



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 06:29 pm BST

PDB ID : 7QHM
EMDB ID : EMD-13976
Title : Cytochrome bcc-aa3 supercomplex (respiratory supercomplex III2/IV2) from *Corynebacterium glutamicum* (stigmatellin and azide bound)
Authors : Kao, W.-C.; Hunte, C.
Deposited on : 2021-12-13
Resolution : 2.80 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

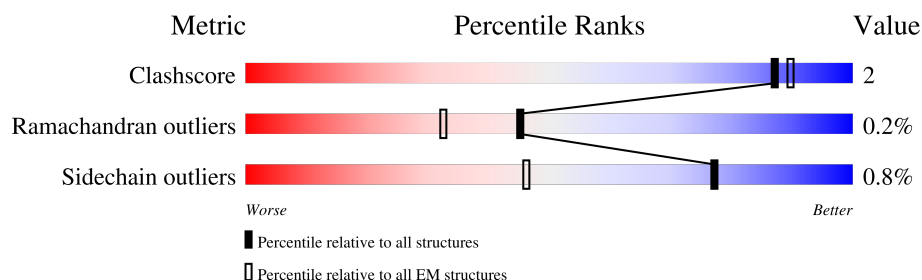
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



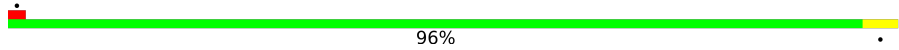
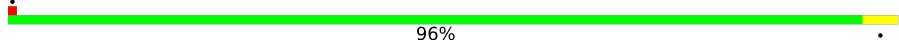
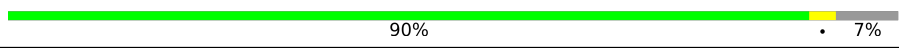
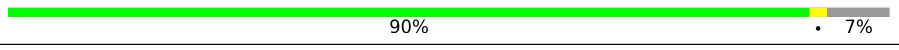
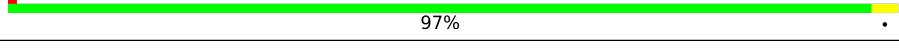
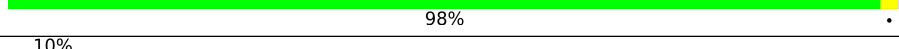
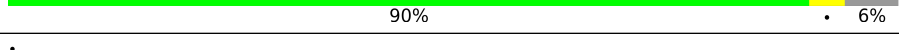
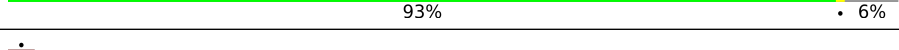
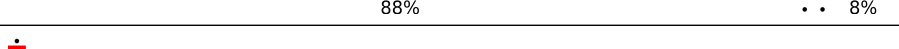
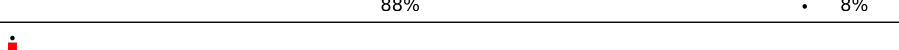

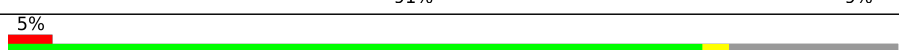

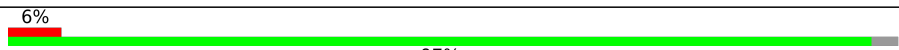
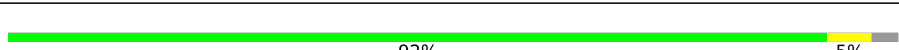



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	408	94% 5% .
1	N	408	93% 6% .
2	B	539	93% 6% .
2	O	539	94% 5% .
3	C	283	77% 5% 18%
3	P	283	78% . 18%
4	D	594	93% . .
4	Q	594	92% 5% .

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Mol	Chain	Length	Quality of chain
5	E	331	
5	R	331	
6	F	205	
6	S	205	
7	G	143	
7	T	143	
8	H	163	
8	U	163	
9	I	147	
9	V	147	
10	J	112	
10	W	112	
11	K	73	
11	X	73	
12	L	65	
12	Y	65	
13	M	168	
13	Z	168	

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
25	HAS	D	601	X	-	-	-
25	HAS	D	602	X	-	-	-
25	HAS	Q	601	X	-	-	-
25	HAS	Q	602	X	-	-	-
29	AZI	D	606	-	-	X	-

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 97775 atoms, of which 48245 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	402	Total	C	H	N	O	S	2	0
			6231	2004	3084	540	587	16		
1	N	401	Total	C	H	N	O	S	4	0
			6224	2004	3079	539	586	16		

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	534	Total	C	H	N	O	S	6	0
			8485	2765	4268	709	721	22		
2	O	534	Total	C	H	N	O	S	0	0
			8425	2746	4239	703	715	22		

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	233	Total	C	H	N	O	S	2	0
			3443	1089	1694	306	344	10		
3	P	233	Total	C	H	N	O	S	0	0
			3418	1083	1680	302	343	10		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	576	Total	C	H	N	O	S	0	0
			9018	3031	4470	735	750	32		
4	Q	576	Total	C	H	N	O	S	2	0
			9034	3036	4477	736	753	32		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	585	ALA	-	expression tag	UNP Q79VD7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	586	ALA	-	expression tag	UNP Q79VD7
D	587	TRP	-	expression tag	UNP Q79VD7
D	588	SER	-	expression tag	UNP Q79VD7
D	589	HIS	-	expression tag	UNP Q79VD7
D	590	PRO	-	expression tag	UNP Q79VD7
D	591	GLN	-	expression tag	UNP Q79VD7
D	592	PHE	-	expression tag	UNP Q79VD7
D	593	GLU	-	expression tag	UNP Q79VD7
D	594	LYS	-	expression tag	UNP Q79VD7
Q	585	ALA	-	expression tag	UNP Q79VD7
Q	586	ALA	-	expression tag	UNP Q79VD7
Q	587	TRP	-	expression tag	UNP Q79VD7
Q	588	SER	-	expression tag	UNP Q79VD7
Q	589	HIS	-	expression tag	UNP Q79VD7
Q	590	PRO	-	expression tag	UNP Q79VD7
Q	591	GLN	-	expression tag	UNP Q79VD7
Q	592	PHE	-	expression tag	UNP Q79VD7
Q	593	GLU	-	expression tag	UNP Q79VD7
Q	594	LYS	-	expression tag	UNP Q79VD7

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	331	Total	C	H	N	O	S	0	0
			5066	1660	2468	429	498	11		
5	R	331	Total	C	H	N	O	S	2	0
			5089	1666	2482	431	499	11		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	190	Total	C	H	N	O	S	0	0
			2981	992	1495	236	251	7		
6	S	190	Total	C	H	N	O	S	0	0
			2980	992	1494	236	251	7		

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	143	Total	C	H	N	O	S	0	0
			2201	728	1106	167	191	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	143	Total	C	H	N	O	S	2	0
			2219	734	1114	170	192	9		

- Molecule 8 is a protein called Uncharacterized protein Cgl2664/cg2949.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	153	Total	C	H	N	O	S	0	0
			2174	684	1054	184	249	3		
8	U	154	Total	C	H	N	O	S	0	0
			2181	686	1057	185	250	3		

- Molecule 9 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	135	Total	C	H	N	O	S	0	0
			2144	691	1071	190	191	1		
9	V	135	Total	C	H	N	O	S	0	0
			2144	691	1071	190	191	1		

- Molecule 10 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	102	Total	C	H	N	O	S	0	0
			1571	506	792	134	136	3		
10	W	102	Total	C	H	N	O	S	0	0
			1571	506	792	134	136	3		

- Molecule 11 is a protein called Actinobacterial supercomplex, subunit C (AscC).

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	59	Total	C	H	N	O		0	0
			901	297	432	81	91			
11	X	57	Total	C	H	N	O		0	0
			864	286	413	78	87			

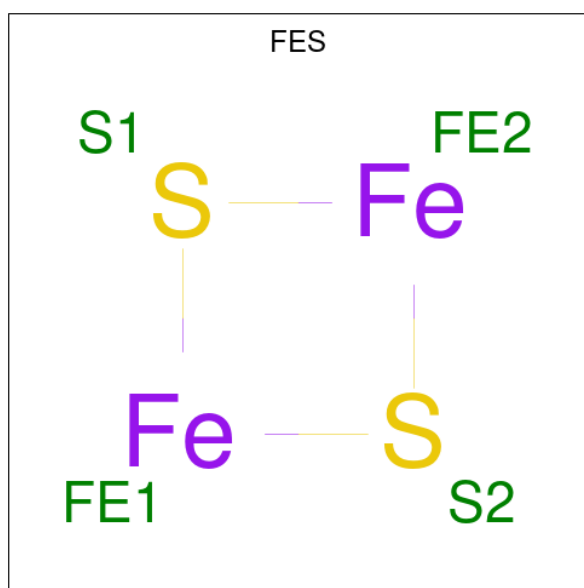
- Molecule 12 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	63	Total	C	H	N	O	S	0	0
			915	294	470	70	78	3		
12	Y	63	Total	C	H	N	O	S	0	0
			915	294	470	70	78	3		

- Molecule 13 is a protein called Thiamine biosynthesis protein X.

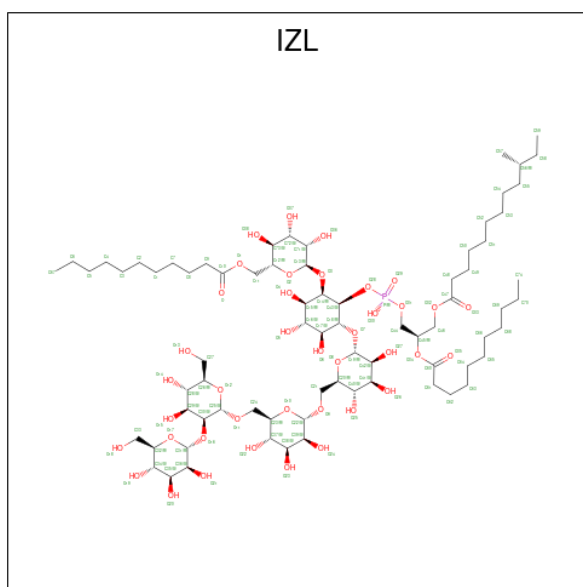
Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	22	Total	C	H	N	O	S	0	0
			330	101	159	32	37	1		
13	Z	24	Total	C	H	N	O	S	0	0
			358	110	172	35	40	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



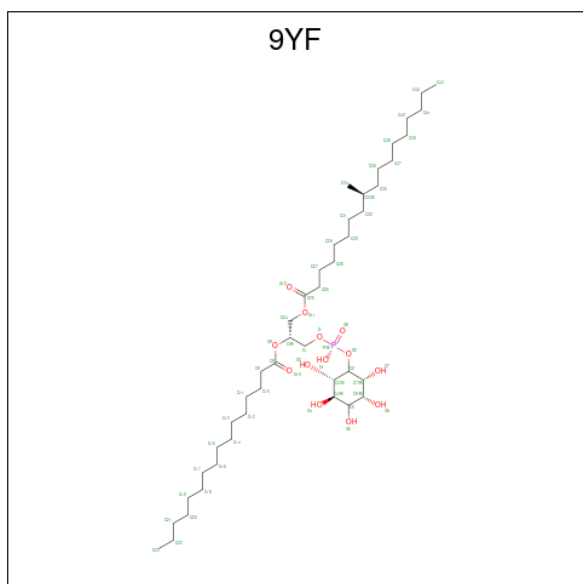
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	Fe	S	0
			4	2	2	
14	N	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is [(2 {R})-3-[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (three-letter code: IZL) (formula: $\text{C}_{74}\text{H}_{133}\text{O}_{39}\text{P}$) (labeled as "Ligand of Interest" by depositor).



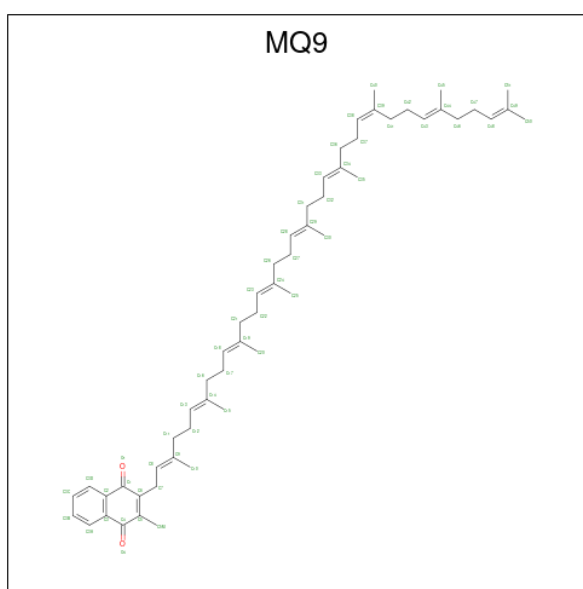
Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	H	O	P	0
			212	63	109	39	1	
15	N	1	Total	C	H	O	P	0
			212	63	109	39	1	

- Molecule 16 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (three-letter code: 9YF) (formula: C₄₄H₈₅O₁₃P) (labeled as "Ligand of Interest" by depositor).



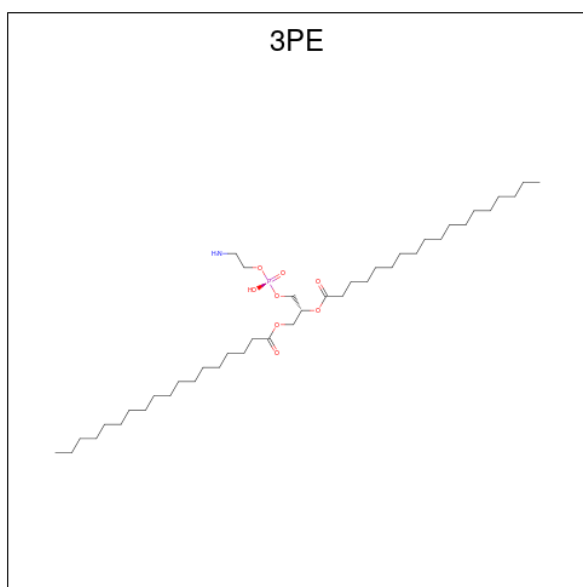
Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	H	O	P	0
			66	22	30	13	1	
16	H	1	Total	C	H	O	P	0
			60	20	26	13	1	
16	N	1	Total	C	H	O	P	0
			66	22	30	13	1	
16	U	1	Total	C	H	O	P	0
			75	25	36	13	1	

- Molecule 17 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	H	O	0
			138	56	80	2	
17	B	1	Total	C	H	O	0
			46	21	23	2	
17	N	1	Total	C	H	O	0
			78	34	42	2	
17	O	1	Total	C	H	O	0
			56	25	29	2	

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



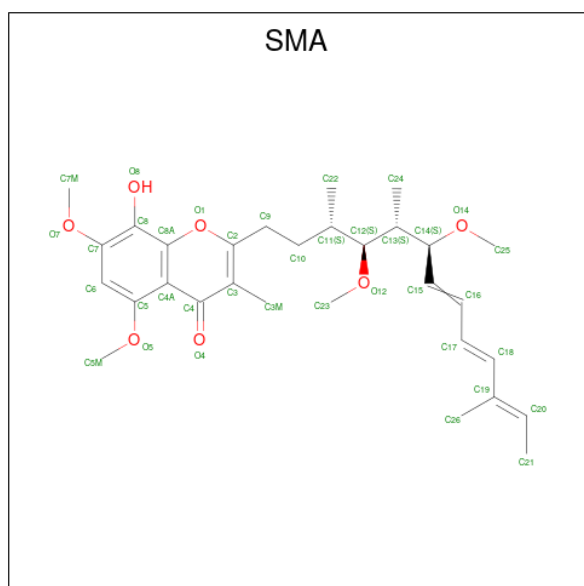
Mol	Chain	Residues	Atoms						AltConf
18	A	1	Total	C	H	N	O	P	0
			76	30	36	1	8	1	
18	C	1	Total	C	H	N	O	P	0
			45	15	20	1	8	1	
18	C	1	Total	C	H	N	O	P	0
			45	15	20	1	8	1	
18	D	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	F	1	Total	C	H	N	O	P	0
			54	22	22	1	8	1	
18	J	1	Total	C	H	N	O	P	0
			111	37	64	1	8	1	
18	L	1	Total	C	H	N	O	P	0
			68	20	38	1	8	1	
18	N	1	Total	C	H	N	O	P	0
			66	28	28	1	8	1	
18	P	1	Total	C	H	N	O	P	0
			45	17	18	1	8	1	
18	Q	1	Total	C	H	N	O	P	0
			71	29	32	1	8	1	
18	R	1	Total	C	H	N	O	P	0
			47	21	16	1	8	1	
18	S	1	Total	C	H	N	O	P	0
			95	33	52	1	8	1	
18	T	1	Total	C	H	N	O	P	0
			50	16	24	1	8	1	
18	T	1	Total	C	H	N	O	P	0
			86	32	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
18	T	1	Total	C	H	N	O	P
			74	28	36	1	8	1
18	T	1	Total	C	H	N	O	P
			84	30	44	1	8	1
18	W	1	Total	C	H	N	O	P
			115	37	68	1	8	1

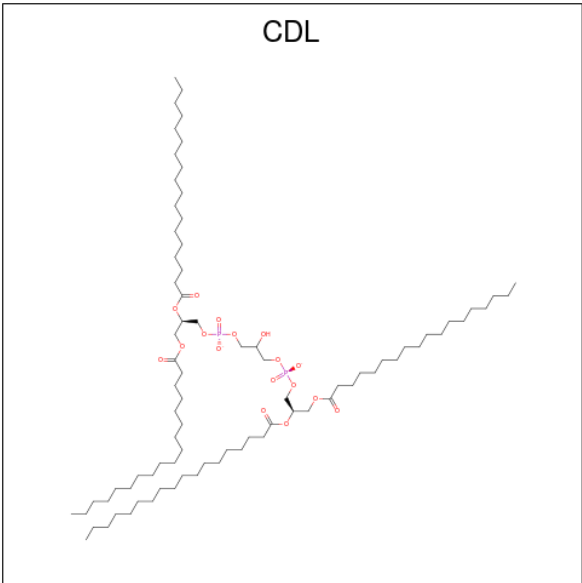
- Molecule 19 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$) (labeled as "Ligand of Interest" by depositor).





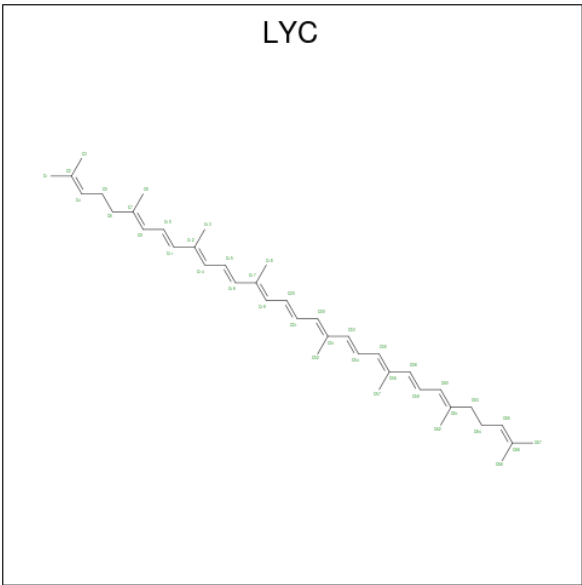
Mol	Chain	Residues	Atoms						AltConf
20	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
20	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
20	O	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
20	O	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 21 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



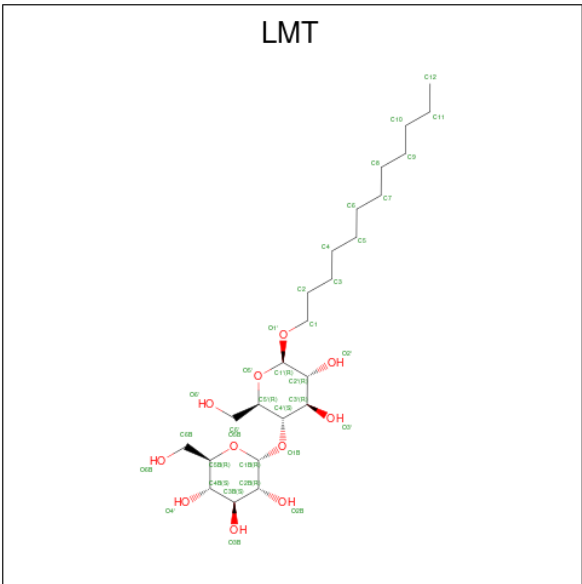
Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	H	O	P	0
			95	37	39	17	2	
21	B	1	Total	C	H	O	P	0
			72	26	27	17	2	
21	B	1	Total	C	H	O	P	0
			126	51	56	17	2	
21	D	1	Total	C	H	O	P	0
			161	58	84	17	2	
21	D	1	Total	C	H	O	P	0
			128	44	65	17	2	
21	F	1	Total	C	H	O	P	0
			94	38	37	17	2	
21	G	1	Total	C	H	O	P	0
			154	56	79	17	2	
21	G	1	Total	C	H	O	P	0
			125	50	56	17	2	
21	I	1	Total	C	H	O	P	0
			107	38	50	17	2	
21	O	1	Total	C	H	O	P	0
			145	47	79	17	2	
21	Q	1	Total	C	H	O	P	0
			183	64	100	17	2	
21	Q	1	Total	C	H	O	P	0
			145	47	79	17	2	
21	S	1	Total	C	H	O	P	0
			135	46	70	17	2	
21	T	1	Total	C	H	O	P	0
			175	61	95	17	2	
21	T	1	Total	C	H	O	P	0
			111	46	46	17	2	
21	V	1	Total	C	H	O	P	0
			159	50	90	17	2	

- Molecule 22 is LYCOPENE (three-letter code: LYC) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	H	0
			96	40	56	
22	O	1	Total	C	H	0
			96	40	56	

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



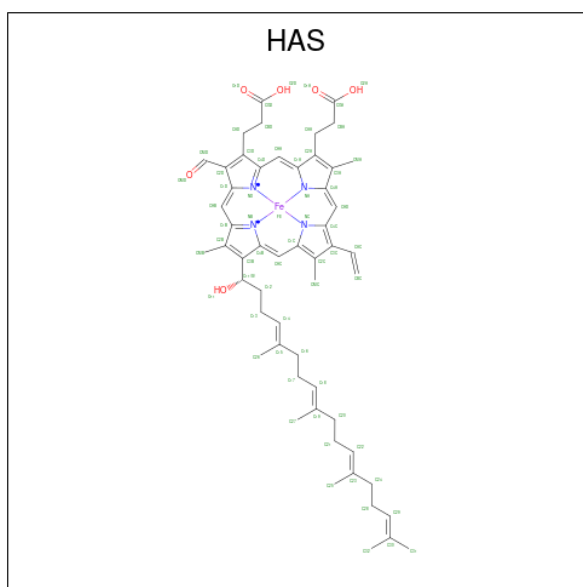
Mol	Chain	Residues	Atoms				AltConf
23	B	1	Total	C	H	O	0
			71	21	39	11	

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Mol	Chain	Residues	Atoms				AltConf
23	O	1	Total	C	H	O	0
			71	21	39	11	

-
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and functional groups, such as hydroxyl groups (OH) and carboxylic acid groups (COOH). The atoms are labeled with letters and numbers, indicating their positions within the molecule.

- Molecule 25 is HEME-AS (three-letter code: HAS) (formula: $\text{C}_{54}\text{H}_{64}\text{FeN}_4\text{O}_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
25	D	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	D	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	Q	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	Q	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	

- Molecule 26 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Cu	0
			1	1	
26	Q	1	Total	Cu	0
			1	1	

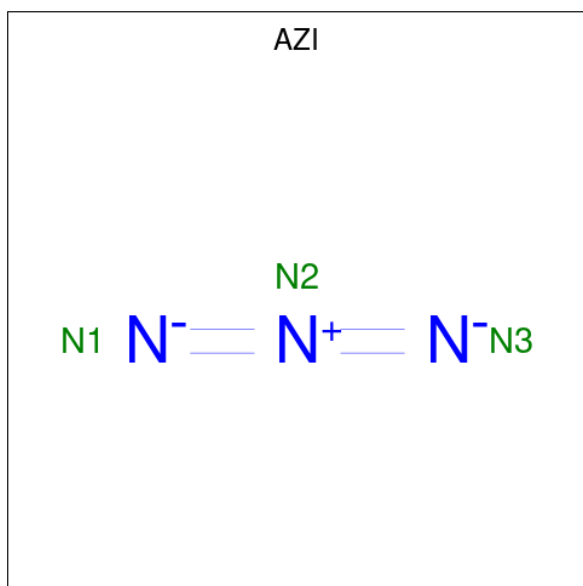
- Molecule 27 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	D	1	Total	Mn	0
			1	1	
27	R	1	Total	Mn	0
			1	1	

- Molecule 28 is CALCIUM ION (three-letter code: CA) (formula: Ca).

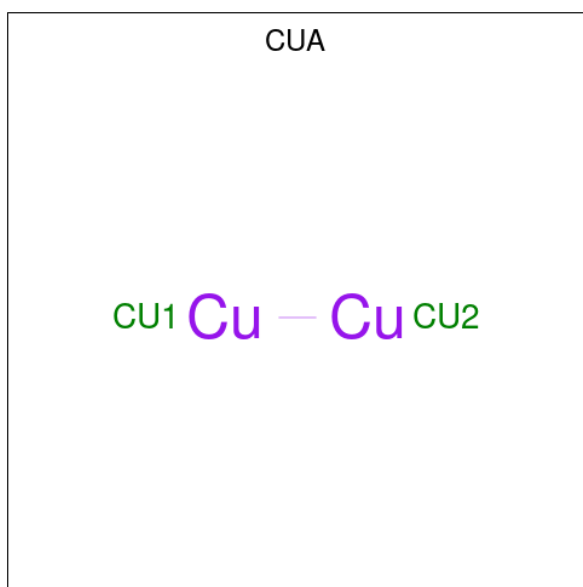
Mol	Chain	Residues	Atoms		AltConf
28	D	1	Total	Ca	0
			1	1	
28	Q	1	Total	Ca	0
			1	1	

- Molecule 29 is AZIDE ION (three-letter code: AZI) (formula: N₃) (labeled as "Ligand of Interest" by depositor).



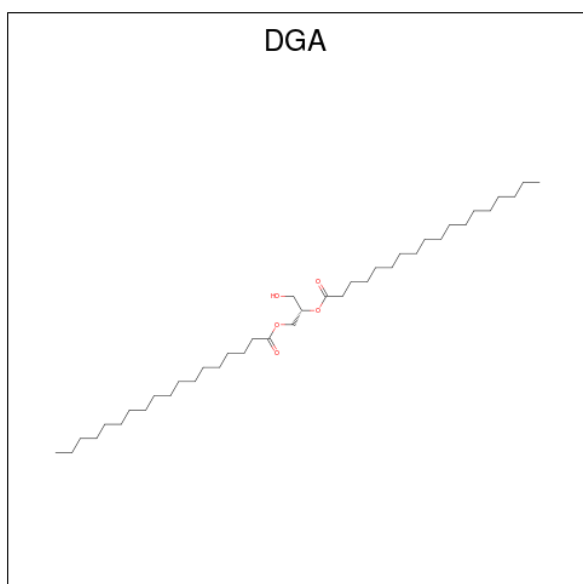
Mol	Chain	Residues	Atoms		AltConf
29	D	1	Total	N	0
			3	3	
29	Q	1	Total	N	0
			3	3	

- Molecule 30 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



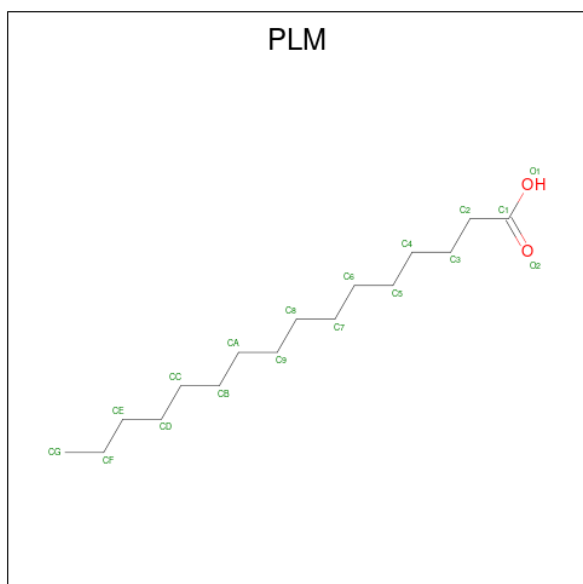
Mol	Chain	Residues	Atoms		AltConf
30	E	1	Total	Cu	0
			1	1	
30	E	1	Total	Cu	0
			1	1	
30	R	1	Total	Cu	0
			1	1	
30	R	1	Total	Cu	0
			1	1	

- Molecule 31 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	E	1	Total	C	O	0
			20	16	4	
31	H	1	Total	C	O	0
			17	13	4	
31	M	1	Total	C	O	0
			22	18	4	
31	R	1	Total	C	O	0
			25	21	4	
31	U	1	Total	C	O	0
			27	23	4	
31	Z	1	Total	C	O	0
			29	25	4	

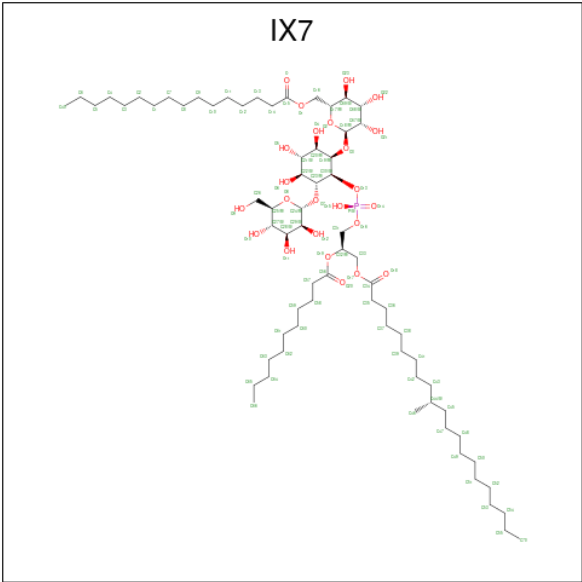
- Molecule 32 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
32	H	1	Total	C	H	O	0
			41	16	24	1	
32	M	1	Total	C	H	O	0
			9	4	4	1	
32	U	1	Total	C	H	O	0
			45	16	28	1	
32	Z	1	Total	C	H	O	0
			9	4	4	1	

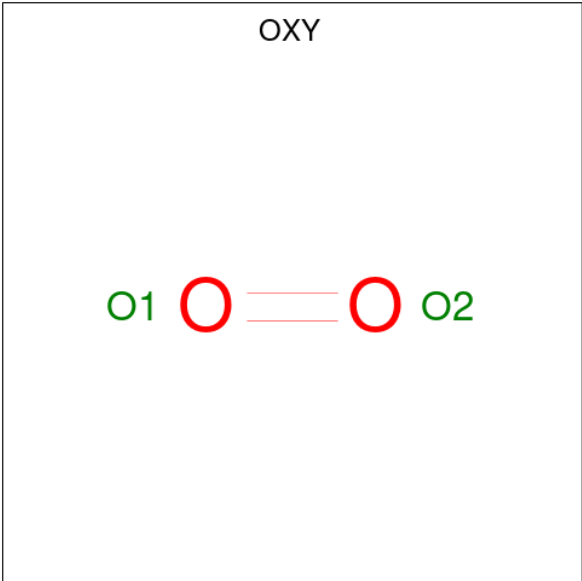
- Molecule 33 is [(2 {R})-3-[(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {

S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {S})-10-methylhenicosanoate (three-letter code: IX7) (formula: C₇₀H₁₃₁O₂₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	H	1	Total	C	H	O	P	0
			155	47	83	24	1	
33	U	1	Total	C	H	O	P	0
			155	47	83	24	1	

- Molecule 34 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
34	Q	1	Total	O	0
			2	2	

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	A	31	Total	O	0
			31	31	
35	B	56	Total	O	0
			56	56	
35	C	26	Total	O	0
			26	26	
35	D	21	Total	O	0
			21	21	
35	E	13	Total	O	0
			13	13	
35	F	3	Total	O	0
			3	3	
35	G	6	Total	O	0
			6	6	
35	K	3	Total	O	0
			3	3	
35	N	31	Total	O	0
			31	31	
35	O	46	Total	O	0
			46	46	
35	P	49	Total	O	0
			49	49	
35	Q	53	Total	O	0
			53	53	
35	R	44	Total	O	0
			44	44	
35	S	5	Total	O	0
			5	5	
35	T	13	Total	O	0
			13	13	
35	U	12	Total	O	0
			12	12	
35	V	2	Total	O	0
			2	2	
35	X	2	Total	O	0
			2	2	

3 Residue-property plots [i](#)

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

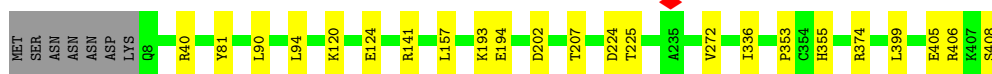
- Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A: 



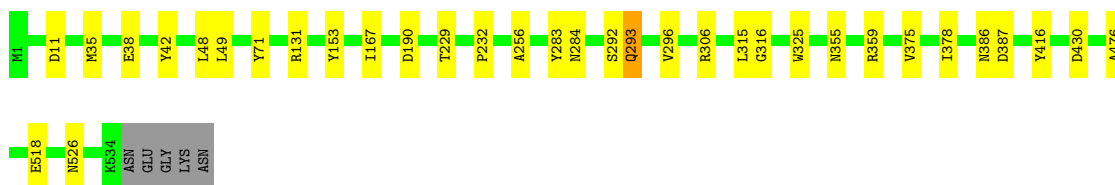
- Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain N: 



- Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain B: 




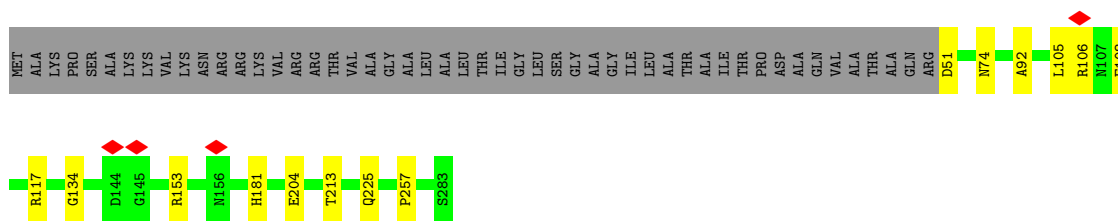
- Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain O: 



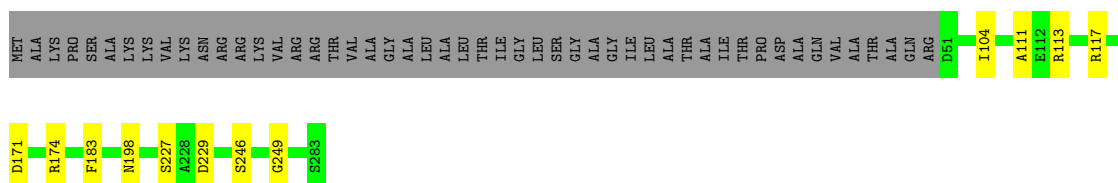
- Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain C: 



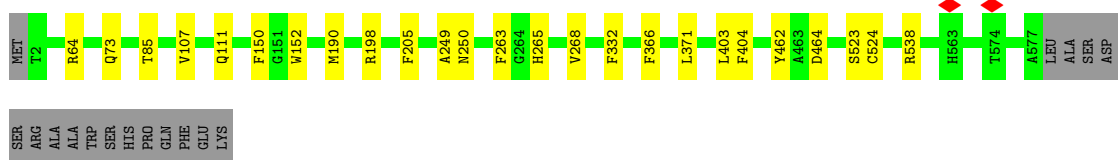
- Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain P: 78% 18%



- Molecule 4: Cytochrome c oxidase subunit 1

Chain D: 93% 5%



- Molecule 4: Cytochrome c oxidase subunit 1

Chain Q: 92% 5%



- Molecule 5: Cytochrome c oxidase subunit 2

Chain E: 96% 5%



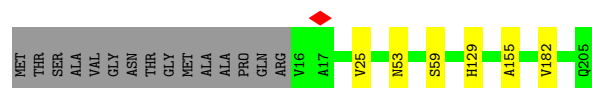
- Molecule 5: Cytochrome c oxidase subunit 2

Chain R: 96% 5%



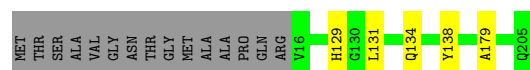
- Molecule 6: Cytochrome c oxidase subunit 3

Chain F: 90% 7%



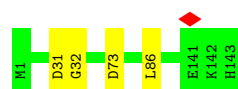
- Molecule 6: Cytochrome c oxidase subunit 3

Chain S: 90% 7%



- Molecule 7: Cytochrome c oxidase polypeptide 4

Chain G: 97%



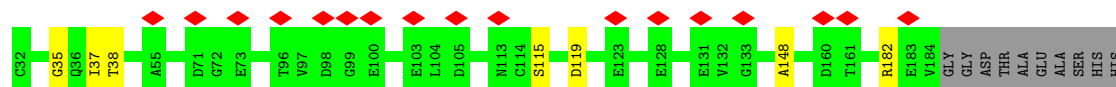
- Molecule 7: Cytochrome c oxidase polypeptide 4

Chain T: 98%



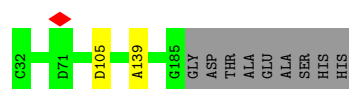
- Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain H: 10% 90% 6%




- Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain U: 93% 6%




- Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211

Chain I:  88% 8%




- Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211

Chain V:  88% 8%




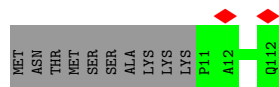
- Molecule 10: Hypothetical membrane protein

Chain J:  89% 9%




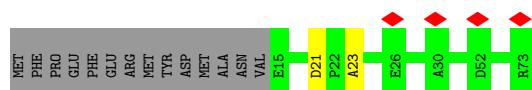
- Molecule 10: Hypothetical membrane protein

Chain W:  91% 9%



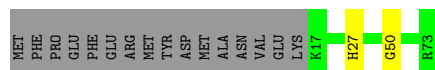
- Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

Chain K:  5% 78% 19%



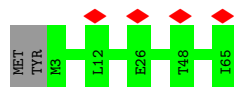
- Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

Chain X:  75% 22%

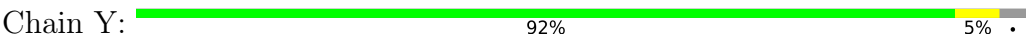


- Molecule 12: Hypothetical membrane protein

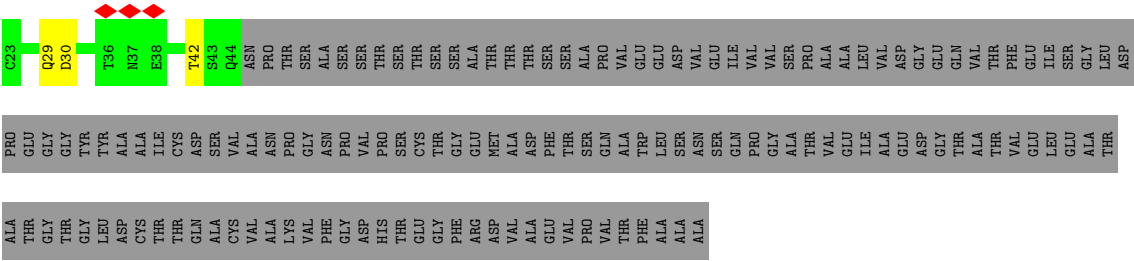
Chain L:  6% 97%



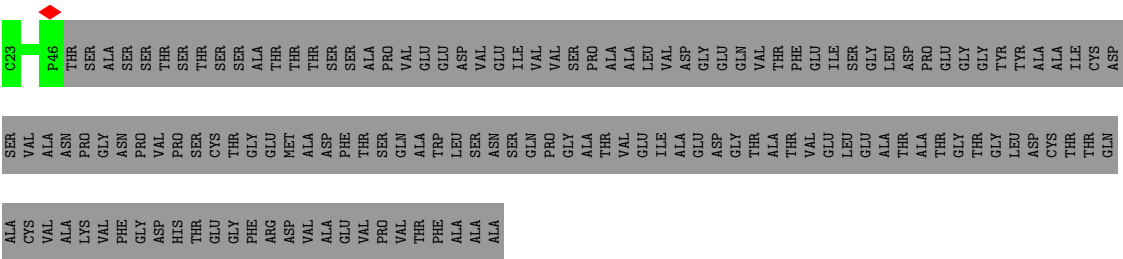
● Molecule 12: Hypothetical membrane protein



