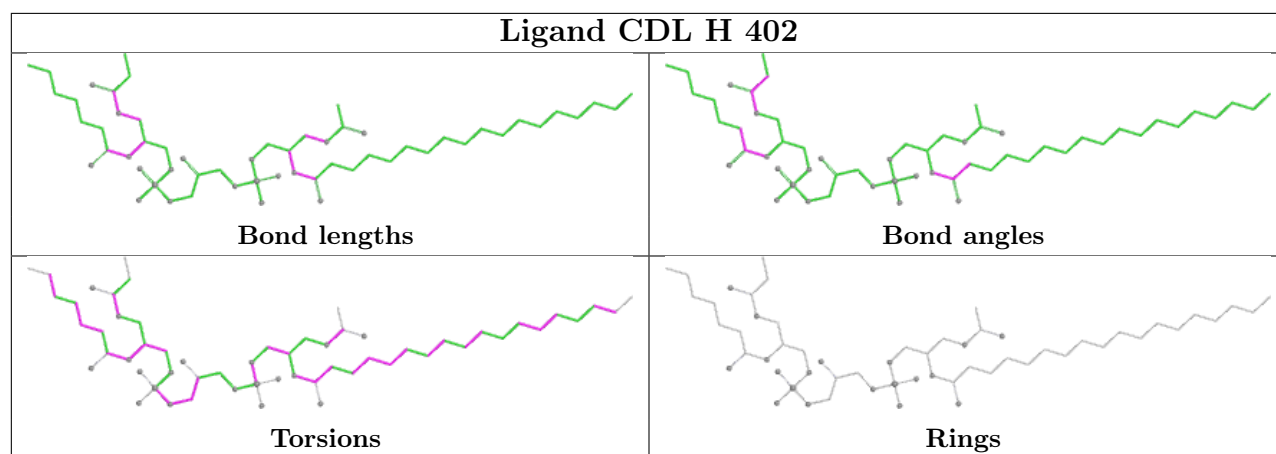
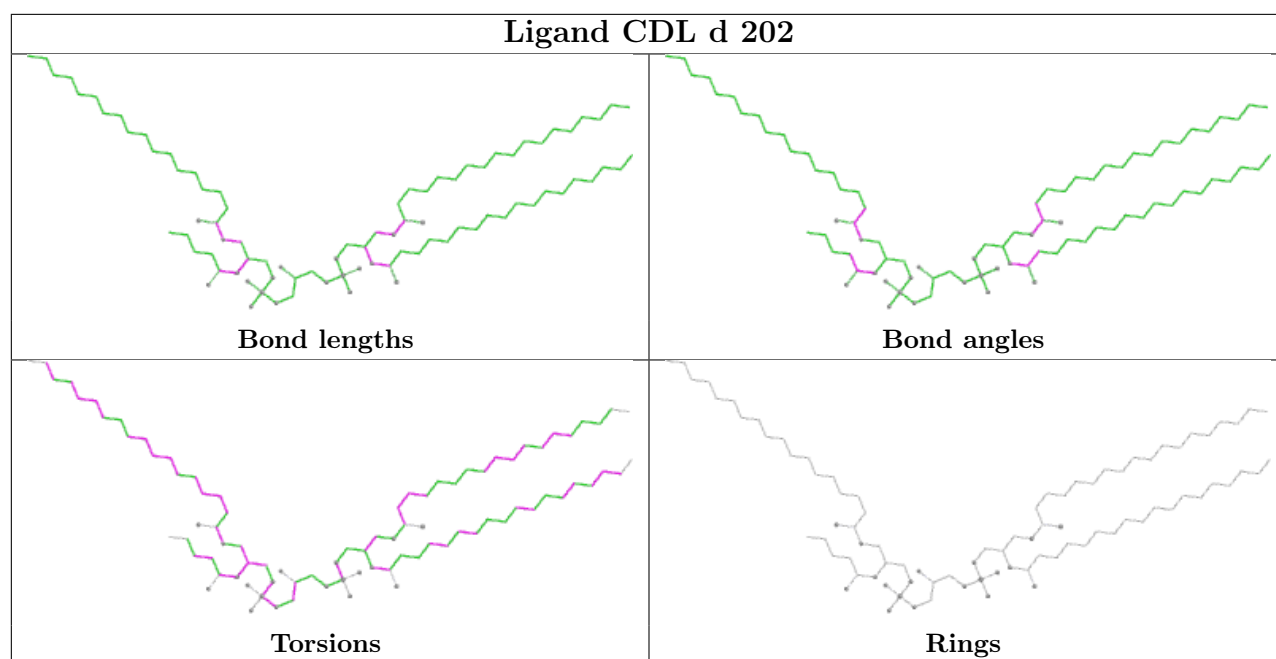


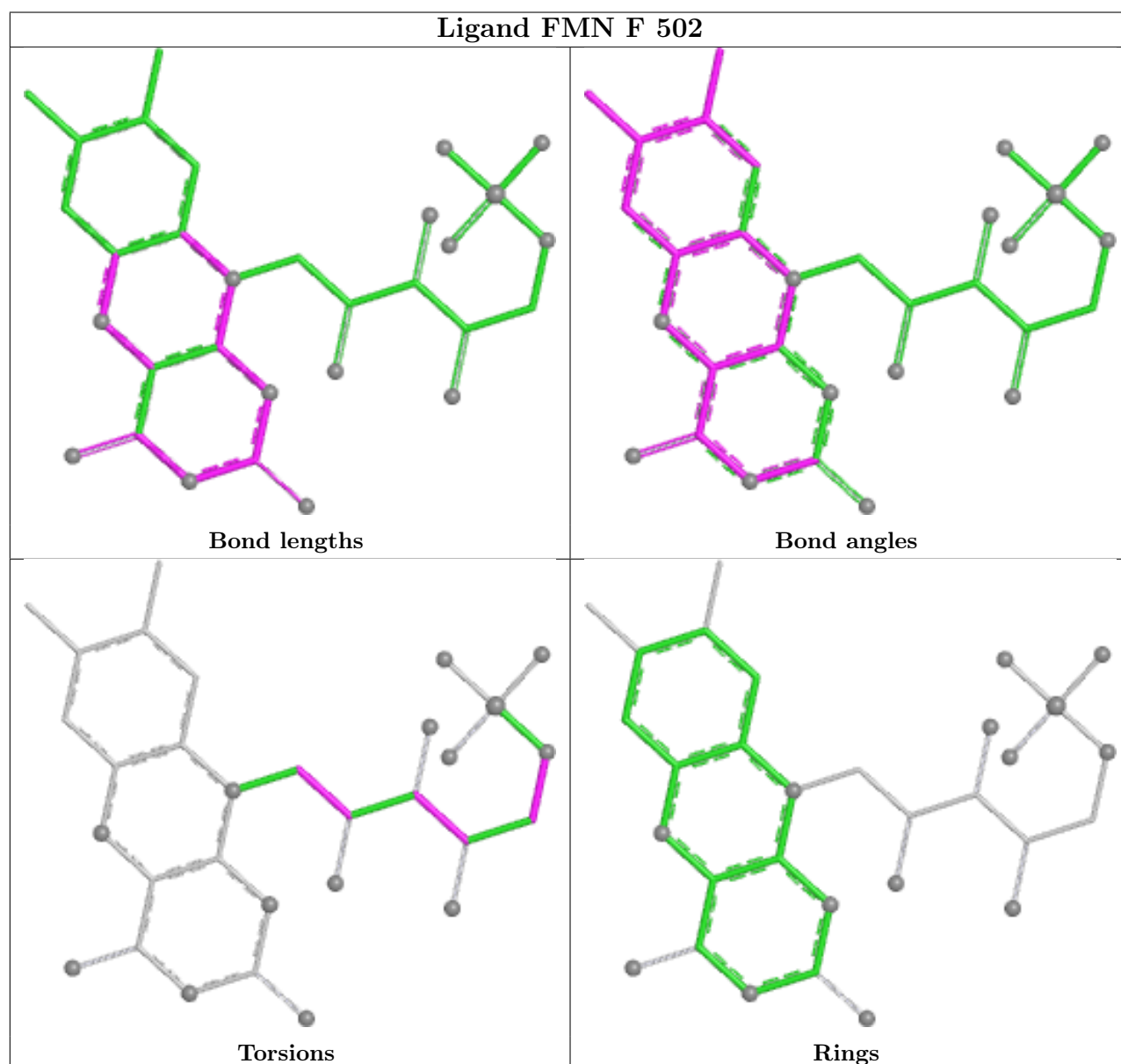
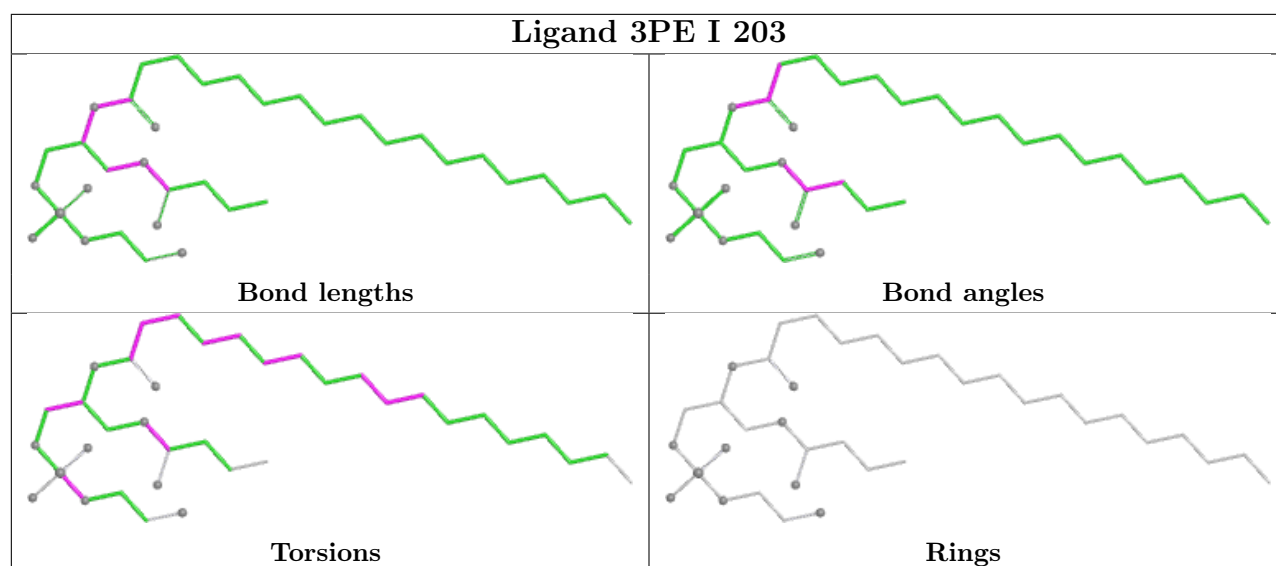


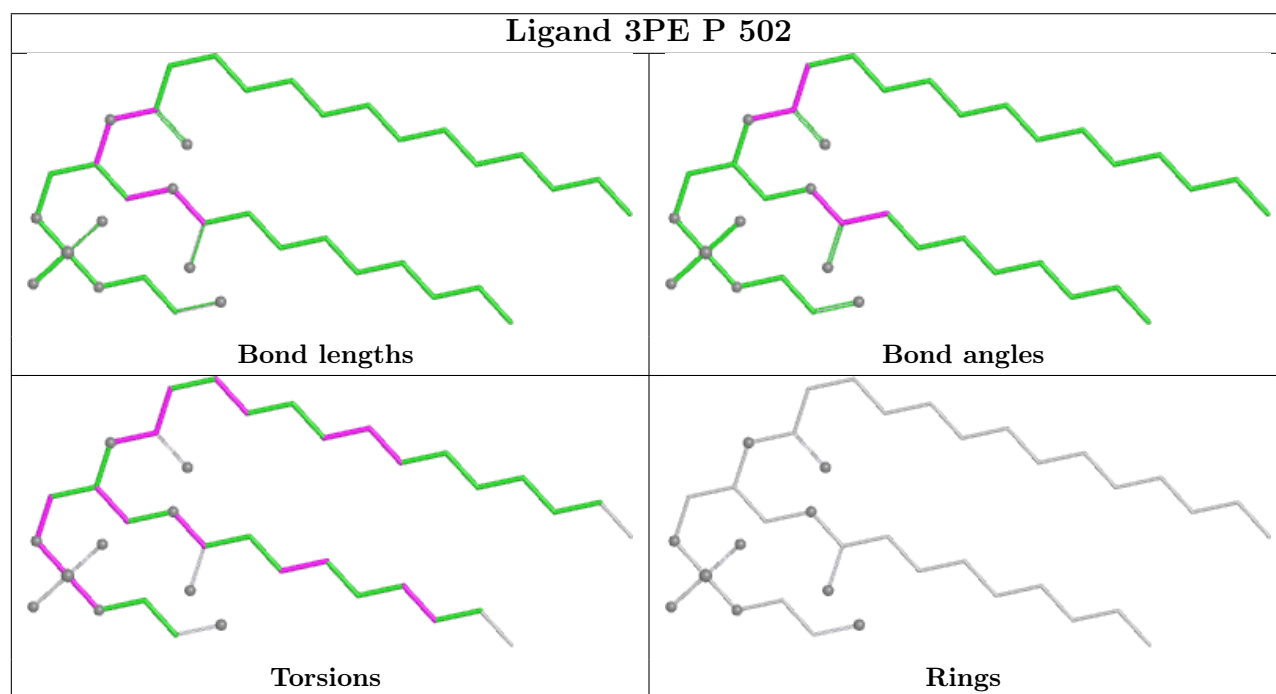
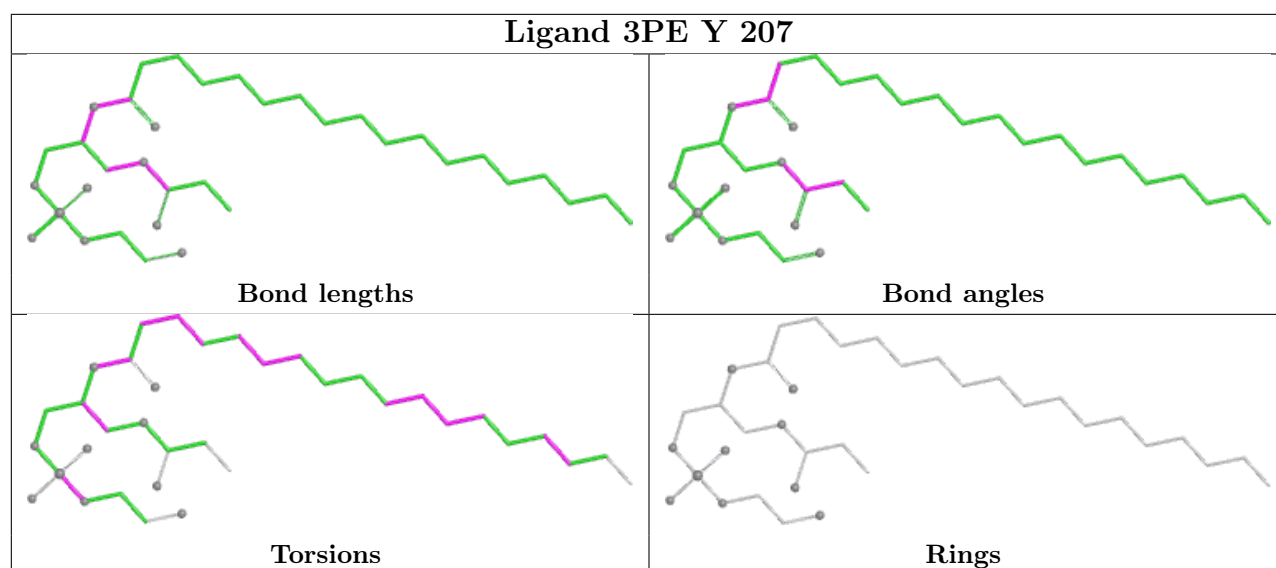


