



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:34 PM UTC

PDB ID : 7PQD / pdb_00007pqd
EMDB ID : EMD-13590
Title : Cryo-EM structure of the dimeric Rhodobacter sphaeroides RC-LH1 core complex at 2.9 Å: the structural basis for dimerisation
Authors : Qian, P.; Hunter, C.N.
Deposited on : 2021-09-17
Resolution : 2.90 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

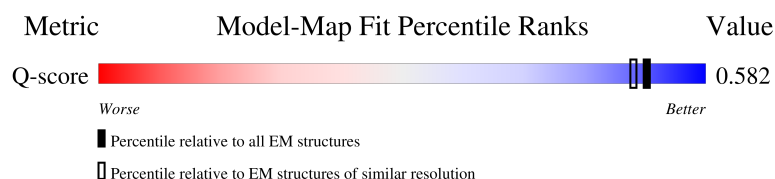
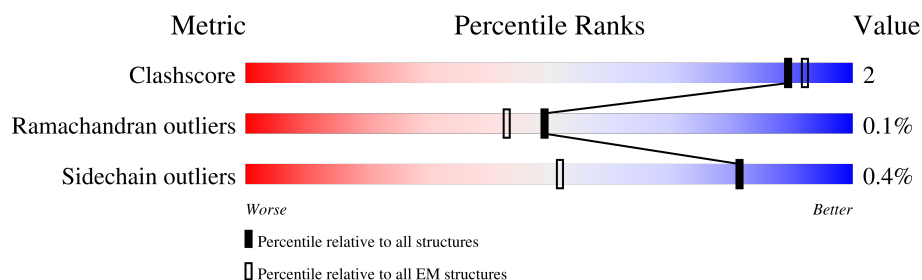
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



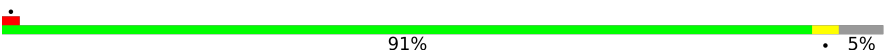
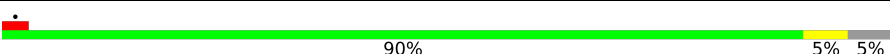
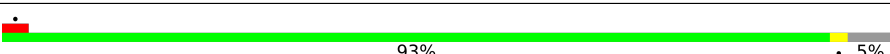
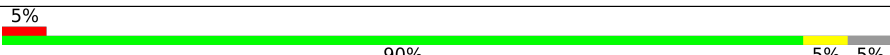
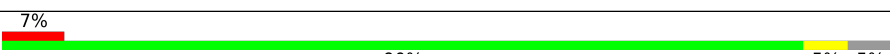
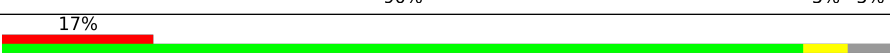
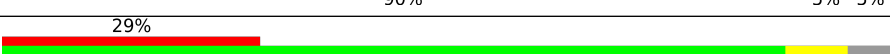
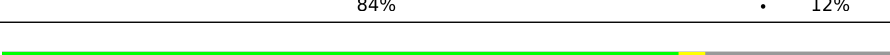
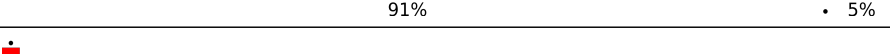
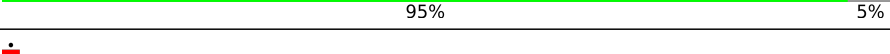
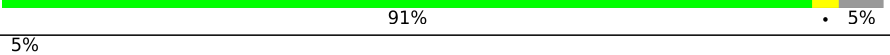
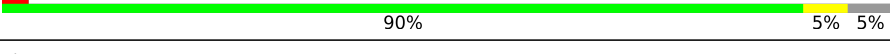
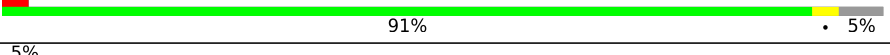
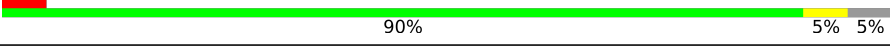
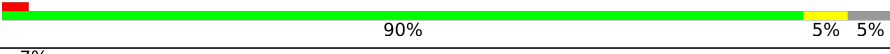
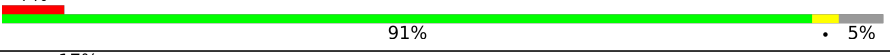
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	AA	58	 72% 7% 21%
1	AB	58	 91% 5%
1	AC	58	 95% 5%
1	AD	58	 90% 5% 5%

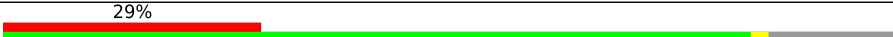
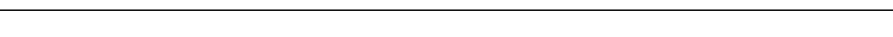
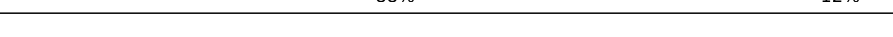
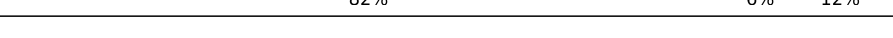
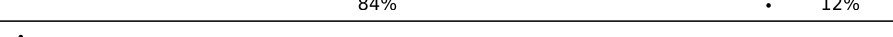
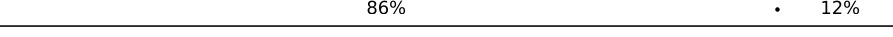
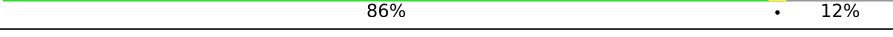
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Mol	Chain	Length	Quality of chain
1	AE	58	
1	AF	58	
1	AG	58	
1	AH	58	
1	AI	58	
1	AJ	58	
1	AK	58	
1	AL	58	
1	AM	58	
1	AN	58	
1	aa	58	
1	ab	58	
1	ac	58	
1	ad	58	
1	ae	58	
1	af	58	
1	ag	58	
1	ah	58	
1	ai	58	
1	aj	58	
1	ak	58	
1	al	58	
1	am	58	
1	an	58	
2	BA	49	

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Mol	Chain	Length	Quality of chain
2	BB	49	
2	BC	49	
2	BD	49	
2	BE	49	
2	BF	49	
2	BG	49	
2	BH	49	
2	BI	49	
2	BJ	49	
2	BK	49	
2	BL	49	
2	BM	49	
2	BN	49	
2	ba	49	
2	bb	49	
2	bc	49	
2	bd	49	
2	be	49	
2	bf	49	
2	bg	49	
2	bh	49	
2	bi	49	
2	bj	49	
2	bk	49	
2	bl	49	

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Mol	Chain	Length	Quality of chain
2	bm	49	
2	bn	49	
3	H	246	
3	h	246	
4	L	281	
4	l	281	
5	M	307	
5	m	307	
6	UA	31	
6	UB	31	
6	ua	31	
6	ub	31	
7	UU	49	
7	uu	49	
8	X	55	
8	x	55	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 45952 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 LH1-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	46	Total	C	N	O	S	0	0
			394	272	60	59	3		
1	AB	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AC	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AD	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AE	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AF	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AG	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AH	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AI	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AJ	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AK	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AL	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AM	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	AN	51	Total	C	N	O	S	0	0
			432	296	69	65	2		
1	aa	46	Total	C	N	O	S	0	0
			394	272	60	59	3		
1	ab	55	Total	C	N	O	S	0	0
			462	314	74	71	3		
1	ac	55	Total	C	N	O	S	0	0
			462	314	74	71	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ad	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	ae	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	af	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	ag	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	ah	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	ai	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	aj	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	ak	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	al	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	am	55	Total 462	C 314	N 74	O 71	S 3	0	0
1	an	51	Total 432	C 296	N 69	O 65	S 2	0	0

- Molecule 2 is a protein called LH1-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	BB	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	BC	42	Total 343	C 230	N 54	O 58	S 1	0	0
2	BD	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	BE	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	BF	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	BG	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	BH	43	Total 351	C 236	N 55	O 59	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BI	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	BJ	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	BK	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
2	BL	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
2	BM	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
2	BN	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
2	ba	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	bb	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	bc	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
2	bd	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	be	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	bf	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	bg	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	bh	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	bi	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	bj	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	bk	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
2	bl	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
2	bm	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
2	bn	37	Total	C	N	O	S	0	0
			308	207	49	51	1		

- Molecule 3 is a protein called RC-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total	C	N	O	S	0	0
			1866	1196	316	344	10		
3	h	246	Total	C	N	O	S	0	0
			1866	1196	316	344	10		

- Molecule 4 is a protein called RC-L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	281	Total	C	N	O	S	0	0
			2231	1507	355	361	8		
4	l	281	Total	C	N	O	S	0	0
			2231	1507	355	361	8		

- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	307	Total	C	N	O	S	0	0
			2444	1630	400	403	11		
5	m	307	Total	C	N	O	S	0	0
			2444	1630	400	403	11		

- Molecule 6 is a protein called PufZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UA	31	Total	C	N	O	S	0	0
			244	165	39	35	5		
6	UB	31	Total	C	N	O	S	0	0
			244	165	39	35	5		
6	ua	31	Total	C	N	O	S	0	0
			244	165	39	35	5		
6	ub	31	Total	C	N	O	S	0	0
			244	165	39	35	5		

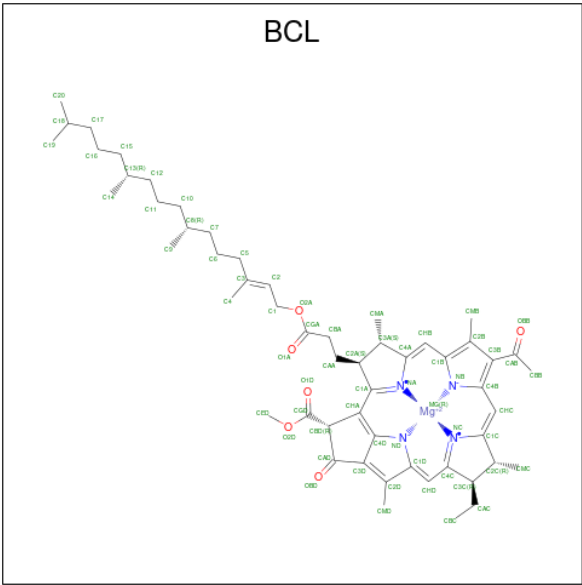
- Molecule 7 is a protein called PufY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UU	49	Total	C	N	O	S	0	0
			362	247	56	56	3		
7	uu	49	Total	C	N	O	S	0	0
			362	247	56	56	3		

- Molecule 8 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	55	Total	C	N	O	S	0	0
			424	281	74	66	3		
8	x	55	Total	C	N	O	S	0	0
			424	281	74	66	3		

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	AA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	AB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	AC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	AD	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	AE	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	AF	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	AG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	AH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	AI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
9	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BC	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BH	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BJ	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BM	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	BN	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0

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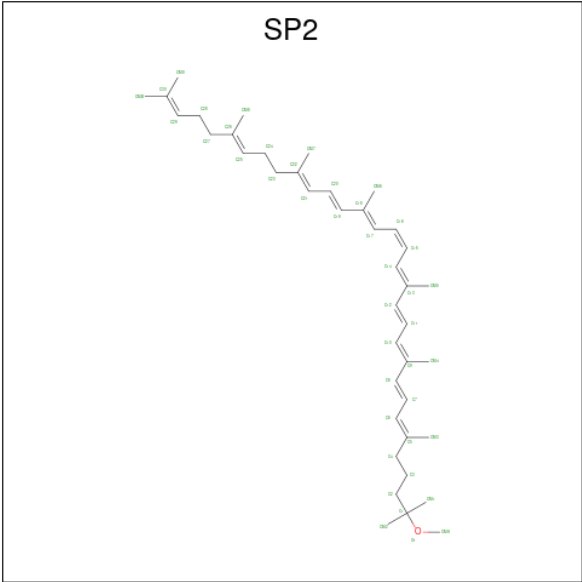
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9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	aa	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ac	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ad	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ae	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	af	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ag	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ah	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ai	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	aj	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ak	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	al	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	am	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	an	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	ba	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bb	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bc	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bd	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	be	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
9	bf	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bg	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bh	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bi	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bj	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bk	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bl	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bm	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	bn	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	m	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 10 is 3,4-DIHYDROSPHEROIDENE (CCD ID: SP2) (formula: C₄₁H₆₂O).



Mol	Chain	Residues	Atoms			AltConf
10	AA	1	Total	C	O	0
			42	41	1	
10	AB	1	Total	C	O	0
			42	41	1	
10	AB	1	Total	C	O	0
			42	41	1	
10	AB	1	Total	C	O	0
			42	41	1	
10	AC	1	Total	C	O	0
			42	41	1	
10	AC	1	Total	C	O	0
			42	41	1	
10	AE	1	Total	C	O	0
			42	41	1	
10	AF	1	Total	C	O	0
			42	41	1	
10	AF	1	Total	C	O	0
			42	41	1	
10	AG	1	Total	C	O	0
			42	41	1	
10	AH	1	Total	C	O	0
			42	41	1	
10	AI	1	Total	C	O	0
			42	41	1	
10	AI	1	Total	C	O	0
			42	41	1	
10	AJ	1	Total	C	O	0
			42	41	1	

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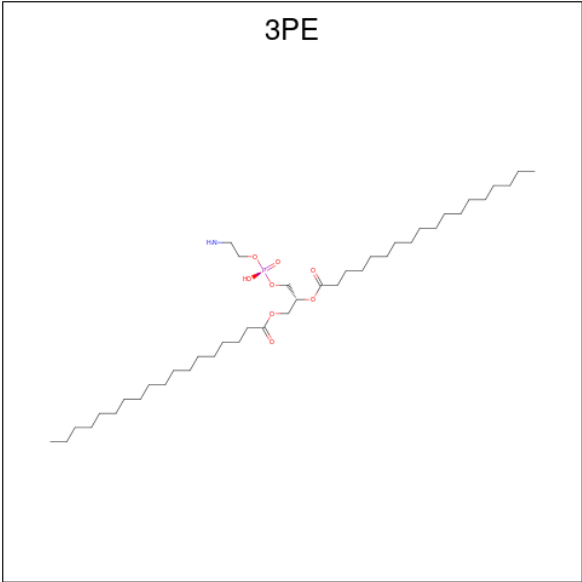
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	AJ	1	42	41	1	0
10	AK	1	42	41	1	0
10	AM	1	42	41	1	0
10	BA	1	42	41	1	0
10	BC	1	42	41	1	0
10	BE	1	42	41	1	0
10	BF	1	42	41	1	0
10	BH	1	42	41	1	0
10	BJ	1	42	41	1	0
10	BK	1	42	41	1	0
10	BL	1	42	41	1	0
10	BL	1	42	41	1	0
10	M	1	42	41	1	0
10	ab	1	42	41	1	0
10	ab	1	42	41	1	0
10	ab	1	42	41	1	0
10	ac	1	42	41	1	0
10	ac	1	42	41	1	0
10	ad	1	42	41	1	0
10	ae	1	42	41	1	0
10	ae	1	42	41	1	0

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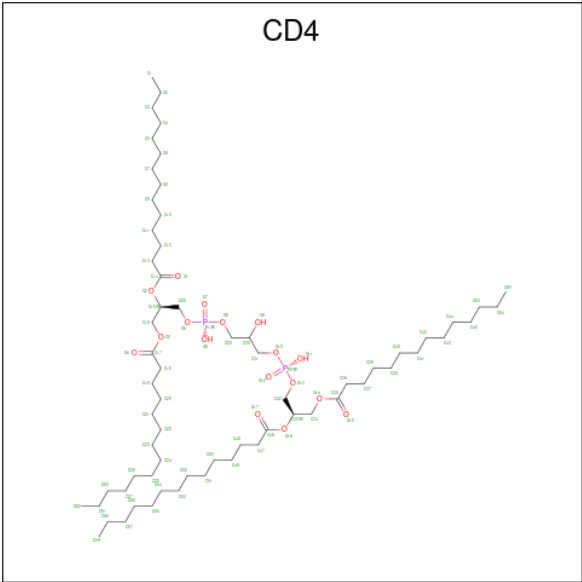
Mol	Chain	Residues	Atoms			AltConf
10	af	1	Total	C	O	0
			42	41	1	
10	af	1	Total	C	O	0
			42	41	1	
10	af	1	Total	C	O	0
			42	41	1	
10	ah	1	Total	C	O	0
			42	41	1	
10	ai	1	Total	C	O	0
			42	41	1	
10	ai	1	Total	C	O	0
			42	41	1	
10	aj	1	Total	C	O	0
			42	41	1	
10	aj	1	Total	C	O	0
			42	41	1	
10	ak	1	Total	C	O	0
			42	41	1	
10	al	1	Total	C	O	0
			42	41	1	
10	am	1	Total	C	O	0
			42	41	1	
10	ba	1	Total	C	O	0
			42	41	1	
10	bb	1	Total	C	O	0
			42	41	1	
10	bf	1	Total	C	O	0
			42	41	1	
10	bh	1	Total	C	O	0
			42	41	1	
10	bj	1	Total	C	O	0
			42	41	1	
10	bk	1	Total	C	O	0
			42	41	1	
10	bl	1	Total	C	O	0
			42	41	1	
10	m	1	Total	C	O	0
			42	41	1	

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



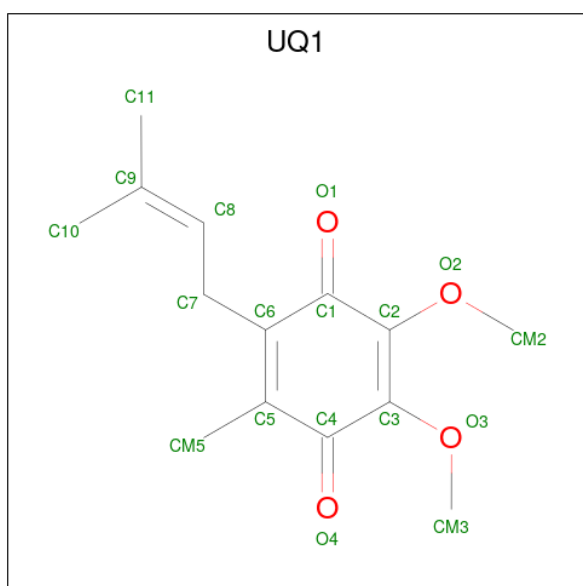
Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	ac	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	h	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 12 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: C₆₅H₁₂₆O₁₇P₂).



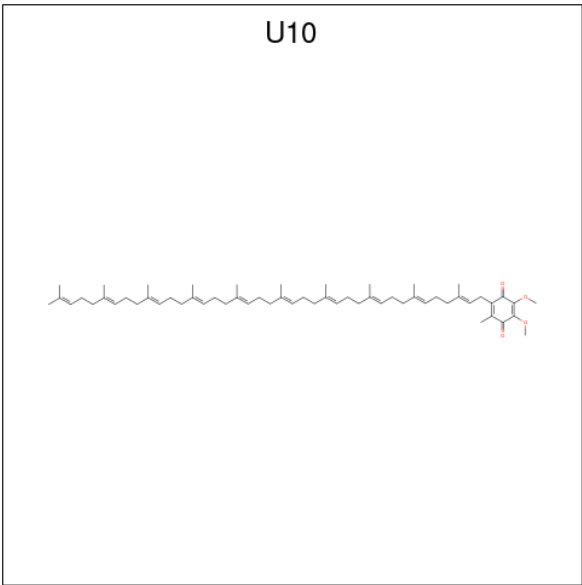
Mol	Chain	Residues	Atoms				AltConf
12	H	1	Total	C	O	P	0
			84	65	17	2	
12	M	1	Total	C	O	P	0
			84	65	17	2	
12	h	1	Total	C	O	P	0
			84	65	17	2	
12	m	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 13 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



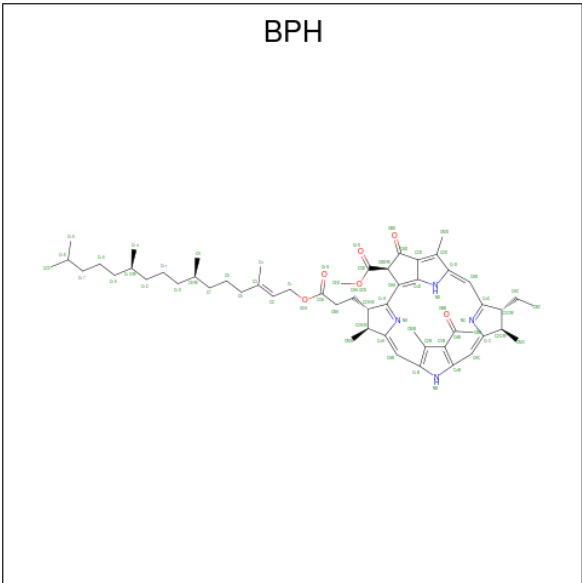
Mol	Chain	Residues	Atoms				AltConf
13	L	1	Total	C	O		0
			18	14	4		
13	l	1	Total	C	O		0
			18	14	4		

- Molecule 14 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



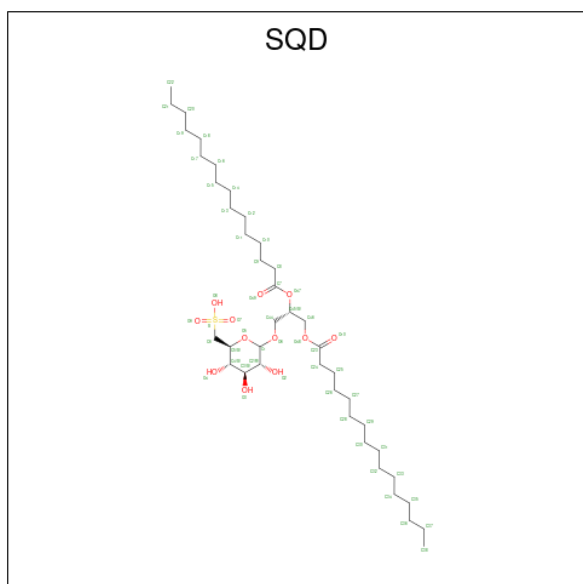
Mol	Chain	Residues	Atoms			AltConf
14	L	1	Total	C	O	0
			63	59	4	
14	M	1	Total	C	O	0
			63	59	4	
14	l	1	Total	C	O	0
			63	59	4	
14	m	1	Total	C	O	0
			63	59	4	

- Molecule 15 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total	C	N	O	0
			65	55	4	6	
15	M	1	Total	C	N	O	0
			65	55	4	6	
15	l	1	Total	C	N	O	0
			65	55	4	6	
15	m	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total	C	O	S	0
			54	41	12	1	
16	x	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 17 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
17	M	1	Total 35	C 24	O 11	0
17	m	1	Total 35	C 24	O 11	0

- Molecule 18 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
18	M	1	Total 1	Fe 1	0
18	m	1	Total 1	Fe 1	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	AB	2	Total 2	O 2	0
19	BB	1	Total 1	O 1	0
19	H	18	Total 18	O 18	0
19	L	27	Total 27	O 27	0
19	M	19	Total 19	O 19	0

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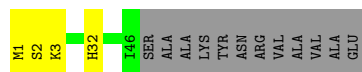
Mol	Chain	Residues	Atoms		AltConf
19	X	5	Total 5	O 5	0
19	ab	3	Total 3	O 3	0
19	h	18	Total 18	O 18	0
19	l	27	Total 27	O 27	0
19	m	19	Total 19	O 19	0
19	x	5	Total 5	O 5	0

3 Residue-property plots [i](#)

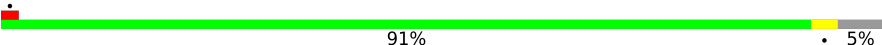
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

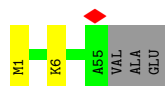
- Molecule 1: LH1-alpha

Chain AA:  72% 7% 21%

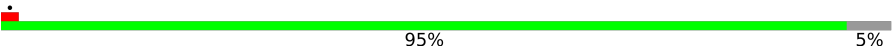


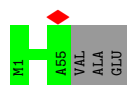
- Molecule 1: LH1-alpha

Chain AB:  91% 5%



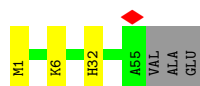
- Molecule 1: LH1-alpha

Chain AC:  95% 5%



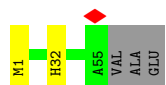
- Molecule 1: LH1-alpha

Chain AD:  90% 5% 5%

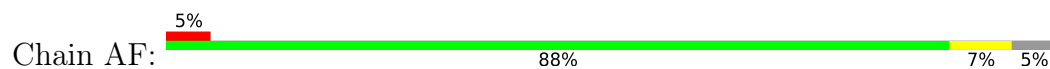


- Molecule 1: LH1-alpha

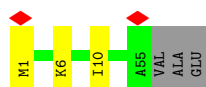
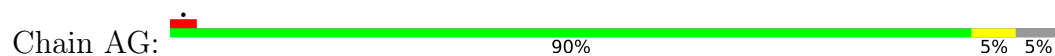
Chain AE:  91% 5%



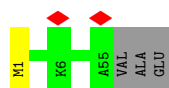
● Molecule 1: LH1-alpha



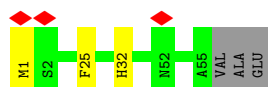
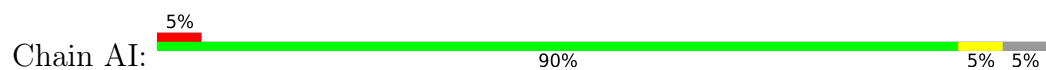
● Molecule 1: LH1-alpha