● Molecule 13: Thiamine biosynthesis protein X



● Molecule 13: Thiamine biosynthesis protein X



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	200424	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 ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.641	Depositor
Minimum map value	-1.574	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	281.49, 203.01399, 150.981	wwPDB
Map dimensions	177, 238, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.853, 0.853, 0.85300004	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: AZI, DGA, CDL, LMT, IX7, HEM, OXY, FES, CUA, LYC, IZL, HAS, SMA, PLM, MN, HEC, CU, 3PE, 9YF, MQ9, CA

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	0.39	0/3238	0.62	0/4403
1	N	0.41	0/3244	0.62	0/4414
2	B	0.41	0/4359	0.62	0/5937
2	O	0.44	0/4301	0.62	0/5860
3	C	0.35	0/1785	0.60	0/2413
3	P	0.42	0/1770	0.60	0/2394
4	D	0.40	0/4718	0.58	0/6438
4	Q	0.44	0/4734	0.60	0/6460
5	E	0.36	0/2671	0.58	0/3642
5	R	0.42	0/2686	0.58	0/3661
6	F	0.37	0/1528	0.56	0/2081
6	S	0.42	0/1528	0.57	0/2081
7	G	0.35	0/1126	0.53	0/1529
7	T	0.40	0/1144	0.52	0/1554
8	H	0.32	0/1134	0.58	0/1553
8	U	0.35	0/1138	0.58	0/1558
9	I	0.32	0/1103	0.58	0/1508
9	V	0.35	0/1103	0.60	0/1508
10	J	0.32	0/799	0.56	0/1087
10	W	0.37	0/799	0.63	0/1087
11	K	0.38	0/486	0.53	0/663
11	X	0.41	0/468	0.56	0/640
12	L	0.28	0/453	0.49	0/616
12	Y	0.33	0/453	0.54	0/616
13	M	0.27	0/174	0.57	0/238
13	Z	0.30	0/190	0.60	0/261
All	All	0.39	0/47132	0.59	0/64202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3147	3084	3070	17	0
1	N	3145	3079	3063	16	0
2	B	4217	4268	4238	26	0
2	O	4186	4239	4238	20	0
3	C	1749	1694	1690	7	0
3	P	1738	1680	1680	7	0
4	D	4548	4470	4471	15	0
4	Q	4557	4477	4468	18	0
5	E	2598	2468	2468	6	0
5	R	2607	2482	2476	10	0
6	F	1486	1495	1494	5	0
6	S	1486	1494	1494	3	0
7	G	1095	1106	1106	2	0
7	T	1105	1114	1104	1	0
8	H	1120	1054	1054	5	0
8	U	1124	1057	1057	1	0
9	I	1073	1071	1071	4	0
9	V	1073	1071	1071	3	0
10	J	779	792	792	1	0
10	W	779	792	792	0	0
11	K	469	432	432	1	0
11	X	451	413	413	0	0
12	L	445	470	469	0	0
12	Y	445	470	469	2	0
13	M	171	159	159	2	0
13	Z	186	172	172	0	0
14	A	4	0	0	0	0
14	N	4	0	0	0	0
15	A	103	109	0	3	0
15	N	103	109	0	0	0
16	A	36	30	0	0	0
16	H	34	26	0	0	0
16	N	36	30	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	U	39	36	0	2	0
17	A	58	80	80	3	0
17	B	23	23	21	3	0
17	N	36	42	42	2	0
17	O	27	29	29	3	0
18	A	40	36	57	1	0
18	C	50	40	48	2	0
18	D	31	26	36	0	0
18	F	32	22	38	1	0
18	J	47	64	71	0	0
18	L	30	38	34	0	0
18	N	38	28	53	1	0
18	P	27	18	28	2	0
18	Q	39	32	55	3	0
18	R	31	16	36	3	0
18	S	43	52	60	0	0
18	T	146	148	191	1	0
18	W	47	68	68	0	0
19	B	37	42	41	1	0
19	O	37	42	41	1	0
20	B	86	60	60	3	0
20	O	86	60	60	3	0
21	B	171	122	174	2	0
21	D	140	149	171	1	0
21	F	57	37	58	1	0
21	G	144	135	179	2	0
21	I	57	50	61	0	0
21	O	66	79	79	0	0
21	Q	149	179	195	4	0
21	S	65	70	74	0	0
21	T	145	141	181	1	0
21	V	69	90	90	0	0
22	B	40	56	56	0	0
22	O	40	56	56	1	0
23	B	32	39	37	0	0
23	O	32	39	37	0	0
24	C	86	60	60	2	0
24	P	86	60	60	1	0
25	D	130	124	124	5	0
25	Q	130	124	124	4	0
26	D	1	0	0	0	0
26	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	D	1	0	0	0	0
27	R	1	0	0	0	0
28	D	1	0	0	0	0
28	Q	1	0	0	0	0
29	D	3	0	0	2	0
29	Q	3	0	0	0	0
30	E	2	0	0	0	0
30	R	2	0	0	0	0
31	E	20	0	21	0	0
31	H	17	0	15	2	0
31	M	22	0	25	1	0
31	R	25	0	31	0	0
31	U	27	0	35	3	0
31	Z	29	0	39	0	0
32	H	17	24	31	0	0
32	M	5	4	4	0	0
32	U	17	28	31	0	0
32	Z	5	4	4	0	0
33	H	72	83	0	2	0
33	U	72	83	0	2	0
34	Q	2	0	0	0	0
35	A	31	0	0	8	0
35	B	56	0	0	10	0
35	C	26	0	0	1	0
35	D	21	0	0	1	0
35	E	13	0	0	4	0
35	F	3	0	0	1	0
35	G	6	0	0	0	0
35	K	3	0	0	0	0
35	N	31	0	0	5	0
35	O	46	0	0	3	0
35	P	49	0	0	1	0
35	Q	53	0	0	8	0
35	R	44	0	0	2	0
35	S	5	0	0	0	0
35	T	13	0	0	0	0
35	U	12	0	0	0	0
35	V	2	0	0	0	0
35	X	2	0	0	0	0
All	All	49530	48245	48212	187	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 2.

The worst 5 of 187 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)
4:Q:238:ASP:OD2	35:Q:701:HOH:O	2.04	0.75
1:N:353:PRO:O	35:N:601:HOH:O	2.05	0.75
4:D:205:PHE:O	35:D:701:HOH:O	2.04	0.74
6:F:59:SER:O	35:F:401:HOH:O	2.07	0.73
3:C:257:PRO:O	35:C:401:HOH:O	2.08	0.72

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	402/408 (98%)	382 (95%)	20 (5%)	0	100	100
1	N	403/408 (99%)	388 (96%)	14 (4%)	1 (0%)	44	73
2	B	538/539 (100%)	519 (96%)	16 (3%)	3 (1%)	22	51
2	O	532/539 (99%)	518 (97%)	14 (3%)	0	100	100
3	C	233/283 (82%)	217 (93%)	13 (6%)	3 (1%)	10	32
3	P	231/283 (82%)	214 (93%)	17 (7%)	0	100	100
4	D	574/594 (97%)	553 (96%)	21 (4%)	0	100	100
4	Q	576/594 (97%)	553 (96%)	22 (4%)	1 (0%)	44	73
5	E	329/331 (99%)	313 (95%)	14 (4%)	2 (1%)	22	51
5	R	331/331 (100%)	318 (96%)	13 (4%)	0	100	100
6	F	188/205 (92%)	185 (98%)	3 (2%)	0	100	100
6	S	188/205 (92%)	182 (97%)	6 (3%)	0	100	100
7	G	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
7	T	143/143 (100%)	137 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	151/163 (93%)	147 (97%)	4 (3%)	0	100	100
8	U	152/163 (93%)	146 (96%)	6 (4%)	0	100	100
9	I	133/147 (90%)	124 (93%)	8 (6%)	1 (1%)	16	44
9	V	133/147 (90%)	126 (95%)	6 (4%)	1 (1%)	16	44
10	J	100/112 (89%)	97 (97%)	3 (3%)	0	100	100
10	W	100/112 (89%)	95 (95%)	5 (5%)	0	100	100
11	K	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
11	X	55/73 (75%)	53 (96%)	1 (2%)	1 (2%)	7	24
12	L	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
12	Y	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
13	M	20/168 (12%)	16 (80%)	4 (20%)	0	100	100
13	Z	22/168 (13%)	20 (91%)	2 (9%)	0	100	100
All	All	5854/6462 (91%)	5608 (96%)	233 (4%)	13 (0%)	45	73

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	292	SER
4	Q	575	ALA
9	V	30	GLY
2	B	71	TYR
3	C	181	HIS

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	328/332 (99%)	327 (100%)	1 (0%)	91	97
1	N	329/332 (99%)	326 (99%)	3 (1%)	75	92
2	B	443/441 (100%)	440 (99%)	3 (1%)	81	94
2	O	437/441 (99%)	436 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	178/212 (84%)	176 (99%)	2 (1%)	70	90
3	P	177/212 (84%)	176 (99%)	1 (1%)	84	95
4	D	473/488 (97%)	466 (98%)	7 (2%)	60	86
4	Q	475/488 (97%)	468 (98%)	7 (2%)	60	86
5	E	274/274 (100%)	269 (98%)	5 (2%)	54	83
5	R	276/274 (101%)	274 (99%)	2 (1%)	81	94
6	F	156/166 (94%)	156 (100%)	0	100	100
6	S	156/166 (94%)	155 (99%)	1 (1%)	84	95
7	G	114/114 (100%)	113 (99%)	1 (1%)	75	92
7	T	116/114 (102%)	114 (98%)	2 (2%)	56	84
8	H	127/133 (96%)	126 (99%)	1 (1%)	79	93
8	U	127/133 (96%)	127 (100%)	0	100	100
9	I	116/125 (93%)	116 (100%)	0	100	100
9	V	116/125 (93%)	115 (99%)	1 (1%)	75	92
10	J	81/90 (90%)	80 (99%)	1 (1%)	67	89
10	W	81/90 (90%)	81 (100%)	0	100	100
11	K	50/63 (79%)	50 (100%)	0	100	100
11	X	48/63 (76%)	47 (98%)	1 (2%)	48	80
12	L	43/45 (96%)	43 (100%)	0	100	100
12	Y	43/45 (96%)	43 (100%)	0	100	100
13	M	22/135 (16%)	22 (100%)	0	100	100
13	Z	24/135 (18%)	24 (100%)	0	100	100
All	All	4810/5236 (92%)	4770 (99%)	40 (1%)	77	93

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	189	ASN
6	S	129	HIS
4	Q	263	PHE
4	Q	404	PHE
7	T	113	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	R	318	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 6 are monoatomic and 4 are modelled with single atom - leaving 78 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	$\# Z > 2$
24	HEC	P	301	3	32,50,50	1.47	2 (6%)	24,82,82	1.91	6 (25%)
18	3PE	L	101	-	29,29,50	0.41	0	32,34,55	0.57	0
23	LMT	O	601	-	33,33,36	0.16	0	44,44,47	1.04	2 (4%)
18	3PE	T	206	-	39,39,50	0.35	0	42,44,55	0.72	1 (2%)
31	DGA	H	201	-	16,16,43	0.30	0	18,18,45	0.19	0
21	CDL	O	606	-	65,65,99	0.39	0	71,77,111	0.59	1 (1%)
17	MQ9	B	604	-	24,24,59	0.72	1 (4%)	30,33,75	1.36	2 (6%)
16	9YF	H	203	-	34,34,58	0.32	0	44,46,71	0.47	1 (2%)
20	HEM	B	602	2	41,50,50	1.13	2 (4%)	45,82,82	1.42	8 (17%)
21	CDL	B	605	-	55,55,99	0.40	0	61,67,111	0.53	0
24	HEC	P	302	3	32,50,50	1.42	2 (6%)	24,82,82	1.71	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CDL	Q	607	-	82,82,99	0.35	0	88,94,111	0.40	0
19	SMA	B	601	-	38,38,38	0.66	2 (5%)	48,52,52	0.80	2 (4%)
33	IX7	H	204	-	74,74,97	0.39	0	97,99,123	1.07	6 (6%)
21	CDL	B	606	-	44,44,99	0.43	0	50,56,111	0.38	0
32	PLM	U	202	8	16,16,17	0.16	0	15,15,17	0.21	0
18	3PE	F	301	-	31,31,50	0.39	0	34,36,55	0.85	1 (2%)
18	3PE	A	505	-	39,39,50	0.33	0	42,44,55	0.55	0
20	HEM	B	603	2	41,50,50	1.20	4 (9%)	45,82,82	1.09	4 (8%)
17	MQ9	A	504	-	59,59,59	0.55	1 (1%)	72,75,75	0.94	5 (6%)
24	HEC	C	301	3	32,50,50	1.43	2 (6%)	24,82,82	1.45	4 (16%)
21	CDL	D	607	-	76,76,99	0.36	0	82,88,111	0.54	1 (1%)
24	HEC	C	302	3	32,50,50	1.34	2 (6%)	24,82,82	1.62	5 (20%)
31	DGA	E	403	-	19,19,43	0.28	0	21,21,45	0.18	0
32	PLM	H	202	8	16,16,17	0.18	0	15,15,17	0.24	0
31	DGA	M	201	-	21,21,43	0.26	0	23,23,45	0.24	0
18	3PE	T	203	-	41,41,50	0.34	0	44,46,55	0.41	0
21	CDL	T	201	-	79,79,99	0.35	0	85,91,111	0.47	1 (1%)
21	CDL	G	202	-	68,68,99	0.36	0	74,80,111	0.64	2 (2%)
29	AZI	Q	605	26	0,2,2	-	-	0,1,1	-	-
19	SMA	O	602	-	38,38,38	0.44	1 (2%)	48,52,52	0.41	0
25	HAS	Q	601	4	69,72,72	1.20	4 (5%)	73,109,109	1.51	12 (16%)
18	3PE	W	201	-	46,46,50	0.34	0	49,51,55	0.93	3 (6%)
21	CDL	B	609	-	69,69,99	0.37	0	75,81,111	0.46	0
15	IZL	N	504	-	108,108,119	0.41	0	150,152,163	1.11	15 (10%)
18	3PE	T	205	-	37,37,50	0.36	0	40,42,55	0.41	0
31	DGA	R	404	-	24,24,43	0.28	0	26,26,45	0.19	0
20	HEM	O	604	2	41,50,50	1.15	2 (4%)	45,82,82	1.04	3 (6%)
18	3PE	S	301	-	42,42,50	0.39	0	45,47,55	0.58	1 (2%)
21	CDL	V	201	-	68,68,99	0.37	0	72,79,111	0.45	0
21	CDL	T	204	-	64,64,99	0.38	0	70,76,111	0.67	1 (1%)
32	PLM	M	202	13	4,4,17	0.33	0	3,3,17	0.27	0
18	3PE	C	303	-	24,24,50	0.45	0	27,29,55	0.62	0
18	3PE	N	502	-	37,37,50	0.34	0	40,42,55	0.43	0
20	HEM	O	603	2	41,50,50	1.18	3 (7%)	45,82,82	1.56	9 (20%)
25	HAS	D	602	29,4	69,72,72	1.19	5 (7%)	73,109,109	1.71	14 (19%)
21	CDL	Q	608	-	65,65,99	0.38	0	71,77,111	0.42	0
14	FES	N	503	1	0,4,4	-	-	-	-	-
17	MQ9	O	605	-	28,28,59	0.57	1 (3%)	34,37,75	1.21	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	HAS	D	601	4	69,72,72	1.24	5 (7%)	73,109,109	1.75	15 (20%)
34	OXY	Q	606	-	1,1,1	0.16	0	-		
17	MQ9	N	501	-	37,37,59	0.50	1 (2%)	45,48,75	0.84	3 (6%)
18	3PE	R	405	-	30,30,50	0.37	0	33,35,55	0.47	0
21	CDL	I	201	-	56,56,99	0.39	0	62,68,111	0.45	0
18	3PE	D	609	-	30,30,50	0.39	0	33,35,55	0.38	0
18	3PE	C	304	-	24,24,50	0.43	0	27,29,55	0.63	0
33	IX7	U	204	-	74,74,97	0.34	0	97,99,123	0.94	4 (4%)
21	CDL	G	201	-	74,74,99	0.35	0	80,86,111	0.59	1 (1%)
18	3PE	J	201	-	46,46,50	0.33	0	49,51,55	0.64	1 (2%)
16	9YF	N	505	-	36,36,58	0.34	0	46,48,71	0.41	0
22	LYC	O	607	-	39,39,39	0.37	0	44,46,46	0.47	0
29	AZI	D	606	25,26	0,2,2	-	-	0,1,1	-	-
16	9YF	A	503	-	36,36,58	0.42	0	46,48,71	0.50	1 (2%)
21	CDL	D	608	-	62,62,99	0.39	0	68,74,111	0.56	0
31	DGA	Z	201	-	28,28,43	0.24	0	30,30,45	0.35	0
21	CDL	F	302	-	56,56,99	0.40	0	62,68,111	0.60	1 (1%)
18	3PE	T	202	-	25,25,50	0.42	0	28,30,55	0.48	0
31	DGA	U	201	-	26,26,43	0.29	0	28,28,45	0.34	0
18	3PE	Q	609	-	38,38,50	0.35	0	41,43,55	0.43	0
14	FES	A	501	1	0,4,4	-	-	-		
18	3PE	P	303	-	26,26,50	0.44	0	29,31,55	0.73	2 (6%)
23	LMT	B	608	-	33,33,36	0.14	0	44,44,47	0.59	0
21	CDL	S	302	-	64,64,99	0.38	0	70,76,111	0.58	1 (1%)
25	HAS	Q	602	4	69,72,72	1.18	5 (7%)	73,109,109	1.84	17 (23%)
32	PLM	Z	202	13	4,4,17	0.30	0	3,3,17	0.34	0
22	LYC	B	607	-	39,39,39	0.22	0	44,46,46	0.31	0
15	IZL	A	502	-	108,108,119	0.34	0	150,152,163	1.04	9 (6%)
16	9YF	U	203	-	39,39,58	0.32	0	49,51,71	0.43	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
33	IX7	H	204	-	-	28/58/122/146	0/3/3/3
21	CDL	B	606	-	-	11/54/54/110	-
21	CDL	T	204	-	-	28/75/75/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	3PE	F	301	-	-	20/35/35/54	-
32	PLM	U	202	8	-	2/13/14/15	-
32	PLM	M	202	13	-	0/1/2/15	-
18	3PE	A	505	-	-	16/43/43/54	-
18	3PE	C	303	-	-	12/28/28/54	-
18	3PE	N	502	-	-	8/41/41/54	-
20	HEM	O	603	2	-	5/12/54/54	-
20	HEM	B	603	2	-	2/12/54/54	-
24	HEC	P	301	3	-	3/10/54/54	-
17	MQ9	A	504	-	-	21/53/73/73	0/2/2/2
18	3PE	D	609	-	-	13/34/34/54	-
24	HEC	C	301	3	-	2/10/54/54	-
21	CDL	D	607	-	-	39/87/87/110	-
18	3PE	C	304	-	-	10/28/28/54	-
25	HAS	D	602	29,4	1/1/18/18	19/40/82/82	-
24	HEC	C	302	3	-	2/10/54/54	-
31	DGA	E	403	-	-	2/20/20/45	-
21	CDL	G	201	-	-	33/85/85/110	-
21	CDL	Q	608	-	-	19/76/76/110	-
32	PLM	H	202	8	-	1/13/14/15	-
18	3PE	L	101	-	-	14/33/33/54	-
33	IX7	U	204	-	-	25/58/122/146	0/3/3/3
14	FES	N	503	1	-	-	0/1/1/1
18	3PE	J	201	-	-	27/50/50/54	-
23	LMT	O	601	-	-	11/18/58/61	0/2/2/2
16	9YF	N	505	-	-	5/31/55/78	0/1/1/1
31	DGA	M	201	-	-	3/22/22/45	-
18	3PE	T	206	-	-	23/43/43/54	-
22	LYC	O	607	-	-	1/43/43/43	-
16	9YF	A	503	-	-	15/31/55/78	0/1/1/1
17	MQ9	O	605	-	-	8/16/36/73	0/2/2/2
18	3PE	T	203	-	-	17/45/45/54	-
25	HAS	D	601	4	1/1/18/18	13/40/82/82	-
21	CDL	D	608	-	-	32/73/73/110	-
21	CDL	T	201	-	-	42/90/90/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CDL	G	202	-	-	24/79/79/110	-
31	DGA	Z	201	-	-	5/29/29/45	-
19	SMA	O	602	-	-	11/34/34/34	0/2/2/2
25	HAS	Q	601	4	1/1/18/18	10/40/82/82	-
18	3PE	T	202	-	-	13/29/29/54	-
21	CDL	F	302	-	-	27/67/67/110	-
31	DGA	U	201	-	-	6/27/27/45	-
31	DGA	H	201	-	-	0/17/17/45	-
17	MQ9	N	501	-	-	7/27/47/73	0/2/2/2
18	3PE	Q	609	-	-	15/42/42/54	-
18	3PE	W	201	-	-	25/50/50/54	-
21	CDL	O	606	-	-	37/76/76/110	-
17	MQ9	B	604	-	-	3/11/31/73	0/2/2/2
21	CDL	B	609	-	-	31/80/80/110	-
14	FES	A	501	1	-	-	0/1/1/1
16	9YF	H	203	-	-	5/29/53/78	0/1/1/1
15	IZL	N	504	-	-	31/73/197/208	0/6/6/6
18	3PE	T	205	-	-	14/41/41/54	-
18	3PE	P	303	-	-	15/30/30/54	-
23	LMT	B	608	-	-	8/18/58/61	0/2/2/2
31	DGA	R	404	-	-	2/25/25/45	-
18	3PE	R	405	-	-	16/34/34/54	-
20	HEM	B	602	2	-	3/12/54/54	-
21	CDL	S	302	-	-	37/75/75/110	-
25	HAS	Q	602	4	1/1/18/18	11/40/82/82	-
21	CDL	B	605	-	-	25/66/66/110	-
20	HEM	O	604	2	-	2/12/54/54	-
18	3PE	S	301	-	-	21/46/46/54	-
32	PLM	Z	202	13	-	0/1/2/15	-
21	CDL	I	201	-	-	27/67/67/110	-
22	LYC	B	607	-	-	4/43/43/43	-
21	CDL	V	201	-	-	37/78/78/110	-
15	IZL	A	502	-	-	29/73/197/208	0/6/6/6
21	CDL	Q	607	-	-	30/93/93/110	-
19	SMA	B	601	-	-	9/34/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	HEC	P	302	3	-	2/10/54/54	-
16	9YF	U	203	-	-	3/34/58/78	0/1/1/1

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	301	HEC	C2B-C3B	-5.31	1.35	1.40
24	C	301	HEC	C2B-C3B	-5.24	1.35	1.40
25	D	601	HAS	OMD-CMD	5.05	1.33	1.22
24	P	302	HEC	C2B-C3B	-5.04	1.35	1.40
24	P	301	HEC	C3C-C2C	-4.88	1.35	1.40

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	604	MQ9	C8-C7-C6	6.17	128.68	112.05
25	Q	602	HAS	C26-C15-C16	6.00	125.37	115.27
25	D	601	HAS	C25-C23-C24	5.14	123.92	115.27
25	D	602	HAS	CMC-C2C-C1C	-5.14	120.57	128.46
25	D	601	HAS	C27-C19-C20	4.90	123.51	115.27

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	D	601	HAS	NA
25	D	602	HAS	NA
25	Q	601	HAS	NA
25	Q	602	HAS	NA

5 of 1077 torsion outliers are listed below:

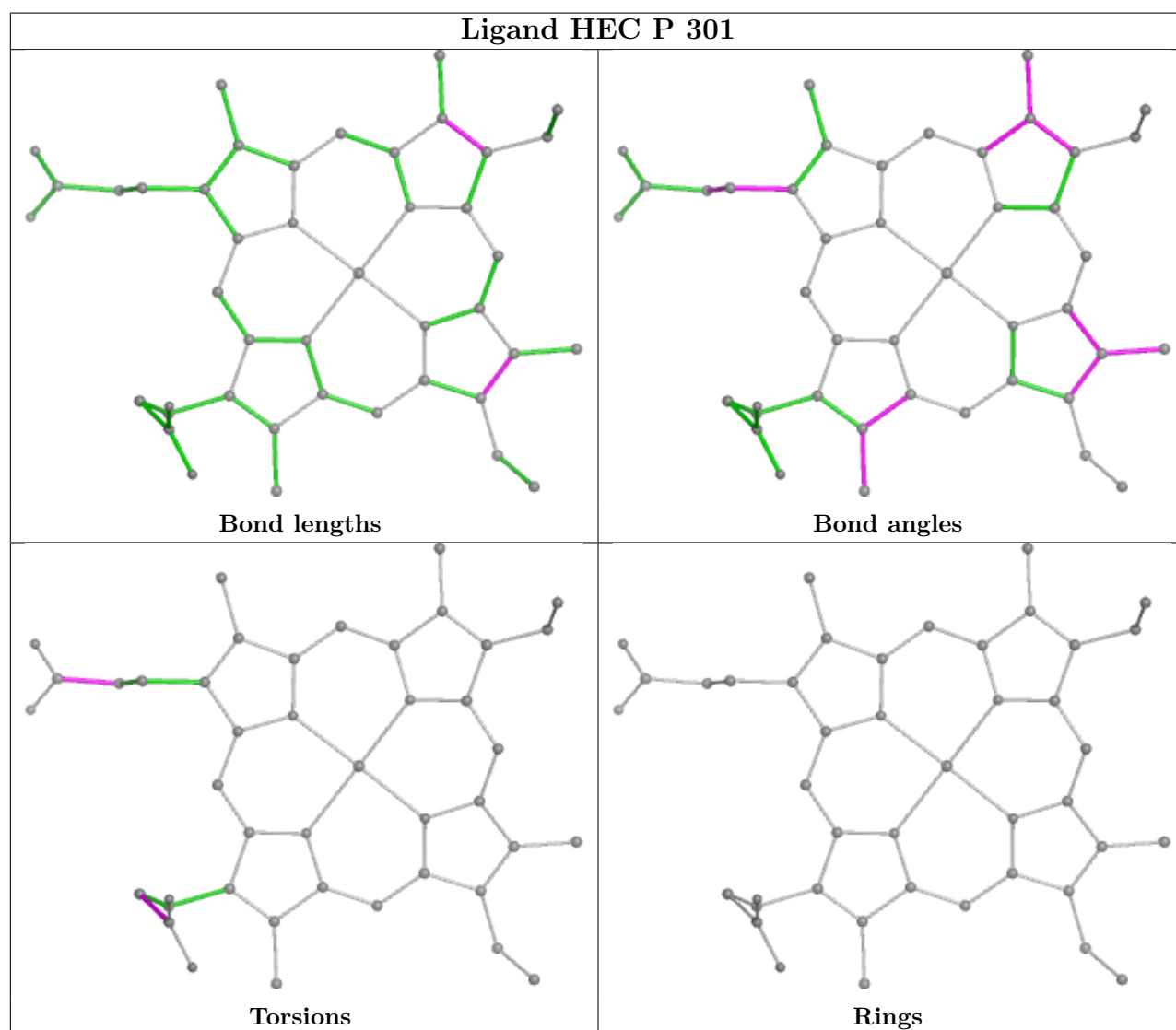
Mol	Chain	Res	Type	Atoms
15	A	502	IZL	C44-O31-P-O30
15	N	504	IZL	O10-C22-O9-C21
15	N	504	IZL	C61-C60-O34-C45
16	A	503	9YF	C2-O2-P-O1
16	A	503	9YF	C1-O-P-O1

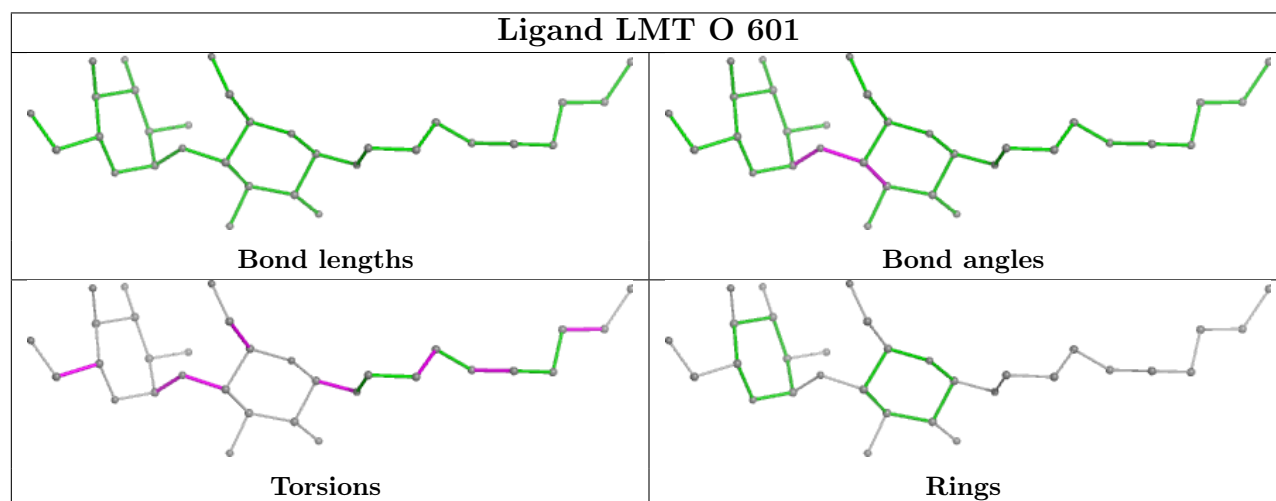
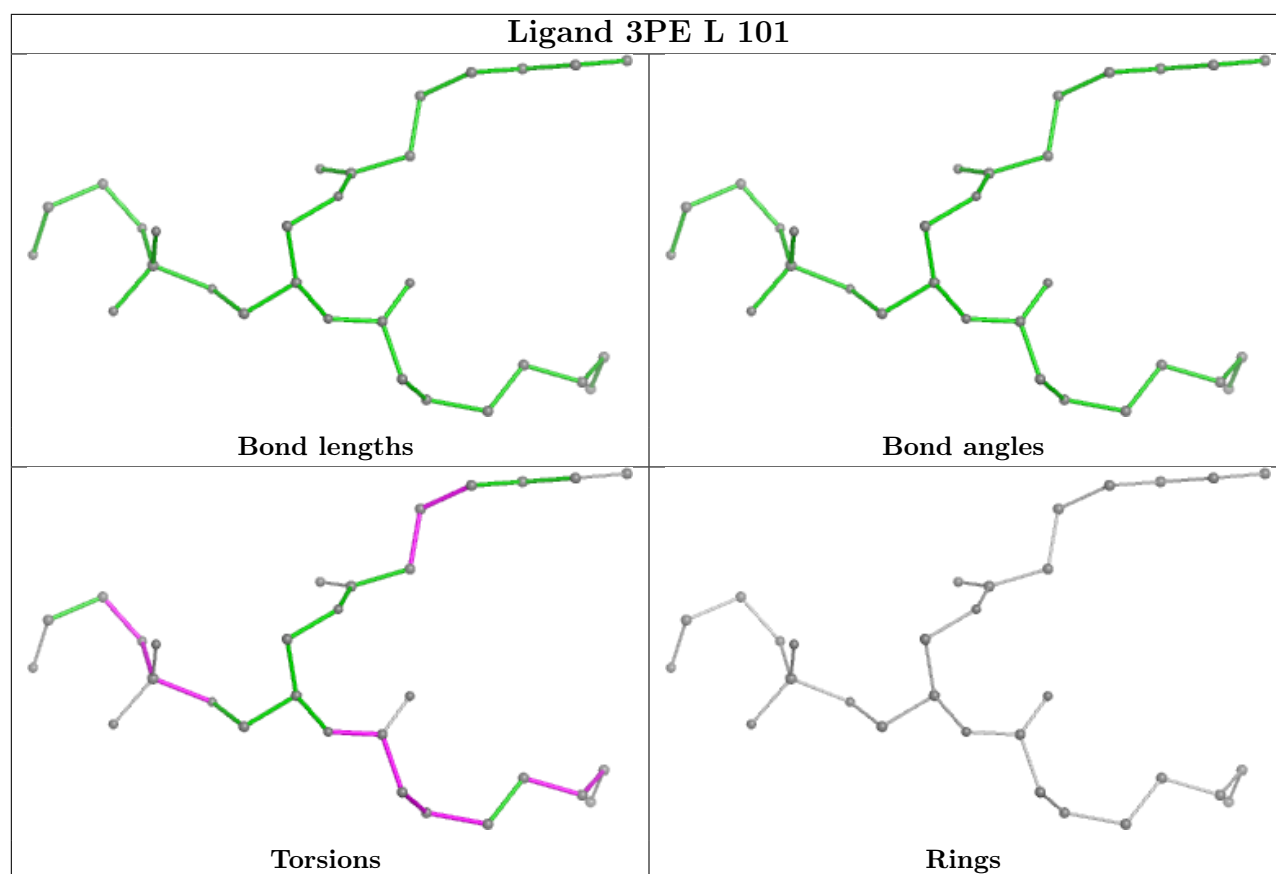
There are no ring outliers.