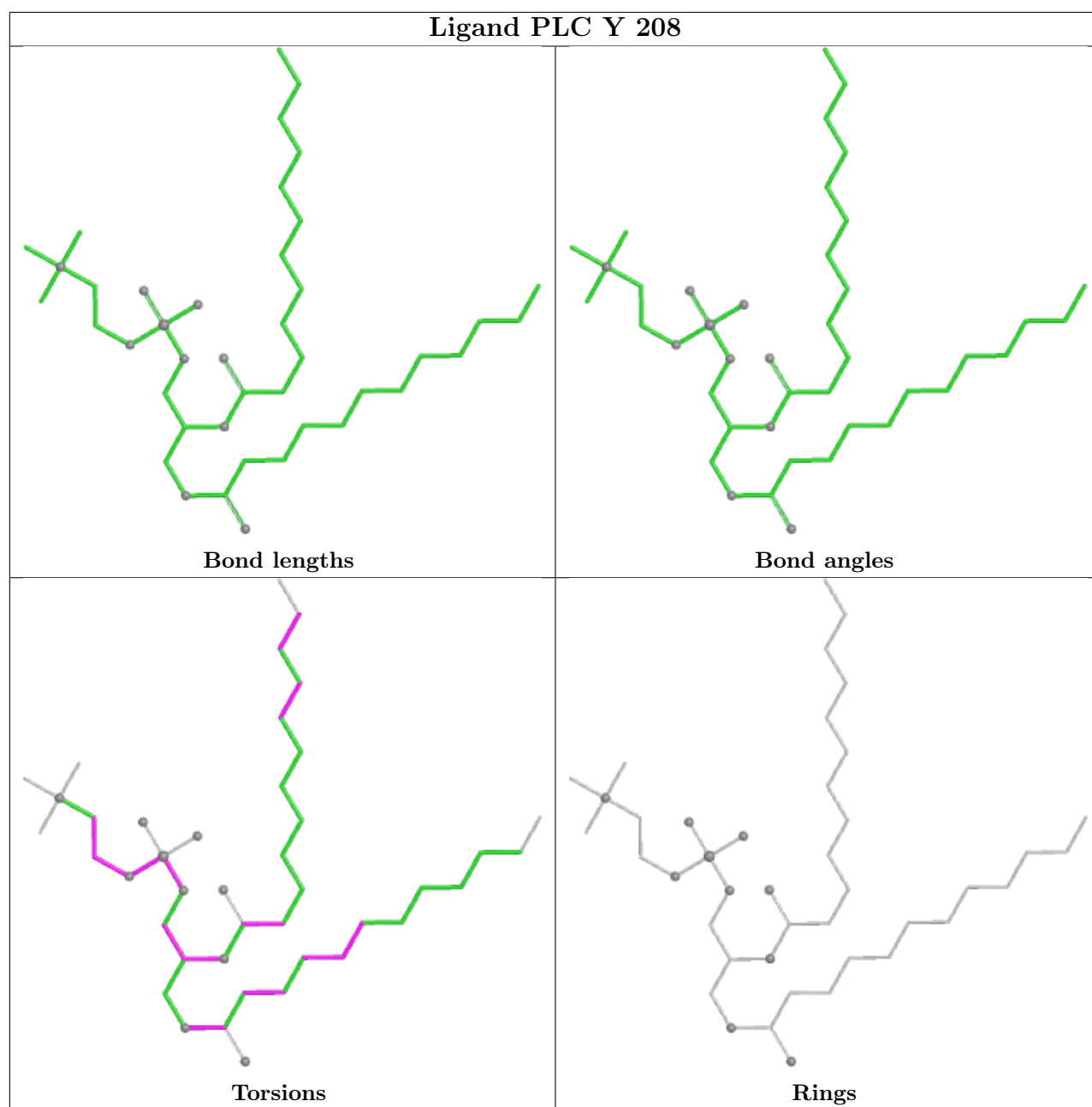


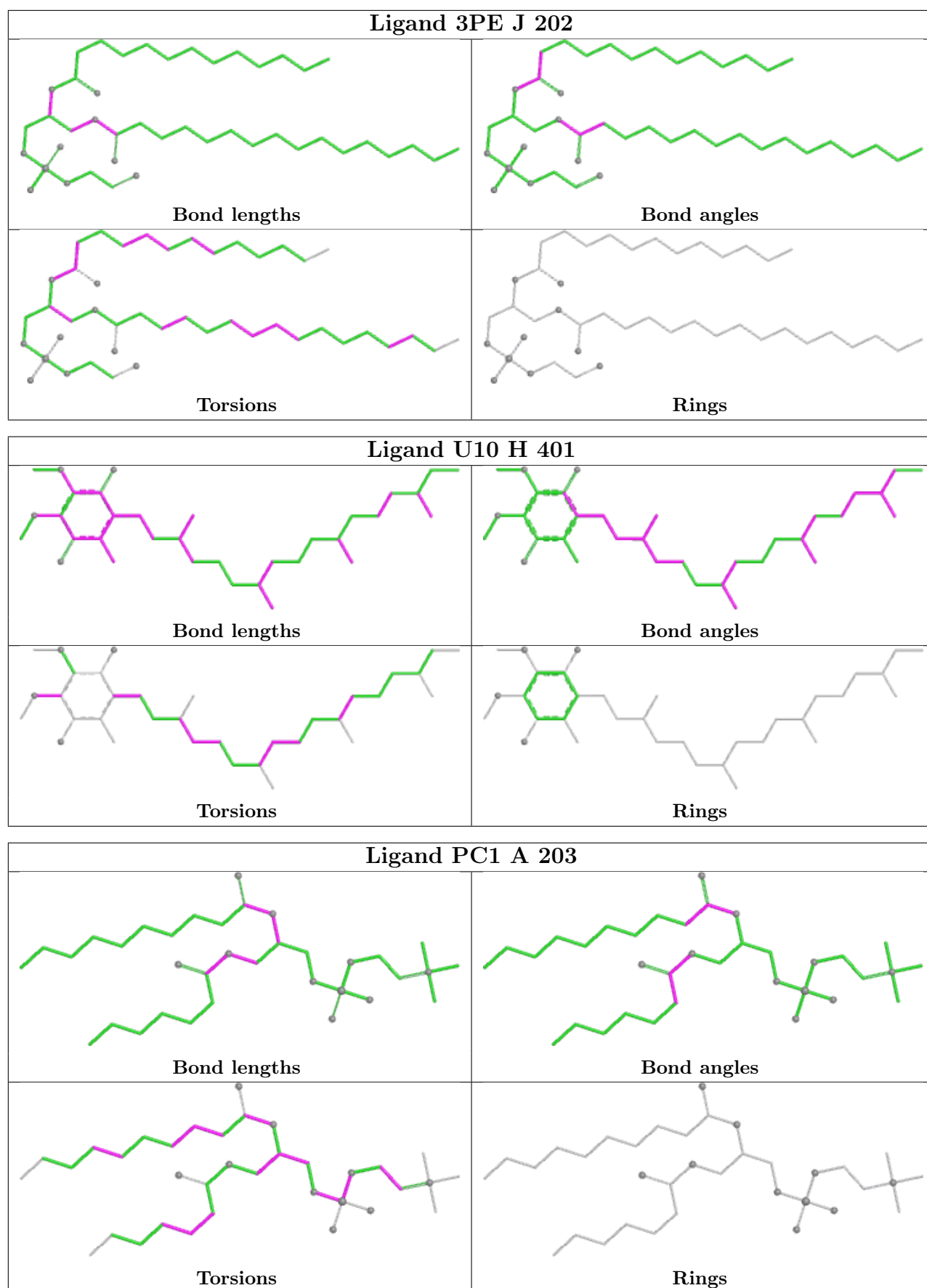


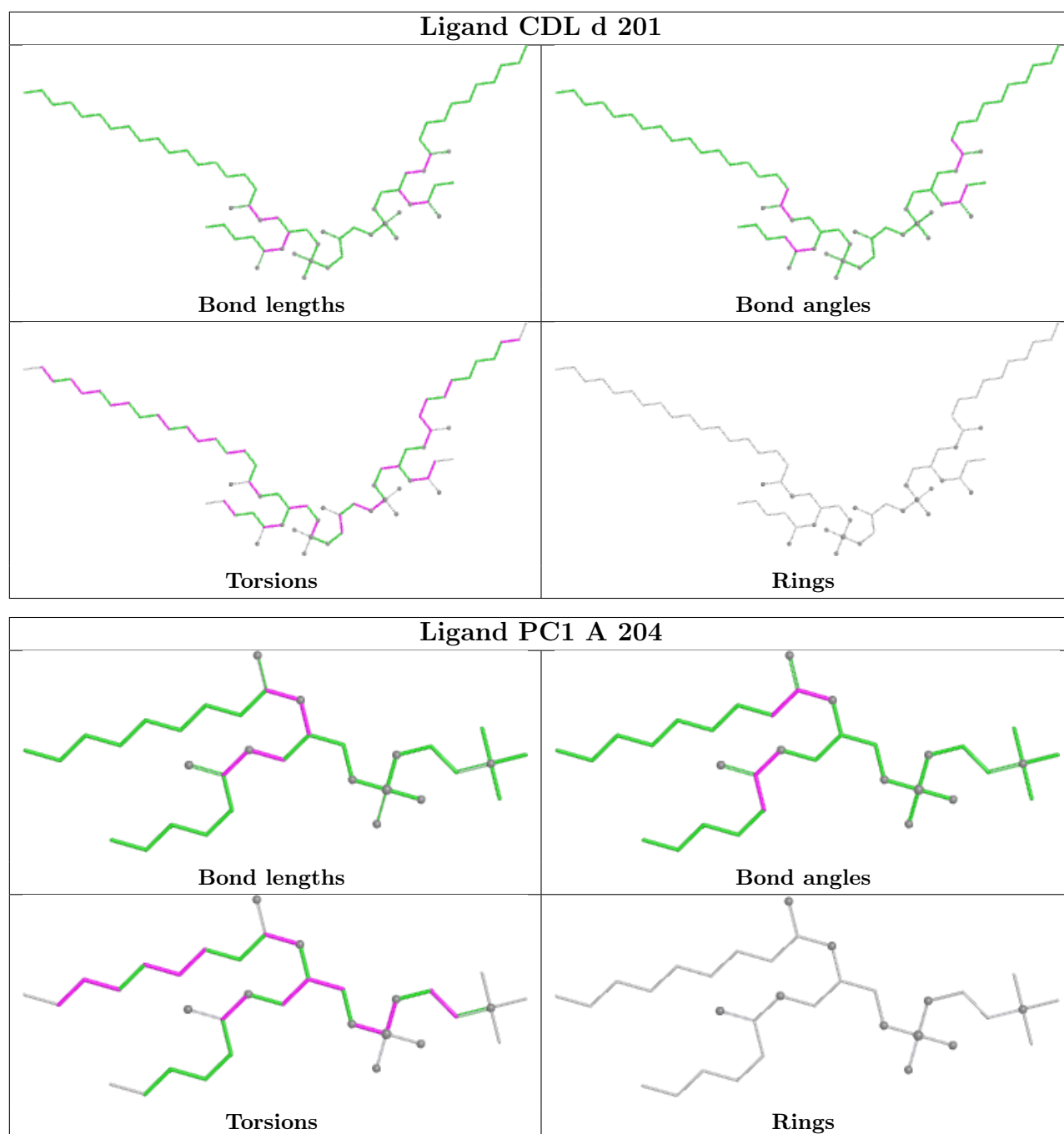


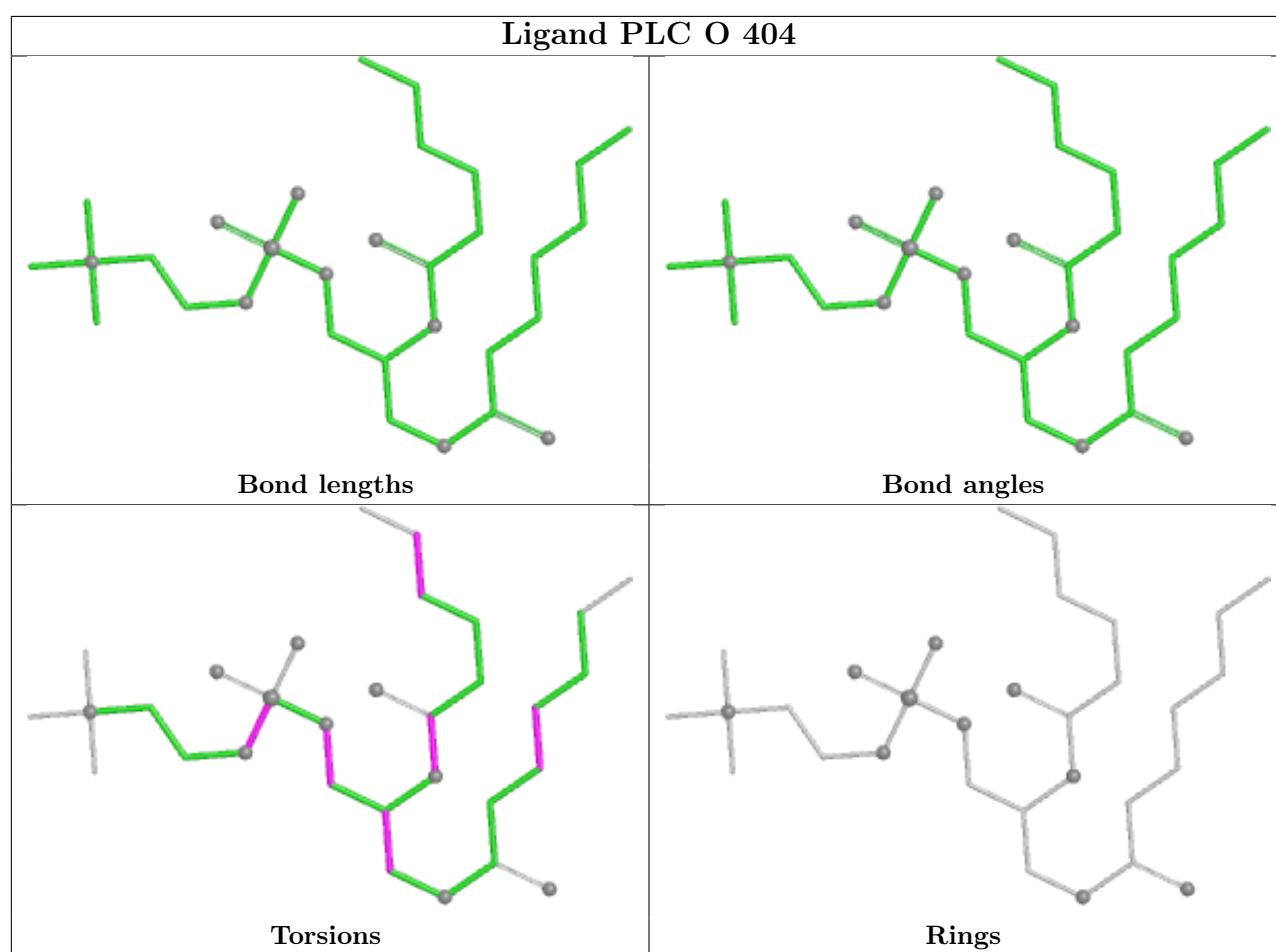
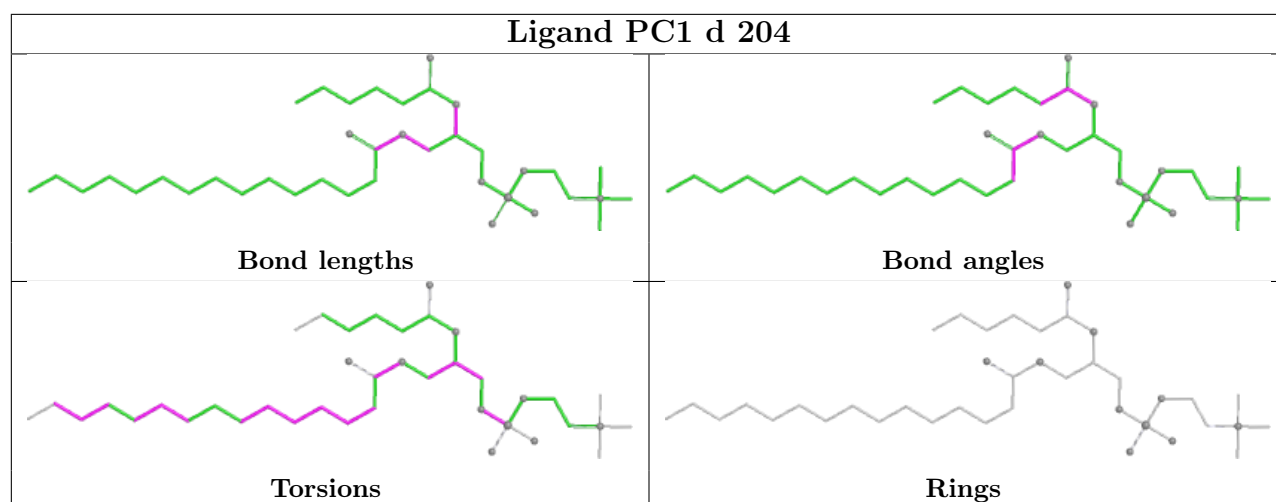