● Molecule 1: LH1-alpha



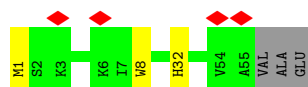
● Molecule 1: LH1-alpha



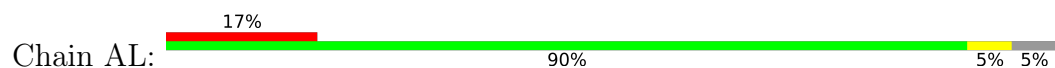
● Molecule 1: LH1-alpha

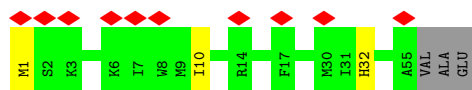


● Molecule 1: LH1-alpha

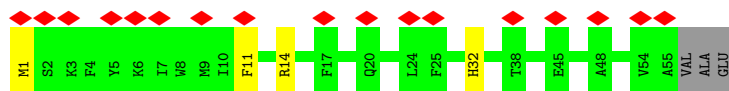
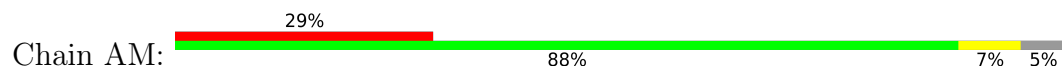


● Molecule 1: LH1-alpha

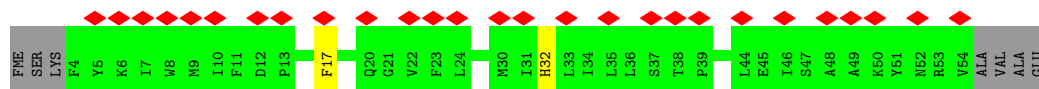
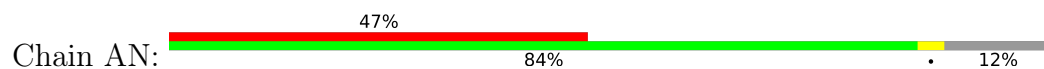




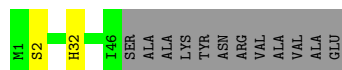
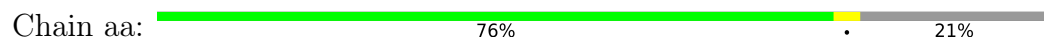
- Molecule 1: LH1-alpha



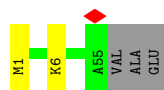
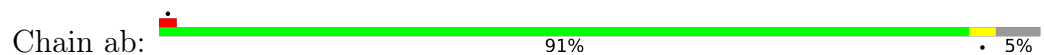
- Molecule 1: LH1-alpha



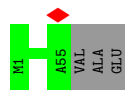
- Molecule 1: LH1-alpha



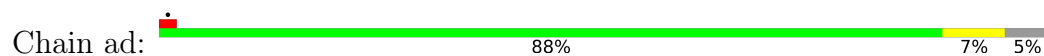
- Molecule 1: LH1-alpha



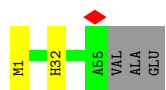
- Molecule 1: LH1-alpha



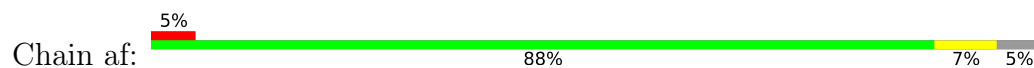
- Molecule 1: LH1-alpha



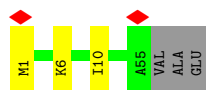
- Molecule 1: LH1-alpha



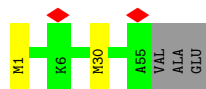
- Molecule 1: LH1-alpha



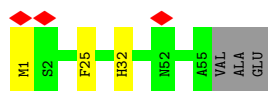
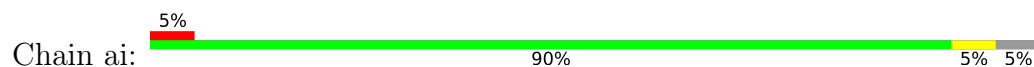
- Molecule 1: LH1-alpha



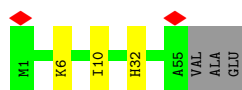
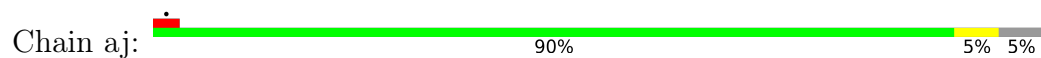
- Molecule 1: LH1-alpha



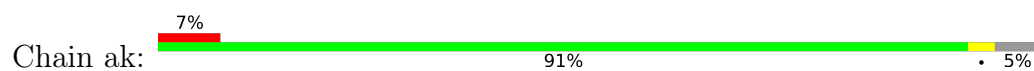
- Molecule 1: LH1-alpha

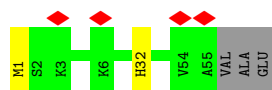


- Molecule 1: LH1-alpha

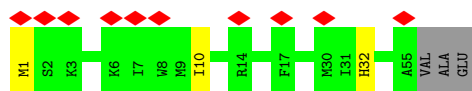
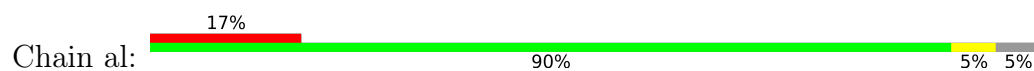


- Molecule 1: LH1-alpha

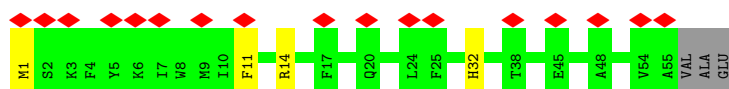
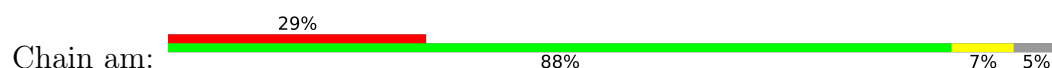




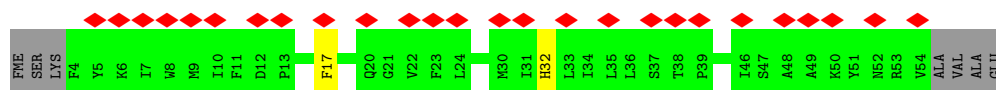
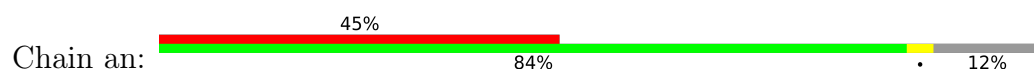
- Molecule 1: LH1-alpha



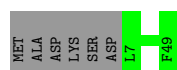
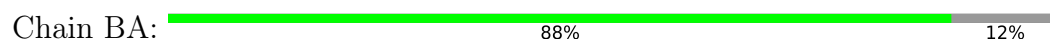
- Molecule 1: LH1-alpha



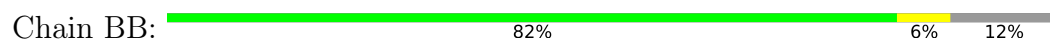
- Molecule 1: LH1-alpha



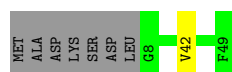
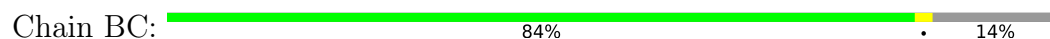
- Molecule 2: LH1-beta



- Molecule 2: LH1-beta

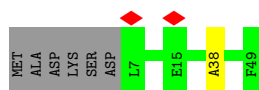


- Molecule 2: LH1-beta

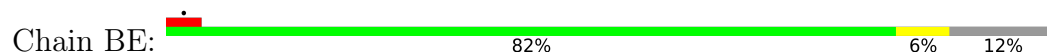


- Molecule 2: LH1-beta

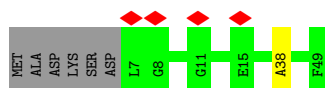
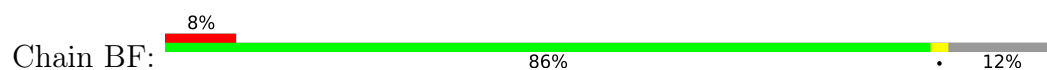




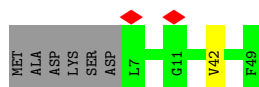
- Molecule 2: LH1-beta



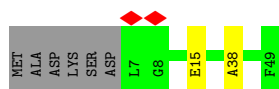
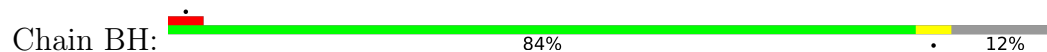
- Molecule 2: LH1-beta



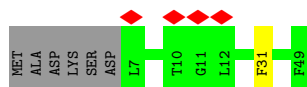
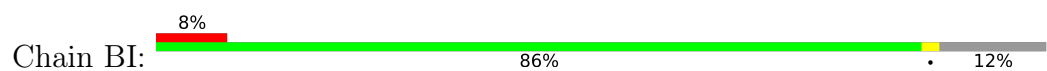
- Molecule 2: LH1-beta



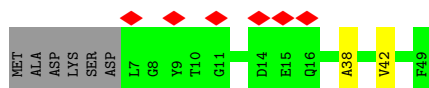
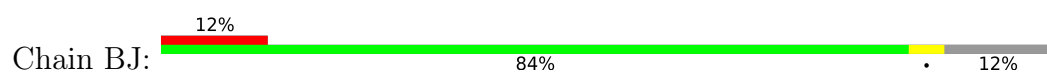
- Molecule 2: LH1-beta



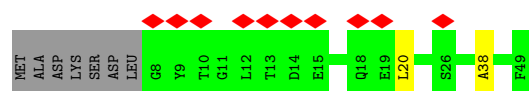
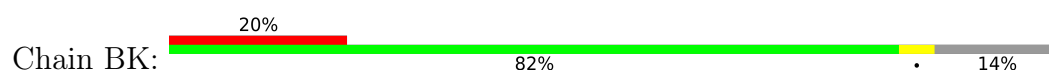
- Molecule 2: LH1-beta



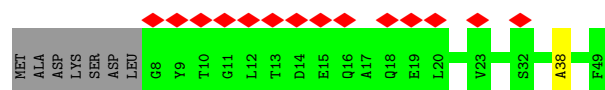
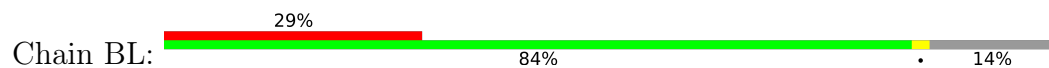
- Molecule 2: LH1-beta



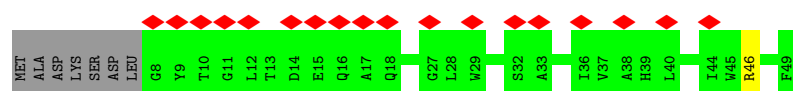
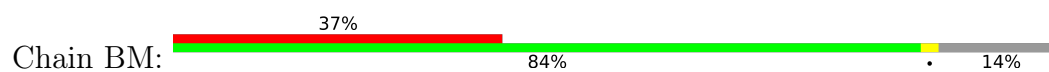
- Molecule 2: LH1-beta



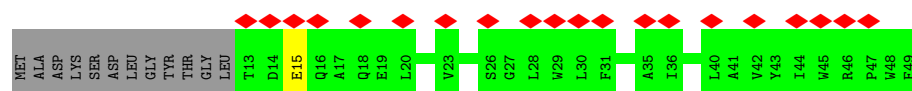
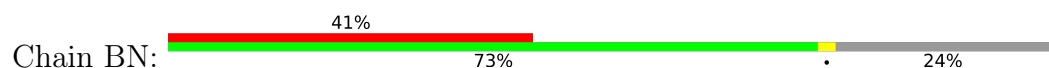
- Molecule 2: LH1-beta



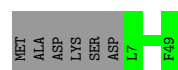
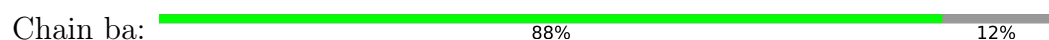
- Molecule 2: LH1-beta



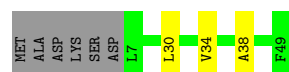
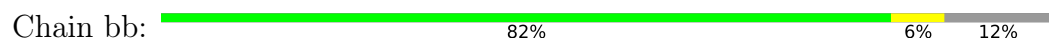
- Molecule 2: LH1-beta



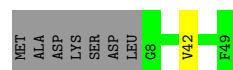
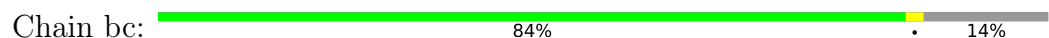
- Molecule 2: LH1-beta



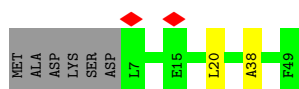
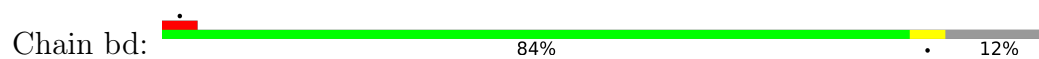
- Molecule 2: LH1-beta



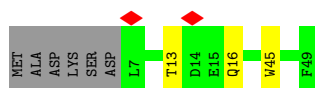
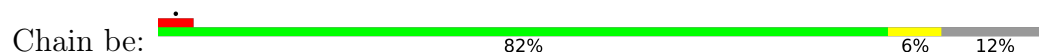
- Molecule 2: LH1-beta



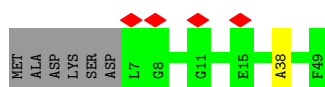
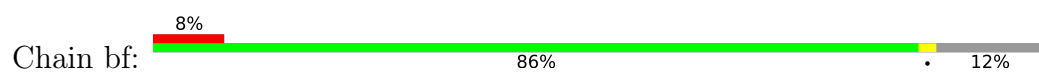
- Molecule 2: LH1-beta



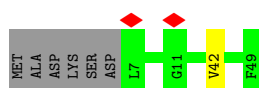
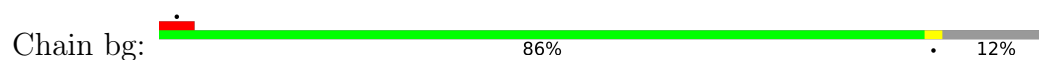
- Molecule 2: LH1-beta



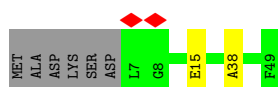
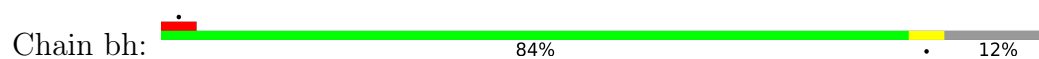
- Molecule 2: LH1-beta



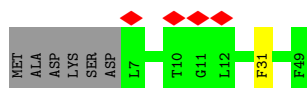
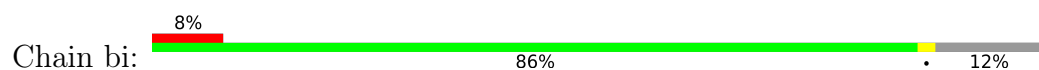
- Molecule 2: LH1-beta



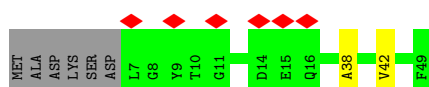
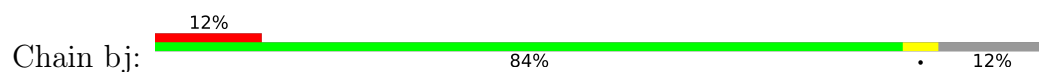
- Molecule 2: LH1-beta



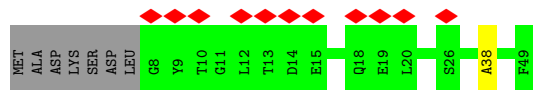
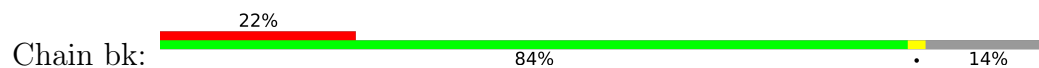
- Molecule 2: LH1-beta



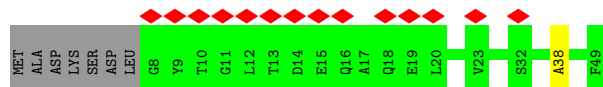
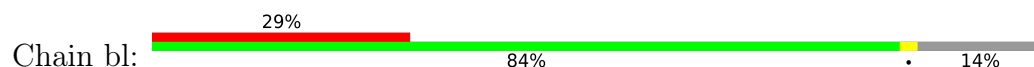
- Molecule 2: LH1-beta



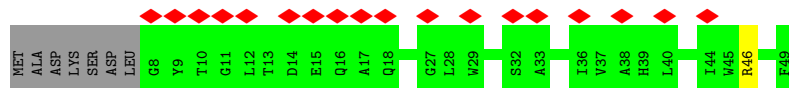
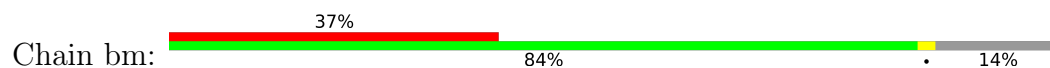
- Molecule 2: LH1-beta



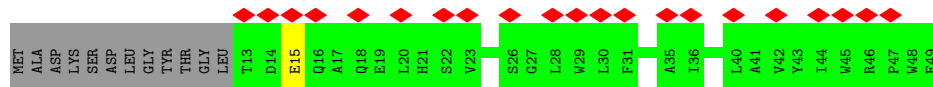
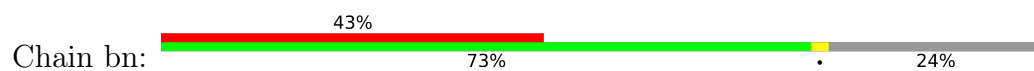
- Molecule 2: LH1-beta



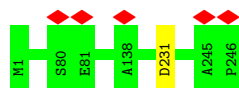
- Molecule 2: LH1-beta



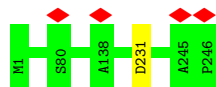
- Molecule 2: LH1-beta



- Molecule 3: RC-H



- Molecule 3: RC-H



- Molecule 4: RC-L



- Molecule 4: RC-L

Chain l:  97%



- Molecule 5: Reaction center protein M chain

Chain M:  97%

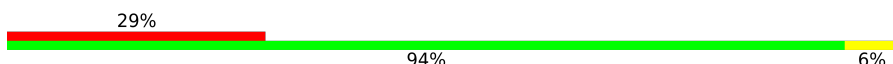


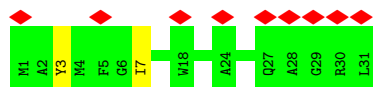
- Molecule 5: Reaction center protein M chain

Chain m:  97%



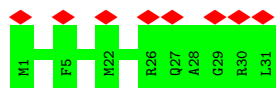
- Molecule 6: PufZ

Chain UA:  29% 94% 6%

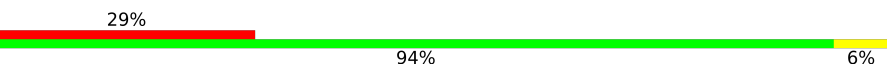


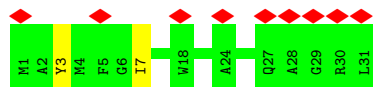
- Molecule 6: PufZ

Chain UB:  26% 100%



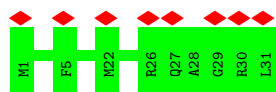
- Molecule 6: PufZ

Chain ua:  29% 94% 6%

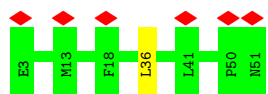


- Molecule 6: PufZ

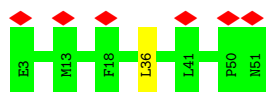
Chain ub:  26% 100%



- Molecule 7: PufY



- Molecule 7: PufY



- Molecule 8: PufX



There are no outlier residues recorded for this chain.

- Molecule 8: PufX



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	58945	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 ($e^-/\text{\AA}^2$)	45.36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0222	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD4, BCL, U10, 3PE, BPH, LMT, SP2, FME, SQD, FE, UQ1

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	AA	0.16	0/397	0.41	0/539
1	AB	0.15	0/466	0.41	0/632
1	AC	0.15	0/466	0.44	0/632
1	AD	0.16	0/466	0.42	0/632
1	AE	0.16	0/466	0.45	0/632
1	AF	0.16	0/466	0.42	0/632
1	AG	0.16	0/466	0.47	0/632
1	AH	0.18	0/466	0.50	0/632
1	AI	0.16	0/466	0.43	0/632
1	AJ	0.18	0/466	0.43	0/632
1	AK	0.18	0/466	0.46	0/632
1	AL	0.18	0/466	0.46	0/632
1	AM	0.15	0/466	0.42	0/632
1	AN	0.16	0/446	0.44	0/606
1	aa	0.16	0/397	0.40	0/539
1	ab	0.15	0/466	0.41	0/632
1	ac	0.16	0/466	0.44	0/632
1	ad	0.16	0/466	0.42	0/632
1	ae	0.16	0/466	0.44	0/632
1	af	0.17	0/466	0.41	0/632
1	ag	0.15	0/466	0.48	0/632
1	ah	0.18	0/466	0.49	0/632
1	ai	0.16	0/466	0.44	0/632
1	aj	0.17	0/466	0.43	0/632
1	ak	0.18	0/466	0.45	0/632
1	al	0.18	0/466	0.46	0/632
1	am	0.15	0/466	0.42	0/632
1	an	0.16	0/446	0.44	0/606
2	BA	0.14	0/364	0.39	0/499
2	BB	0.12	0/364	0.37	0/499
2	BC	0.13	0/356	0.38	0/488
2	BD	0.13	0/364	0.39	0/499

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BE	0.12	0/364	0.40	0/499
2	BF	0.14	0/364	0.43	0/499
2	BG	0.12	0/364	0.35	0/499
2	BH	0.11	0/364	0.37	0/499
2	BI	0.13	0/364	0.38	0/499
2	BJ	0.12	0/364	0.42	0/499
2	BK	0.14	0/356	0.45	0/488
2	BL	0.13	0/356	0.41	0/488
2	BM	0.12	0/356	0.37	0/488
2	BN	0.14	0/320	0.37	0/439
2	ba	0.15	0/364	0.40	0/499
2	bb	0.12	0/364	0.37	0/499
2	bc	0.13	0/356	0.38	0/488
2	bd	0.13	0/364	0.38	0/499
2	be	0.12	0/364	0.40	0/499
2	bf	0.14	0/364	0.43	0/499
2	bg	0.12	0/364	0.36	0/499
2	bh	0.11	0/364	0.38	0/499
2	bi	0.13	0/364	0.38	0/499
2	bj	0.11	0/364	0.40	0/499
2	bk	0.14	0/356	0.41	0/488
2	bl	0.13	0/356	0.41	0/488
2	bm	0.12	0/356	0.36	0/488
2	bn	0.14	0/320	0.37	0/439
3	H	0.12	0/1916	0.37	0/2609
3	h	0.12	0/1916	0.37	0/2609
4	L	0.14	0/2319	0.39	0/3175
4	l	0.14	0/2319	0.39	0/3175
5	M	0.13	0/2537	0.40	0/3464
5	m	0.13	0/2537	0.40	0/3464
6	UA	0.12	0/250	0.37	0/334
6	UB	0.13	0/250	0.36	0/334
6	ua	0.12	0/250	0.37	0/334
6	ub	0.12	0/250	0.37	0/334
7	UU	0.11	0/373	0.35	0/505
7	uu	0.11	0/373	0.35	0/505
8	X	0.15	0/436	0.50	0/589
8	x	0.15	0/436	0.50	0/589
All	All	0.14	0/39072	0.41	0/53242

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	BM	0	1
2	bm	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BM	46	ARG	Sidechain
2	bm	46	ARG	Sidechain

