



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 03:25 PM EDT

PDB ID : 7JRP / pdb_00007jrp
EMDB ID : EMD-22448
Title : Plant Mitochondrial complex SC III2+IV from Vigna radiata
Authors : Maldonado, M.; Letts, J.A.
Deposited on : 2020-08-12
Resolution : 3.80 Å(reported)
Based on initial models : 6Q9E, 6HU9

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

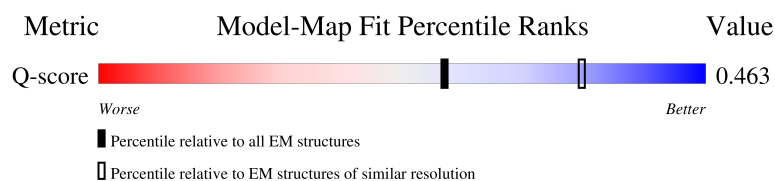
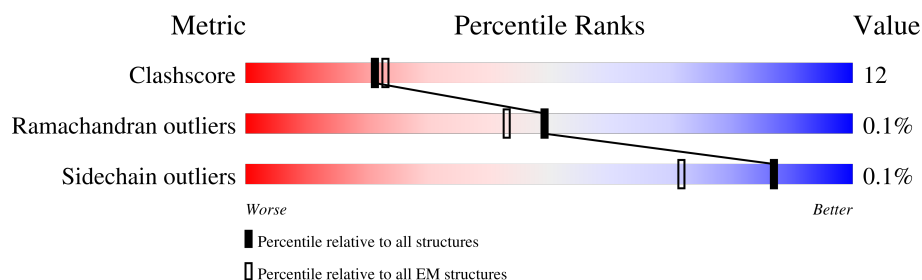
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



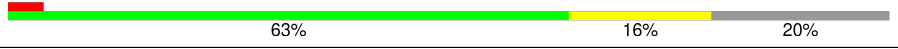
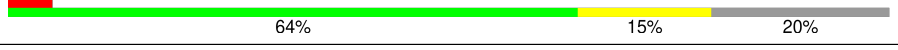
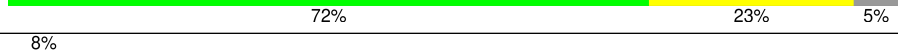
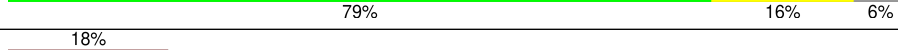
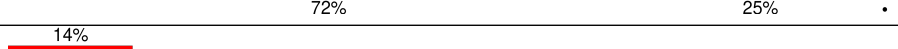
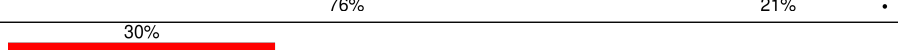
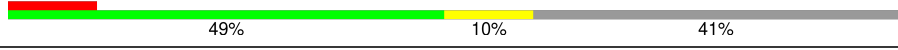
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	527	
1	M	527	
2	B	506	
2	N	506	

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Mol	Chain	Length	Quality of chain
3	C	393	
3	O	393	
4	D	306	
4	P	306	
5	E	271	
5	Q	271	
6	F	122	
6	R	122	
7	G	72	
7	S	72	
8	H	69	
8	T	69	
9	J	72	
9	V	72	
10	K	81	
10	W	81	
11	a	527	
12	b	251	
13	c	265	
14	d	79	
15	e	150	
16	f	100	
17	g	181	
18	h	64	
19	i	67	

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Mol	Chain	Length	Quality of chain
20	j	96	

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
26	HEC	D	501	X	-	-	-
26	HEC	P	402	X	-	-	-

2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 45166 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 Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3838	2409	678	736	15		
1	M	487	Total	C	N	O	S	0	0
			3838	2409	678	736	15		

- Molecule 2 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	457	Total	C	N	O	S	0	0
			3471	2196	588	675	12		
2	N	455	Total	C	N	O	S	0	0
			3456	2187	585	672	12		

- Molecule 3 is a protein called COB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	388	Total	C	N	O	S	0	0
			3104	2088	487	515	14		
3	O	388	Total	C	N	O	S	0	0
			3104	2088	487	515	14		

- Molecule 4 is a protein called cytochrome c1-2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	244	Total	C	N	O	S	0	0
			1910	1214	327	358	11		
4	P	244	Total	C	N	O	S	0	0
			1910	1214	327	358	11		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	74	Total	C	N	O	S	0	0
			574	375	97	101	1		
5	Q	74	Total	C	N	O	S	0	0
			574	375	97	101	1		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	116	Total	C	N	O	S	0	0
			965	616	173	172	4		
6	R	115	Total	C	N	O	S	0	0
			959	613	172	170	4		

- Molecule 7 is a protein called cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			578	382	97	98	1		
7	S	70	Total	C	N	O	S	0	0
			578	382	97	98	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			536	344	90	96	6		
8	T	64	Total	C	N	O	S	0	0
			527	339	89	93	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	60	Total	C	N	O	S	0	0
			480	313	83	83	1		
9	V	59	Total	C	N	O	S	0	0
			476	311	82	82	1		

- Molecule 10 is a protein called QCR10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	31	Total	C	N	O	S	0	0
			218	144	35	38	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	32	Total	C	N	O	S	0	0
			226	150	36	39	1		

- Molecule 11 is a protein called COX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	524	Total	C	N	O	S	0	0
			4074	2726	640	684	24		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	239	Total	C	N	O	S	0	0
			1915	1249	308	348	10		

- Molecule 13 is a protein called COX3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	265	Total	C	N	O	S	0	0
			2134	1445	335	347	7		

- Molecule 14 is a protein called COX4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	76	Total	C	N	O	S	0	0
			595	387	97	109	2		

- Molecule 15 is a protein called cytochrome c oxidase subunit 5b-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	94	Total	C	N	O	S	0	0
			733	464	124	142	3		

- Molecule 16 is a protein called cytochrome c oxidase subunit 6a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	59	Total	C	N	O	S	0	0
			480	315	76	88	1		

- Molecule 17 is a protein called cytochrome c oxidase subunit 6b-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	74	Total	C	N	O	S	0	0
			612	385	110	113	4		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 5C.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	49	Total	C	N	O	S	0	0
			391	255	67	68	1		

- Molecule 19 is a protein called COX7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	64	Total	C	N	O	S	0	0
			510	331	91	87	1		

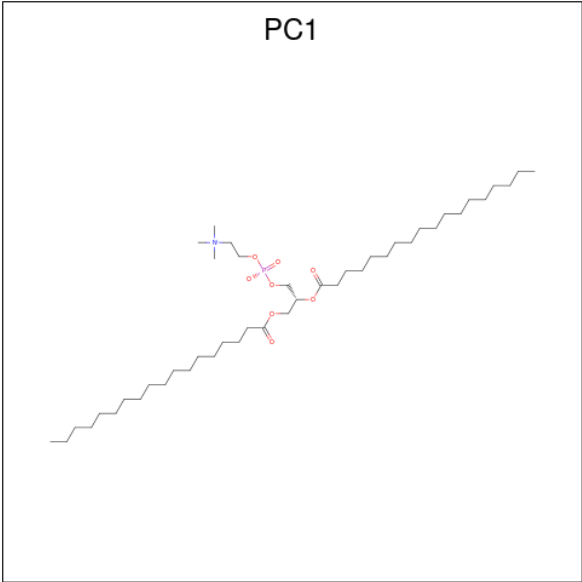
- Molecule 20 is a protein called COX7c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	47	Total	C	N	O	S	0	0
			384	254	67	60	3		

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

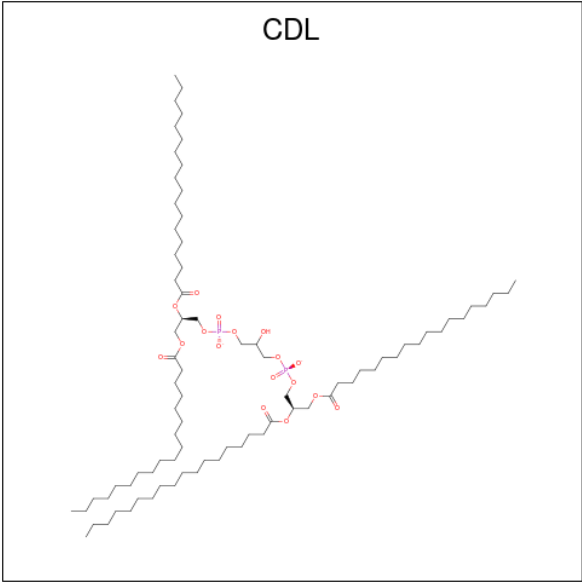
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Zn	0
			1	1	
21	M	1	Total	Zn	0
			1	1	
21	e	1	Total	Zn	0
			1	1	

- Molecule 22 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



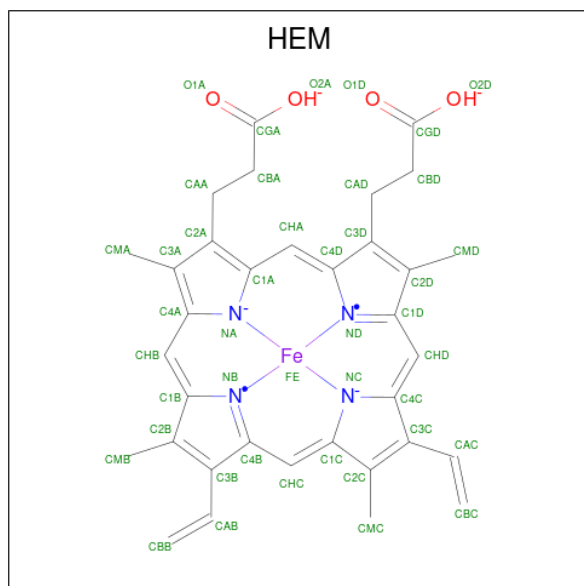
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
22	M	1	Total	C	N	O	P	0
			27	17	1	8	1	
22	S	1	Total	C	N	O	P	0
			28	18	1	8	1	
22	a	1	Total	C	N	O	P	0
			39	29	1	8	1	
22	i	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 23 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total 51	C 32	O 17	P 2	0
23	C	1	Total 54	C 35	O 17	P 2	0
23	C	1	Total 55	C 36	O 17	P 2	0
23	D	1	Total 41	C 22	O 17	P 2	0
23	M	1	Total 53	C 34	O 17	P 2	0
23	O	1	Total 54	C 35	O 17	P 2	0
23	P	1	Total 48	C 29	O 17	P 2	0
23	S	1	Total 50	C 31	O 17	P 2	0
23	a	1	Total 67	C 48	O 17	P 2	0

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



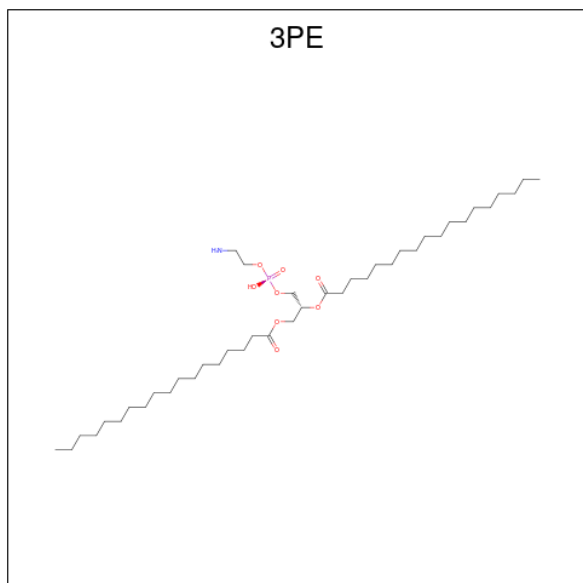
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
24	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
24	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



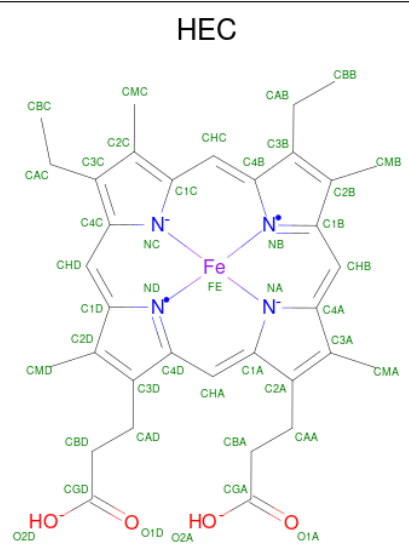
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	C	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	G	1	Total	C	N	O	P	0
			20	10	1	8	1	
25	O	1	Total	C	N	O	P	0
			24	14	1	8	1	
25	O	1	Total	C	N	O	P	0
			26	16	1	8	1	

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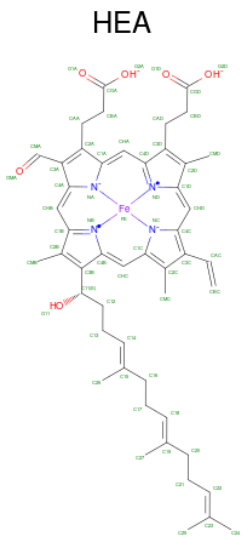
Mol	Chain	Residues	Atoms					AltConf
25	O	1	Total	C	N	O	P	0
			33	23	1	8	1	
25	O	1	Total	C	N	O	P	0
			26	16	1	8	1	
25	P	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	a	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	a	1	Total	C	N	O	P	0
			39	29	1	8	1	
25	b	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	b	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	b	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	c	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	c	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	d	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	i	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 26 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
26	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
26	P	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 27 is HEME-A (CCD ID: HEA) (formula: $\text{C}_{49}\text{H}_{56}\text{FeN}_4\text{O}_6$).



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

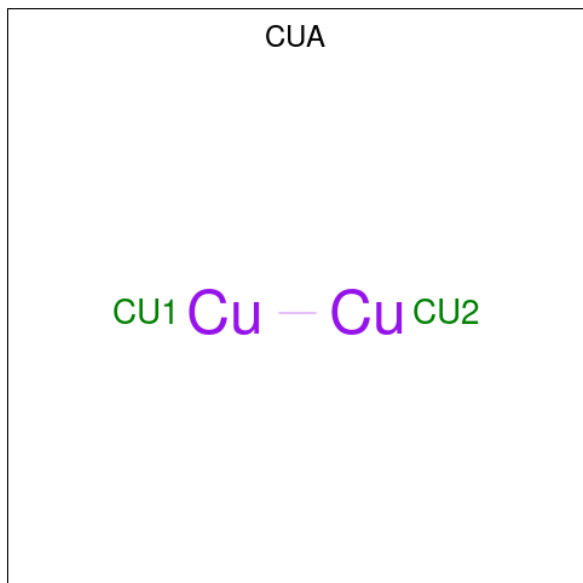
- Molecule 28 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
28	a	1	Total	Cu	0
			1	1	

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

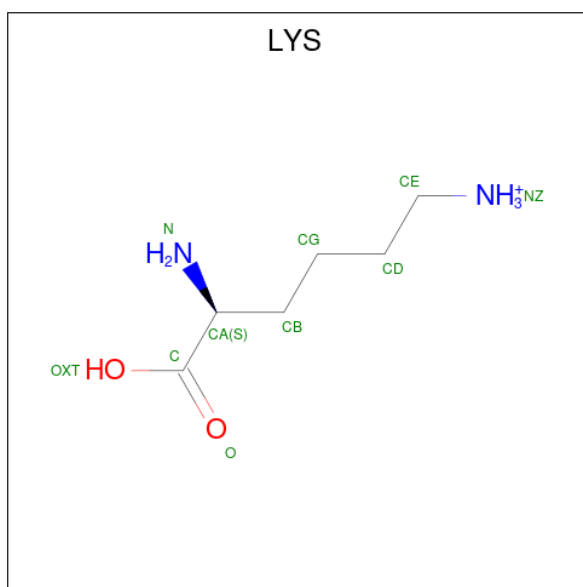
Mol	Chain	Residues	Atoms		AltConf
29	a	1	Total	Mg	0
			1	1	

- Molecule 30 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

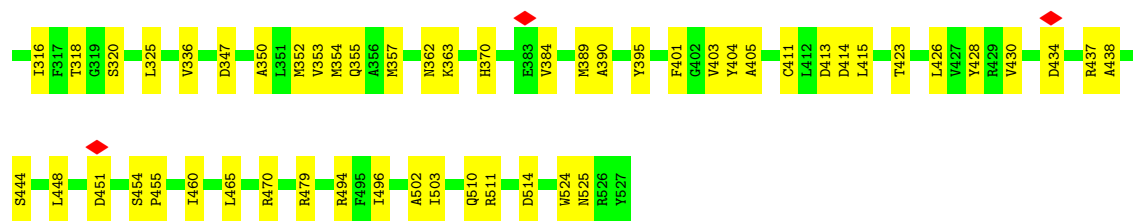


Mol	Chain	Residues	Atoms		AltConf
30	b	1	Total	Cu	0
			2	2	

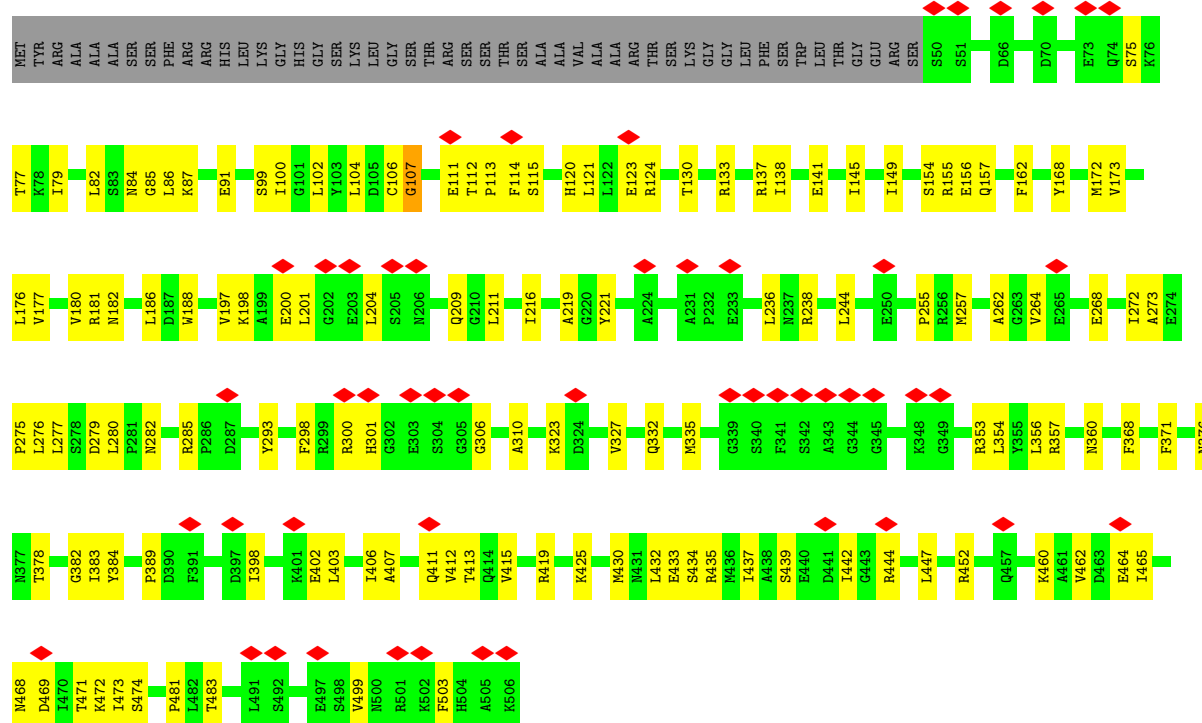
- Molecule 31 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



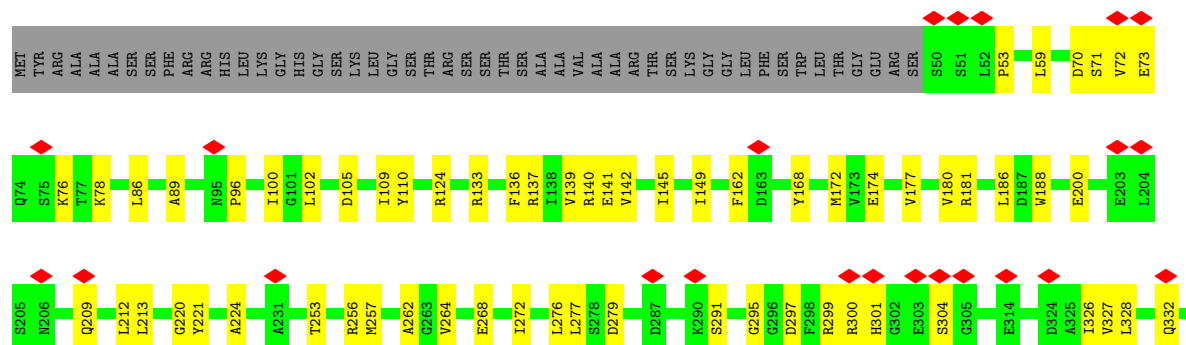
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	i	1	9	6	2	1	0

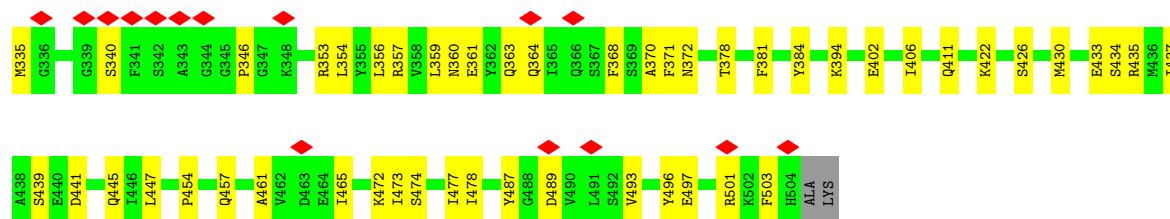


• Molecule 2: Alpha-MPP



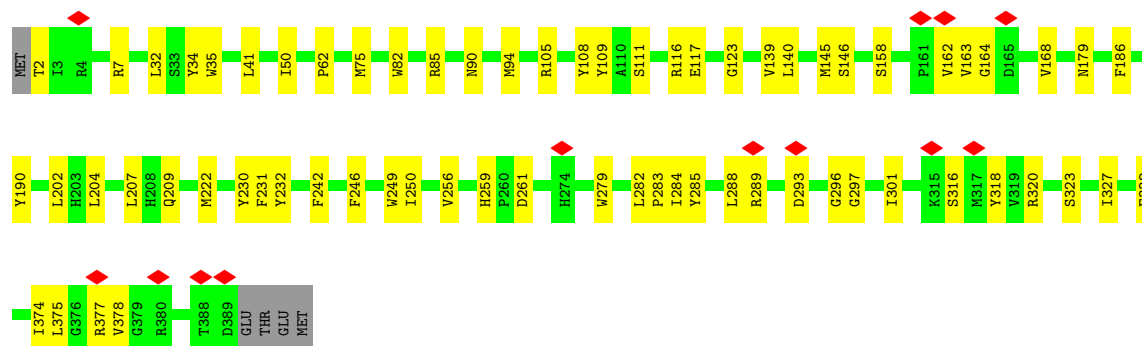
• Molecule 2: Alpha-MPP





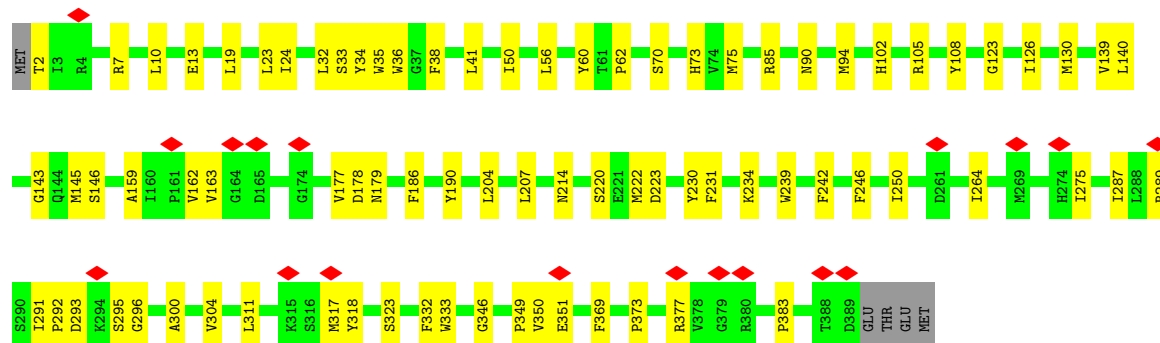
- Molecule 3: COB

Chain C: 81% 17%



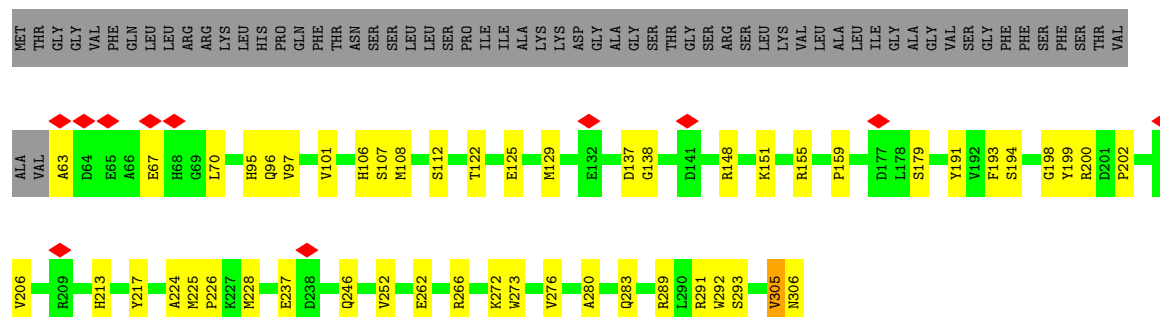
- Molecule 3: COB

Chain O: 5% 78% 21%

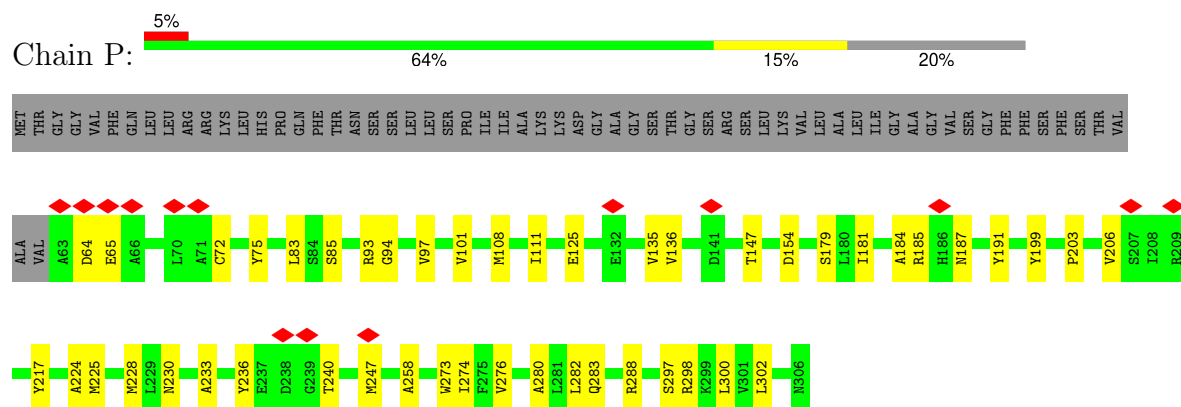


- Molecule 4: cytochrome c1-2, heme protein, mitochondrial

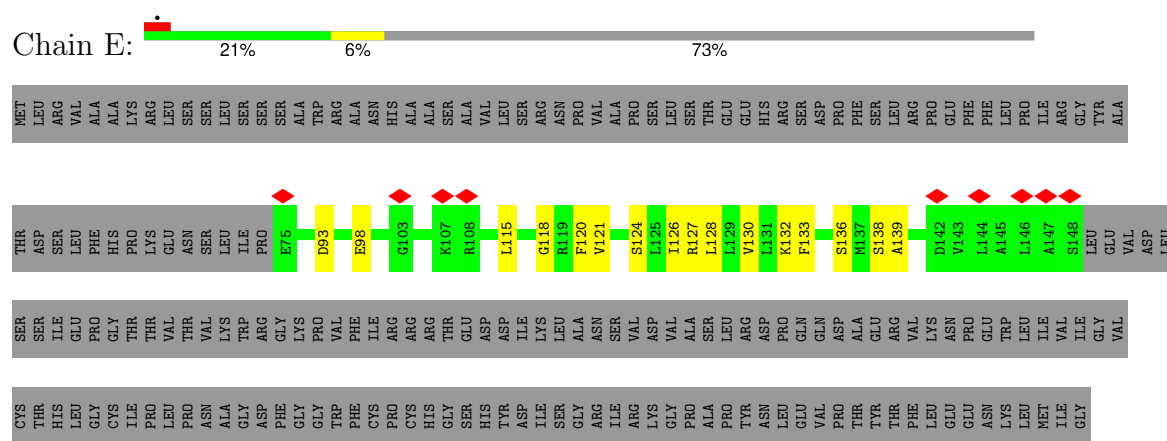
Chain D: 63% 16% 20%



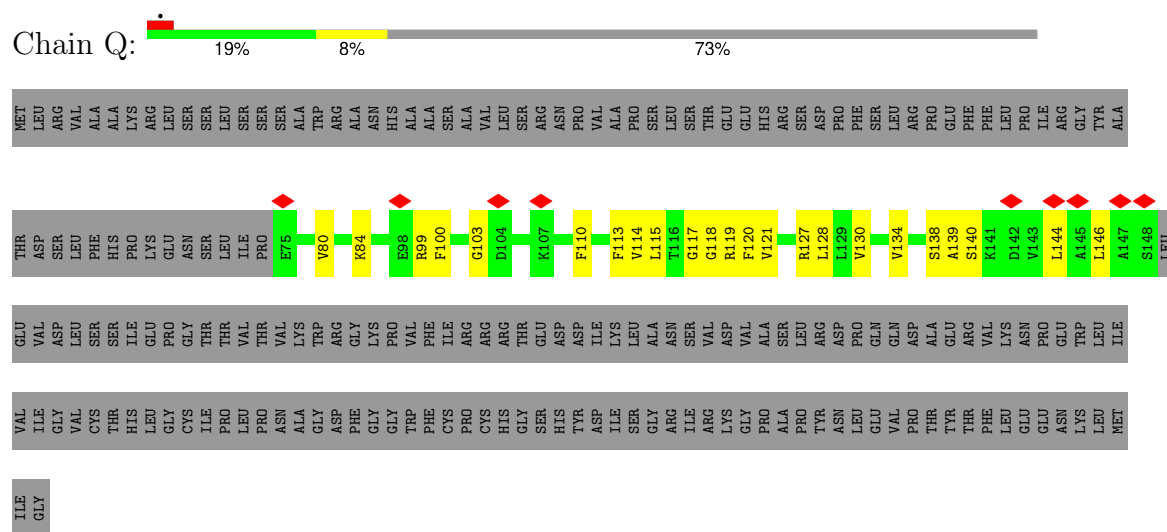
- Molecule 4: cytochrome c1-2, heme protein, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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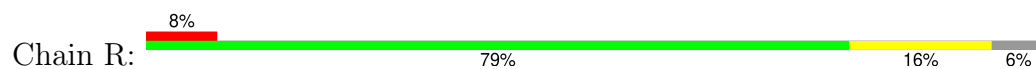