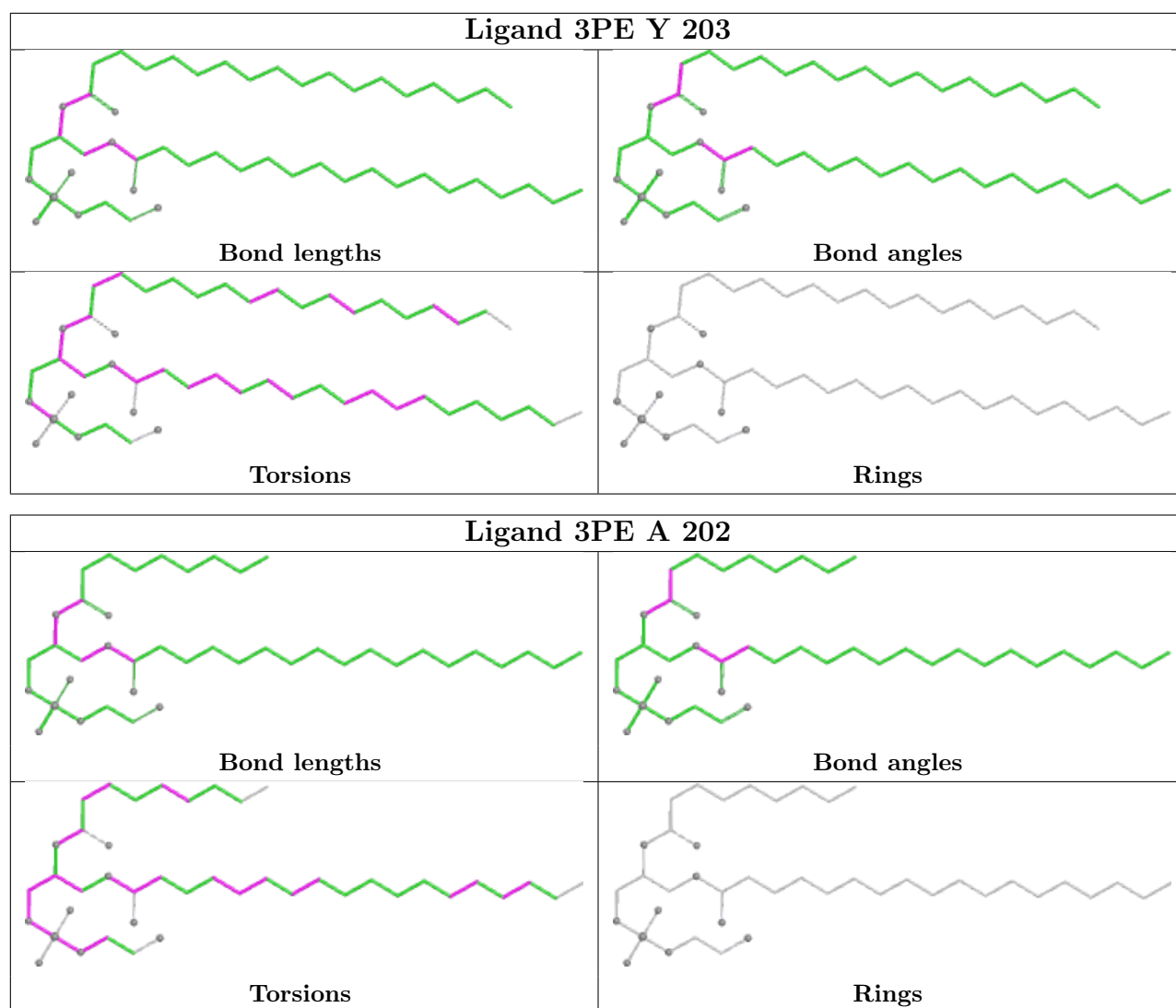


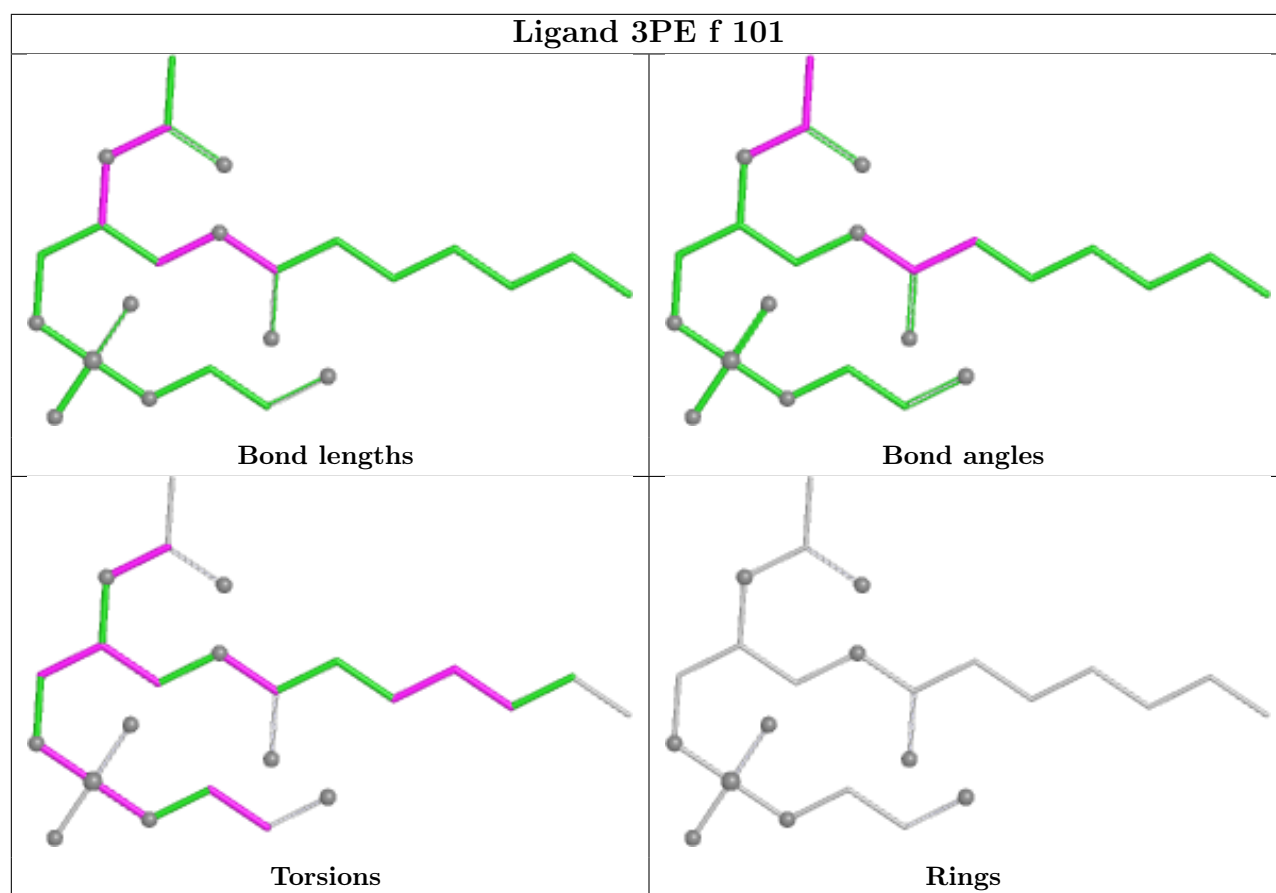


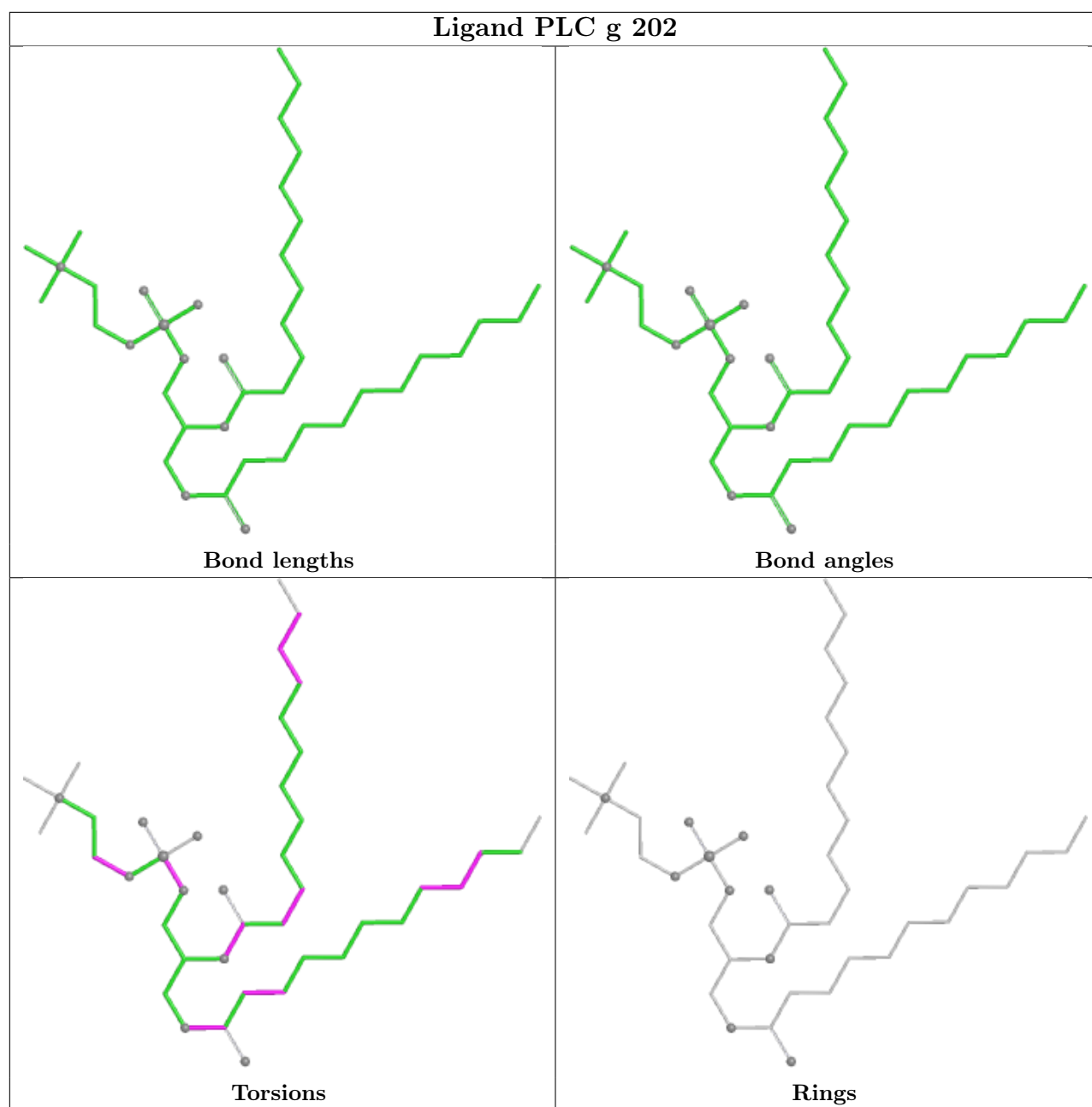


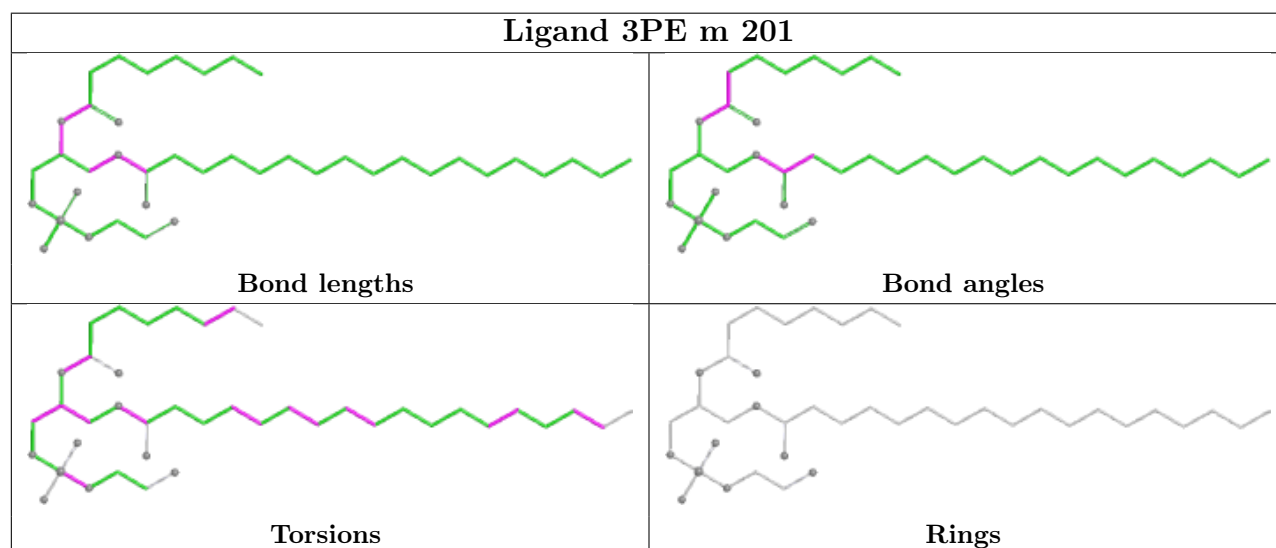
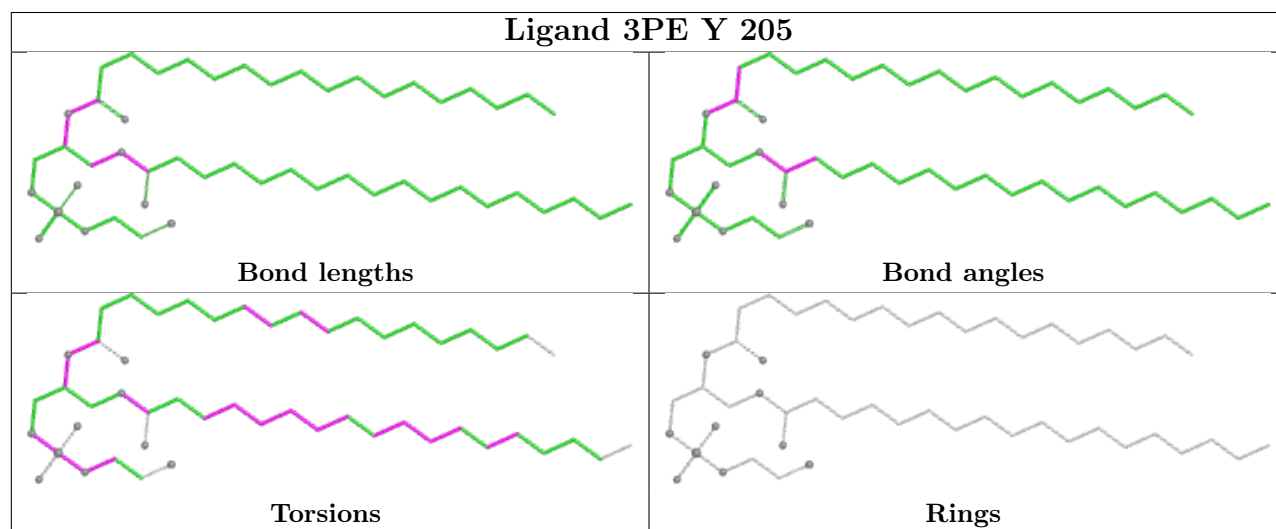
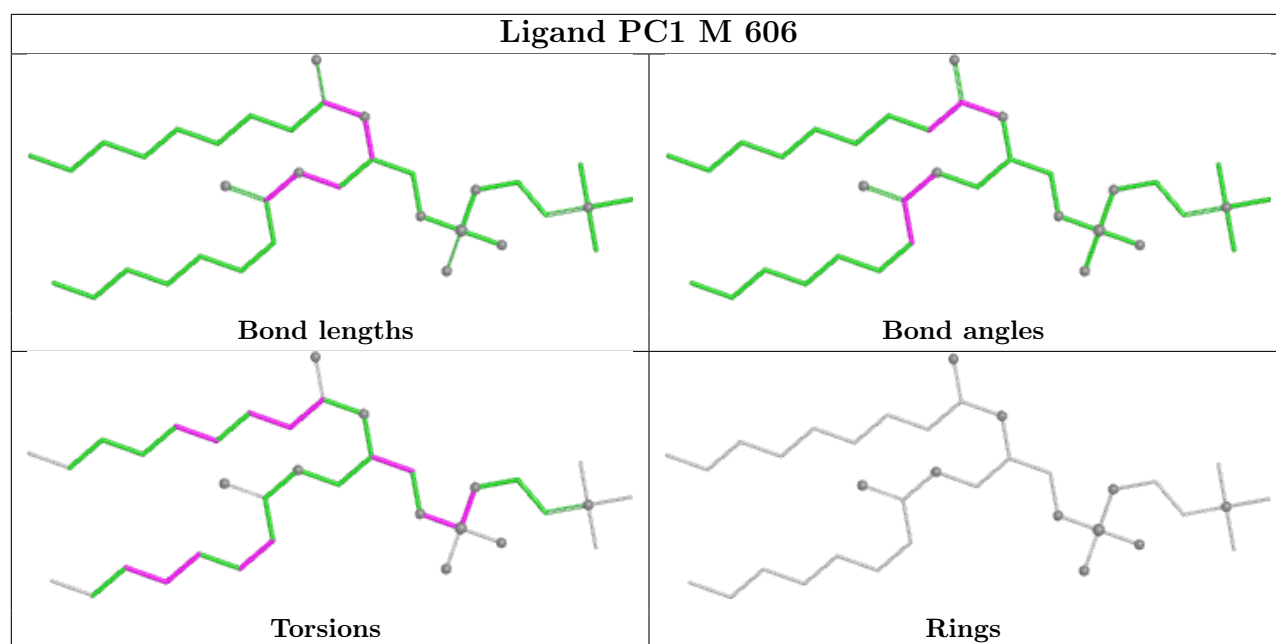


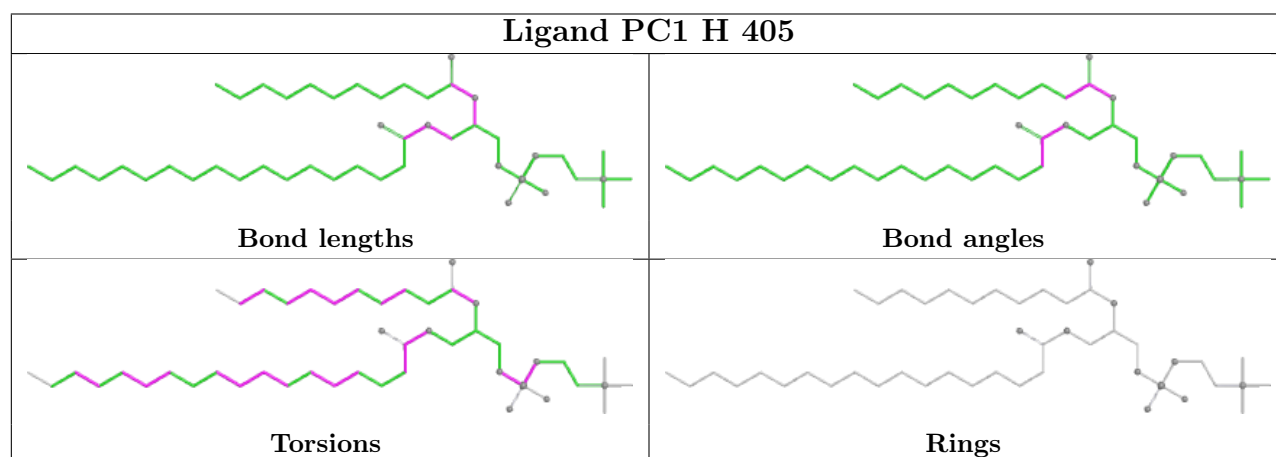
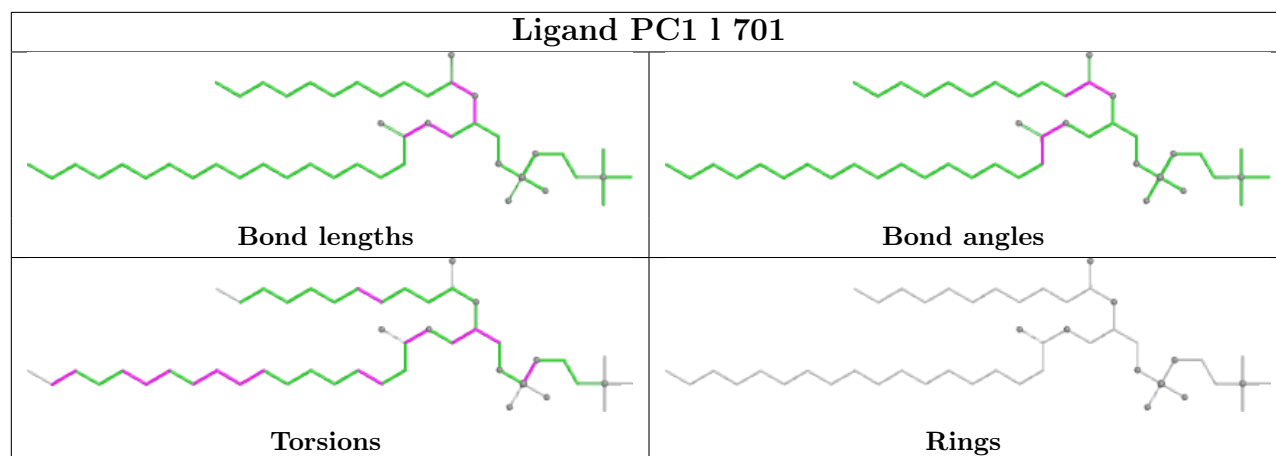
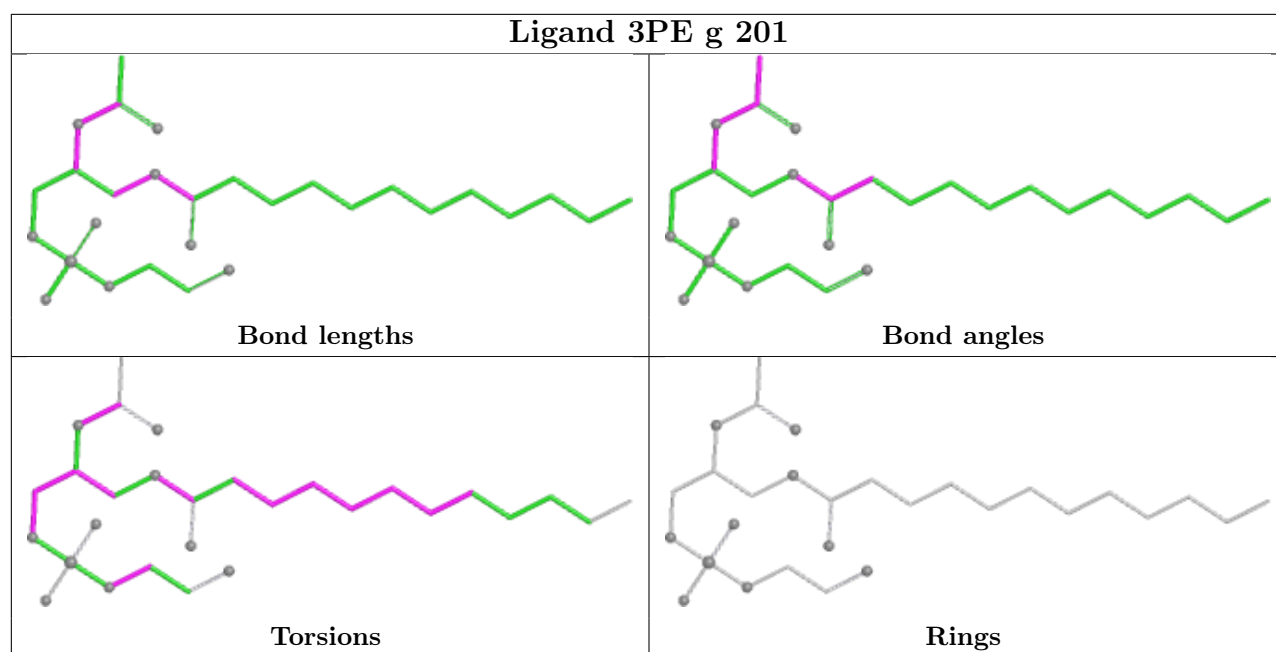