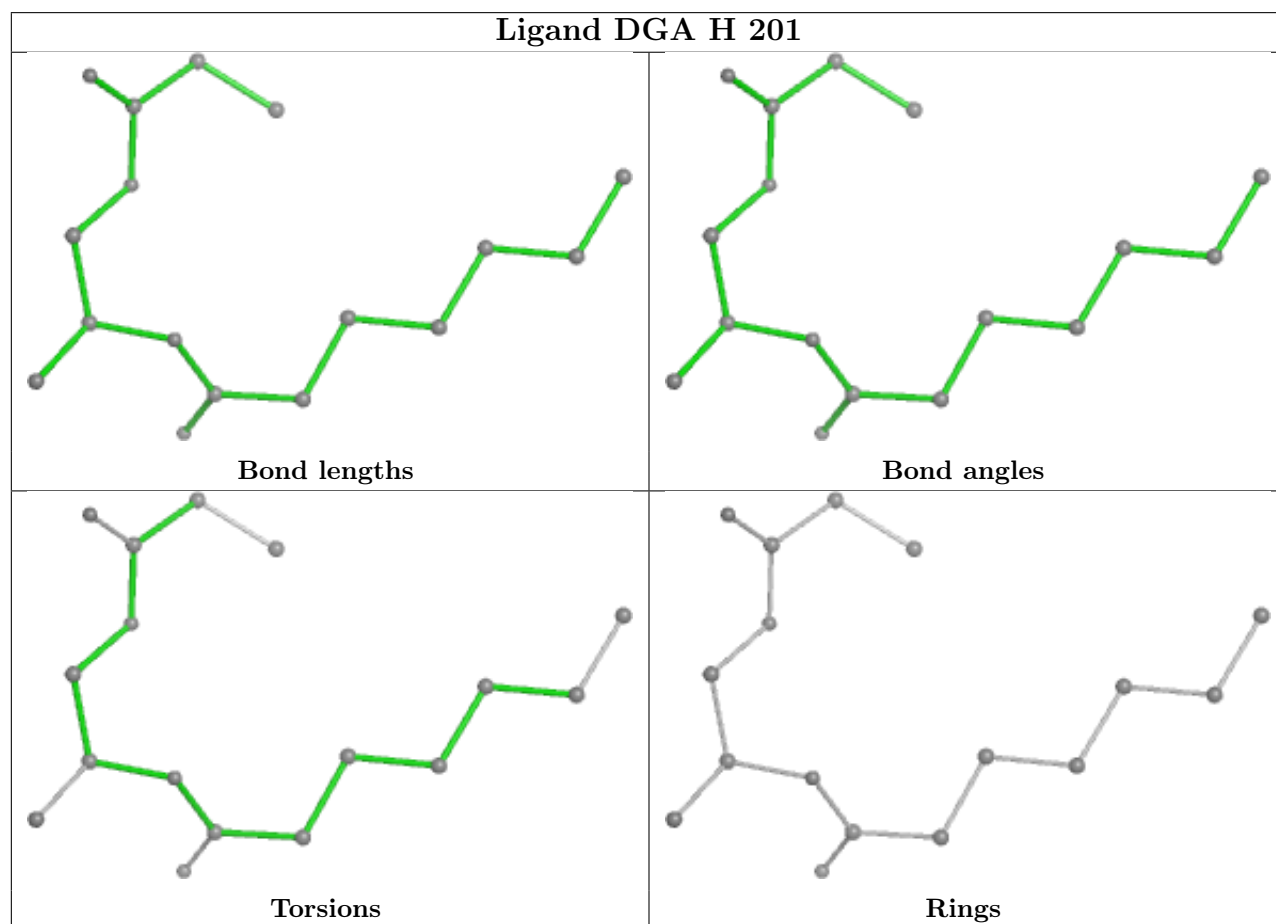
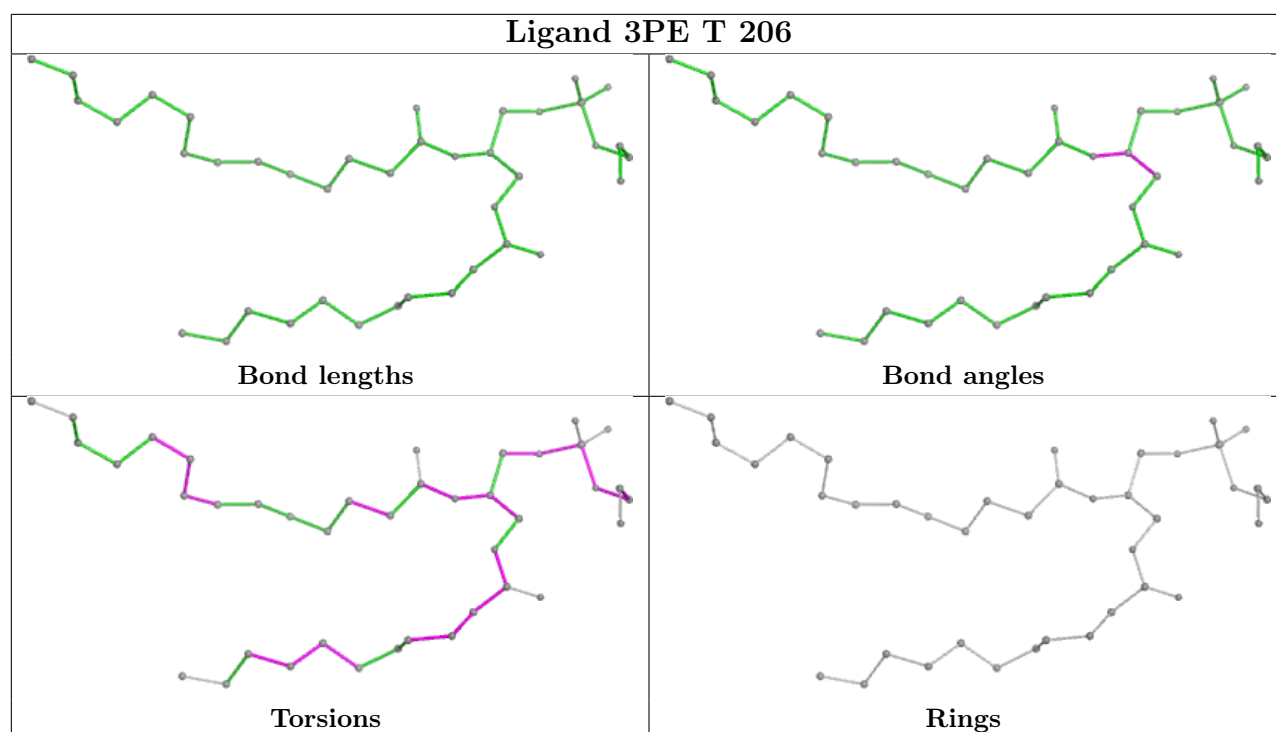
43 monomers are involved in 69 short contacts:

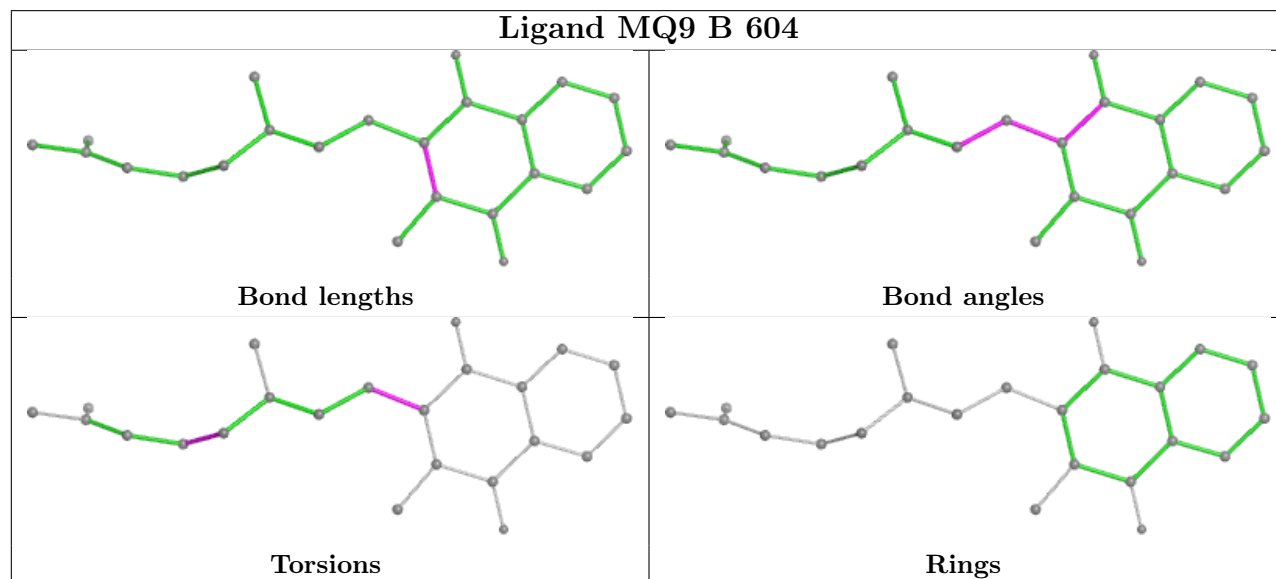
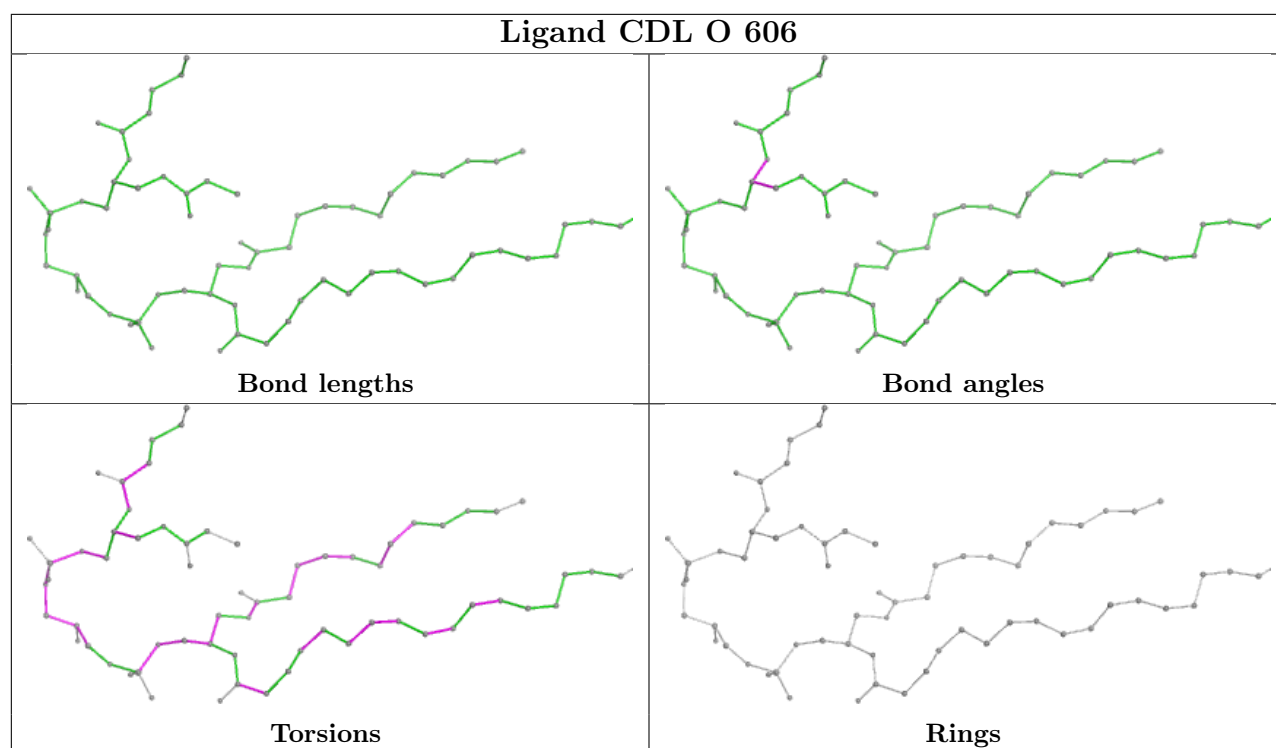
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	H	201	DGA	2	0
17	B	604	MQ9	3	0
20	B	602	HEM	2	0
21	B	605	CDL	1	0
24	P	302	HEC	1	0
21	Q	607	CDL	1	0
19	B	601	SMA	1	0
33	H	204	IX7	2	0
18	F	301	3PE	1	0
18	A	505	3PE	1	0
20	B	603	HEM	1	0
17	A	504	MQ9	3	0
24	C	301	HEC	1	0
21	D	607	CDL	1	0
24	C	302	HEC	1	0
31	M	201	DGA	1	0
18	T	203	3PE	1	0
21	T	201	CDL	1	0
21	G	202	CDL	1	0
19	O	602	SMA	1	0
25	Q	601	HAS	2	0
21	B	609	CDL	1	0
20	O	604	HEM	1	0
18	C	303	3PE	2	0
18	N	502	3PE	1	0
20	O	603	HEM	2	0
25	D	602	HAS	4	0
21	Q	608	CDL	3	0
17	O	605	MQ9	3	0
25	D	601	HAS	1	0
17	N	501	MQ9	2	0
18	R	405	3PE	3	0
33	U	204	IX7	2	0
21	G	201	CDL	1	0
22	O	607	LYC	1	0
29	D	606	AZI	2	0
21	F	302	CDL	1	0
31	U	201	DGA	3	0
18	Q	609	3PE	3	0
18	P	303	3PE	2	0
25	Q	602	HAS	2	0
15	A	502	IZL	3	0
16	U	203	9YF	2	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.

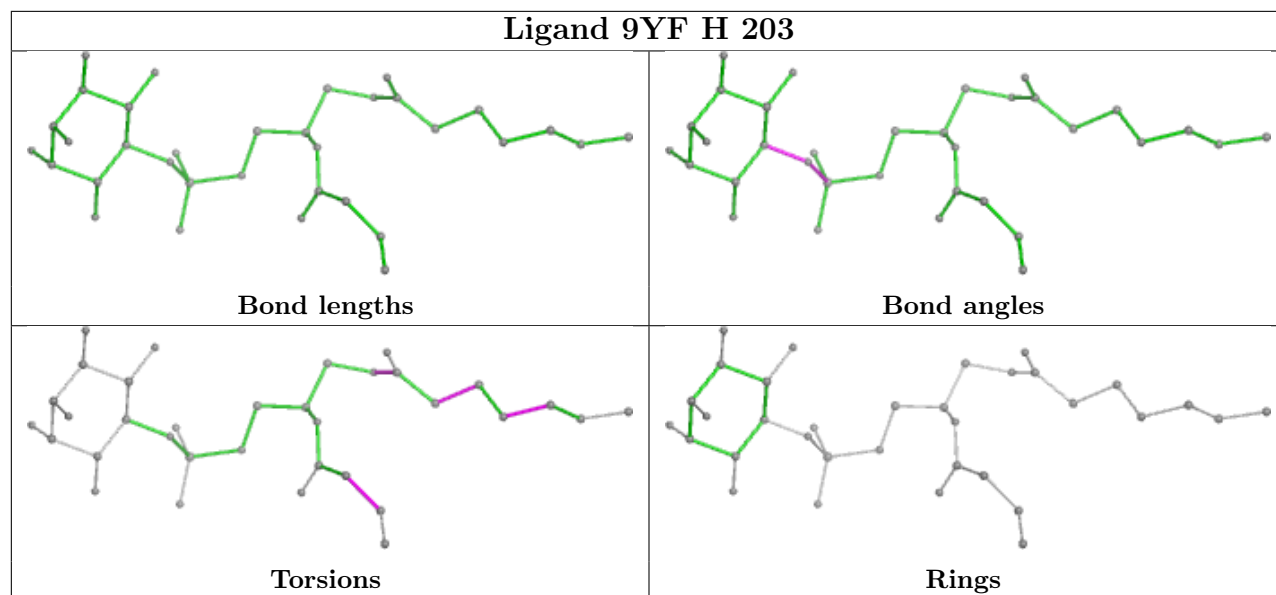




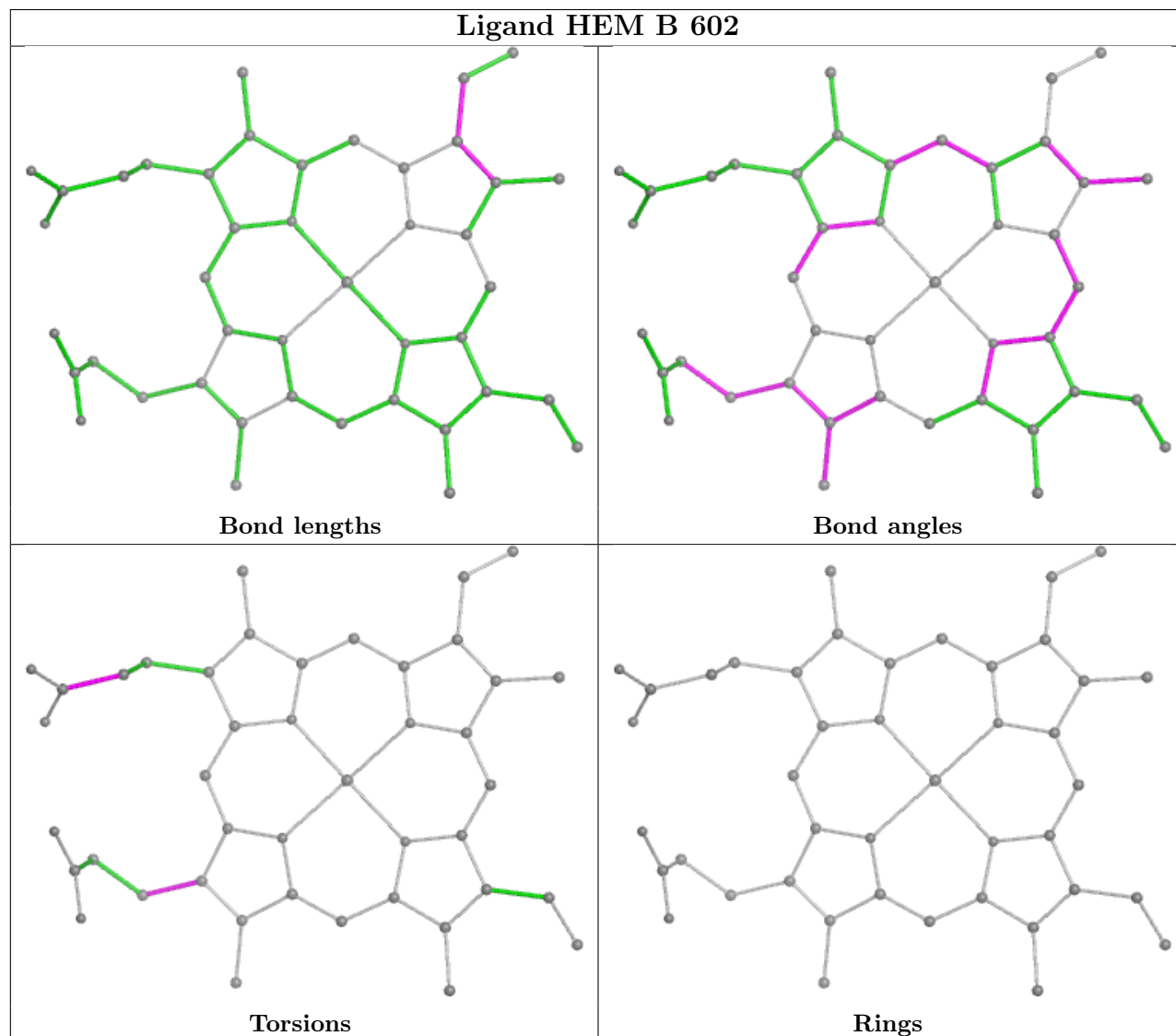


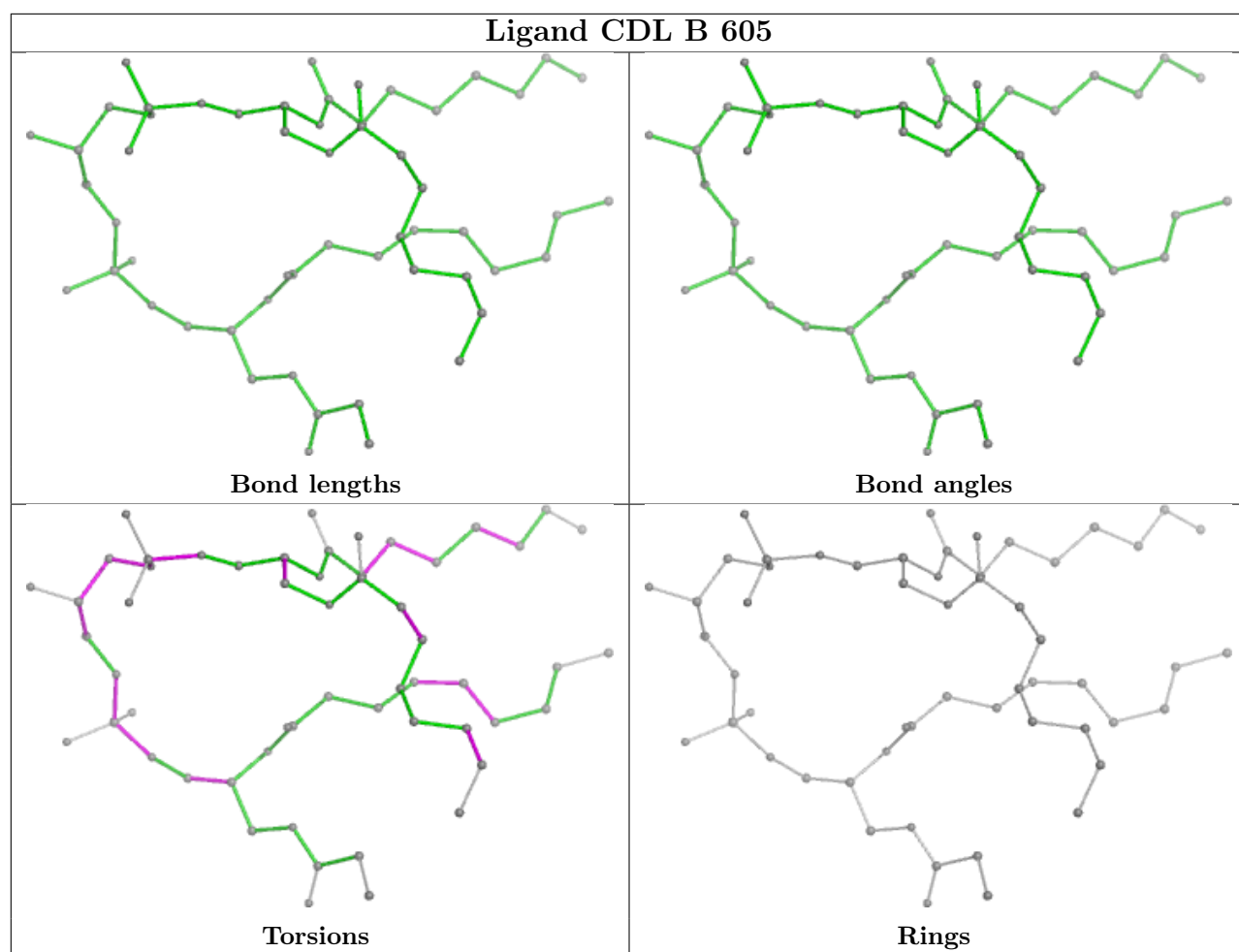


Ligand 9YF H 203

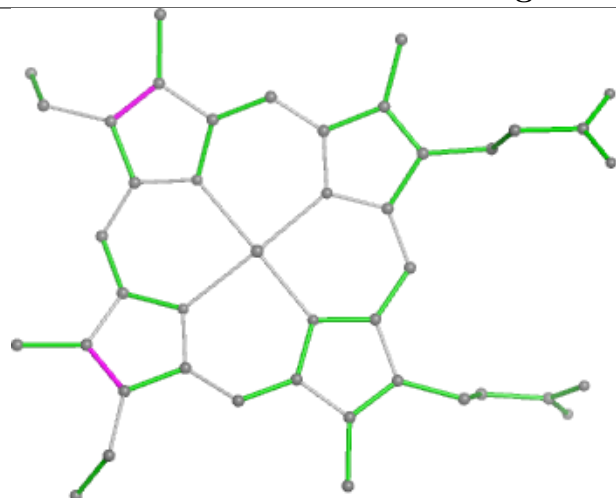


Ligand HEM B 602

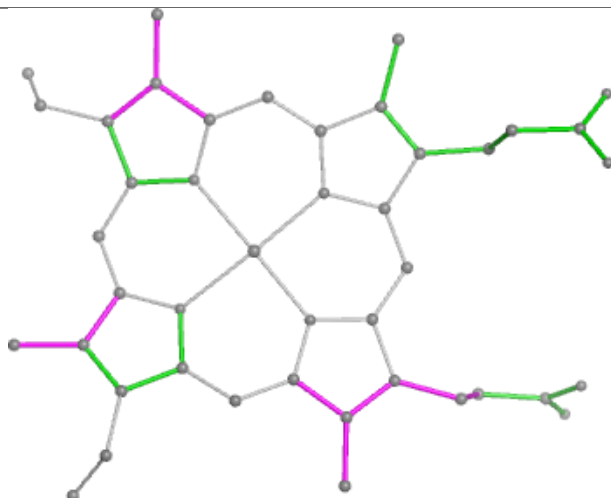




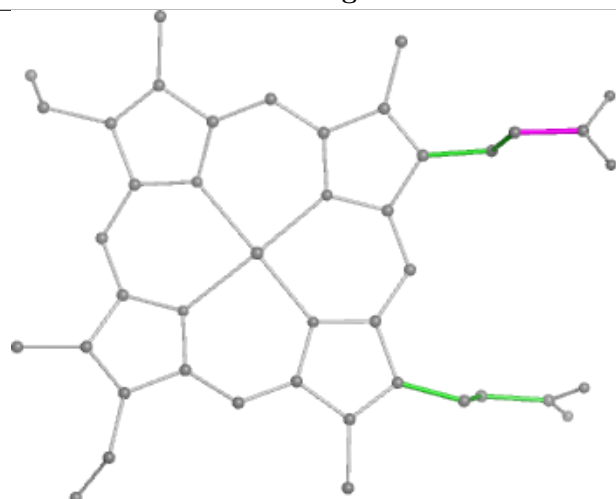
Ligand HEC P 302



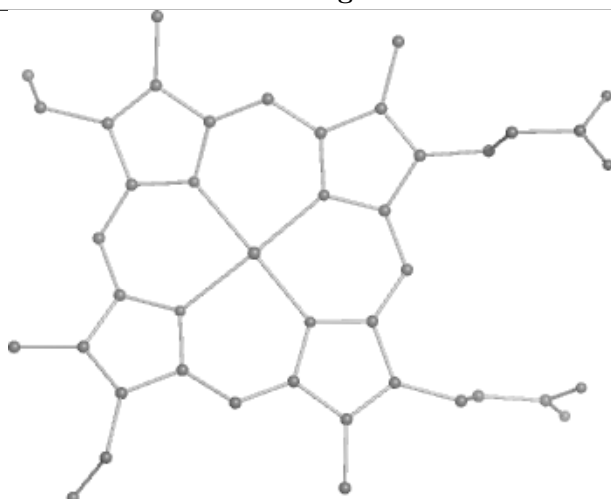
Bond lengths



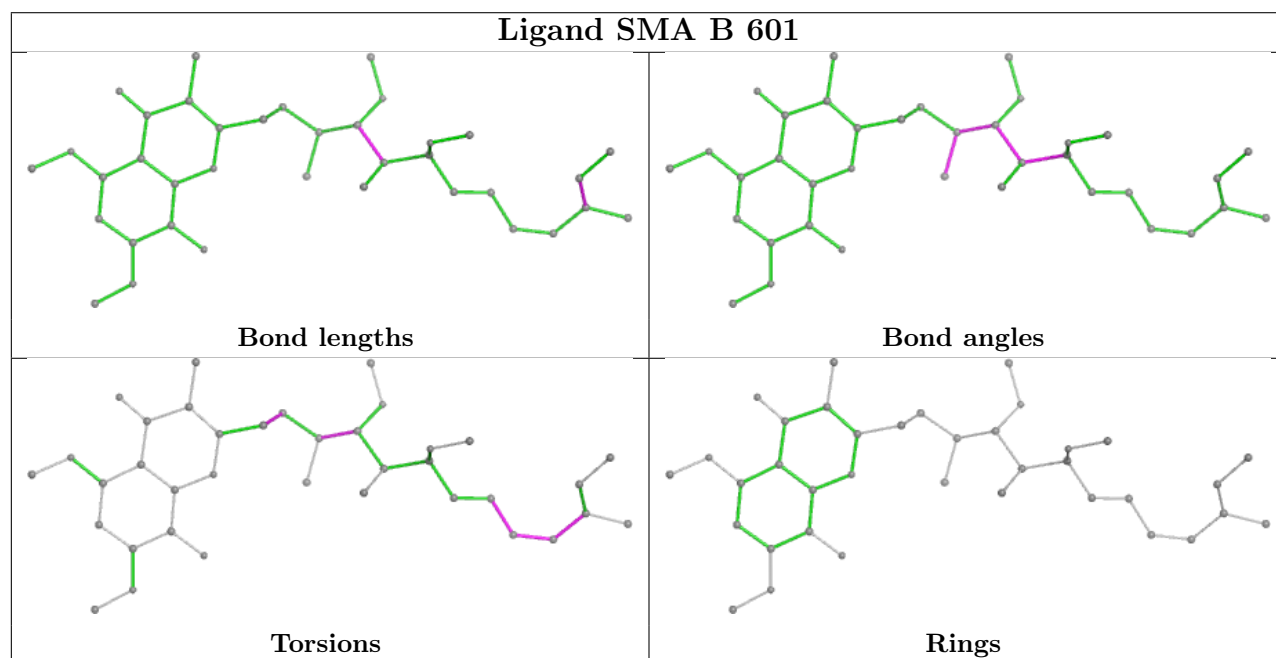
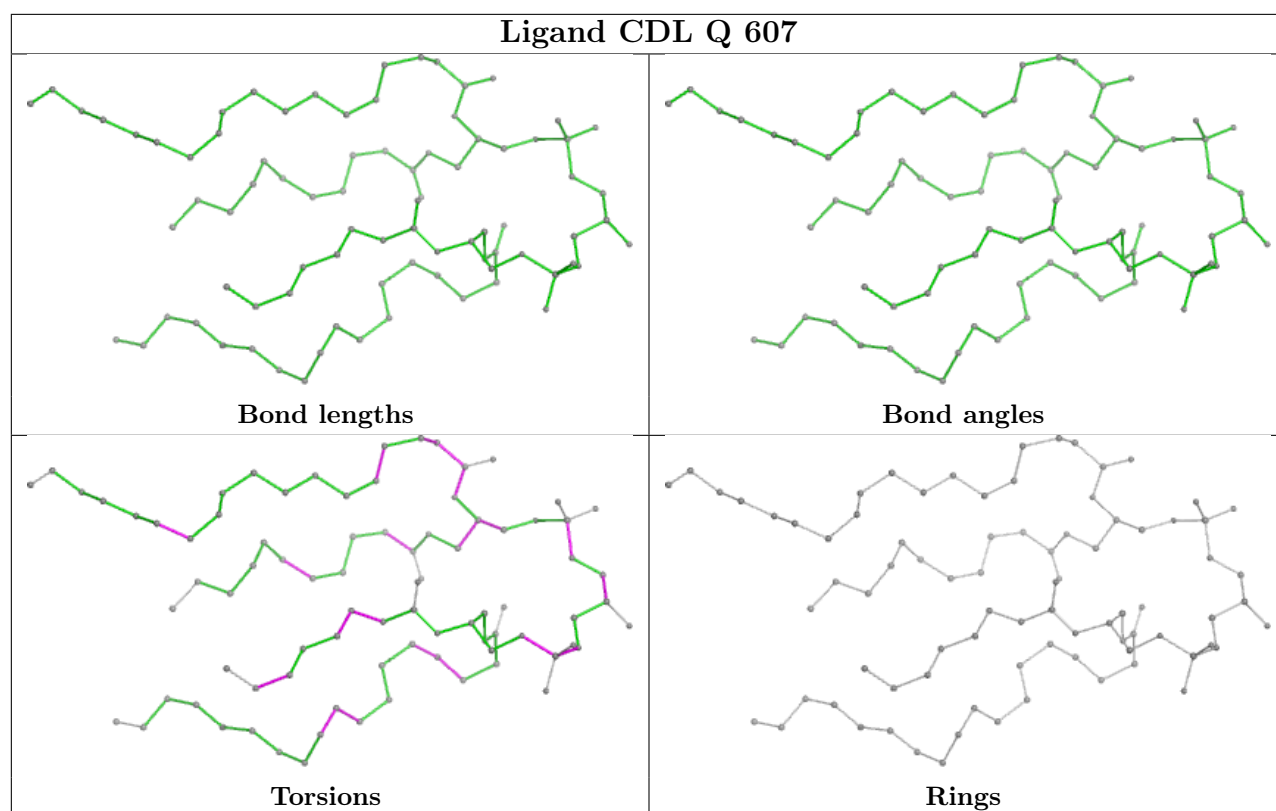
Bond angles