- Molecule 6: Cytochrome b-c1 complex subunit 7

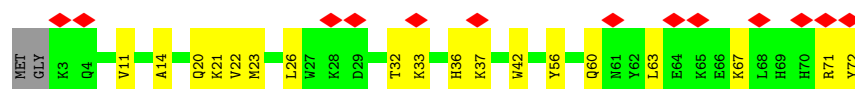




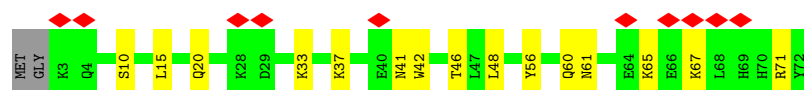
- Molecule 6: Cytochrome b-c1 complex subunit 7



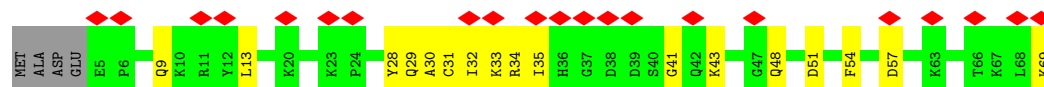
- Molecule 7: cytochrome b-c1 complex subunit 8



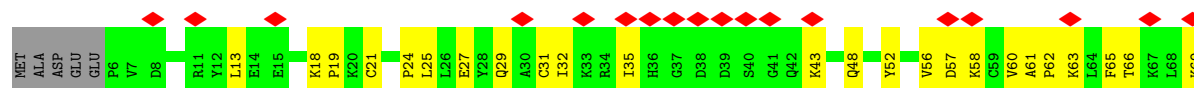
- Molecule 7: cytochrome b-c1 complex subunit 8



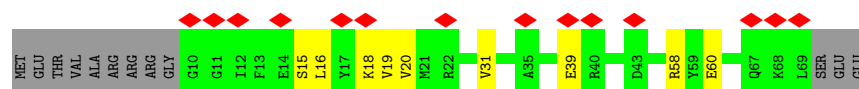
- Molecule 8: Cytochrome b-c1 complex subunit 6



- Molecule 8: Cytochrome b-c1 complex subunit 6



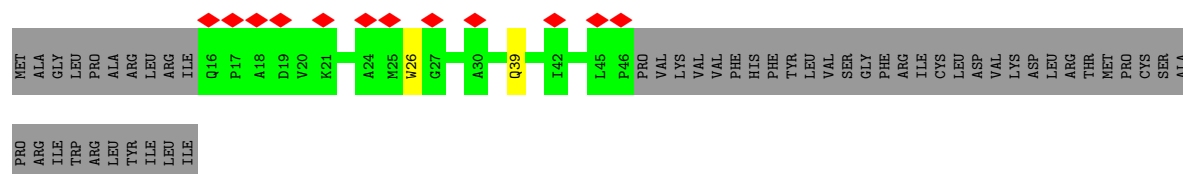
- Molecule 9: cytochrome b-c1 complex subunit 9



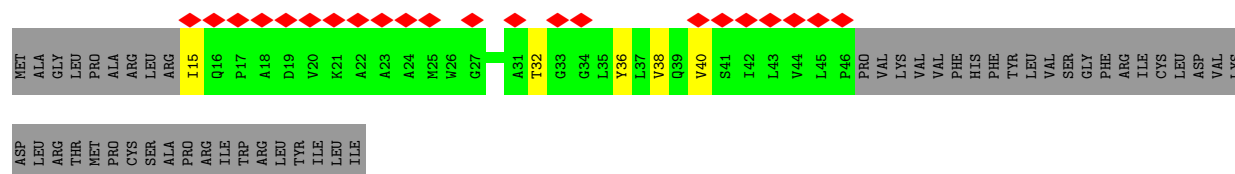
- Molecule 9: cytochrome b-c1 complex subunit 9



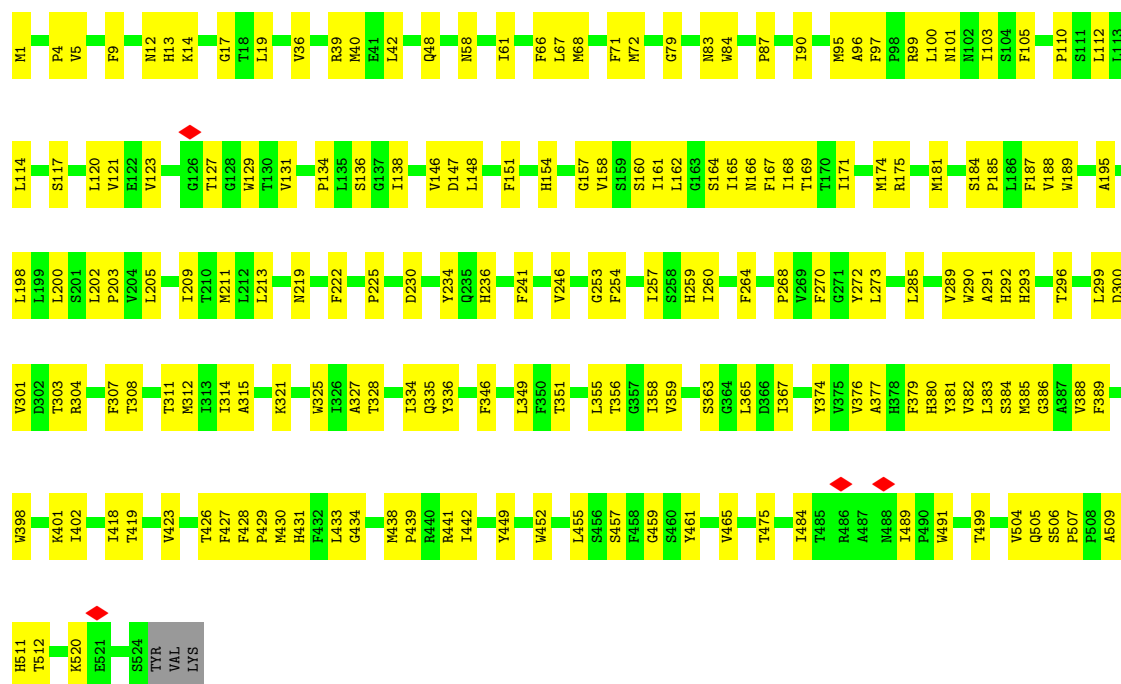
Chain K: 15% 36% 62%



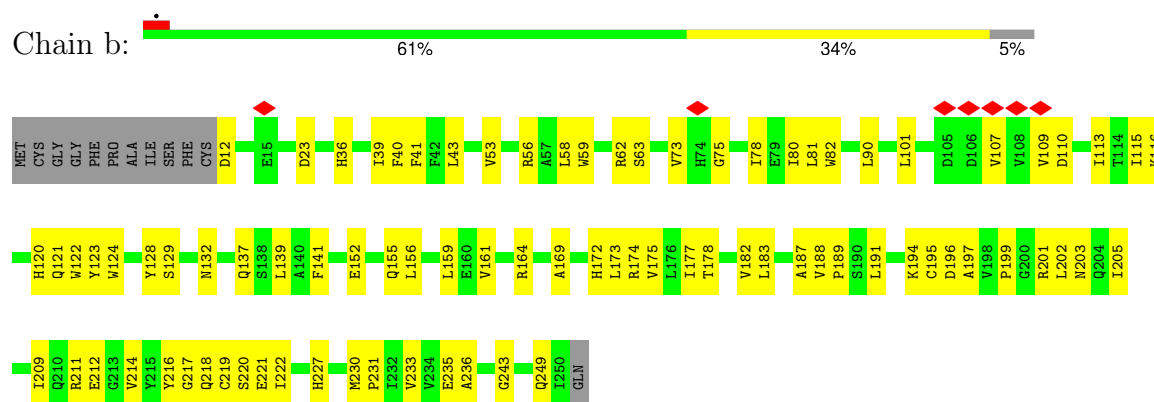
Chain W:



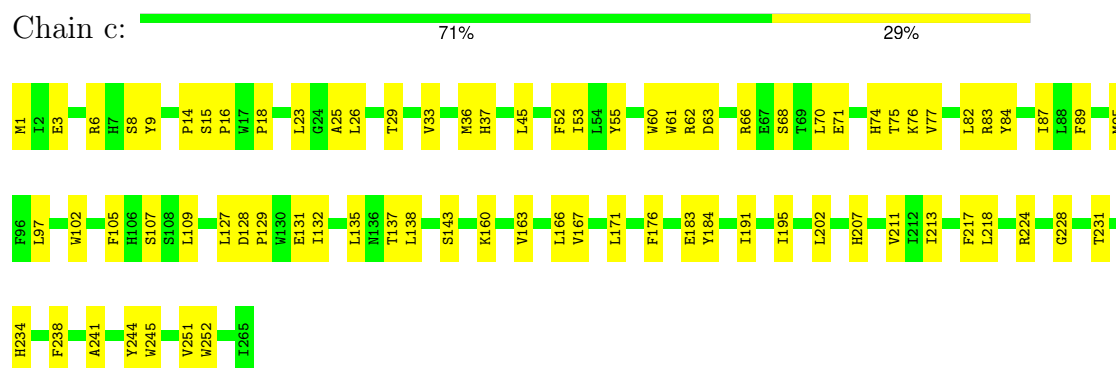
Chain a: 64% 35%



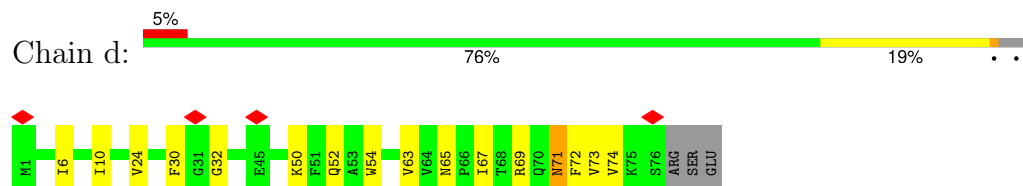
- Molecule 12: Cytochrome c oxidase subunit 2



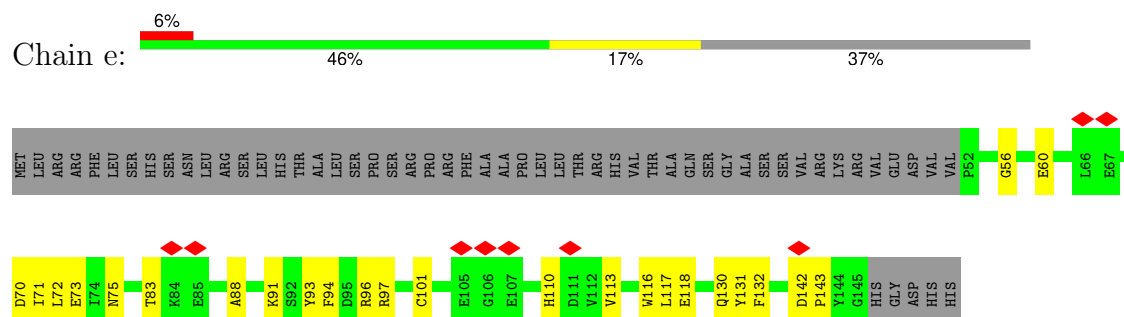
- Molecule 13: COX3



- Molecule 14: COX4

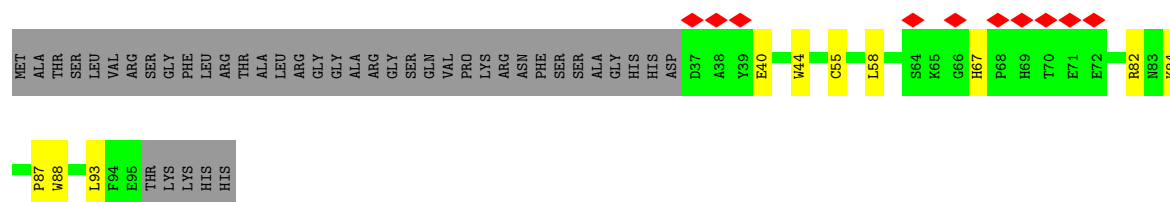


- Molecule 15: cytochrome c oxidase subunit 5b-2, mitochondrial

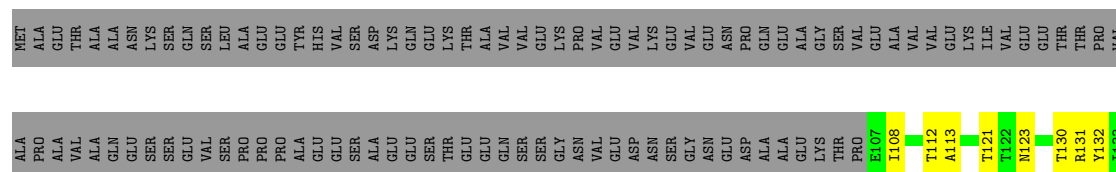


- Molecule 16: cytochrome c oxidase subunit 6a, mitochondrial





• Molecule 17: cytochrome c oxidase subunit 6b-1



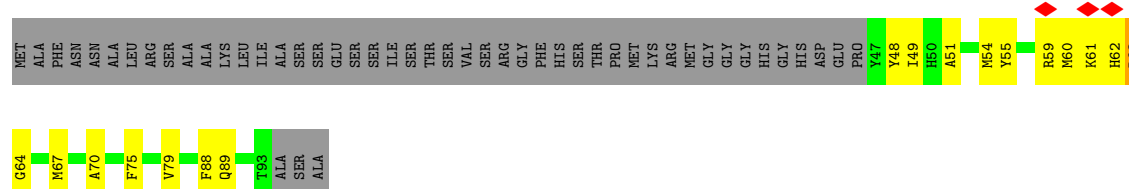
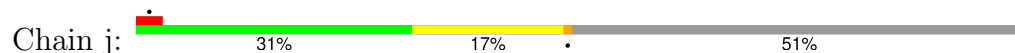
• Molecule 18: Cytochrome c oxidase subunit 5C



• Molecule 19: COX7a



• Molecule 20: COX7c



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29348	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 ($e^-/\text{\AA}^2$)	86.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60010	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.662	Depositor
Minimum map value	-36.912	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.159	Depositor
Recommended contour level	6	Depositor
Map size (Å)	426.5984, 426.5984, 426.5984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8332, 0.8332, 0.8332	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CUA, HEC, HEA, ZN, HEM, CDL, 3PE, CU, PC1

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	0.24	0/3914	0.41	0/5309
1	M	0.24	0/3914	0.41	0/5309
2	B	0.22	0/3541	0.41	1/4803 (0.0%)
2	N	0.22	0/3526	0.41	0/4785
3	C	0.28	0/3220	0.40	0/4413
3	O	0.29	0/3220	0.42	0/4413
4	D	0.23	0/1962	0.36	0/2663
4	P	0.24	0/1962	0.37	0/2663
5	E	0.22	0/588	0.37	0/797
5	Q	0.23	0/588	0.42	0/797
6	F	0.25	0/986	0.37	0/1326
6	R	0.25	0/980	0.38	0/1318
7	G	0.20	0/595	0.36	0/807
7	S	0.19	0/595	0.34	0/807
8	H	0.18	0/550	0.35	0/737
8	T	0.19	0/541	0.45	0/724
9	J	0.19	0/490	0.38	0/660
9	V	0.21	0/486	0.43	0/655
10	K	0.16	0/222	0.33	0/305
10	W	0.18	0/230	0.31	0/316
11	a	0.30	0/4214	0.50	0/5758
12	b	0.26	0/1971	0.46	0/2697
13	c	0.27	0/2217	0.39	0/3030
14	d	0.23	0/612	0.44	0/832
15	e	0.22	0/756	0.40	0/1026
16	f	0.17	0/499	0.42	0/682
17	g	0.28	0/631	0.62	0/853
18	h	0.25	0/399	0.44	0/538
19	i	0.24	0/524	0.50	0/705
20	j	0.23	0/394	0.51	0/528
All	All	0.25	0/44327	0.42	1/60256 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	107	GLY	N-CA-C	5.73	117.62	110.29

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	3838	0	3797	78	0
1	M	3838	0	3797	94	0
2	B	3471	0	3471	98	0
2	N	3456	0	3453	85	0
3	C	3104	0	3070	70	0
3	O	3104	0	3070	71	0
4	D	1910	0	1843	48	0
4	P	1910	0	1843	49	0
5	E	574	0	591	16	0
5	Q	574	0	591	30	0
6	F	965	0	982	28	0
6	R	959	0	977	15	0
7	G	578	0	599	17	0
7	S	578	0	599	13	0
8	H	536	0	528	15	0
8	T	527	0	521	26	0
9	J	480	0	486	7	0
9	V	476	0	483	17	0
10	K	218	0	230	2	0
10	W	226	0	241	7	0
11	a	4074	0	4063	187	0
12	b	1915	0	1876	73	0
13	c	2134	0	2098	74	0
14	d	595	0	596	23	0
15	e	733	0	677	16	0
16	f	480	0	452	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	g	612	0	563	12	0
18	h	391	0	405	8	0
19	i	510	0	528	19	0
20	j	384	0	398	16	0
21	A	1	0	0	0	0
21	M	1	0	0	0	0
21	e	1	0	0	0	0
22	A	29	0	32	1	0
22	M	27	0	28	1	0
22	S	28	0	30	2	0
22	a	39	0	52	1	0
22	i	36	0	46	4	0
23	A	51	0	46	1	0
23	C	109	0	106	5	0
23	D	41	0	26	1	0
23	M	53	0	50	4	0
23	O	54	0	55	2	0
23	P	48	0	40	2	0
23	S	50	0	44	2	0
23	a	67	0	78	1	0
24	C	86	0	60	7	0
24	O	86	0	60	9	0
25	C	158	0	189	10	0
25	F	32	0	38	2	0
25	G	20	0	14	0	0
25	O	109	0	114	7	0
25	P	28	0	30	2	0
25	a	227	0	301	7	0
25	b	108	0	141	4	0
25	c	200	0	270	13	0
25	d	35	0	44	1	0
25	h	38	0	50	2	0
25	i	35	0	44	2	0
26	D	43	0	30	8	0
26	P	43	0	30	3	0
27	a	120	0	108	11	0
28	a	1	0	0	0	0
29	a	1	0	0	0	0
30	b	2	0	0	0	0
31	i	9	0	12	0	0
All	All	45166	0	44996	1062	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 12.

The worst 5 of 1062 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:P:283:GLN:NE2	5:Q:115:LEU:CA	1.87	1.37
4:P:283:GLN:NE2	5:Q:115:LEU:HA	0.94	1.26
4:P:283:GLN:HE21	5:Q:115:LEU:CA	1.43	1.23
9:V:32:ILE:HG21	10:W:32:THR:HG22	1.25	1.10
11:a:90:ILE:HD11	11:a:175:ARG:HG2	1.21	1.08

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	485/527 (92%)	450 (93%)	35 (7%)	0	100	100
1	M	485/527 (92%)	451 (93%)	34 (7%)	0	100	100
2	B	455/506 (90%)	411 (90%)	42 (9%)	2 (0%)	30	62
2	N	453/506 (90%)	406 (90%)	47 (10%)	0	100	100
3	C	386/393 (98%)	365 (95%)	21 (5%)	0	100	100
3	O	386/393 (98%)	363 (94%)	23 (6%)	0	100	100
4	D	242/306 (79%)	234 (97%)	8 (3%)	0	100	100
4	P	242/306 (79%)	229 (95%)	13 (5%)	0	100	100
5	E	72/271 (27%)	68 (94%)	4 (6%)	0	100	100
5	Q	72/271 (27%)	66 (92%)	6 (8%)	0	100	100
6	F	114/122 (93%)	111 (97%)	3 (3%)	0	100	100
6	R	113/122 (93%)	109 (96%)	4 (4%)	0	100	100
7	G	68/72 (94%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	S	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
8	H	63/69 (91%)	59 (94%)	4 (6%)	0	100	100
8	T	62/69 (90%)	55 (89%)	7 (11%)	0	100	100
9	J	58/72 (81%)	54 (93%)	4 (7%)	0	100	100
9	V	57/72 (79%)	55 (96%)	2 (4%)	0	100	100
10	K	29/81 (36%)	25 (86%)	4 (14%)	0	100	100
10	W	30/81 (37%)	28 (93%)	2 (7%)	0	100	100
11	a	522/527 (99%)	471 (90%)	51 (10%)	0	100	100
12	b	237/251 (94%)	206 (87%)	31 (13%)	0	100	100
13	c	263/265 (99%)	249 (95%)	14 (5%)	0	100	100
14	d	74/79 (94%)	67 (90%)	7 (10%)	0	100	100
15	e	92/150 (61%)	83 (90%)	9 (10%)	0	100	100
16	f	57/100 (57%)	54 (95%)	3 (5%)	0	100	100
17	g	72/181 (40%)	63 (88%)	9 (12%)	0	100	100
18	h	47/64 (73%)	46 (98%)	1 (2%)	0	100	100
19	i	62/67 (92%)	57 (92%)	5 (8%)	0	100	100
20	j	45/96 (47%)	39 (87%)	5 (11%)	1 (2%)	5	30
All	All	5411/6618 (82%)	5007 (92%)	401 (7%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	j	63	ARG
2	B	435	ARG
2	B	113	PRO

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	407/438 (93%)	407 (100%)	0	100	100
1	M	407/438 (93%)	407 (100%)	0	100	100
2	B	378/414 (91%)	378 (100%)	0	100	100
2	N	377/414 (91%)	377 (100%)	0	100	100
3	C	333/338 (98%)	332 (100%)	1 (0%)	86	84
3	O	333/338 (98%)	333 (100%)	0	100	100
4	D	198/247 (80%)	197 (100%)	1 (0%)	81	81
4	P	198/247 (80%)	197 (100%)	1 (0%)	81	81
5	E	62/233 (27%)	62 (100%)	0	100	100
5	Q	62/233 (27%)	62 (100%)	0	100	100
6	F	102/107 (95%)	102 (100%)	0	100	100
6	R	101/107 (94%)	101 (100%)	0	100	100
7	G	64/65 (98%)	64 (100%)	0	100	100
7	S	64/65 (98%)	64 (100%)	0	100	100
8	H	60/63 (95%)	60 (100%)	0	100	100
8	T	59/63 (94%)	59 (100%)	0	100	100
9	J	49/59 (83%)	49 (100%)	0	100	100
9	V	49/59 (83%)	48 (98%)	1 (2%)	48	65
10	K	21/66 (32%)	21 (100%)	0	100	100
10	W	22/66 (33%)	22 (100%)	0	100	100
11	a	433/436 (99%)	433 (100%)	0	100	100
12	b	213/222 (96%)	213 (100%)	0	100	100
13	c	219/219 (100%)	219 (100%)	0	100	100
14	d	65/68 (96%)	64 (98%)	1 (2%)	57	69
15	e	77/126 (61%)	77 (100%)	0	100	100
16	f	50/82 (61%)	50 (100%)	0	100	100
17	g	63/153 (41%)	63 (100%)	0	100	100
18	h	42/52 (81%)	42 (100%)	0	100	100
19	i	55/58 (95%)	55 (100%)	0	100	100
20	j	40/77 (52%)	40 (100%)	0	100	100
All	All	4603/5553 (83%)	4598 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	259	HIS
4	D	305	VAL
4	P	282	LEU
9	V	31	VAL
14	d	71	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
11	a	259	HIS
17	g	171	GLN
11	a	370	HIS
12	b	18	GLN
4	D	95	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 5 are monoatomic - leaving 53 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
22	PC1	M	603	-	26,26,53	0.38	0	32,34,61	0.41	0
25	3PE	i	103	-	34,34,50	0.36	0	37,39,55	0.30	0
23	CDL	M	602	-	52,52,99	0.39	0	58,64,111	0.43	0
26	HEC	D	501	4	50,50,50	1.34	6 (12%)	68,82,82	1.24	5 (7%)
26	HEC	P	402	4	50,50,50	1.35	6 (12%)	68,82,82	1.18	4 (5%)
25	3PE	a	609	-	37,37,50	0.35	0	40,42,55	0.41	0
31	LYS	i	102	-	7,8,9	0.48	0	3,8,10	0.39	0
25	3PE	a	610	-	39,39,50	0.34	0	42,44,55	0.32	0
25	3PE	C	404	-	37,37,50	0.35	0	40,42,55	0.37	0
23	CDL	P	403	-	47,47,99	0.40	0	53,59,111	0.50	0
23	CDL	C	401	-	53,53,99	0.40	0	59,65,111	0.36	0
23	CDL	O	402	-	53,53,99	0.38	0	59,65,111	0.47	0
23	CDL	S	102	-	49,49,99	0.41	0	55,61,111	0.40	0
25	3PE	a	606	-	31,31,50	0.37	0	34,36,55	0.39	0
23	CDL	a	608	-	66,66,99	0.36	0	72,78,111	0.37	0
22	PC1	S	101	-	27,27,53	1.13	2 (7%)	33,35,61	1.16	3 (9%)
24	HEM	C	402	3	50,50,50	1.36	7 (14%)	67,82,82	1.69	15 (22%)
25	3PE	O	401	-	23,23,50	1.17	2 (8%)	26,28,55	1.18	2 (7%)
23	CDL	A	603	-	50,50,99	0.38	0	56,62,111	0.36	0
23	CDL	D	502	-	40,40,99	0.43	0	46,52,111	0.44	0
25	3PE	b	304	-	42,42,50	0.32	0	45,47,55	0.33	0
30	CUA	b	301	12	0,1,1	-	-	-	-	-
22	PC1	A	602	-	28,28,53	1.39	2 (7%)	34,36,61	1.31	3 (8%)
25	3PE	b	303	-	28,28,50	0.40	0	31,33,55	0.44	0
22	PC1	i	101	-	35,35,53	0.35	0	41,43,61	0.42	0
25	3PE	F	201	-	31,31,50	0.39	0	34,36,55	0.55	0
25	3PE	O	405	-	25,25,50	1.30	2 (8%)	28,30,55	1.30	3 (10%)
25	3PE	P	401	-	27,27,50	1.08	2 (7%)	30,32,55	1.15	2 (6%)
23	CDL	C	409	-	54,54,99	0.38	0	60,66,111	0.35	0
27	HEA	a	602	11	67,67,67	1.25	9 (13%)	81,103,103	1.41	14 (17%)
25	3PE	C	408	-	27,27,50	0.40	0	30,32,55	0.37	0
25	3PE	a	611	-	37,37,50	0.35	0	40,42,55	0.31	0
24	HEM	O	404	3	50,50,50	1.39	7 (14%)	67,82,82	1.63	14 (20%)
25	3PE	C	407	-	34,34,50	0.34	0	37,39,55	0.47	0
25	3PE	a	607	-	39,39,50	0.34	0	42,44,55	0.33	0
25	3PE	c	305	-	39,39,50	0.34	0	42,44,55	0.33	0
25	3PE	c	304	-	42,42,50	0.35	0	45,47,55	0.46	0
25	3PE	c	301	-	39,39,50	0.35	0	42,44,55	0.38	0
25	3PE	G	101	-	19,19,50	1.27	2 (10%)	22,24,55	1.08	2 (9%)
22	PC1	a	605	-	38,38,53	0.35	0	44,46,61	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	3PE	b	302	-	35,35,50	0.36	0	38,40,55	0.34	0
25	3PE	c	302	-	39,39,50	0.35	0	42,44,55	0.50	0
25	3PE	O	407	-	25,25,50	0.41	0	28,30,55	0.43	0
25	3PE	h	101	-	37,37,50	0.35	0	40,42,55	0.33	0
25	3PE	c	303	-	36,36,50	0.35	0	39,41,55	0.35	0
24	HEM	O	403	3	50,50,50	1.37	6 (12%)	67,82,82	1.68	15 (22%)
27	HEA	a	601	11	67,67,67	1.24	8 (11%)	81,103,103	1.79	20 (24%)
25	3PE	C	406	-	28,28,50	0.40	0	31,33,55	0.41	0
25	3PE	a	612	-	38,38,50	0.34	0	41,43,55	0.32	0
25	3PE	C	405	-	27,27,50	1.26	2 (7%)	30,32,55	1.26	3 (10%)
25	3PE	O	406	-	32,32,50	0.37	0	35,37,55	0.35	0
25	3PE	d	101	-	34,34,50	0.36	0	37,39,55	0.33	0
24	HEM	C	403	3	50,50,50	1.36	7 (14%)	67,82,82	1.64	13 (19%)