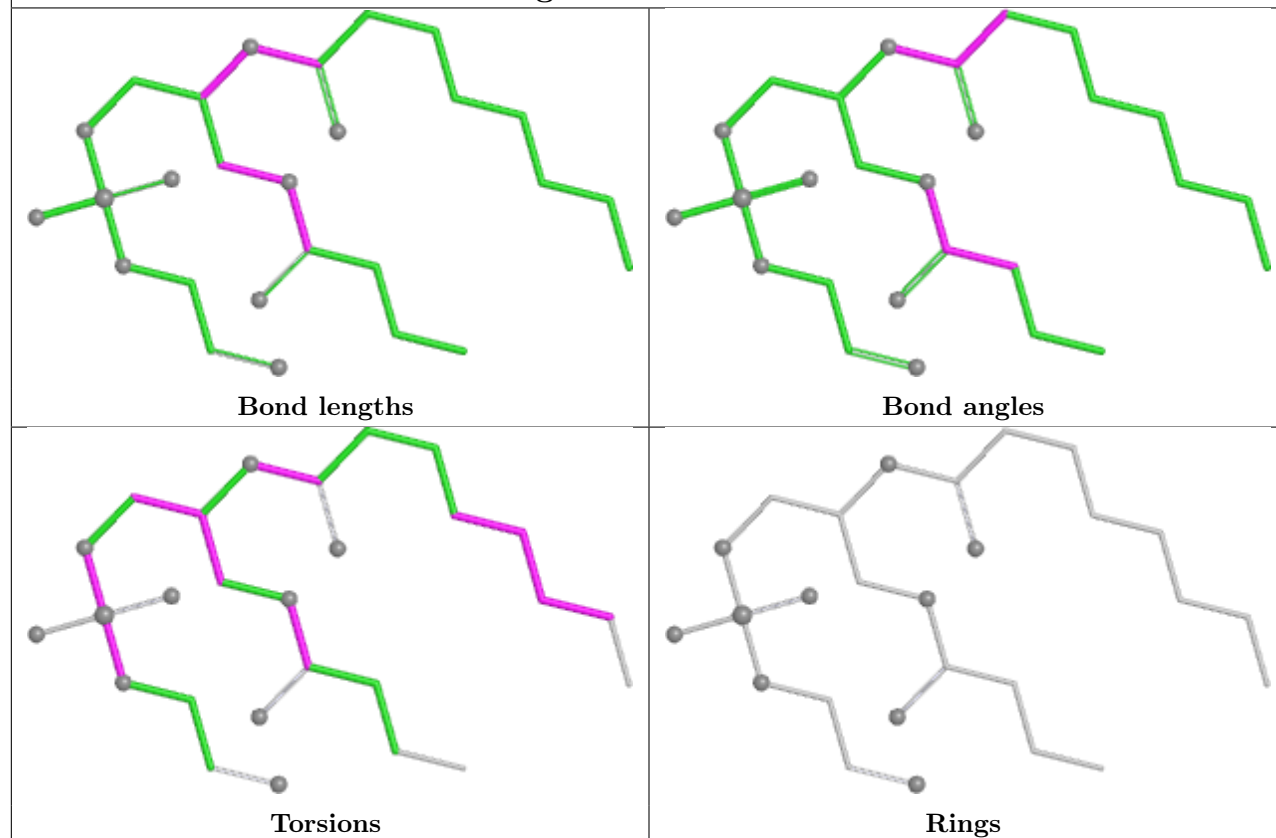




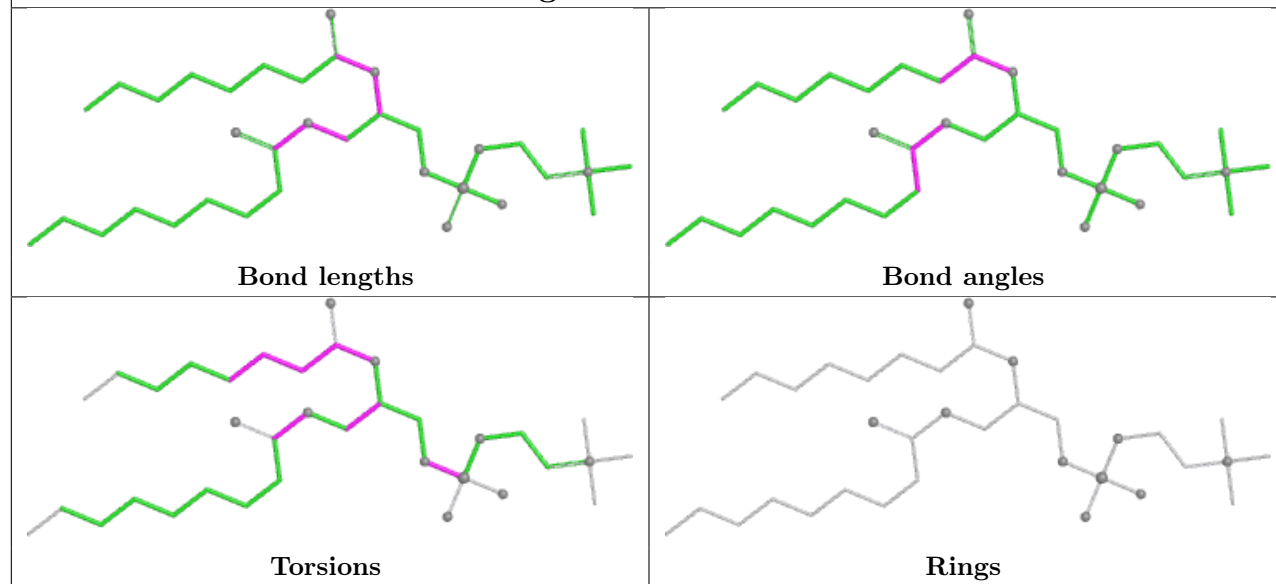


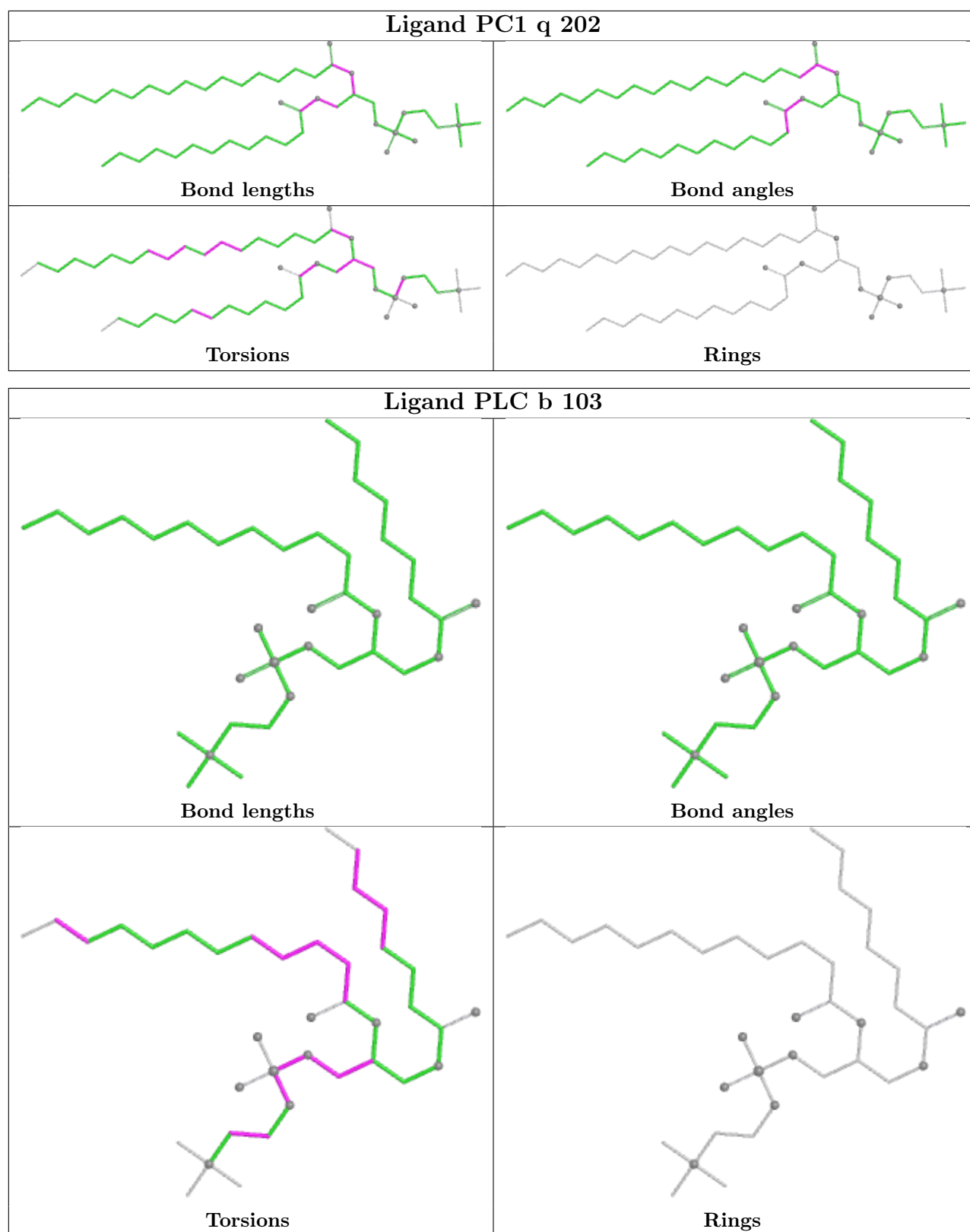


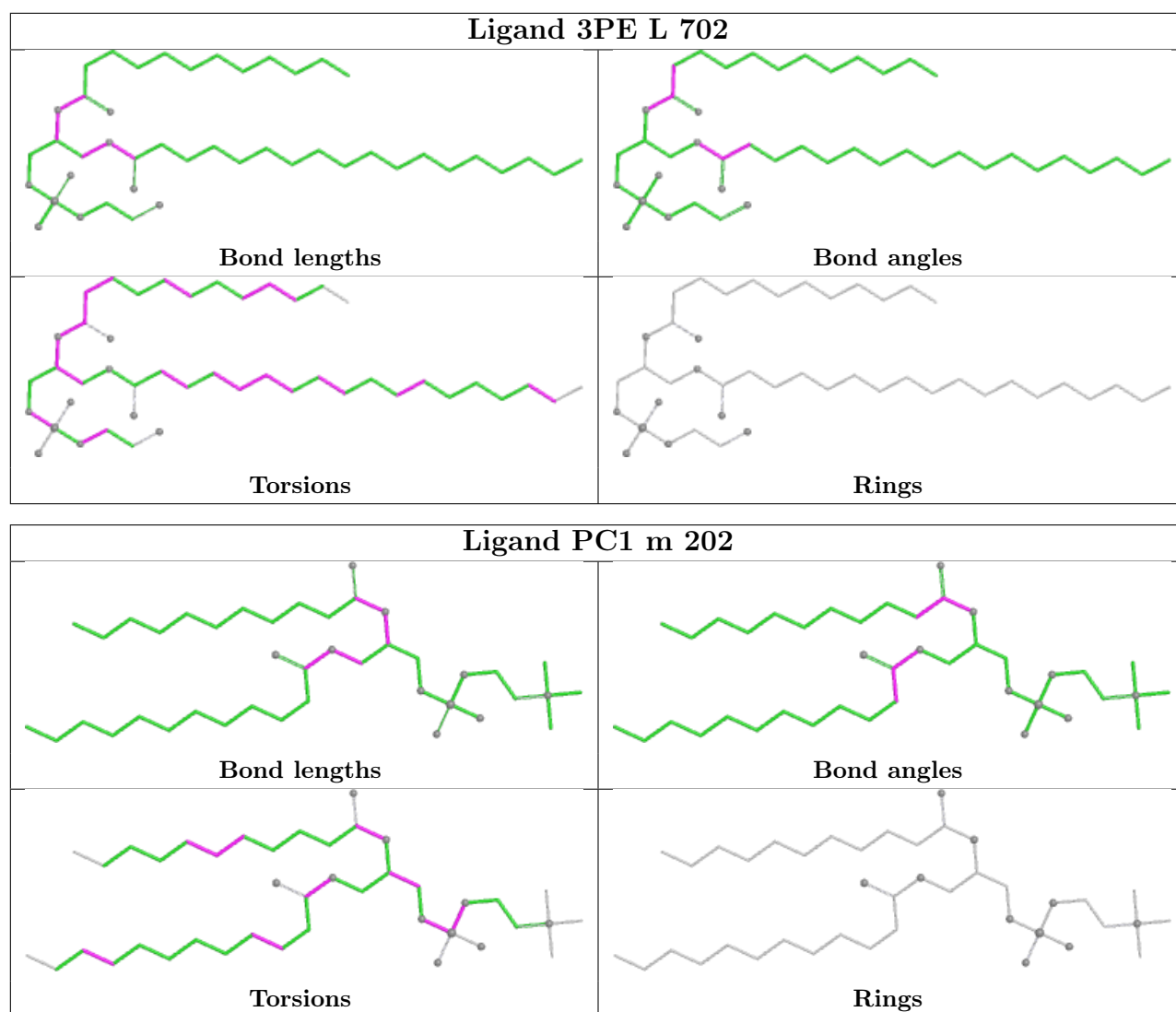
Ligand 3PE Y 202

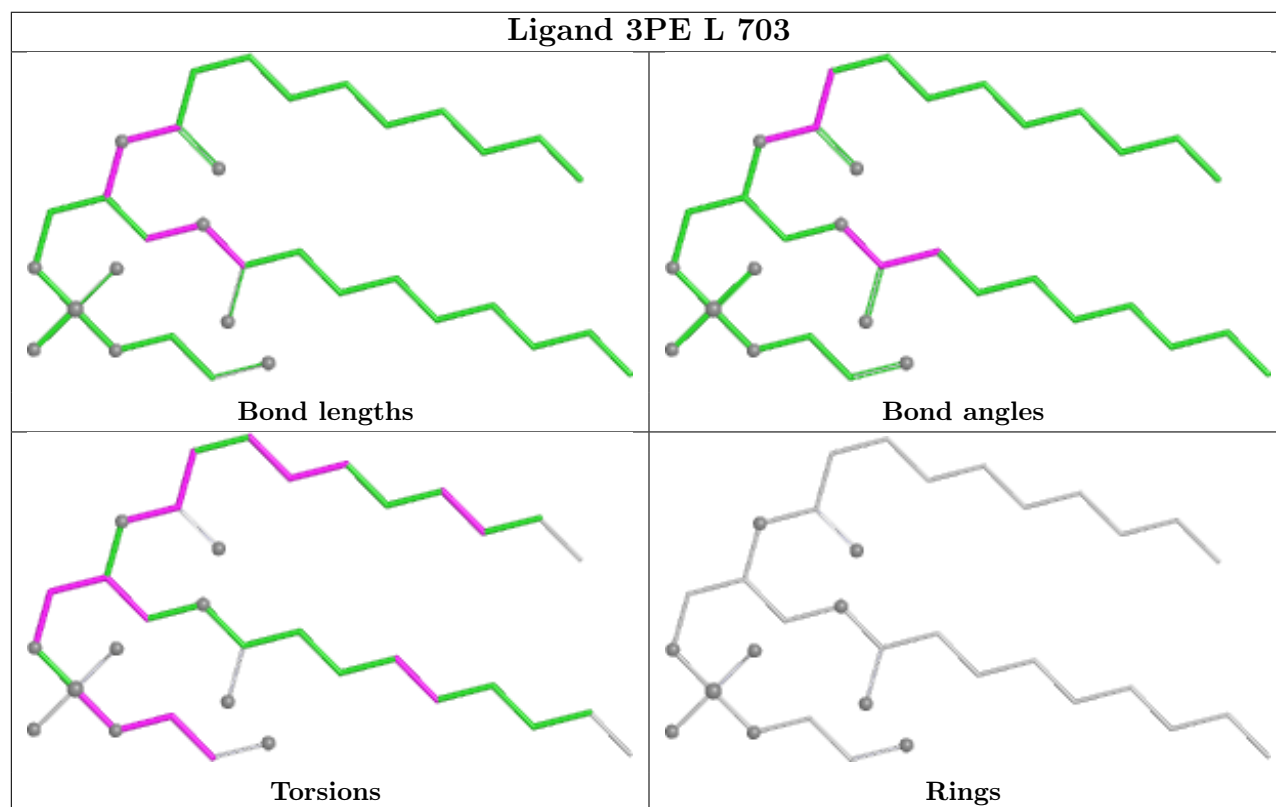
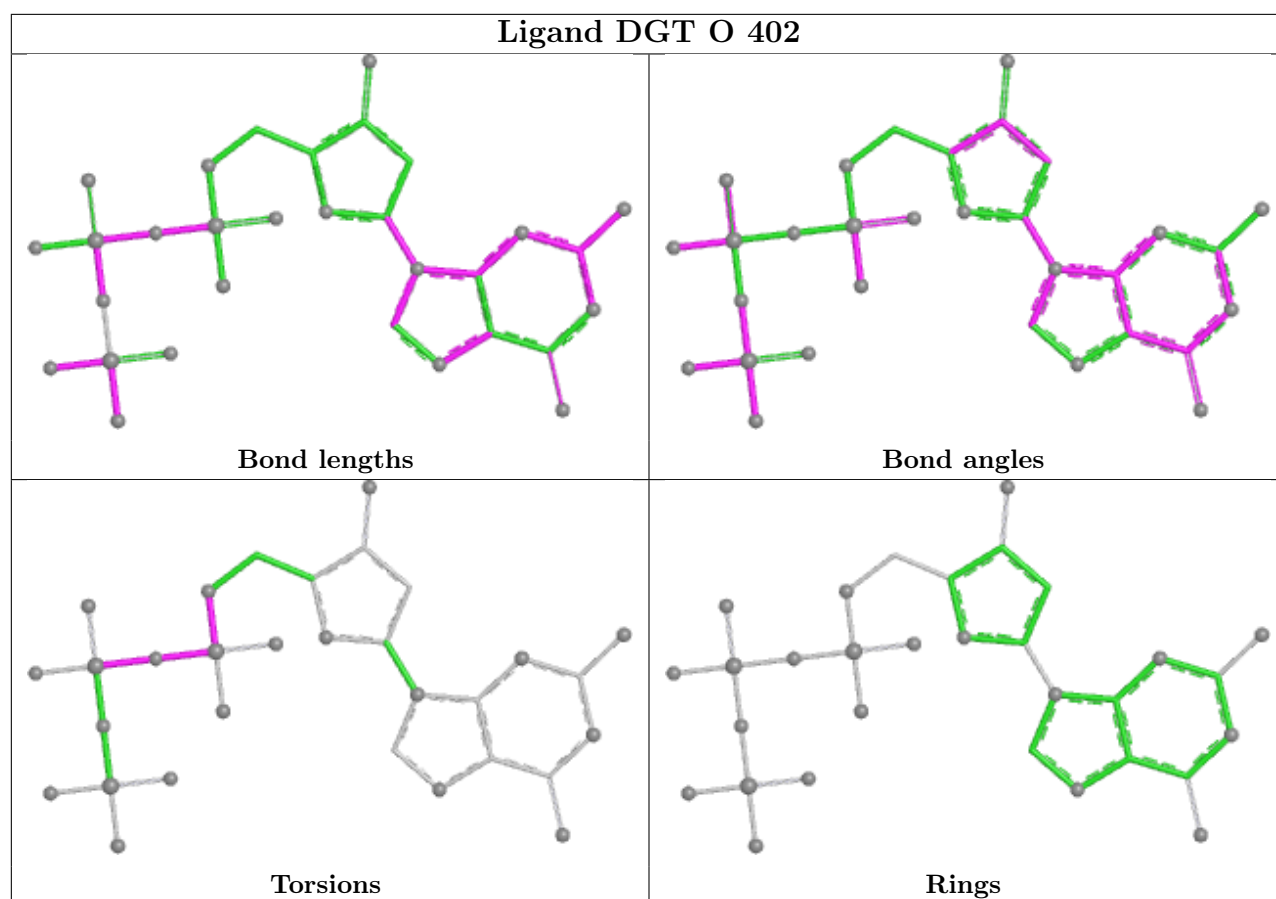