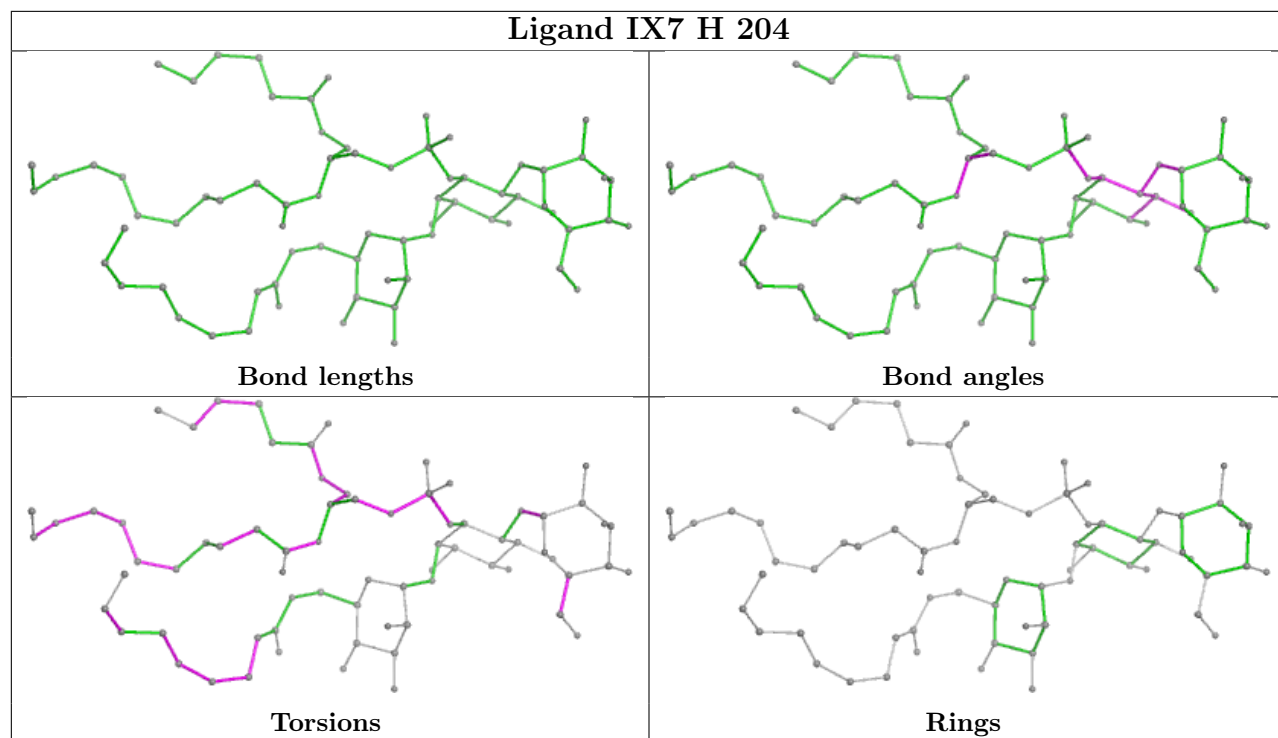


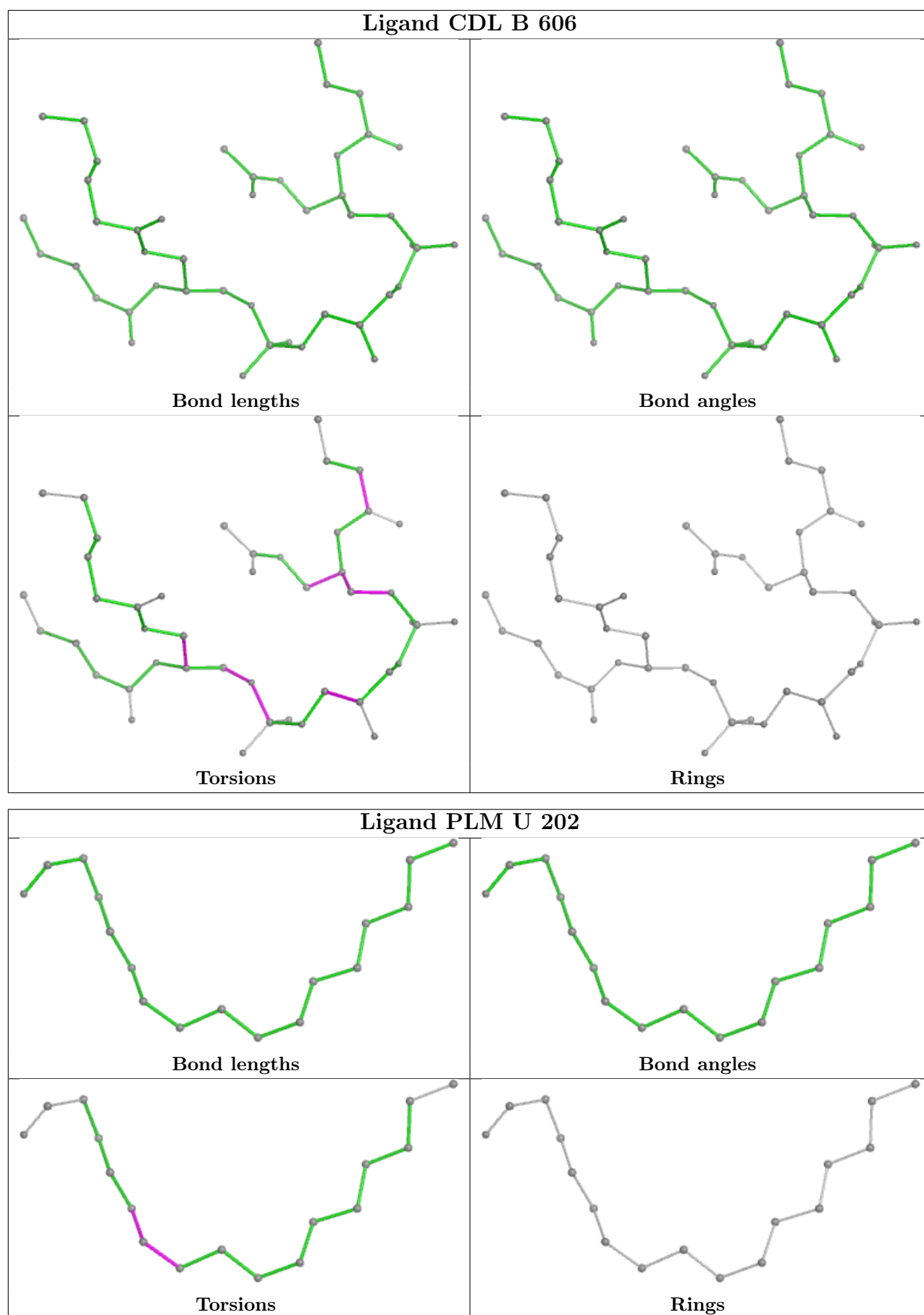
Torsions

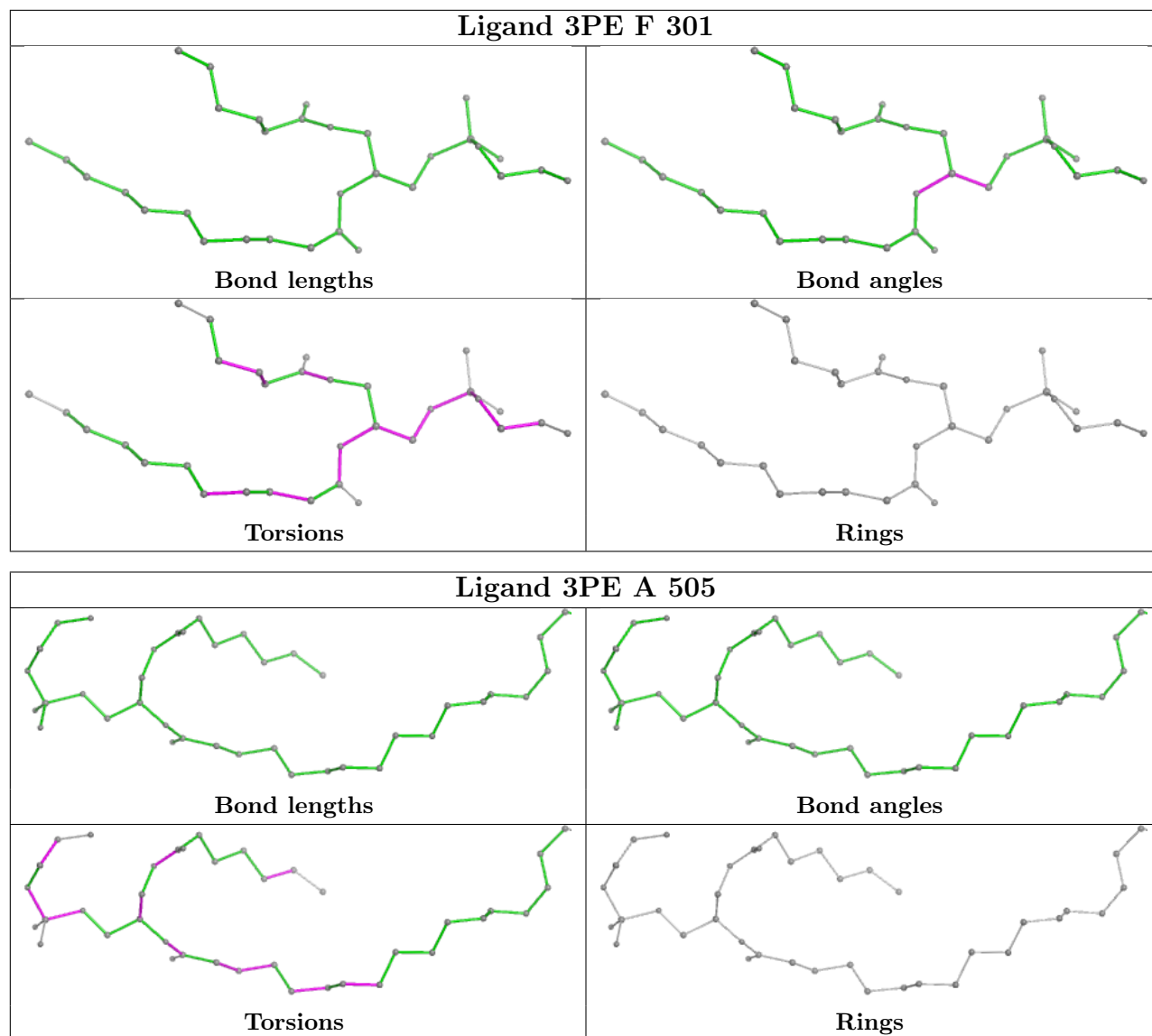


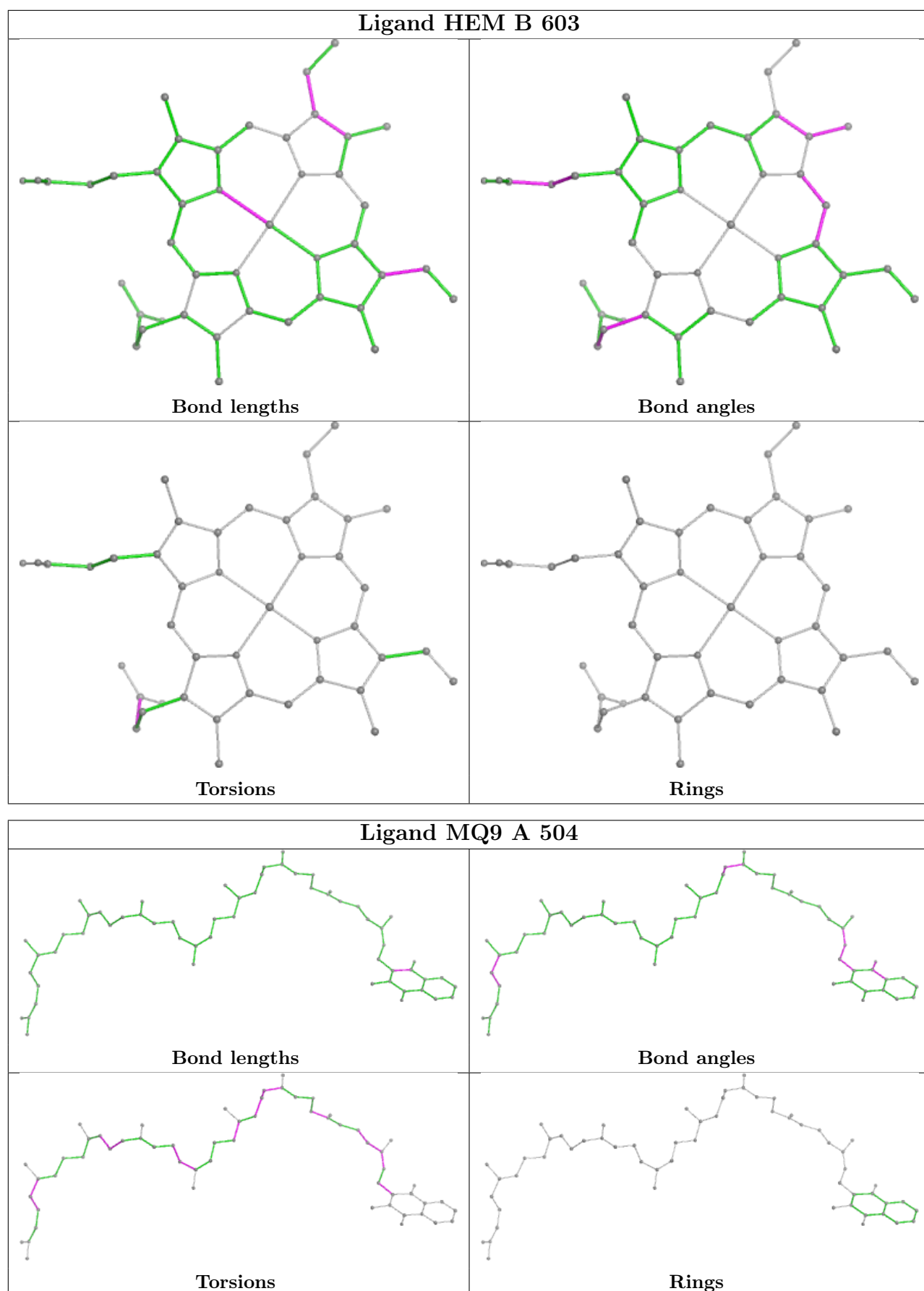
Rings

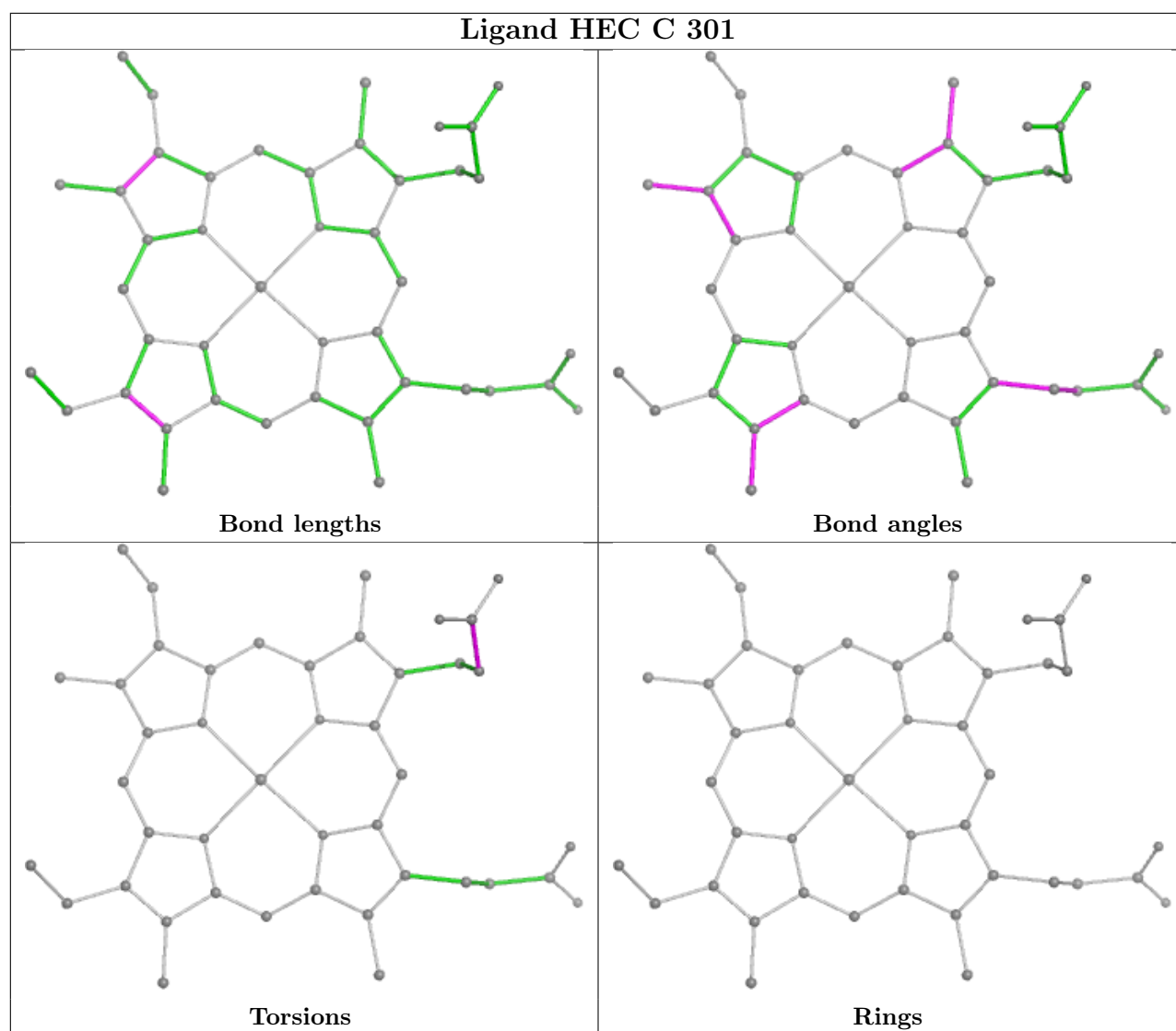


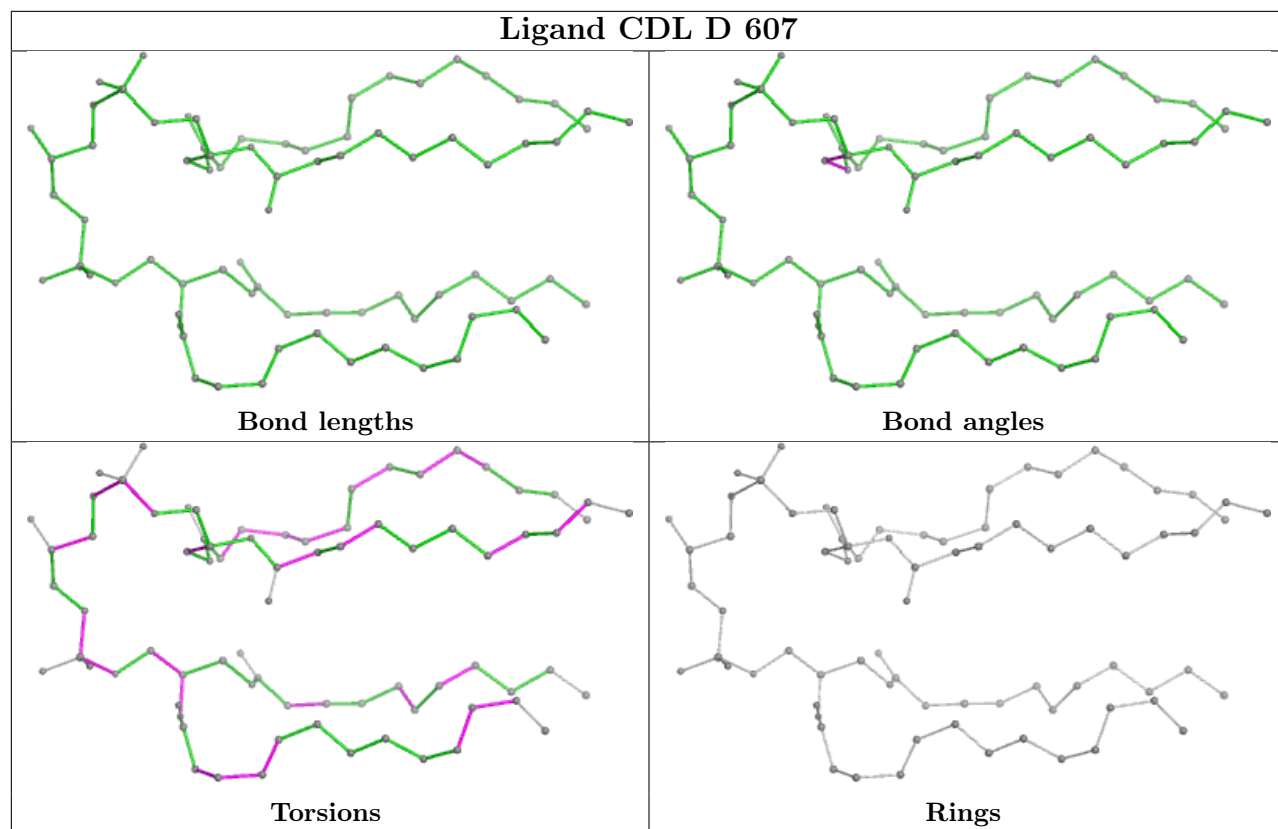


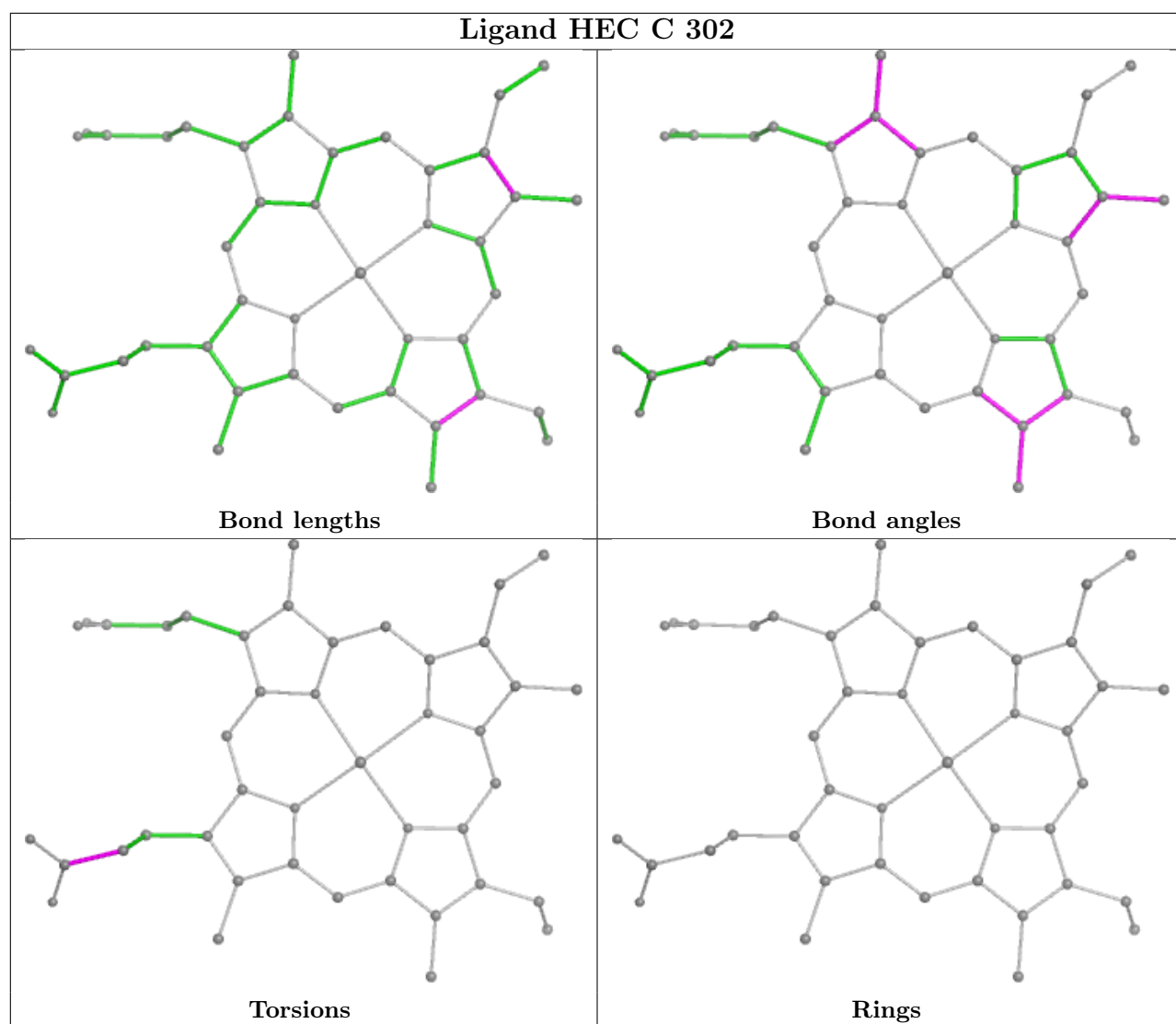


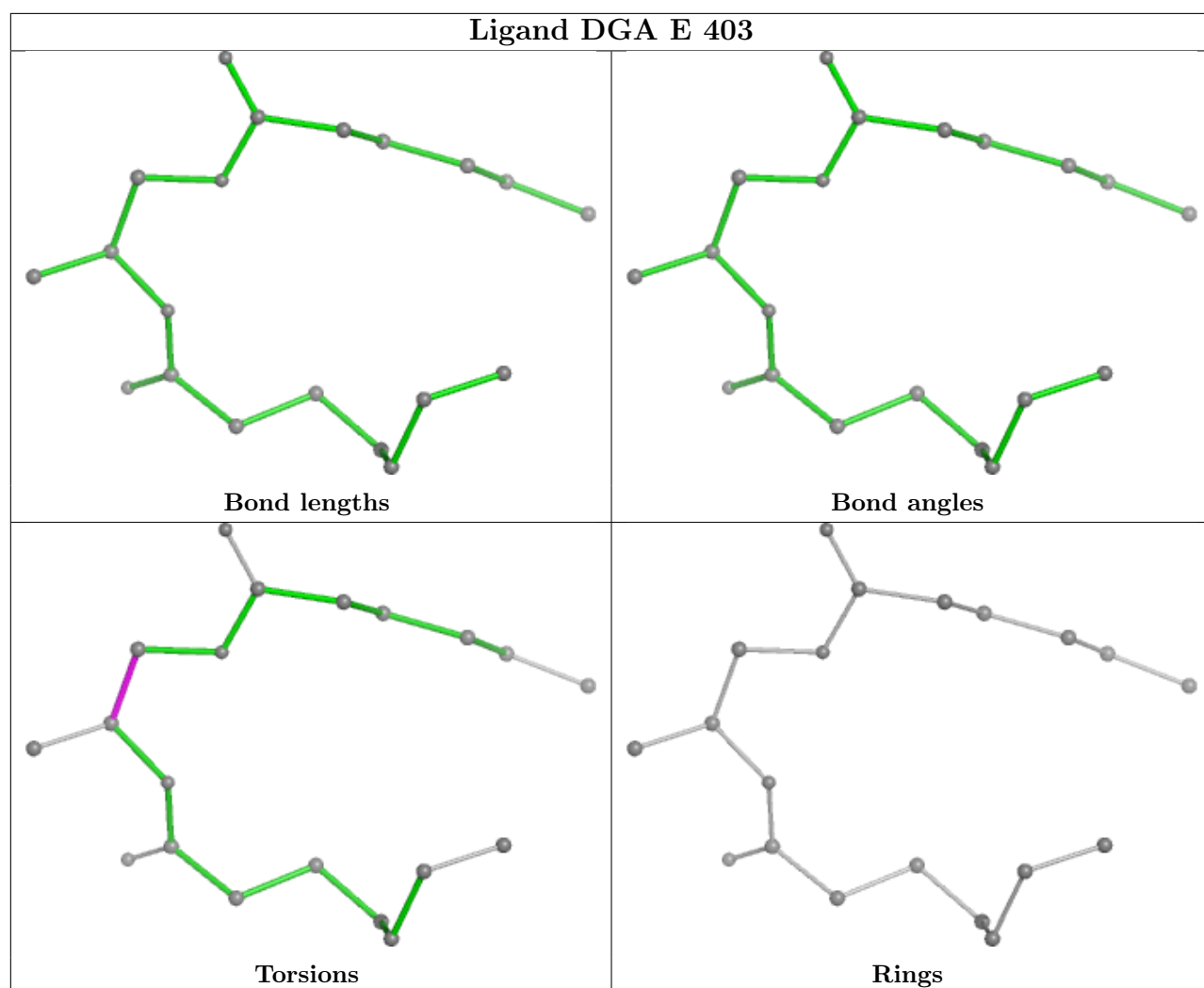


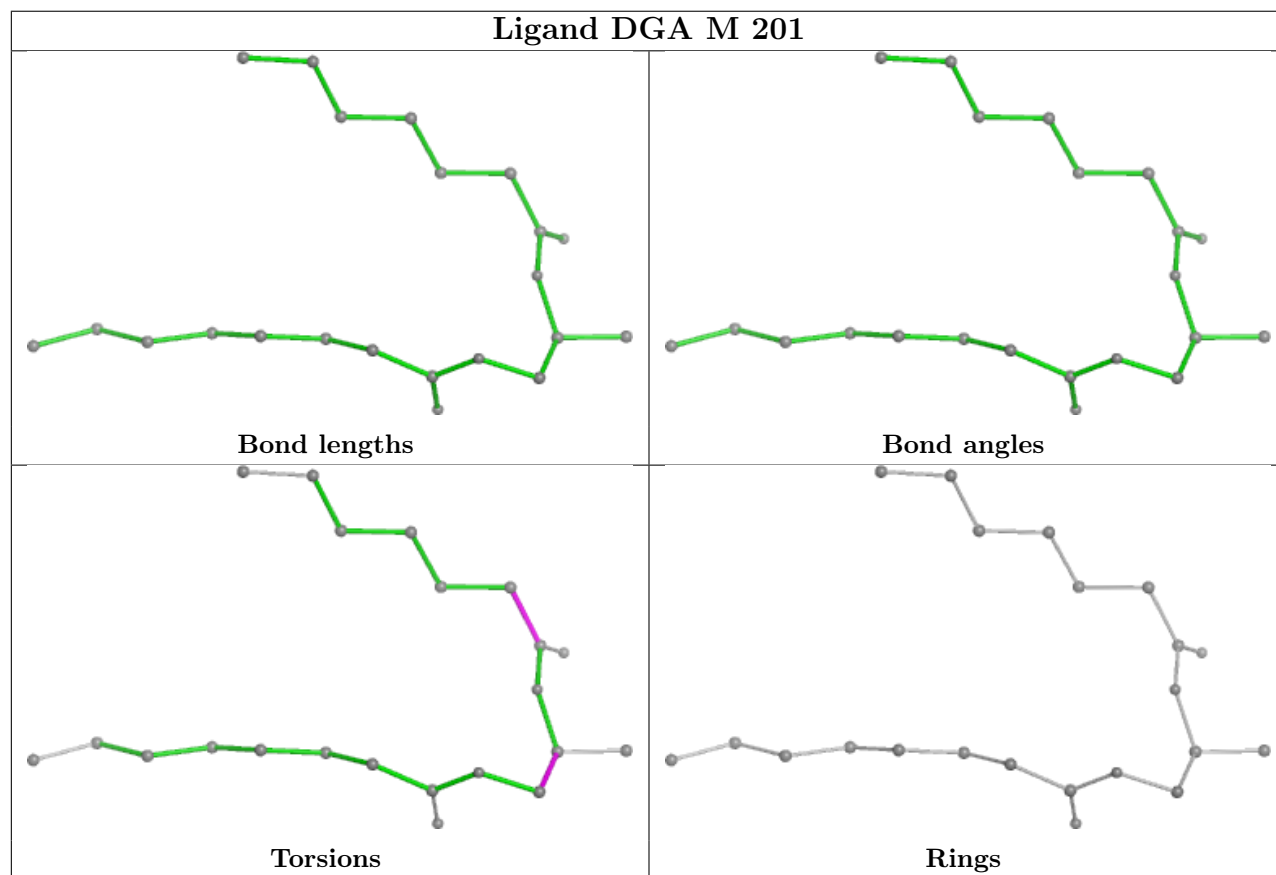
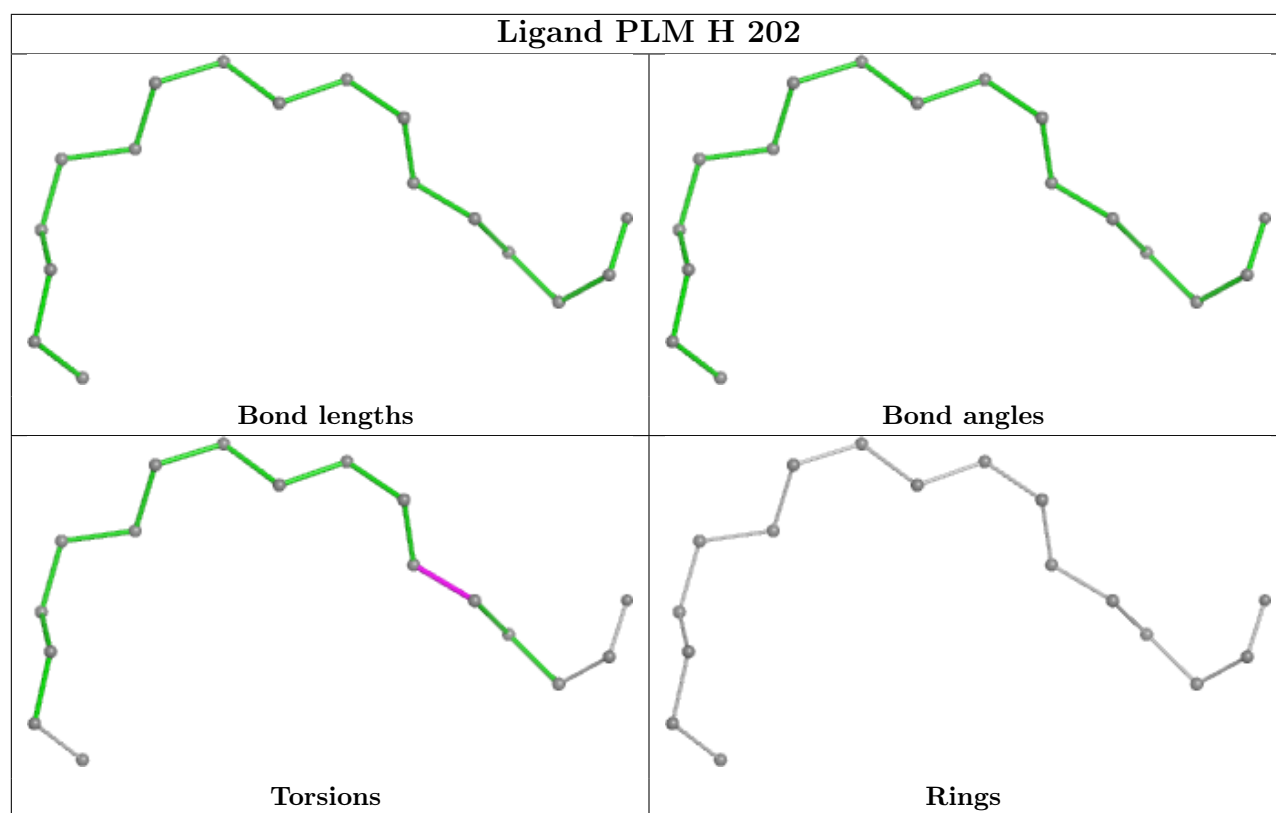


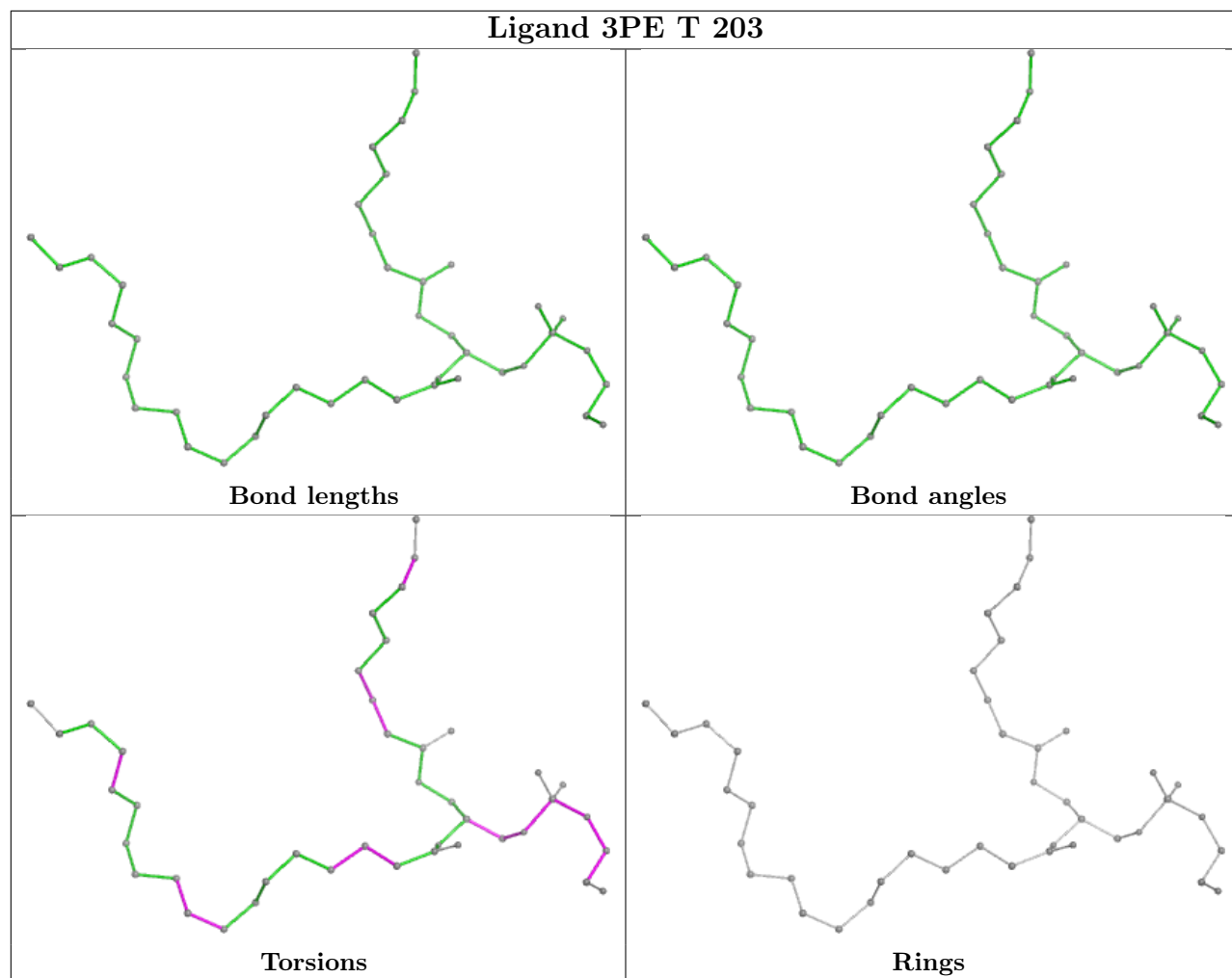


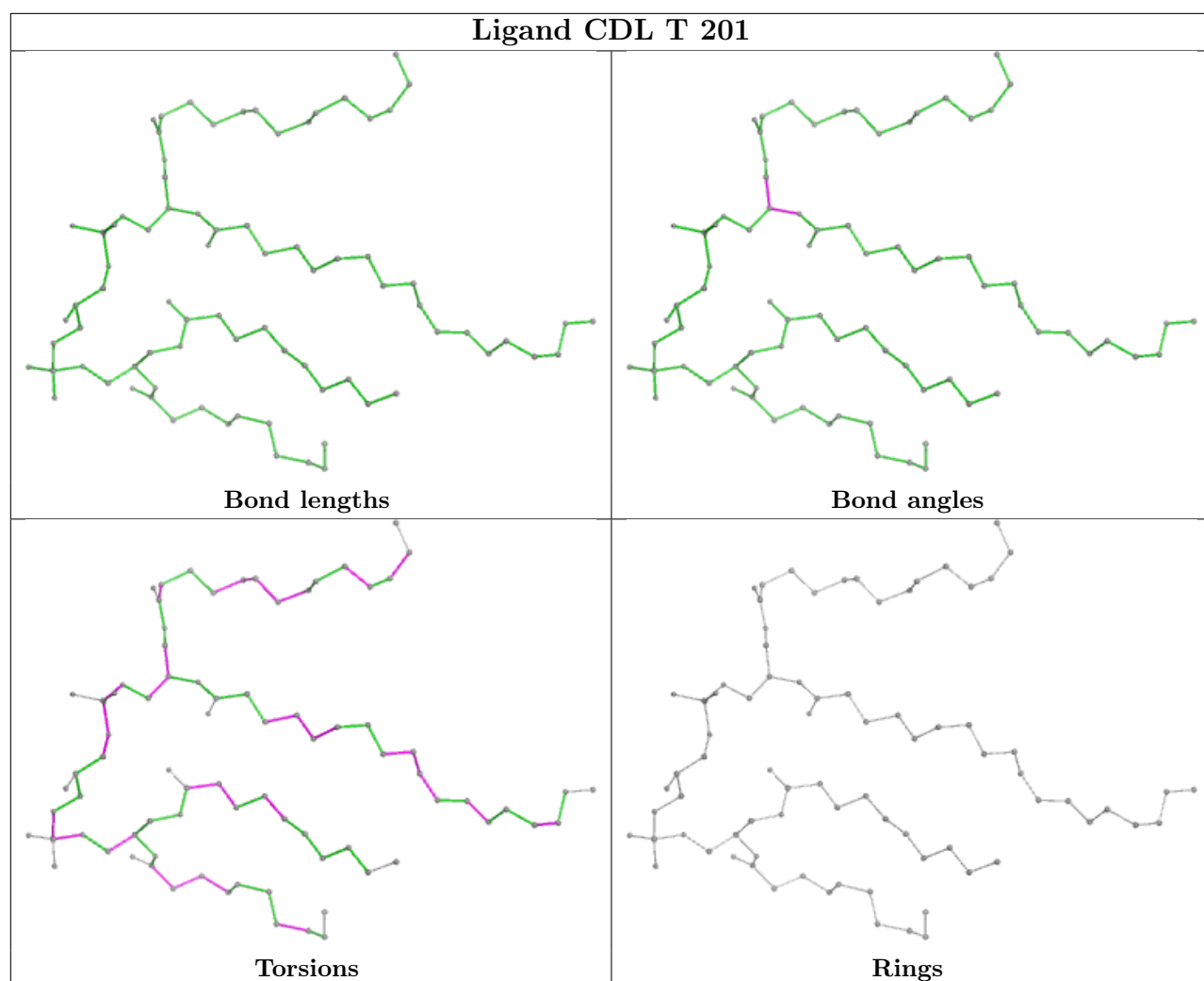


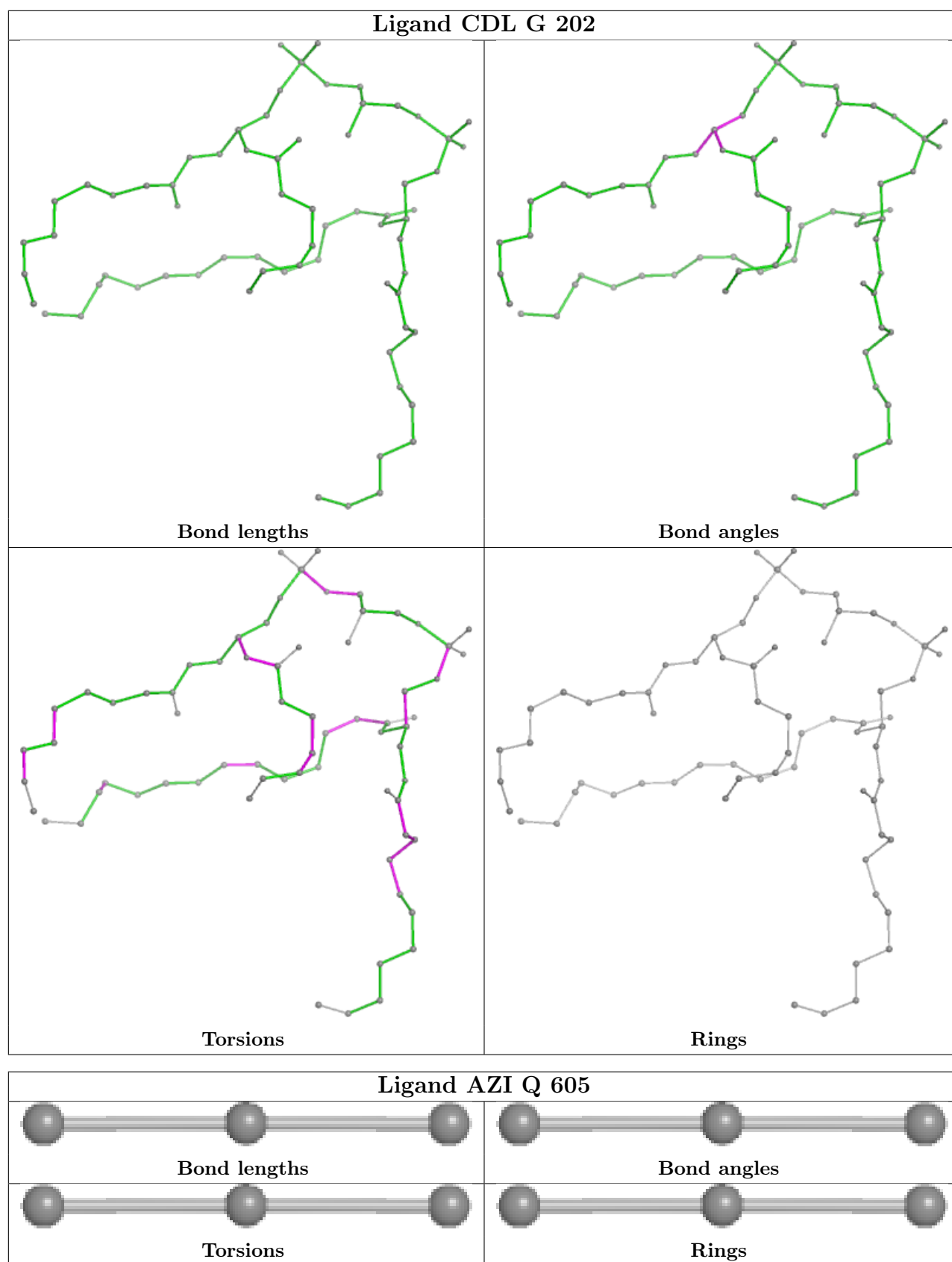


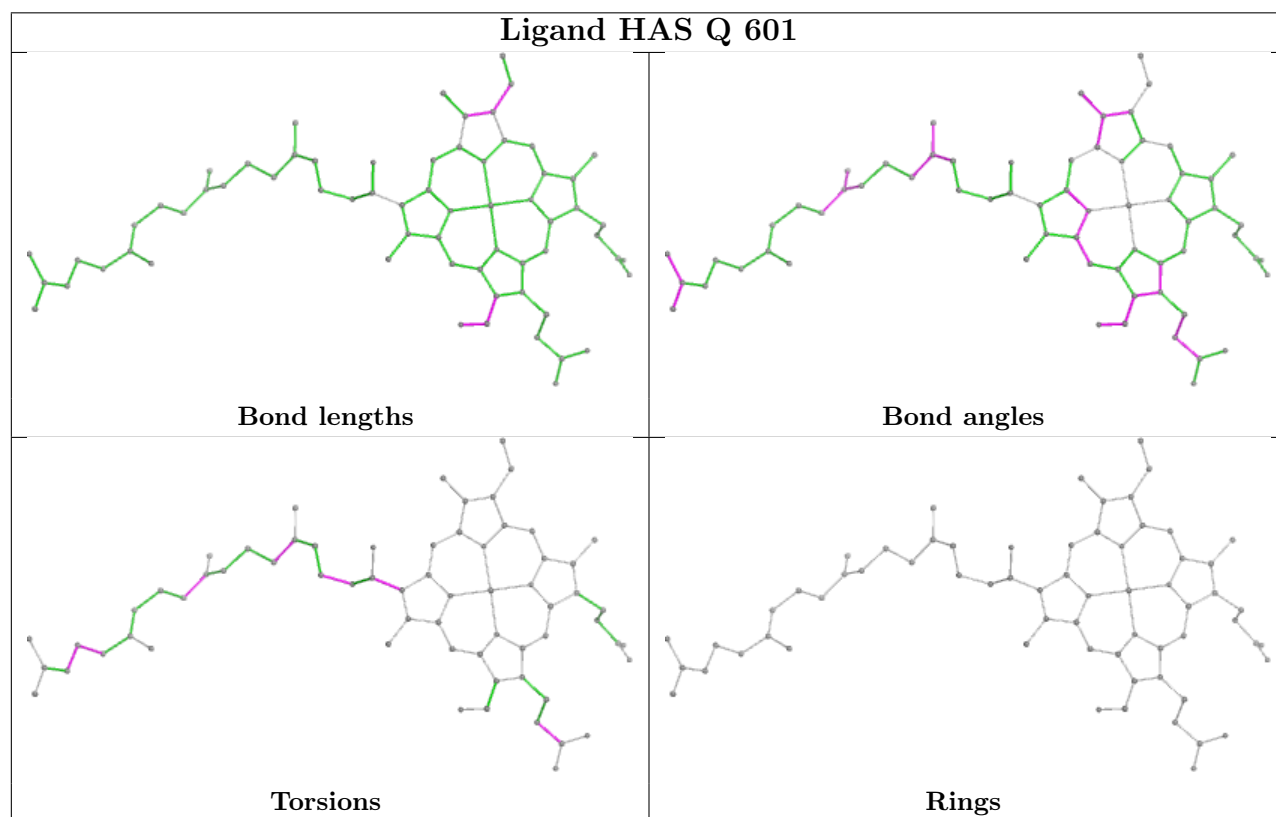
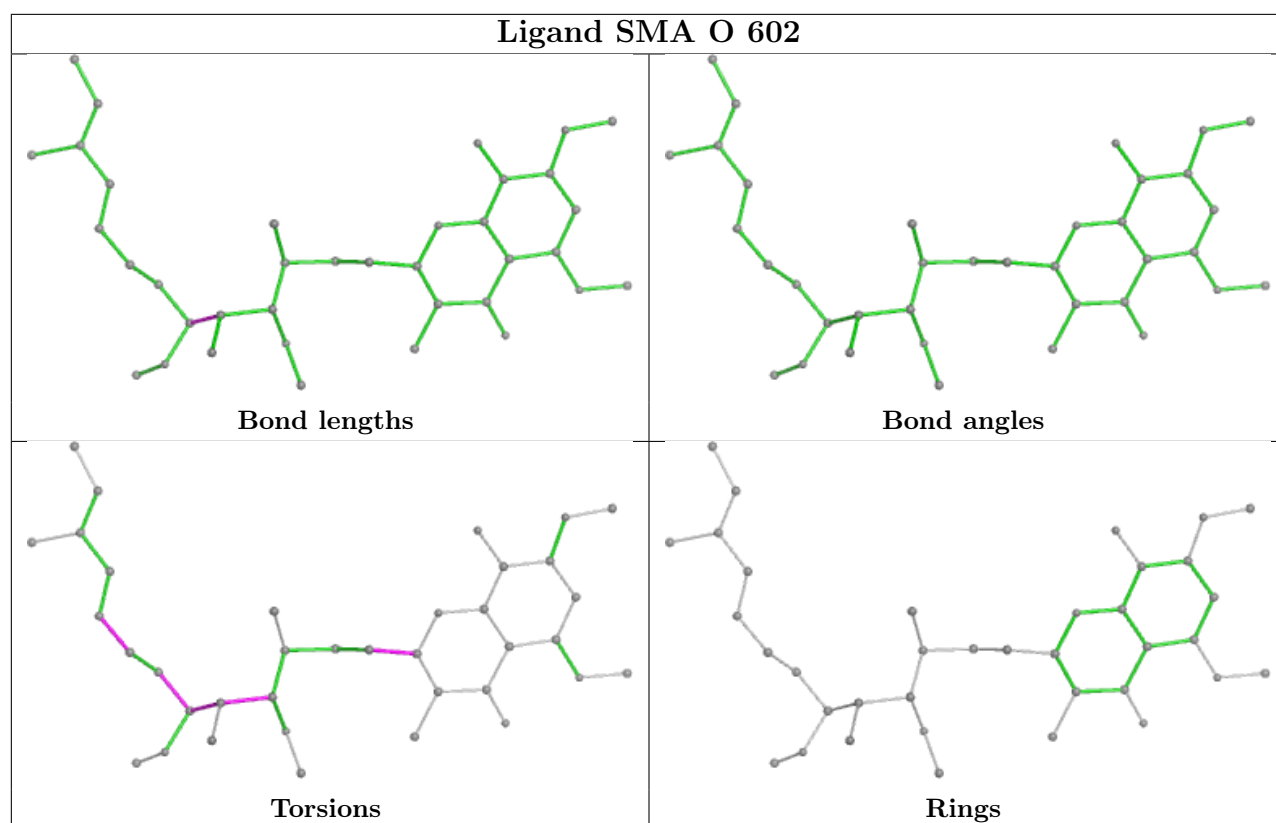