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
26	HEC	P	402	4	1/1/3/7	2/14/54/54	-
22	PC1	M	603	-	-	1/29/29/57	-
23	CDL	M	602	-	-	7/62/62/110	-
26	HEC	D	501	4	1/1/3/7	4/14/54/54	-
25	3PE	i	103	-	-	9/38/38/54	-
25	3PE	a	609	-	-	14/41/41/54	-
31	LYS	i	102	-	-	1/6/7/9	-
25	3PE	a	610	-	-	10/43/43/54	-
25	3PE	C	404	-	-	9/41/41/54	-
23	CDL	P	403	-	-	14/56/56/110	-
23	CDL	C	401	-	-	11/64/64/110	-
23	CDL	O	402	-	-	14/62/62/110	-
23	CDL	S	102	-	-	13/60/60/110	-
25	3PE	a	606	-	-	10/35/35/54	-
23	CDL	a	608	-	-	14/77/77/110	-
22	PC1	S	101	-	-	12/30/30/57	-
24	HEM	C	402	3	-	5/14/54/54	-
25	3PE	O	401	-	-	1/26/26/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CDL	A	603	-	-	13/59/59/110	-
23	CDL	D	502	-	-	14/49/49/110	-
25	3PE	b	304	-	-	6/46/46/54	-
22	PC1	A	602	-	-	5/31/31/57	-
25	3PE	b	303	-	-	9/32/32/54	-
22	PC1	i	101	-	-	5/39/39/57	-
25	3PE	F	201	-	-	9/35/35/54	-
25	3PE	O	405	-	-	9/29/29/54	-
25	3PE	P	401	-	-	9/30/30/54	-
23	CDL	C	409	-	-	7/64/64/110	-
27	HEA	a	602	11	-	8/36/76/76	-
25	3PE	C	408	-	-	5/31/31/54	-
25	3PE	a	611	-	-	5/41/41/54	-
24	HEM	O	404	3	-	9/14/54/54	-
25	3PE	C	407	-	-	12/37/37/54	-
25	3PE	a	607	-	-	4/43/43/54	-
25	3PE	c	305	-	-	7/43/43/54	-
25	3PE	c	304	-	-	12/46/46/54	-
25	3PE	c	301	-	-	11/43/43/54	-
25	3PE	G	101	-	-	6/22/22/54	-
22	PC1	a	605	-	-	14/42/42/57	-
25	3PE	b	302	-	-	8/39/39/54	-
25	3PE	c	302	-	-	8/43/43/54	-
25	3PE	O	407	-	-	2/29/29/54	-
25	3PE	h	101	-	-	2/41/41/54	-
25	3PE	c	303	-	-	8/40/40/54	-
24	HEM	O	403	3	-	10/14/54/54	-
27	HEA	a	601	11	-	12/36/76/76	-
25	3PE	C	406	-	-	6/32/32/54	-
25	3PE	a	612	-	-	5/42/42/54	-
25	3PE	C	405	-	-	14/31/31/54	-
25	3PE	O	406	-	-	7/36/36/54	-
25	3PE	d	101	-	-	15/38/38/54	-
24	HEM	C	403	3	-	8/14/54/54	-

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	602	PC1	O21-C21	4.96	1.46	1.35
25	C	405	3PE	O31-C31	4.30	1.45	1.33
22	A	602	PC1	O31-C31	4.28	1.45	1.33
25	O	405	3PE	O31-C31	4.26	1.45	1.33
25	O	401	3PE	O21-C21	4.18	1.46	1.34

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	O	403	HEM	CHC-C4B-NB	4.91	129.71	124.42
22	A	602	PC1	O21-C21-C22	4.85	119.74	111.09
24	C	402	HEM	CHC-C4B-NB	4.81	129.59	124.42
27	a	601	HEA	C3C-C4C-NC	-4.63	105.90	109.80
24	C	402	HEM	CHD-C4C-NC	4.53	129.38	124.45

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	D	501	HEC	NA
26	P	402	HEC	NA

5 of 435 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	602	PC1	C11-O13-P-O12
22	A	602	PC1	C11-O13-P-O14
22	A	602	PC1	C11-O13-P-O11
22	S	101	PC1	C1-O11-P-O12
22	S	101	PC1	C1-O11-P-O14

There are no ring outliers.

43 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	M	603	PC1	1	0
25	i	103	3PE	2	0
23	M	602	CDL	4	0
26	D	501	HEC	8	0
26	P	402	HEC	3	0
25	a	610	3PE	1	0
23	P	403	CDL	2	0

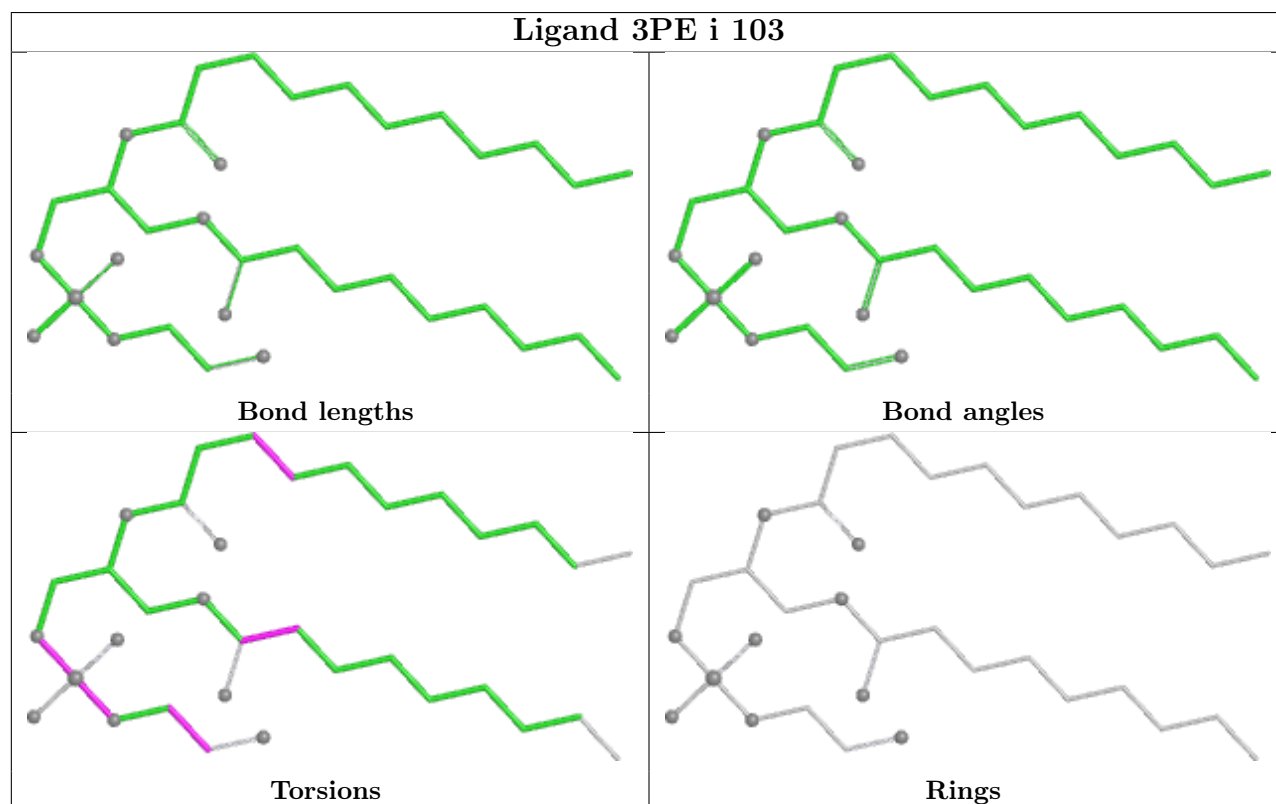
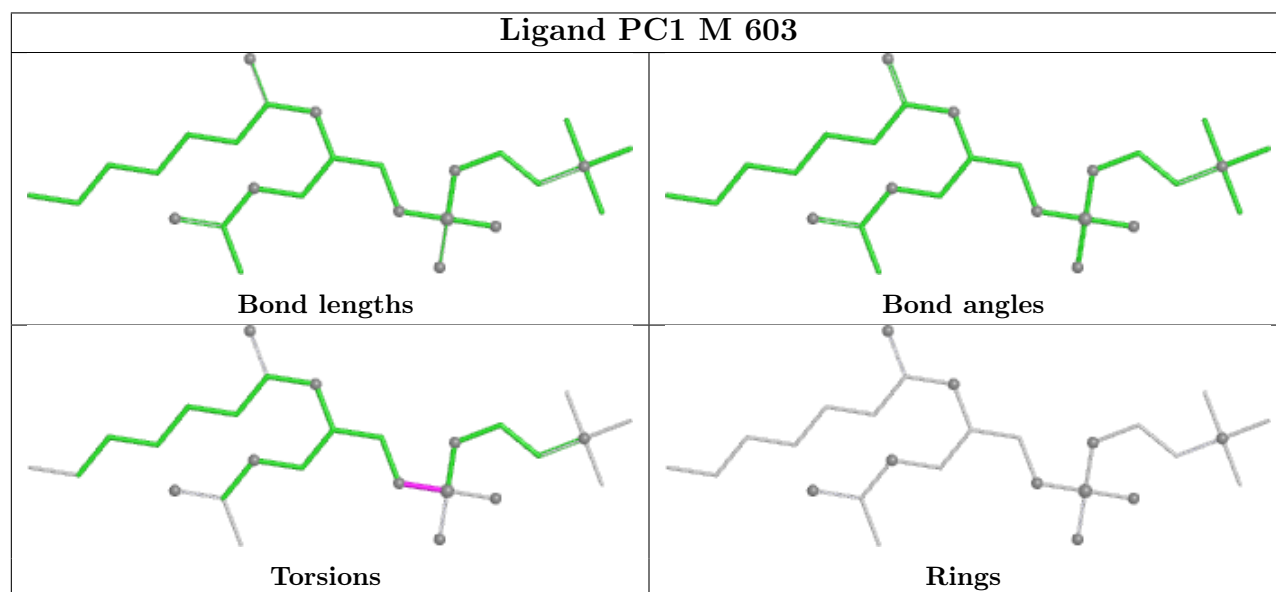
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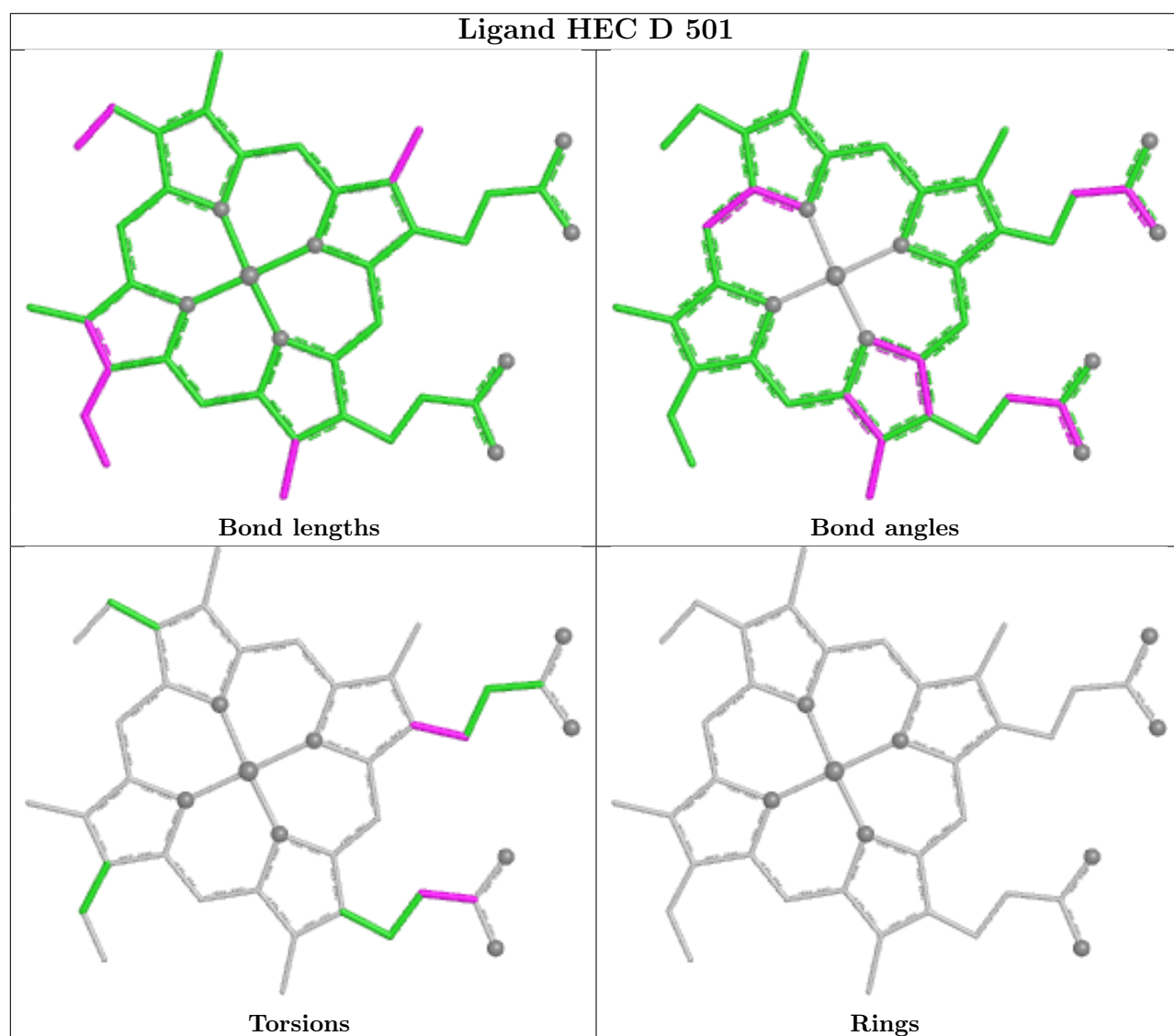
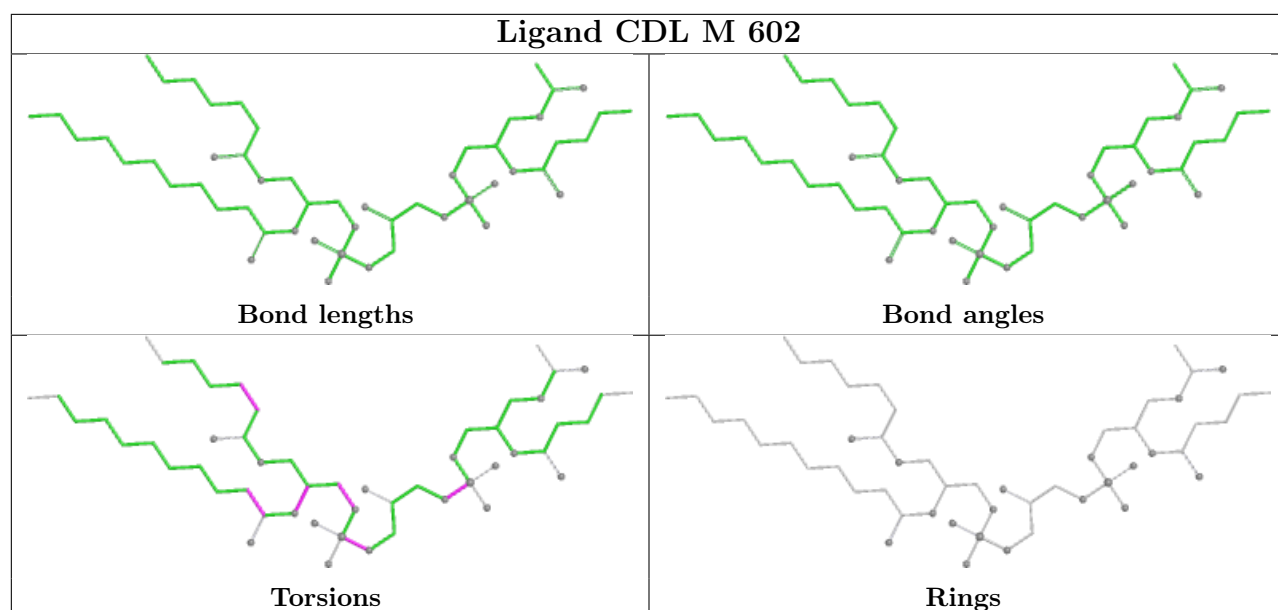
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	401	CDL	3	0
23	O	402	CDL	2	0
23	S	102	CDL	2	0
23	a	608	CDL	1	0
22	S	101	PC1	2	0
24	C	402	HEM	2	0
25	O	401	3PE	7	0
23	A	603	CDL	1	0
23	D	502	CDL	1	0
25	b	304	3PE	1	0
22	A	602	PC1	1	0
25	b	303	3PE	2	0
22	i	101	PC1	4	0
25	F	201	3PE	2	0
25	P	401	3PE	2	0
23	C	409	CDL	2	0
27	a	602	HEA	6	0
25	C	408	3PE	1	0
24	O	404	HEM	6	0
25	C	407	3PE	3	0
25	a	607	3PE	5	0
25	c	305	3PE	1	0
25	c	304	3PE	1	0
25	c	301	3PE	4	0
22	a	605	PC1	1	0
25	b	302	3PE	1	0
25	c	302	3PE	3	0
25	h	101	3PE	2	0
25	c	303	3PE	4	0
24	O	403	HEM	3	0
27	a	601	HEA	5	0
25	C	406	3PE	4	0
25	a	612	3PE	1	0
25	C	405	3PE	2	0
25	d	101	3PE	1	0
24	C	403	HEM	5	0

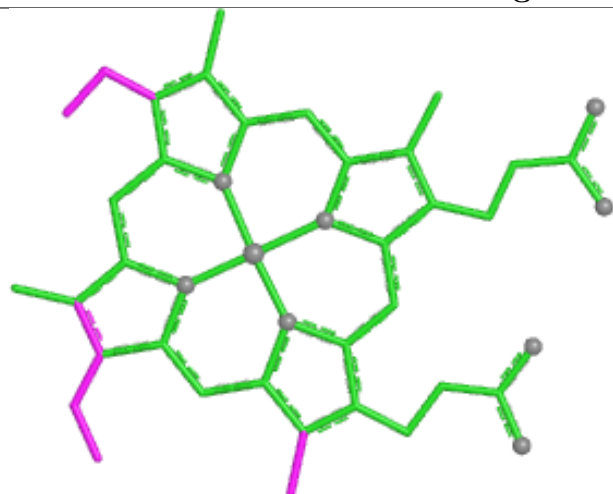
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