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	AA	394	0	411	2	0
1	AB	462	0	481	1	0
1	AC	462	0	481	0	0
1	AD	462	0	481	2	0
1	AE	462	0	481	1	0
1	AF	462	0	481	3	0
1	AG	462	0	481	2	0
1	AH	462	0	481	0	0
1	AI	462	0	481	2	0
1	AJ	462	0	481	3	0
1	AK	462	0	481	2	0
1	AL	462	0	481	2	0
1	AM	462	0	481	3	0
1	AN	432	0	447	2	0
1	aa	394	0	411	1	0
1	ab	462	0	481	1	0
1	ac	462	0	481	0	0
1	ad	462	0	481	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	ae	462	0	481	1	0
1	af	462	0	481	3	0
1	ag	462	0	481	2	0
1	ah	462	0	481	1	0
1	ai	462	0	481	2	0
1	aj	462	0	481	3	0
1	ak	462	0	481	1	0
1	al	462	0	481	2	0
1	am	462	0	481	3	0
1	an	432	0	447	2	0
2	BA	351	0	336	0	0
2	BB	351	0	336	4	0
2	BC	343	0	325	2	0
2	BD	351	0	336	1	0
2	BE	351	0	336	2	0
2	BF	351	0	336	1	0
2	BG	351	0	336	1	0
2	BH	351	0	336	1	0
2	BI	351	0	336	1	0
2	BJ	351	0	336	2	0
2	BK	343	0	325	2	0
2	BL	343	0	325	1	0
2	BM	343	0	325	0	0
2	BN	308	0	292	0	0
2	ba	351	0	336	0	0
2	bb	351	0	336	4	0
2	bc	343	0	325	2	0
2	bd	351	0	336	2	0
2	be	351	0	336	2	0
2	bf	351	0	336	1	0
2	bg	351	0	336	1	0
2	bh	351	0	336	1	0
2	bi	351	0	336	1	0
2	bj	351	0	336	2	0
2	bk	343	0	325	1	0
2	bl	343	0	325	1	0
2	bm	343	0	325	0	0
2	bn	308	0	292	0	0
3	H	1866	0	1864	0	0
3	h	1866	0	1864	0	0
4	L	2231	0	2187	6	0
4	l	2231	0	2187	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	2444	0	2359	3	0
5	m	2444	0	2359	3	0
6	UA	244	0	250	1	0
6	UB	244	0	250	0	0
6	ua	244	0	250	1	0
6	ub	244	0	250	0	0
7	UU	362	0	358	1	0
7	uu	362	0	358	1	0
8	X	424	0	438	0	0
8	x	424	0	438	0	0
9	AA	66	0	74	0	0
9	AB	66	0	74	3	0
9	AC	66	0	74	1	0
9	AD	66	0	74	1	0
9	AE	66	0	74	0	0
9	AF	66	0	74	1	0
9	AG	66	0	74	0	0
9	AH	66	0	74	1	0
9	AI	66	0	74	4	0
9	AJ	66	0	74	3	0
9	AK	66	0	74	3	0
9	AL	66	0	74	0	0
9	AM	66	0	74	1	0
9	AN	66	0	74	0	0
9	BA	66	0	74	2	0
9	BB	66	0	74	0	0
9	BC	66	0	74	1	0
9	BD	66	0	74	1	0
9	BE	66	0	74	1	0
9	BF	66	0	74	1	0
9	BG	66	0	74	0	0
9	BH	66	0	74	1	0
9	BI	66	0	74	1	0
9	BJ	66	0	74	1	0
9	BK	66	0	74	1	0
9	BL	66	0	74	2	0
9	BM	66	0	74	1	0
9	BN	66	0	74	1	0
9	L	132	0	148	0	0
9	M	132	0	148	0	0
9	aa	66	0	74	1	0
9	ab	66	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	ac	66	0	74	1	0
9	ad	66	0	74	0	0
9	ae	66	0	74	0	0
9	af	66	0	74	0	0
9	ag	66	0	74	0	0
9	ah	66	0	74	1	0
9	ai	66	0	74	4	0
9	aj	66	0	74	2	0
9	ak	66	0	74	3	0
9	al	66	0	74	0	0
9	am	66	0	74	2	0
9	an	66	0	74	0	0
9	ba	66	0	74	2	0
9	bb	66	0	74	0	0
9	bc	66	0	74	1	0
9	bd	66	0	74	1	0
9	be	66	0	74	1	0
9	bf	66	0	74	1	0
9	bg	66	0	74	0	0
9	bh	66	0	74	1	0
9	bi	66	0	74	2	0
9	bj	66	0	74	1	0
9	bk	66	0	74	1	0
9	bl	66	0	74	2	0
9	bm	66	0	74	1	0
9	bn	66	0	74	1	0
9	l	132	0	148	0	0
9	m	132	0	148	0	0
10	AA	42	0	62	1	0
10	AB	126	0	186	4	0
10	AC	84	0	124	3	0
10	AE	42	0	62	1	0
10	AF	84	0	124	2	0
10	AG	42	0	62	4	0
10	AH	42	0	62	3	0
10	AI	84	0	124	2	0
10	AJ	84	0	124	3	0
10	AK	42	0	62	3	0
10	AM	42	0	62	1	0
10	BA	42	0	62	1	0
10	BC	42	0	62	3	0
10	BE	42	0	62	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BF	42	0	62	3	0
10	BH	42	0	62	3	0
10	BJ	42	0	62	0	0
10	BK	42	0	62	1	0
10	BL	84	0	124	2	0
10	M	42	0	62	0	0
10	ab	126	0	186	3	0
10	ac	84	0	124	4	0
10	ad	42	0	62	1	0
10	ae	84	0	124	3	0
10	af	126	0	186	5	0
10	ah	42	0	62	3	0
10	ai	84	0	124	2	0
10	aj	84	0	124	6	0
10	ak	42	0	62	3	0
10	al	42	0	62	3	0
10	am	42	0	62	0	0
10	ba	42	0	62	0	0
10	bb	42	0	62	1	0
10	bf	42	0	62	3	0
10	bh	42	0	62	2	0
10	bj	42	0	62	0	0
10	bk	42	0	62	2	0
10	bl	42	0	62	1	0
10	m	42	0	62	2	0
11	AC	51	0	82	1	0
11	H	51	0	82	0	0
11	ac	51	0	82	1	0
11	h	51	0	82	0	0
12	H	84	0	124	0	0
12	M	84	0	124	1	0
12	h	84	0	124	0	0
12	m	84	0	124	1	0
13	L	18	0	18	0	0
13	l	18	0	18	1	0
14	L	63	0	90	3	0
14	M	63	0	90	2	0
14	l	63	0	90	2	0
14	m	63	0	90	2	0
15	L	65	0	76	1	0
15	M	65	0	76	1	0
15	l	65	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	m	65	0	76	0	0
16	L	54	0	78	1	0
16	x	54	0	78	0	0
17	M	35	0	45	0	0
17	m	35	0	45	0	0
18	M	1	0	0	0	0
18	m	1	0	0	0	0
19	AB	2	0	0	0	0
19	BB	1	0	0	0	0
19	H	18	0	0	0	0
19	L	27	0	0	0	0
19	M	19	0	0	0	0
19	X	5	0	0	0	0
19	ab	3	0	0	0	0
19	h	18	0	0	0	0
19	l	27	0	0	0	0
19	m	19	0	0	0	0
19	x	5	0	0	0	0
All	All	45952	0	47758	171	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 171 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)
9:ai:102:BCL:H72	9:ai:102:BCL:H41	1.77	0.66
9:BA:102:BCL:H203	2:BB:34:VAL:HG22	1.79	0.65
10:ak:102:SP2:HM62	2:bk:38:ALA:HB1	1.78	0.65
10:AK:102:SP2:HM62	2:BK:38:ALA:HB1	1.79	0.64
9:ba:102:BCL:H203	2:bb:34:VAL:HG22	1.79	0.64

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	44/58 (76%)	43 (98%)	0	1 (2%)	5	19
1	AB	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AC	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AD	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AE	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AF	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AG	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AH	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AI	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AJ	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AK	53/58 (91%)	53 (100%)	0	0	100	100
1	AL	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AM	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	AN	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
1	aa	44/58 (76%)	43 (98%)	0	1 (2%)	5	19
1	ab	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ac	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ad	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ae	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	af	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ag	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ah	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ai	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	aj	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	ak	53/58 (91%)	53 (100%)	0	0	100	100
1	al	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	am	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
1	an	49/58 (84%)	48 (98%)	1 (2%)	0	100	100
2	BA	41/49 (84%)	41 (100%)	0	0	100	100
2	BB	41/49 (84%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BC	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	BD	41/49 (84%)	41 (100%)	0	0	100	100
2	BE	41/49 (84%)	41 (100%)	0	0	100	100
2	BF	41/49 (84%)	41 (100%)	0	0	100	100
2	BG	41/49 (84%)	41 (100%)	0	0	100	100
2	BH	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	BI	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	BJ	41/49 (84%)	41 (100%)	0	0	100	100
2	BK	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	BL	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	BM	40/49 (82%)	40 (100%)	0	0	100	100
2	BN	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
2	ba	41/49 (84%)	41 (100%)	0	0	100	100
2	bb	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	bc	40/49 (82%)	40 (100%)	0	0	100	100
2	bd	41/49 (84%)	41 (100%)	0	0	100	100
2	be	41/49 (84%)	41 (100%)	0	0	100	100
2	bf	41/49 (84%)	41 (100%)	0	0	100	100
2	bg	41/49 (84%)	41 (100%)	0	0	100	100
2	bh	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	bi	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	bj	41/49 (84%)	41 (100%)	0	0	100	100
2	bk	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	bl	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	bm	40/49 (82%)	40 (100%)	0	0	100	100
2	bn	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
3	H	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
3	h	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
4	L	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	30	59
4	l	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	30	59
5	M	305/307 (99%)	294 (96%)	10 (3%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	m	305/307 (99%)	294 (96%)	10 (3%)	1 (0%)	36	65
6	UA	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
6	UB	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
6	ua	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
6	ub	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
7	UU	47/49 (96%)	47 (100%)	0	0	100	100
7	uu	47/49 (96%)	47 (100%)	0	0	100	100
8	X	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
8	x	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
All	All	4558/4996 (91%)	4453 (98%)	99 (2%)	6 (0%)	49	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	SER
1	aa	2	SER
5	M	195	ASN
5	m	195	ASN
4	L	31	VAL

5.3.2 Protein sidechains [i](#)

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	AA	42/50 (84%)	42 (100%)	0	100	100
1	AB	48/50 (96%)	48 (100%)	0	100	100
1	AC	48/50 (96%)	48 (100%)	0	100	100
1	AD	48/50 (96%)	48 (100%)	0	100	100
1	AE	48/50 (96%)	48 (100%)	0	100	100
1	AF	48/50 (96%)	48 (100%)	0	100	100
1	AG	48/50 (96%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AH	48/50 (96%)	48 (100%)	0	100	100
1	AI	48/50 (96%)	48 (100%)	0	100	100
1	AJ	48/50 (96%)	48 (100%)	0	100	100
1	AK	48/50 (96%)	48 (100%)	0	100	100
1	AL	48/50 (96%)	48 (100%)	0	100	100
1	AM	48/50 (96%)	48 (100%)	0	100	100
1	AN	46/50 (92%)	46 (100%)	0	100	100
1	aa	42/50 (84%)	42 (100%)	0	100	100
1	ab	48/50 (96%)	48 (100%)	0	100	100
1	ac	48/50 (96%)	48 (100%)	0	100	100
1	ad	48/50 (96%)	48 (100%)	0	100	100
1	ae	48/50 (96%)	48 (100%)	0	100	100
1	af	48/50 (96%)	48 (100%)	0	100	100
1	ag	48/50 (96%)	48 (100%)	0	100	100
1	ah	48/50 (96%)	48 (100%)	0	100	100
1	ai	48/50 (96%)	48 (100%)	0	100	100
1	aj	48/50 (96%)	48 (100%)	0	100	100
1	ak	48/50 (96%)	48 (100%)	0	100	100
1	al	48/50 (96%)	48 (100%)	0	100	100
1	am	48/50 (96%)	48 (100%)	0	100	100
1	an	46/50 (92%)	46 (100%)	0	100	100
2	BA	35/40 (88%)	35 (100%)	0	100	100
2	BB	35/40 (88%)	35 (100%)	0	100	100
2	BC	34/40 (85%)	34 (100%)	0	100	100
2	BD	35/40 (88%)	35 (100%)	0	100	100
2	BE	35/40 (88%)	35 (100%)	0	100	100
2	BF	35/40 (88%)	35 (100%)	0	100	100
2	BG	35/40 (88%)	35 (100%)	0	100	100
2	BH	35/40 (88%)	34 (97%)	1 (3%)	37	71
2	BI	35/40 (88%)	35 (100%)	0	100	100
2	BJ	35/40 (88%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BK	34/40 (85%)	34 (100%)	0	100	100
2	BL	34/40 (85%)	34 (100%)	0	100	100
2	BM	34/40 (85%)	34 (100%)	0	100	100
2	BN	31/40 (78%)	30 (97%)	1 (3%)	34	68
2	ba	35/40 (88%)	35 (100%)	0	100	100
2	bb	35/40 (88%)	35 (100%)	0	100	100
2	bc	34/40 (85%)	34 (100%)	0	100	100
2	bd	35/40 (88%)	35 (100%)	0	100	100
2	be	35/40 (88%)	35 (100%)	0	100	100
2	bf	35/40 (88%)	35 (100%)	0	100	100
2	bg	35/40 (88%)	35 (100%)	0	100	100
2	bh	35/40 (88%)	34 (97%)	1 (3%)	37	71
2	bi	35/40 (88%)	35 (100%)	0	100	100
2	bj	35/40 (88%)	35 (100%)	0	100	100
2	bk	34/40 (85%)	34 (100%)	0	100	100
2	bl	34/40 (85%)	34 (100%)	0	100	100
2	bm	34/40 (85%)	34 (100%)	0	100	100
2	bn	31/40 (78%)	30 (97%)	1 (3%)	34	68
3	H	198/198 (100%)	197 (100%)	1 (0%)	81	93
3	h	198/198 (100%)	197 (100%)	1 (0%)	81	93
4	L	220/220 (100%)	218 (99%)	2 (1%)	70	90
4	l	220/220 (100%)	218 (99%)	2 (1%)	70	90
5	M	240/240 (100%)	238 (99%)	2 (1%)	73	90
5	m	240/240 (100%)	238 (99%)	2 (1%)	73	90
6	UA	22/22 (100%)	22 (100%)	0	100	100
6	UB	22/22 (100%)	22 (100%)	0	100	100
6	ua	22/22 (100%)	22 (100%)	0	100	100
6	ub	22/22 (100%)	22 (100%)	0	100	100
7	UU	33/33 (100%)	33 (100%)	0	100	100
7	uu	33/33 (100%)	33 (100%)	0	100	100
8	X	42/42 (100%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	x	42/42 (100%)	42 (100%)	0	100	100
All	All	3846/4074 (94%)	3832 (100%)	14 (0%)	81	94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	bh	15	GLU
2	bn	15	GLU
5	m	263	GLU
4	l	247	CYS
5	m	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	bc	18	GLN
5	m	259	ASN
5	m	300	ASN
5	m	299	GLN
4	L	183	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	AH	1	1	8,9,10	0.94	0	8,9,11	1.00	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	AI	1	1	8,9,10	0.96	0	8,9,11	1.06	1 (12%)
1	FME	AE	1	1	8,9,10	0.95	0	8,9,11	1.06	1 (12%)
1	FME	ad	1	1	8,9,10	0.92	0	8,9,11	1.13	1 (12%)
1	FME	AD	1	1	8,9,10	0.92	0	8,9,11	1.12	1 (12%)
1	FME	AK	1	1	8,9,10	0.96	0	8,9,11	1.26	2 (25%)
1	FME	AC	1	1	8,9,10	0.99	0	8,9,11	0.90	0
1	FME	ab	1	1	8,9,10	0.95	0	8,9,11	1.22	1 (12%)
1	FME	ah	1	1	8,9,10	0.94	0	8,9,11	0.99	1 (12%)
1	FME	aa	1	1	8,9,10	0.96	0	8,9,11	0.79	0
1	FME	AF	1	1	8,9,10	0.94	0	8,9,11	1.21	1 (12%)
1	FME	aj	1	1	8,9,10	0.98	0	8,9,11	0.94	0
1	FME	AG	1	1	8,9,10	0.93	0	8,9,11	1.35	1 (12%)
1	FME	AM	1	1	8,9,10	0.95	0	8,9,11	1.05	1 (12%)
1	FME	al	1	1	8,9,10	0.93	0	8,9,11	1.14	1 (12%)
1	FME	am	1	1	8,9,10	0.95	0	8,9,11	1.05	1 (12%)
1	FME	af	1	1	8,9,10	0.94	0	8,9,11	1.21	1 (12%)
1	FME	AB	1	1	8,9,10	0.95	0	8,9,11	1.22	1 (12%)
1	FME	ac	1	1	8,9,10	0.98	0	8,9,11	0.88	0
1	FME	AA	1	1	8,9,10	0.95	0	8,9,11	0.88	0
1	FME	ak	1	1	8,9,10	0.96	0	8,9,11	1.25	2 (25%)
1	FME	AL	1	1	8,9,10	0.93	0	8,9,11	1.14	1 (12%)
1	FME	ae	1	1	8,9,10	0.95	0	8,9,11	1.06	1 (12%)
1	FME	ag	1	1	8,9,10	0.93	0	8,9,11	1.34	1 (12%)
1	FME	AJ	1	1	8,9,10	0.98	0	8,9,11	0.95	0
1	FME	ai	1	1	8,9,10	0.96	0	8,9,11	1.06	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	AH	1	1	-	0/7/9/11	-
1	FME	AI	1	1	-	0/7/9/11	-
1	FME	AE	1	1	-	0/7/9/11	-
1	FME	ad	1	1	-	0/7/9/11	-
1	FME	AD	1	1	-	0/7/9/11	-
1	FME	AK	1	1	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	AC	1	1	-	1/7/9/11	-
1	FME	ab	1	1	-	0/7/9/11	-
1	FME	ah	1	1	-	0/7/9/11	-
1	FME	aa	1	1	-	1/7/9/11	-
1	FME	AF	1	1	-	0/7/9/11	-
1	FME	aj	1	1	-	4/7/9/11	-
1	FME	AG	1	1	-	1/7/9/11	-
1	FME	AM	1	1	-	1/7/9/11	-
1	FME	al	1	1	-	3/7/9/11	-
1	FME	am	1	1	-	1/7/9/11	-
1	FME	af	1	1	-	0/7/9/11	-
1	FME	AB	1	1	-	0/7/9/11	-
1	FME	ac	1	1	-	1/7/9/11	-
1	FME	AA	1	1	-	2/7/9/11	-
1	FME	ak	1	1	-	2/7/9/11	-
1	FME	AL	1	1	-	3/7/9/11	-
1	FME	ae	1	1	-	0/7/9/11	-
1	FME	ag	1	1	-	1/7/9/11	-
1	FME	AJ	1	1	-	4/7/9/11	-
1	FME	ai	1	1	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AG	1	FME	C-CA-N	3.08	115.44	109.50
1	ag	1	FME	C-CA-N	3.07	115.42	109.50
1	ab	1	FME	C-CA-N	2.66	114.63	109.50
1	AB	1	FME	C-CA-N	2.66	114.63	109.50
1	AF	1	FME	C-CA-N	2.56	114.44	109.50

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AG	1	FME	O-C-CA-CB
1	AK	1	FME	O-C-CA-CB
1	ag	1	FME	O-C-CA-CB
1	ak	1	FME	O-C-CA-CB
1	AA	1	FME	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 142 ligands modelled in this entry, 2 are monoatomic - leaving 140 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	$\# Z > 2$
9	BCL	ai	102	-	69,74,74	1.20	5 (7%)	79,115,115	1.37	10 (12%)
9	BCL	AG	102	-	69,74,74	1.17	4 (5%)	79,115,115	1.31	9 (11%)
10	SP2	AF	103	-	41,41,41	0.21	0	49,50,50	0.55	2 (4%)
9	BCL	BK	101	-	69,74,74	1.17	5 (7%)	79,115,115	1.29	9 (11%)
10	SP2	BF	102	-	41,41,41	0.19	0	49,50,50	0.58	1 (2%)
10	SP2	ae	102	-	41,41,41	0.25	0	49,50,50	0.39	0
9	BCL	AF	102	-	69,74,74	1.19	4 (5%)	79,115,115	1.32	9 (11%)
10	SP2	AA	1002	-	41,41,41	0.16	0	49,50,50	0.62	1 (2%)
9	BCL	bm	1001	-	69,74,74	1.17	4 (5%)	79,115,115	1.29	9 (11%)
10	SP2	AE	101	-	41,41,41	0.25	0	49,50,50	0.40	0
10	SP2	BH	101	-	41,41,41	0.21	0	49,50,50	0.77	2 (4%)
9	BCL	AK	101	-	69,74,74	1.22	4 (5%)	79,115,115	1.38	11 (13%)
9	BCL	bk	101	-	69,74,74	1.16	5 (7%)	79,115,115	1.30	9 (11%)
10	SP2	aj	102	-	41,41,41	0.18	0	49,50,50	0.49	1 (2%)
9	BCL	AE	102	-	69,74,74	1.17	4 (5%)	79,115,115	1.33	9 (11%)
9	BCL	BH	102	-	69,74,74	1.19	5 (7%)	79,115,115	1.42	13 (16%)
10	SP2	AC	103	-	41,41,41	0.22	0	49,50,50	0.57	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	AI	102	-	69,74,74	1.20	4 (5%)	79,115,115	1.36	9 (11%)
10	SP2	AM	1000	-	41,41,41	0.21	0	49,50,50	0.57	1 (2%)
9	BCL	AL	1001	-	69,74,74	1.21	5 (7%)	79,115,115	1.29	10 (12%)
9	BCL	BJ	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	10 (12%)
10	SP2	AJ	103	-	41,41,41	0.26	0	49,50,50	0.79	2 (4%)
10	SP2	ab	103	-	41,41,41	0.14	0	49,50,50	0.90	2 (4%)
10	SP2	af	103	-	41,41,41	0.25	0	49,50,50	0.49	0
10	SP2	AC	104	-	41,41,41	0.23	0	49,50,50	0.59	1 (2%)
16	SQD	x	100	-	52,54,54	1.40	3 (5%)	62,65,65	1.53	9 (14%)
10	SP2	bf	102	-	41,41,41	0.19	0	49,50,50	0.58	1 (2%)
9	BCL	BE	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.36	10 (12%)
10	SP2	AB	104	-	41,41,41	0.22	0	49,50,50	0.67	2 (4%)
13	UQ1	L	302	-	18,18,18	0.79	0	24,25,25	1.75	6 (25%)
10	SP2	BA	101	-	41,41,41	0.21	0	49,50,50	0.57	1 (2%)
10	SP2	ad	1002	-	41,41,41	0.25	0	49,50,50	0.61	1 (2%)
10	SP2	ak	102	-	41,41,41	0.19	0	49,50,50	0.82	2 (4%)
14	U10	L	303	-	63,63,63	2.77	17 (26%)	78,79,79	1.59	21 (26%)
10	SP2	am	1000	-	41,41,41	0.17	0	49,50,50	0.48	0
10	SP2	BC	102	-	41,41,41	0.28	0	49,50,50	0.66	2 (4%)
11	3PE	ac	101	-	50,50,50	0.52	0	53,55,55	0.67	2 (3%)
10	SP2	BL	101	-	41,41,41	0.22	0	49,50,50	0.60	1 (2%)
9	BCL	bi	101	-	69,74,74	1.18	5 (7%)	79,115,115	1.30	10 (12%)
17	LMT	M	1001	-	36,36,36	1.08	4 (11%)	47,47,47	1.00	1 (2%)
9	BCL	ba	102	-	69,74,74	1.17	5 (7%)	79,115,115	1.39	11 (13%)
10	SP2	AG	101	-	41,41,41	0.22	0	49,50,50	0.51	0
10	SP2	af	104	-	41,41,41	0.22	0	49,50,50	0.56	2 (4%)
9	BCL	ah	101	-	69,74,74	1.20	4 (5%)	79,115,115	1.30	8 (10%)
9	BCL	l	305	-	69,74,74	1.12	4 (5%)	79,115,115	1.34	10 (12%)
9	BCL	L	304	-	69,74,74	1.14	4 (5%)	79,115,115	1.27	9 (11%)
10	SP2	bb	1002	-	41,41,41	0.28	0	49,50,50	0.67	1 (2%)
9	BCL	BF	101	-	69,74,74	1.17	5 (7%)	79,115,115	1.26	9 (11%)
9	BCL	m	1004	-	69,74,74	1.17	6 (8%)	79,115,115	1.35	9 (11%)
10	SP2	AI	103	-	41,41,41	0.35	0	49,50,50	0.82	2 (4%)
9	BCL	BB	1001	-	69,74,74	1.17	5 (7%)	79,115,115	1.38	12 (15%)
12	CD4	H	302	-	83,83,83	0.48	0	89,95,95	0.94	6 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	ak	101	-	69,74,74	1.21	4 (5%)	79,115,115	1.37	11 (13%)
9	BCL	BC	101	-	69,74,74	1.18	5 (7%)	79,115,115	1.49	13 (16%)
10	SP2	ab	101	-	41,41,41	0.18	0	49,50,50	0.65	2 (4%)
15	BPH	L	305	-	59,70,70	1.12	5 (8%)	59,101,101	1.90	10 (16%)
9	BCL	AD	1001	-	69,74,74	1.19	4 (5%)	79,115,115	1.35	9 (11%)
10	SP2	ai	101	-	41,41,41	0.34	0	49,50,50	0.93	2 (4%)
10	SP2	ac	103	-	41,41,41	0.16	0	49,50,50	0.61	1 (2%)
13	UQ1	l	304	-	18,18,18	0.79	0	24,25,25	1.74	6 (25%)
9	BCL	ab	102	-	69,74,74	1.22	7 (10%)	79,115,115	1.38	10 (12%)
9	BCL	an	101	-	69,74,74	1.21	4 (5%)	79,115,115	1.28	9 (11%)
14	U10	m	1003	-	63,63,63	2.73	17 (26%)	78,79,79	1.74	19 (24%)
10	SP2	BL	103	-	41,41,41	0.36	0	49,50,50	0.64	2 (4%)
9	BCL	aj	101	-	69,74,74	1.21	4 (5%)	79,115,115	1.38	11 (13%)
9	BCL	AH	101	-	69,74,74	1.20	4 (5%)	79,115,115	1.29	8 (10%)
9	BCL	ac	102	-	69,74,74	1.18	5 (7%)	79,115,115	1.30	9 (11%)
15	BPH	m	1002	-	59,70,70	1.11	5 (8%)	59,101,101	1.90	10 (16%)
11	3PE	H	301	-	50,50,50	0.53	0	53,55,55	0.50	1 (1%)
9	BCL	AN	101	-	69,74,74	1.21	5 (7%)	79,115,115	1.29	9 (11%)
12	CD4	h	302	-	83,83,83	0.48	0	89,95,95	0.94	6 (6%)
16	SQD	L	306	-	52,54,54	1.40	3 (5%)	62,65,65	1.55	8 (12%)
10	SP2	BE	1002	-	41,41,41	0.18	0	49,50,50	0.68	2 (4%)
14	U10	M	1007	-	63,63,63	2.73	17 (26%)	78,79,79	1.74	20 (25%)
9	BCL	ad	1001	-	69,74,74	1.19	4 (5%)	79,115,115	1.35	9 (11%)
10	SP2	AH	102	-	41,41,41	0.17	0	49,50,50	0.56	2 (4%)
9	BCL	AC	101	-	69,74,74	1.18	5 (7%)	79,115,115	1.31	9 (11%)
9	BCL	BG	101	-	69,74,74	1.17	4 (5%)	79,115,115	1.31	10 (12%)
9	BCL	al	1001	-	69,74,74	1.21	5 (7%)	79,115,115	1.32	10 (12%)
9	BCL	AB	101	-	69,74,74	1.22	7 (10%)	79,115,115	1.40	11 (13%)
10	SP2	ae	103	-	41,41,41	0.19	0	49,50,50	0.69	2 (4%)
9	BCL	be	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.36	10 (12%)
9	BCL	bj	102	-	69,74,74	1.15	5 (7%)	79,115,115	1.30	10 (12%)
10	SP2	bk	102	-	41,41,41	0.23	0	49,50,50	0.58	1 (2%)
10	SP2	m	1007	-	41,41,41	0.12	0	49,50,50	0.48	0
10	SP2	aj	103	-	41,41,41	0.23	0	49,50,50	0.76	1 (2%)
15	BPH	M	1003	-	59,70,70	1.11	5 (8%)	59,101,101	1.90	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SP2	AI	101	-	41,41,41	0.33	0	49,50,50	0.97	3 (6%)
10	SP2	AJ	102	-	41,41,41	0.17	0	49,50,50	0.48	0
10	SP2	AB	102	-	41,41,41	0.15	0	49,50,50	0.87	2 (4%)
9	BCL	bh	102	-	69,74,74	1.19	5 (7%)	79,115,115	1.42	13 (16%)
17	LMT	m	1001	-	36,36,36	1.08	4 (11%)	47,47,47	1.00	1 (2%)
10	SP2	AF	101	-	41,41,41	0.18	0	49,50,50	0.69	1 (2%)
9	BCL	l	301	-	69,74,74	1.14	4 (5%)	79,115,115	1.27	9 (11%)
9	BCL	L	301	-	69,74,74	1.12	4 (5%)	79,115,115	1.34	10 (12%)
9	BCL	ag	101	-	69,74,74	1.17	4 (5%)	79,115,115	1.31	9 (11%)
9	BCL	bf	101	-	69,74,74	1.17	5 (7%)	79,115,115	1.26	9 (11%)
9	BCL	bc	101	-	69,74,74	1.18	5 (7%)	79,115,115	1.50	13 (16%)
9	BCL	bg	101	-	69,74,74	1.17	4 (5%)	79,115,115	1.30	10 (12%)
12	CD4	m	1005	-	83,83,83	0.48	0	89,95,95	1.06	5 (5%)
9	BCL	BA	102	-	69,74,74	1.17	5 (7%)	79,115,115	1.39	11 (13%)
9	BCL	bl	101	-	69,74,74	1.18	4 (5%)	79,115,115	1.27	11 (13%)
9	BCL	bn	101	-	69,74,74	1.19	4 (5%)	79,115,115	1.33	10 (12%)
9	BCL	am	1001	-	69,74,74	1.22	4 (5%)	79,115,115	1.33	8 (10%)
9	BCL	bd	101	-	69,74,74	1.17	5 (7%)	79,115,115	1.31	11 (13%)
10	SP2	ah	102	-	41,41,41	0.18	0	49,50,50	0.54	1 (2%)
10	SP2	ai	103	-	41,41,41	0.36	0	49,50,50	0.84	2 (4%)
9	BCL	BI	101	-	69,74,74	1.18	5 (7%)	79,115,115	1.30	10 (12%)
15	BPH	l	302	-	59,70,70	1.12	5 (8%)	59,101,101	1.91	10 (16%)
9	BCL	BD	101	-	69,74,74	1.17	5 (7%)	79,115,115	1.31	11 (13%)
14	U10	l	303	-	63,63,63	2.77	17 (26%)	78,79,79	1.59	21 (26%)
9	BCL	aa	1001	-	69,74,74	1.18	5 (7%)	79,115,115	1.34	9 (11%)
10	SP2	bj	101	-	41,41,41	0.17	0	49,50,50	0.38	0
9	BCL	AJ	101	-	69,74,74	1.21	4 (5%)	79,115,115	1.38	11 (13%)
10	SP2	ac	104	-	41,41,41	0.25	0	49,50,50	0.57	1 (2%)
10	SP2	ba	101	-	41,41,41	0.18	0	49,50,50	0.56	1 (2%)
9	BCL	BL	102	-	69,74,74	1.18	4 (5%)	79,115,115	1.28	11 (13%)
12	CD4	M	1004	-	83,83,83	0.48	0	89,95,95	1.06	5 (5%)
9	BCL	m	1006	-	69,74,74	1.15	5 (7%)	79,115,115	1.39	10 (12%)
10	SP2	bl	102	-	41,41,41	0.37	0	49,50,50	0.64	2 (4%)
9	BCL	M	1002	-	69,74,74	1.15	5 (7%)	79,115,115	1.39	10 (12%)
9	BCL	bb	1001	-	69,74,74	1.16	5 (7%)	79,115,115	1.38	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	BN	101	-	69,74,74	1.19	4 (5%)	79,115,115	1.33	10 (12%)
9	BCL	af	101	-	69,74,74	1.20	4 (5%)	79,115,115	1.32	9 (11%)
9	BCL	AA	1001	-	69,74,74	1.18	5 (7%)	79,115,115	1.34	9 (11%)
10	SP2	al	1002	-	41,41,41	0.27	0	49,50,50	0.58	1 (2%)
10	SP2	BK	102	-	41,41,41	0.22	0	49,50,50	0.63	2 (4%)
9	BCL	AM	1001	-	69,74,74	1.22	4 (5%)	79,115,115	1.34	8 (10%)
10	SP2	BJ	101	-	41,41,41	0.16	0	49,50,50	0.51	1 (2%)
11	3PE	AC	102	-	50,50,50	0.52	0	53,55,55	0.67	2 (3%)
11	3PE	h	301	-	50,50,50	0.53	0	53,55,55	0.50	1 (1%)
10	SP2	AB	103	-	41,41,41	0.23	0	49,50,50	0.60	1 (2%)
9	BCL	M	1008	-	69,74,74	1.17	6 (8%)	79,115,115	1.34	9 (11%)
10	SP2	bh	101	-	41,41,41	0.24	0	49,50,50	0.63	2 (4%)
10	SP2	ab	104	-	41,41,41	0.17	0	49,50,50	0.54	1 (2%)
10	SP2	AK	102	-	41,41,41	0.19	0	49,50,50	0.83	2 (4%)
9	BCL	BM	1001	-	69,74,74	1.17	4 (5%)	79,115,115	1.29	9 (11%)
9	BCL	ae	101	-	69,74,74	1.17	4 (5%)	79,115,115	1.32	9 (11%)
10	SP2	M	1005	-	41,41,41	0.18	0	49,50,50	0.53	0
10	SP2	af	102	-	41,41,41	0.19	0	49,50,50	0.61	1 (2%)