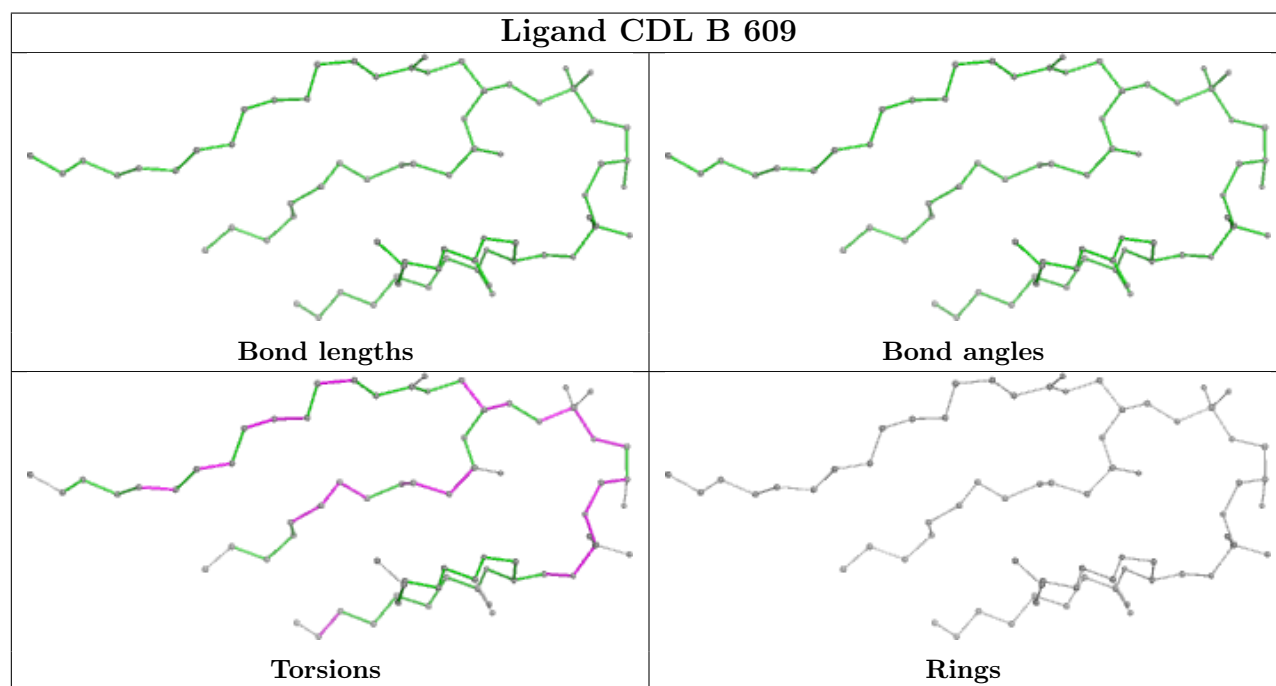
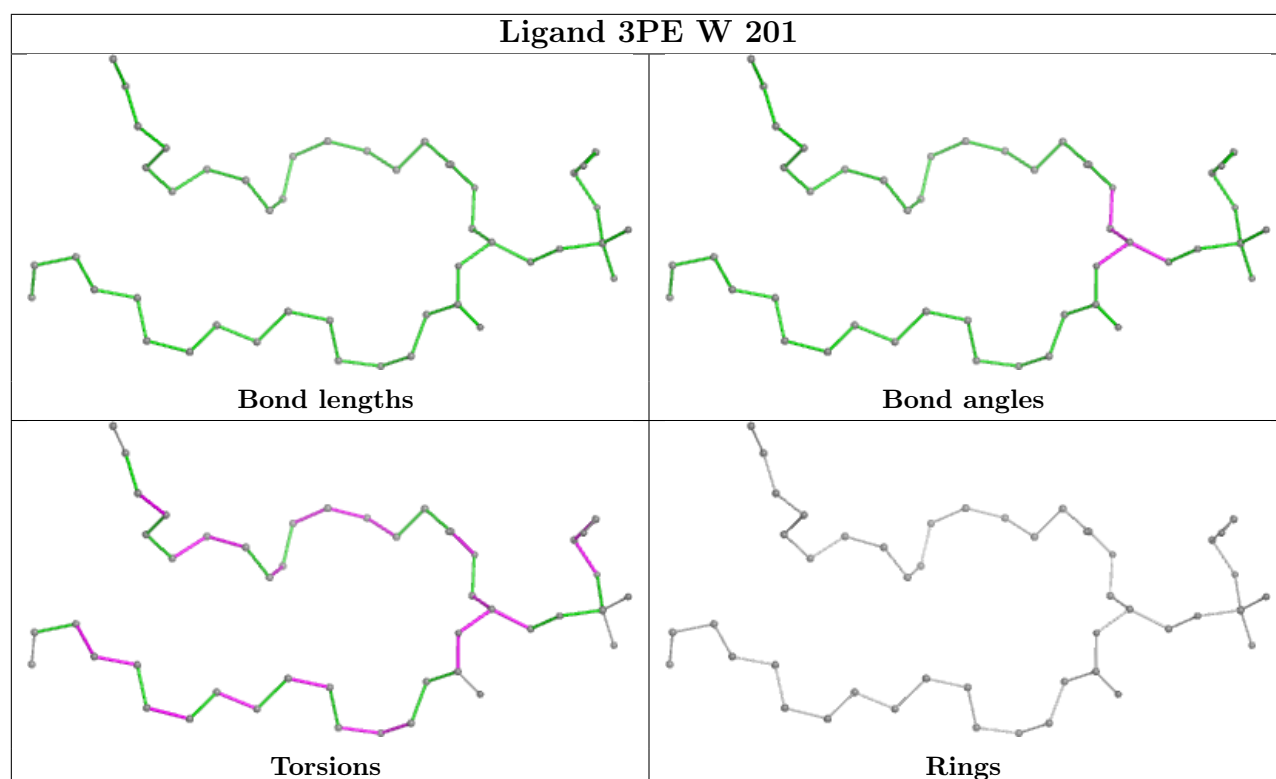


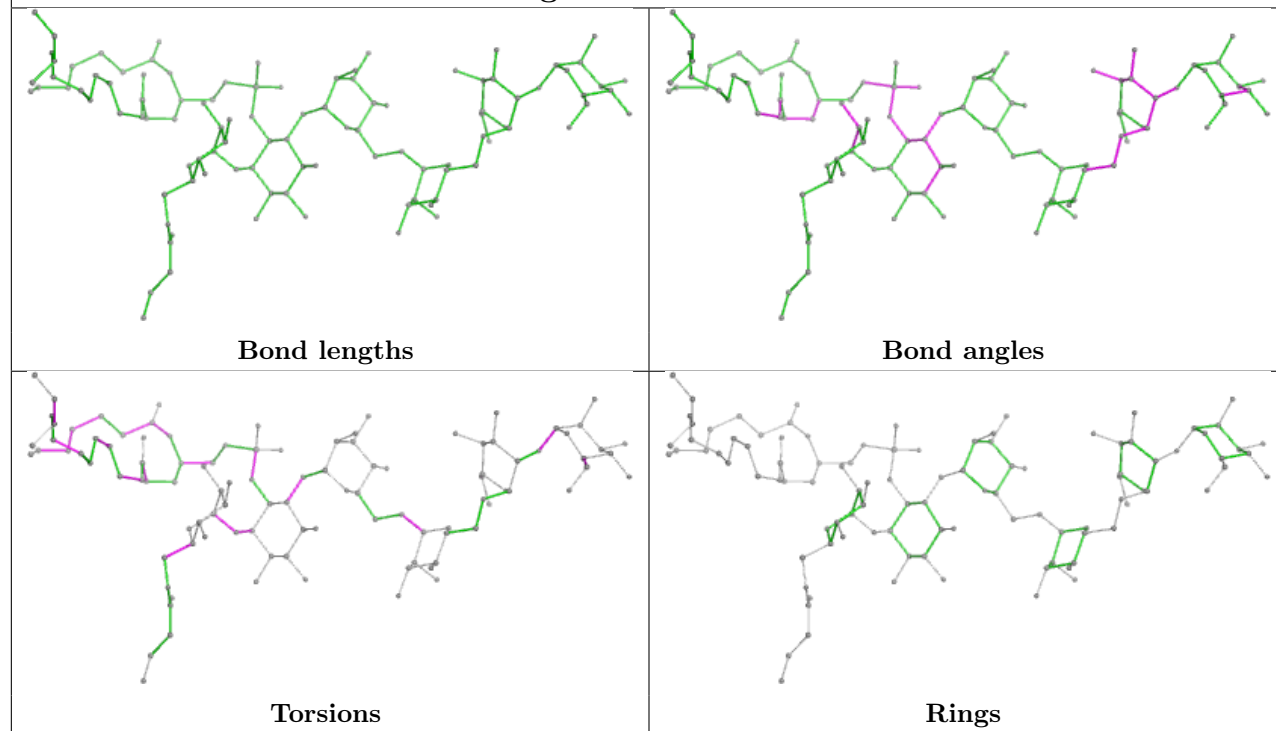
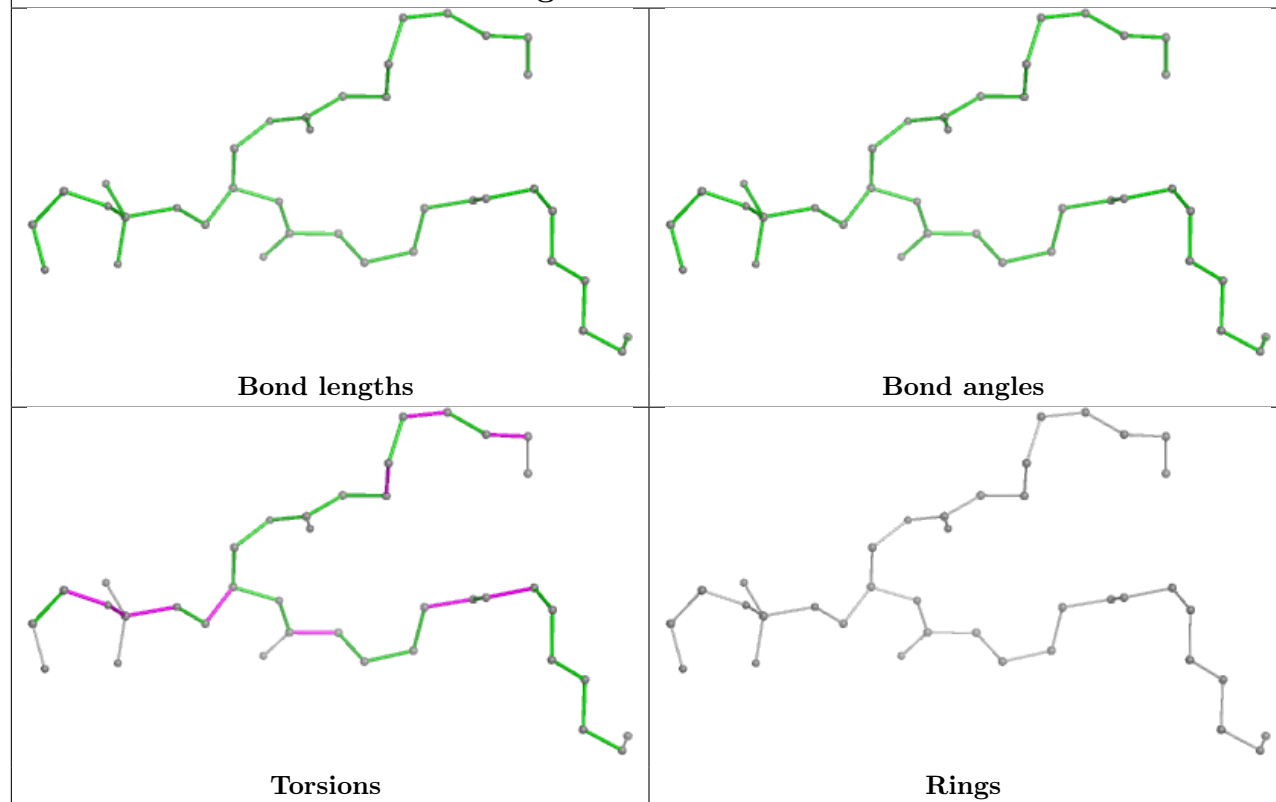


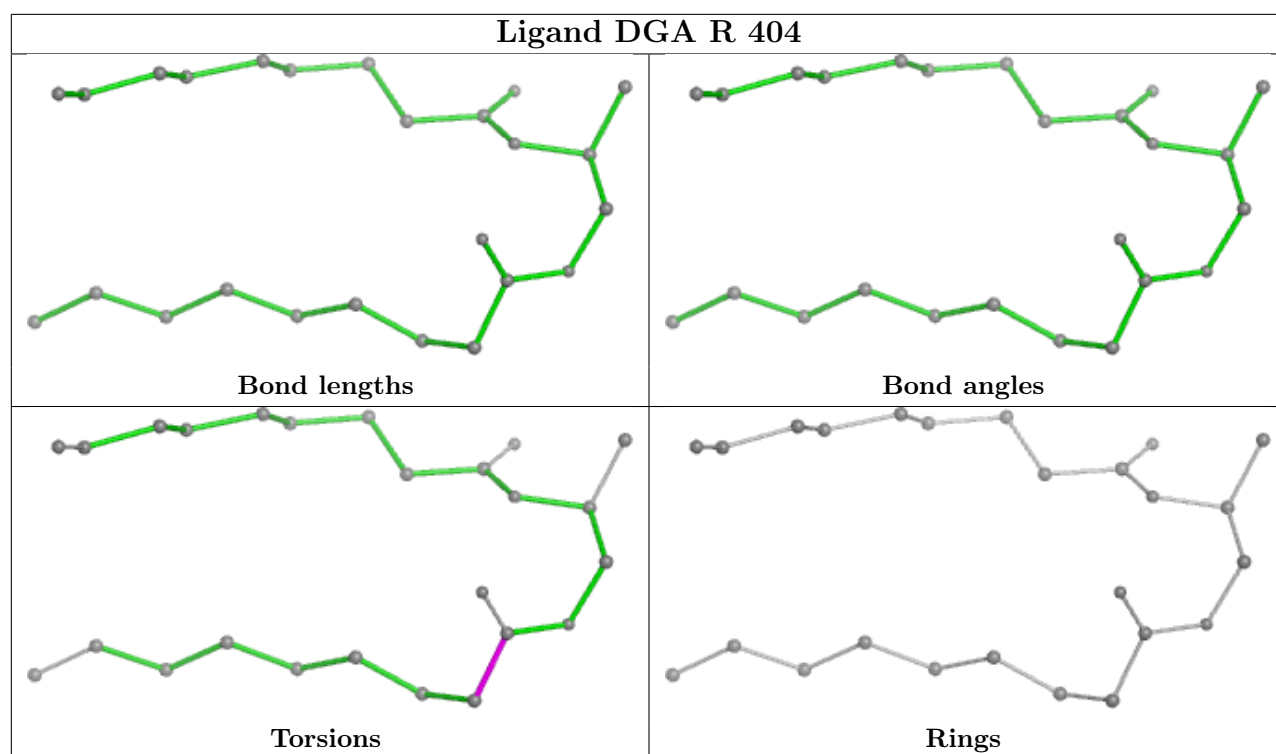


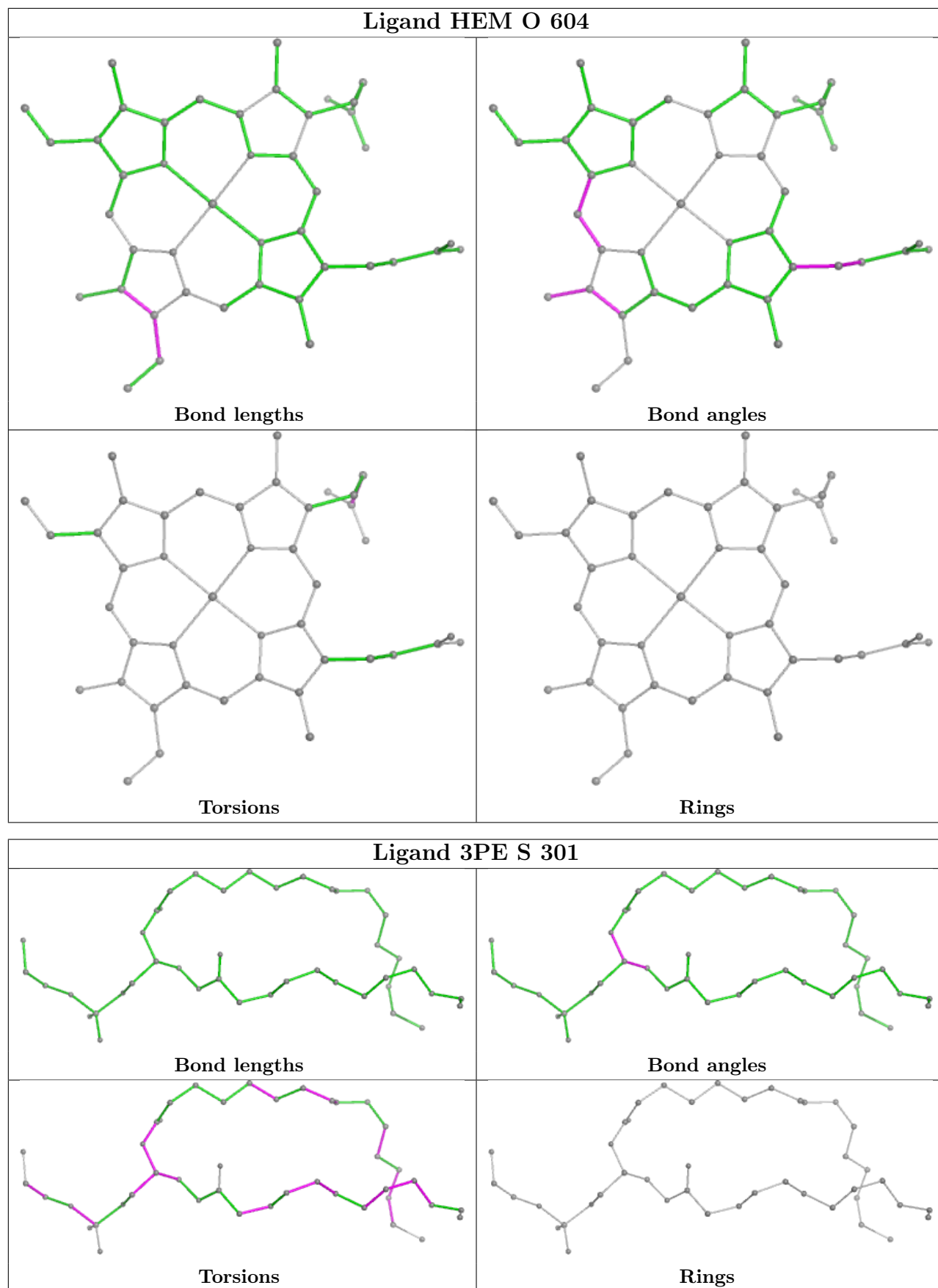


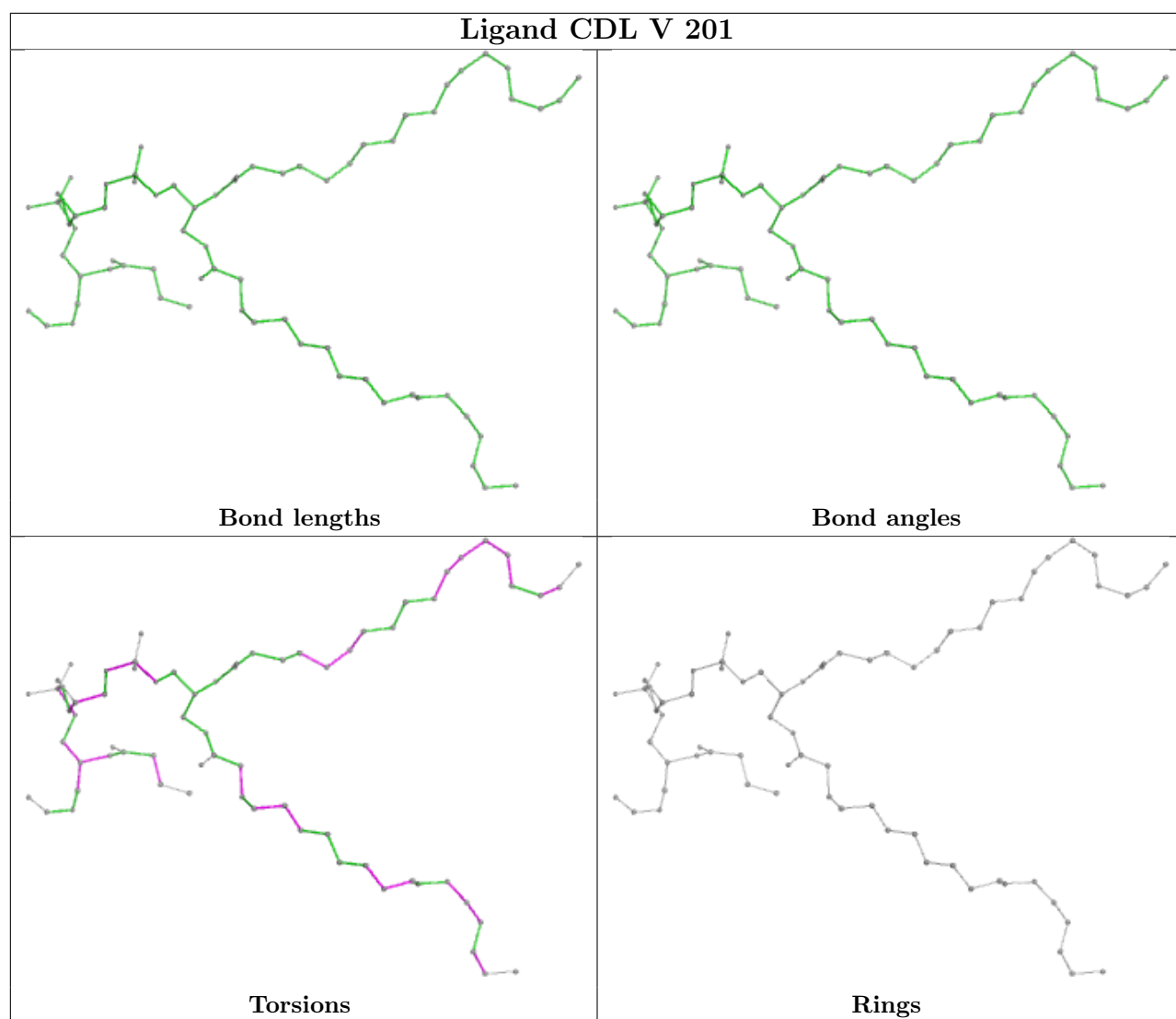


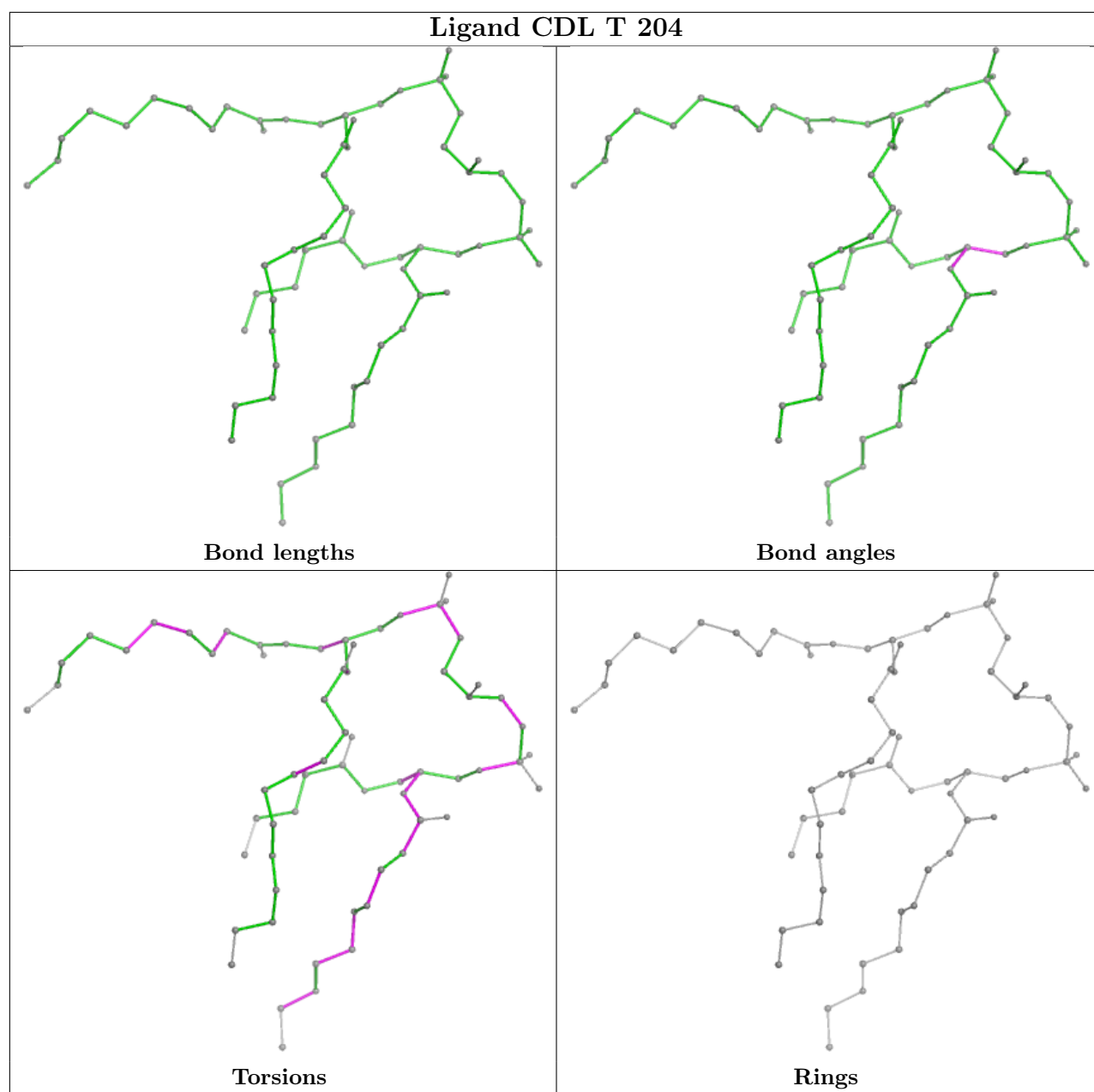


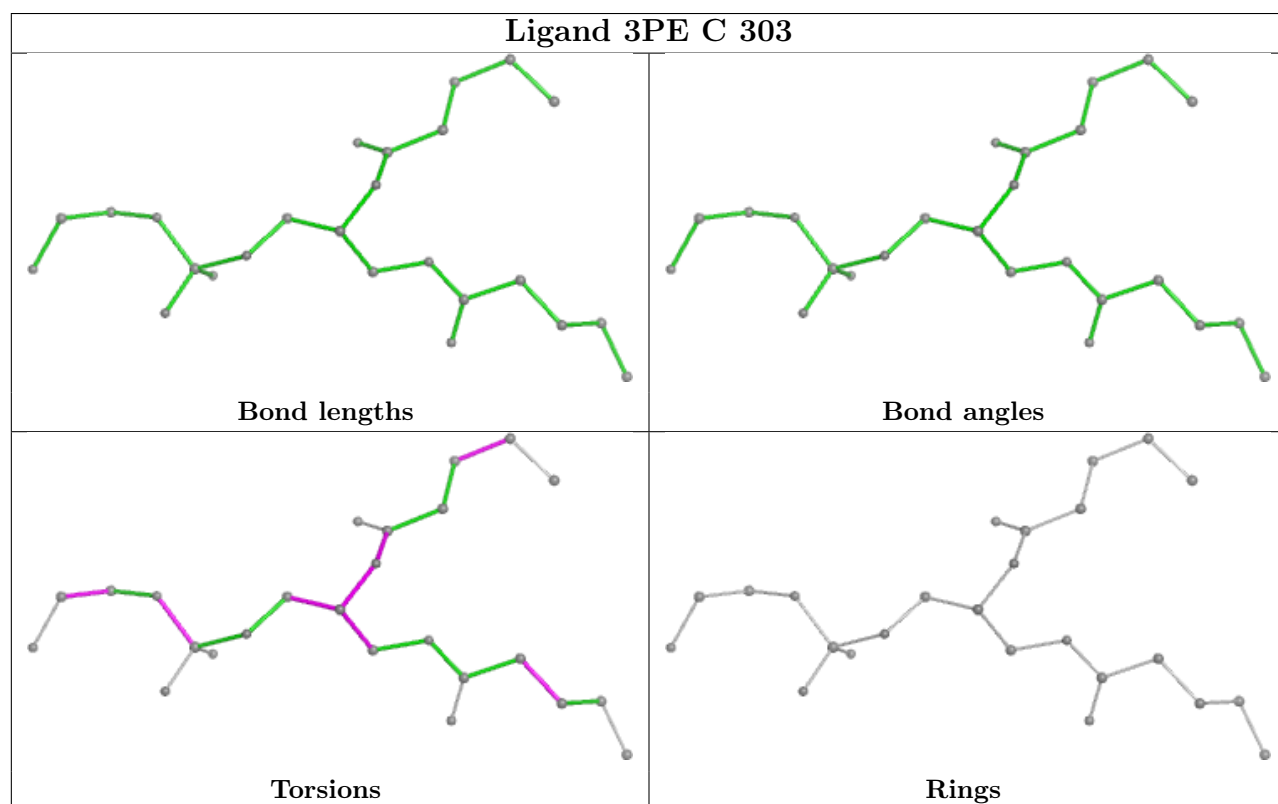
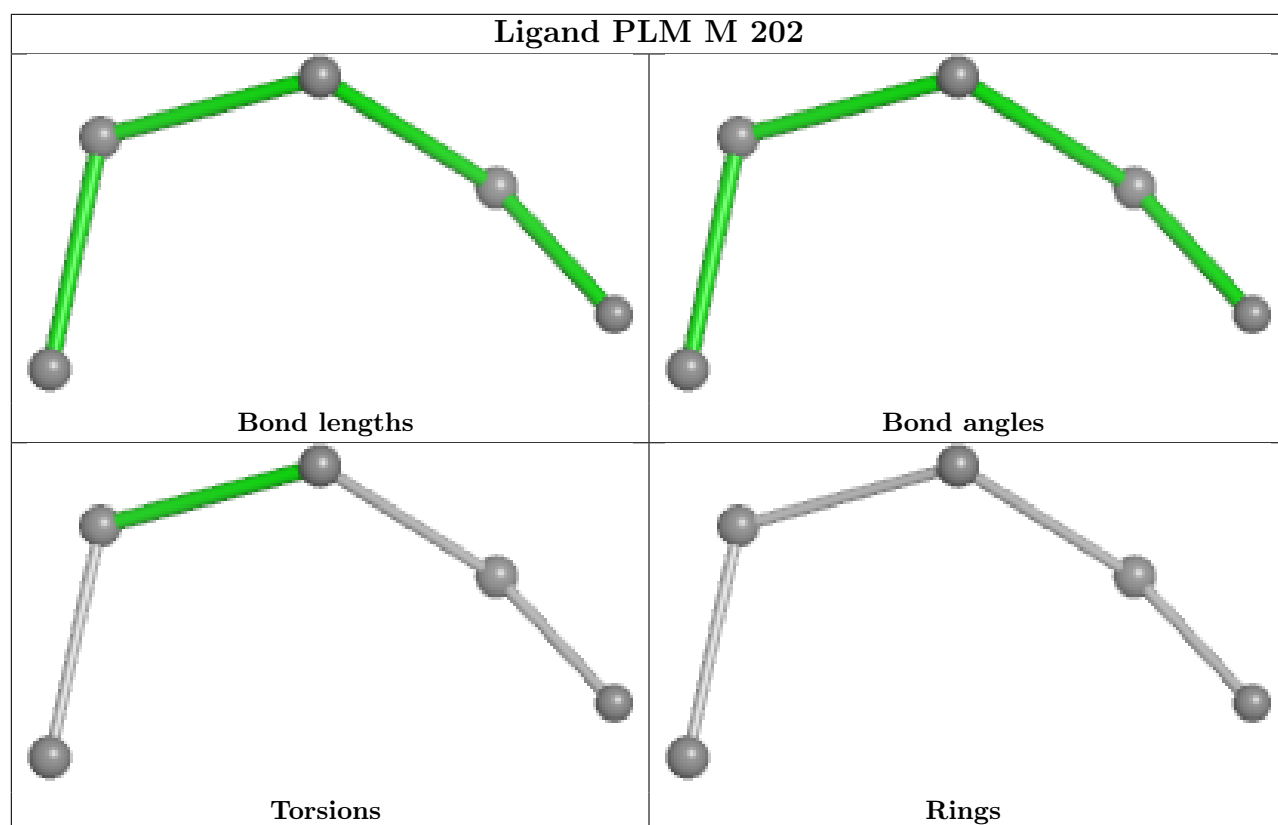
Ligand IZL N 504**Ligand 3PE T 205**

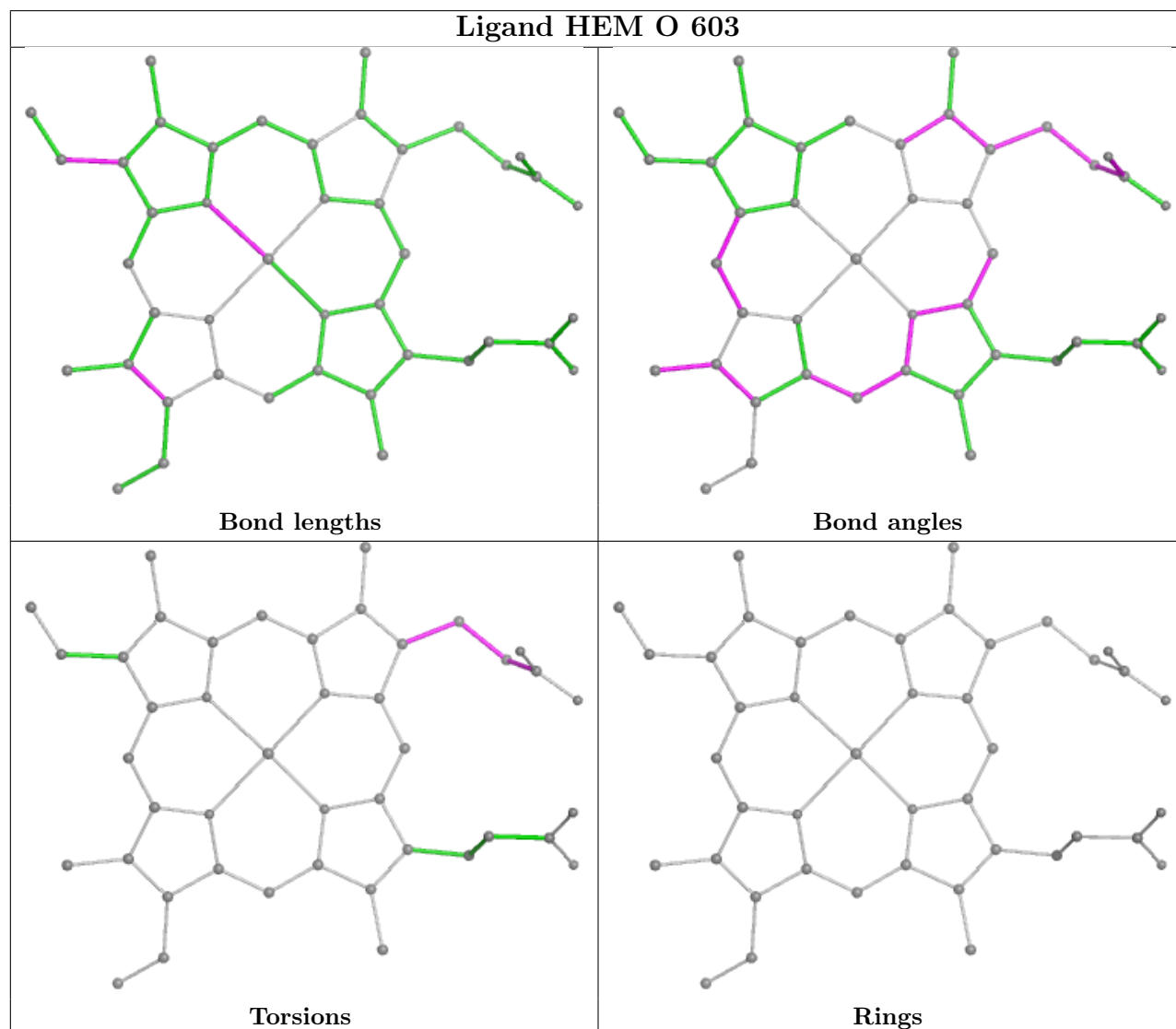
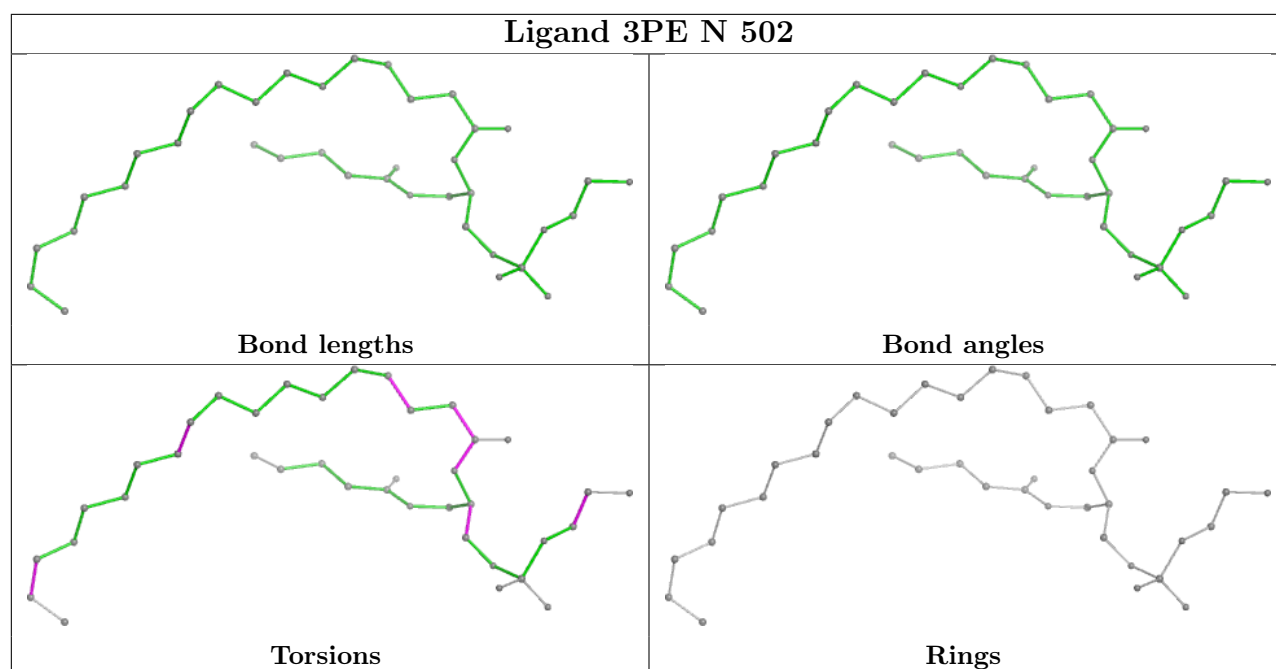