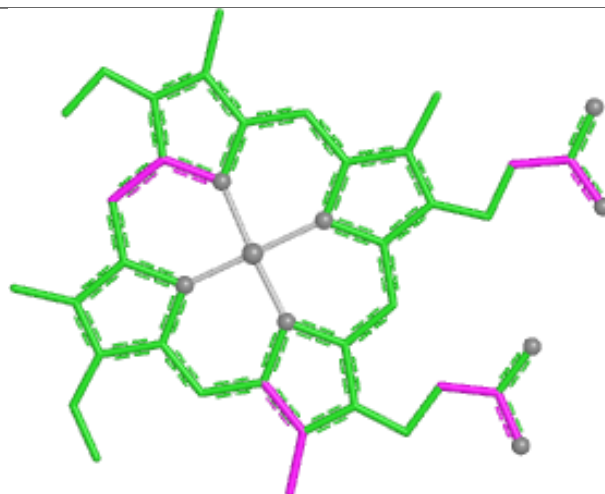




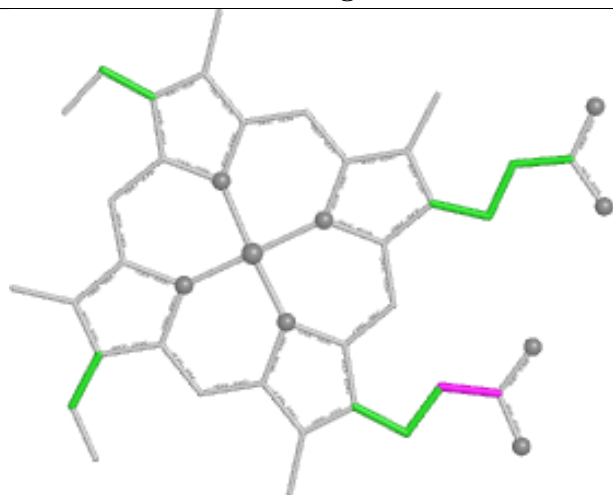
Ligand HEC P 402



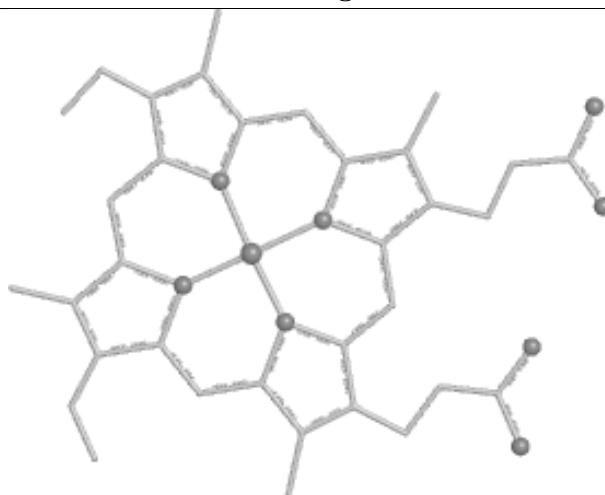
Bond lengths



Bond angles

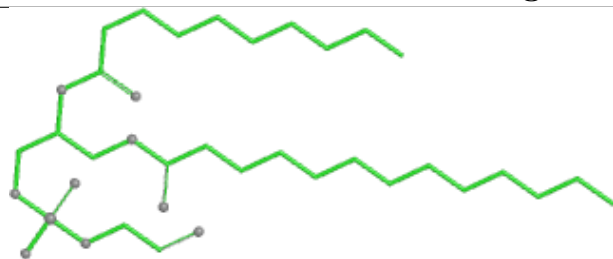


Torsions

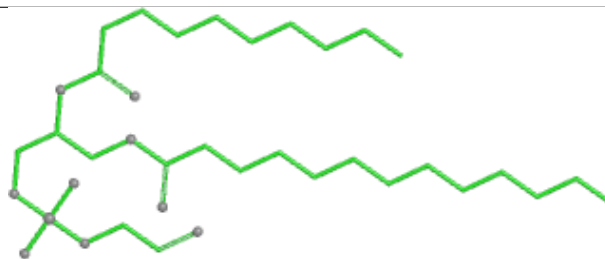


Rings

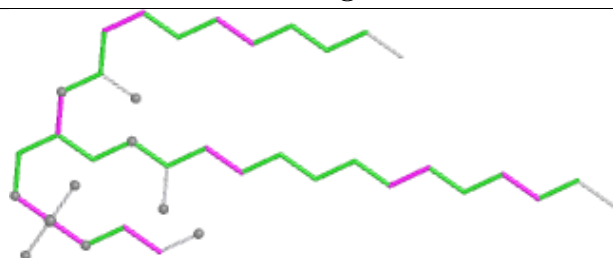
Ligand 3PE a 609



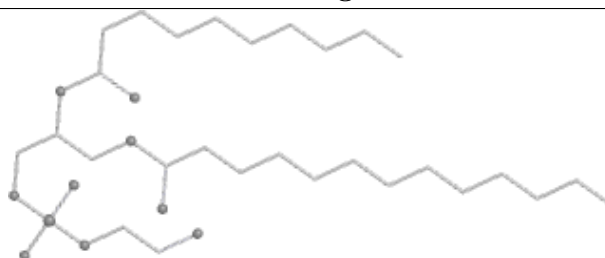
Bond lengths



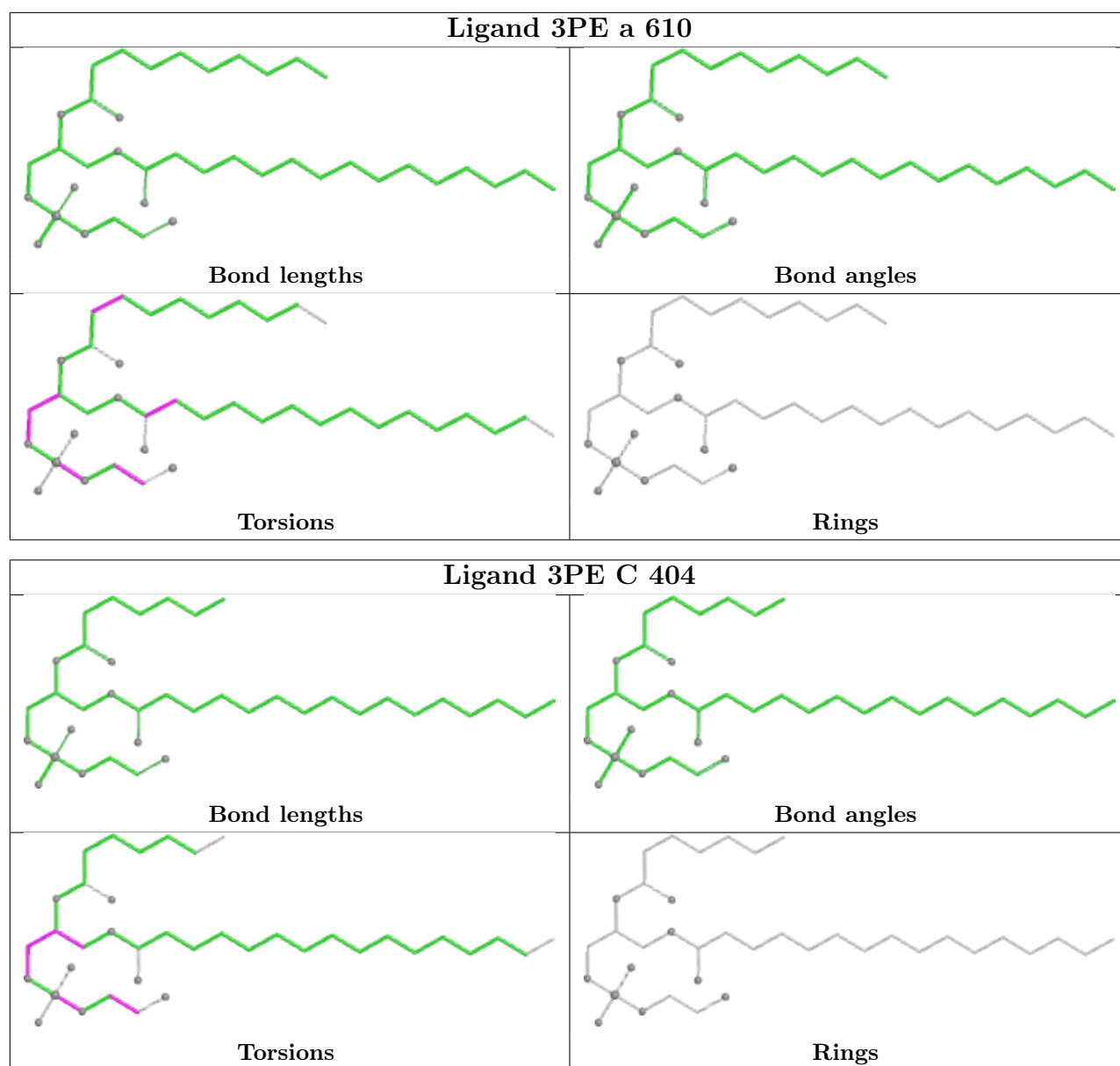
Bond angles

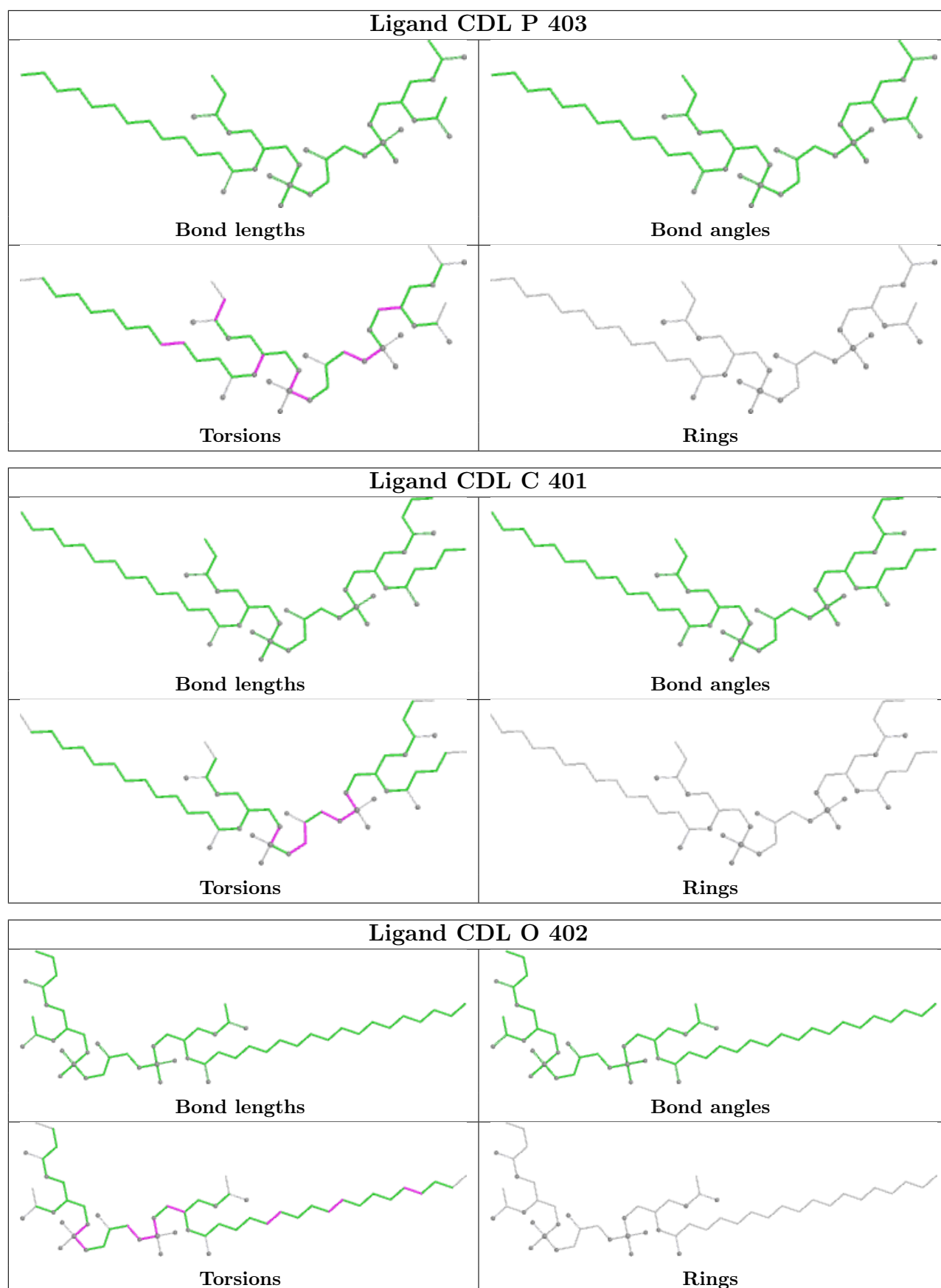


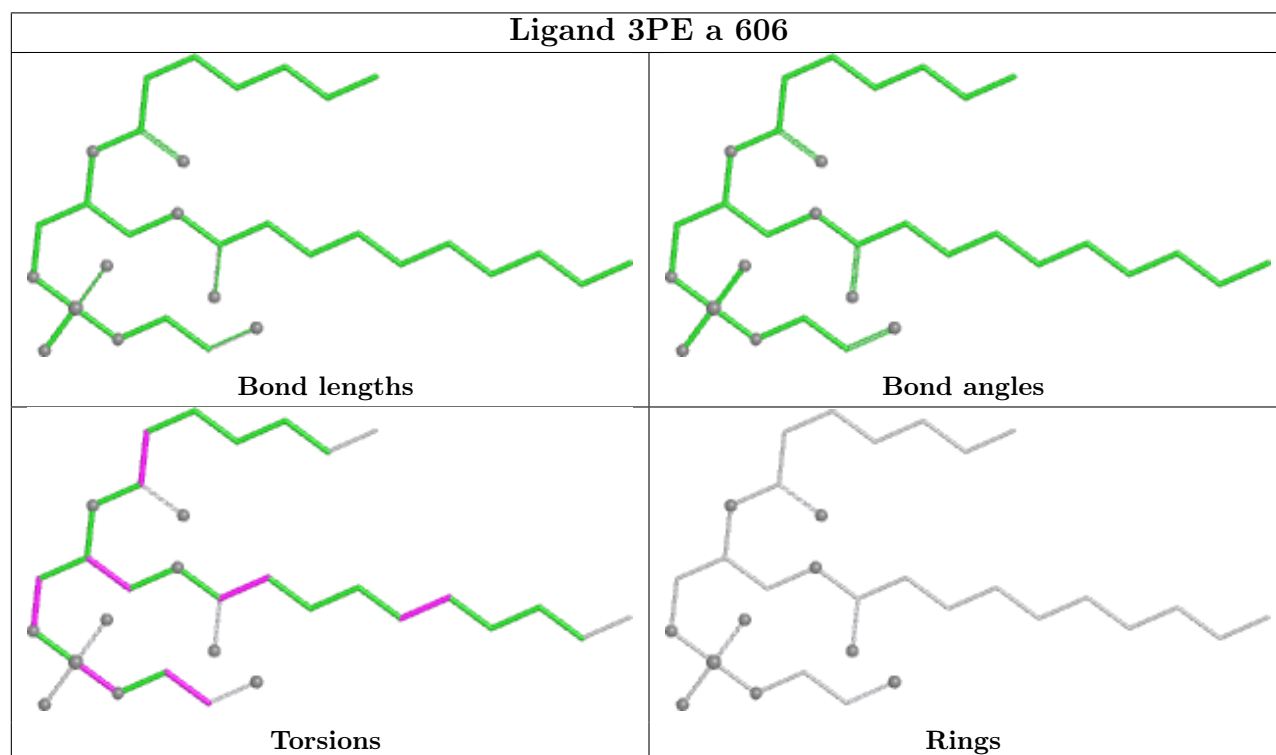
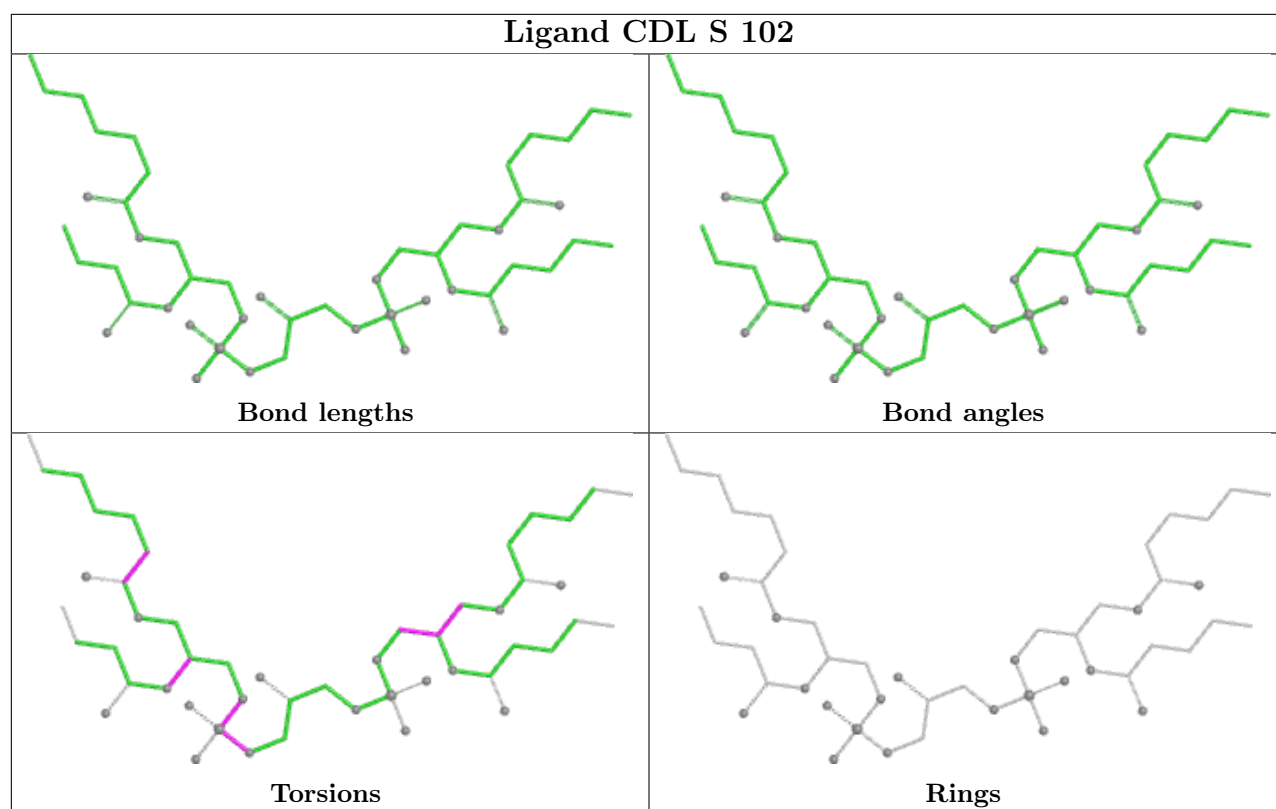
Torsions

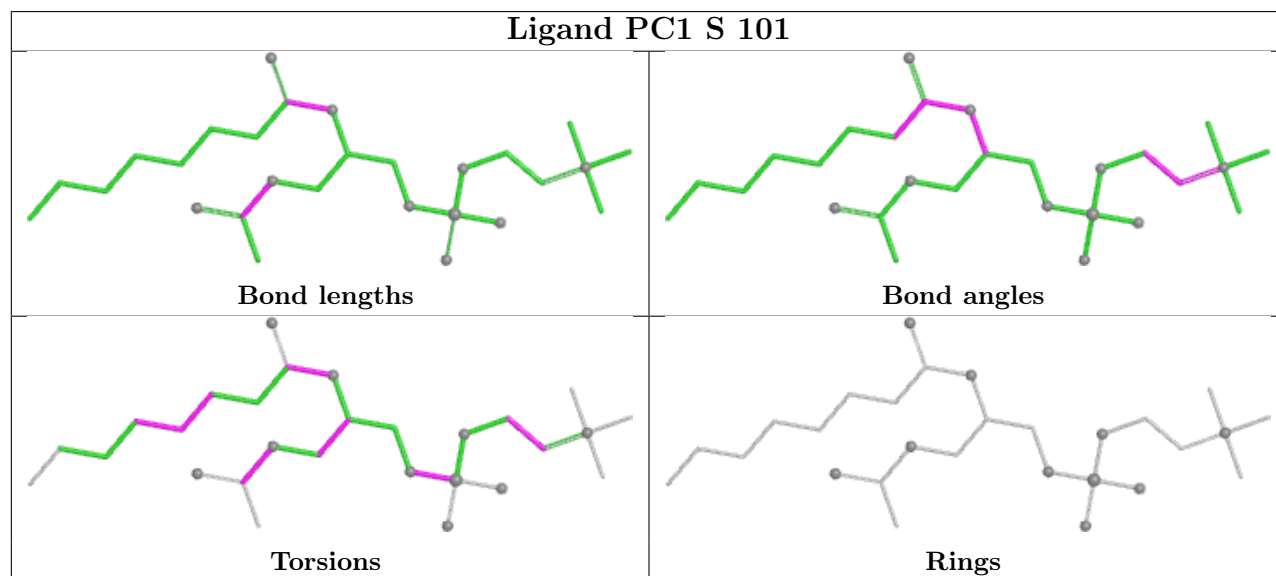
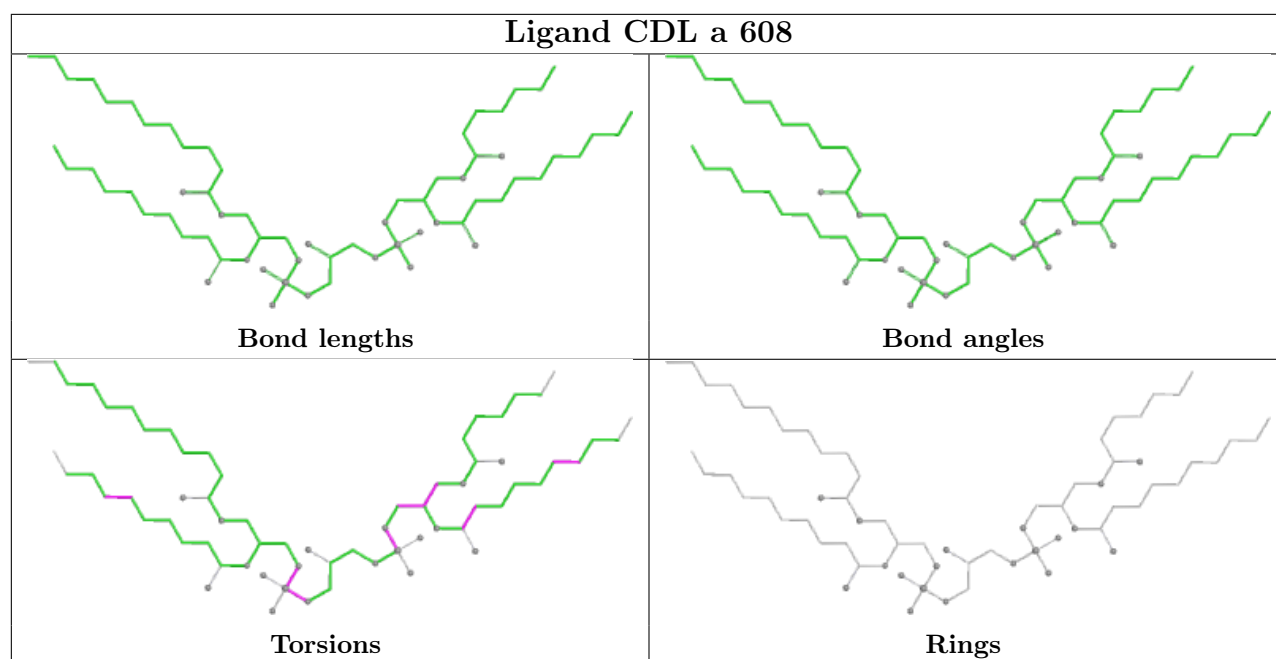


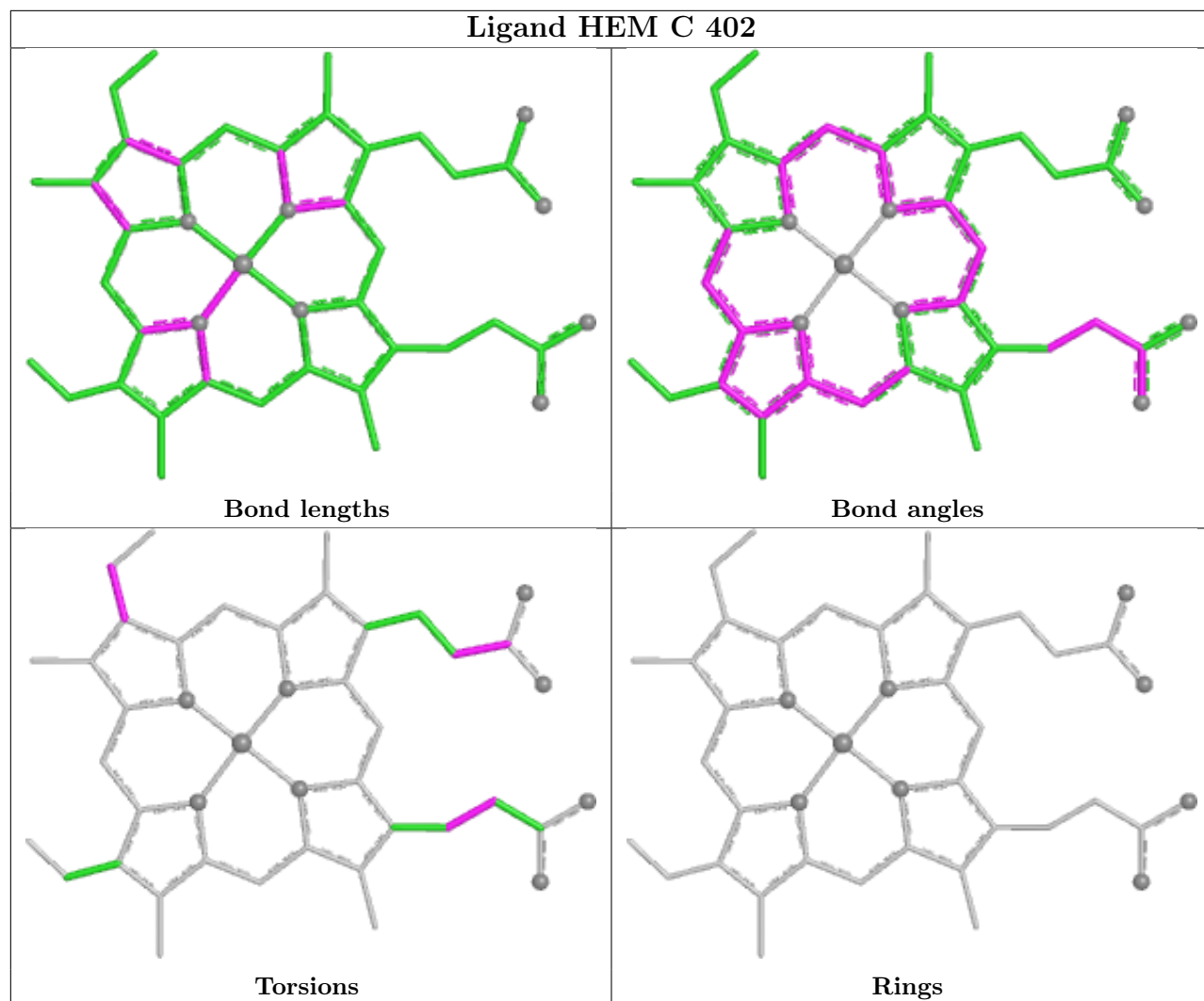
Rings

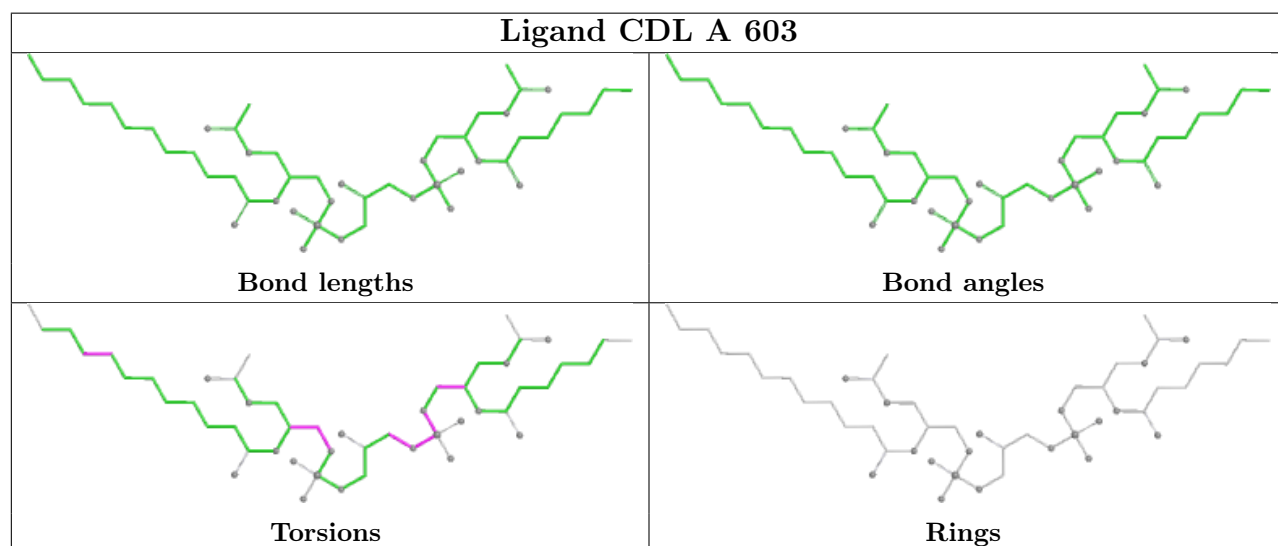
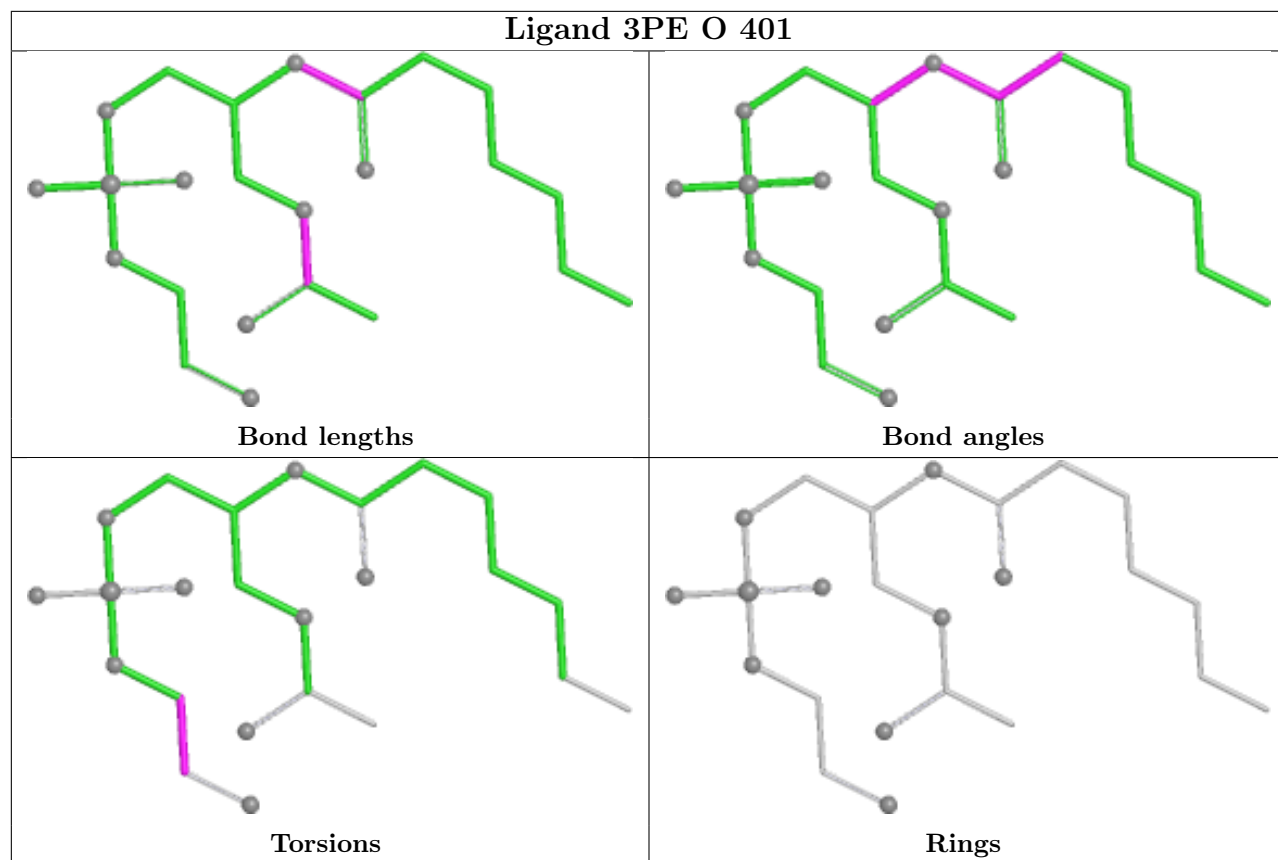