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
9	BCL	ai	102	-	-	7/41/137/137	-
9	BCL	AG	102	-	-	0/41/137/137	-
10	SP2	AF	103	-	-	4/47/47/47	-
9	BCL	BK	101	-	-	4/41/137/137	-
10	SP2	BF	102	-	-	3/47/47/47	-
10	SP2	ae	102	-	-	1/47/47/47	-
9	BCL	AF	102	-	-	6/41/137/137	-
10	SP2	AA	1002	-	-	5/47/47/47	-
9	BCL	bm	1001	-	-	8/41/137/137	-
10	SP2	AE	101	-	-	2/47/47/47	-
10	SP2	BH	101	-	-	5/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AK	101	-	-	4/41/137/137	-
9	BCL	bk	101	-	-	4/41/137/137	-
10	SP2	aj	102	-	-	4/47/47/47	-
9	BCL	AE	102	-	-	4/41/137/137	-
9	BCL	BH	102	-	-	5/41/137/137	-
10	SP2	AC	103	-	-	3/47/47/47	-
9	BCL	AI	102	-	-	7/41/137/137	-
10	SP2	AM	1000	-	-	8/47/47/47	-
9	BCL	AL	1001	-	-	4/41/137/137	-
9	BCL	BJ	102	-	-	6/41/137/137	-
10	SP2	AJ	103	-	-	8/47/47/47	-
10	SP2	ab	103	-	-	6/47/47/47	-
10	SP2	af	103	-	-	8/47/47/47	-
10	SP2	AC	104	-	-	7/47/47/47	-
16	SQD	x	100	-	-	5/49/69/69	0/1/1/1
10	SP2	bf	102	-	-	2/47/47/47	-
9	BCL	BE	1001	-	-	5/41/137/137	-
10	SP2	AB	104	-	-	6/47/47/47	-
13	UQ1	L	302	-	-	4/9/33/33	0/1/1/1
10	SP2	BA	101	-	-	6/47/47/47	-
10	SP2	ad	1002	-	-	5/47/47/47	-
10	SP2	ak	102	-	-	7/47/47/47	-
14	U10	L	303	-	-	16/63/87/87	0/1/1/1
10	SP2	am	1000	-	-	2/47/47/47	-
10	SP2	BC	102	-	-	2/47/47/47	-
11	3PE	ac	101	-	-	22/54/54/54	-
10	SP2	BL	101	-	-	5/47/47/47	-
9	BCL	bi	101	-	-	6/41/137/137	-
17	LMT	M	1001	-	-	3/21/61/61	0/2/2/2
9	BCL	ba	102	-	-	5/41/137/137	-
10	SP2	AG	101	-	-	4/47/47/47	-
10	SP2	af	104	-	-	3/47/47/47	-
9	BCL	ah	101	-	-	0/41/137/137	-
9	BCL	l	305	-	-	0/41/137/137	-
9	BCL	L	304	-	-	0/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SP2	bb	1002	-	-	9/47/47/47	-
9	BCL	BF	101	-	-	5/41/137/137	-
9	BCL	m	1004	-	-	1/41/137/137	-
10	SP2	AI	103	-	-	4/47/47/47	-
9	BCL	BB	1001	-	-	4/41/137/137	-
12	CD4	H	302	-	-	22/94/94/94	-
9	BCL	ak	101	-	-	4/41/137/137	-
9	BCL	BC	101	-	-	8/41/137/137	-
10	SP2	ab	101	-	-	5/47/47/47	-
15	BPH	L	305	-	-	2/37/105/105	0/5/6/6
9	BCL	AD	1001	-	-	3/41/137/137	-
10	SP2	ai	101	-	-	8/47/47/47	-
10	SP2	ac	103	-	-	2/47/47/47	-
13	UQ1	l	304	-	-	4/9/33/33	0/1/1/1
9	BCL	ab	102	-	-	2/41/137/137	-
9	BCL	an	101	-	-	7/41/137/137	-
14	U10	m	1003	-	-	11/63/87/87	0/1/1/1
10	SP2	BL	103	-	-	3/47/47/47	-
9	BCL	aj	101	-	-	2/41/137/137	-
9	BCL	AH	101	-	-	1/41/137/137	-
9	BCL	ac	102	-	-	8/41/137/137	-
15	BPH	m	1002	-	-	2/37/105/105	0/5/6/6
11	3PE	H	301	-	-	11/54/54/54	-
9	BCL	AN	101	-	-	6/41/137/137	-
12	CD4	h	302	-	-	22/94/94/94	-
16	SQD	L	306	-	-	14/49/69/69	0/1/1/1
10	SP2	BE	1002	-	-	6/47/47/47	-
14	U10	M	1007	-	-	11/63/87/87	0/1/1/1
9	BCL	ad	1001	-	-	3/41/137/137	-
10	SP2	AH	102	-	-	4/47/47/47	-
9	BCL	AC	101	-	-	6/41/137/137	-
9	BCL	BG	101	-	-	4/41/137/137	-
9	BCL	al	1001	-	-	4/41/137/137	-
9	BCL	AB	101	-	-	2/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SP2	ae	103	-	-	6/47/47/47	-
9	BCL	be	1001	-	-	5/41/137/137	-
9	BCL	bj	102	-	-	6/41/137/137	-
10	SP2	bk	102	-	-	6/47/47/47	-
10	SP2	m	1007	-	-	5/47/47/47	-
10	SP2	aj	103	-	-	9/47/47/47	-
15	BPH	M	1003	-	-	2/37/105/105	0/5/6/6
10	SP2	AI	101	-	-	2/47/47/47	-
10	SP2	AJ	102	-	-	5/47/47/47	-
10	SP2	AB	102	-	-	4/47/47/47	-
9	BCL	bh	102	-	-	5/41/137/137	-
17	LMT	m	1001	-	-	3/21/61/61	0/2/2/2
10	SP2	AF	101	-	-	6/47/47/47	-
9	BCL	l	301	-	-	0/41/137/137	-
9	BCL	L	301	-	-	0/41/137/137	-
9	BCL	ag	101	-	-	0/41/137/137	-
9	BCL	bf	101	-	-	5/41/137/137	-
9	BCL	bc	101	-	-	8/41/137/137	-
9	BCL	bg	101	-	-	6/41/137/137	-
12	CD4	m	1005	-	-	13/94/94/94	-
9	BCL	BA	102	-	-	5/41/137/137	-
9	BCL	bl	101	-	-	8/41/137/137	-
9	BCL	bn	101	-	-	7/41/137/137	-
9	BCL	am	1001	-	-	0/41/137/137	-
9	BCL	bd	101	-	-	1/41/137/137	-
10	SP2	ah	102	-	-	4/47/47/47	-
10	SP2	ai	103	-	-	3/47/47/47	-
9	BCL	BI	101	-	-	5/41/137/137	-
15	BPH	l	302	-	-	2/37/105/105	0/5/6/6
9	BCL	BD	101	-	-	1/41/137/137	-
14	U10	l	303	-	-	16/63/87/87	0/1/1/1
9	BCL	aa	1001	-	-	2/41/137/137	-
10	SP2	bj	101	-	-	7/47/47/47	-
9	BCL	AJ	101	-	-	4/41/137/137	-
10	SP2	ac	104	-	-	7/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SP2	ba	101	-	-	7/47/47/47	-
9	BCL	BL	102	-	-	8/41/137/137	-
12	CD4	M	1004	-	-	13/94/94/94	-
9	BCL	m	1006	-	-	3/41/137/137	-
10	SP2	bl	102	-	-	2/47/47/47	-
9	BCL	M	1002	-	-	3/41/137/137	-
9	BCL	bb	1001	-	-	4/41/137/137	-
9	BCL	BN	101	-	-	7/41/137/137	-
9	BCL	af	101	-	-	7/41/137/137	-
9	BCL	AA	1001	-	-	2/41/137/137	-
10	SP2	al	1002	-	-	4/47/47/47	-
10	SP2	BK	102	-	-	8/47/47/47	-
9	BCL	AM	1001	-	-	0/41/137/137	-
10	SP2	BJ	101	-	-	7/47/47/47	-
11	3PE	AC	102	-	-	22/54/54/54	-
11	3PE	h	301	-	-	11/54/54/54	-
10	SP2	AB	103	-	-	7/47/47/47	-
9	BCL	M	1008	-	-	1/41/137/137	-
10	SP2	bh	101	-	-	2/47/47/47	-
10	SP2	ab	104	-	-	4/47/47/47	-
10	SP2	AK	102	-	-	7/47/47/47	-
9	BCL	BM	1001	-	-	8/41/137/137	-
9	BCL	ae	101	-	-	4/41/137/137	-
10	SP2	M	1005	-	-	3/47/47/47	-
10	SP2	af	102	-	-	6/47/47/47	-

The worst 5 of 398 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	303	U10	C43-C44	6.41	1.47	1.33
14	L	303	U10	C43-C44	6.40	1.47	1.33
14	M	1007	U10	C38-C39	6.39	1.47	1.33
14	m	1003	U10	C38-C39	6.39	1.47	1.33
14	l	303	U10	C48-C49	6.37	1.47	1.33

The worst 5 of 881 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	1003	BPH	C4D-CHA-CBD	-9.99	103.67	108.45
15	m	1002	BPH	C4D-CHA-CBD	-9.99	103.67	108.45
15	l	302	BPH	C4D-CHA-CBD	-9.94	103.69	108.45
15	L	305	BPH	C4D-CHA-CBD	-9.94	103.69	108.45
16	x	100	SQD	O8-S-C6	-5.69	94.99	105.97

There are no chirality outliers.

5 of 759 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	BA	102	BCL	C3A-C2A-CAA-CBA
9	BB	1001	BCL	C1A-C2A-CAA-CBA
9	BF	101	BCL	C1A-C2A-CAA-CBA
9	BJ	102	BCL	C1A-C2A-CAA-CBA
9	BL	102	BCL	C1A-C2A-CAA-CBA

There are no ring outliers.

98 monomers are involved in 150 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	ai	102	BCL	4	0
10	AF	103	SP2	2	0
9	BK	101	BCL	1	0
10	BF	102	SP2	3	0
10	ae	102	SP2	1	0
9	AF	102	BCL	1	0
10	AA	1002	SP2	1	0
9	bm	1001	BCL	1	0
10	AE	101	SP2	1	0
10	BH	101	SP2	3	0
9	AK	101	BCL	3	0
9	bk	101	BCL	1	0
10	aj	102	SP2	2	0
9	BH	102	BCL	1	0
10	AC	103	SP2	1	0
9	AI	102	BCL	4	0
10	AM	1000	SP2	1	0
9	BJ	102	BCL	1	0
10	AJ	103	SP2	2	0
10	ab	103	SP2	1	0
10	af	103	SP2	3	0
10	AC	104	SP2	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	bf	102	SP2	3	0
9	BE	1001	BCL	1	0
10	AB	104	SP2	2	0
10	BA	101	SP2	1	0
10	ad	1002	SP2	1	0
10	ak	102	SP2	3	0
14	L	303	U10	3	0
10	BC	102	SP2	3	0
11	ac	101	3PE	1	0
9	bi	101	BCL	2	0
9	ba	102	BCL	2	0
10	AG	101	SP2	4	0
10	af	104	SP2	1	0
9	ah	101	BCL	1	0
10	bb	1002	SP2	1	0
9	BF	101	BCL	1	0
9	ak	101	BCL	3	0
9	BC	101	BCL	1	0
10	ab	101	SP2	1	0
15	L	305	BPH	1	0
9	AD	1001	BCL	1	0
10	ai	101	SP2	2	0
10	ac	103	SP2	3	0
13	l	304	UQ1	1	0
9	ab	102	BCL	4	0
14	m	1003	U10	2	0
10	BL	103	SP2	2	0
9	aj	101	BCL	2	0
9	AH	101	BCL	1	0
9	ac	102	BCL	1	0
16	L	306	SQD	1	0
10	BE	1002	SP2	1	0
14	M	1007	U10	2	0
10	AH	102	SP2	3	0
9	AC	101	BCL	1	0
9	AB	101	BCL	3	0
10	ae	103	SP2	2	0
9	be	1001	BCL	1	0
9	bj	102	BCL	1	0
10	bk	102	SP2	2	0
10	m	1007	SP2	2	0
10	aj	103	SP2	4	0

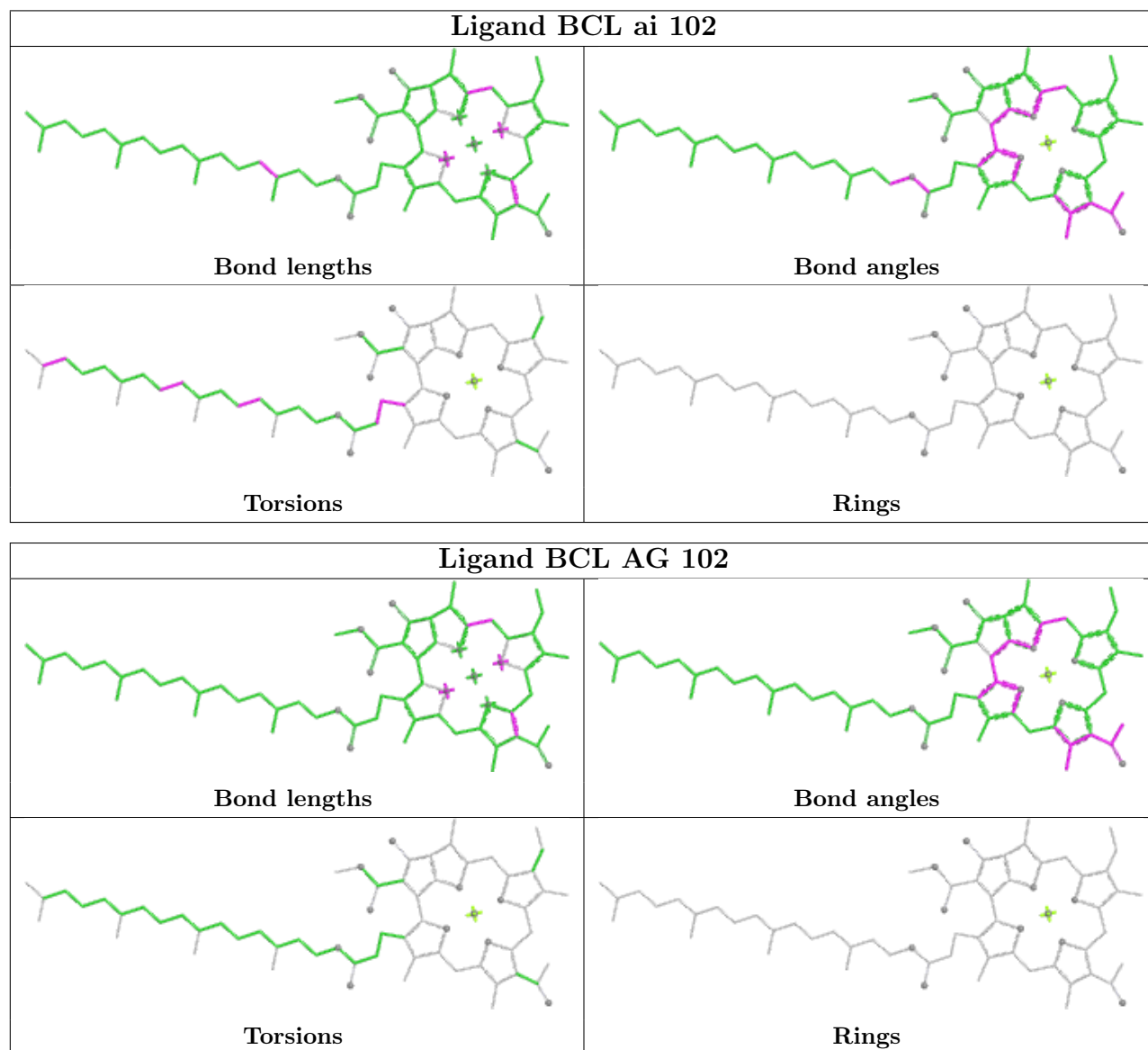
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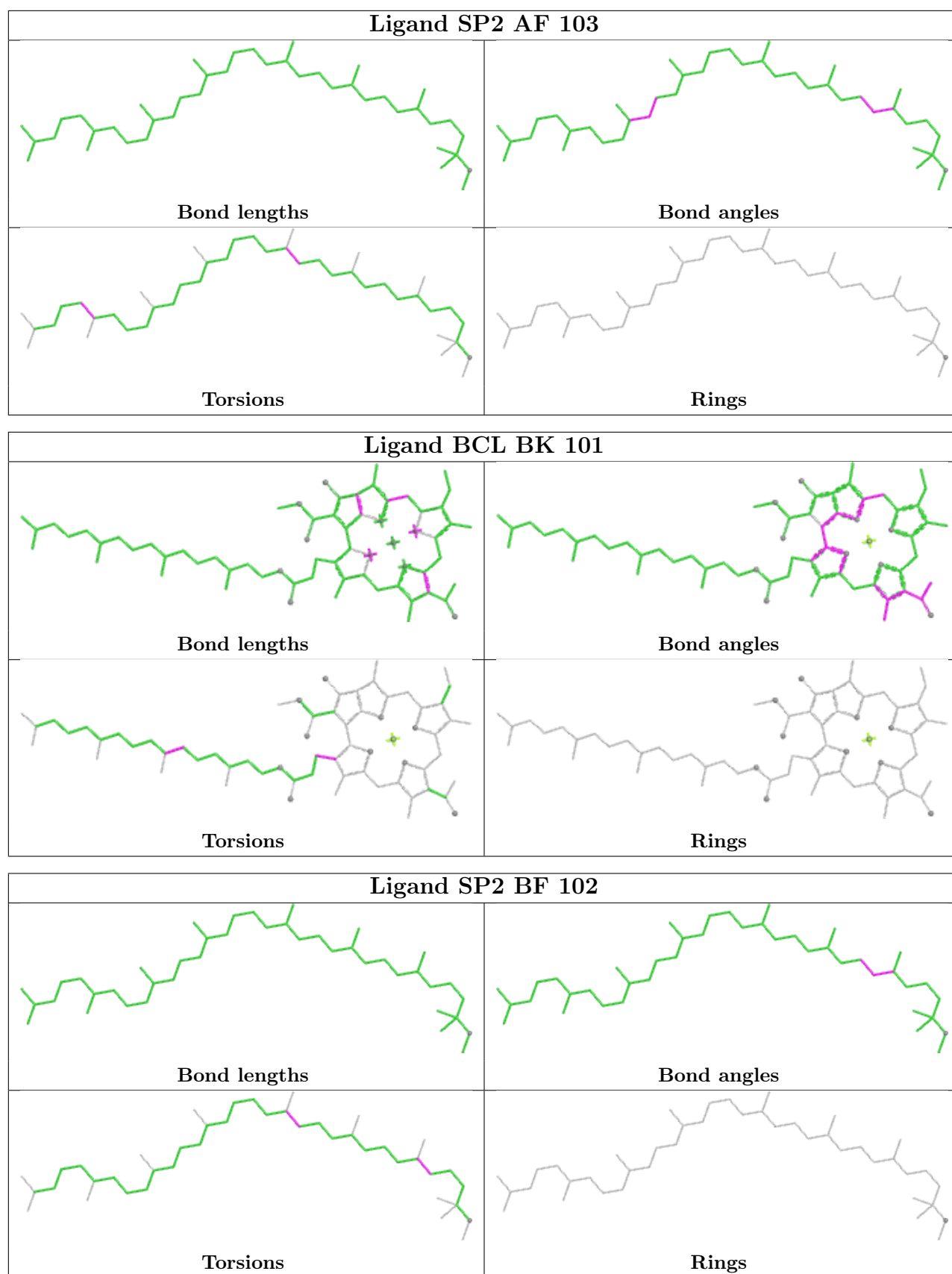
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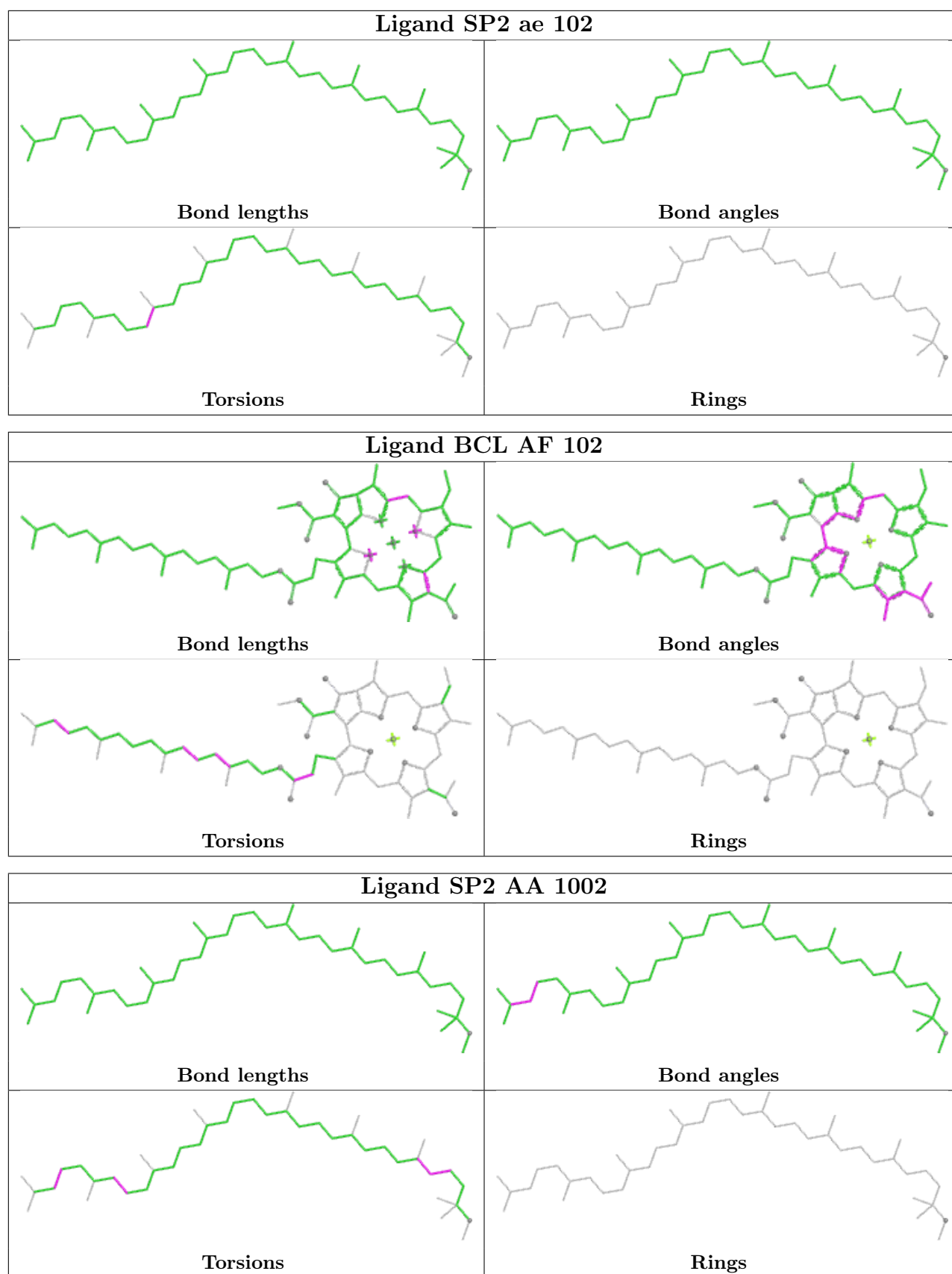
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	M	1003	BPH	1	0
10	AI	101	SP2	2	0
10	AJ	102	SP2	1	0
10	AB	102	SP2	1	0
9	bh	102	BCL	1	0
9	bf	101	BCL	1	0
9	bc	101	BCL	1	0
12	m	1005	CD4	1	0
9	BA	102	BCL	2	0
9	bl	101	BCL	2	0
9	bn	101	BCL	1	0
9	am	1001	BCL	2	0
9	bd	101	BCL	1	0
10	ah	102	SP2	3	0
9	BI	101	BCL	1	0
9	BD	101	BCL	1	0
14	l	303	U10	2	0
9	aa	1001	BCL	1	0
9	AJ	101	BCL	3	0
10	ac	104	SP2	1	0
9	BL	102	BCL	2	0
12	M	1004	CD4	1	0
10	bl	102	SP2	1	0
9	BN	101	BCL	1	0
10	al	1002	SP2	3	0
10	BK	102	SP2	1	0
9	AM	1001	BCL	1	0
11	AC	102	3PE	1	0
10	AB	103	SP2	1	0
10	bh	101	SP2	2	0
10	ab	104	SP2	1	0
10	AK	102	SP2	3	0
9	BM	1001	BCL	1	0
10	af	102	SP2	1	0