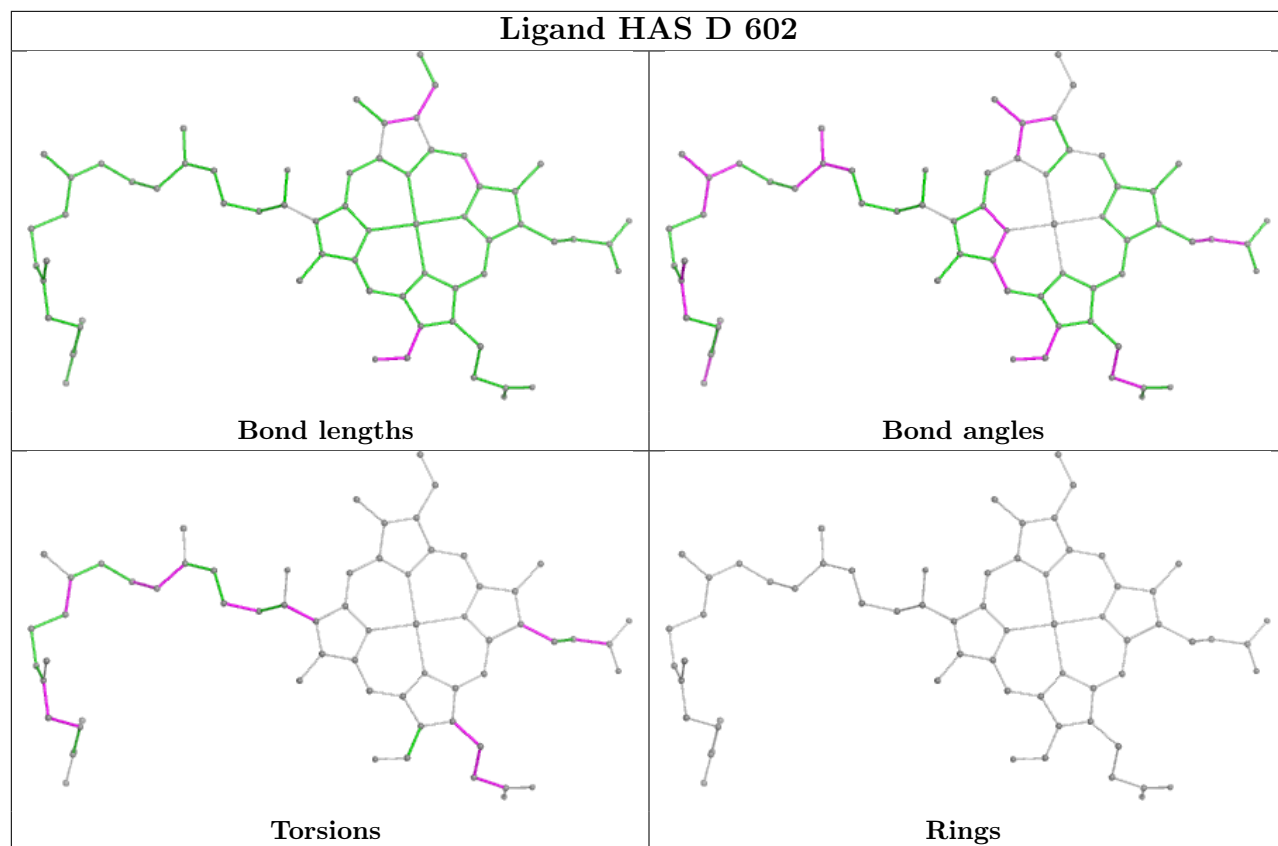


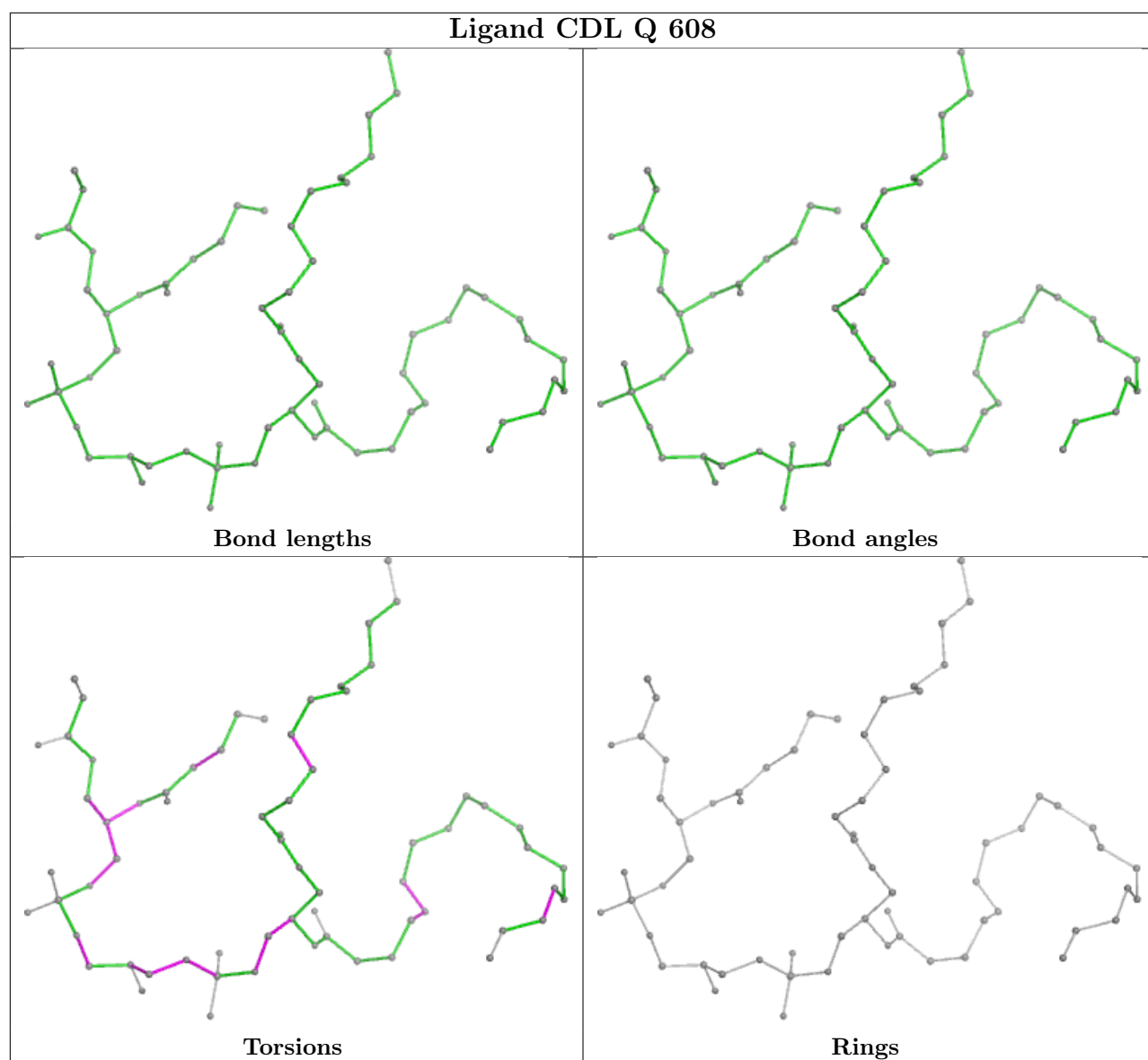


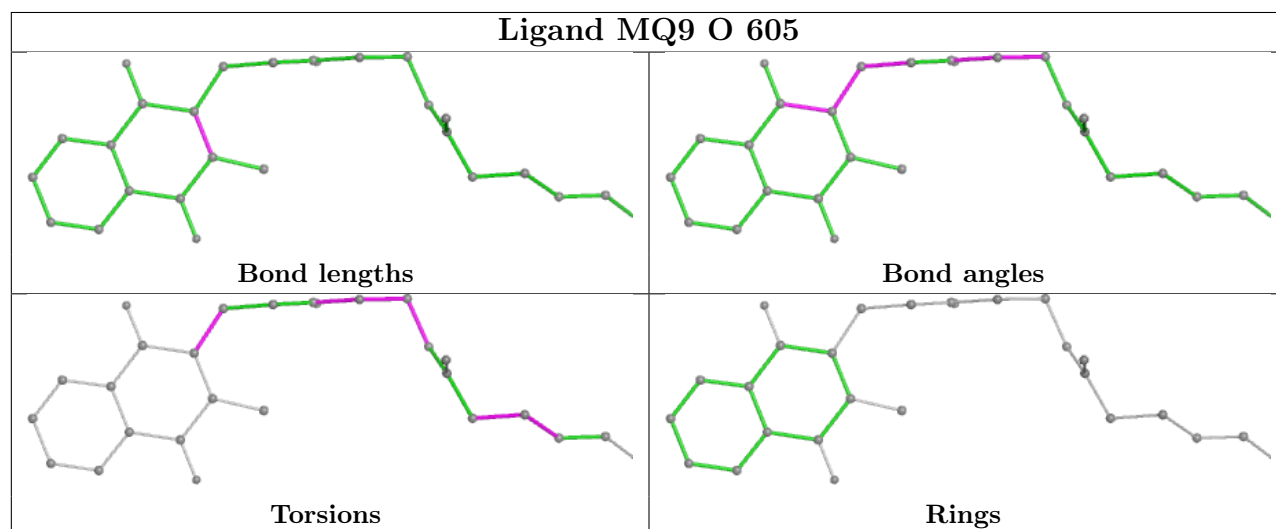
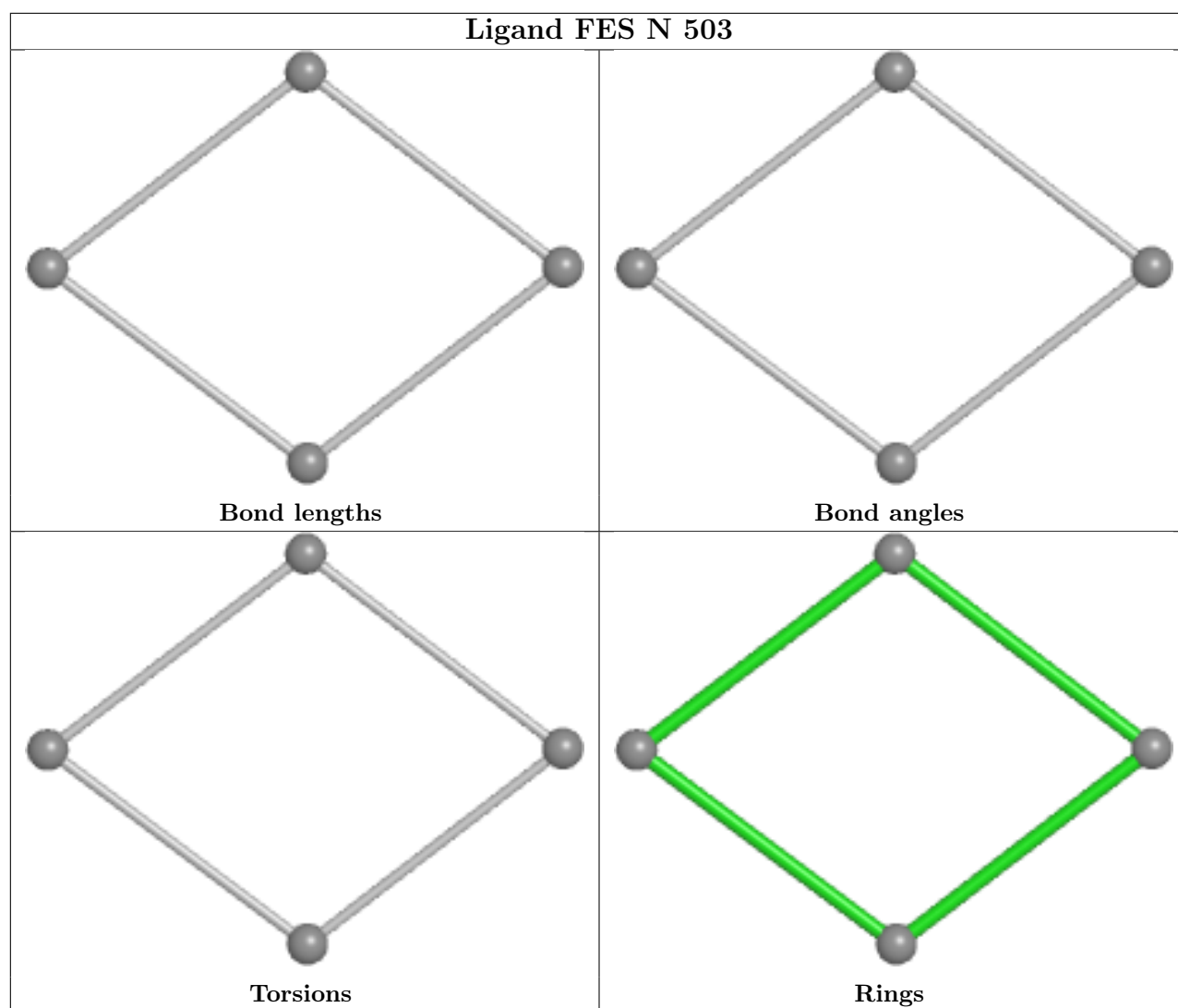


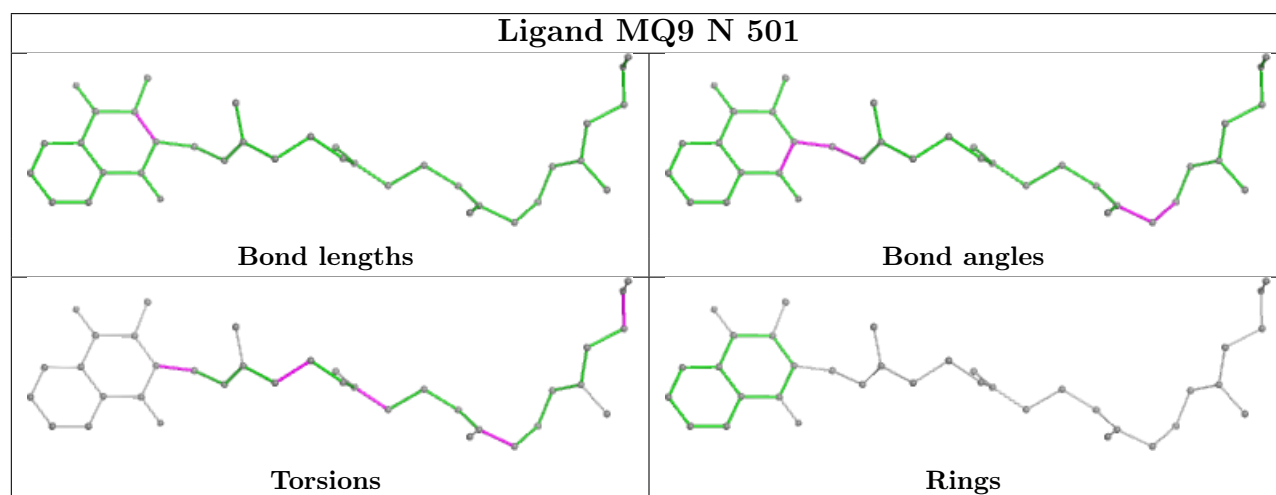
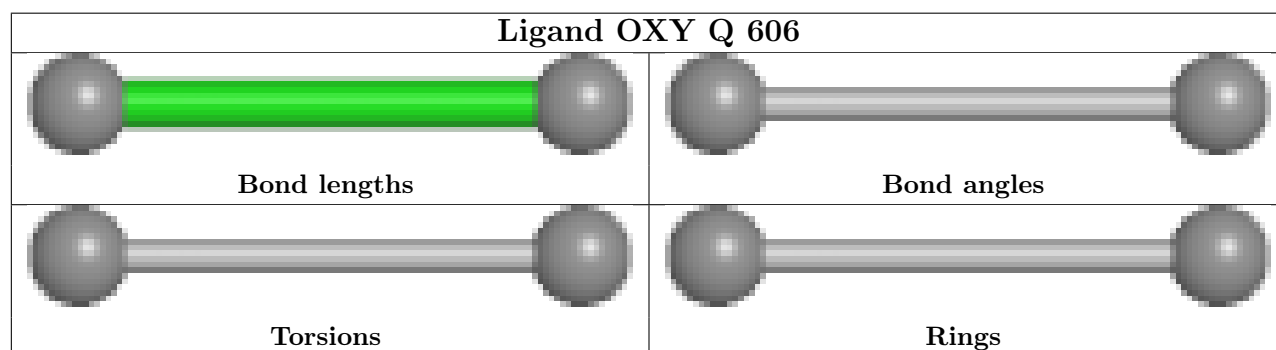
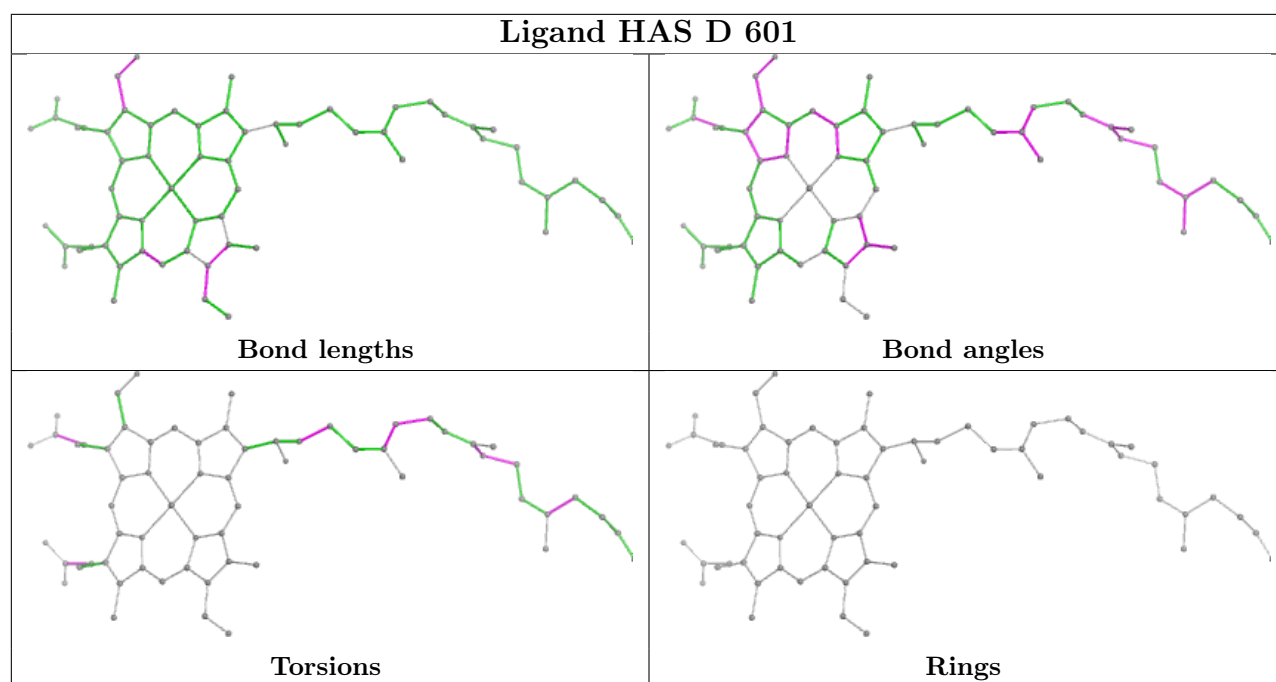


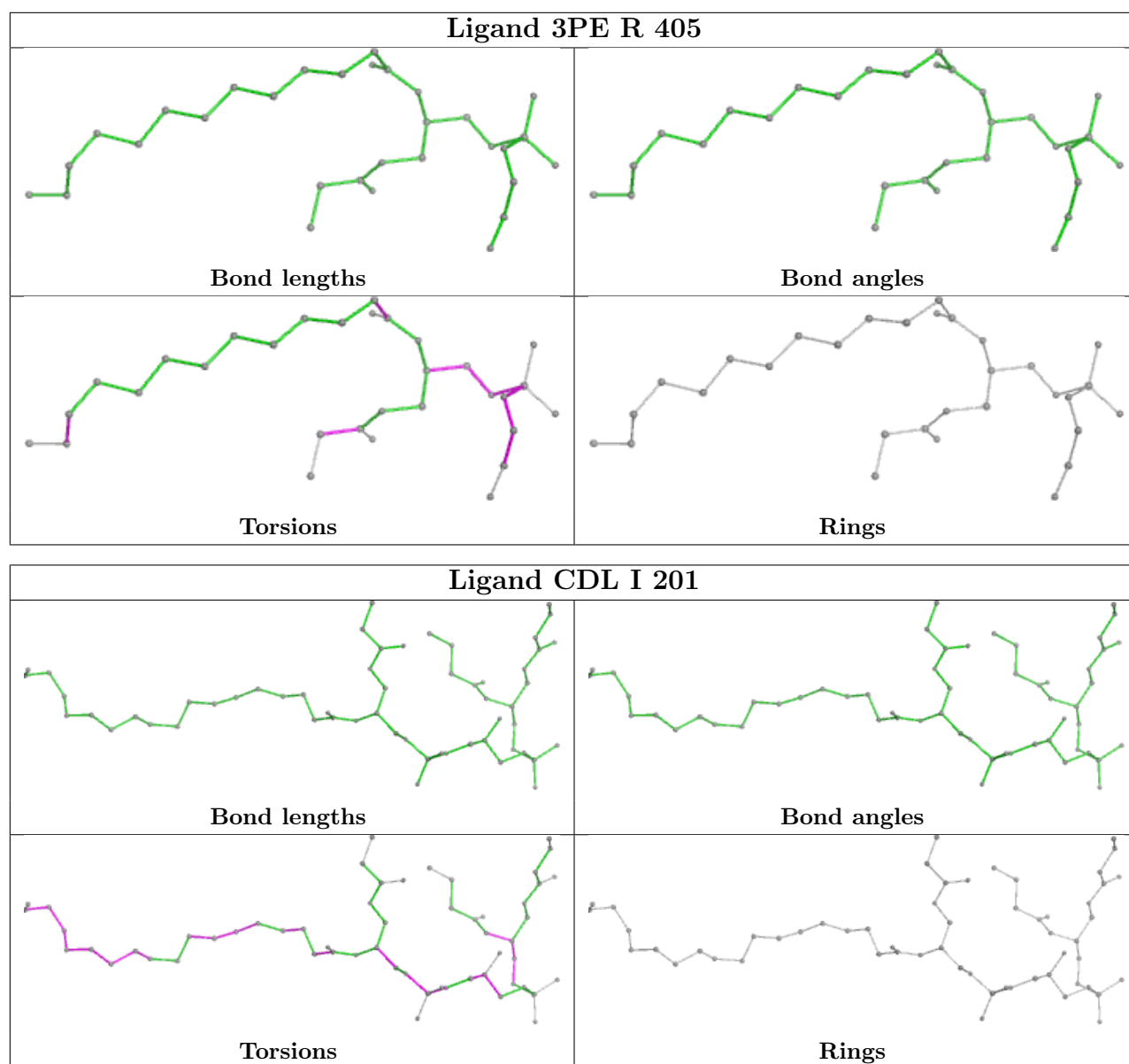


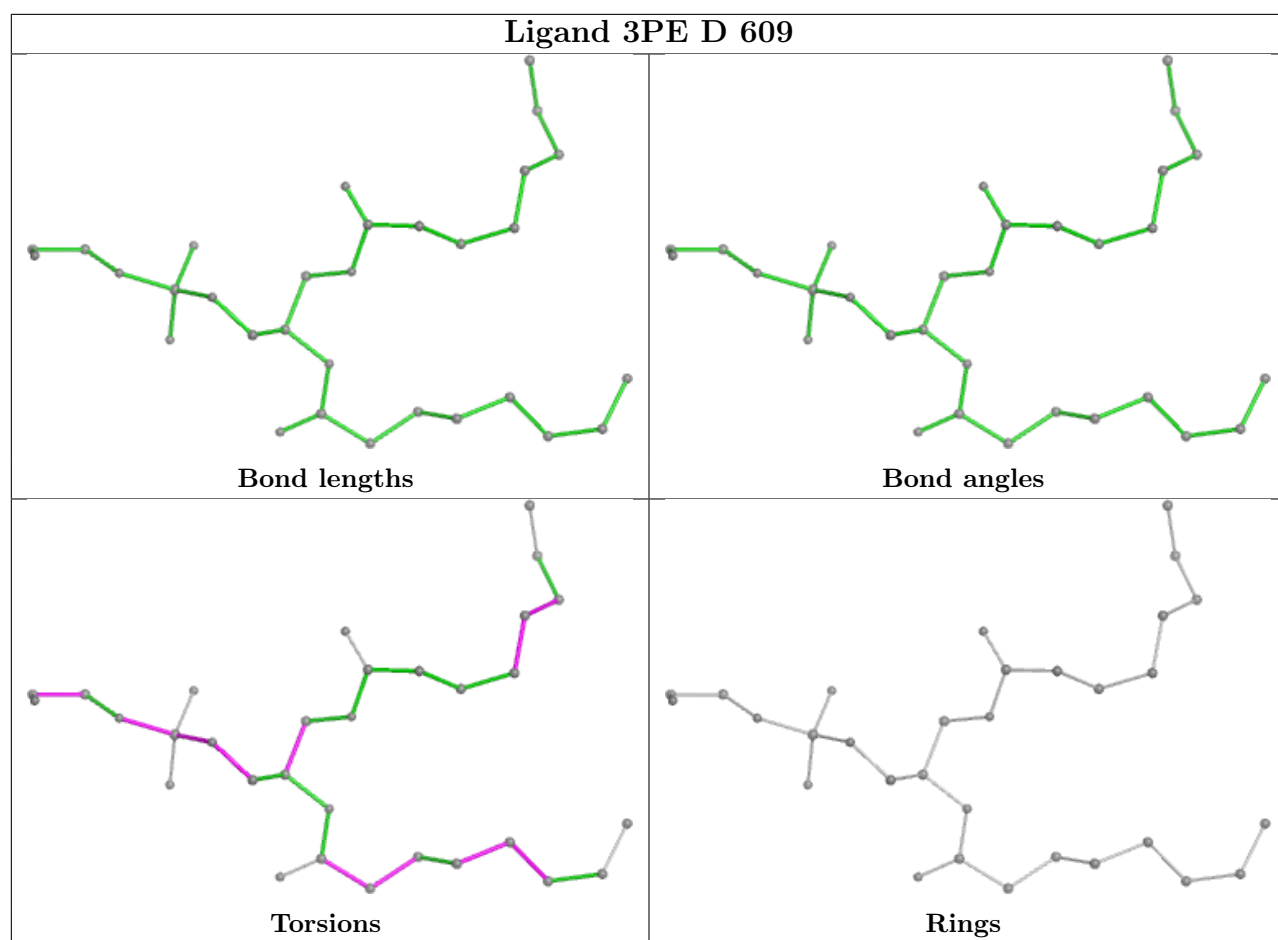


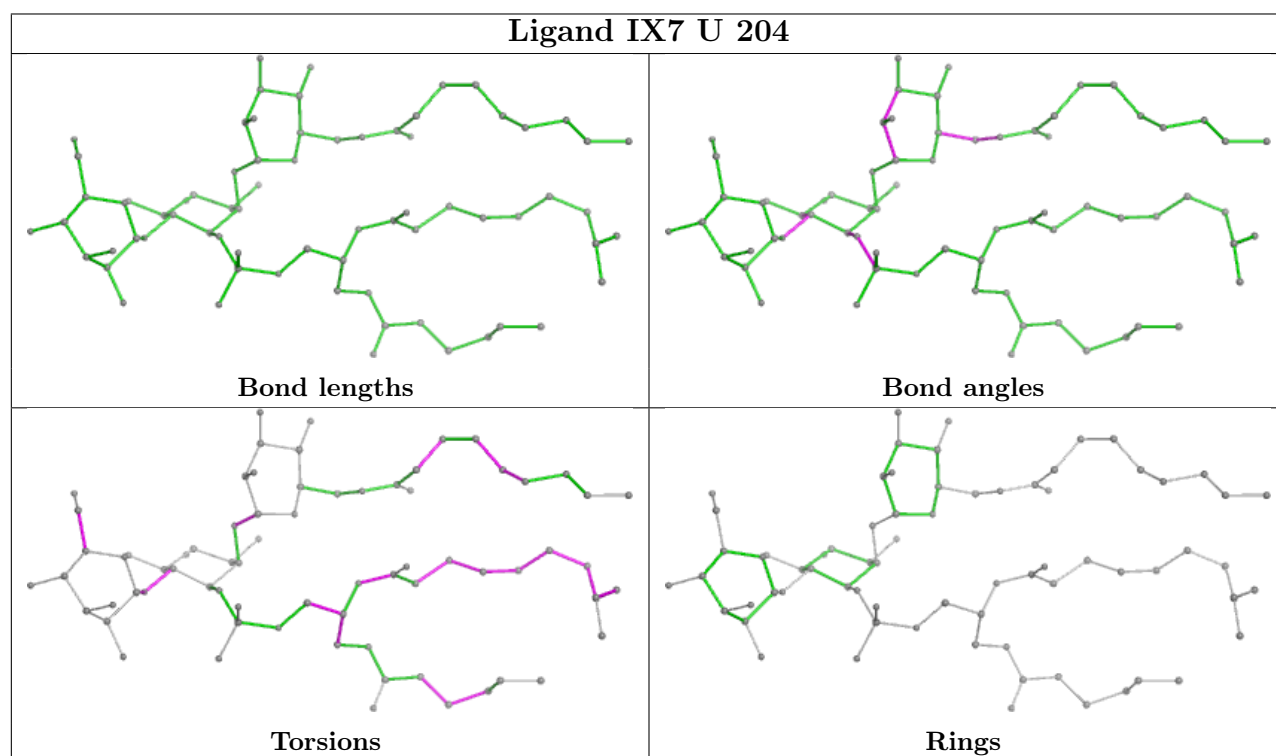
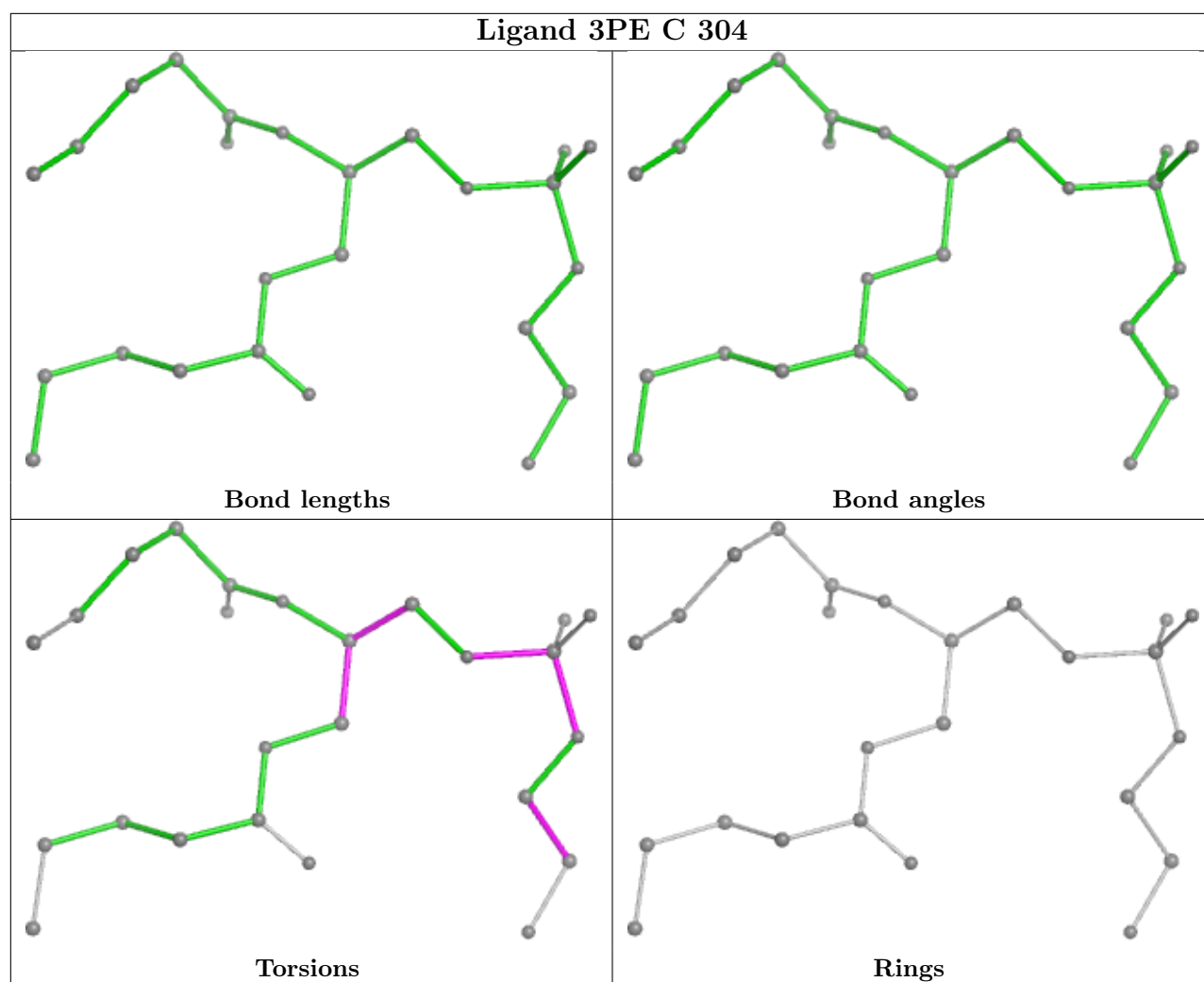


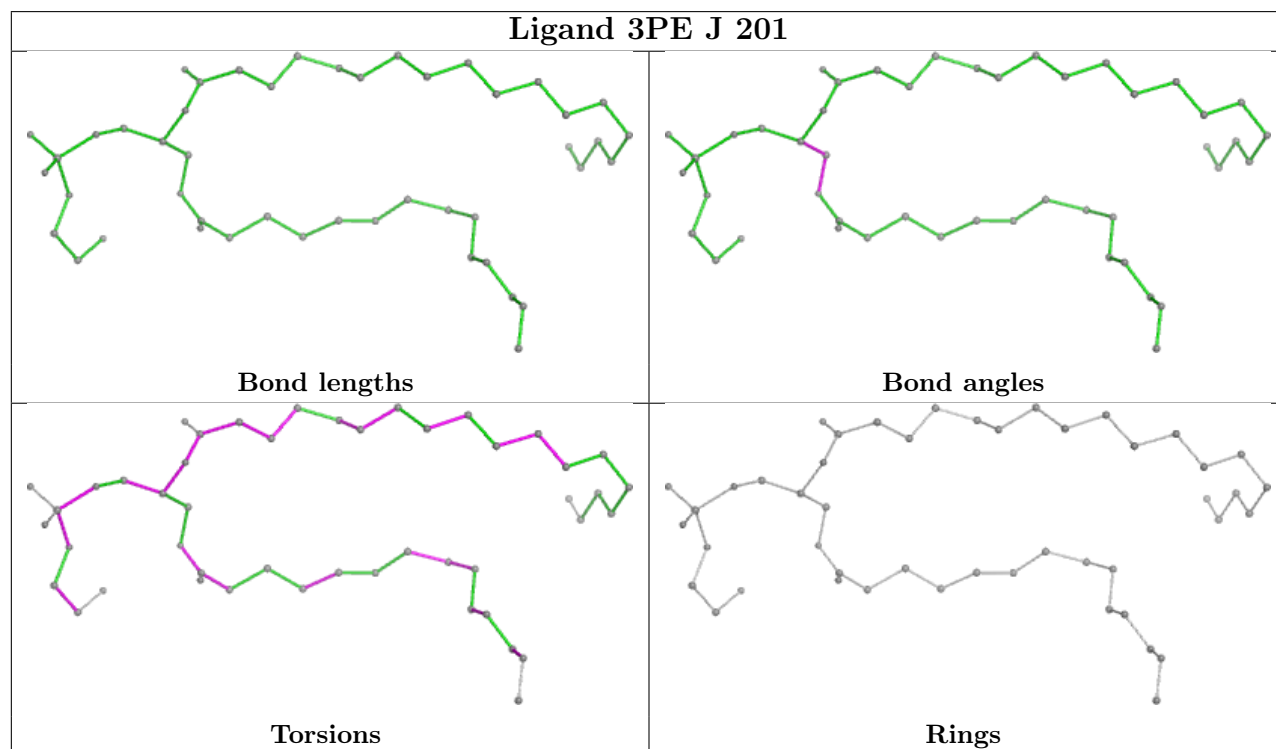
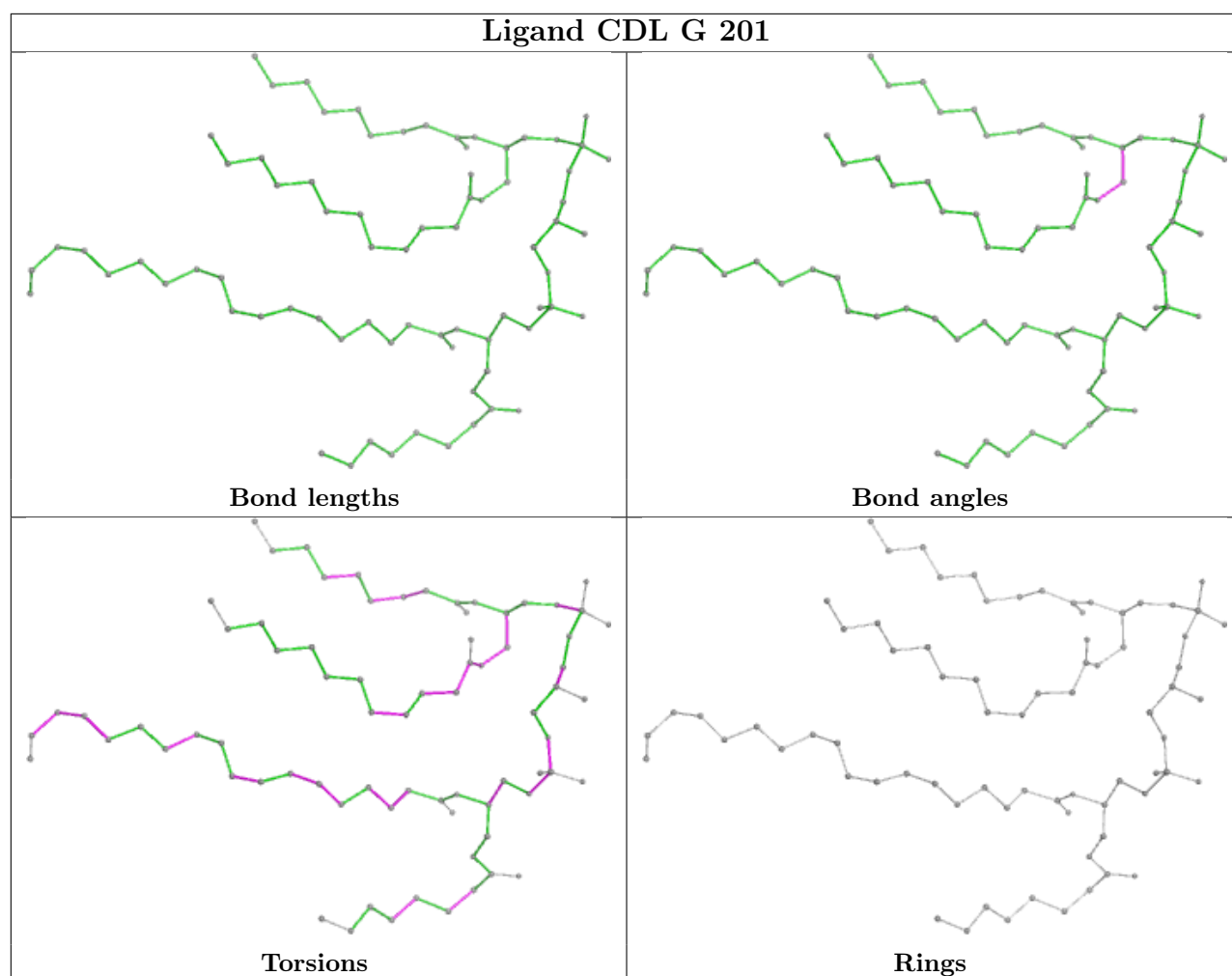