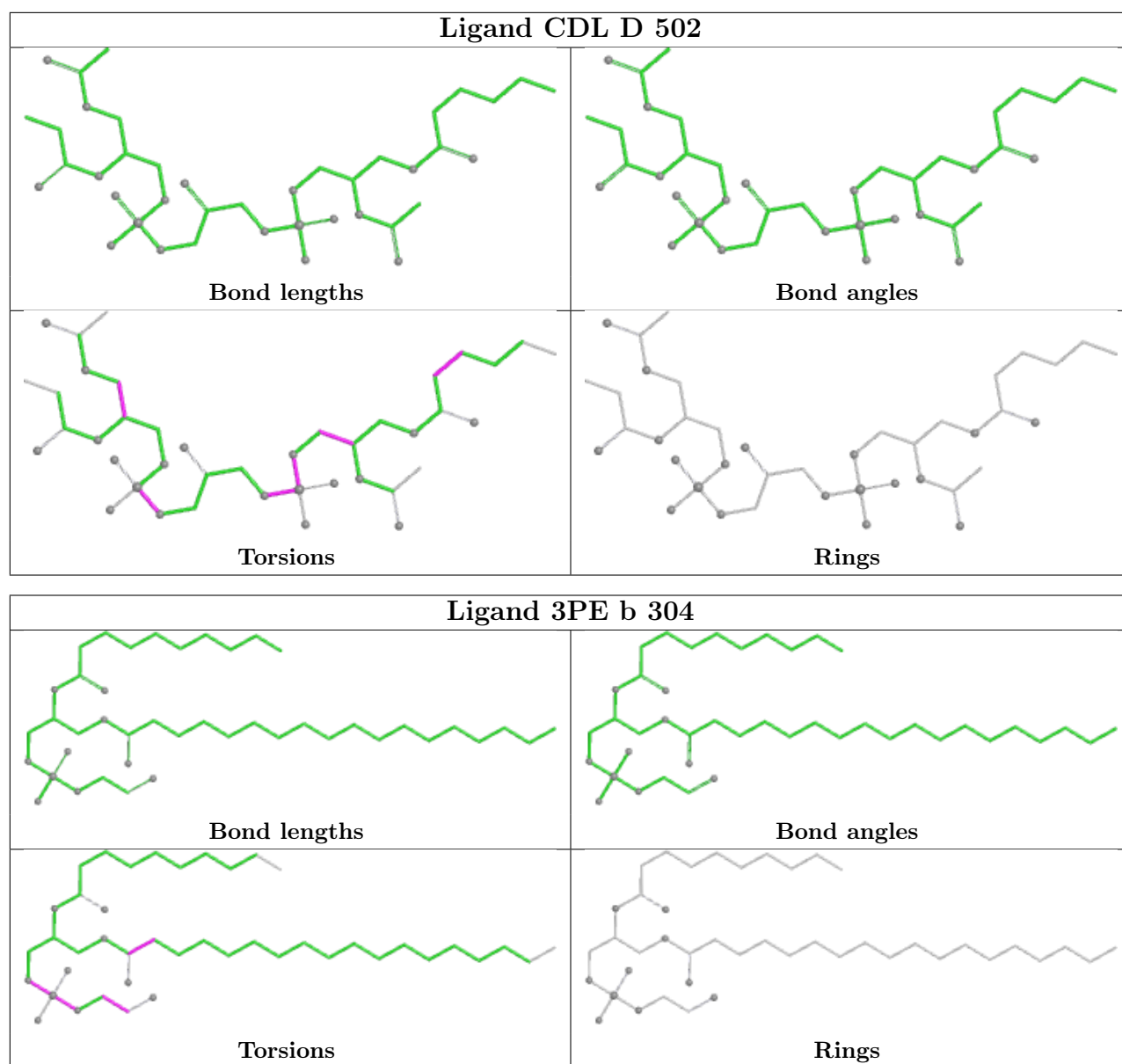


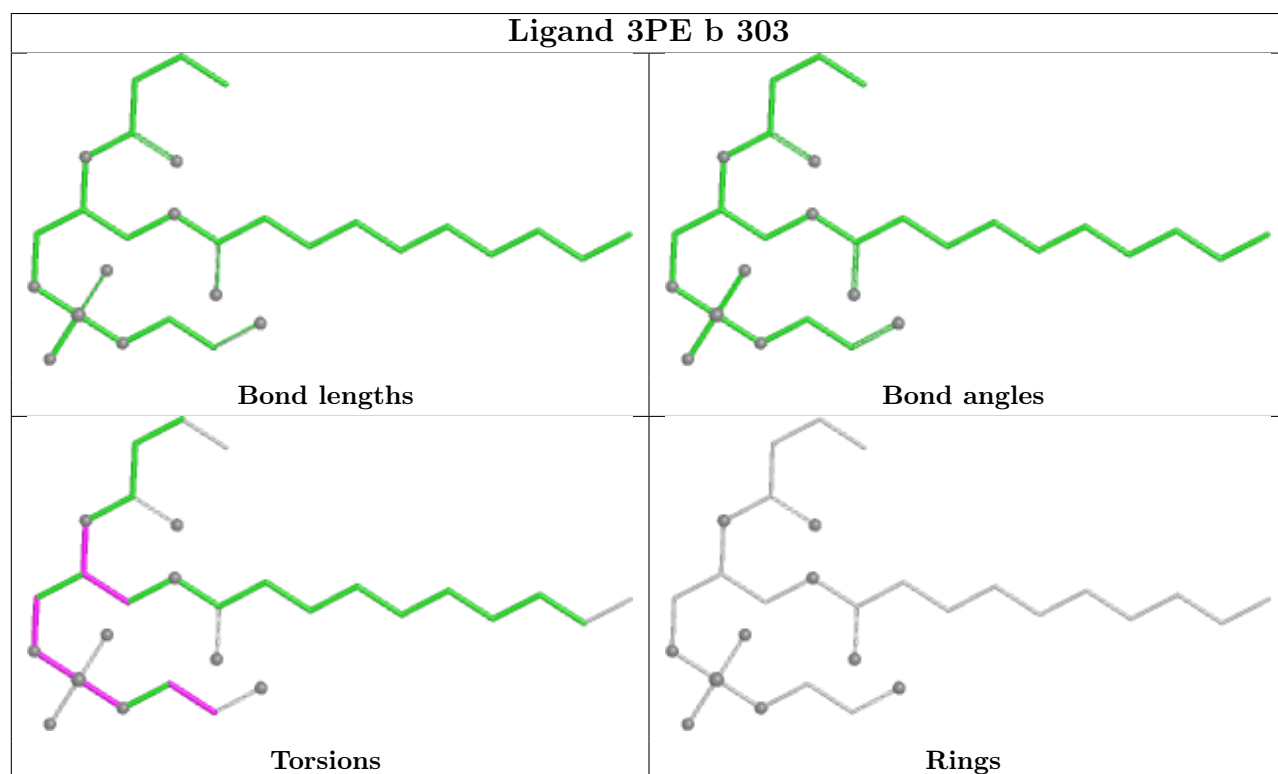
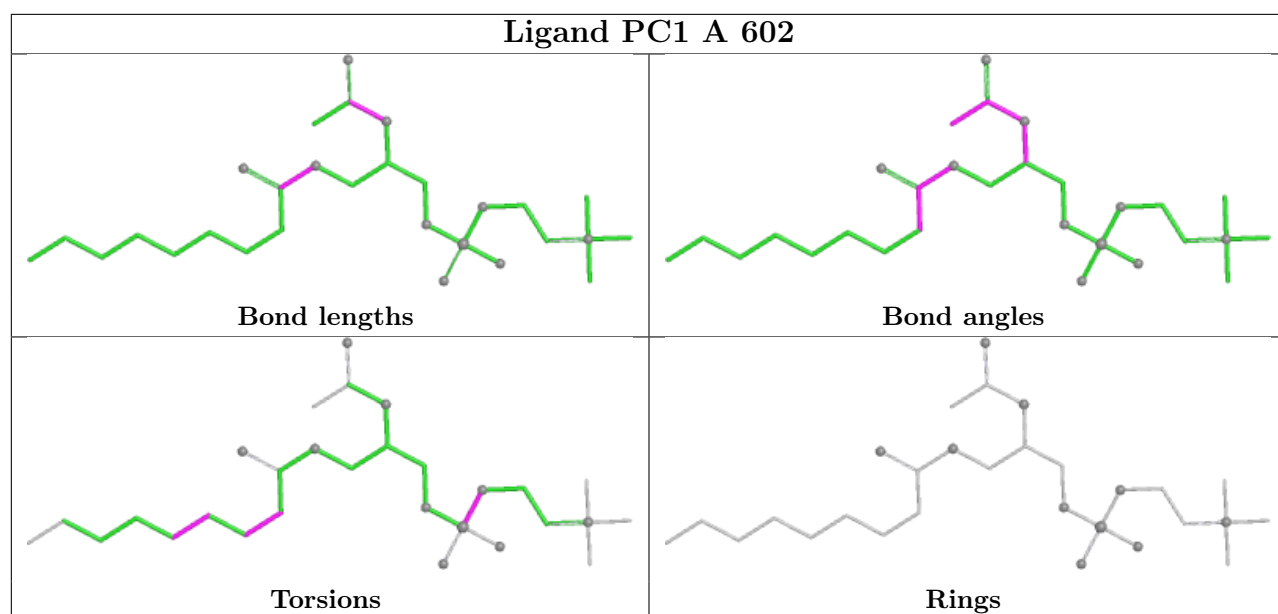


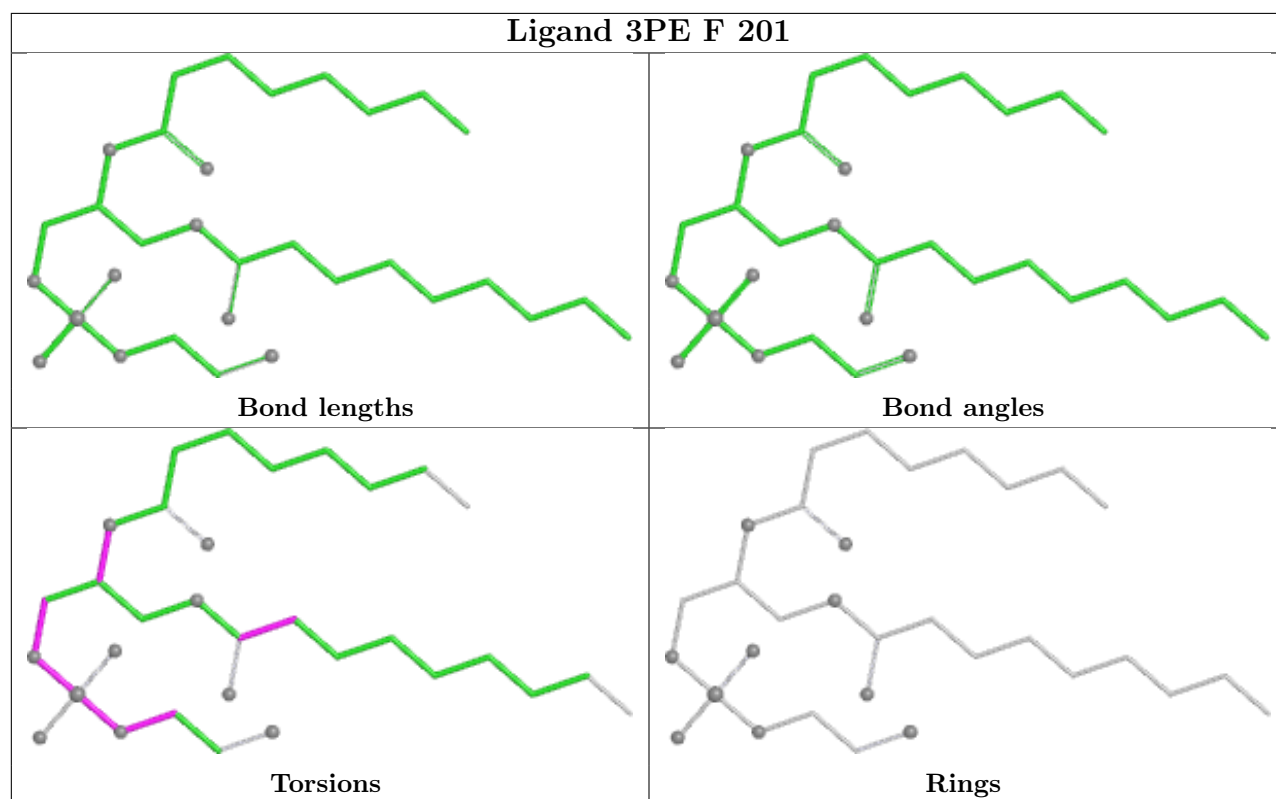
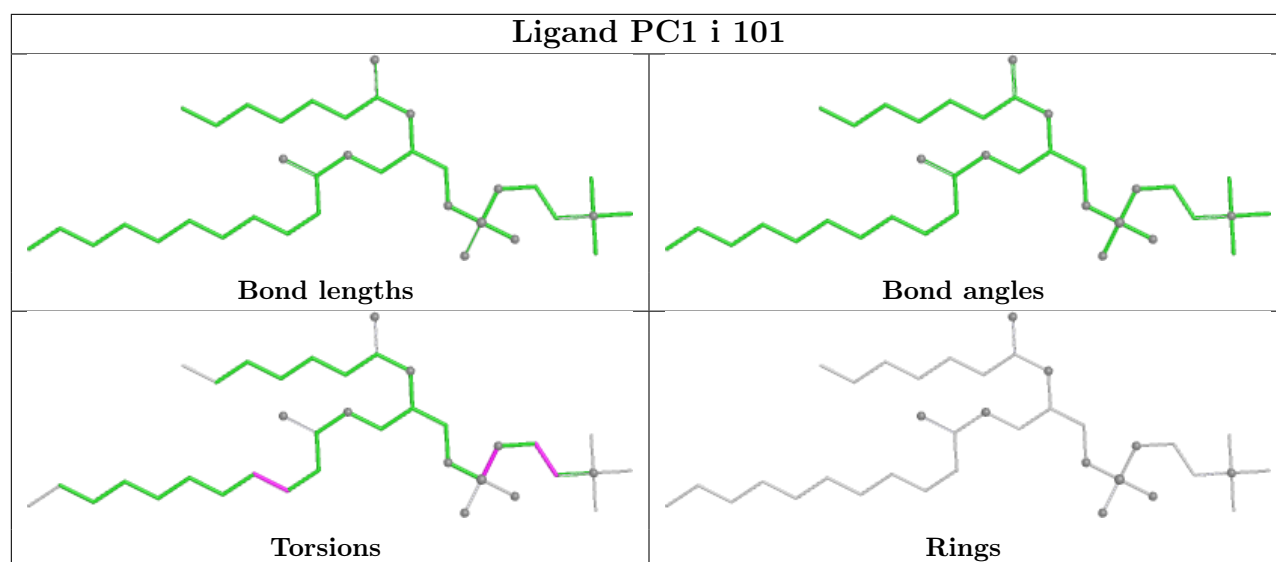




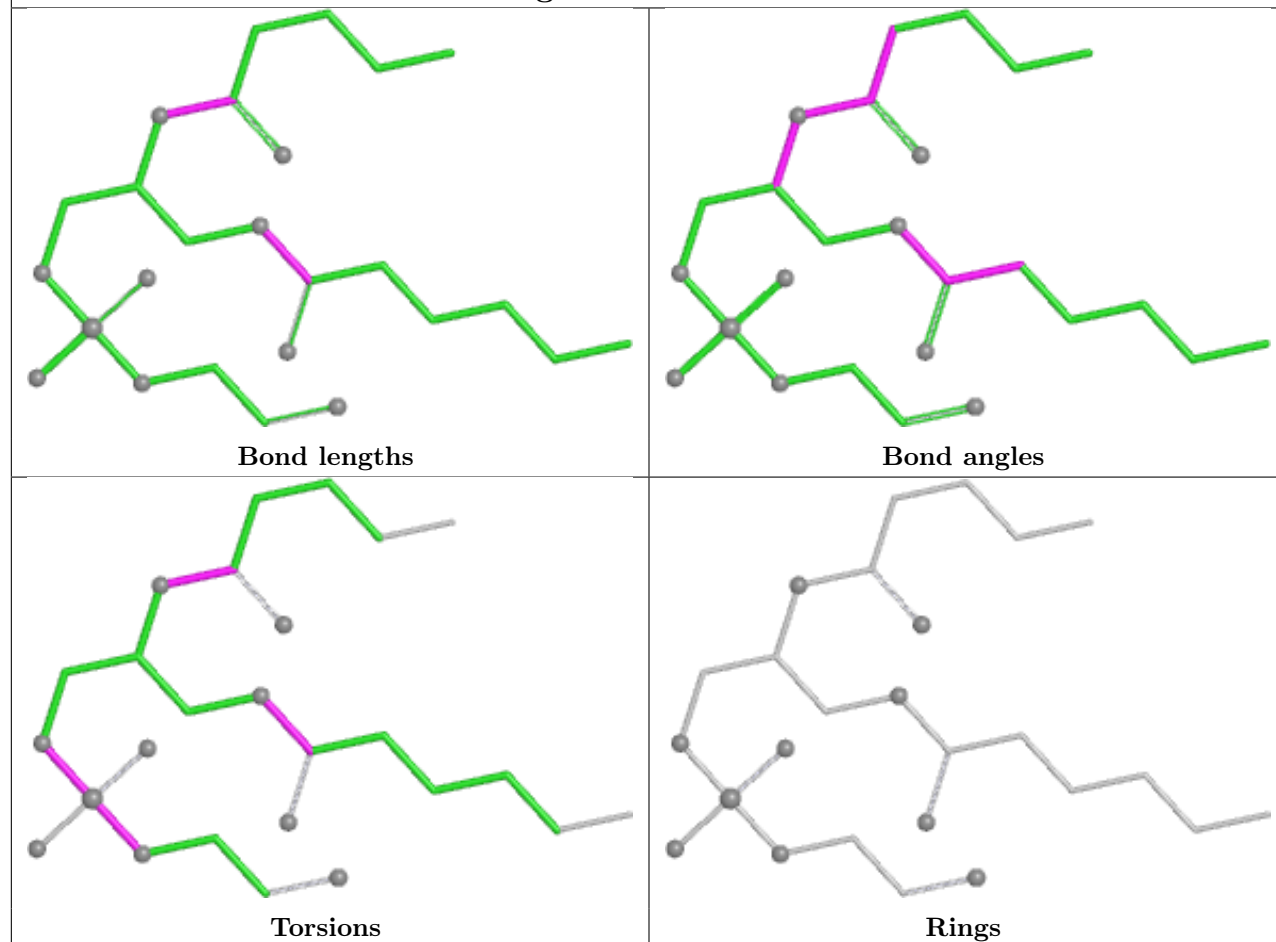




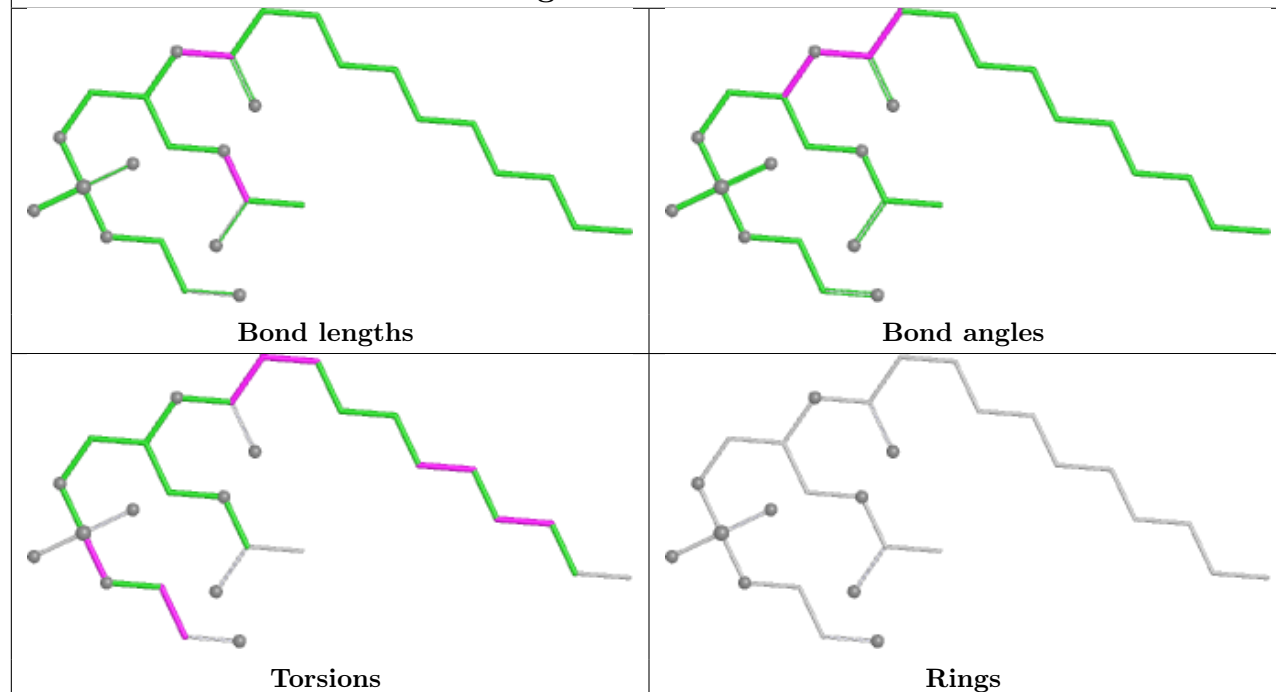


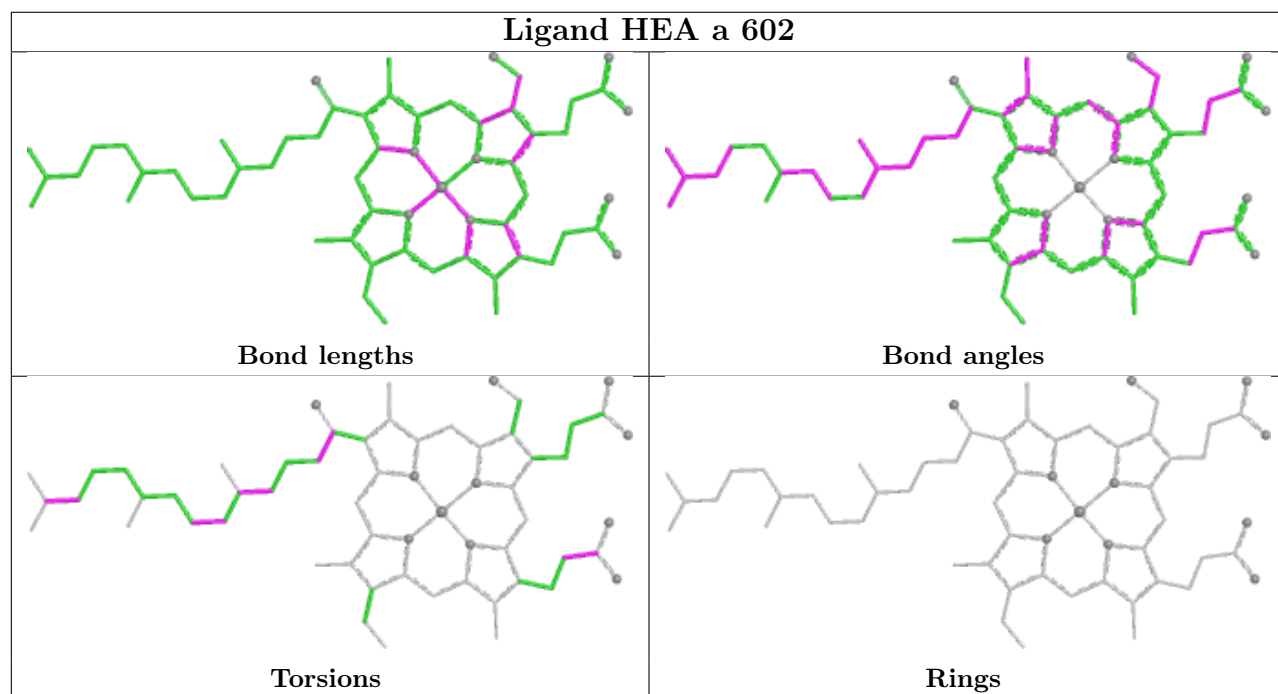
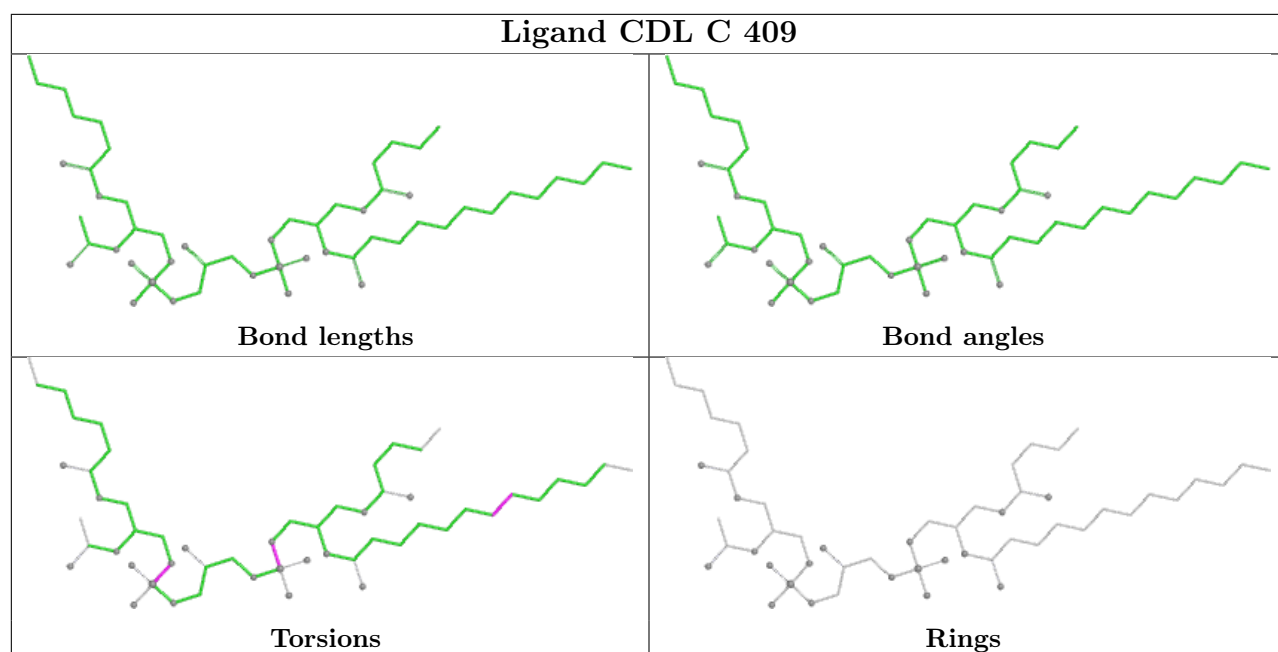


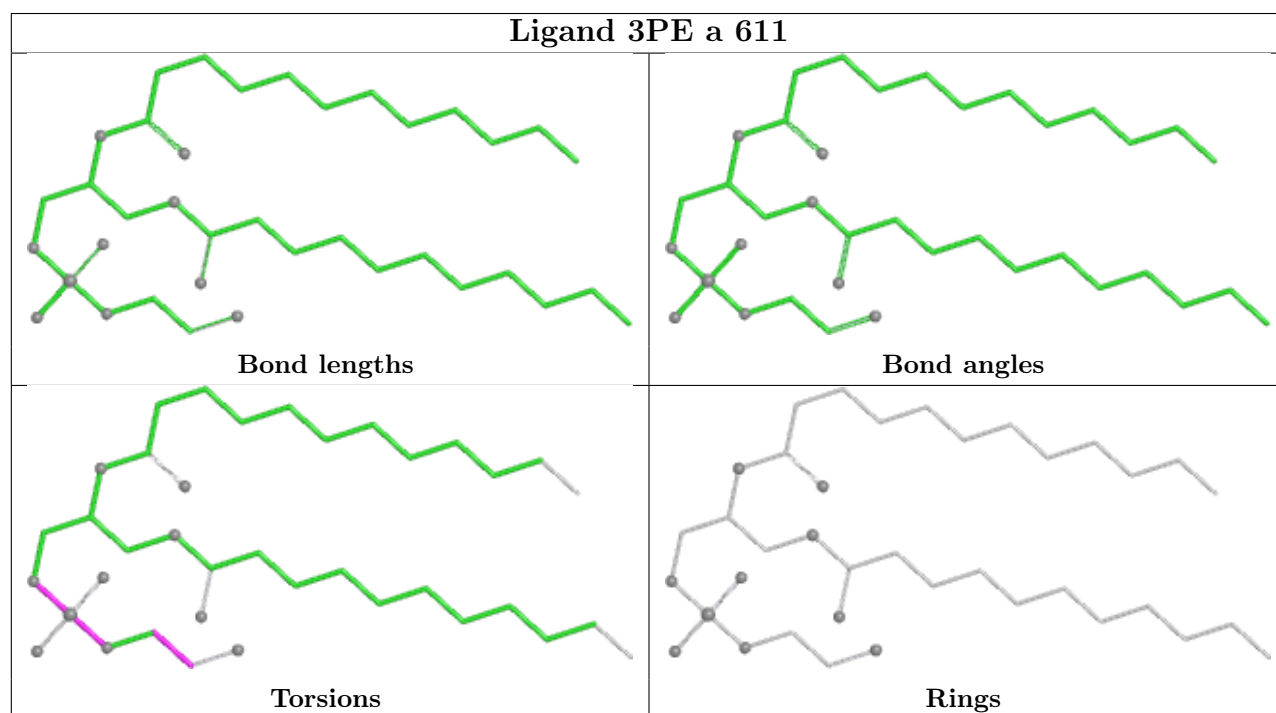
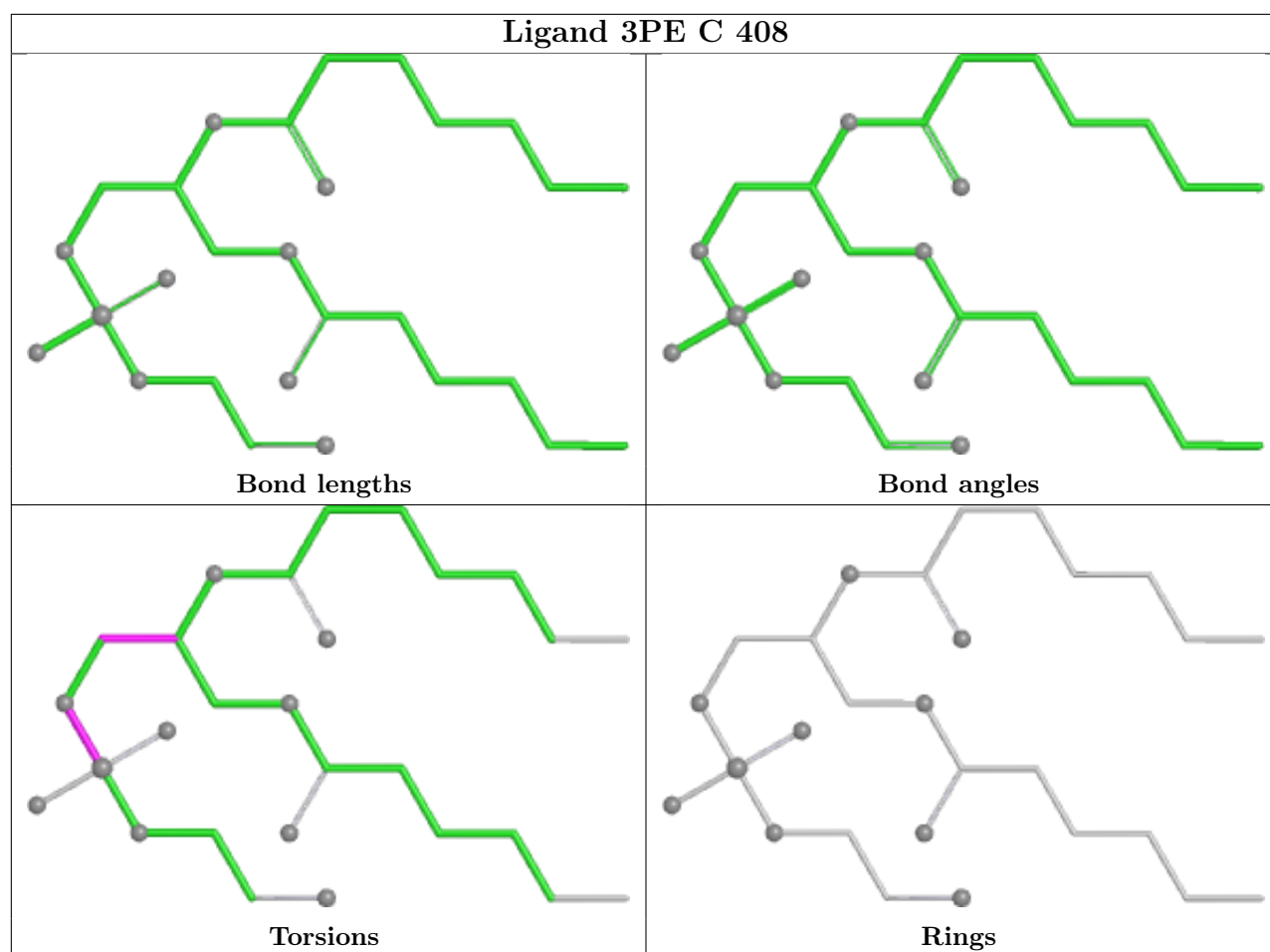
Ligand 3PE O 405