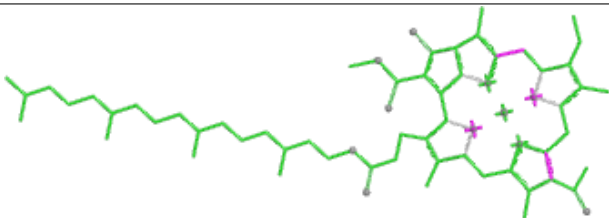
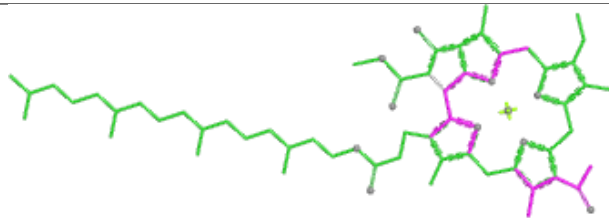
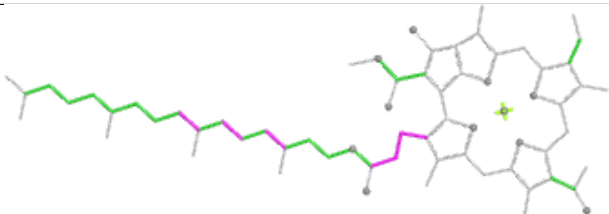
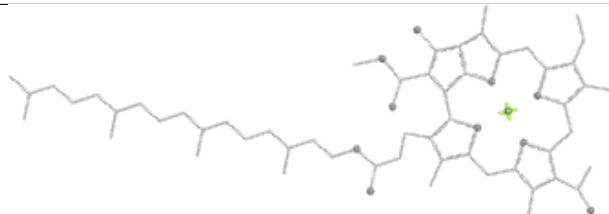
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

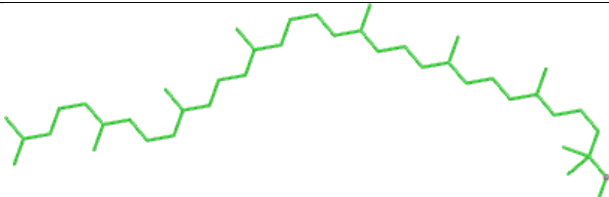
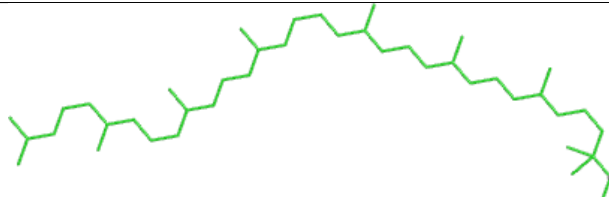
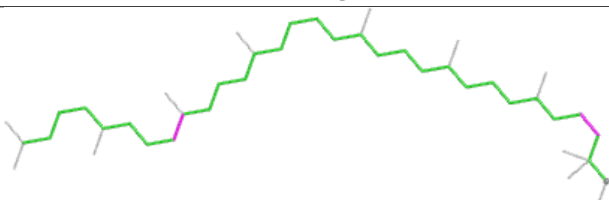
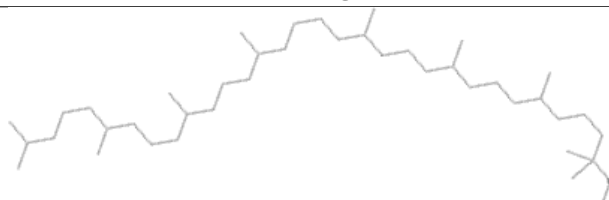
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

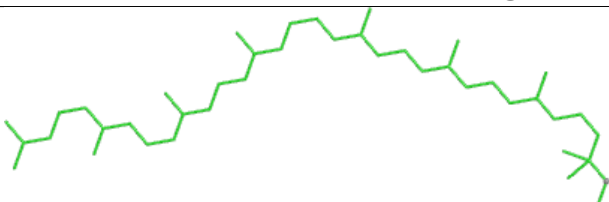
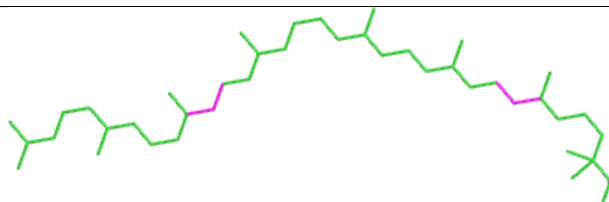
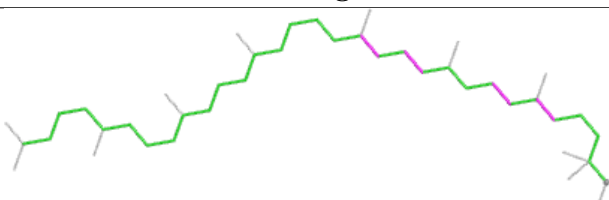
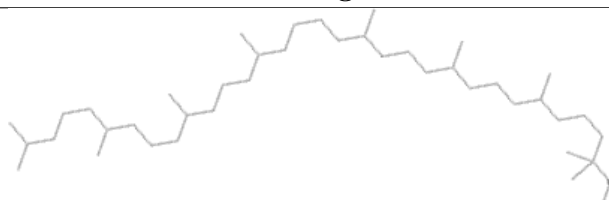


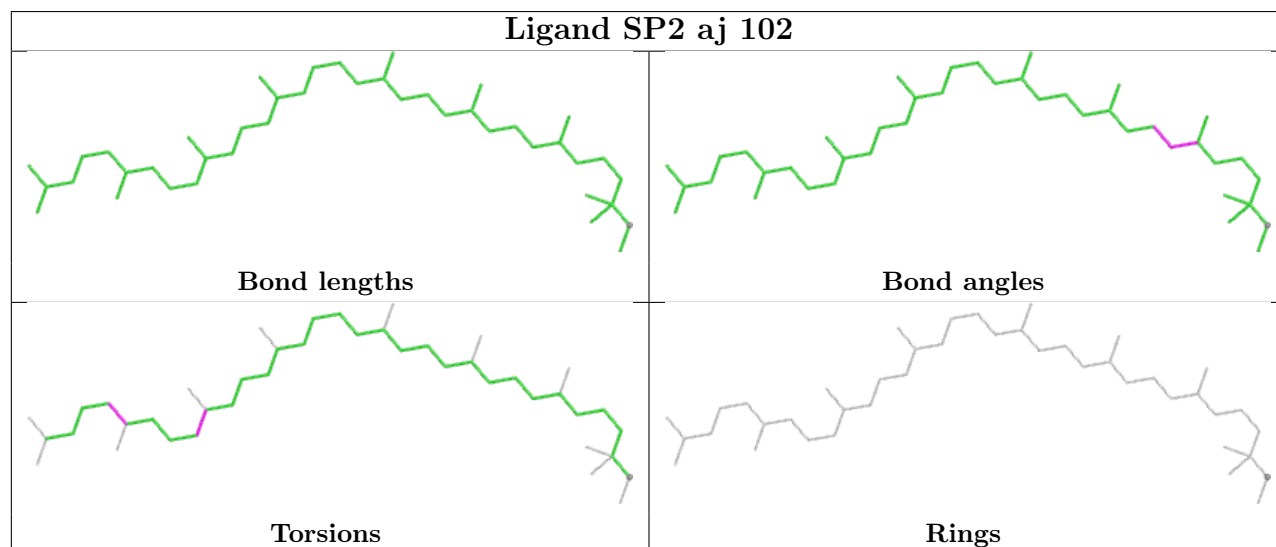
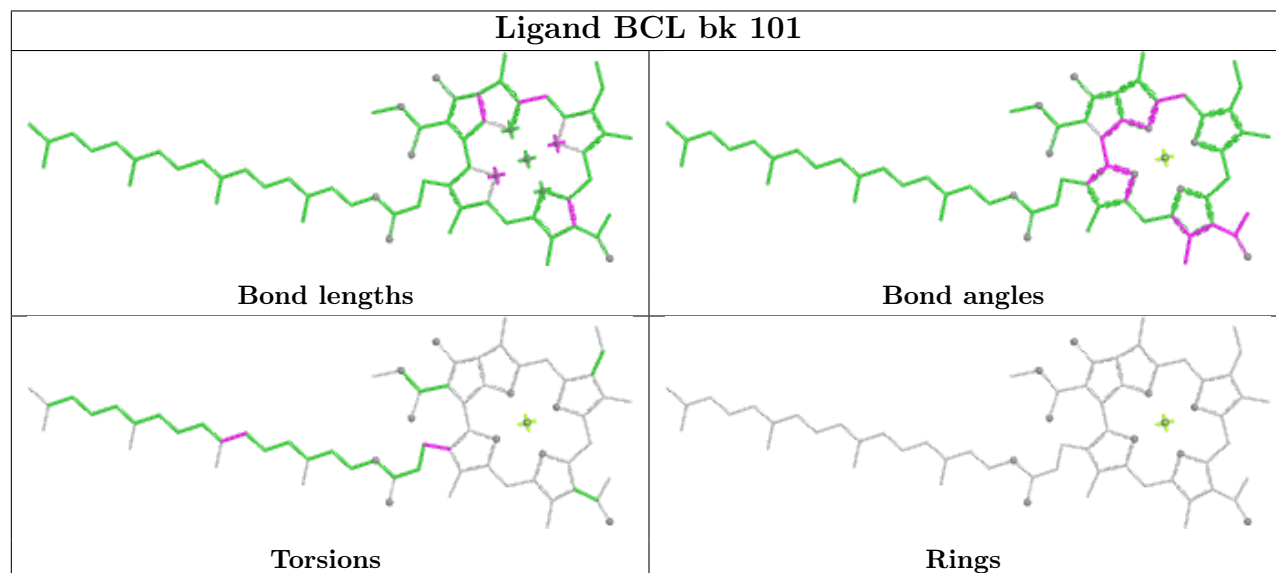
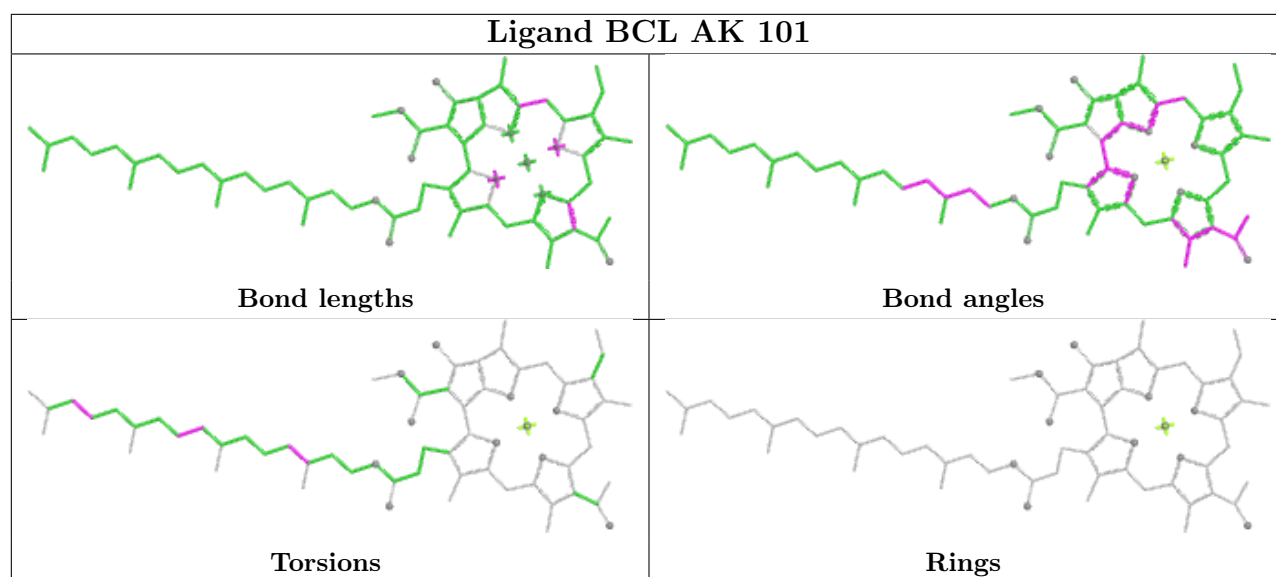


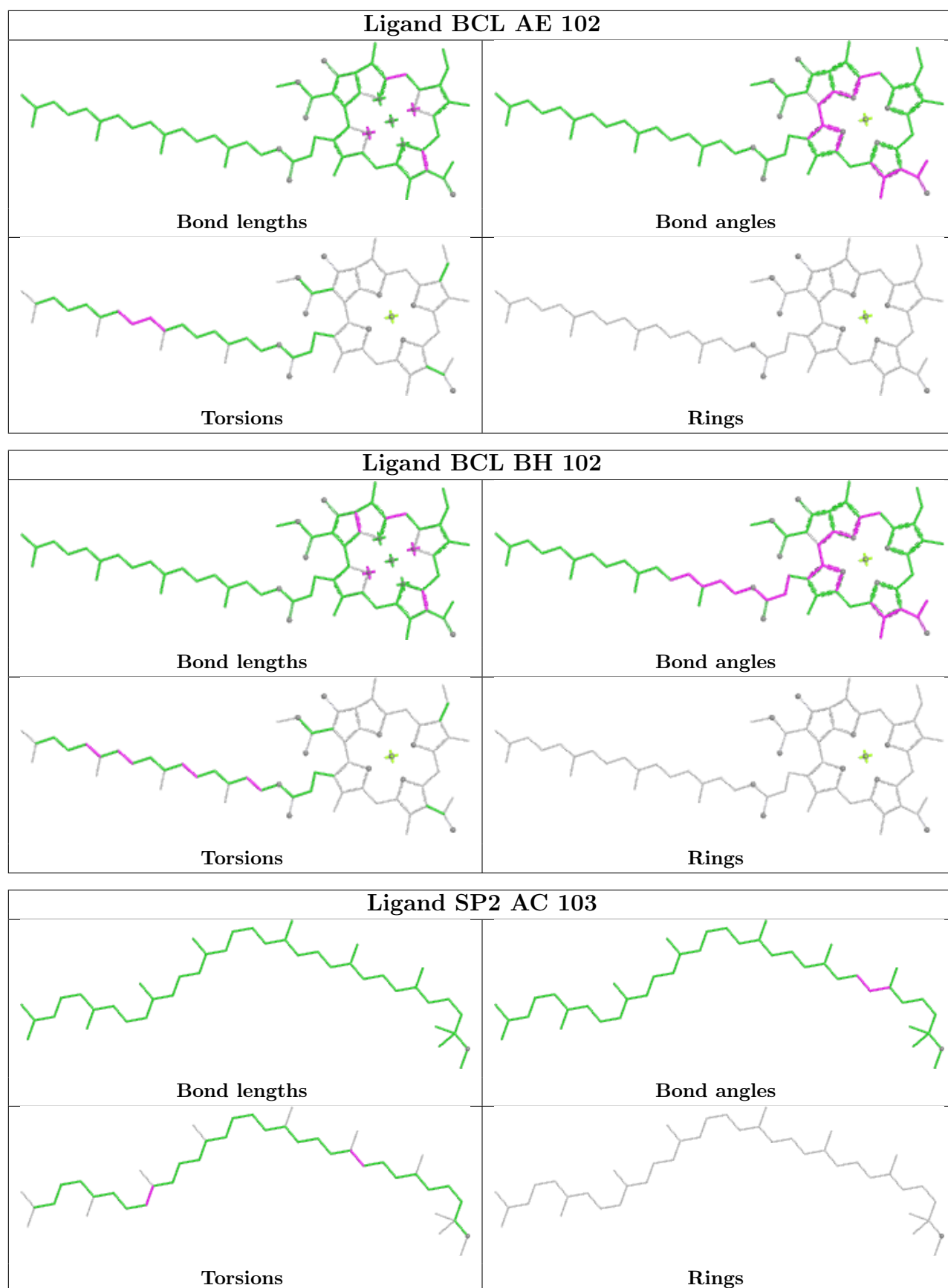


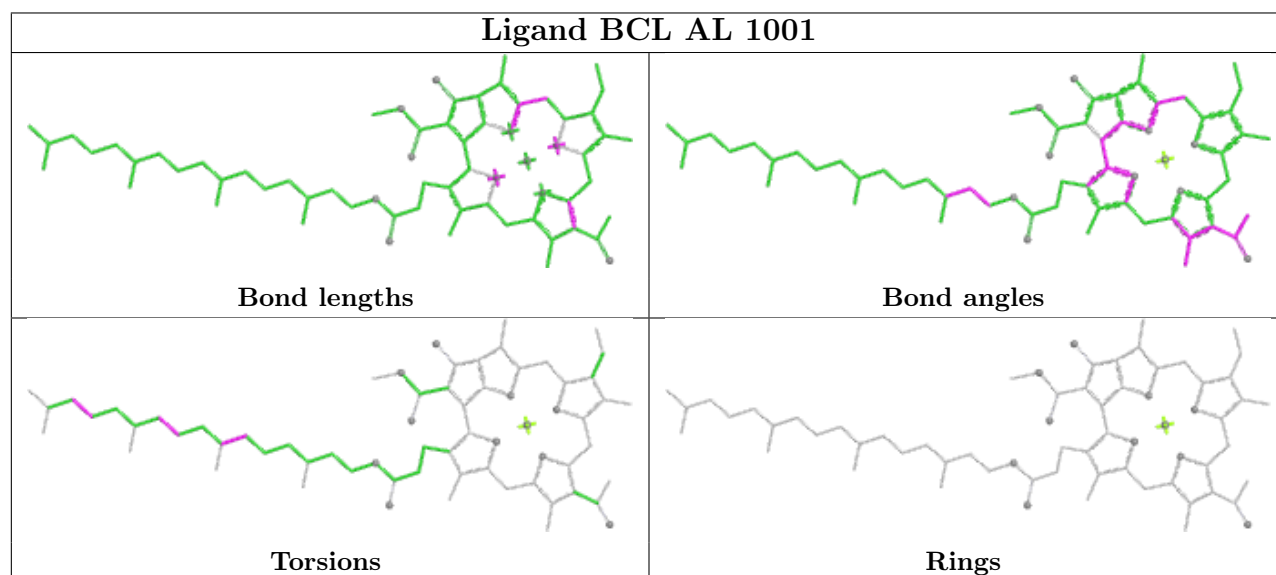
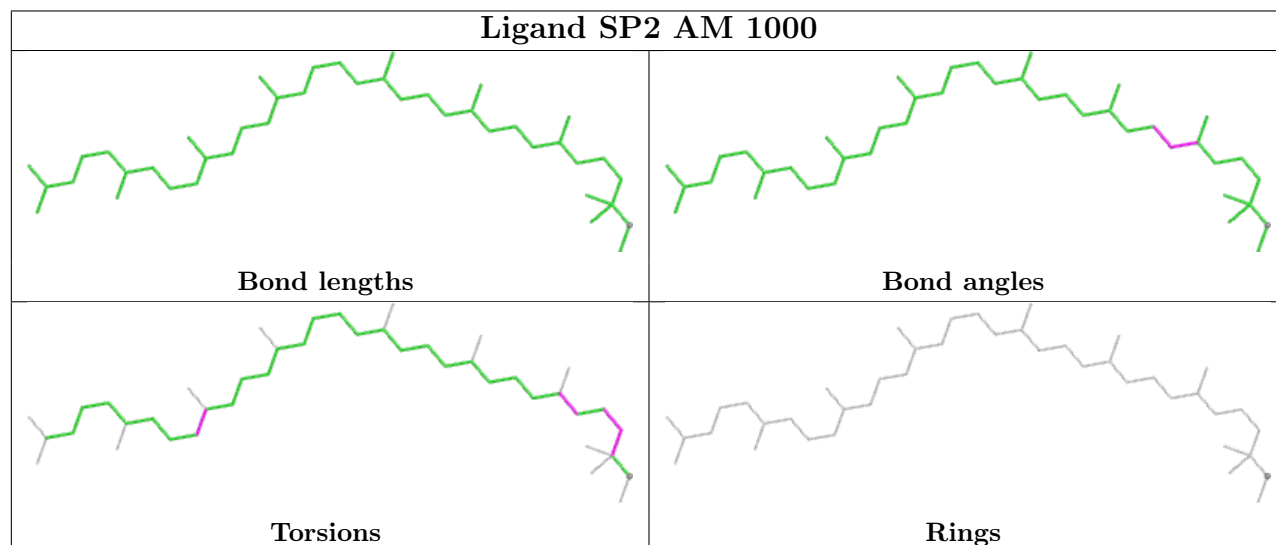
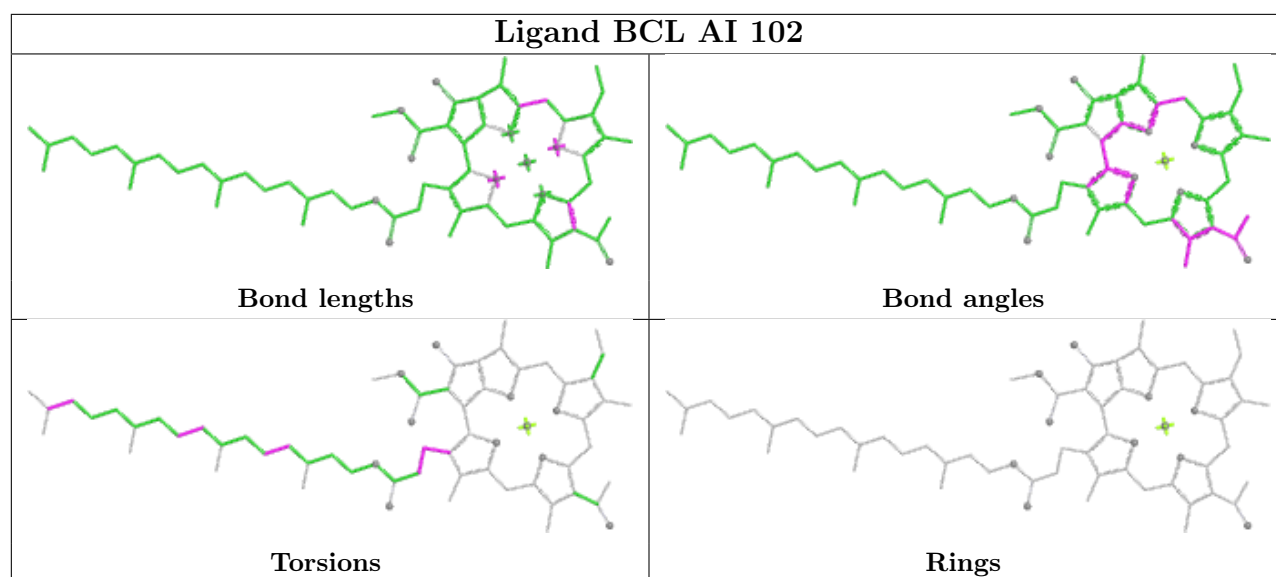
Ligand BCL bm 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