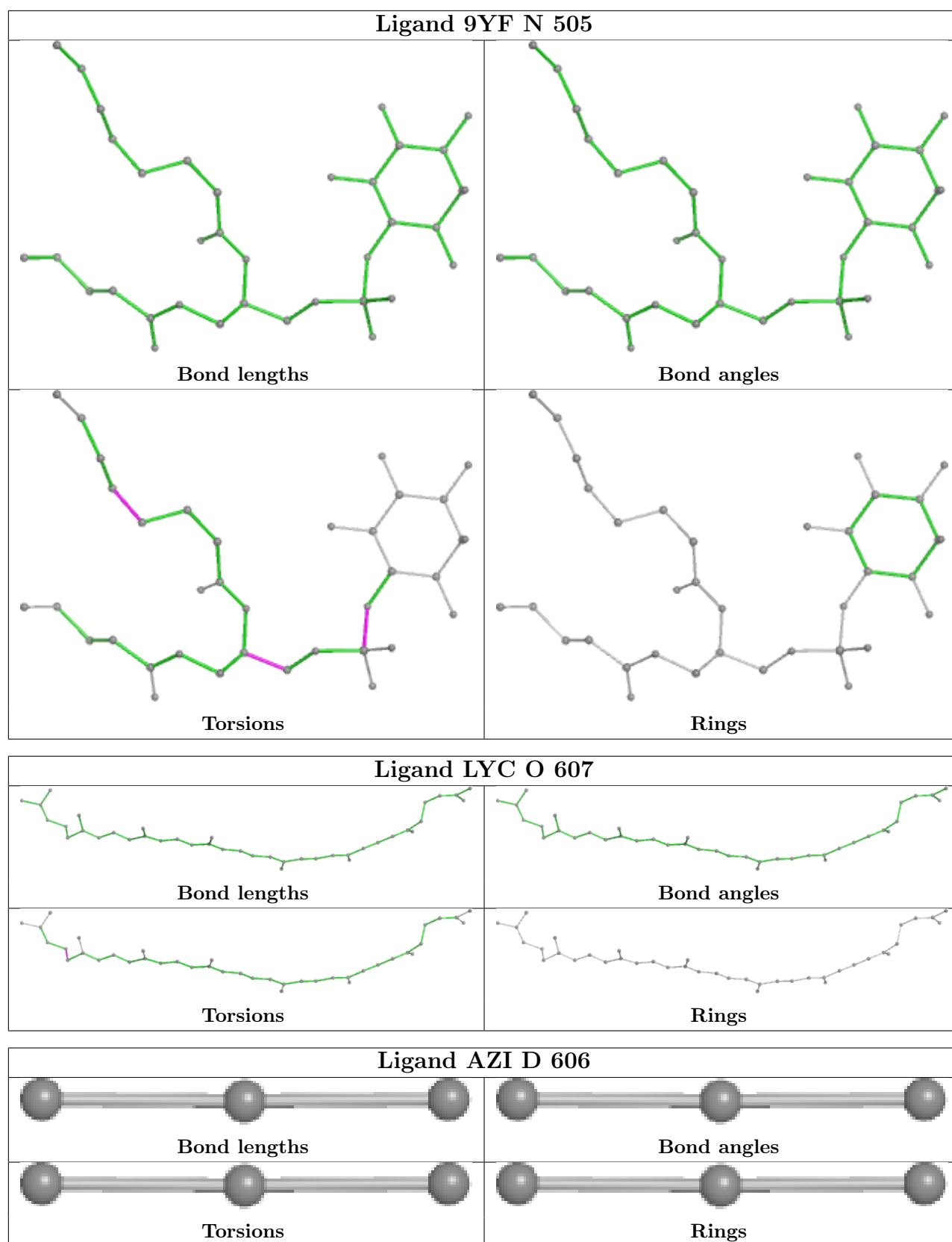


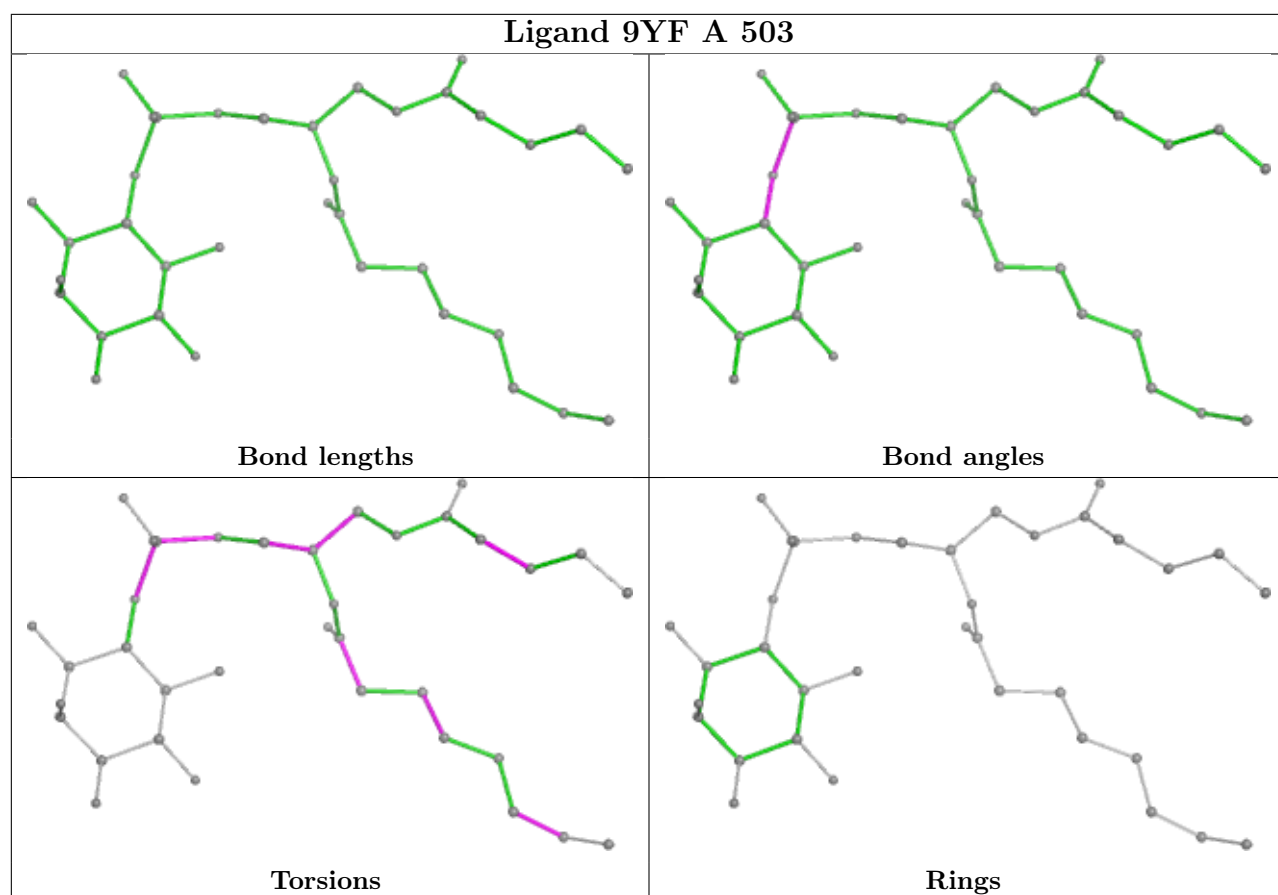


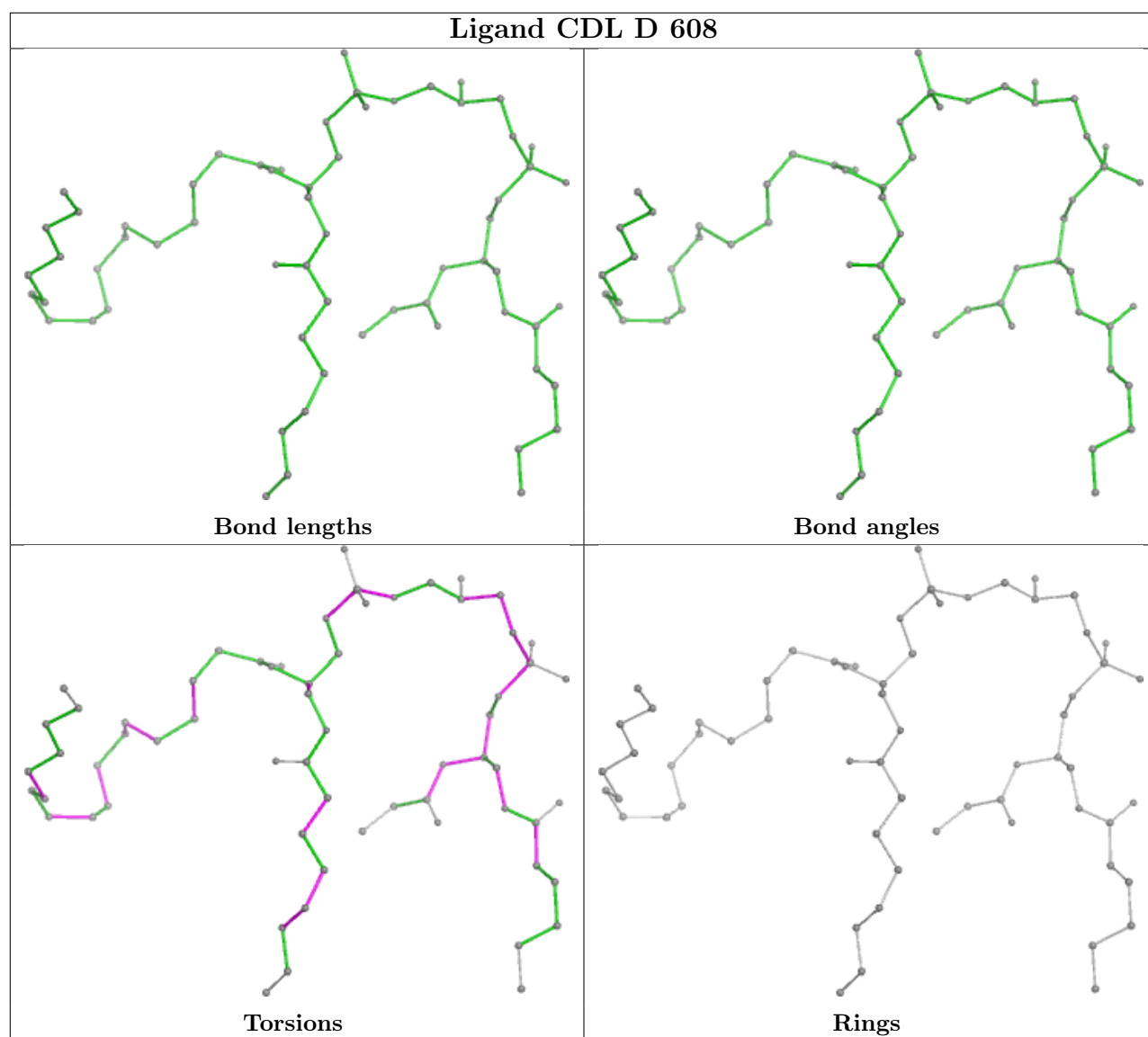


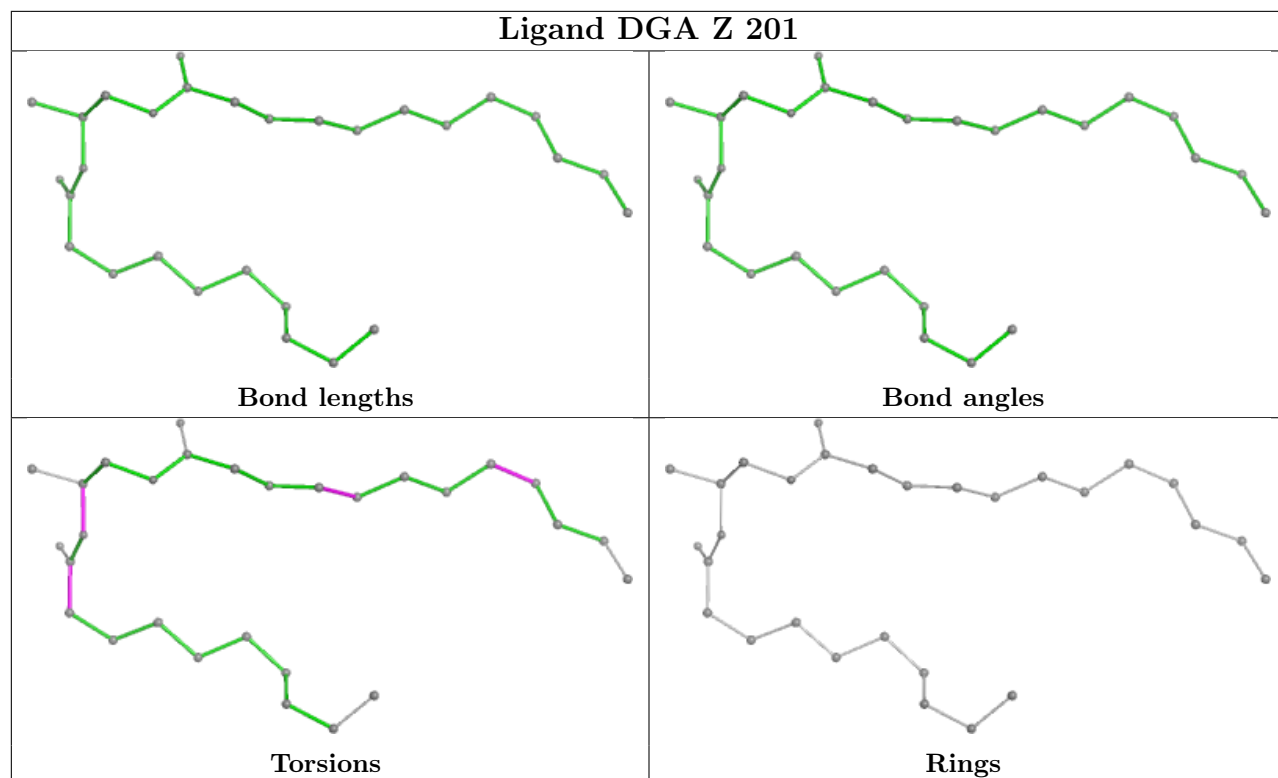


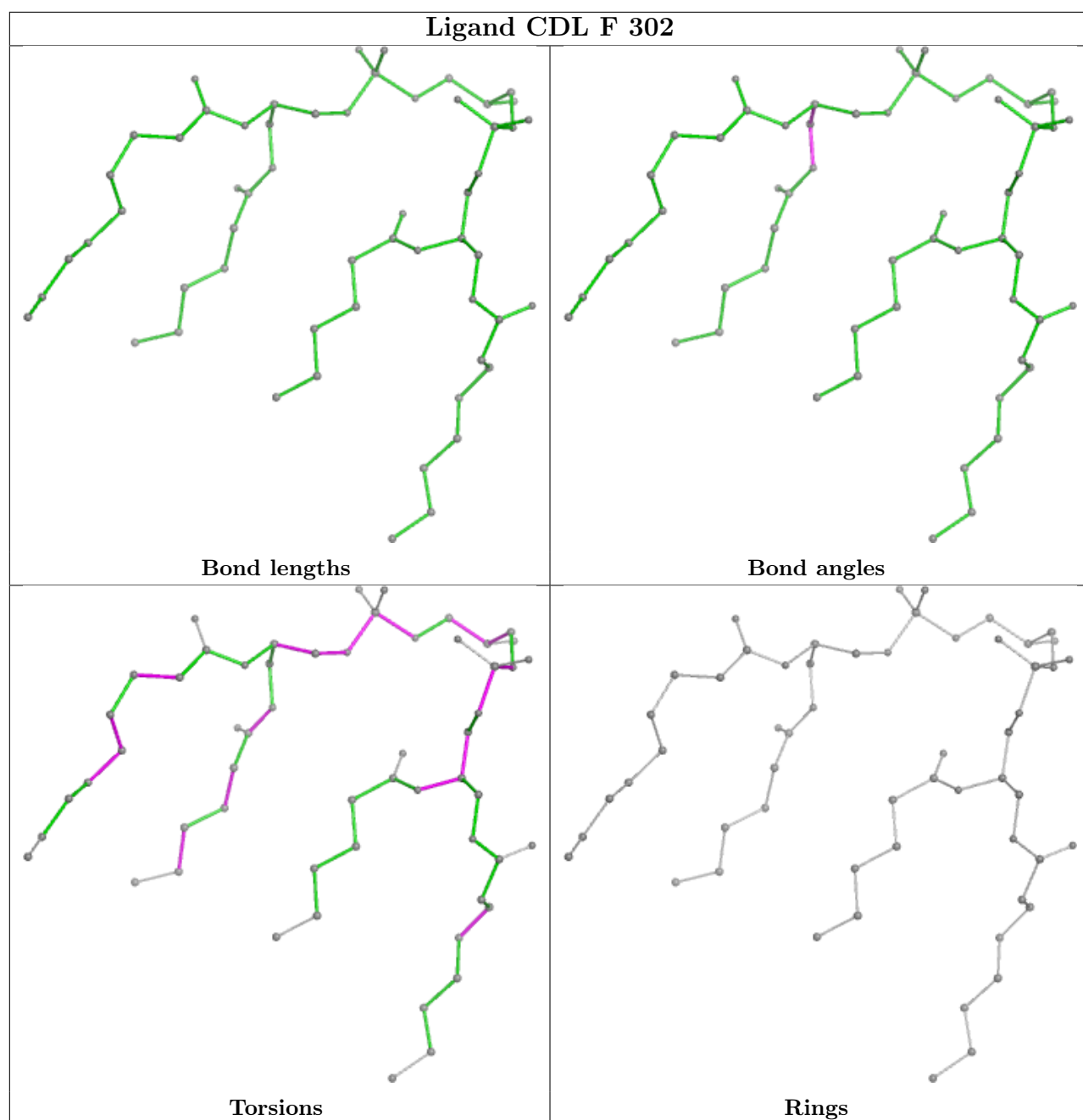


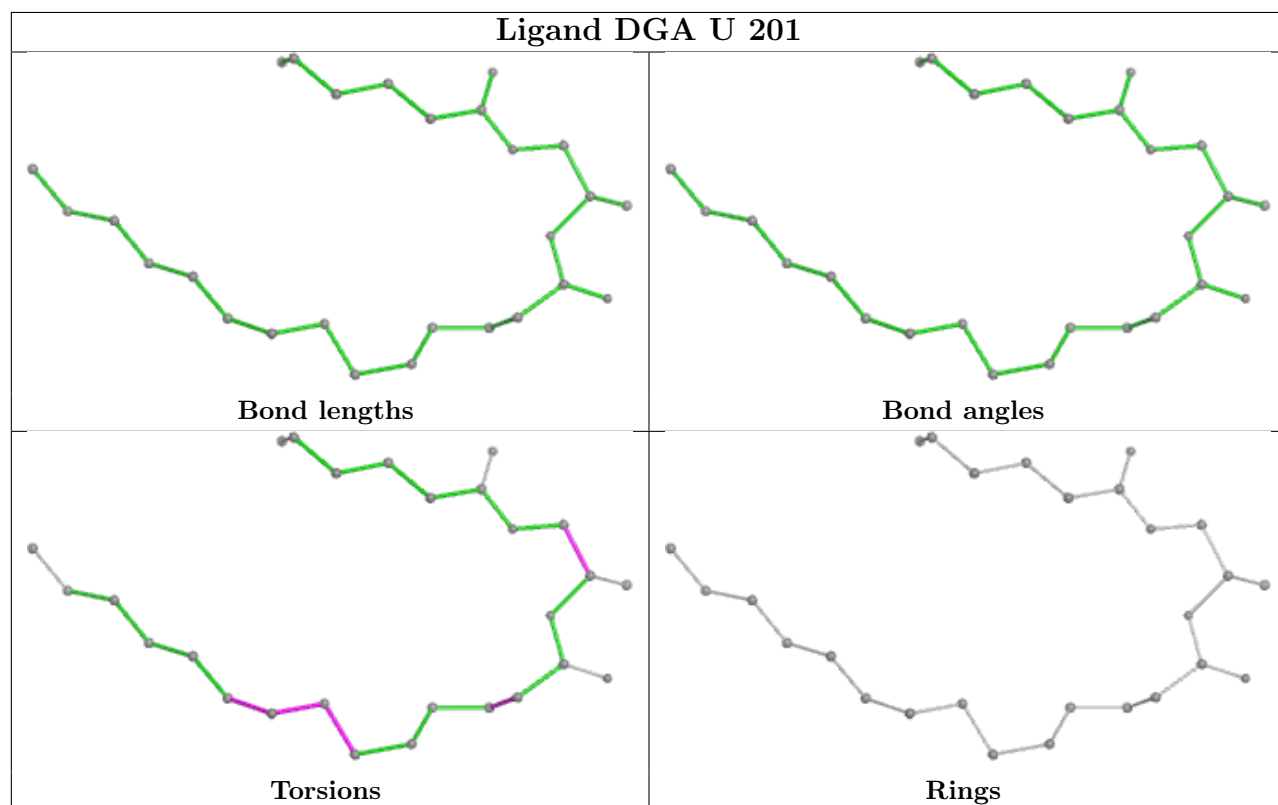
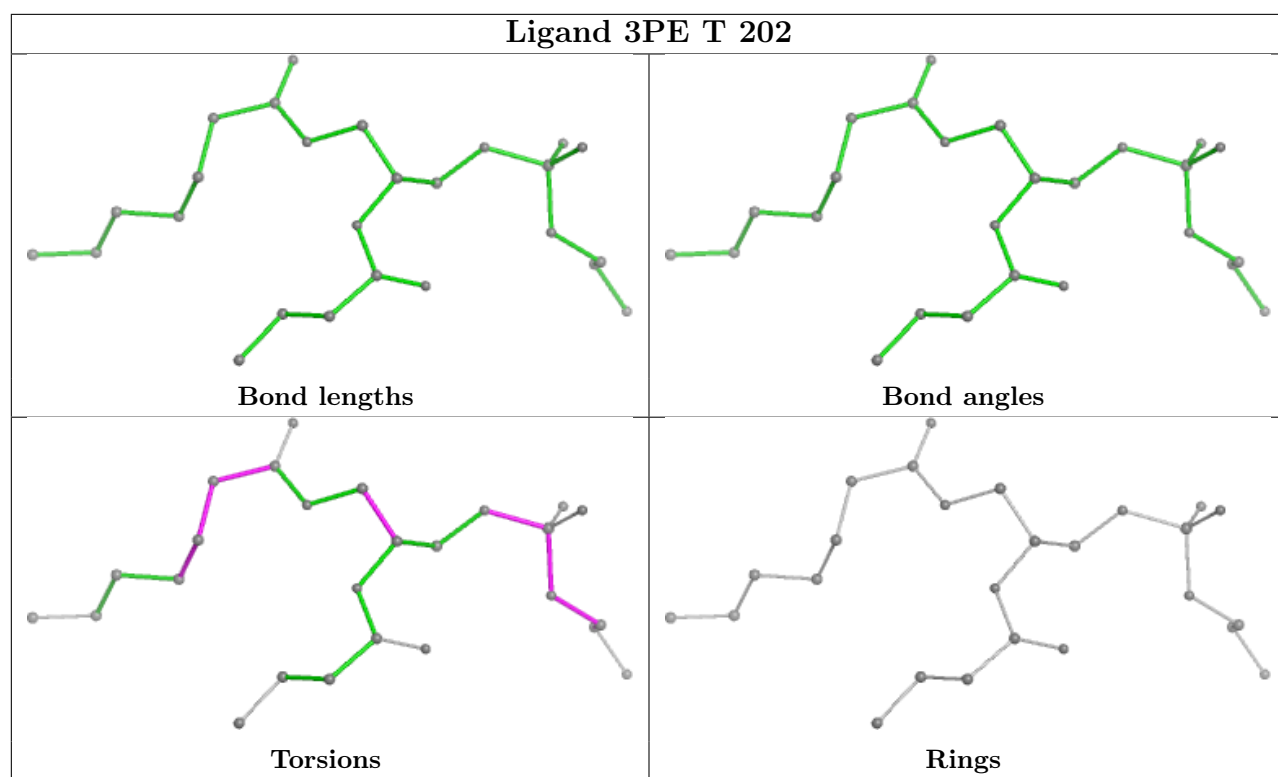


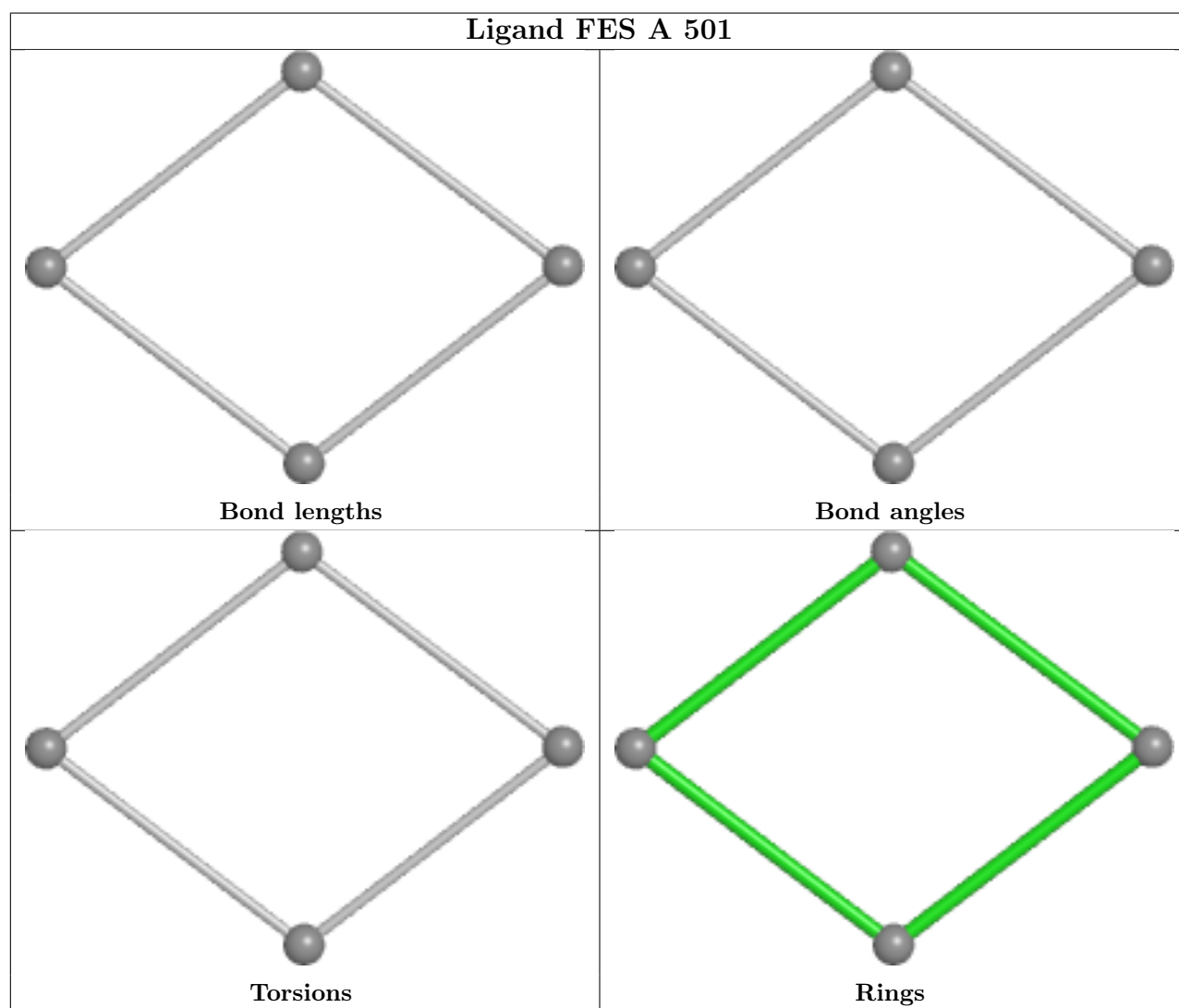
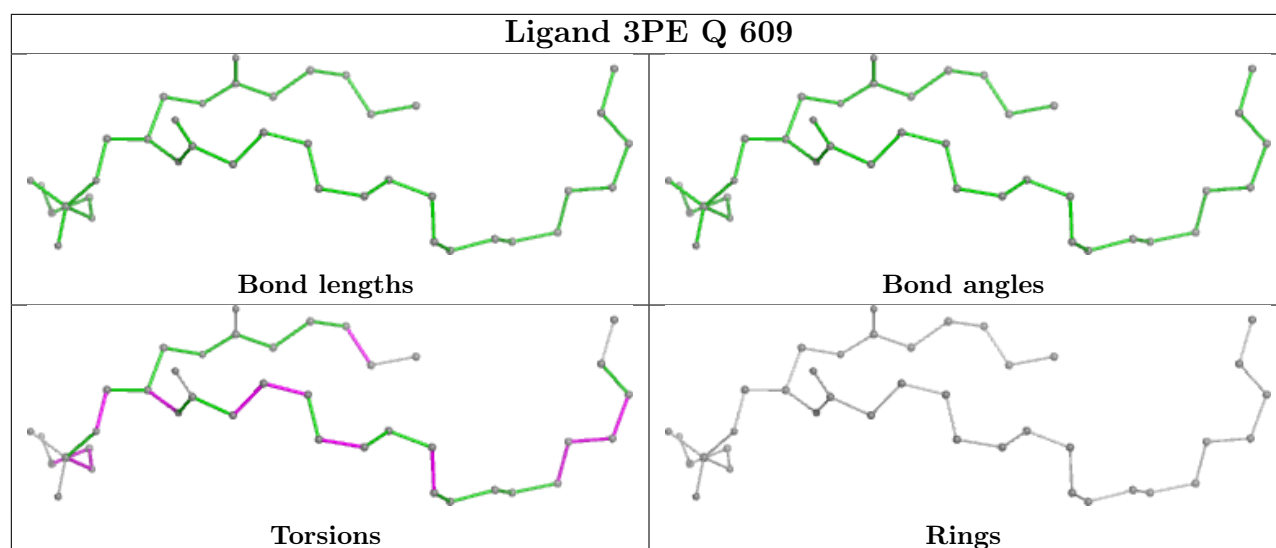


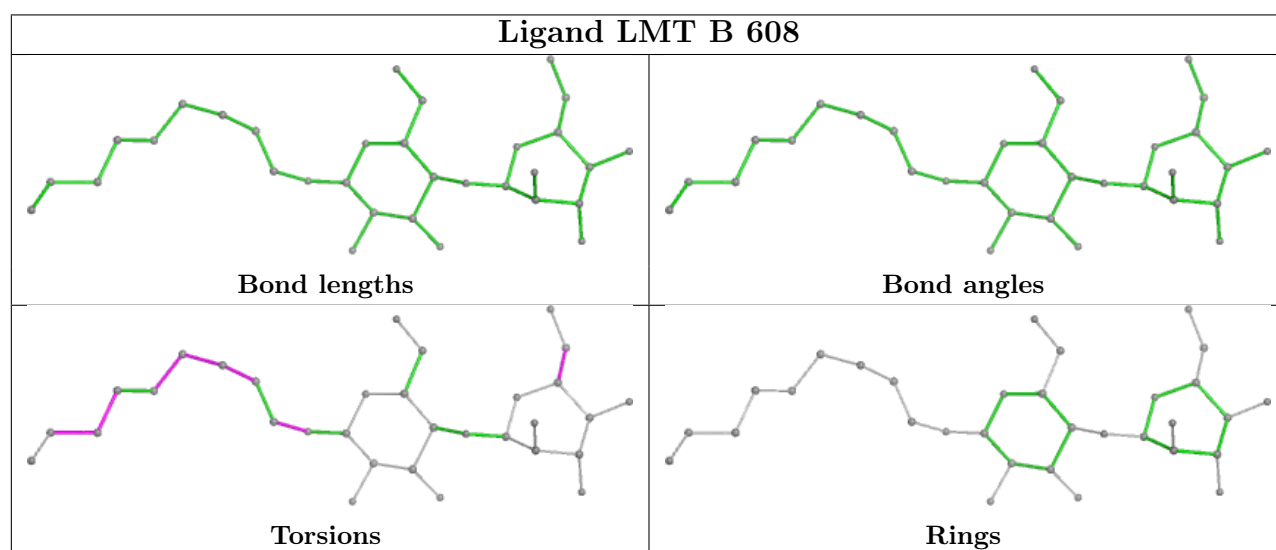
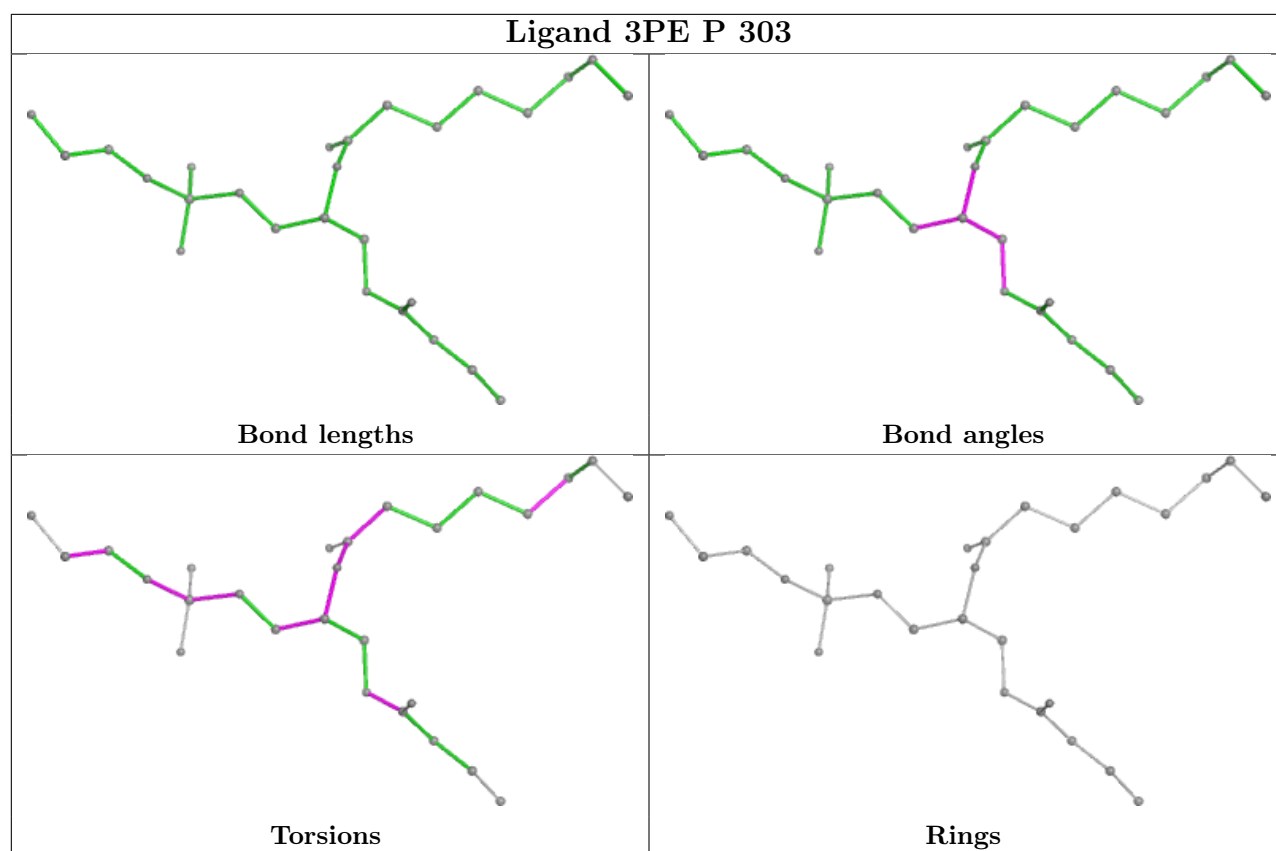