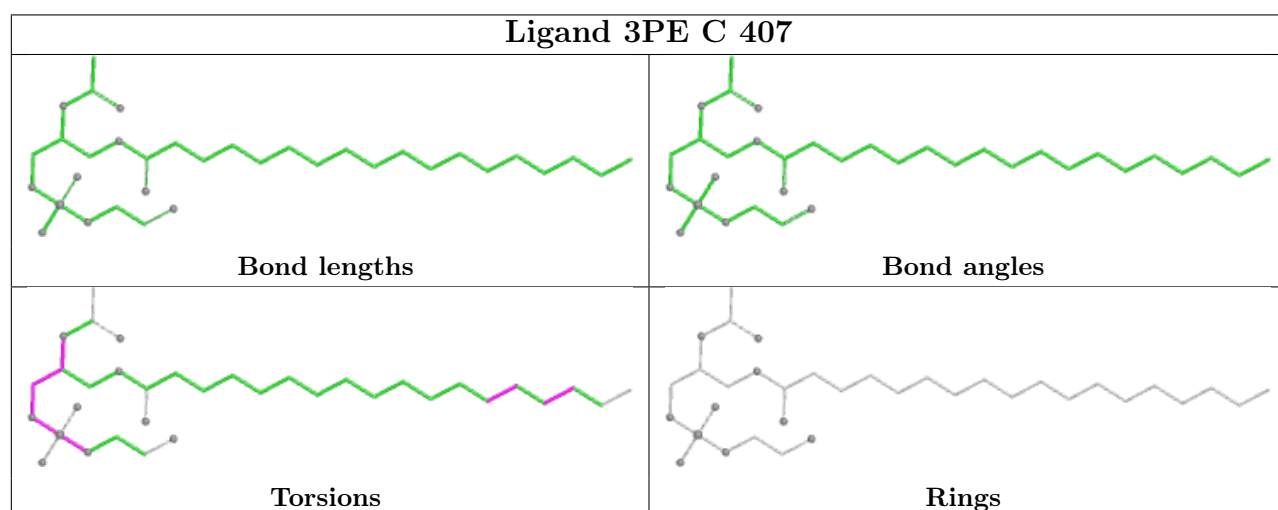
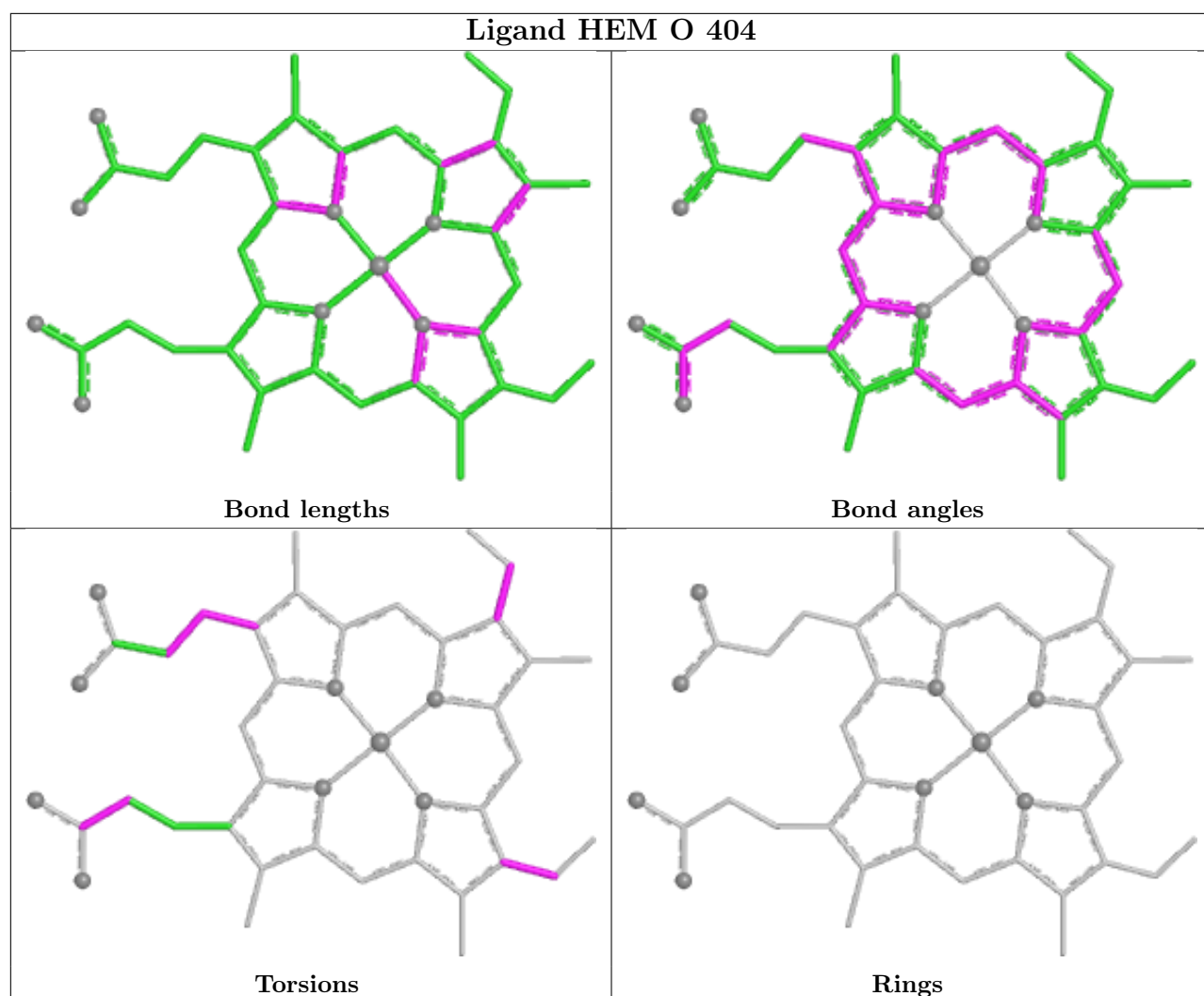


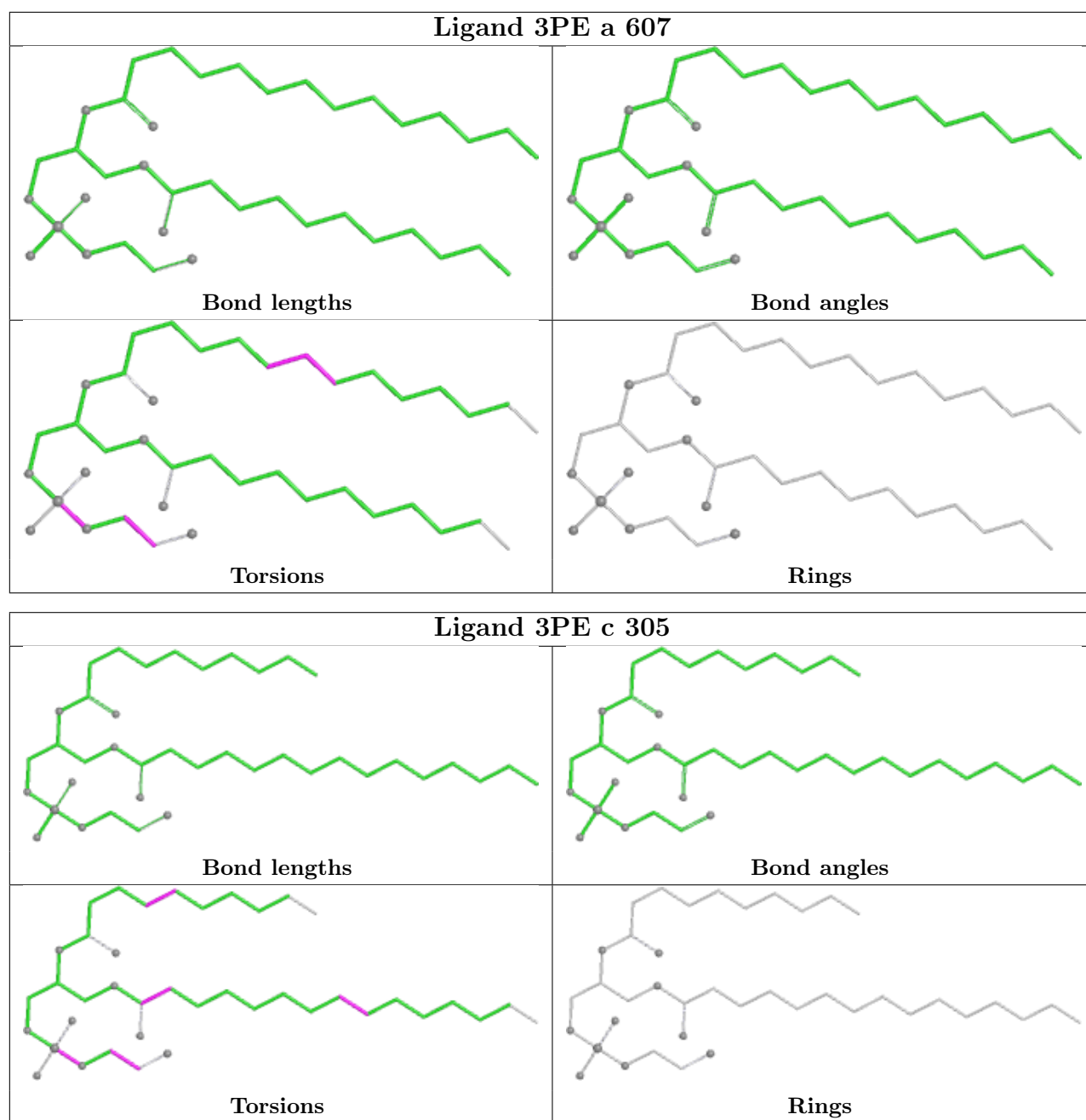
Ligand 3PE P 401

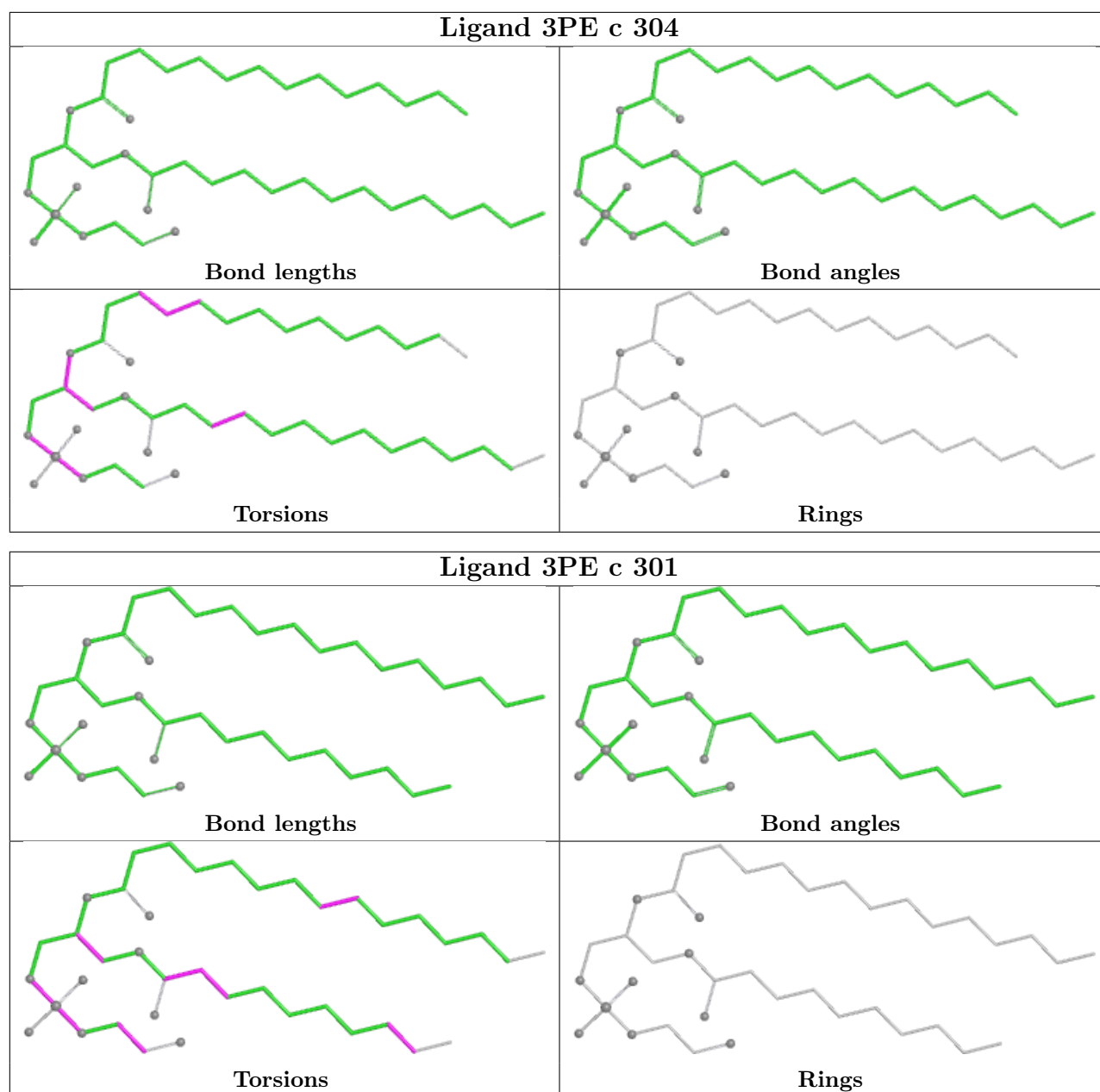


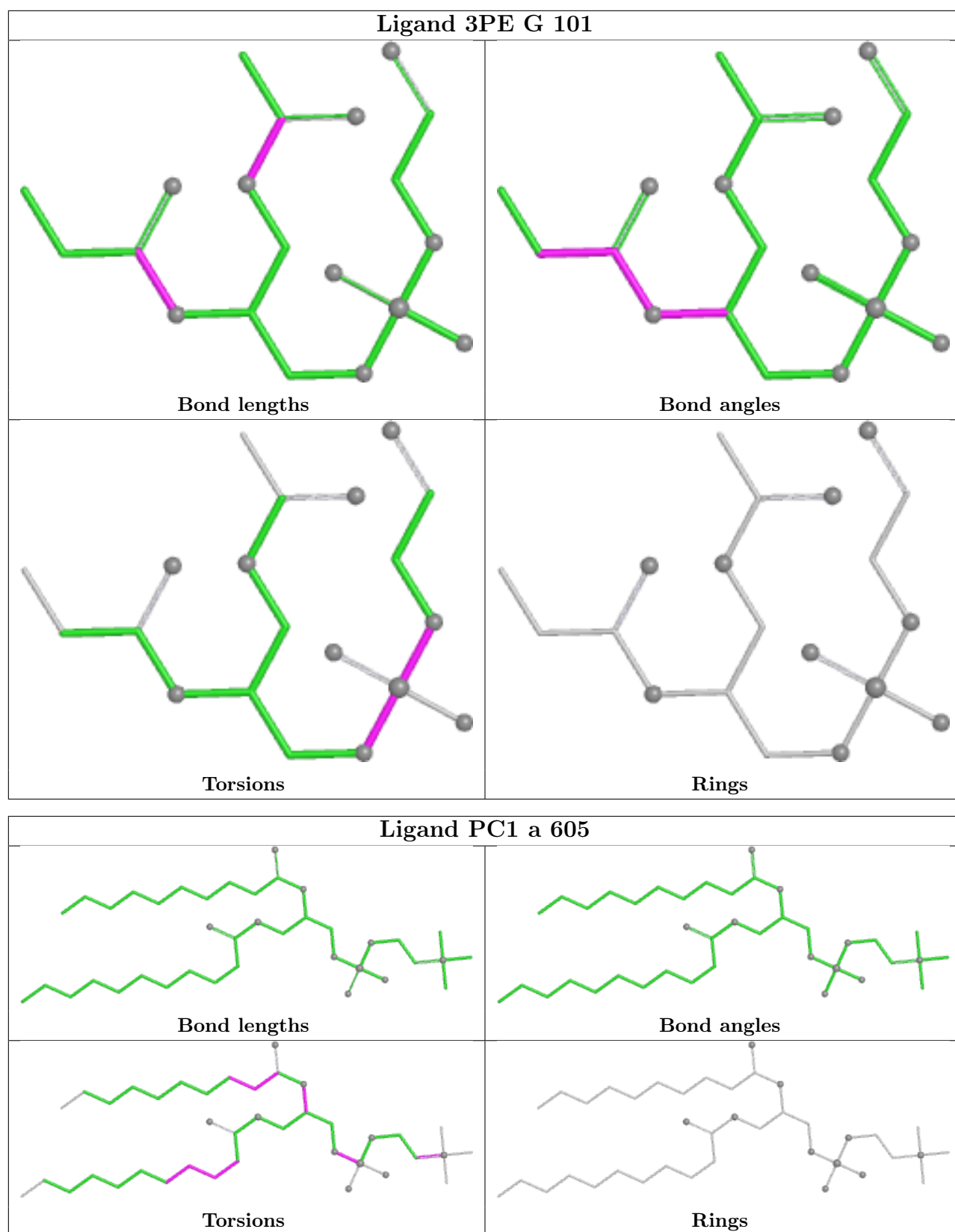


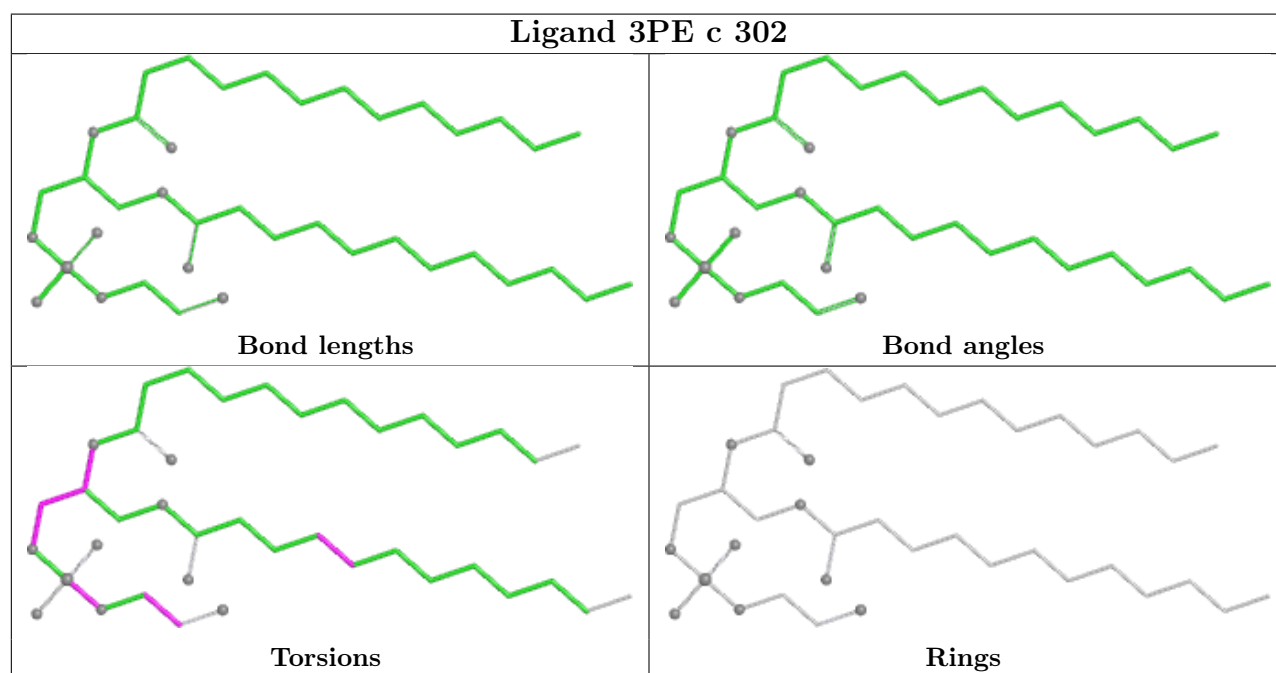
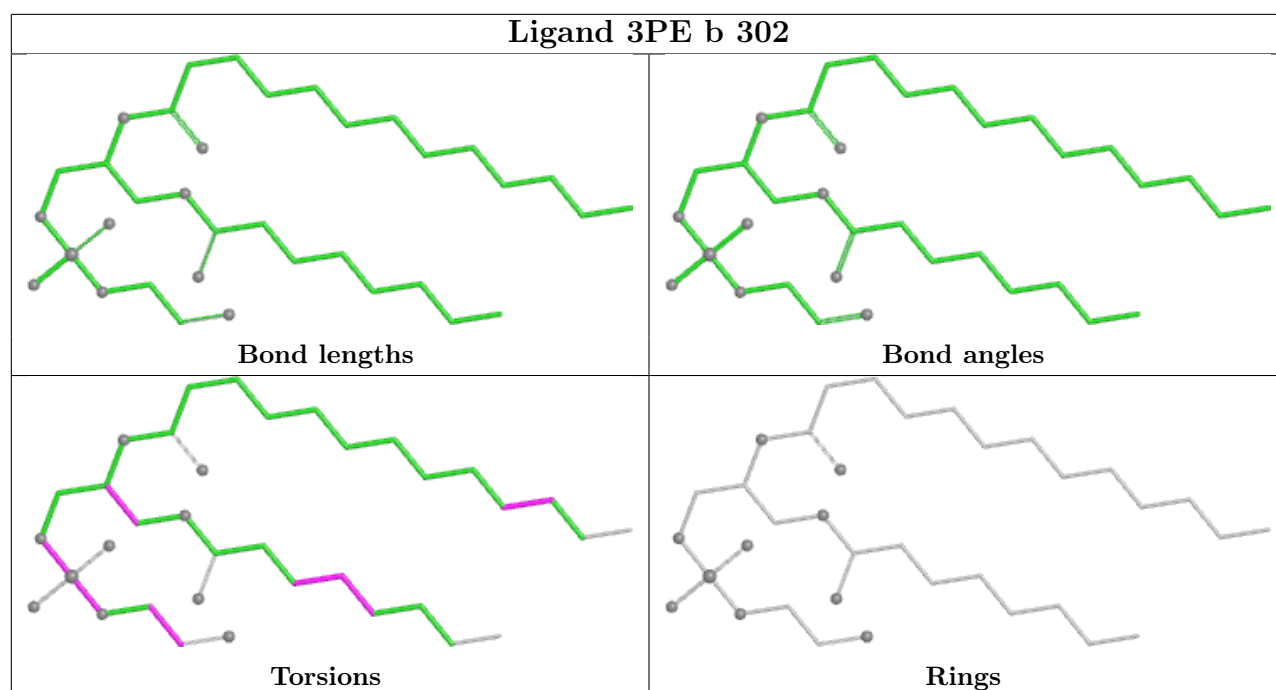


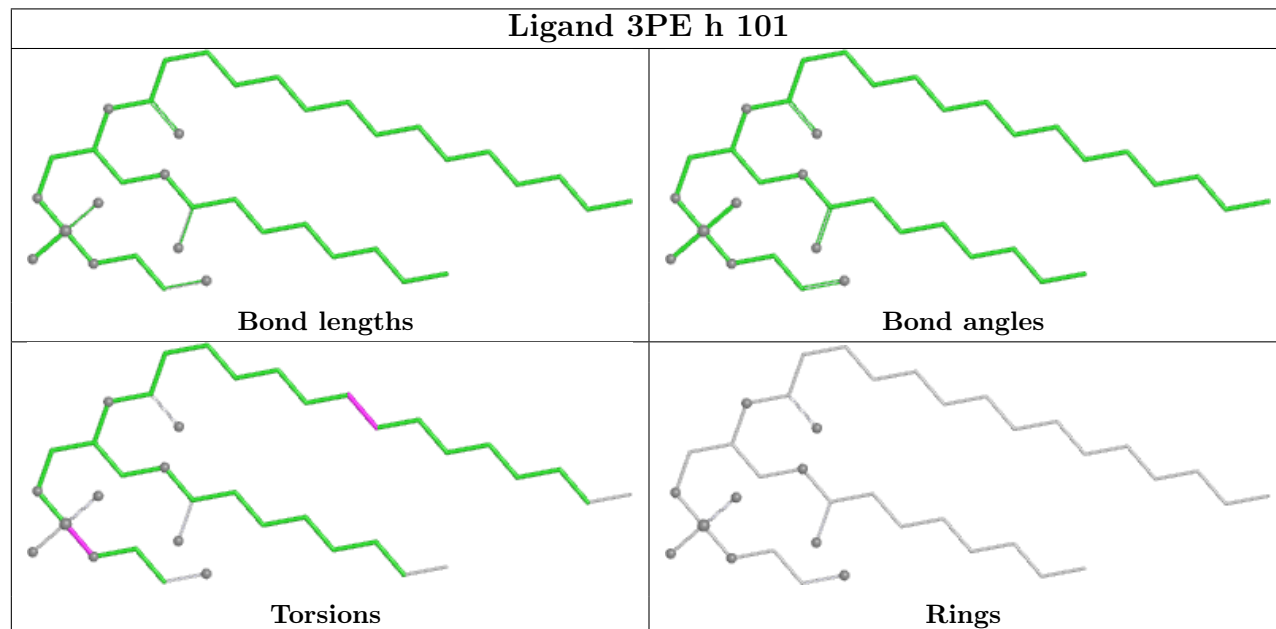
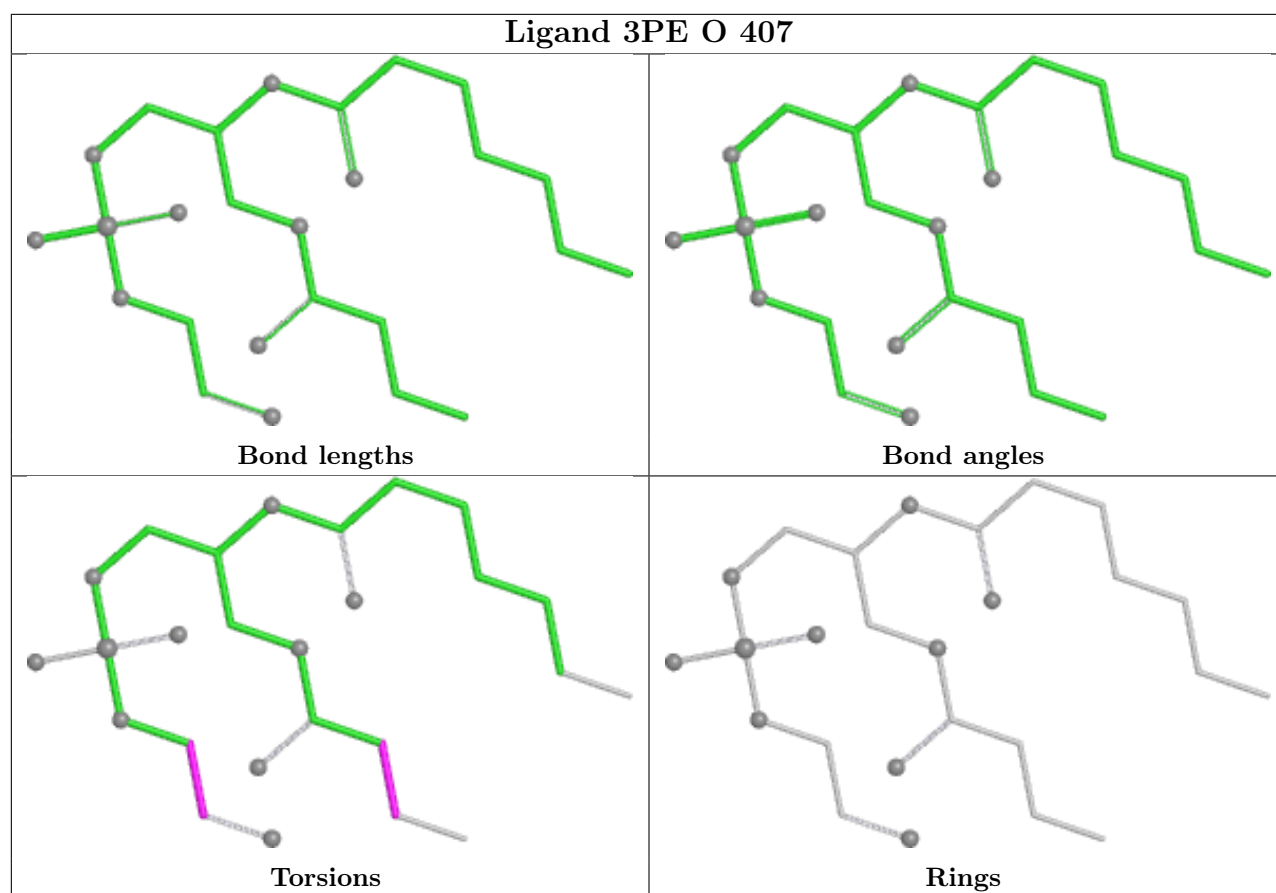