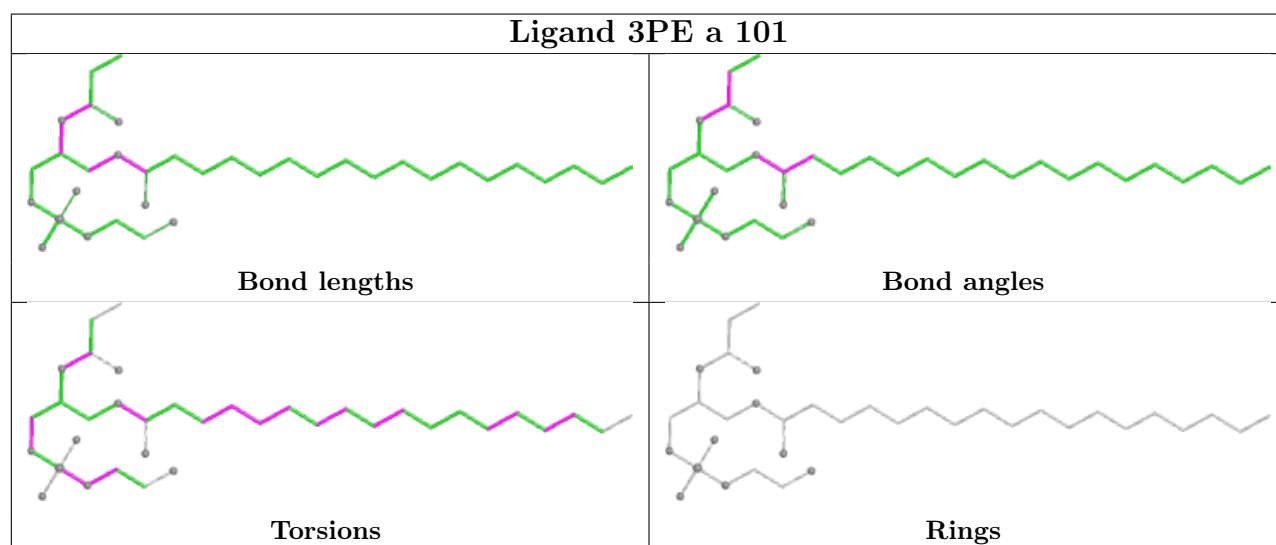
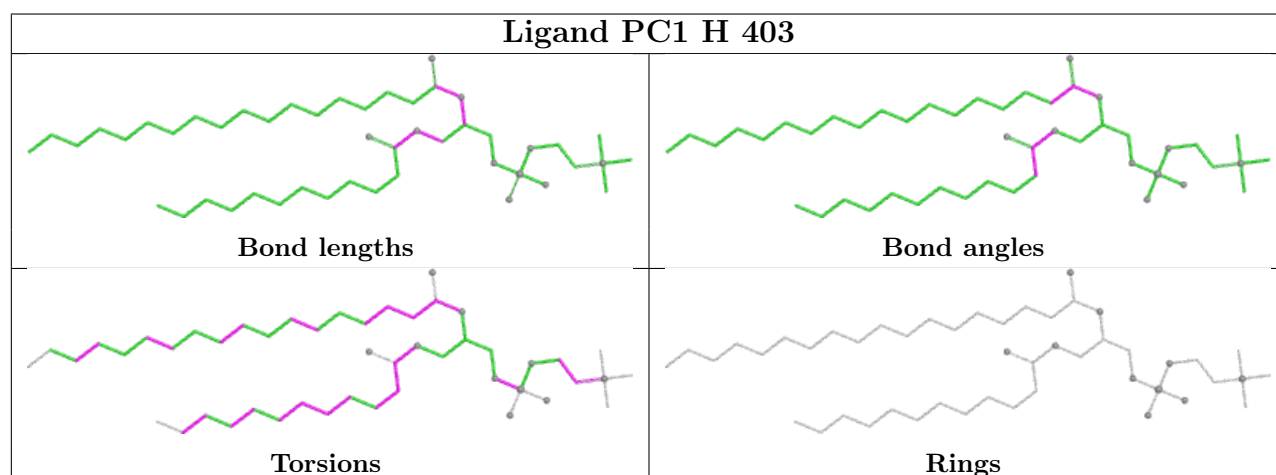
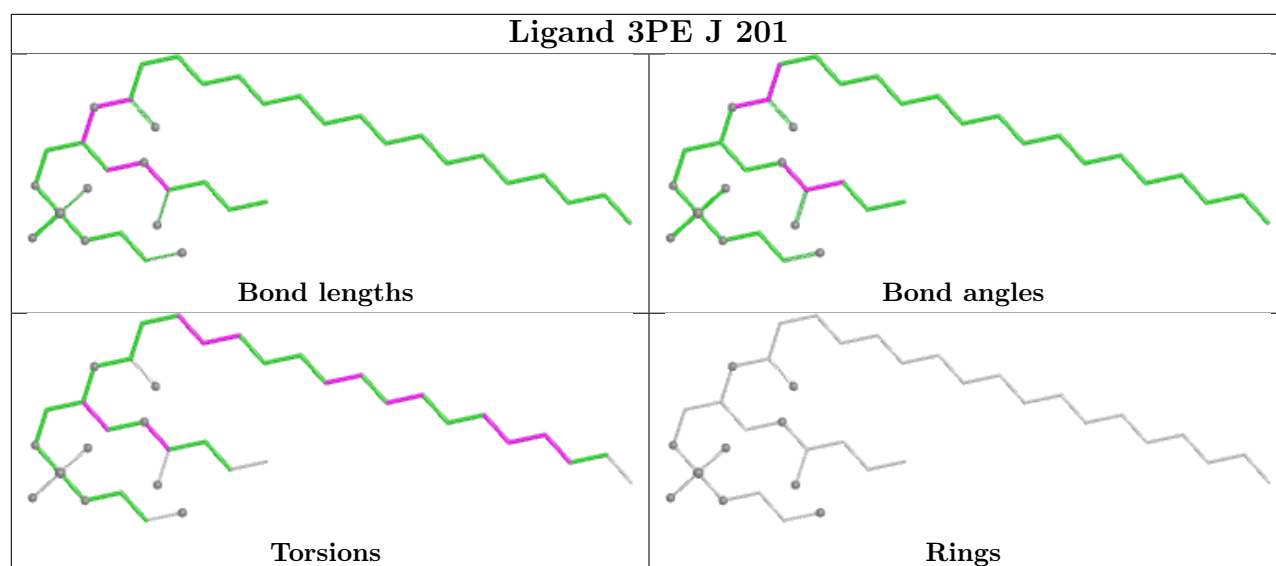
Ligand PC1 J 203

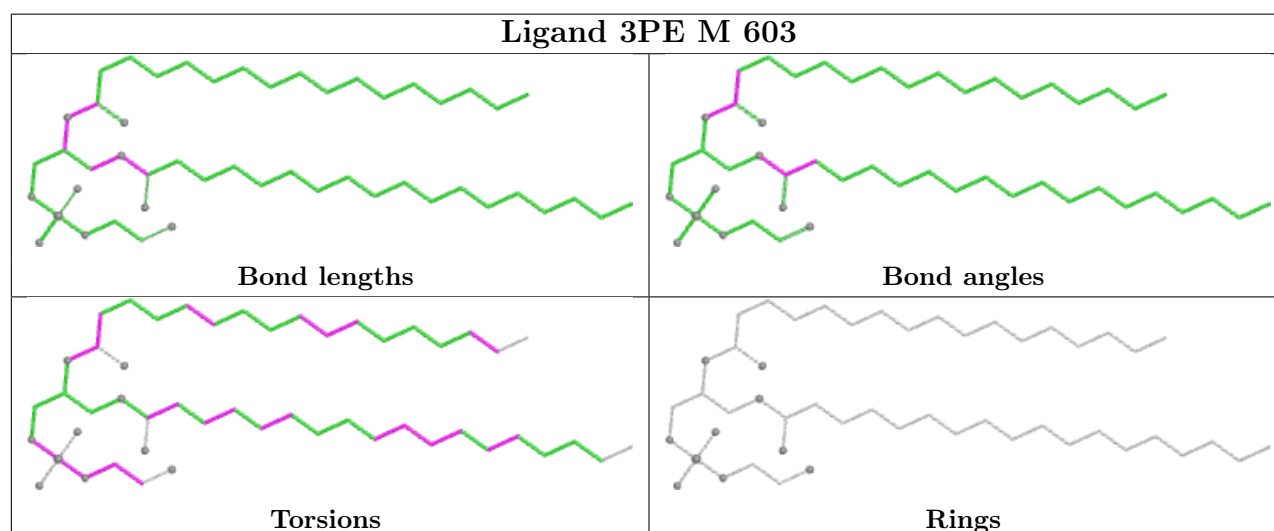
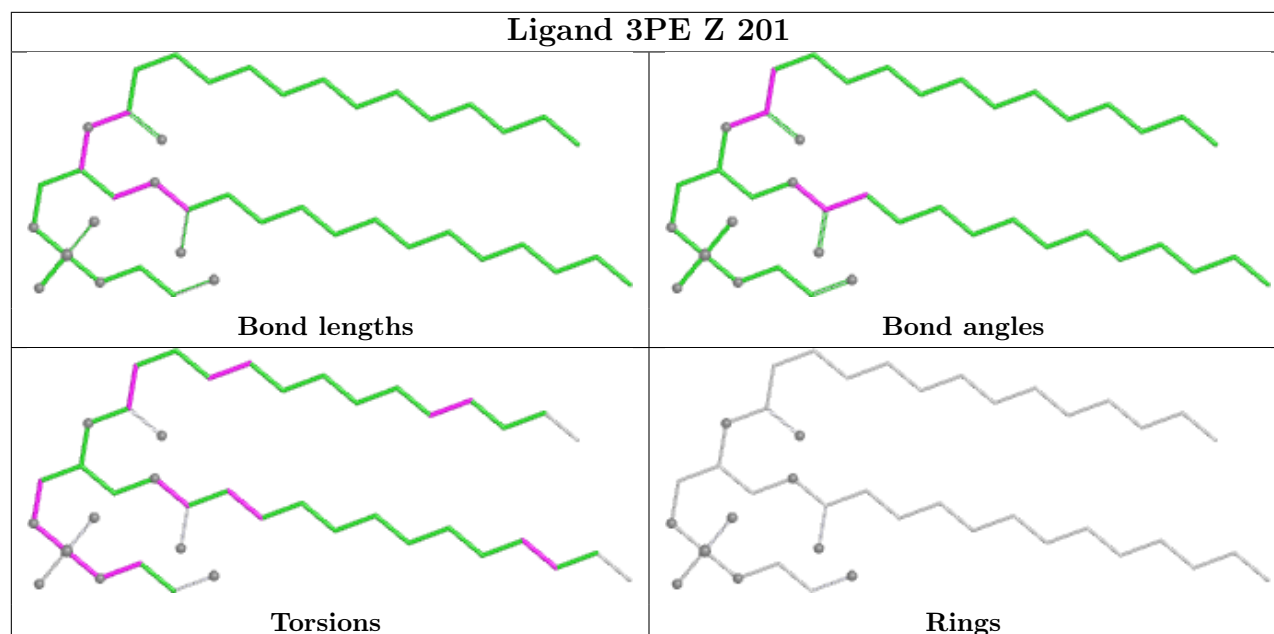
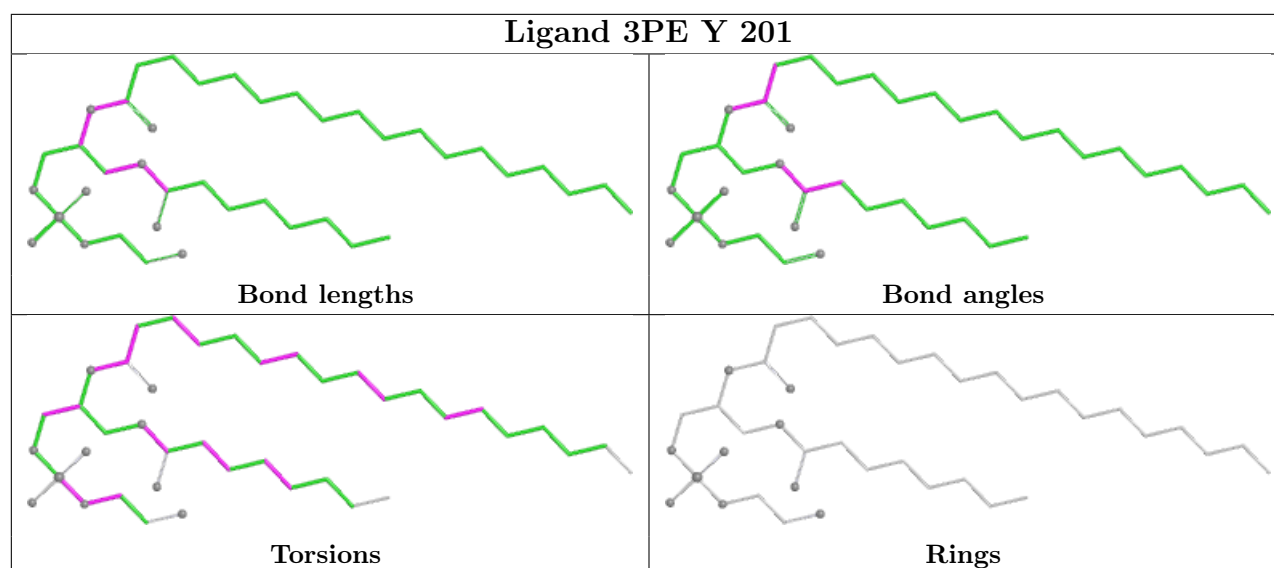