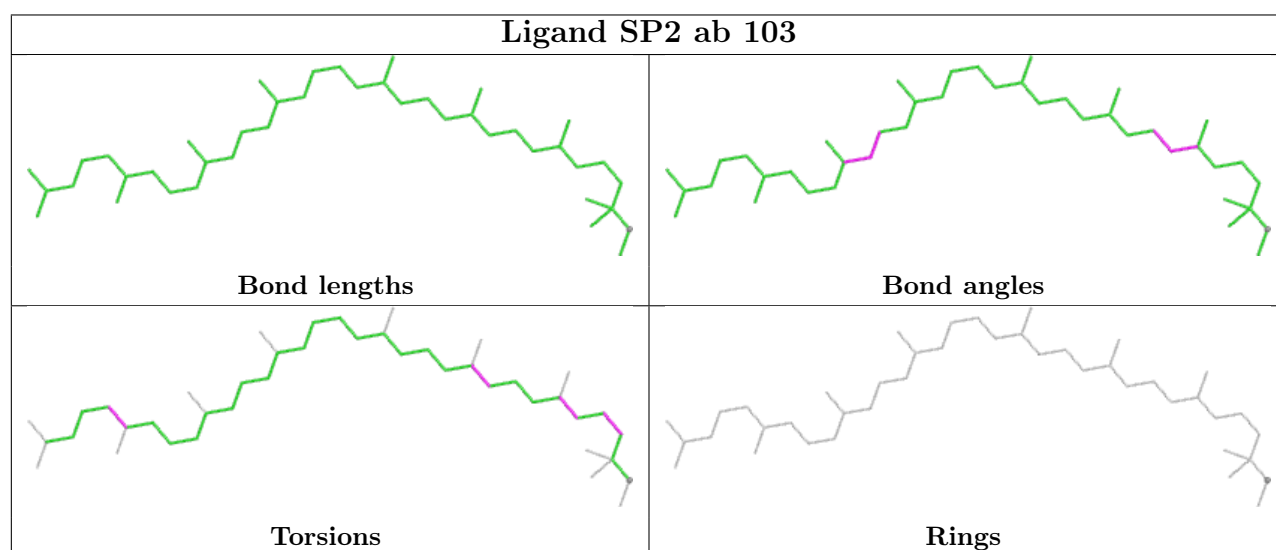
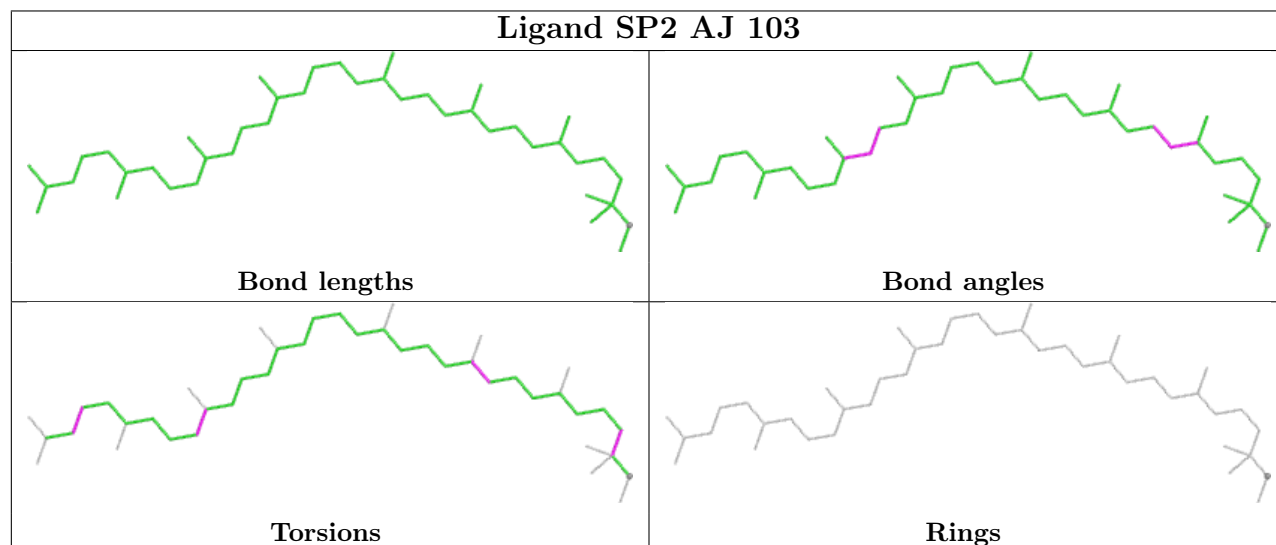
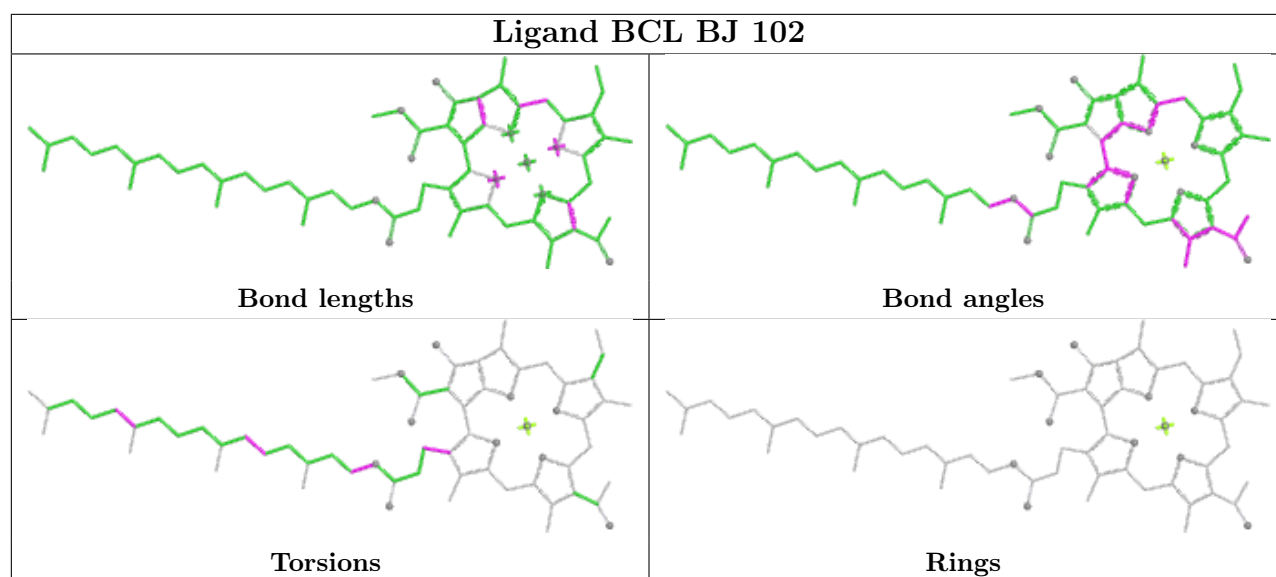
Ligand SP2 AE 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

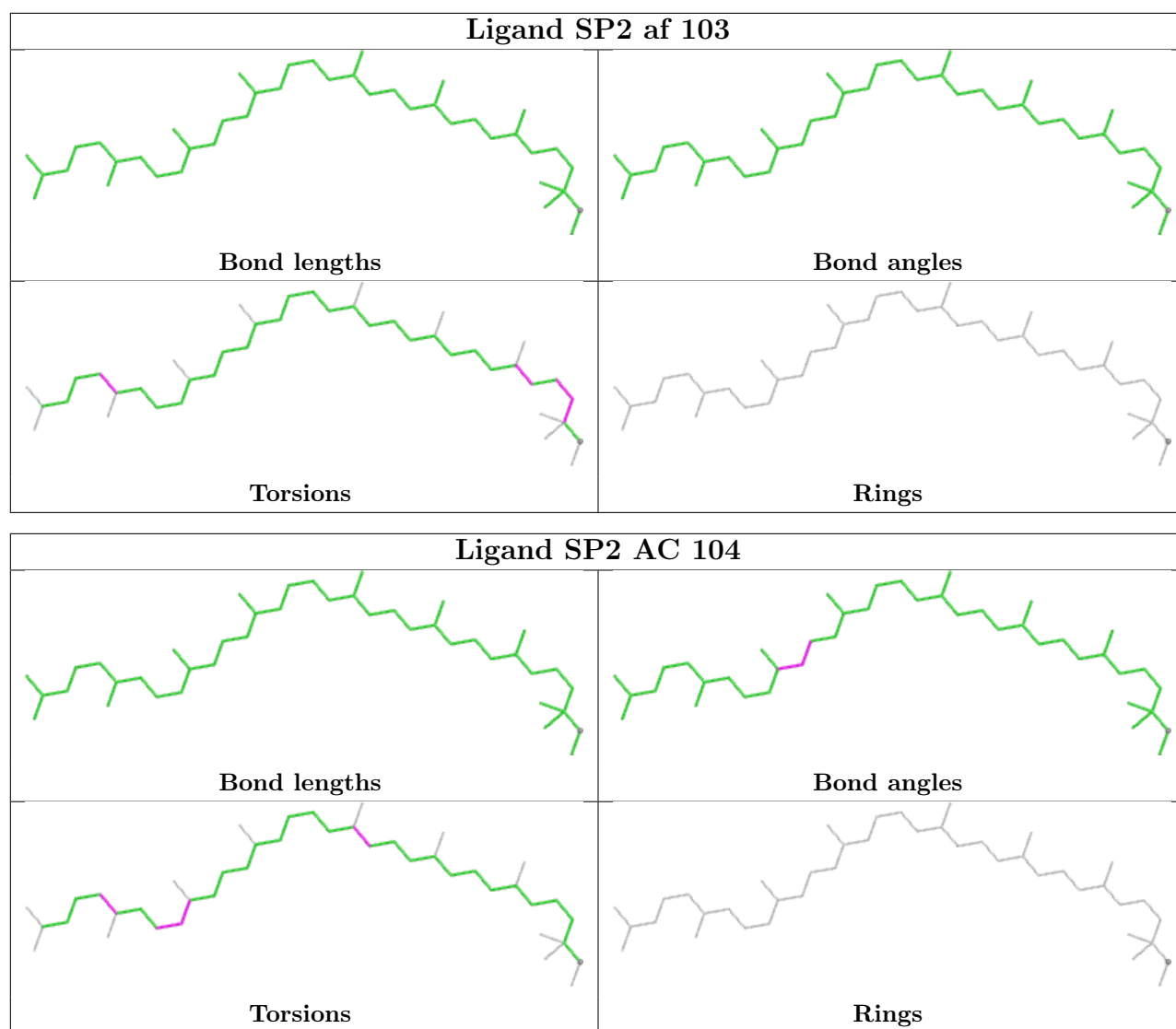
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Bond lengths	Bond angles
	
Torsions	Rings

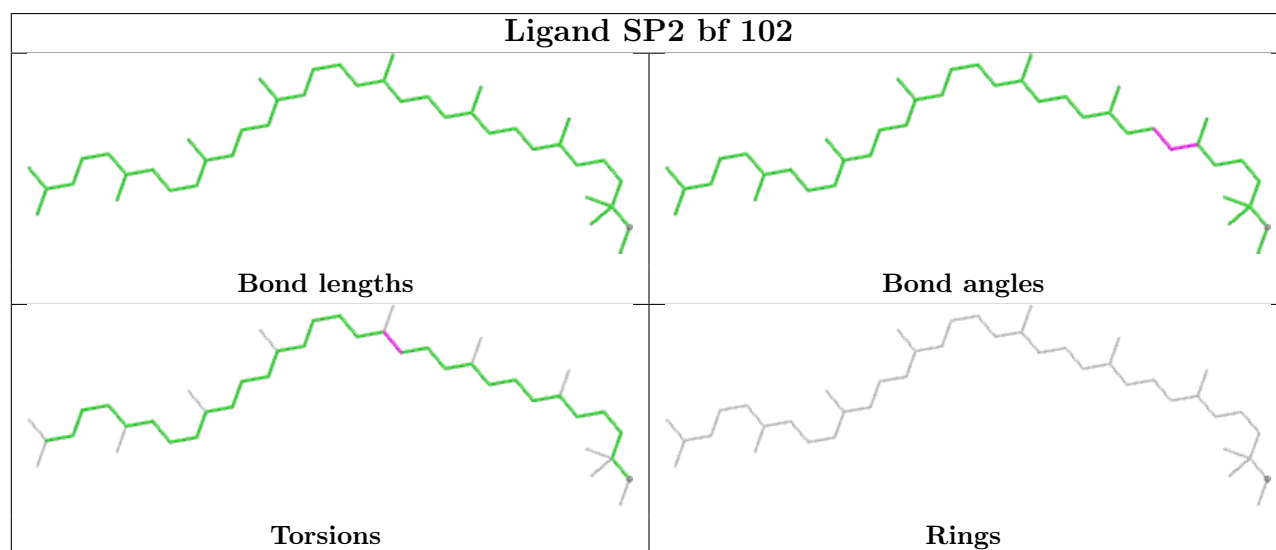
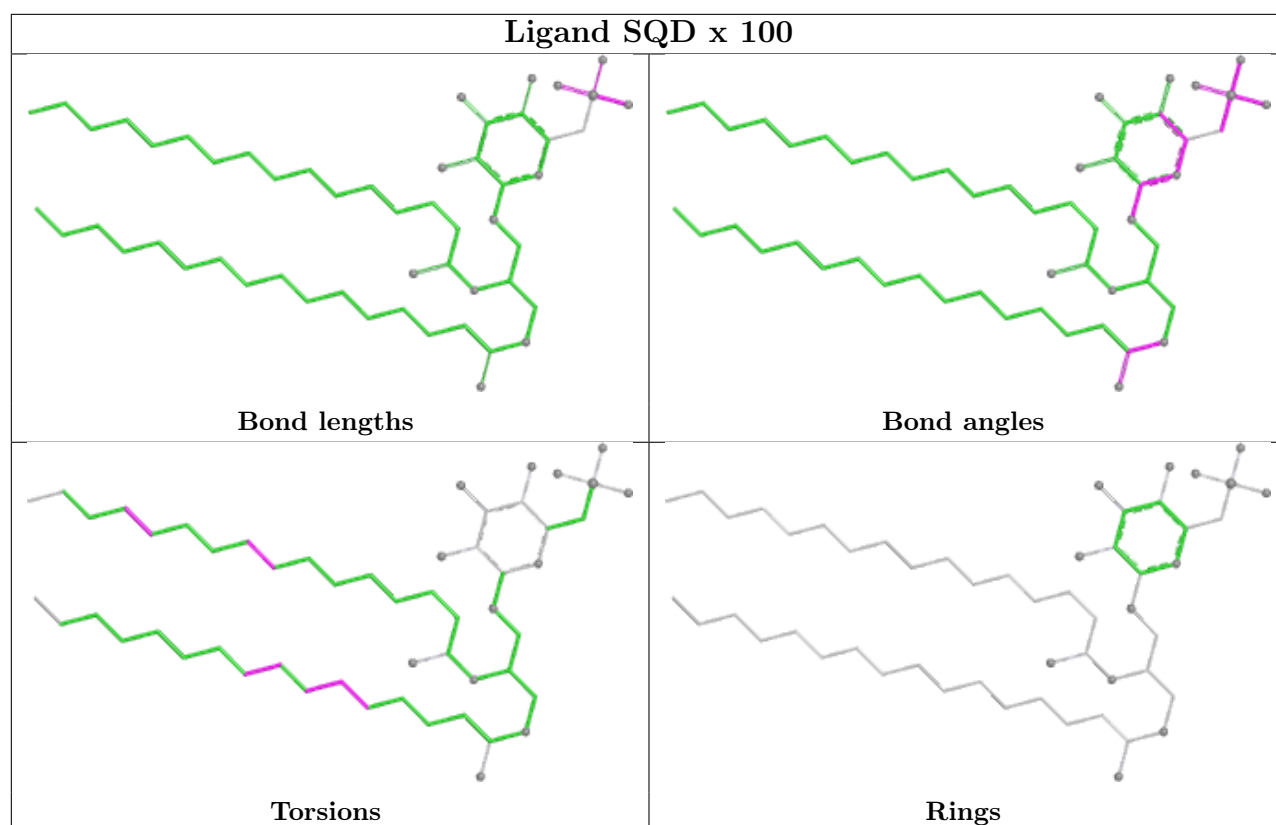