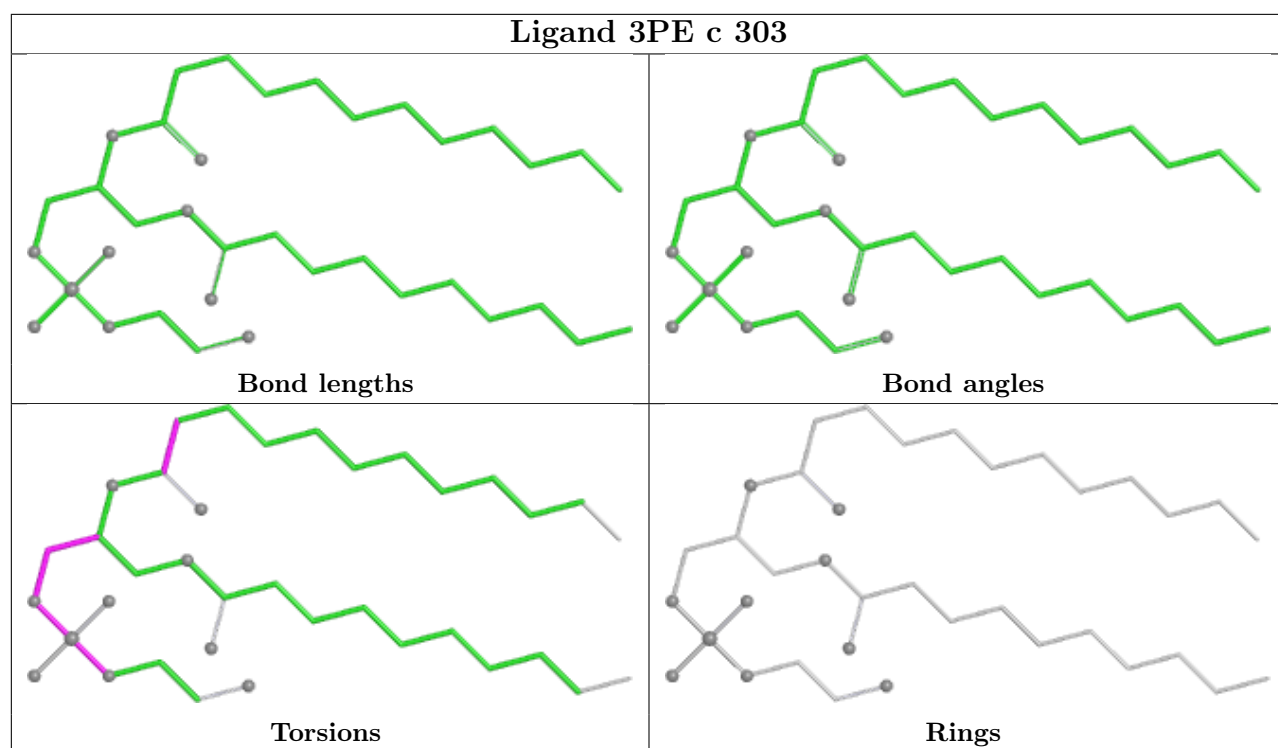


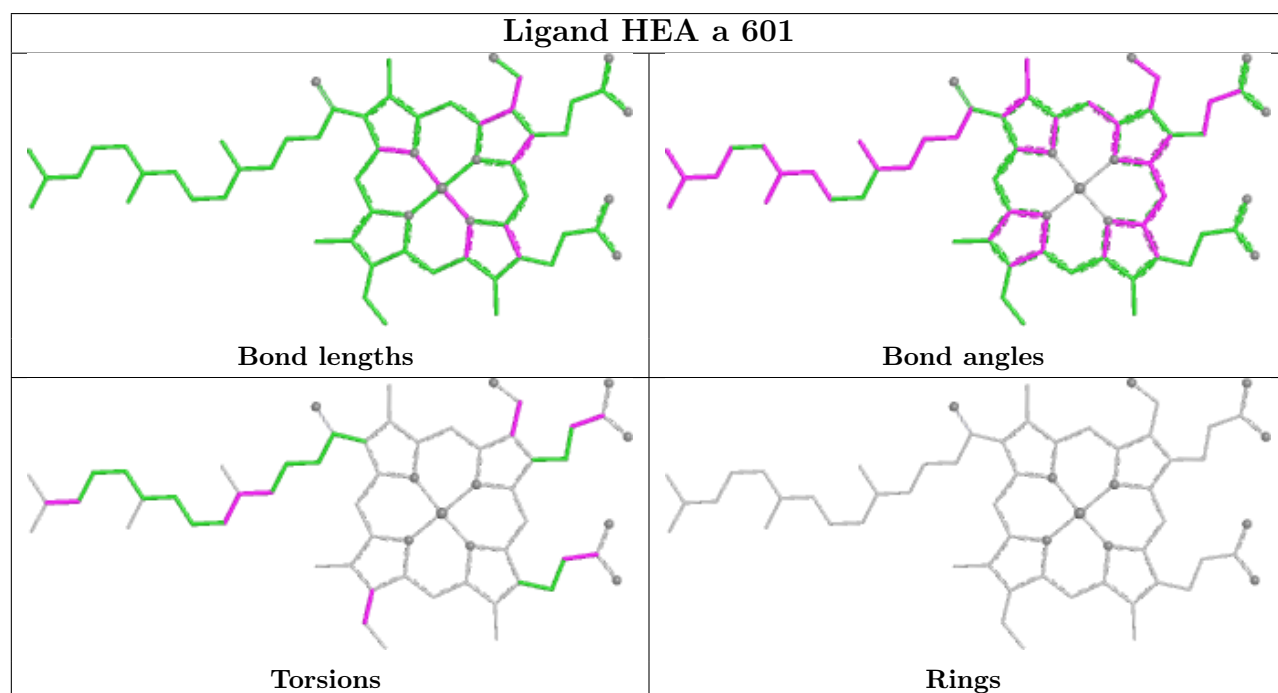
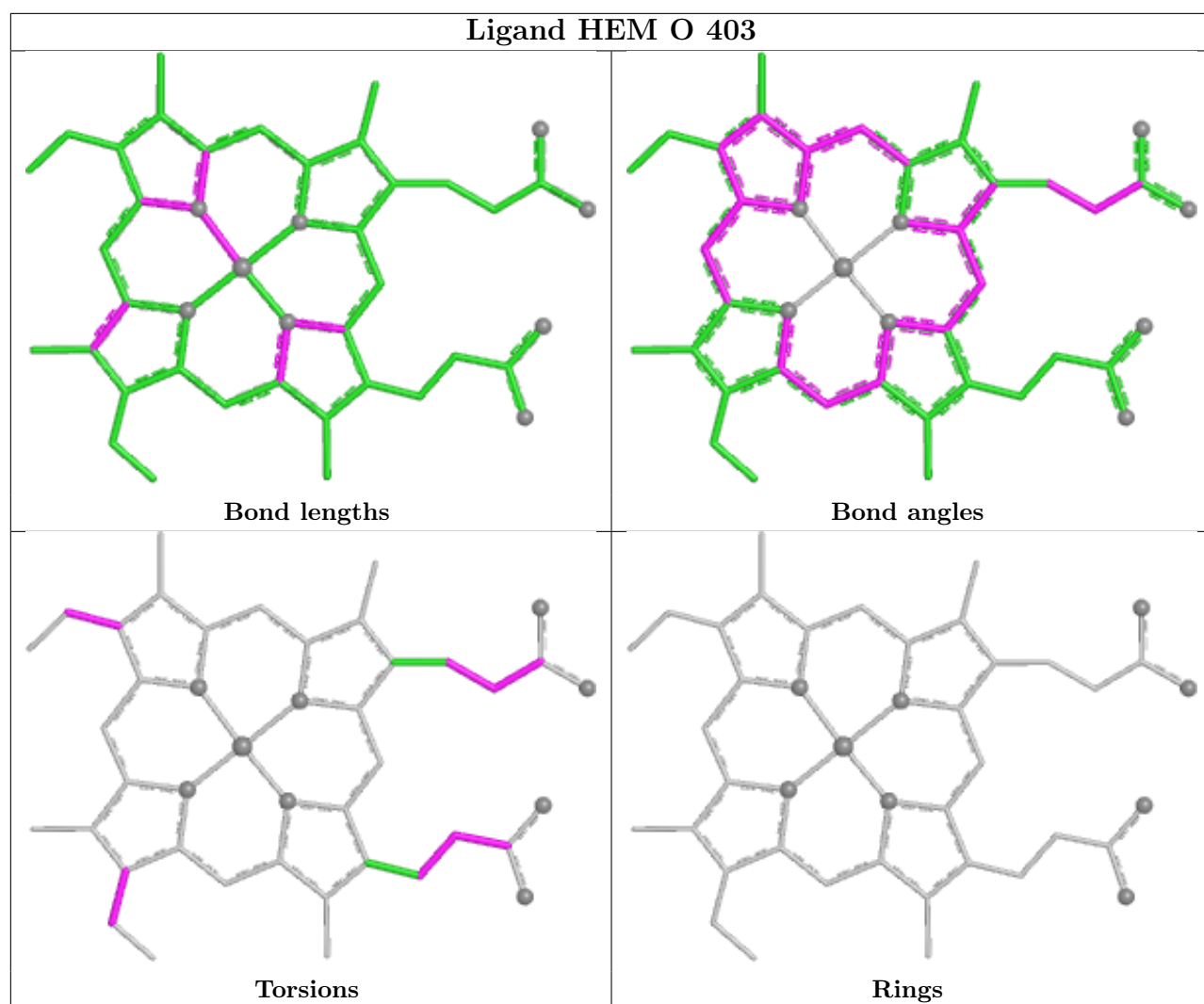


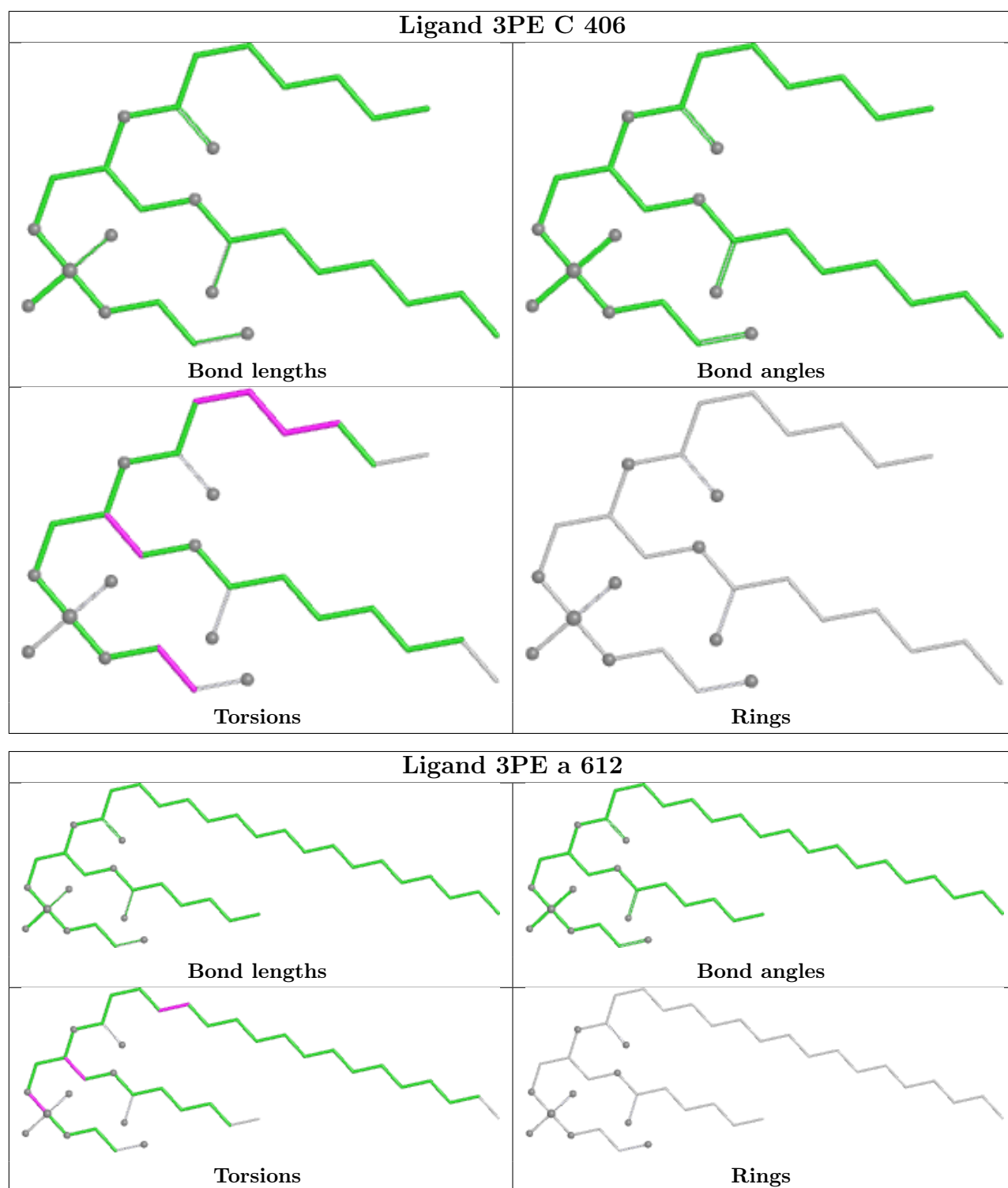


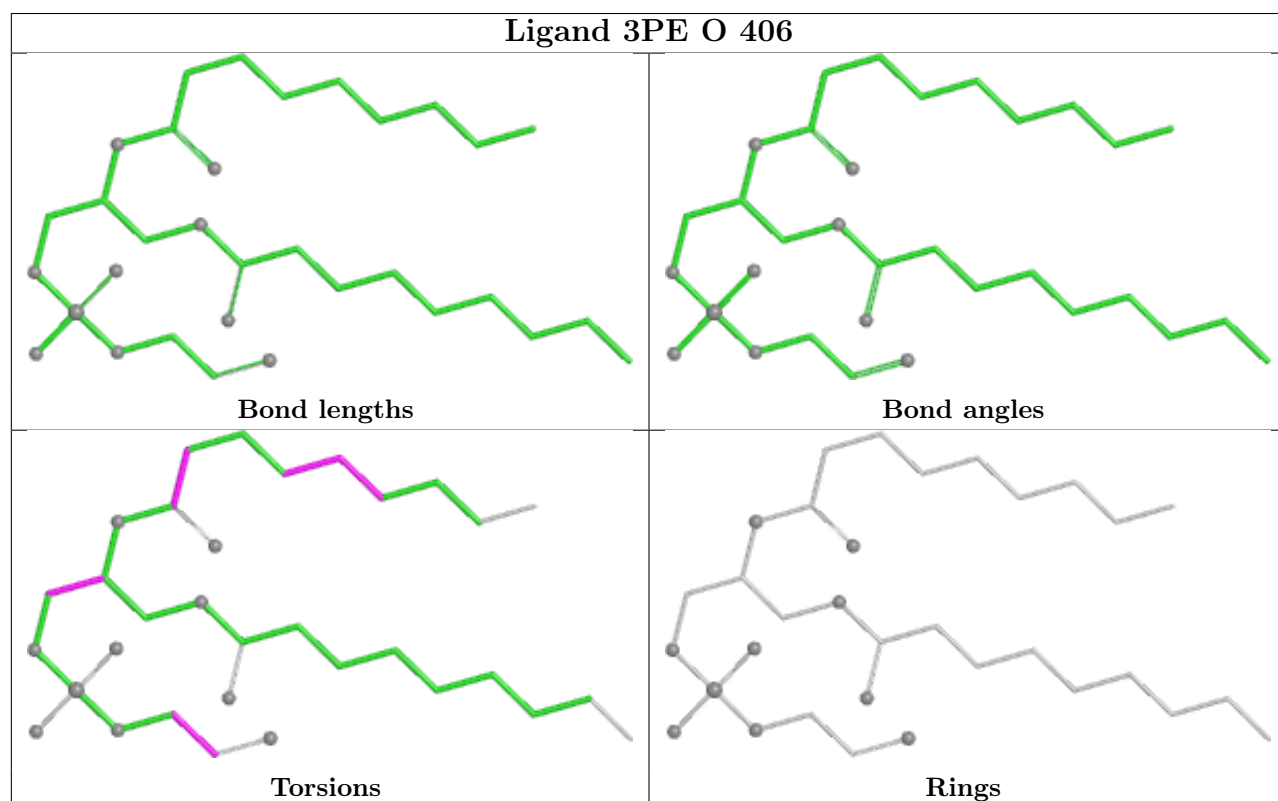
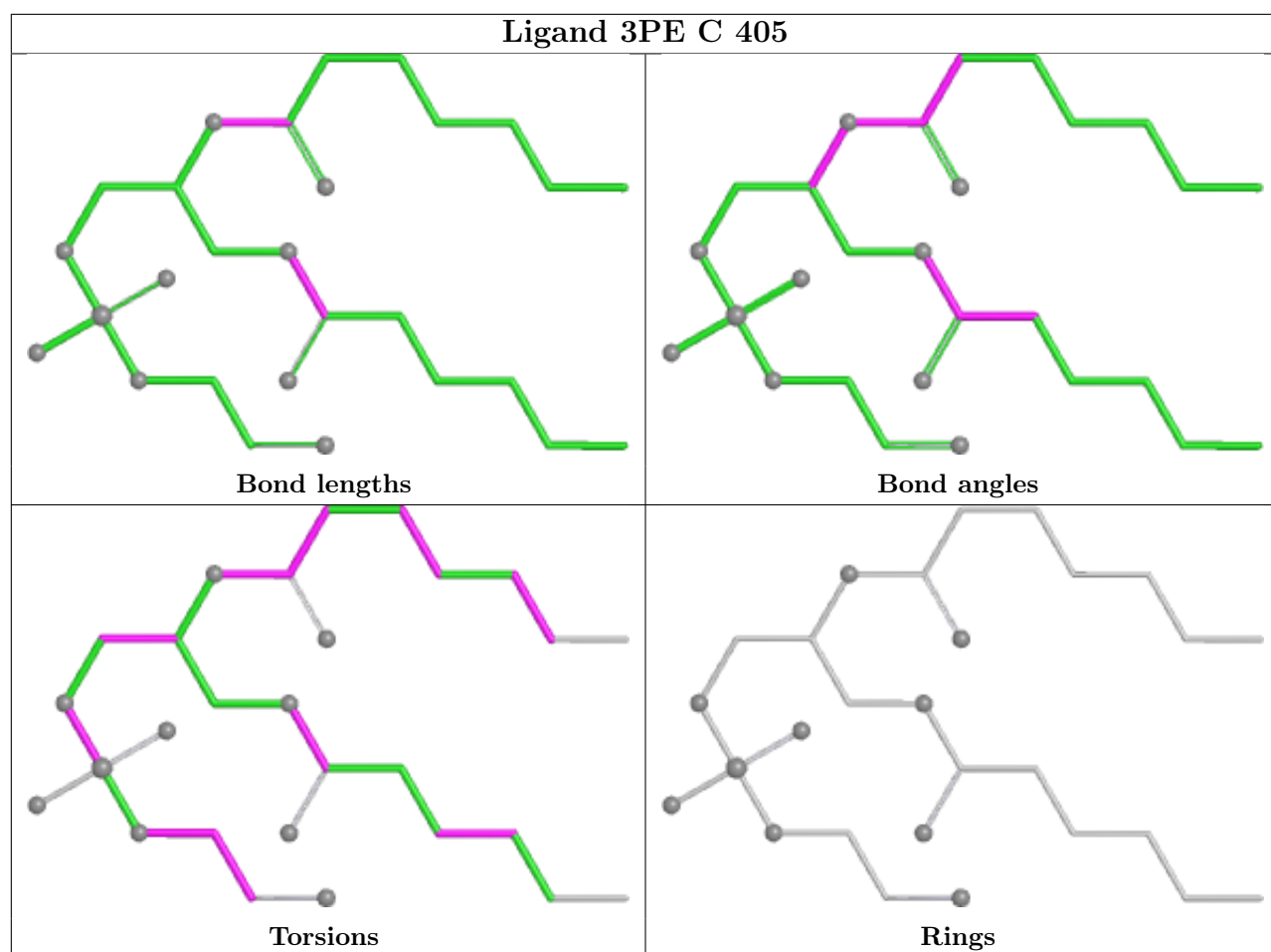


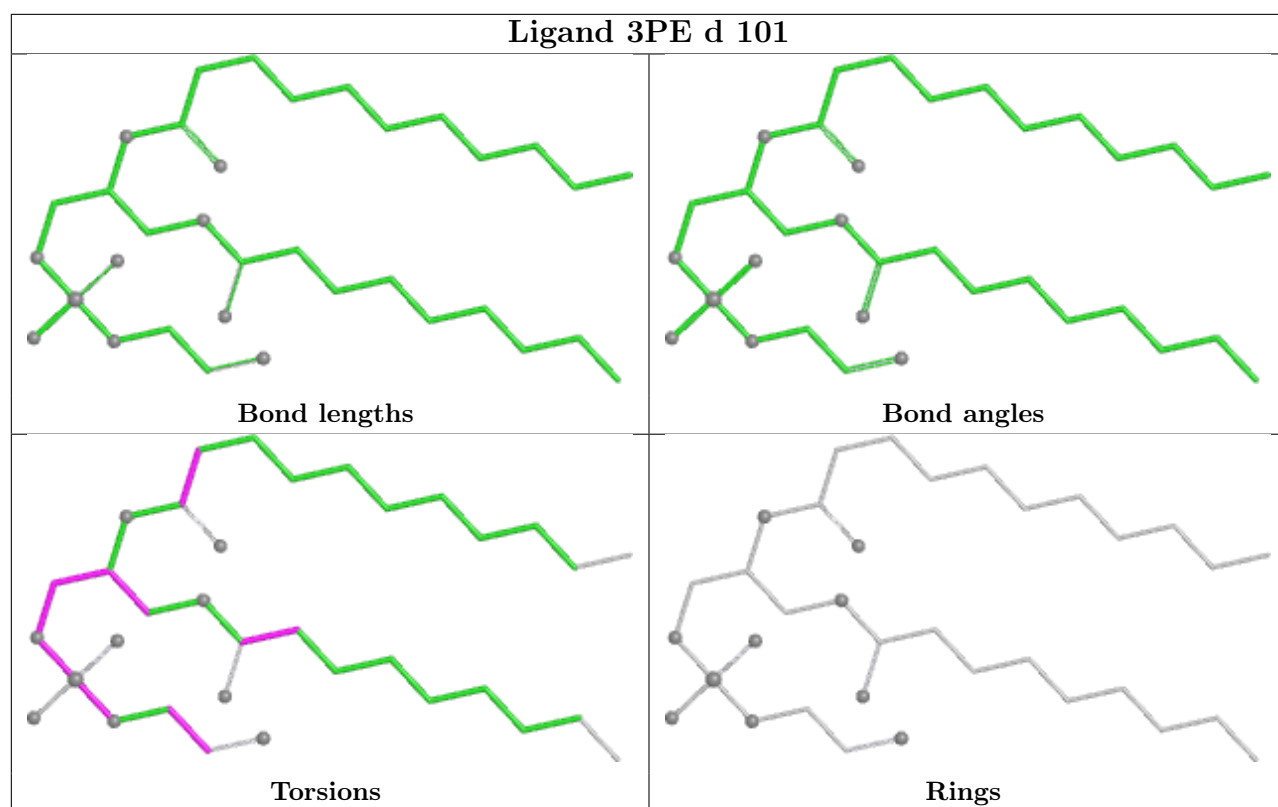


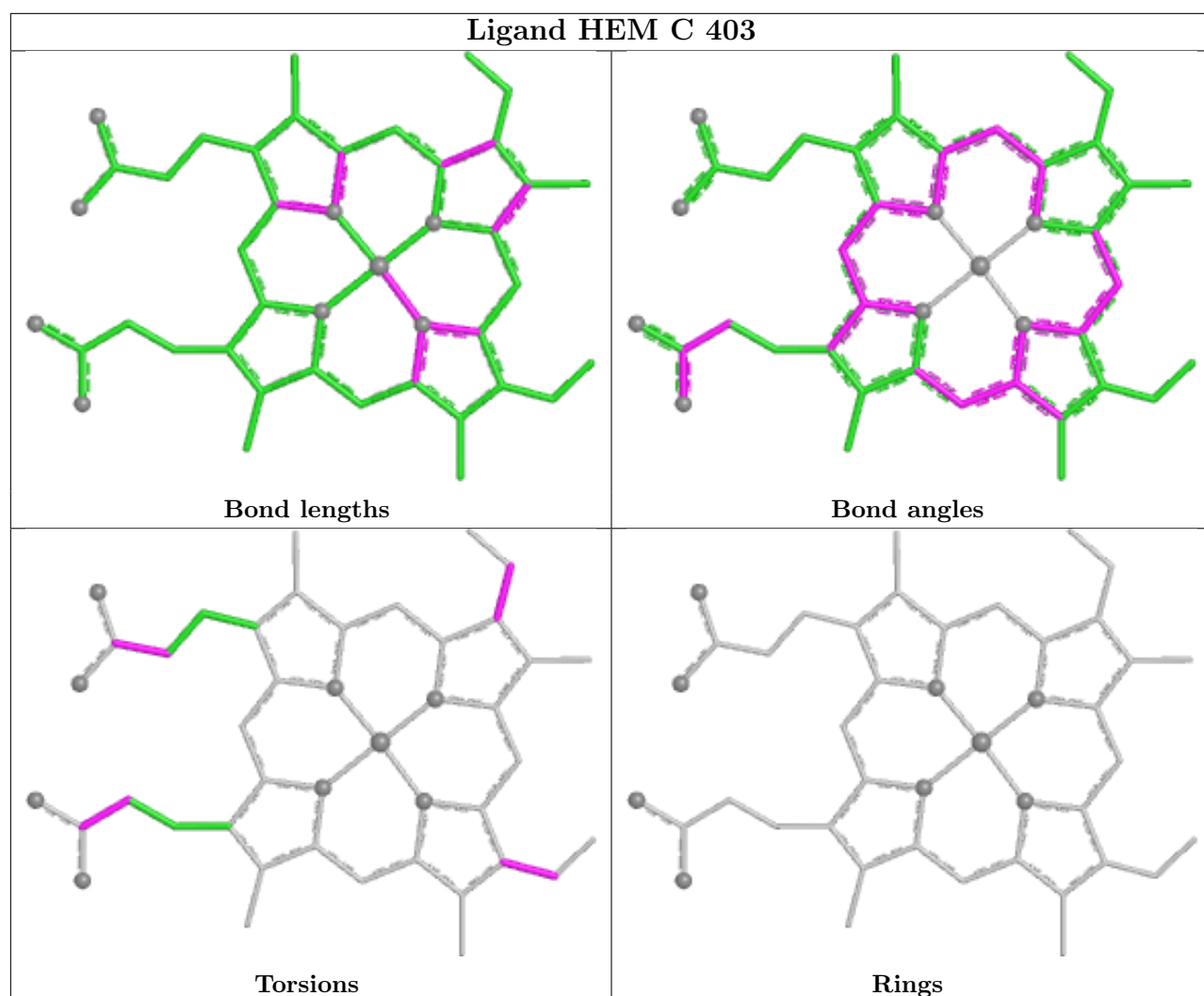












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

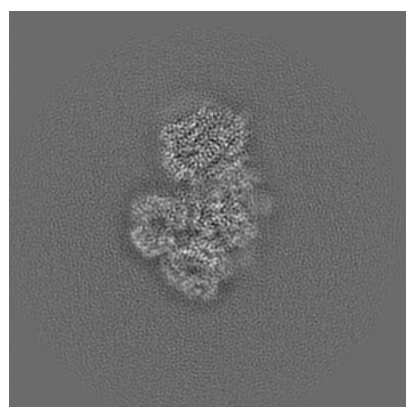
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22448. These allow visual inspection of the internal detail of the map and identification of artifacts.