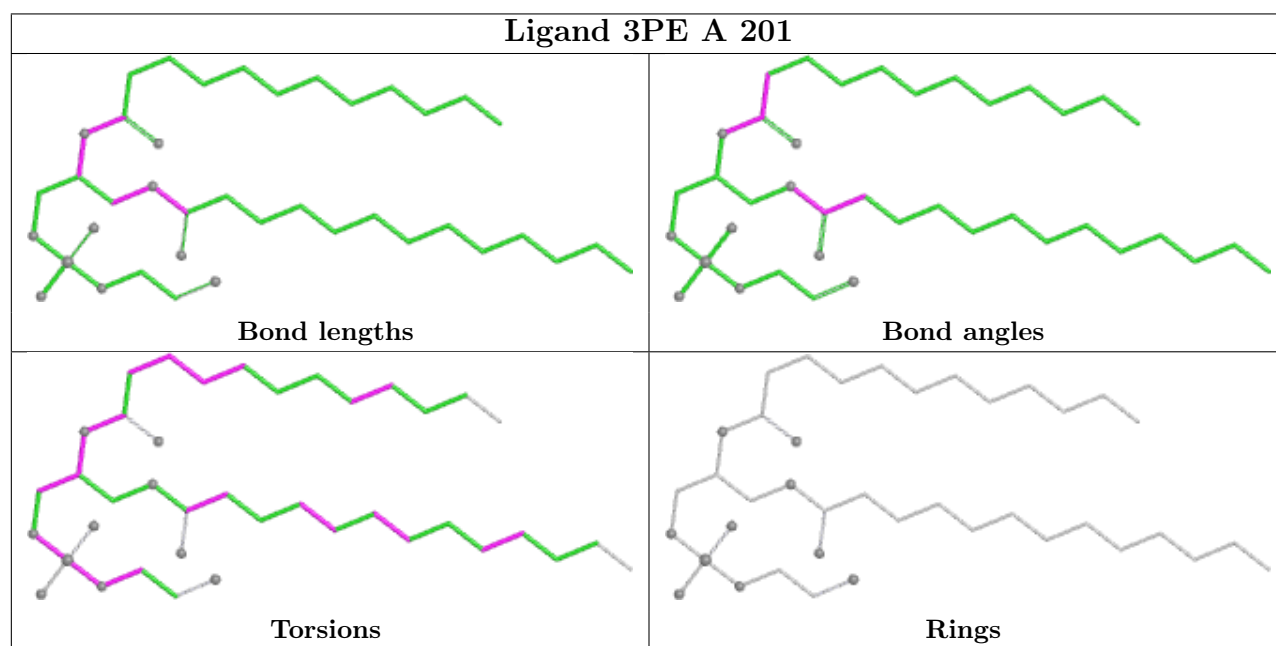
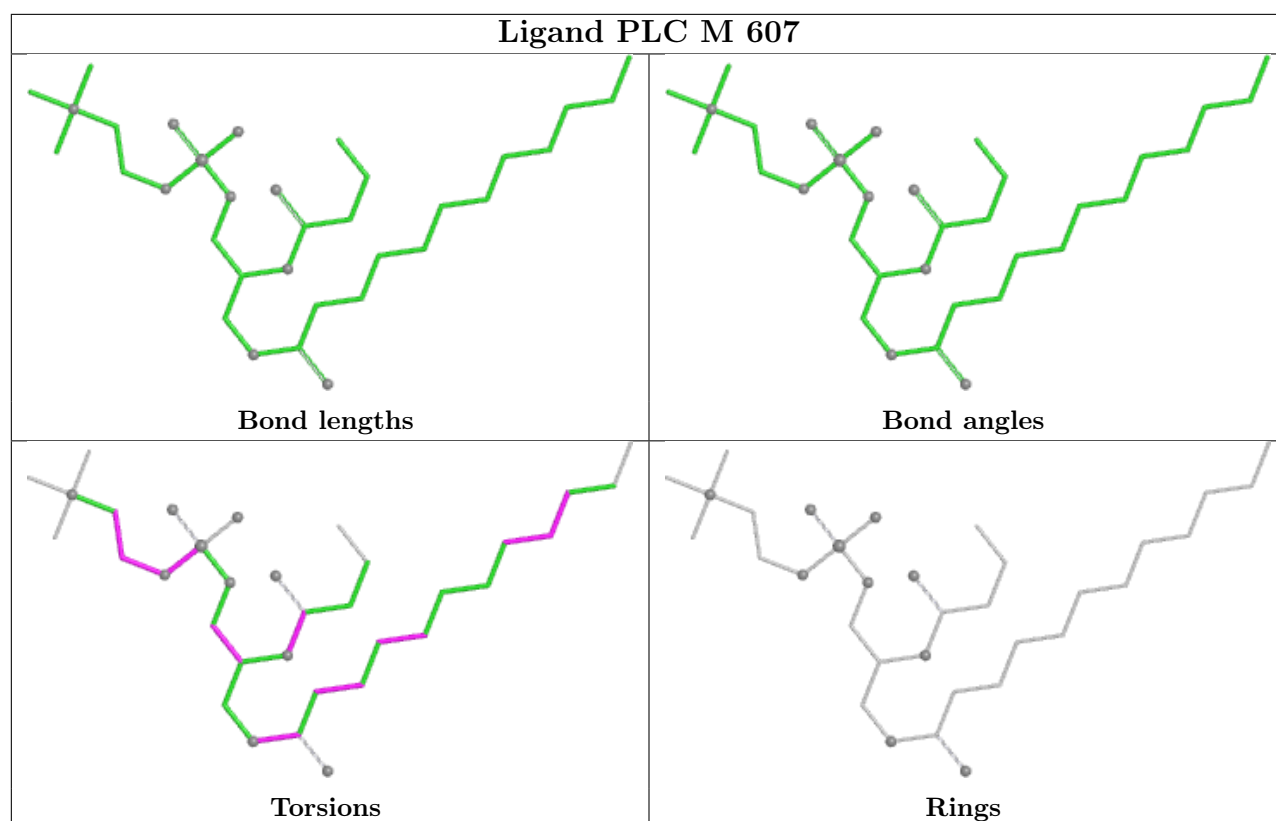


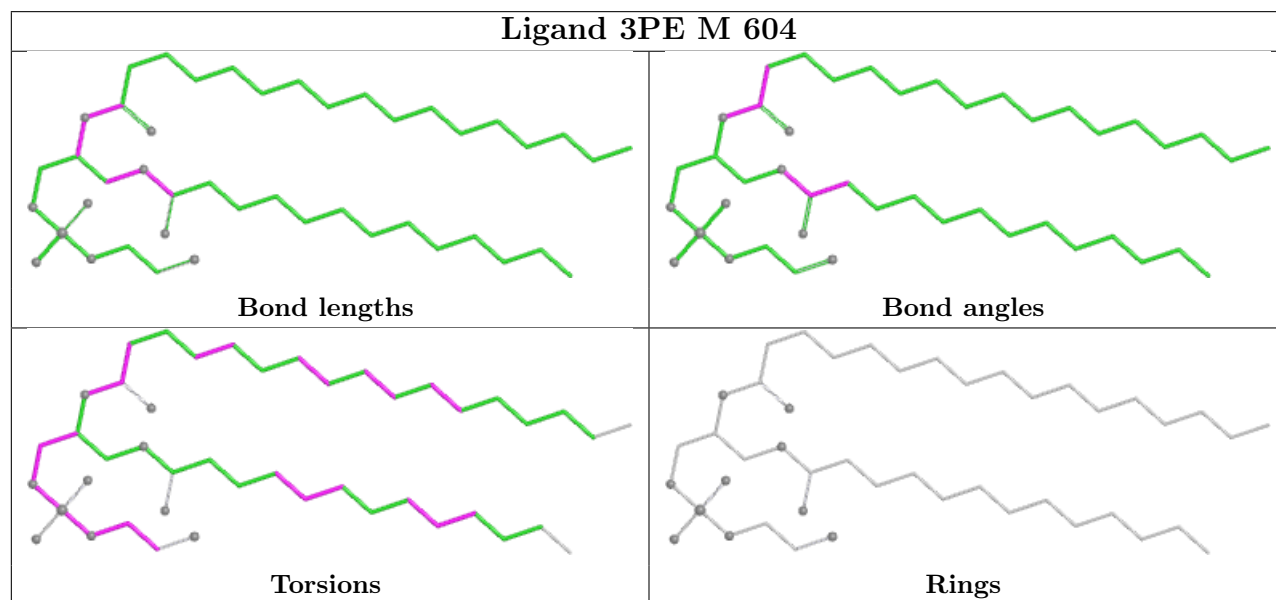
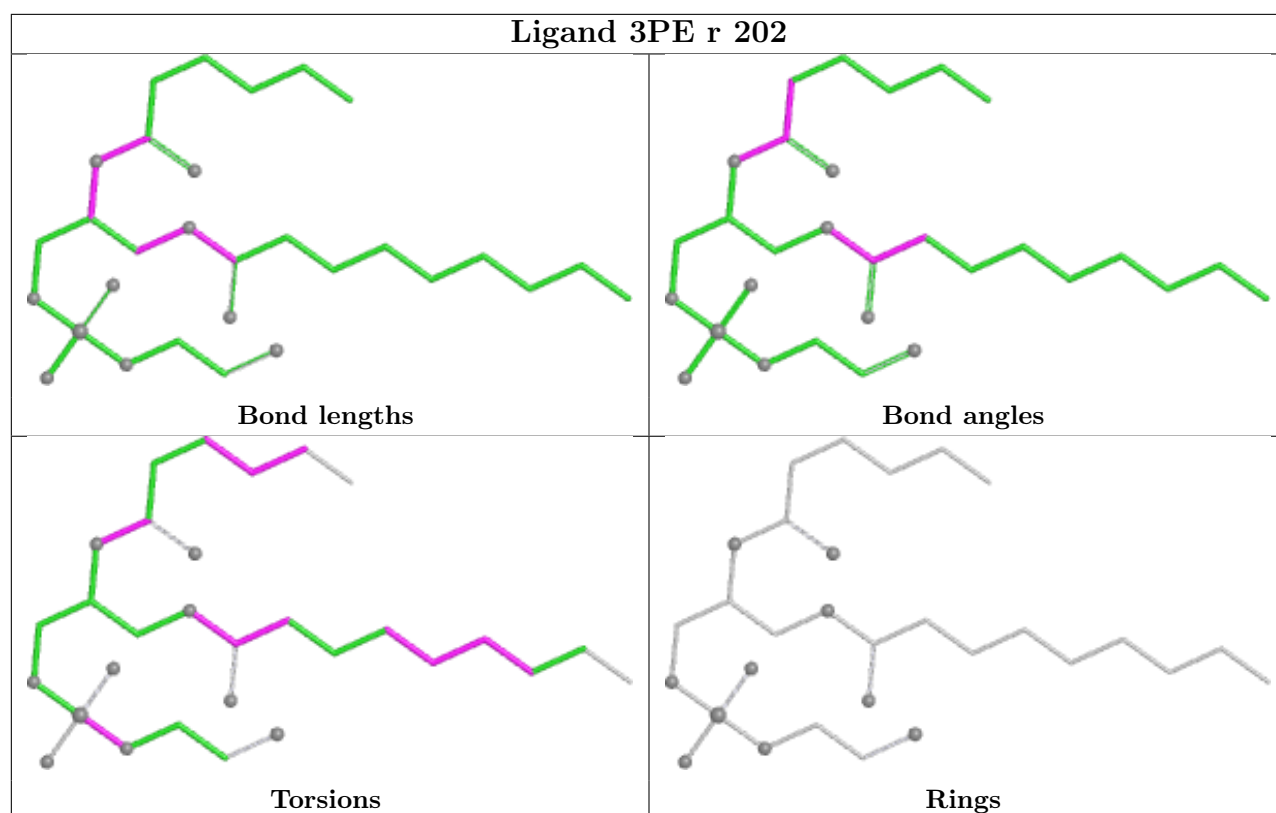


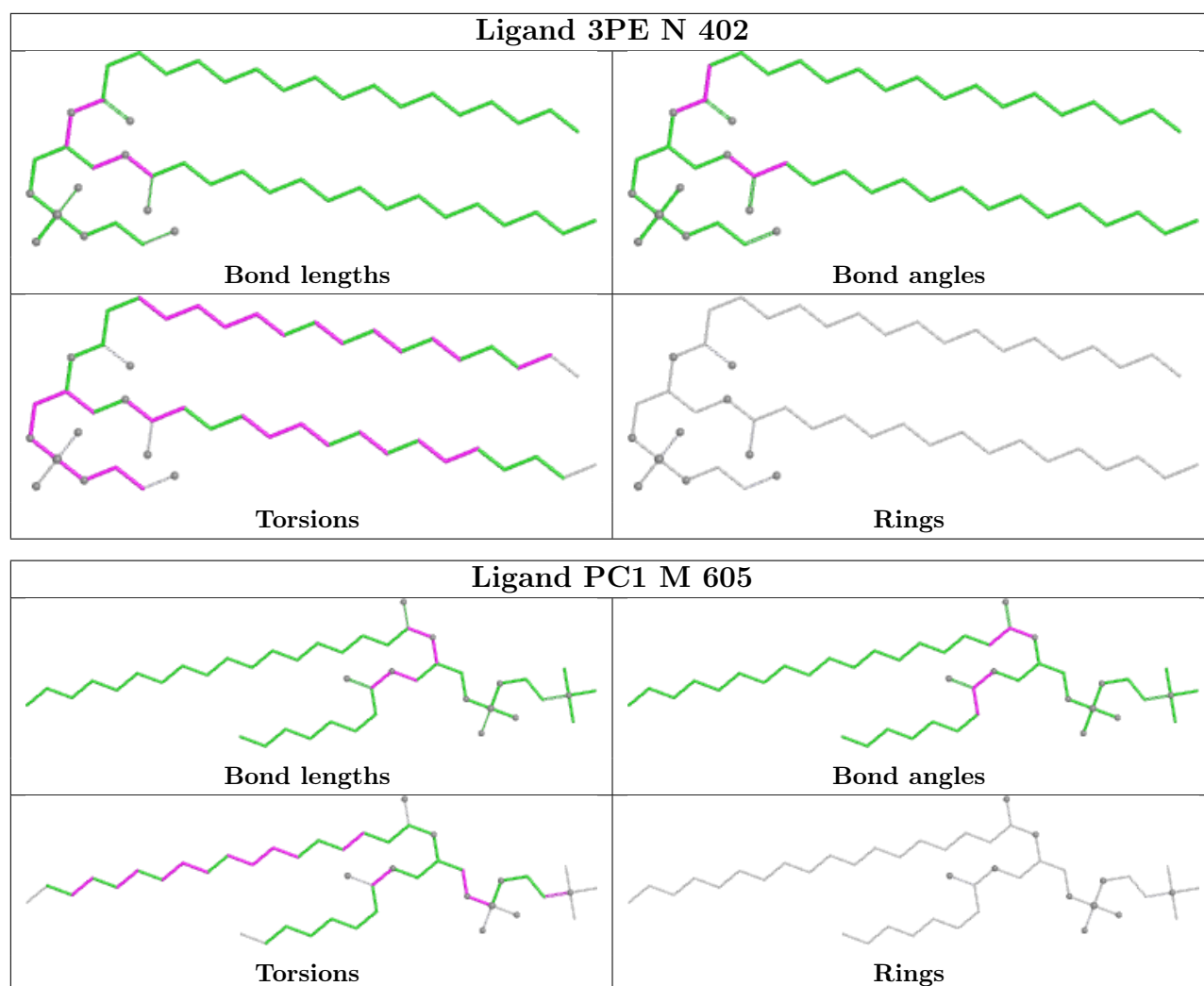


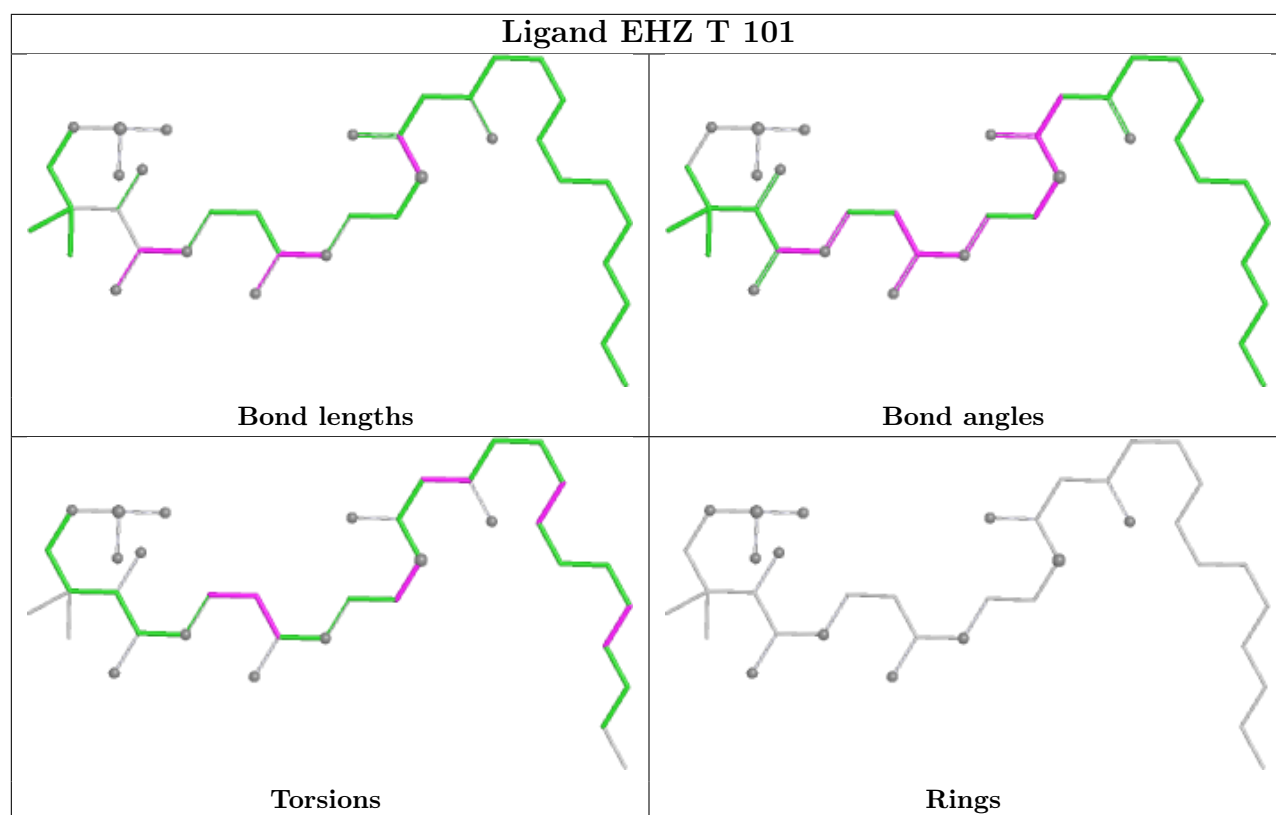












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

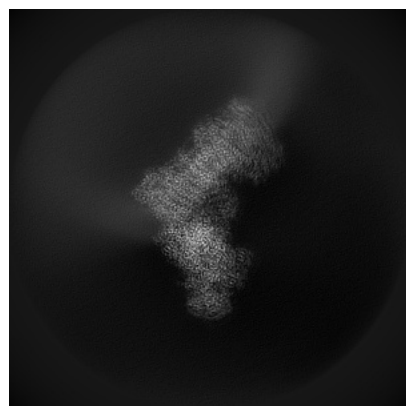
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18069. These allow visual inspection of the internal detail of the map and identification of artifacts.