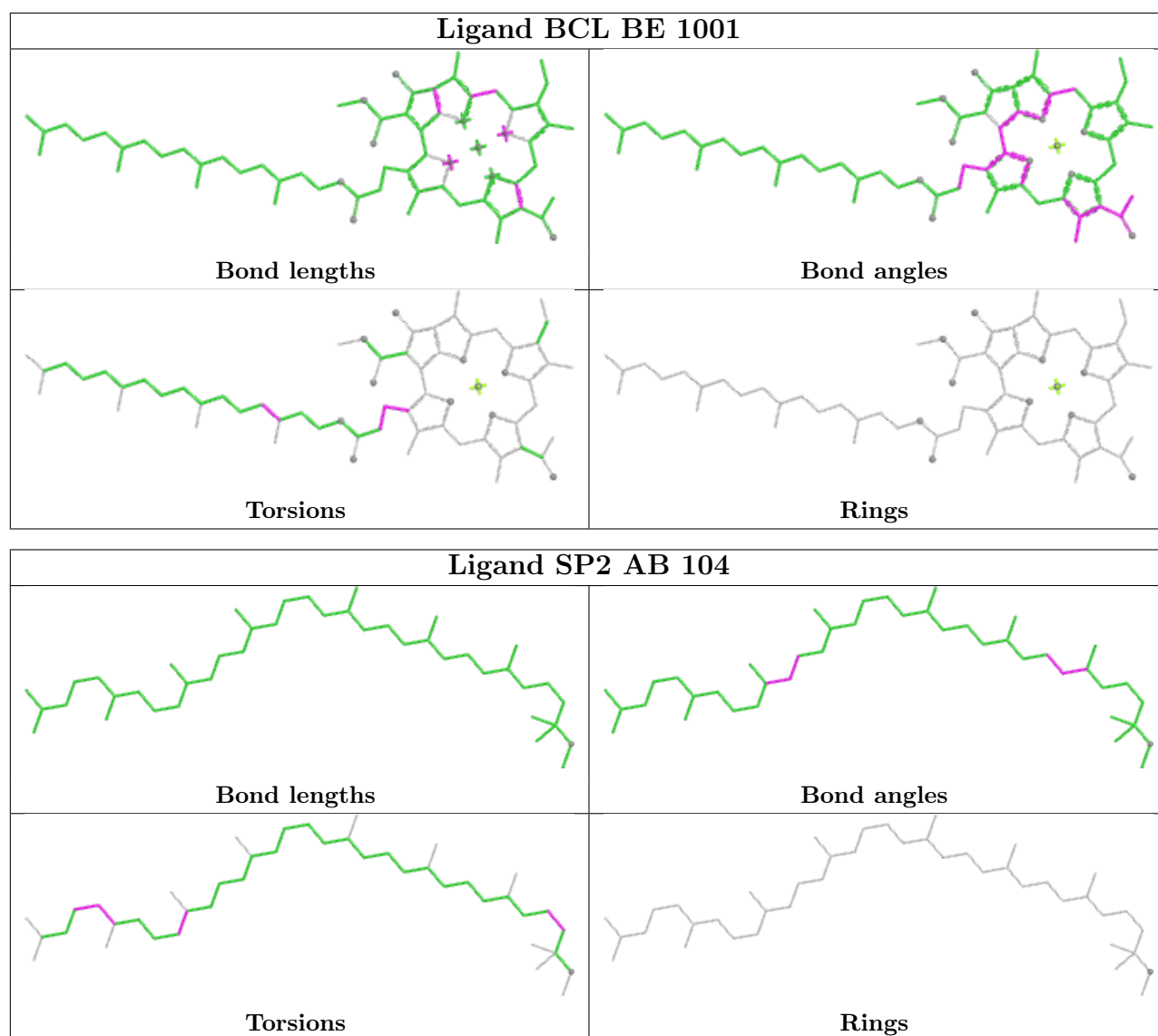




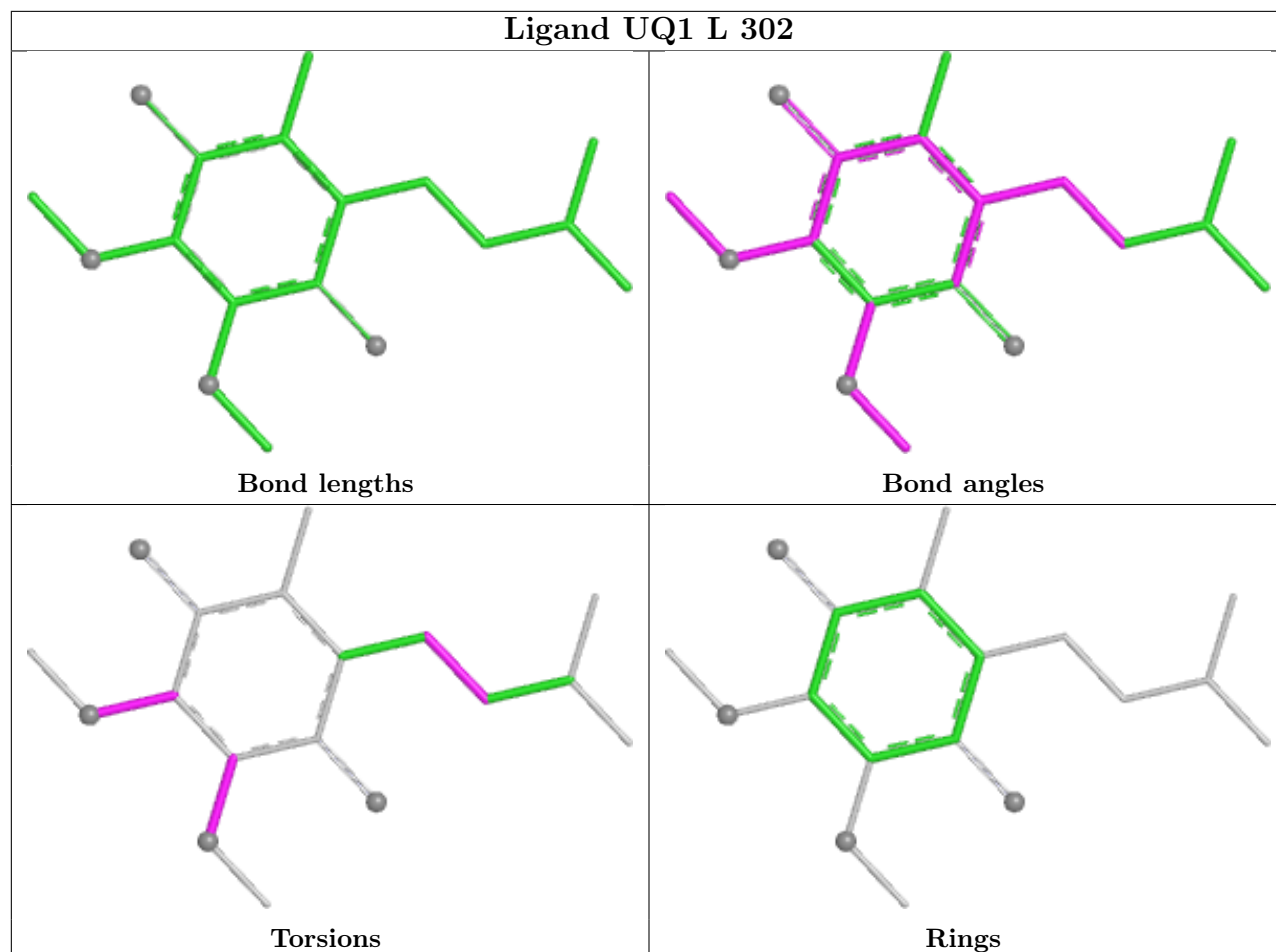




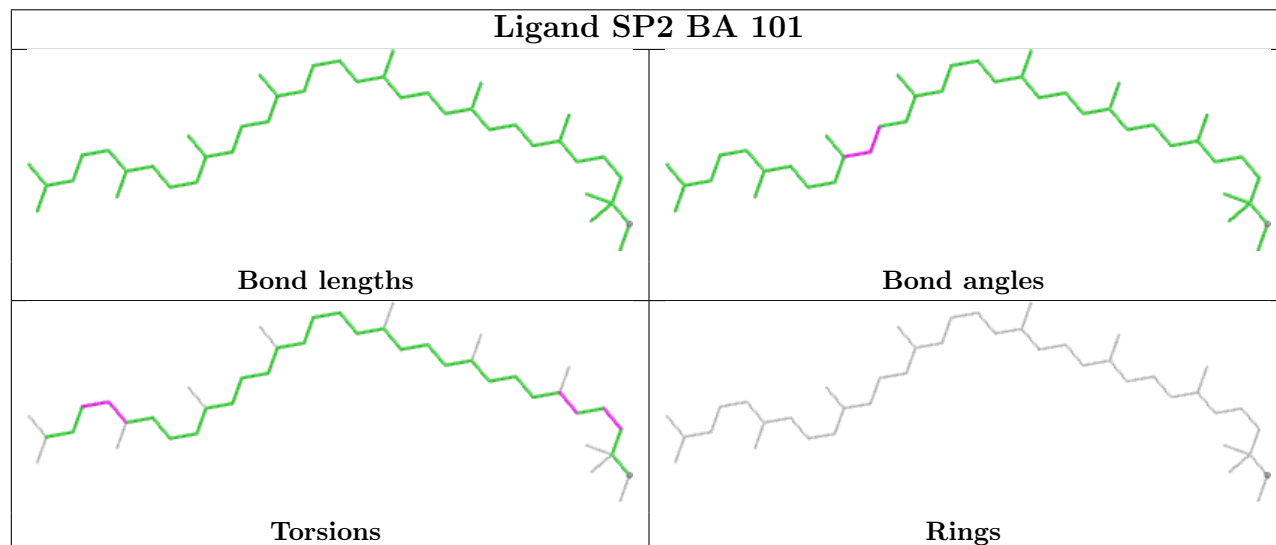


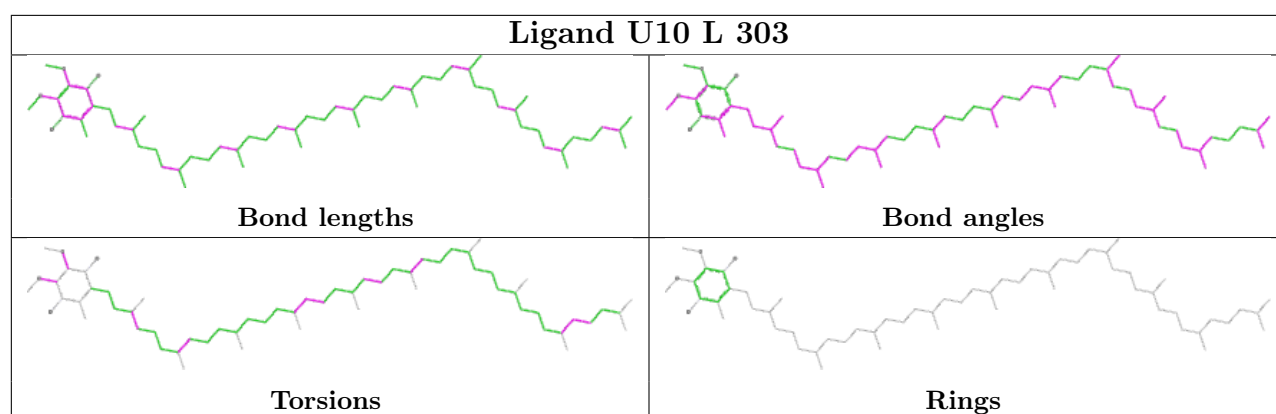
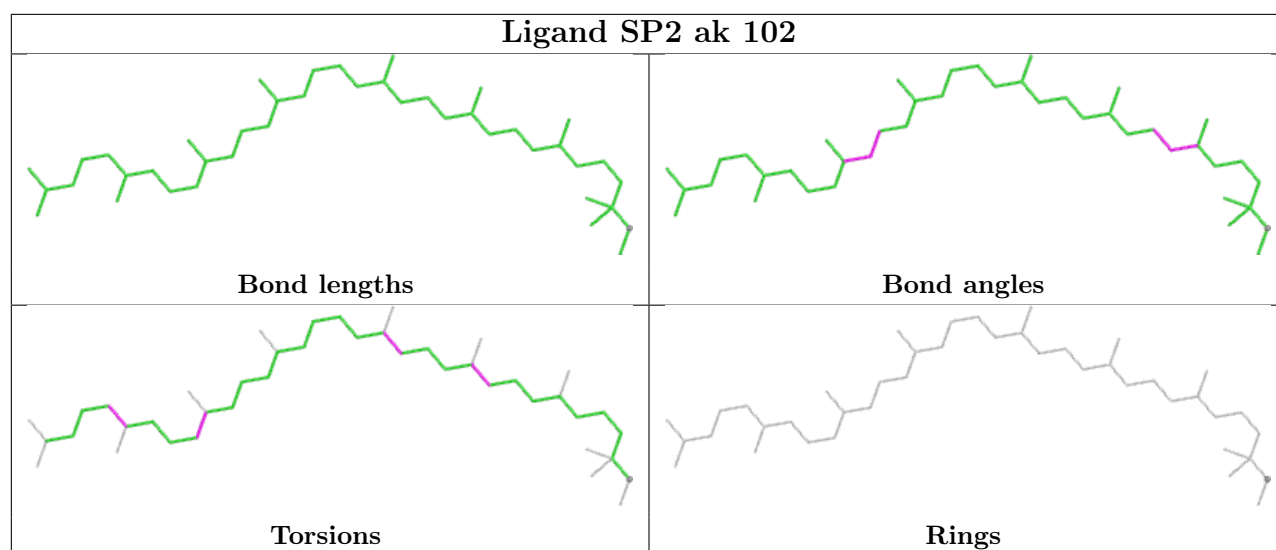
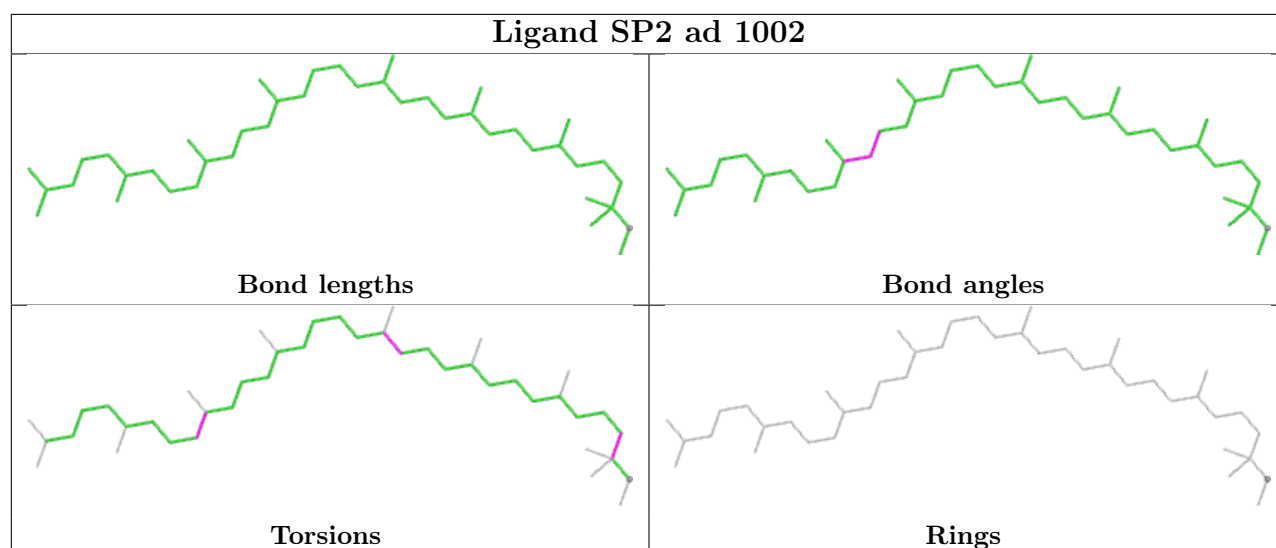


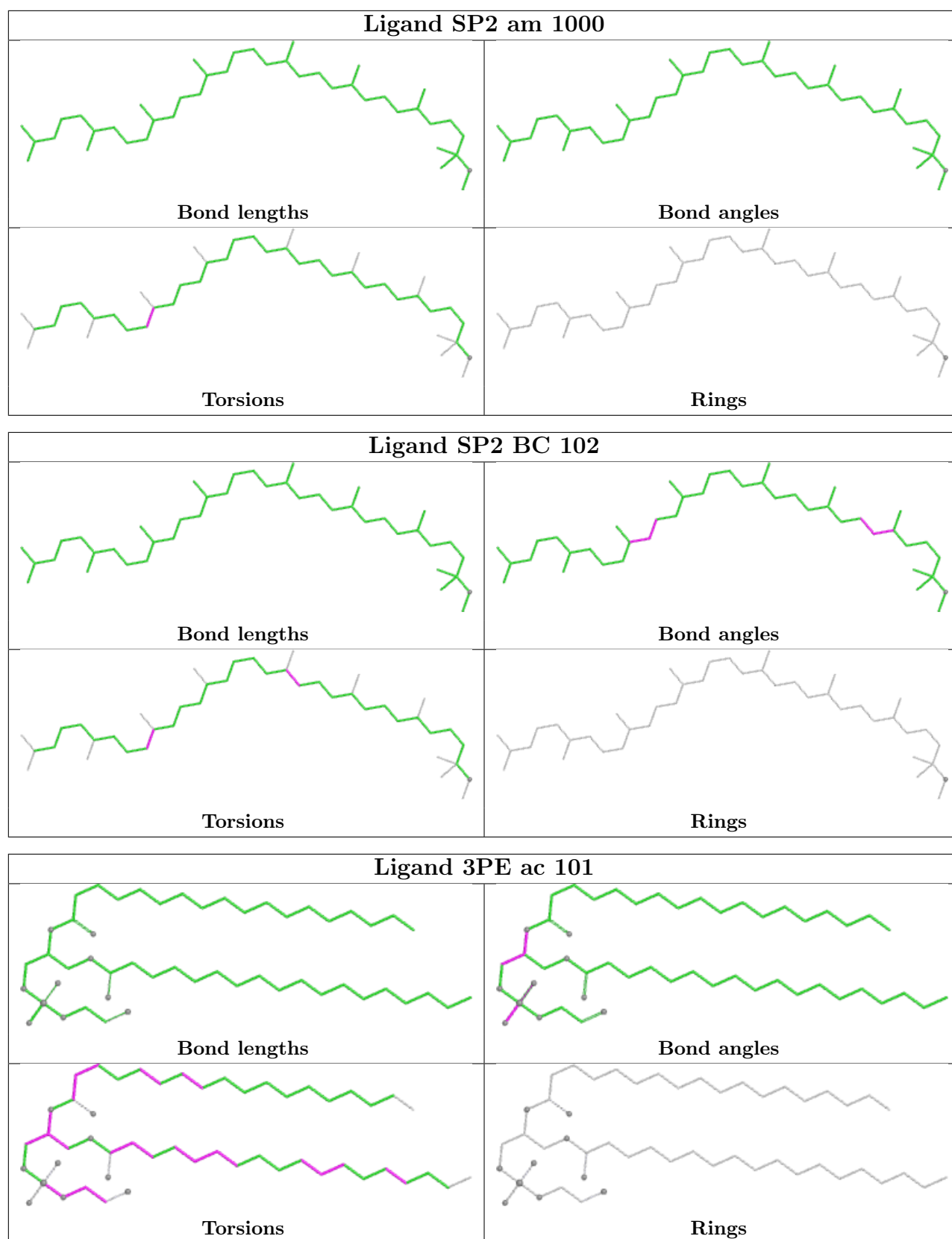
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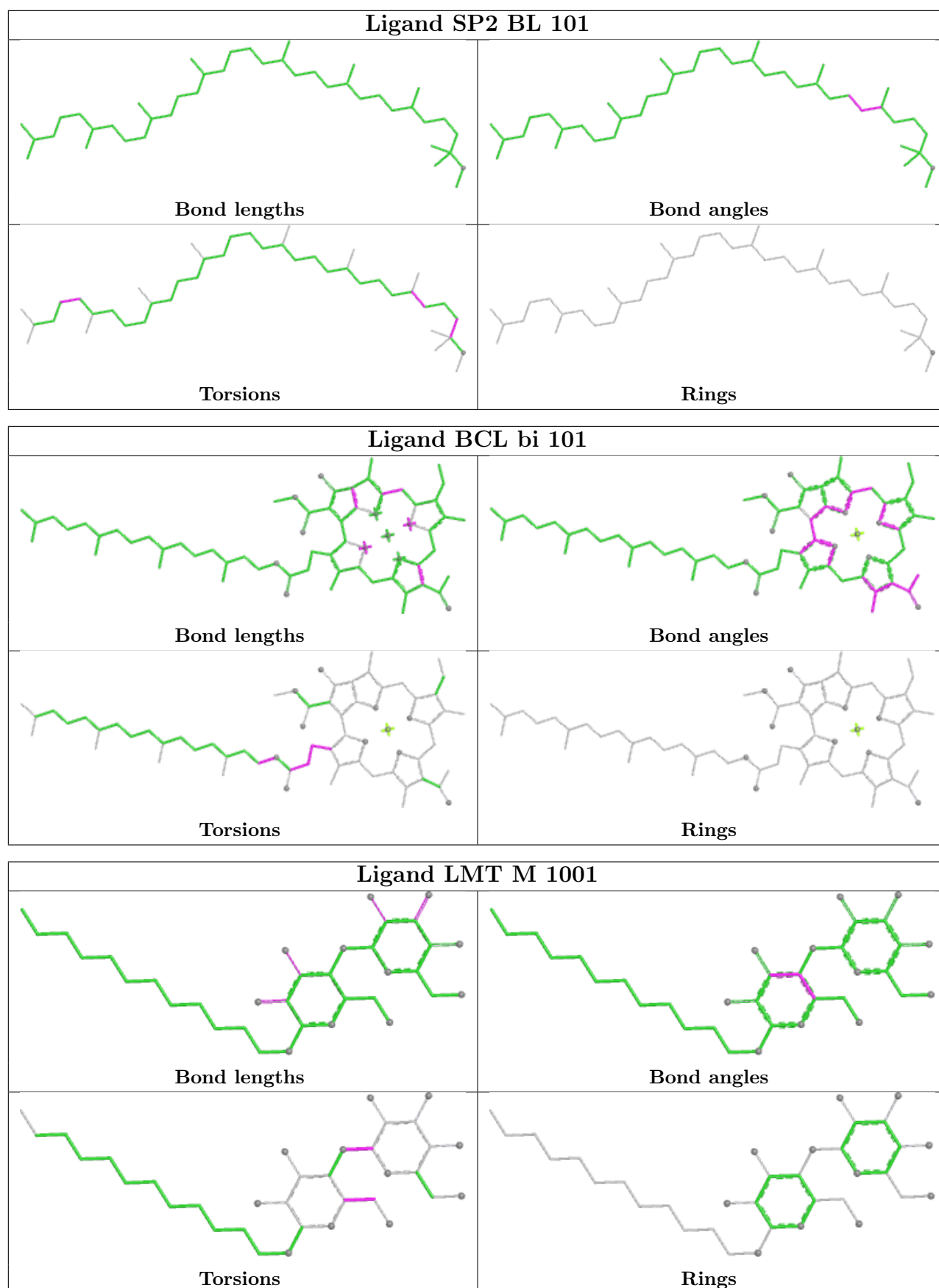


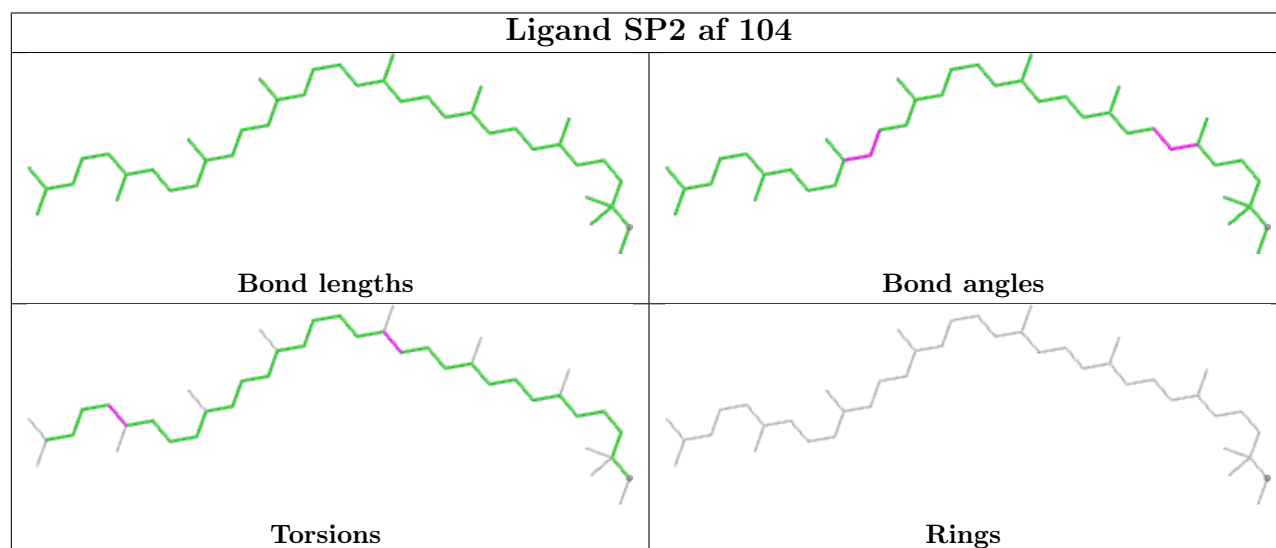
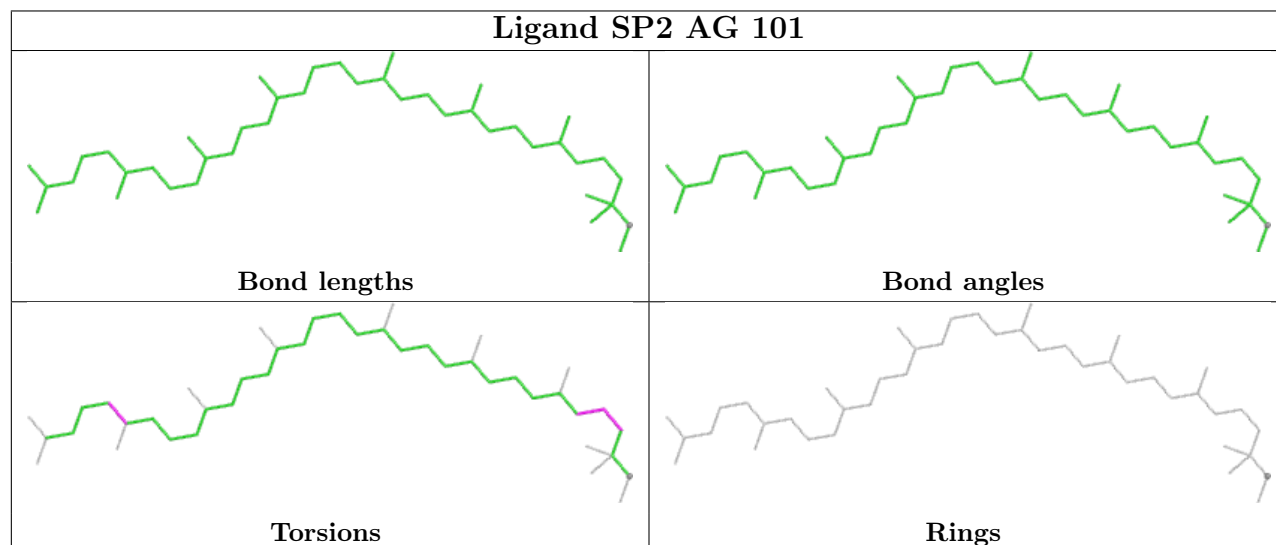
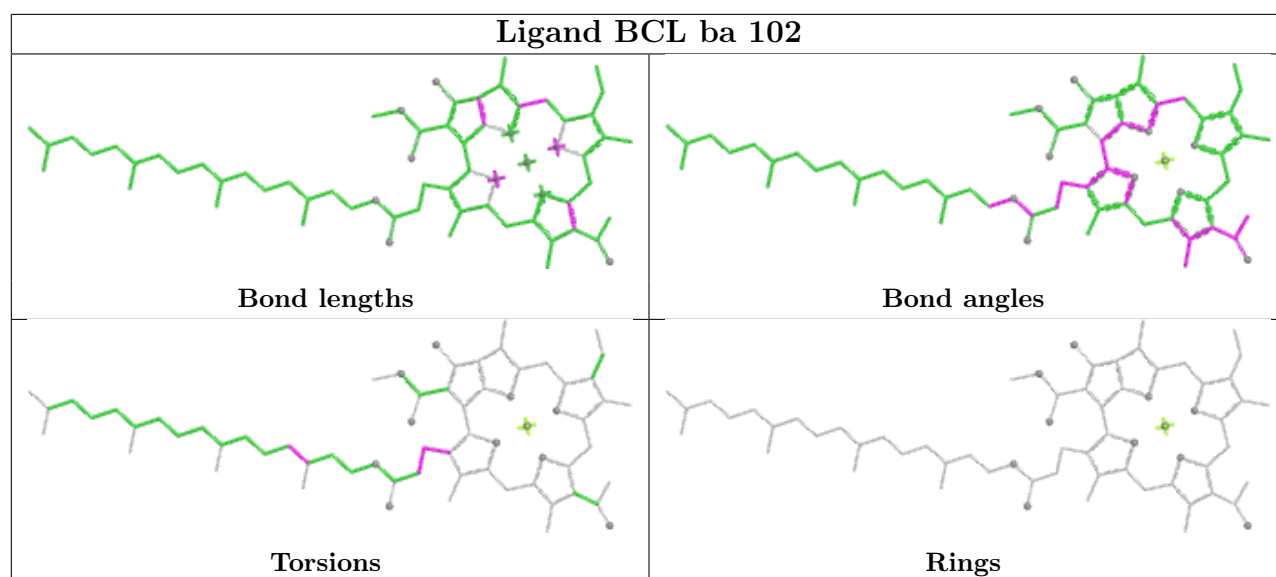
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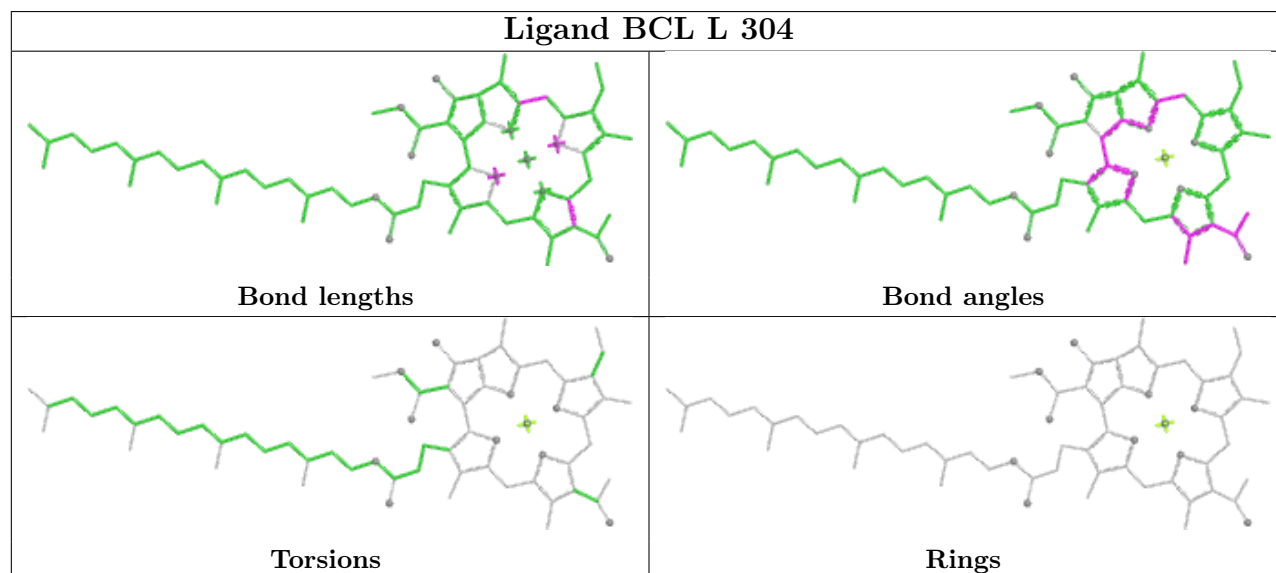
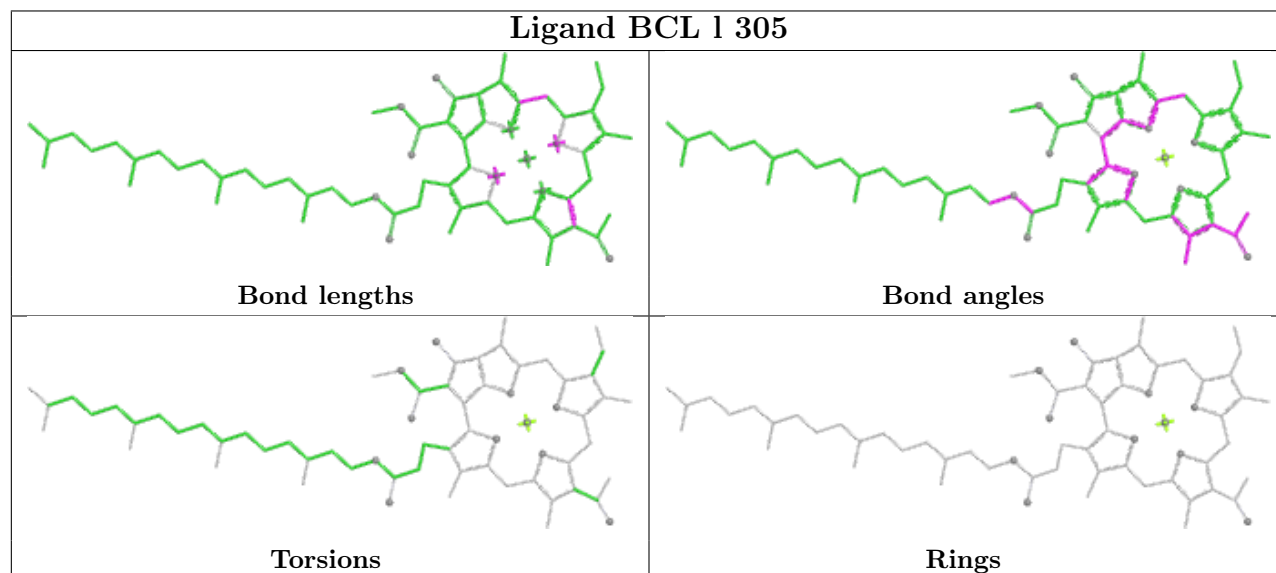
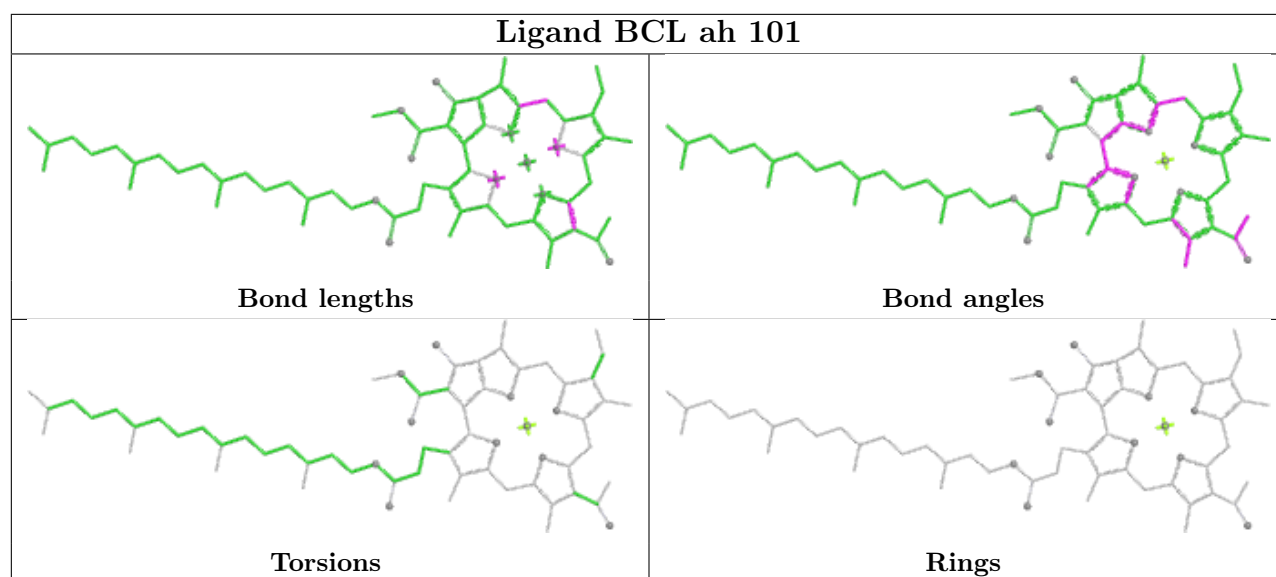