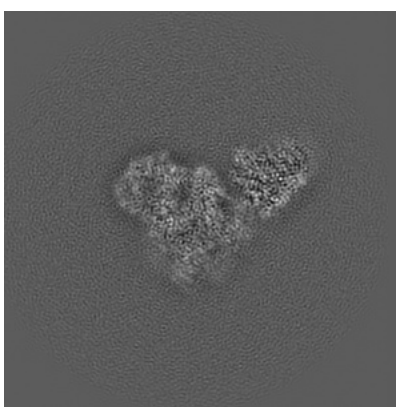
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

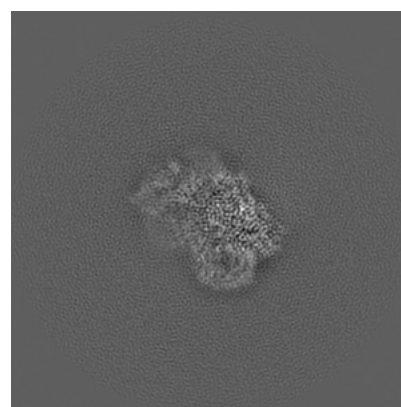
6.1.1 Primary map



X



Y

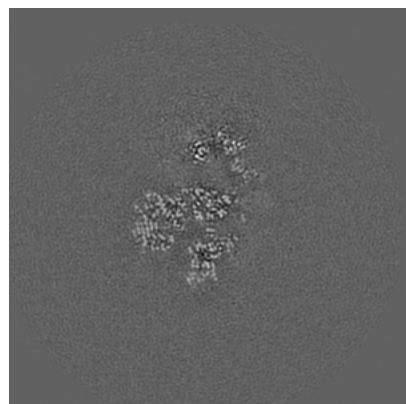


Z

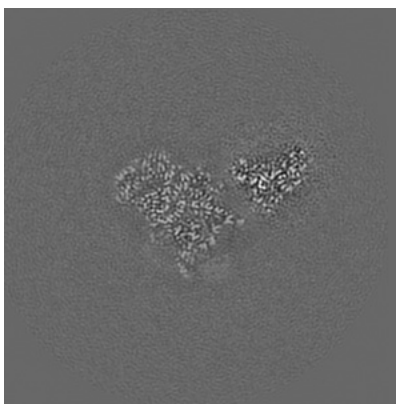
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

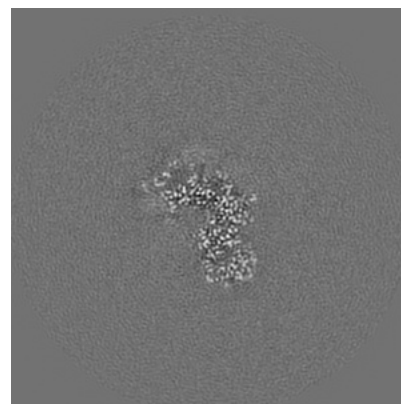
6.2.1 Primary map



X Index: 256



Y Index: 256

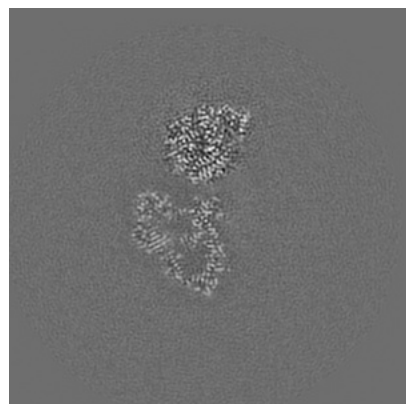


Z Index: 256

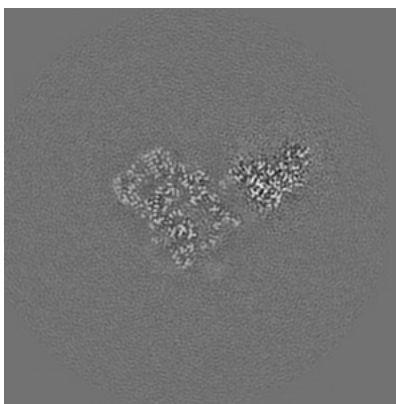
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

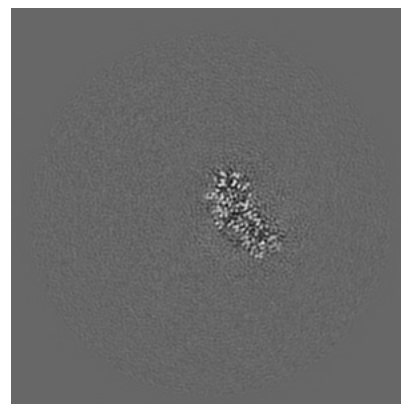
6.3.1 Primary map



X Index: 294



Y Index: 251

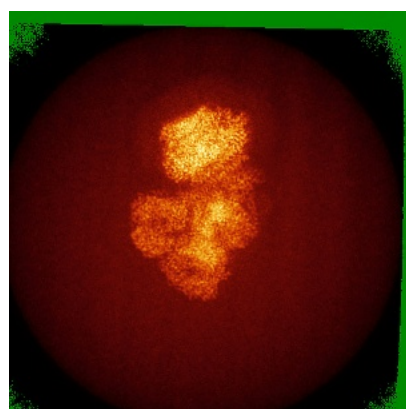


Z Index: 349

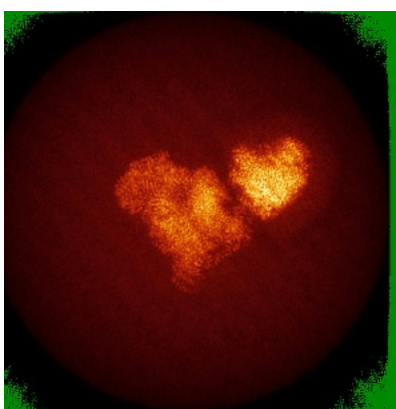
The images above show the largest variance slices of the map in three orthogonal directions.

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

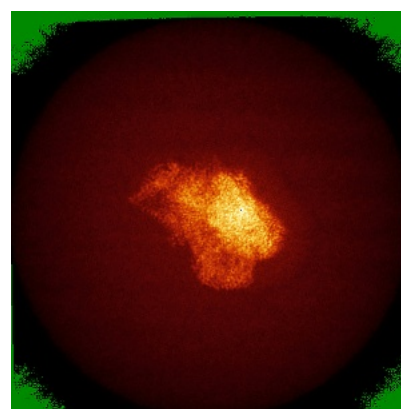
6.4.1 Primary map



X



Y

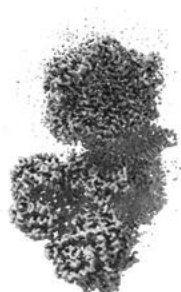


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

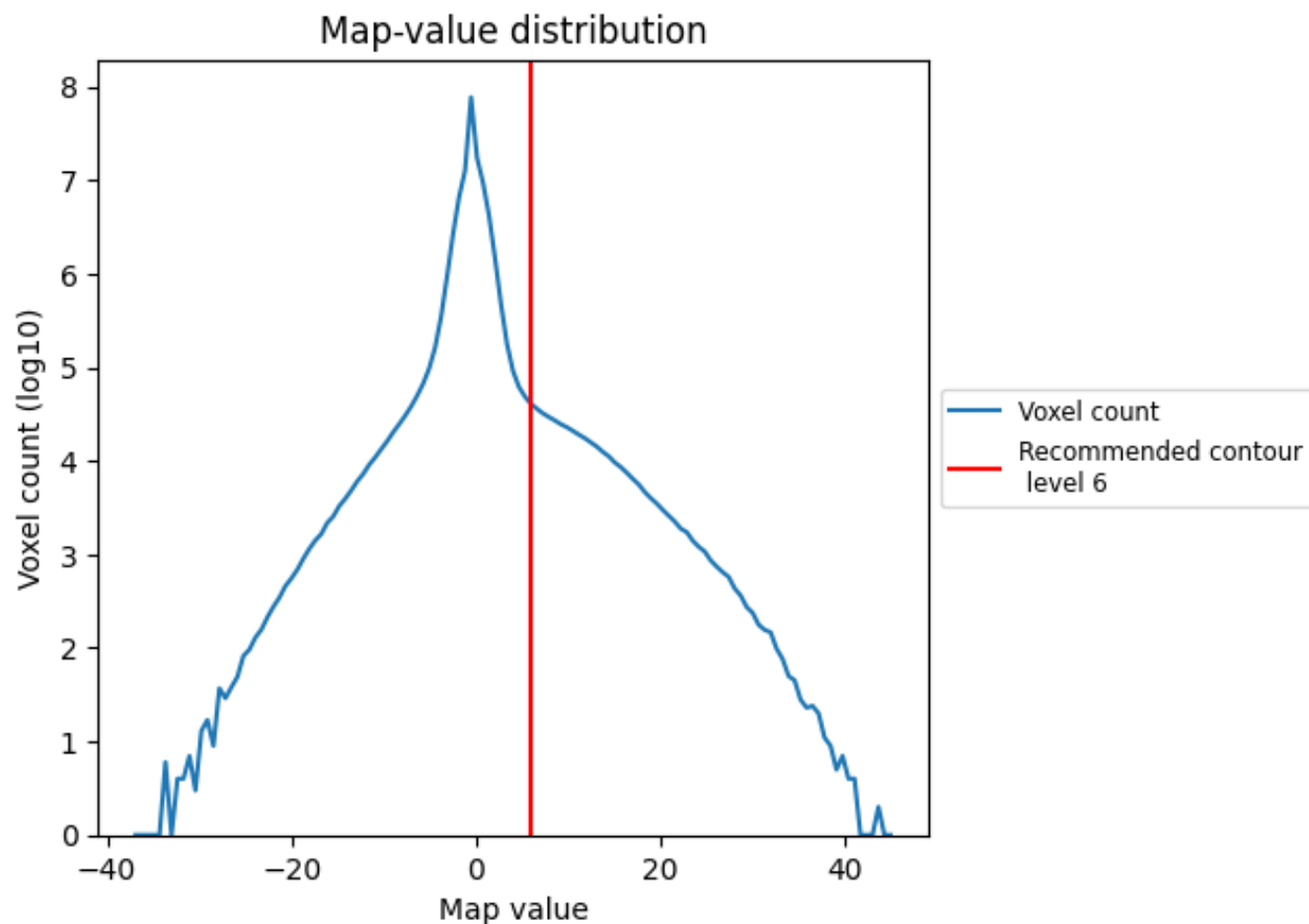
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

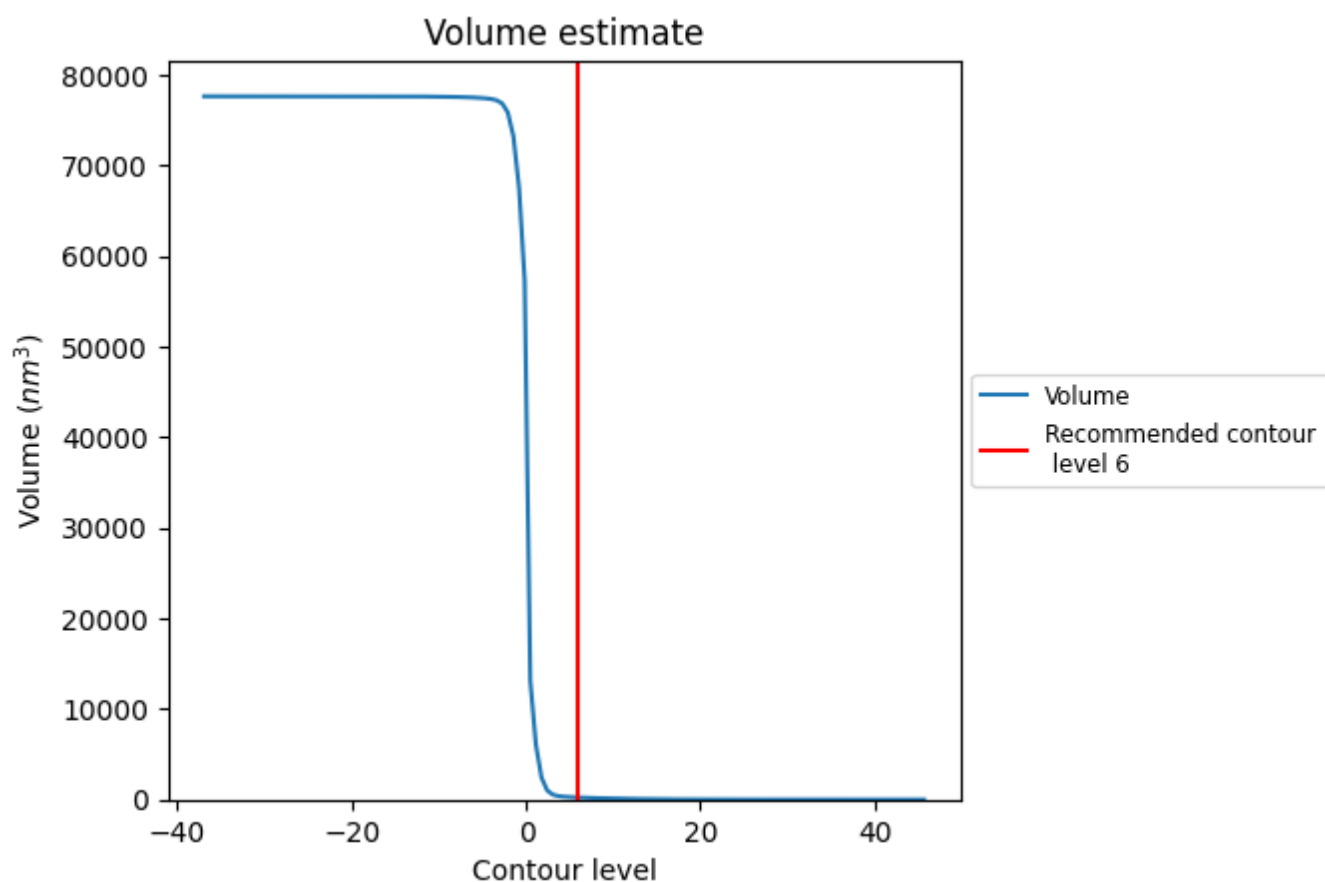
This section contains the results of statistical analysis of the map.

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.

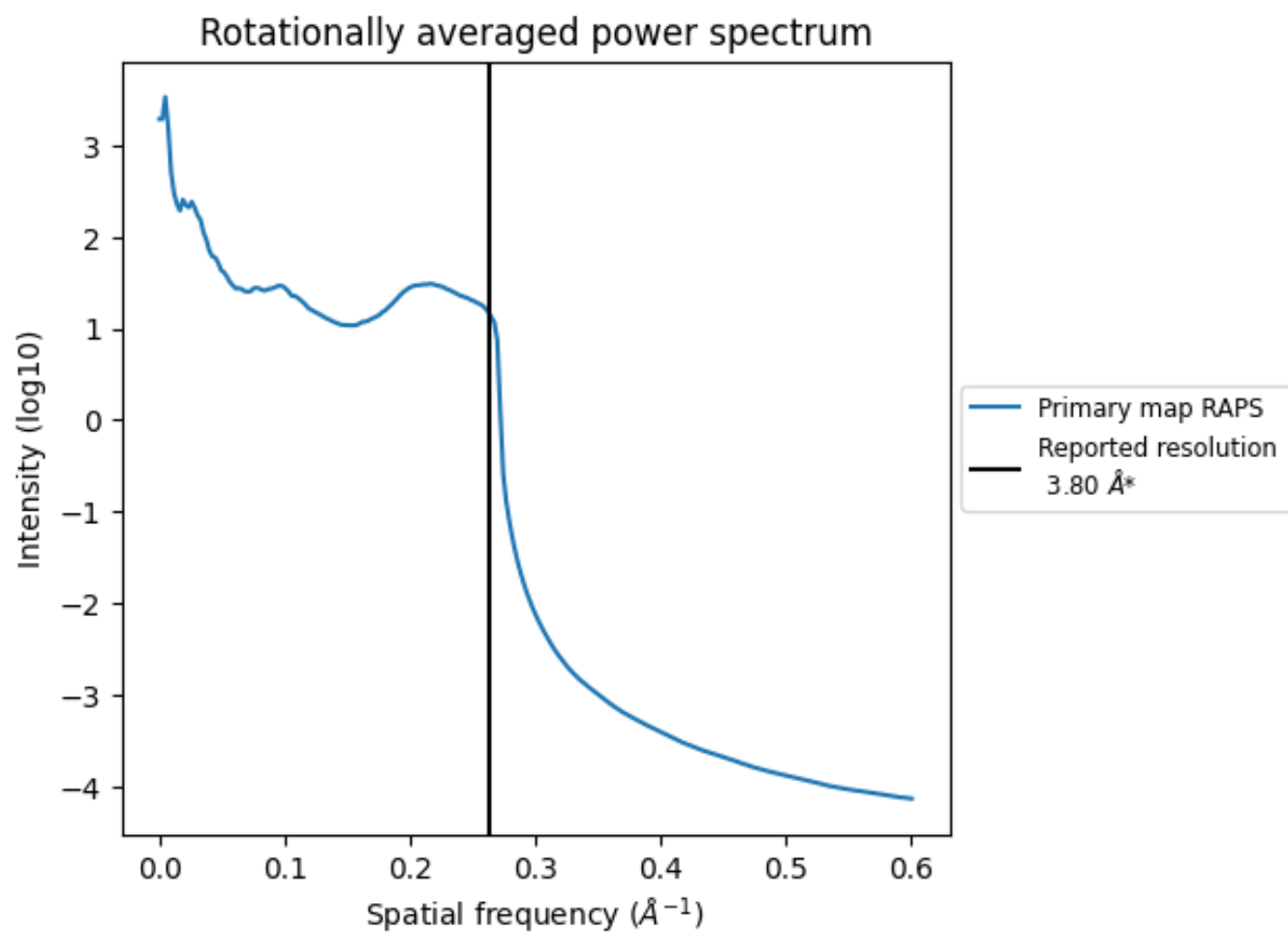
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm^3 ; this corresponds to an approximate mass of 206 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 0.263 Å⁻¹

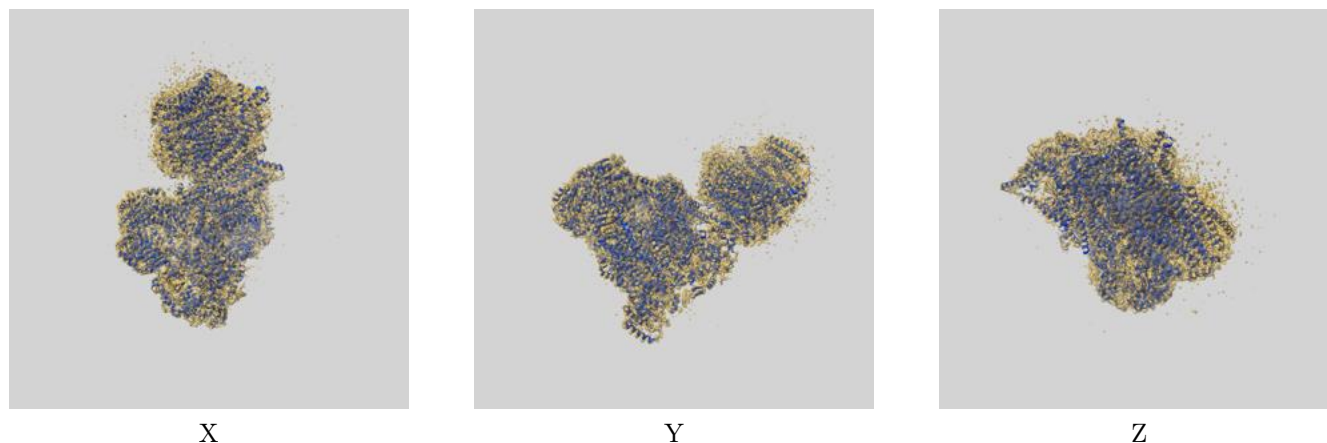
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

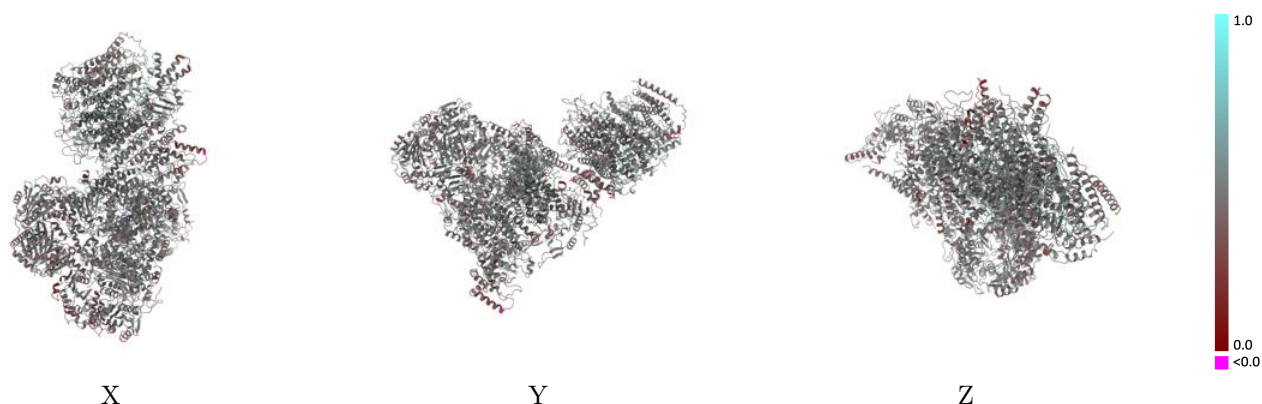
This section contains information regarding the fit between EMDB map EMD-22448 and PDB model 7JRP. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



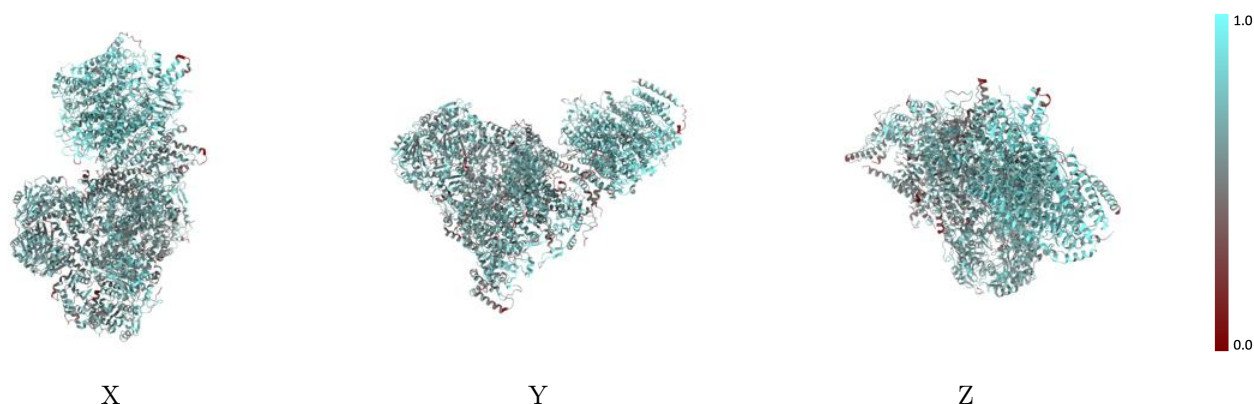
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



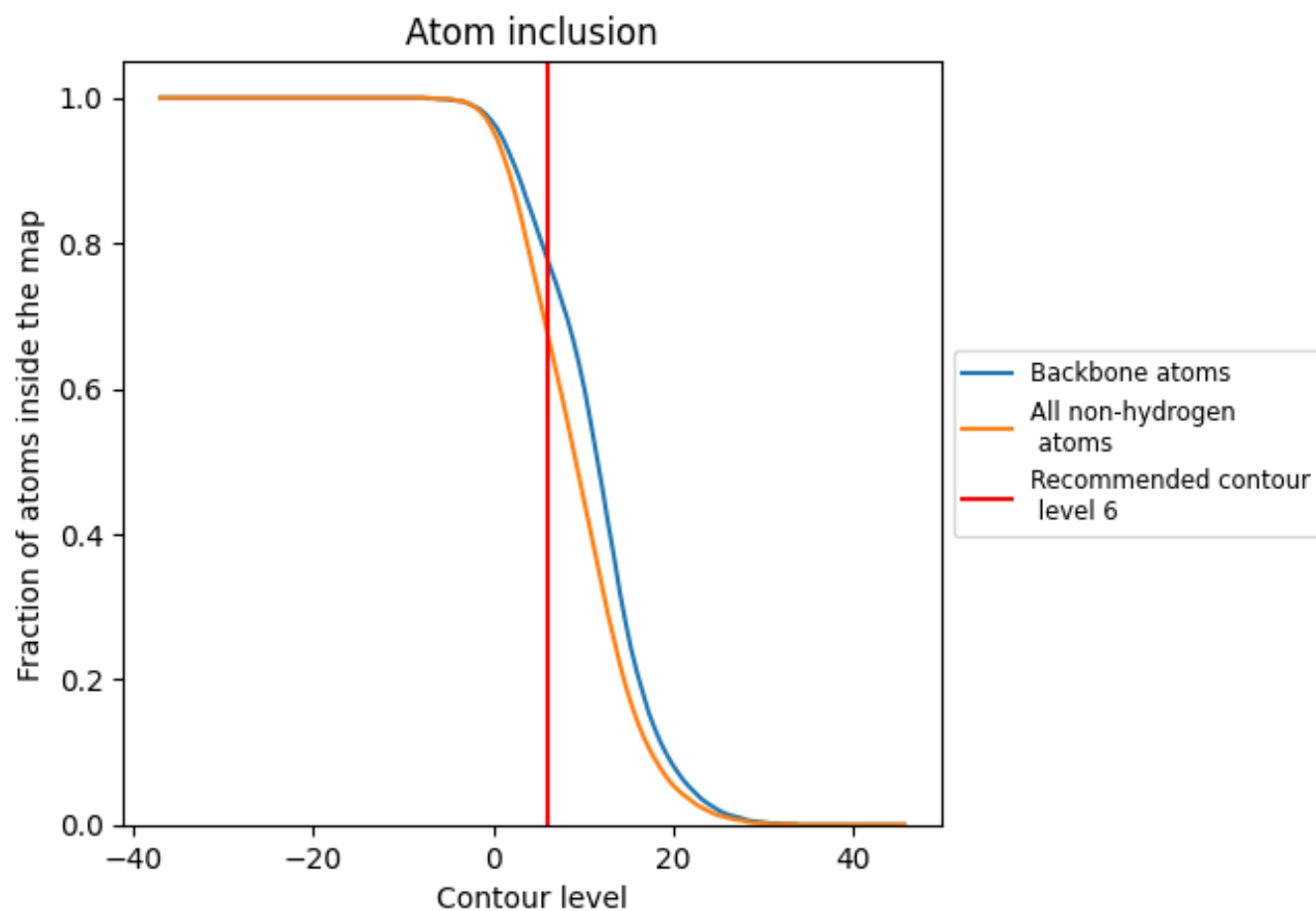
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 68% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.4630
A	 0.6750	 0.4630
B	 0.6150	 0.4340
C	 0.6710	 0.4840
D	 0.6920	 0.4650
E	 0.6020	 0.4600
F	 0.6670	 0.4810
G	 0.5470	 0.4320
H	 0.4820	 0.3410
J	 0.5520	 0.4310
K	 0.4720	 0.3930
M	 0.6630	 0.4590
N	 0.6200	 0.4380
O	 0.6980	 0.4870
P	 0.6670	 0.4690
Q	 0.6000	 0.4640
R	 0.6690	 0.4740
S	 0.5660	 0.4600
T	 0.5000	 0.3520
V	 0.5510	 0.4110
W	 0.3480	 0.3550
a	 0.7970	 0.4960
b	 0.7670	 0.4900
c	 0.7920	 0.4890
d	 0.7210	 0.4550
e	 0.7490	 0.4440
f	 0.6790	 0.4400
g	 0.7650	 0.4530
h	 0.6820	 0.4370
i	 0.7530	 0.4730
j	 0.7500	 0.4690