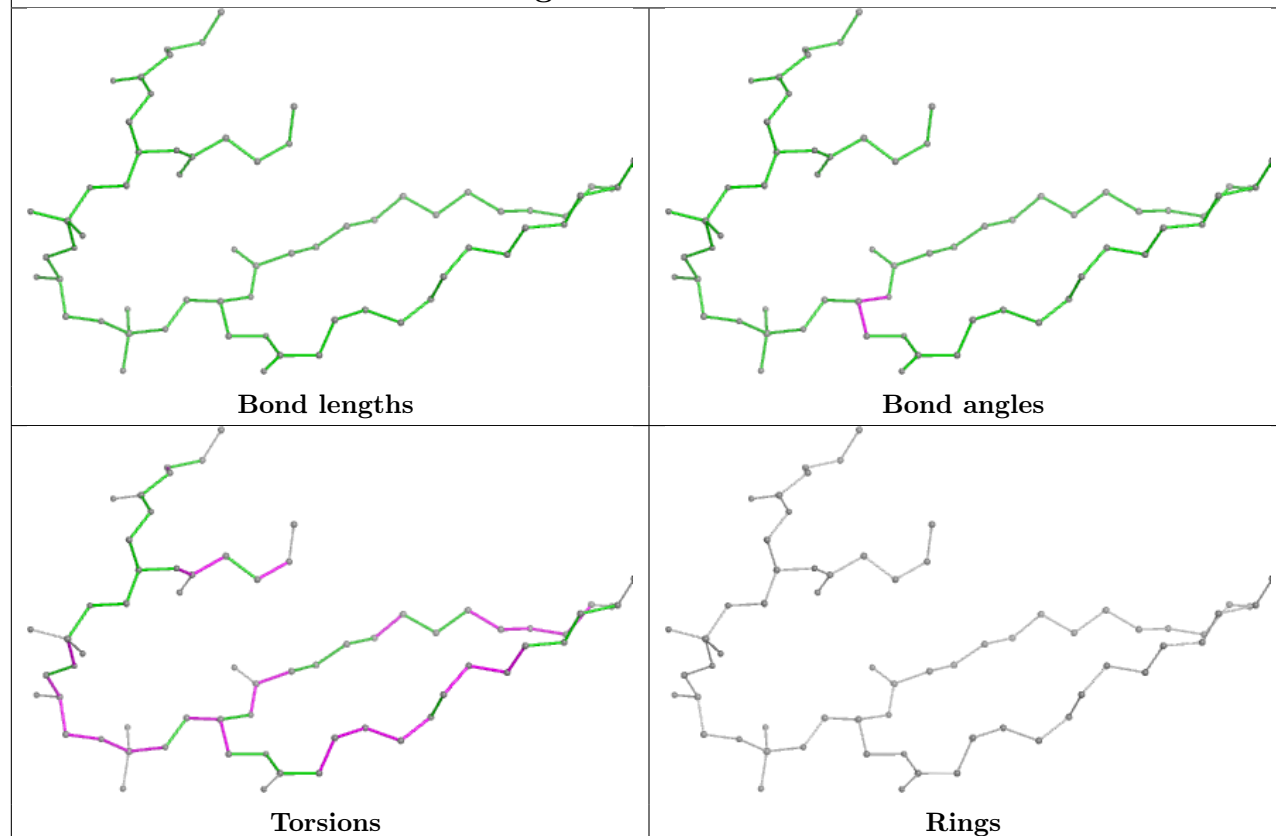
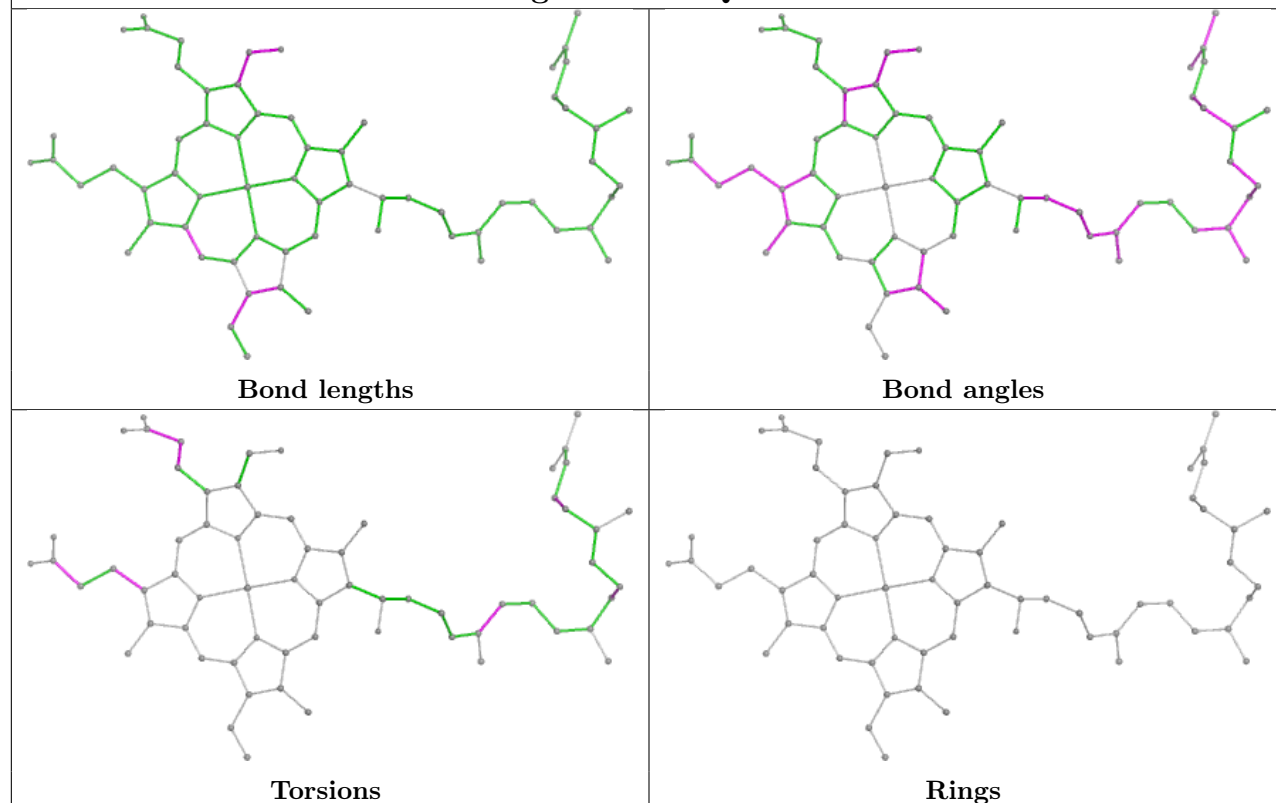


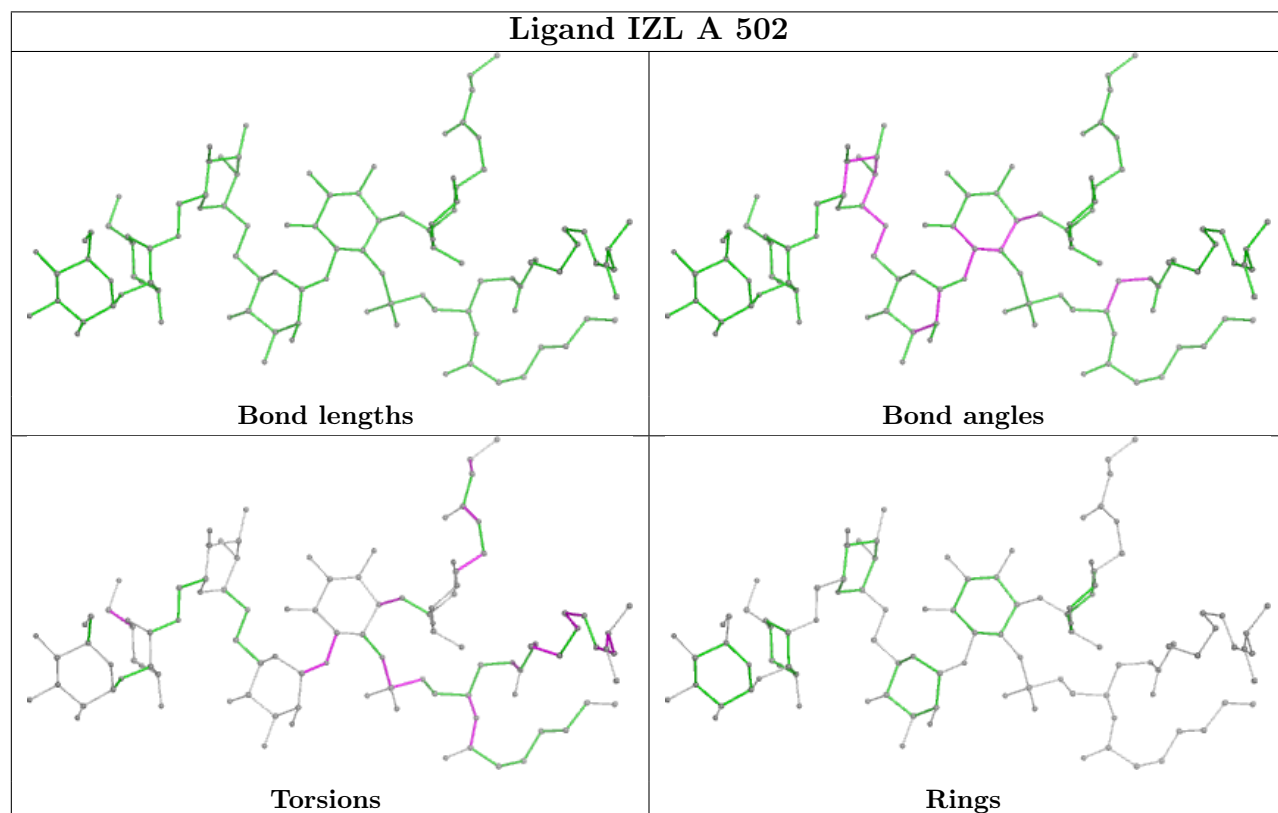
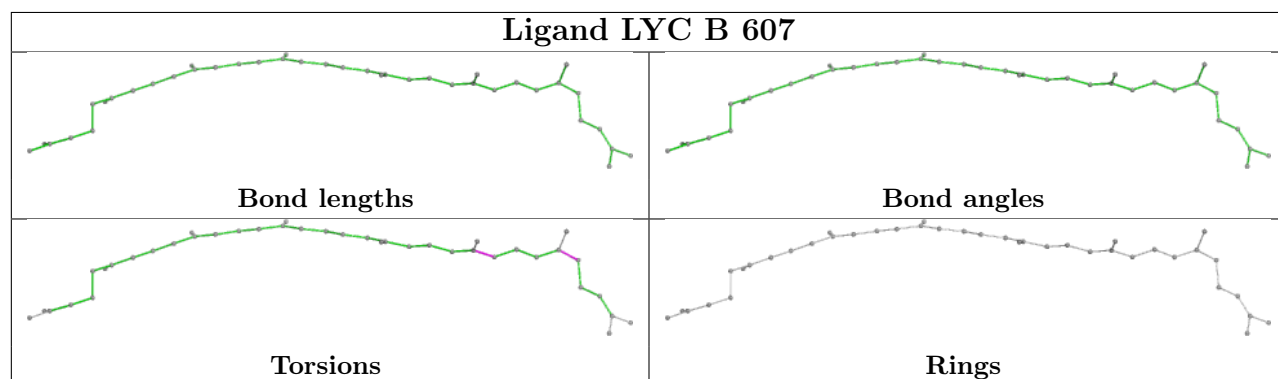
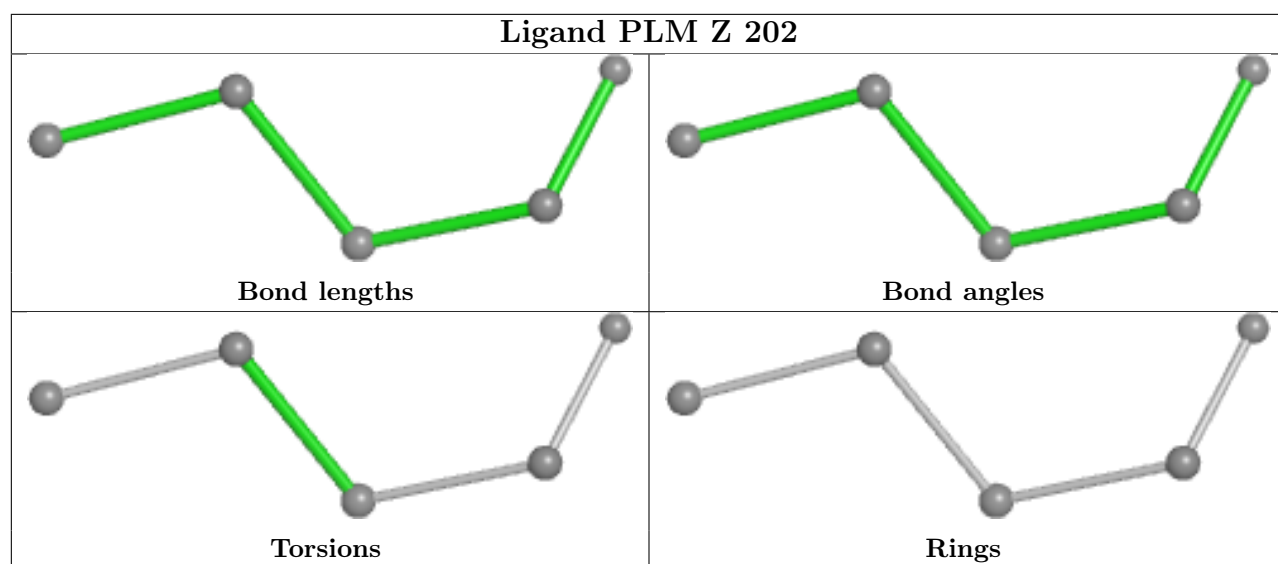


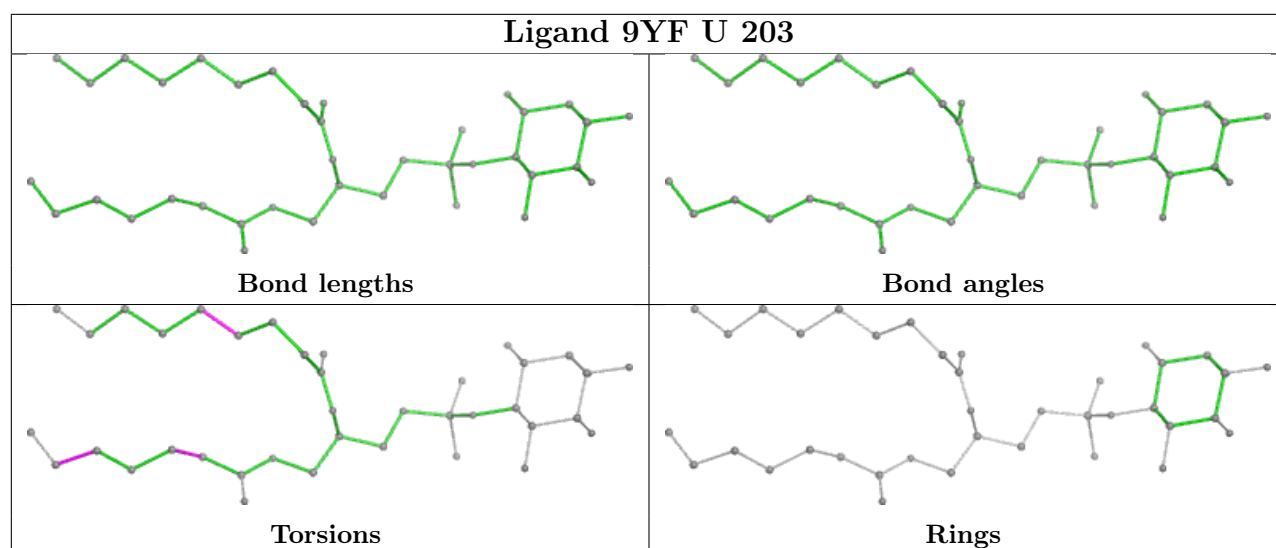






Ligand CDL S 302**Ligand HAS Q 602**





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.

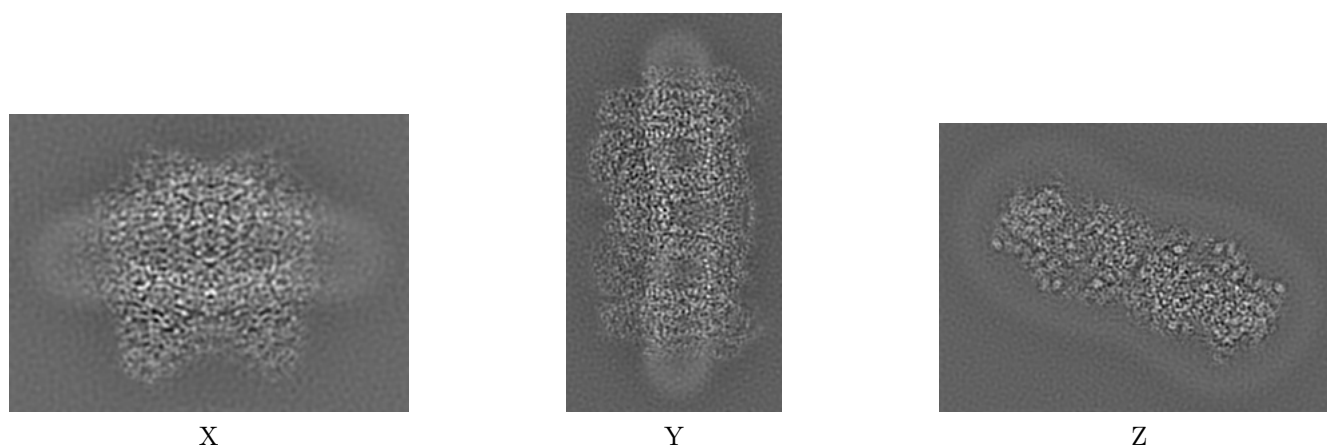
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13976. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

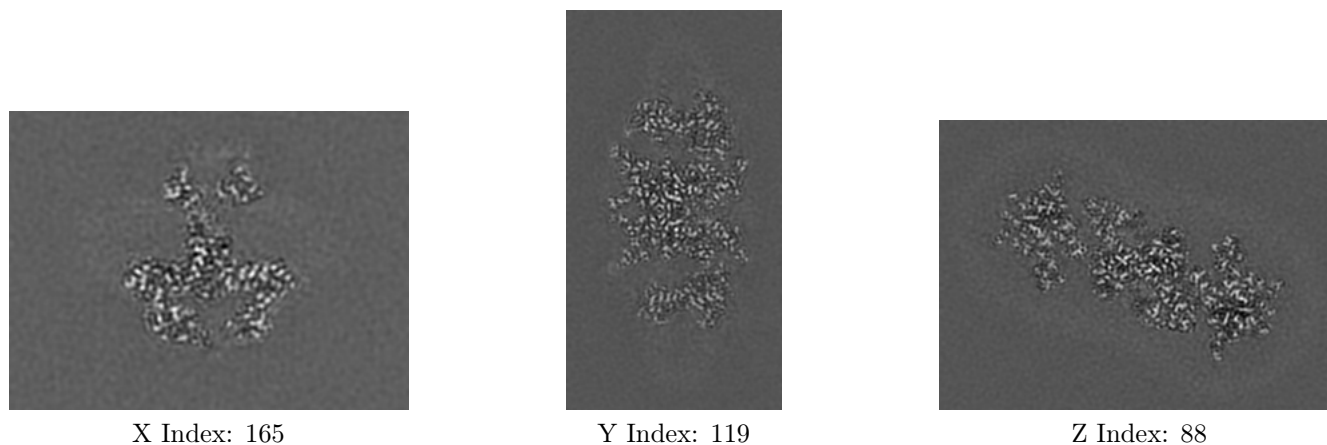
6.1.1 Primary map



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

6.2 Central slices [i](#)

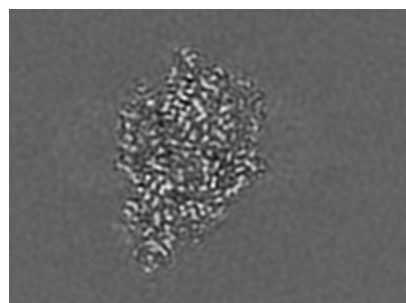
6.2.1 Primary map



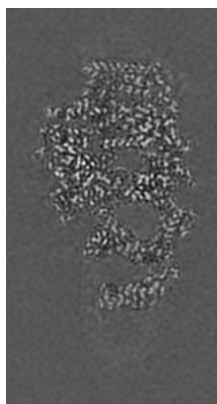
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

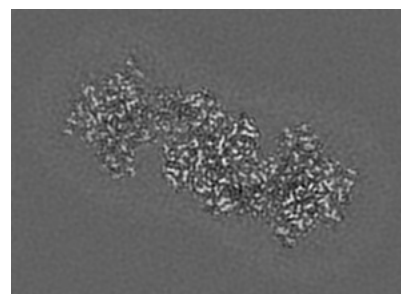
6.3.1 Primary map



X Index: 190



Y Index: 102

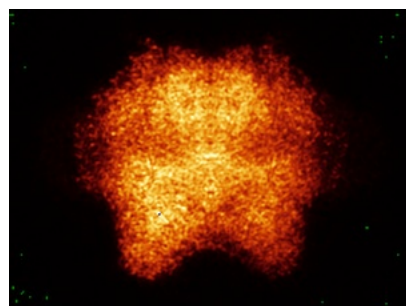


Z Index: 80

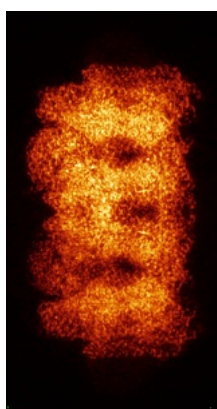
The images above show the largest variance slices of the map in three orthogonal directions.

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

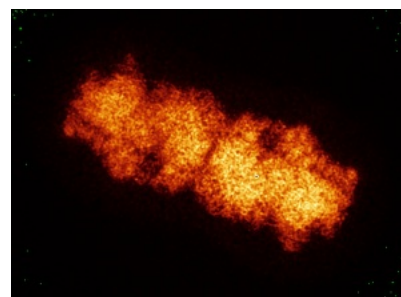
6.4.1 Primary map



X



Y

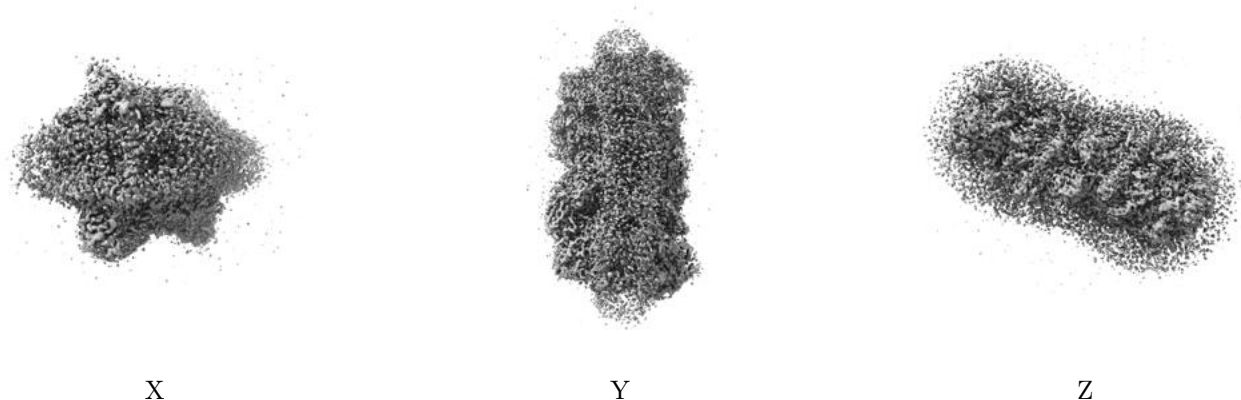


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

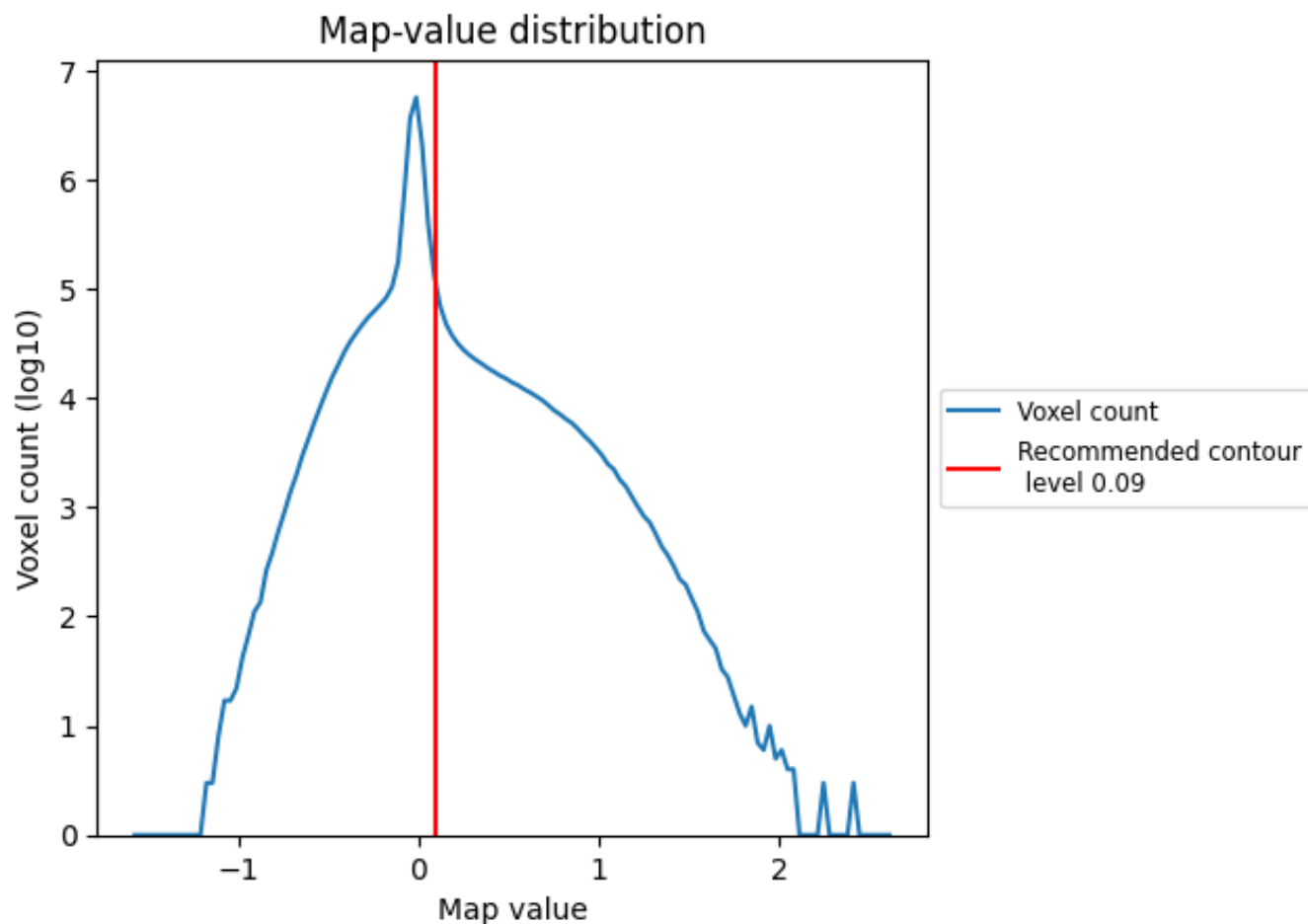
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

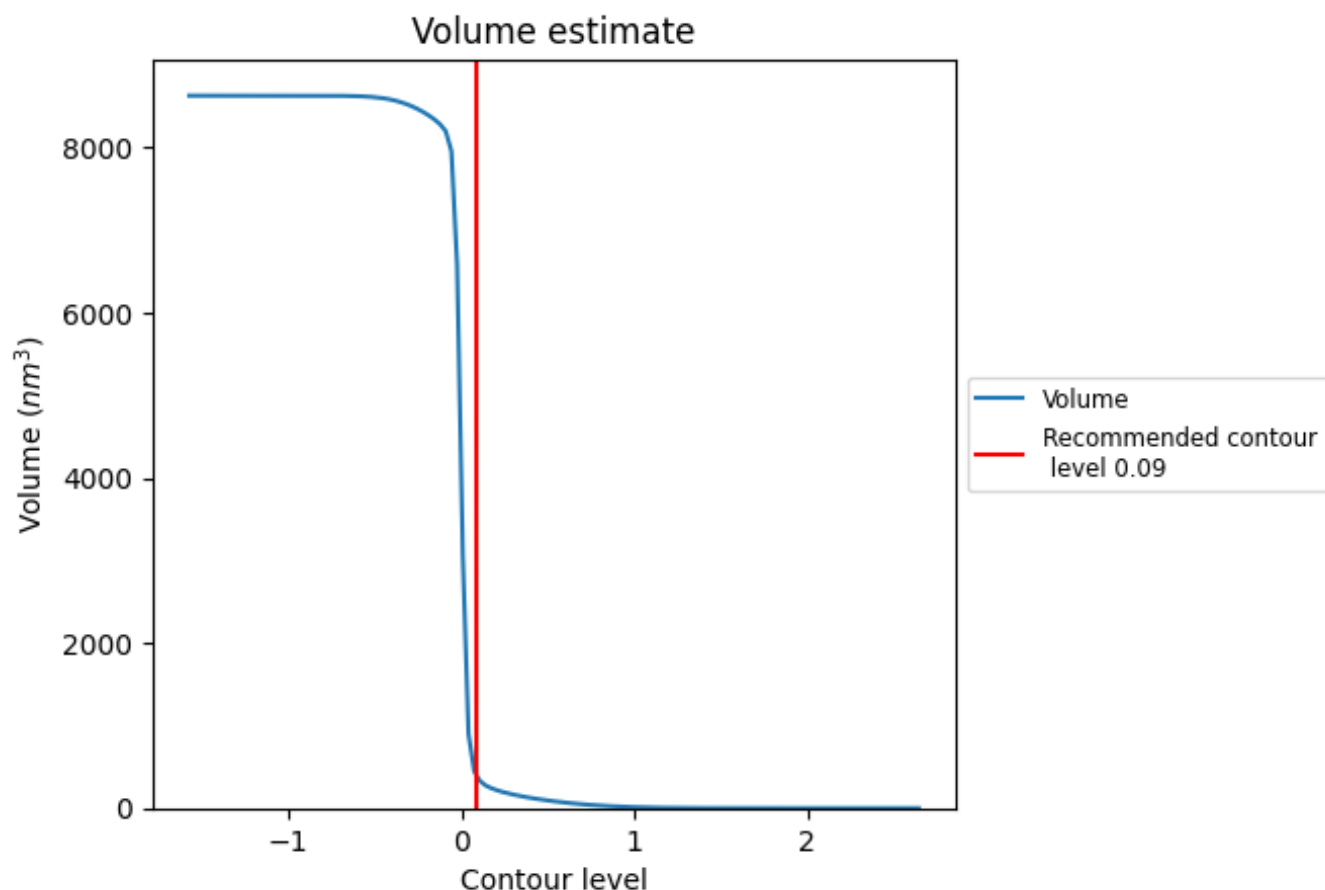
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 385 nm³; this corresponds to an approximate mass of 348 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

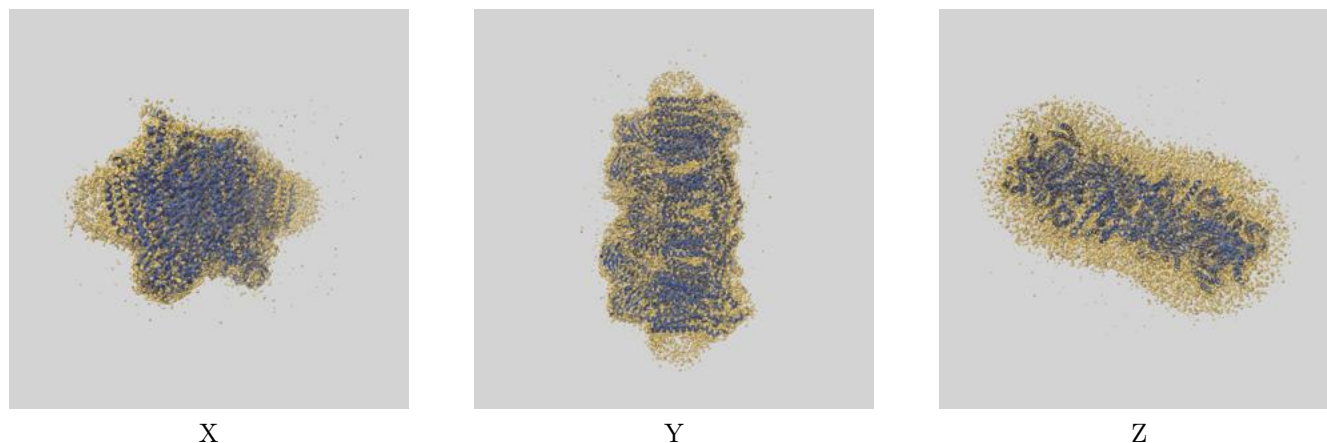
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

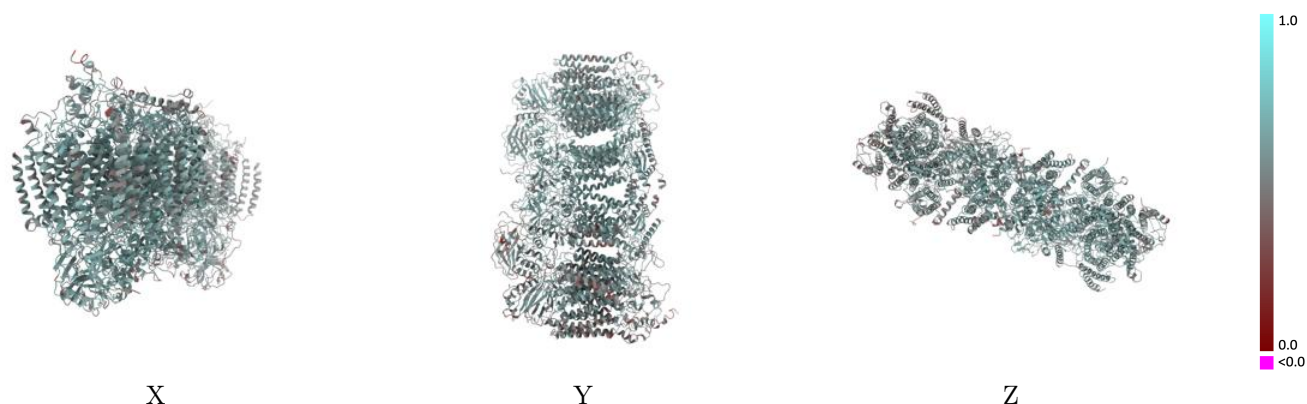
This section contains information regarding the fit between EMDB map EMD-13976 and PDB model 7QHM. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



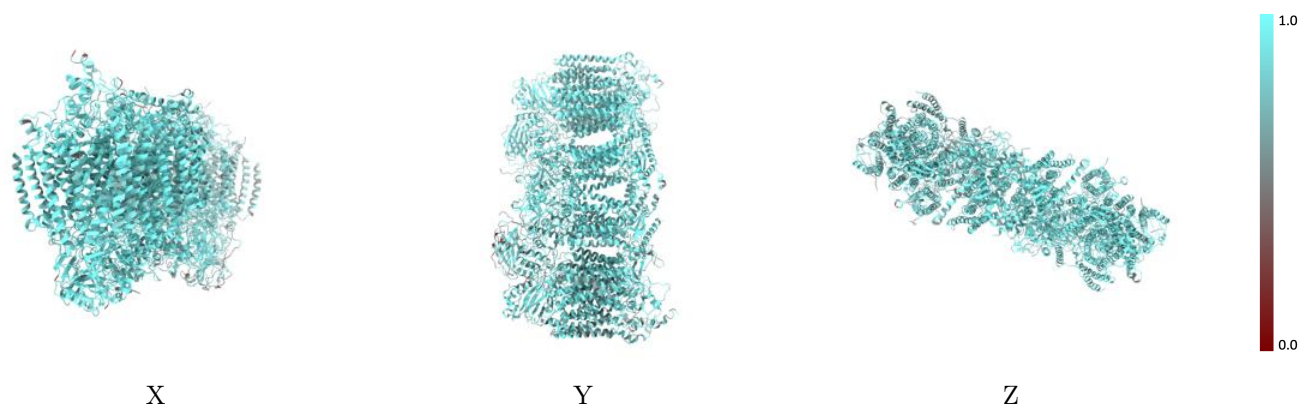
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



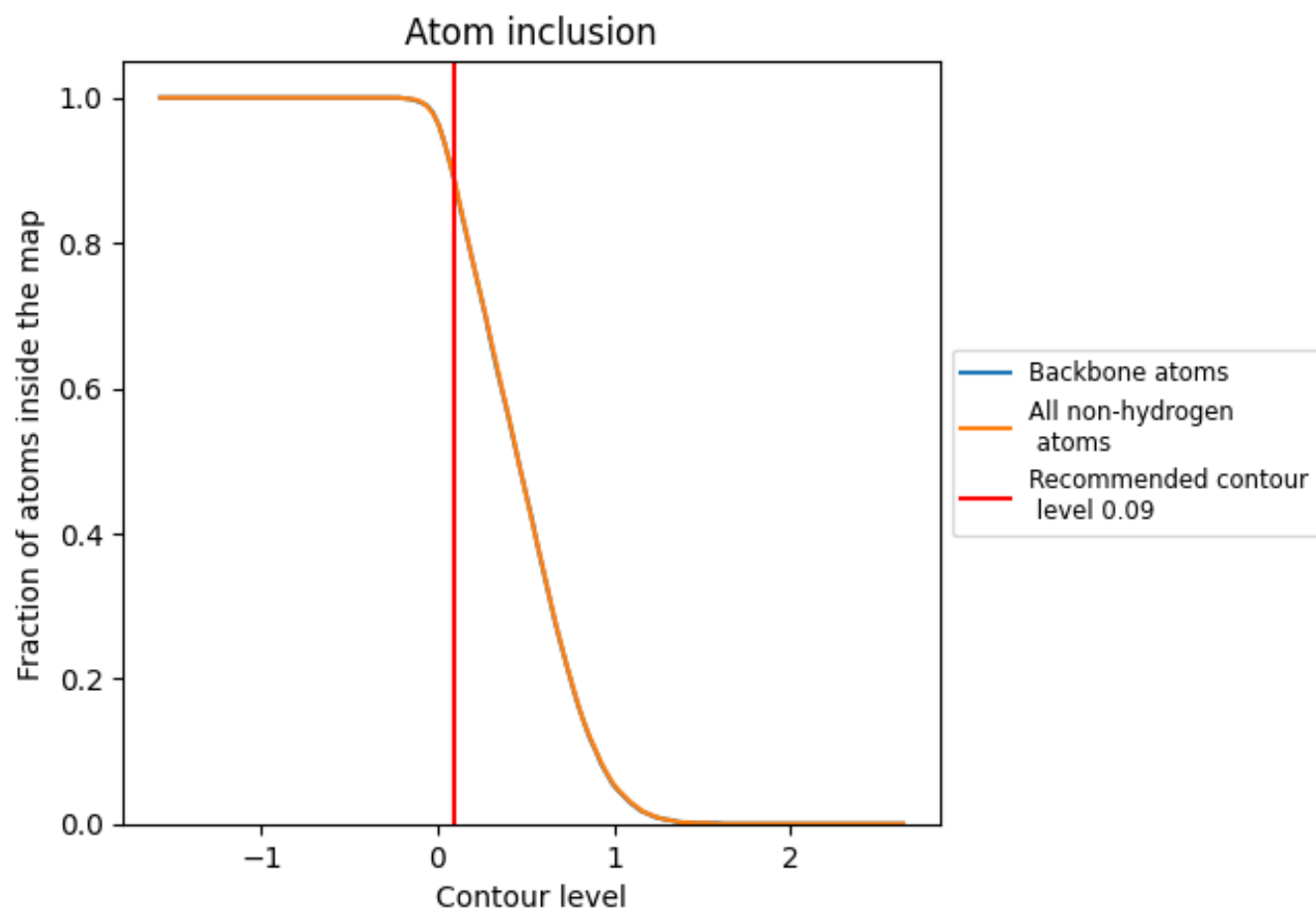
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.5670
A	 0.9130	 0.5720
B	 0.9320	 0.5910
C	 0.8600	 0.5460
D	 0.9010	 0.5660
E	 0.8130	 0.5050
F	 0.8760	 0.5400
G	 0.8600	 0.5310
H	 0.6890	 0.4700
I	 0.7980	 0.4840
J	 0.7720	 0.4750
K	 0.8110	 0.5110
L	 0.6790	 0.4380
M	 0.6380	 0.4570
N	 0.9290	 0.5880
O	 0.9530	 0.6140
P	 0.9440	 0.6130
Q	 0.9450	 0.6050
R	 0.9120	 0.5790
S	 0.9250	 0.5840
T	 0.8990	 0.5740
U	 0.9110	 0.5730
V	 0.8990	 0.5600
W	 0.8640	 0.5230
X	 0.8940	 0.5600
Y	 0.8550	 0.5380
Z	 0.7750	 0.4850