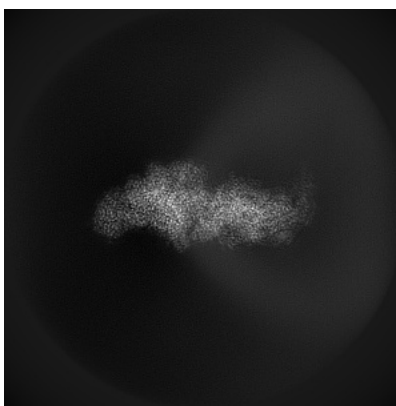
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

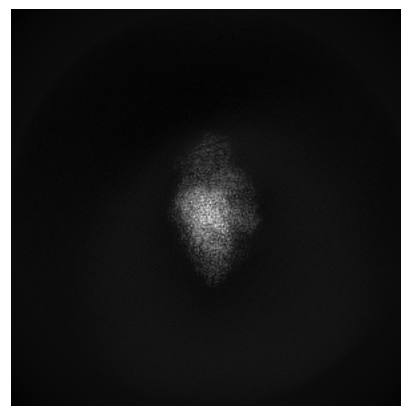
6.1.1 Primary map



X

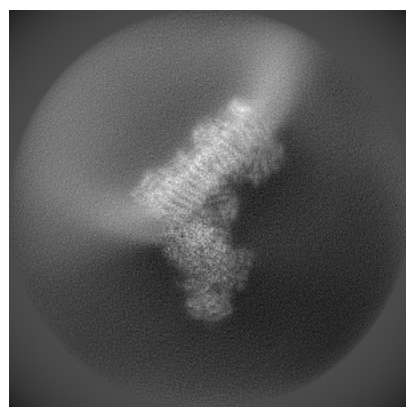


Y

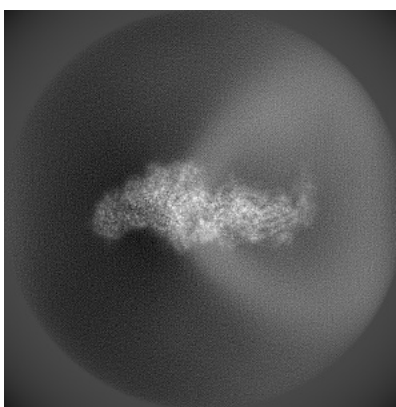


Z

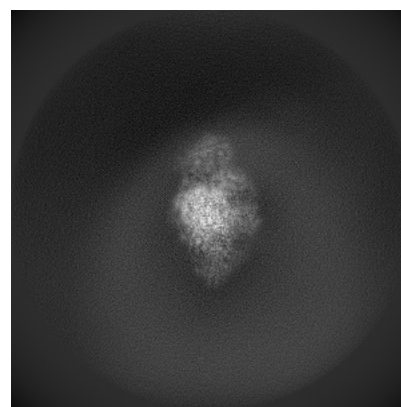
6.1.2 Raw map



X



Y



Z

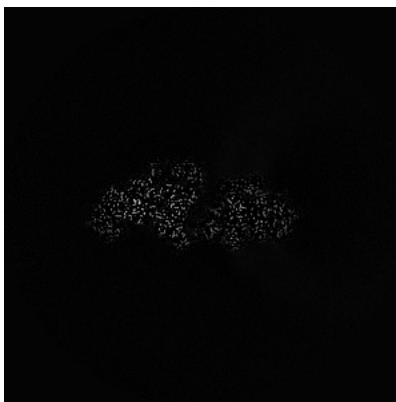
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

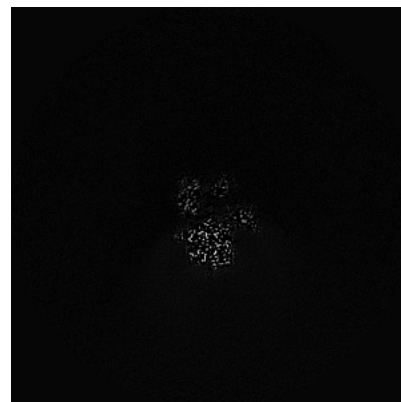
6.2.1 Primary map



X Index: 240

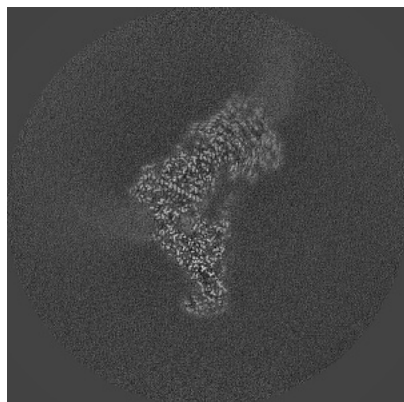


Y Index: 240

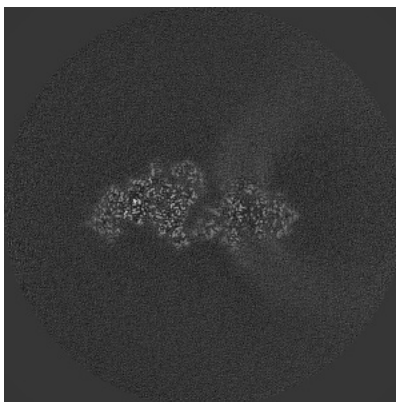


Z Index: 240

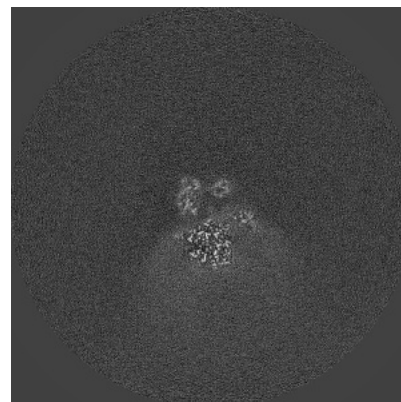
6.2.2 Raw map



X Index: 240



Y Index: 240

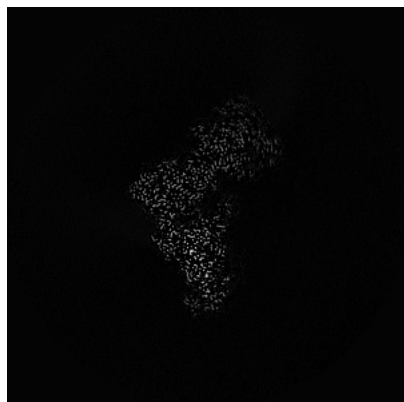


Z Index: 240

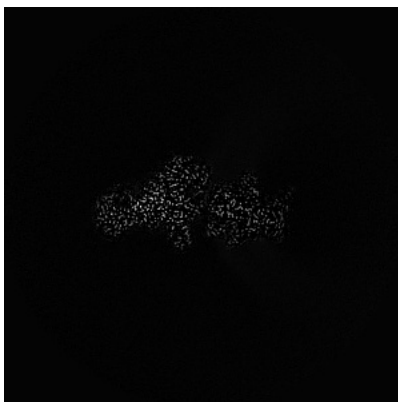
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 247

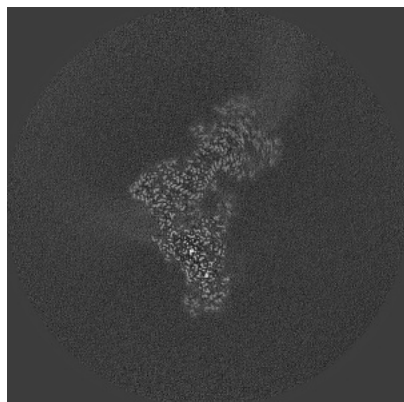


Y Index: 227

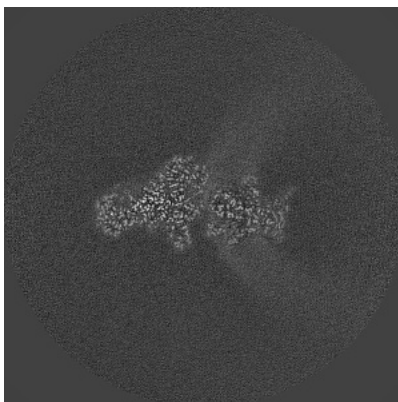


Z Index: 198

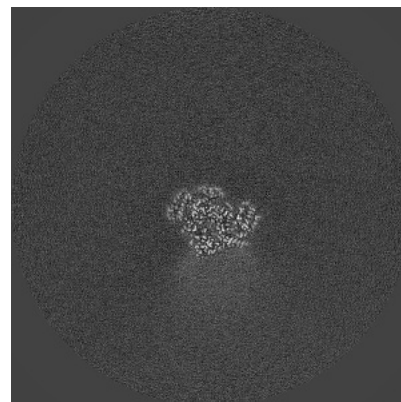
6.3.2 Raw map



X Index: 247



Y Index: 227

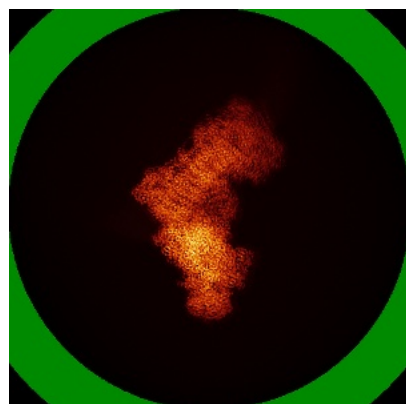


Z Index: 212

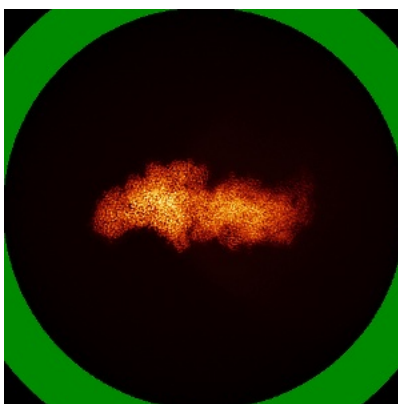
The images above show the largest variance slices of the map in three orthogonal directions.

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

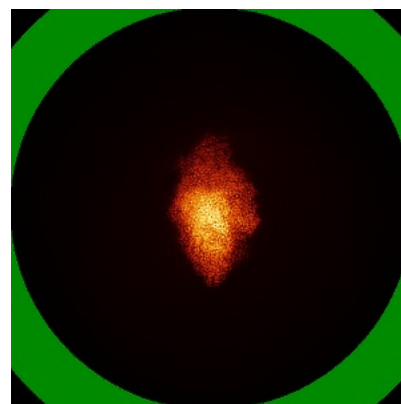
6.4.1 Primary map



X

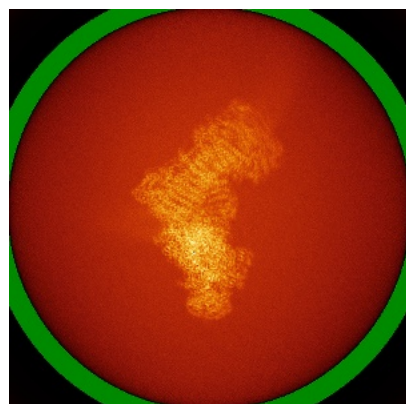


Y

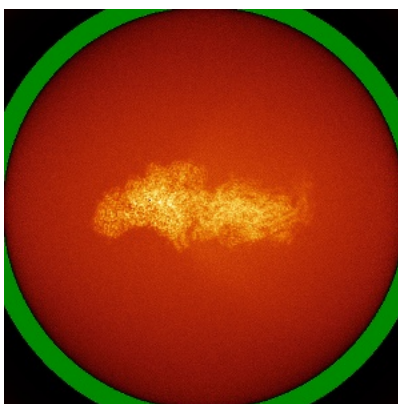


Z

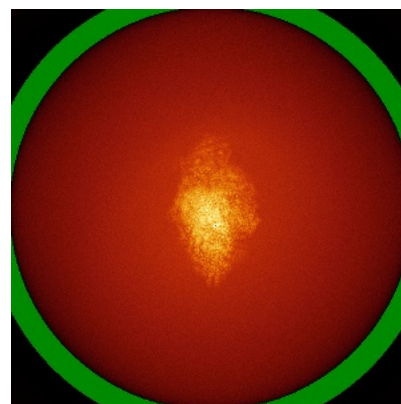
6.4.2 Raw map



X



Y



Z

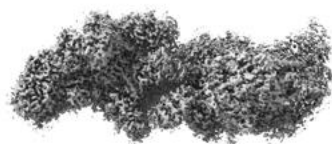
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



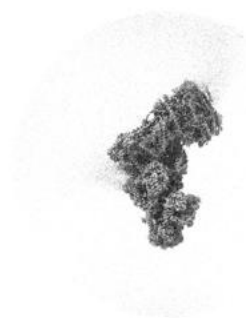
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

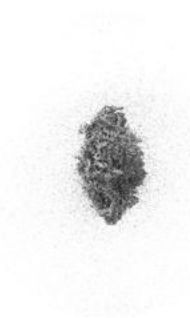
6.5.2 Raw map



X



Y



Z

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

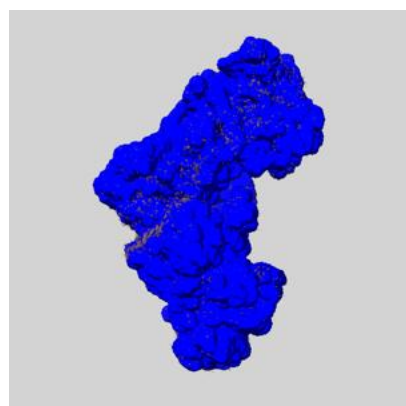
6.6 Mask visualisation [i](#)

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

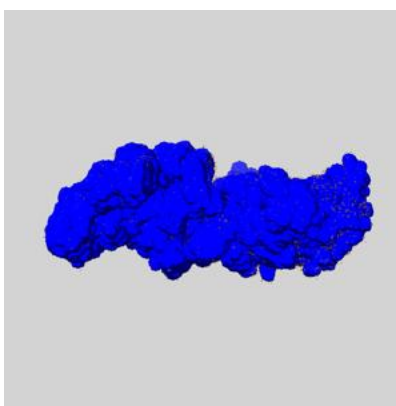
A mask typically either:

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

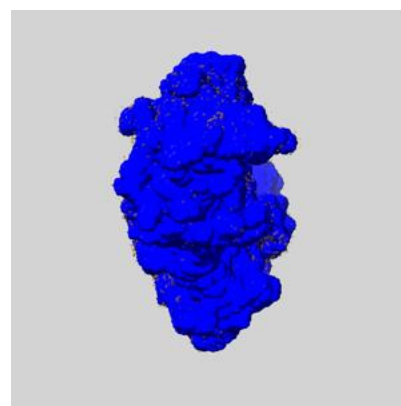
6.6.1 emd_18069_msk_1.map [i](#)



X



Y

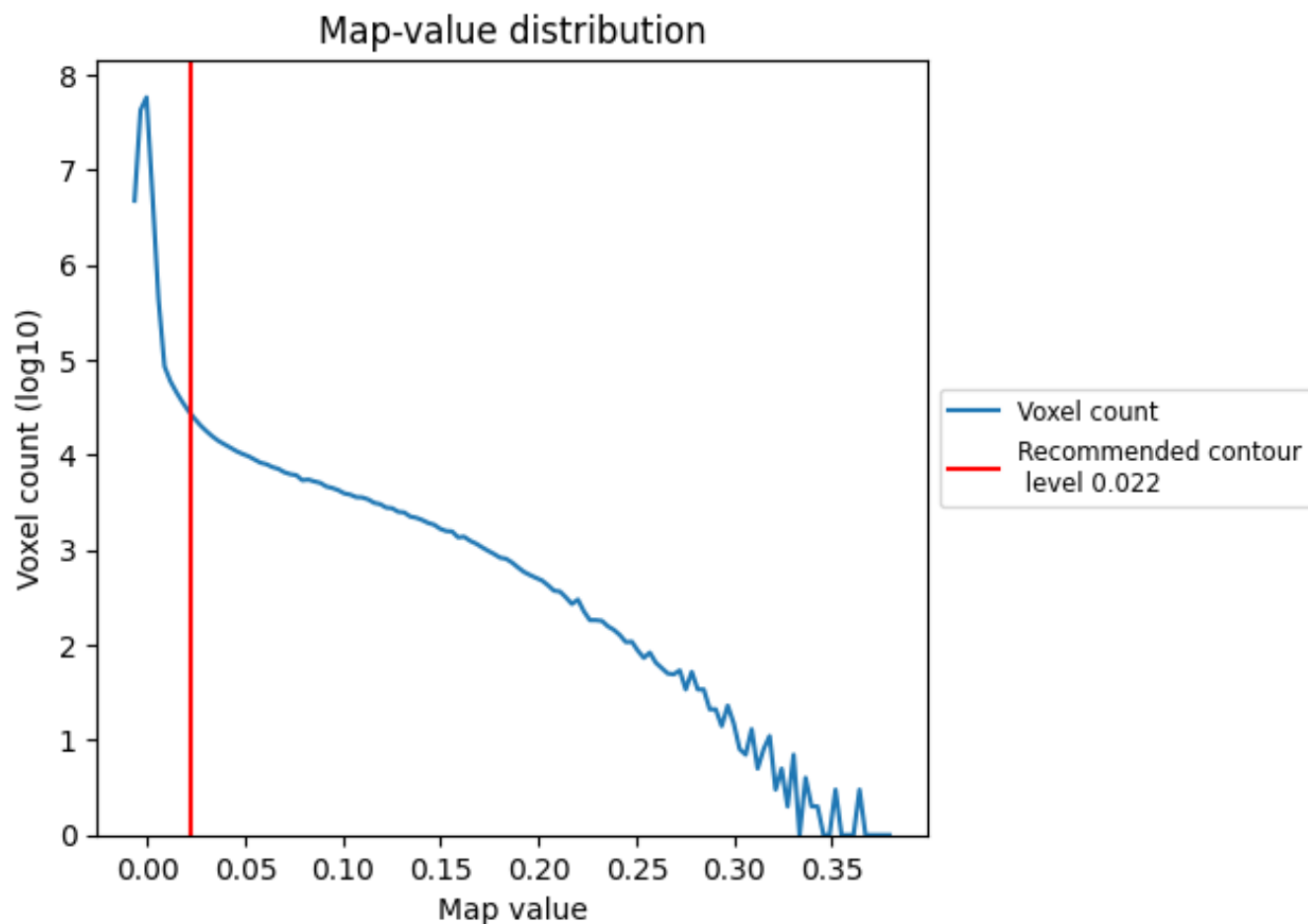


Z

7 Map analysis [i](#)

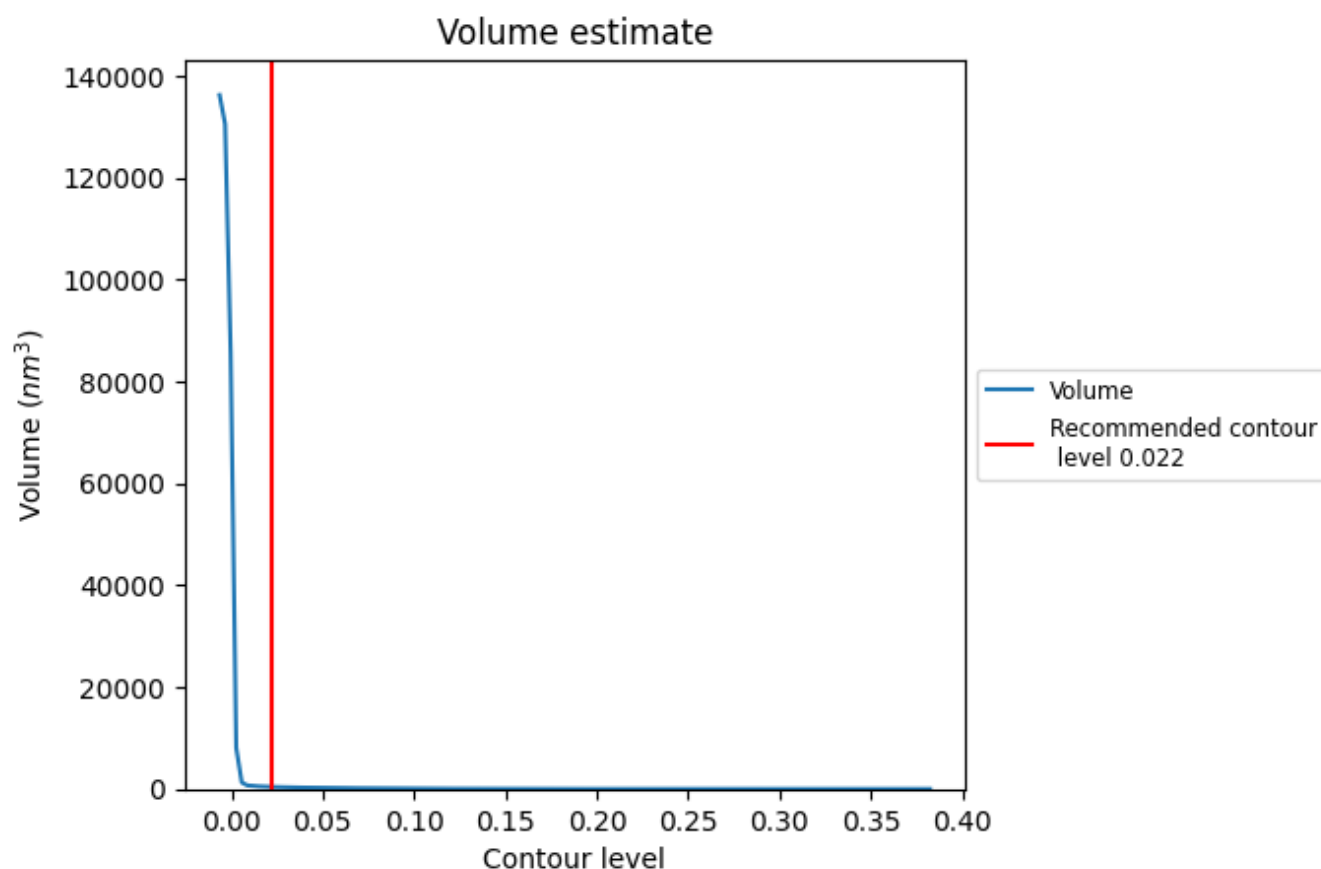
This section contains the results of statistical analysis of the map.

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.

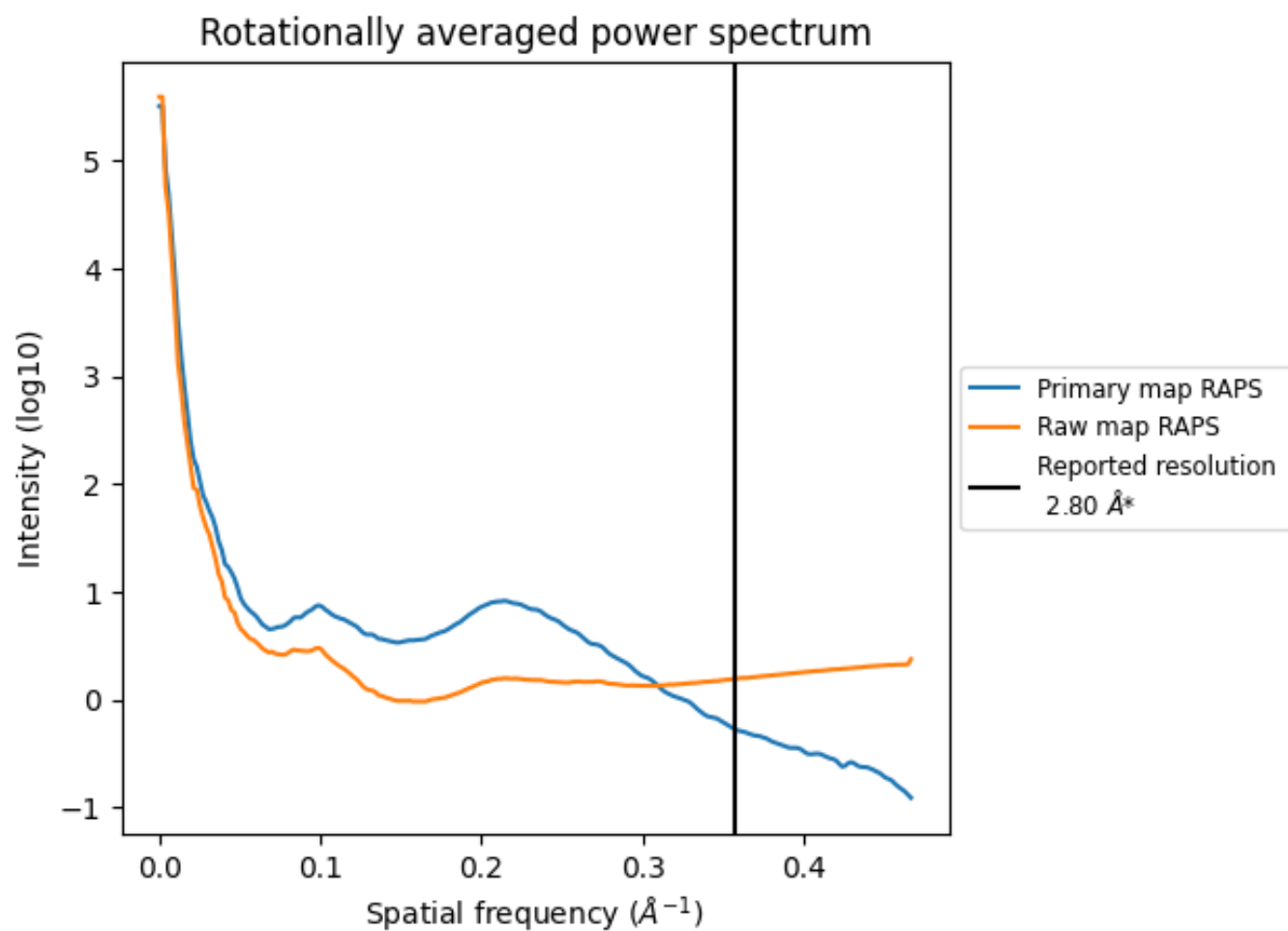
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm^3 ; this corresponds to an approximate mass of 365 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 ⓘ

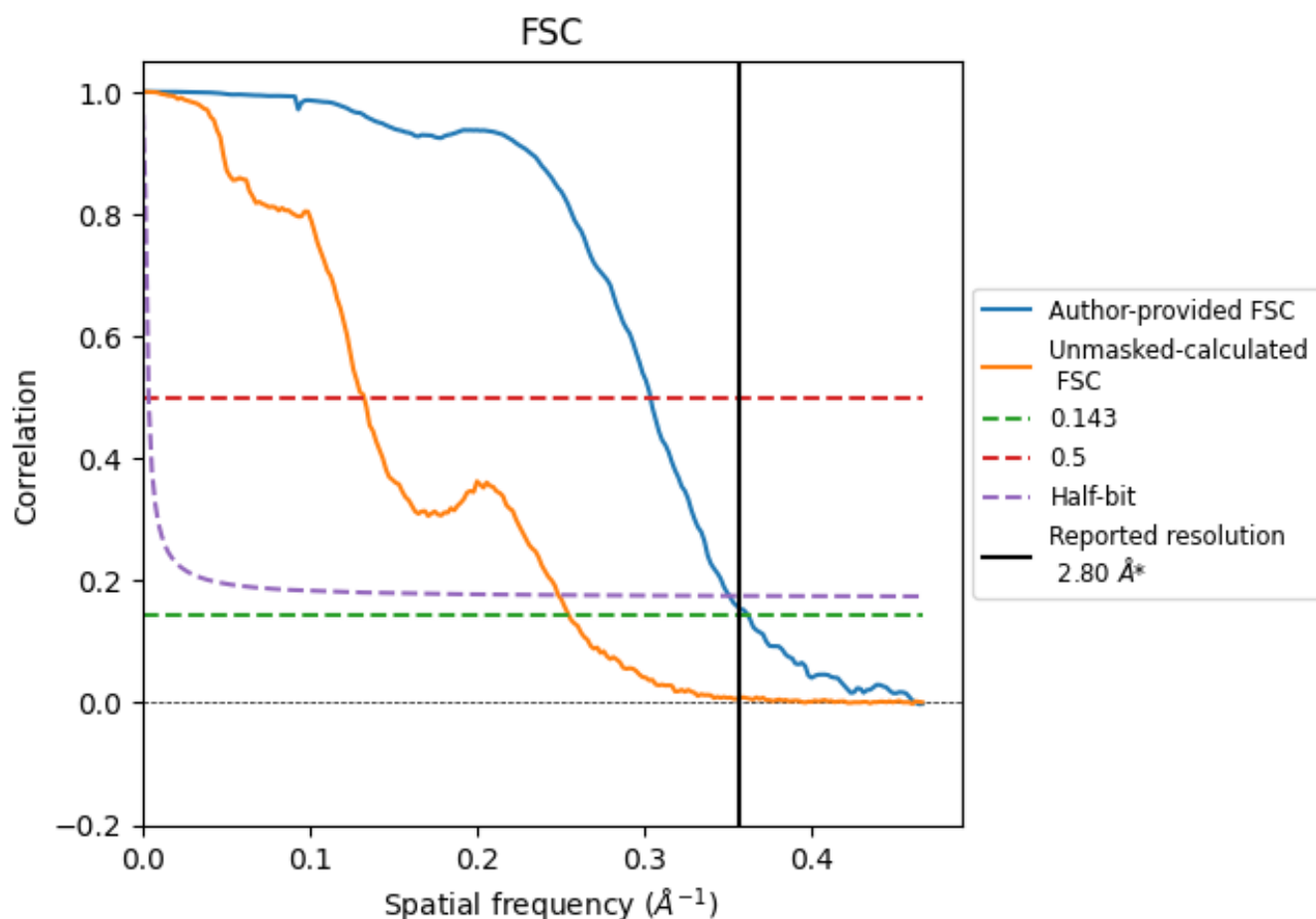


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

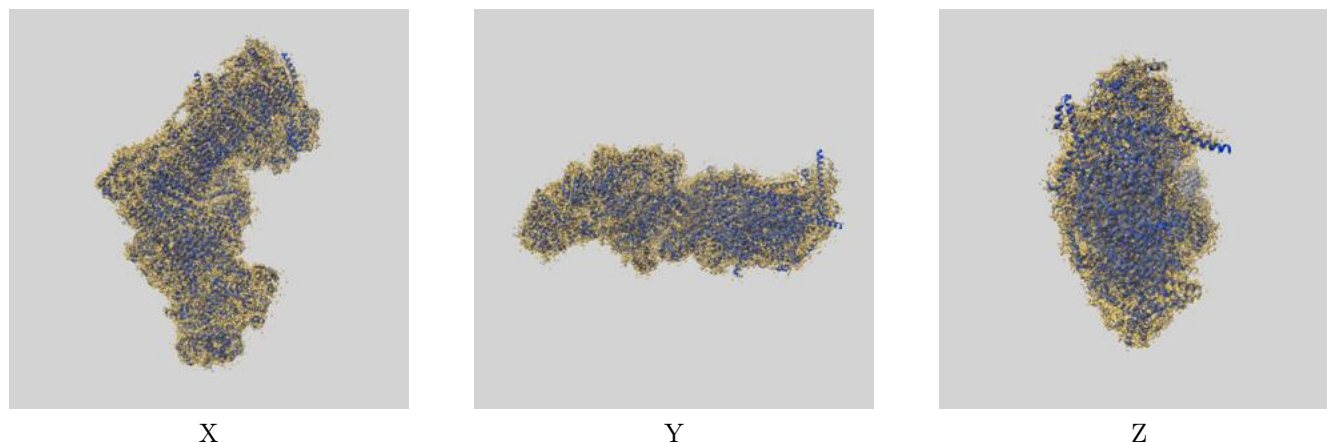
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.29	2.85
Unmasked-calculated*	3.92	7.55	4.02

*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 3.92 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

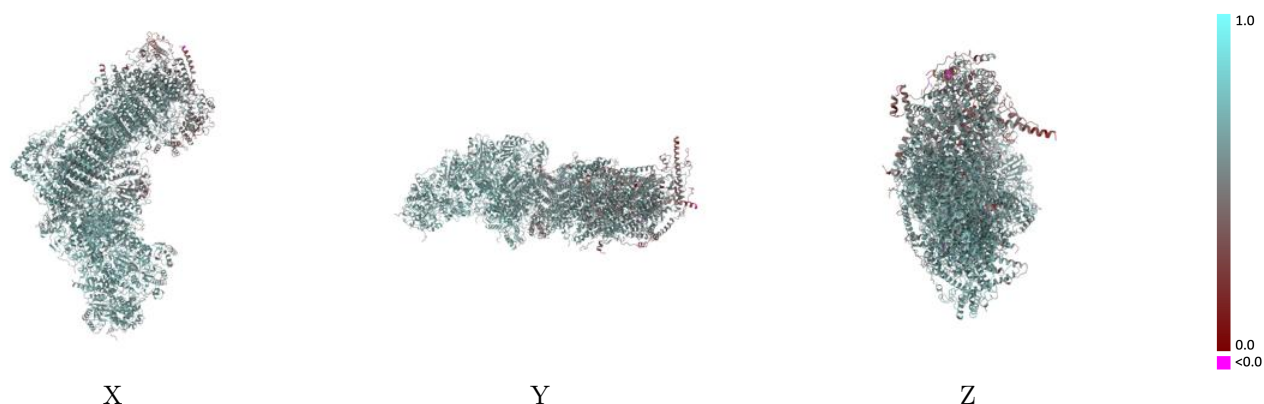
This section contains information regarding the fit between EMDB map EMD-18069 and PDB model 8Q25. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

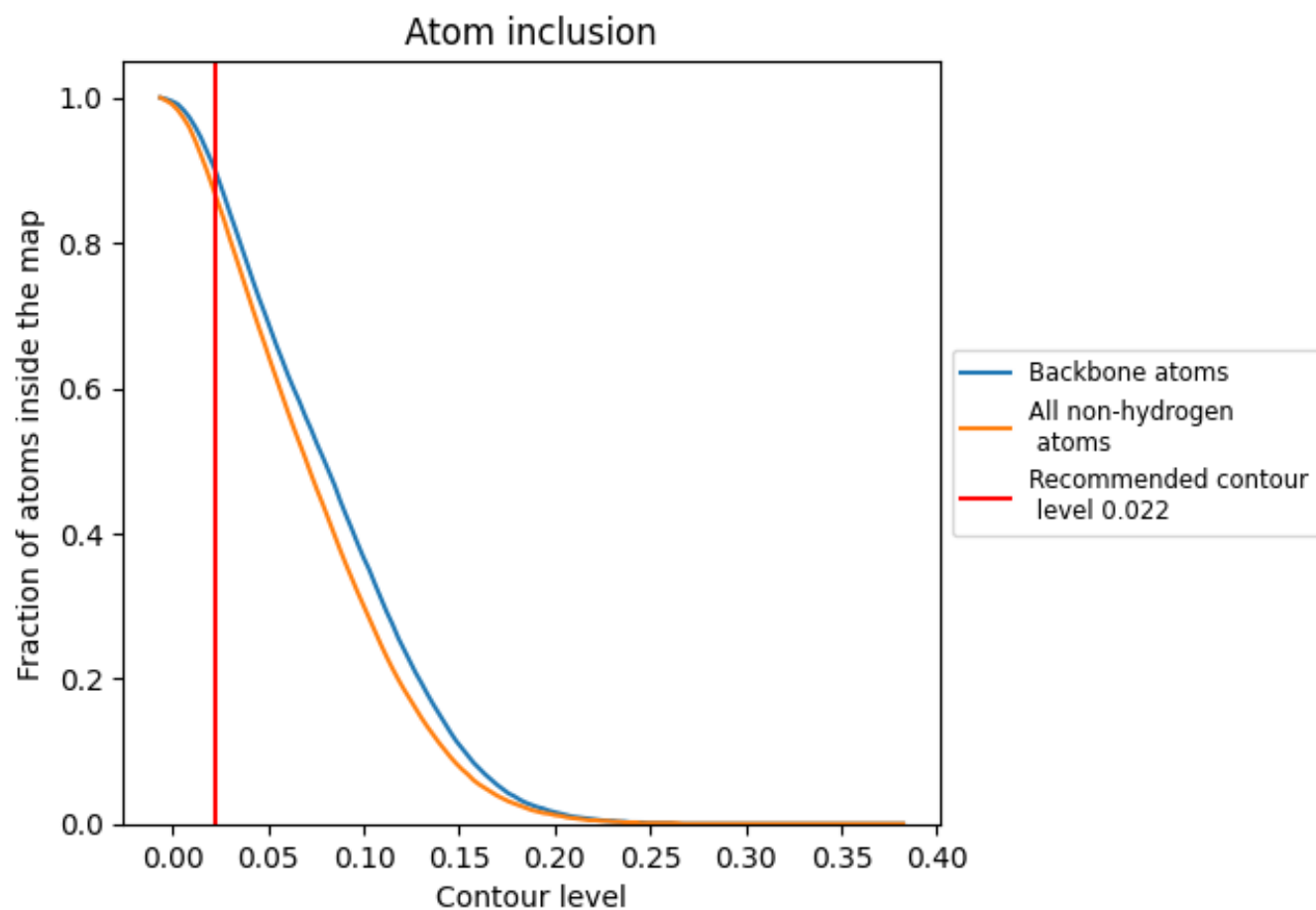


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.5970
A	 0.8980	 0.6190
B	 0.9580	 0.6580
C	 0.9680	 0.6650
D	 0.9580	 0.6630
E	 0.8860	 0.5980
F	 0.9120	 0.6170
G	 0.9280	 0.6370
H	 0.9400	 0.6390
I	 0.9590	 0.6690
J	 0.8900	 0.6010
K	 0.9590	 0.6480
L	 0.8370	 0.5630
M	 0.9350	 0.6330
N	 0.9570	 0.6540
O	 0.8160	 0.5560
P	 0.9020	 0.6180
Q	 0.9270	 0.6500
R	 0.9110	 0.6340
S	 0.7930	 0.5560
T	 0.6820	 0.4770
U	 0.6190	 0.4390
V	 0.8890	 0.6050
W	 0.9140	 0.6360
X	 0.9020	 0.6190
Y	 0.8460	 0.5860
Z	 0.8900	 0.6140
a	 0.9330	 0.6310
b	 0.8680	 0.5980
c	 0.8350	 0.5750
d	 0.9000	 0.6120
e	 0.8730	 0.6090
f	 0.7060	 0.5350
g	 0.8010	 0.5550
h	 0.8840	 0.6010



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.5930	 0.4400
j	 0.5620	 0.4110
k	 0.4960	 0.3830
l	 0.7760	 0.5140
m	 0.7880	 0.5470
n	 0.7330	 0.4970
o	 0.5330	 0.3980
p	 0.7700	 0.5260
q	 0.8980	 0.6300
r	 0.9160	 0.6420
s	 0.8090	 0.5600