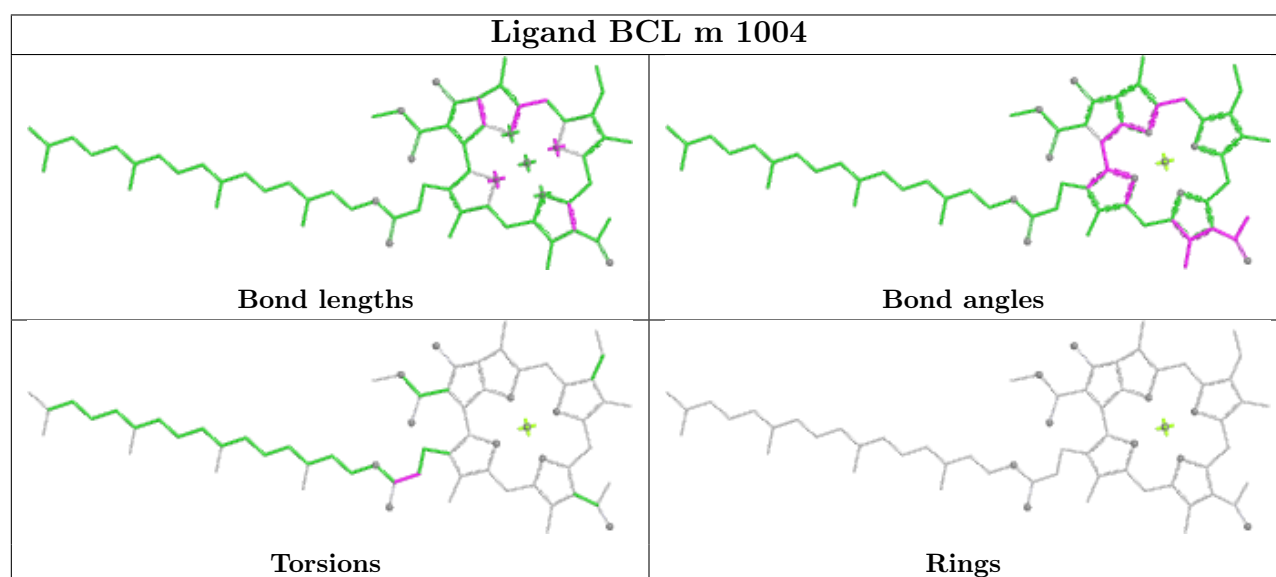
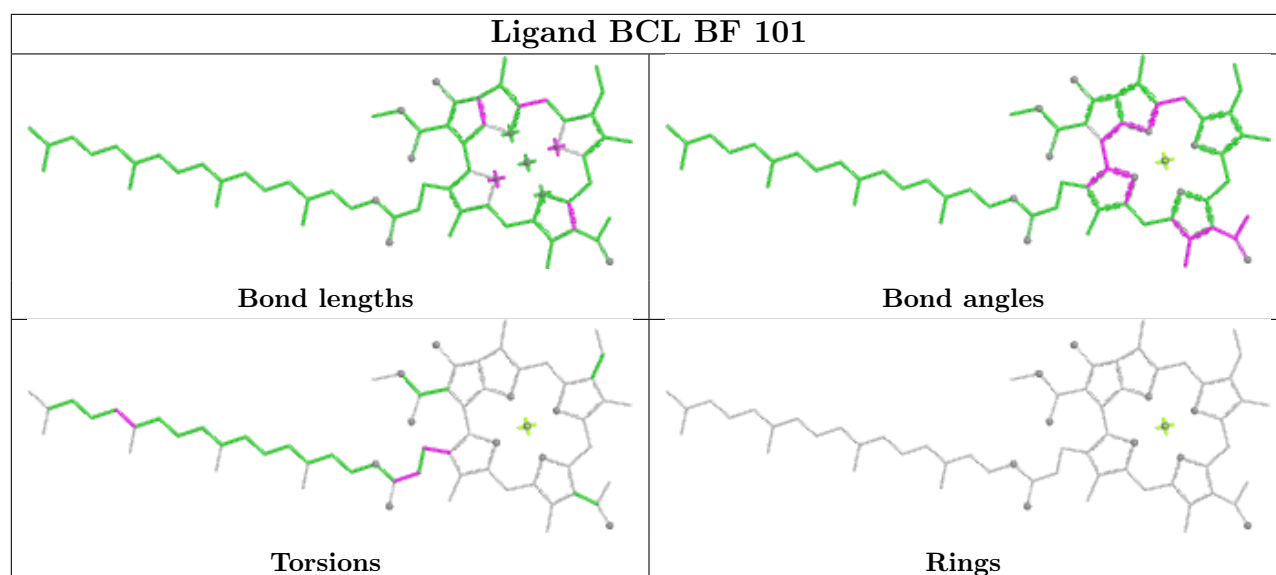
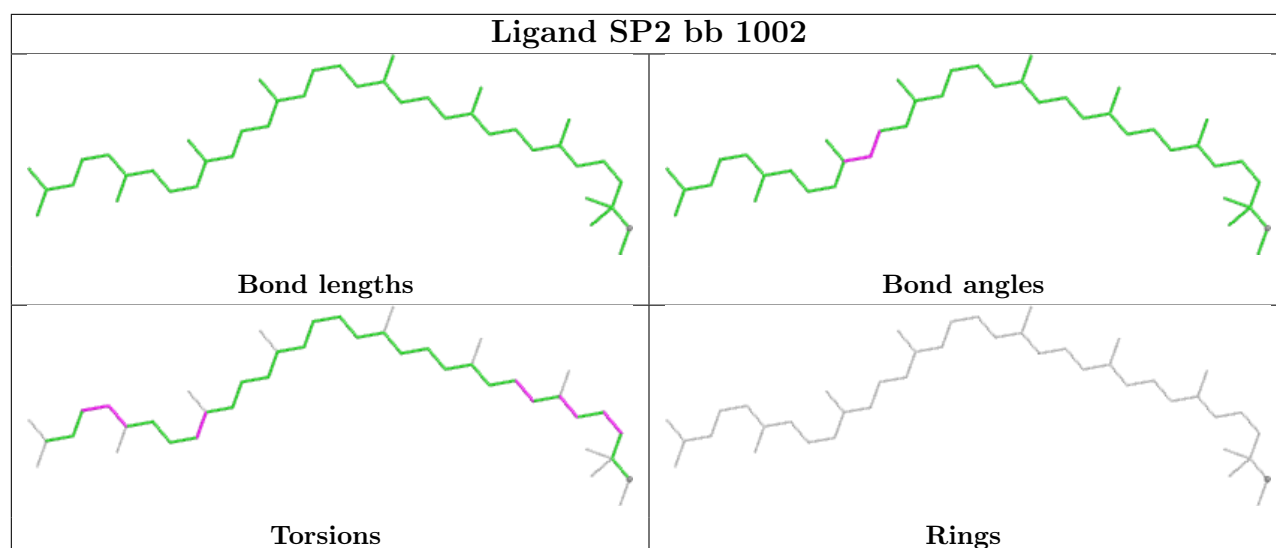


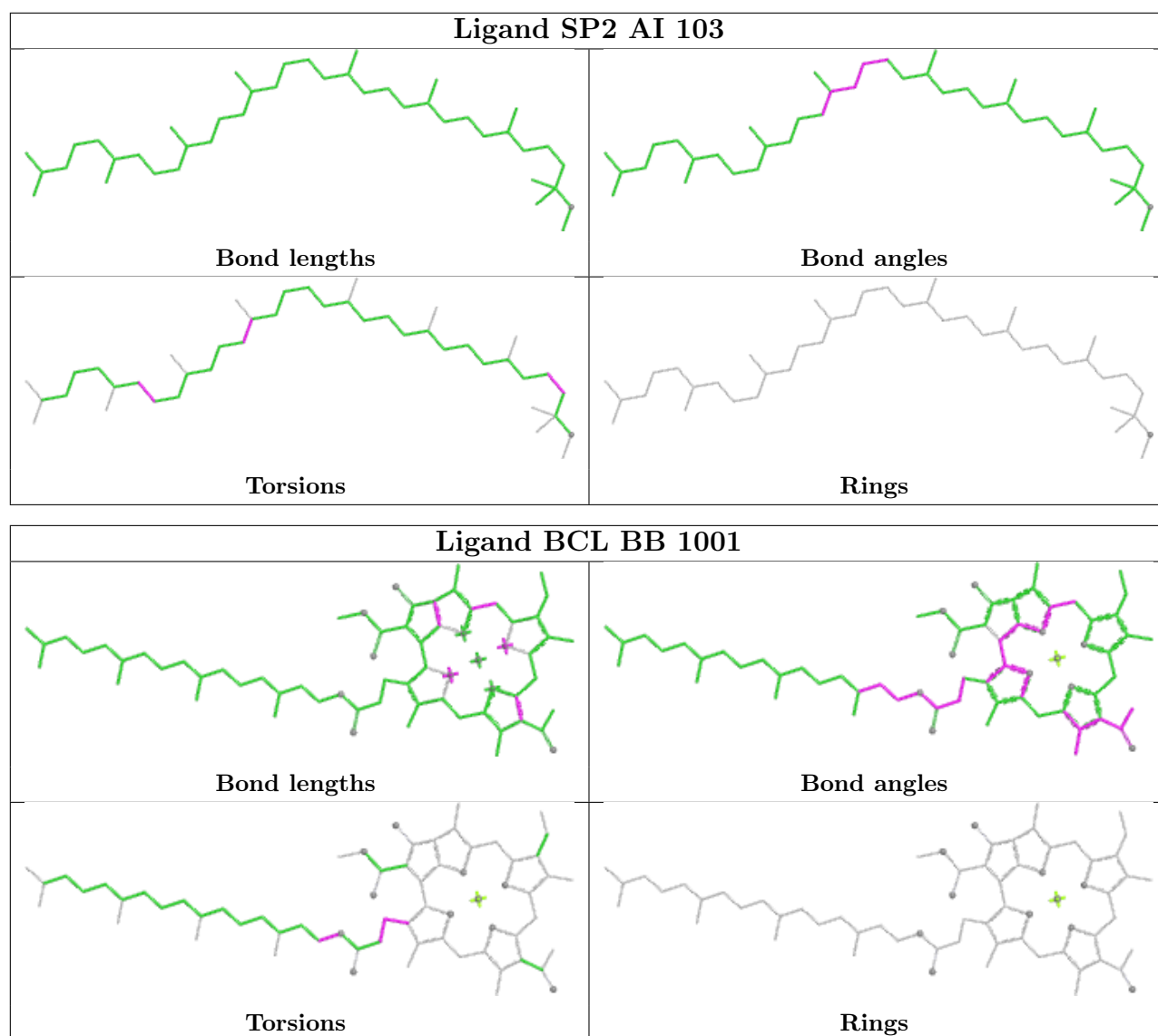


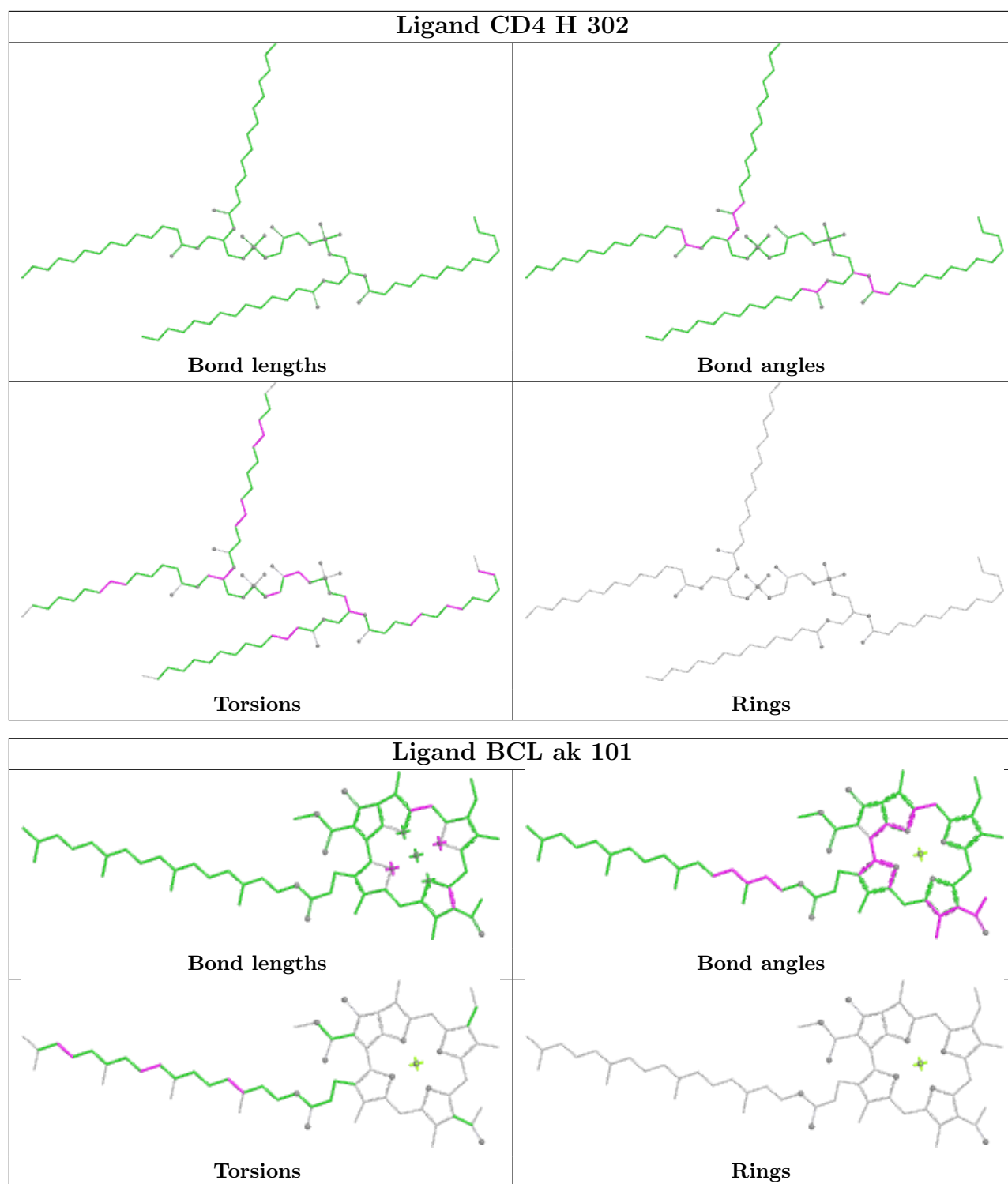


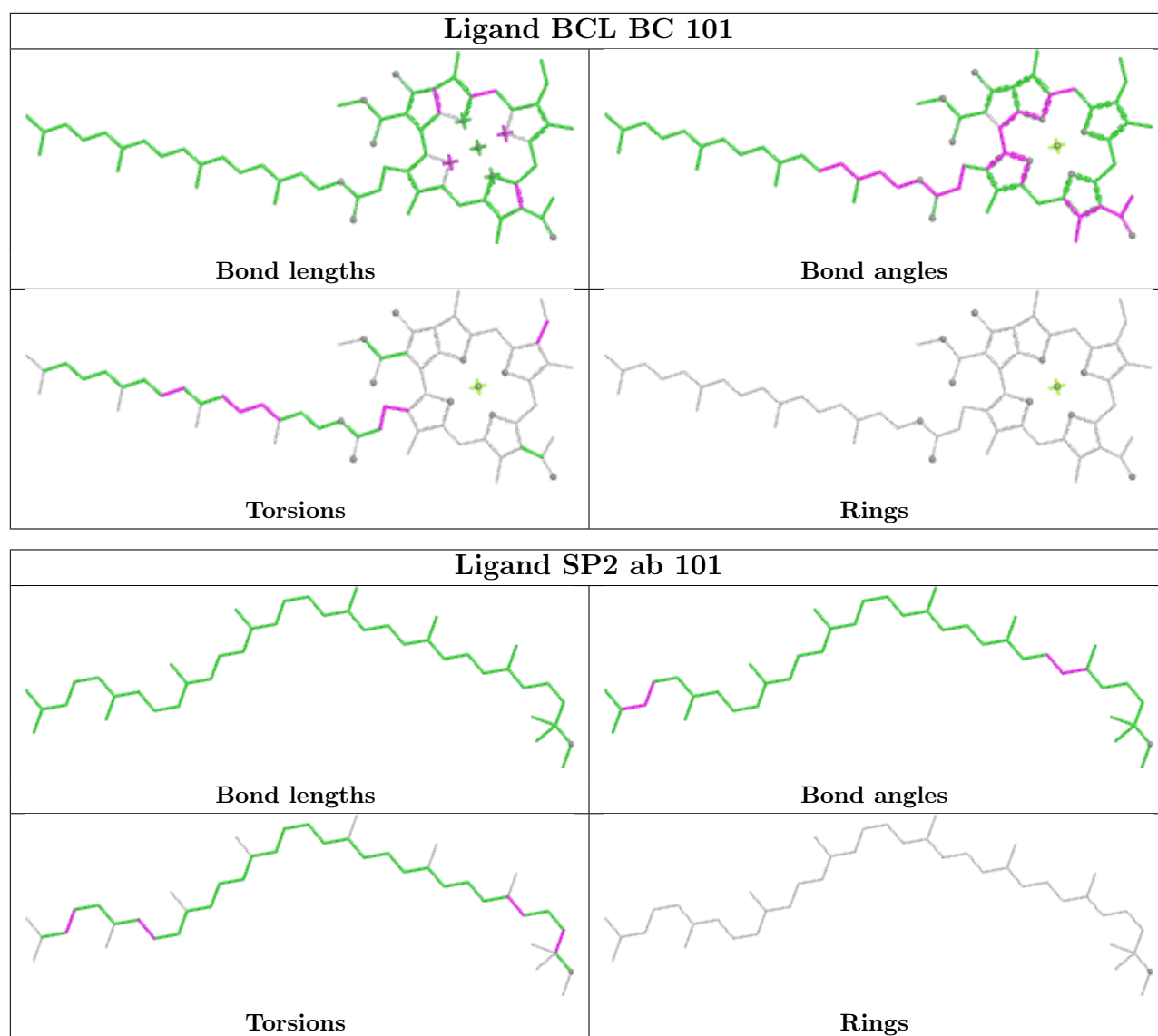


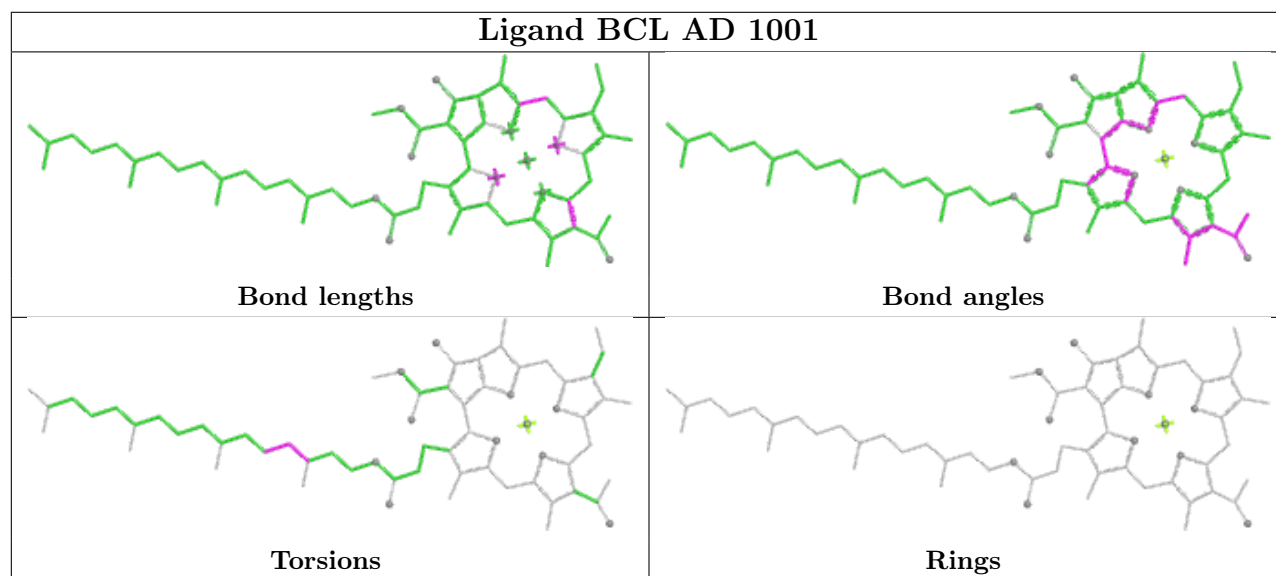
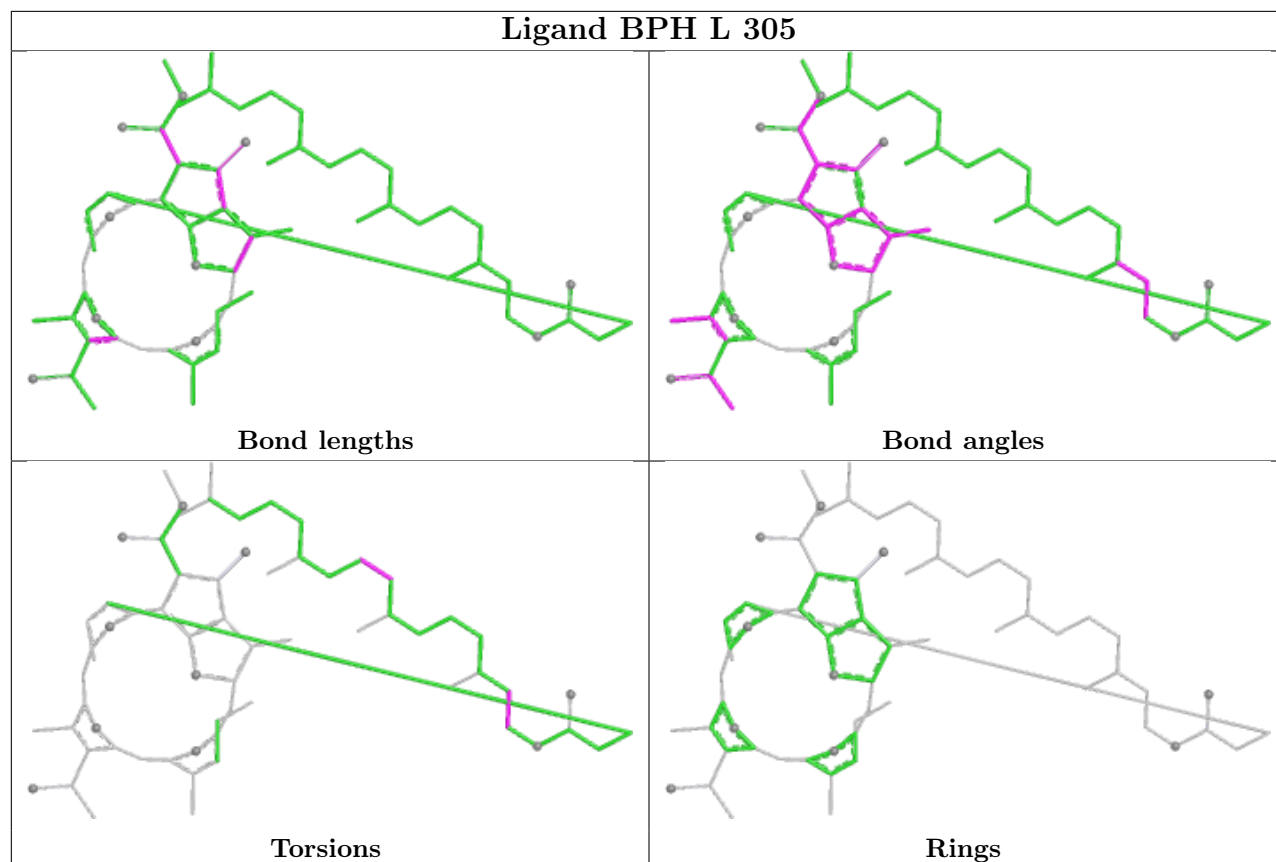


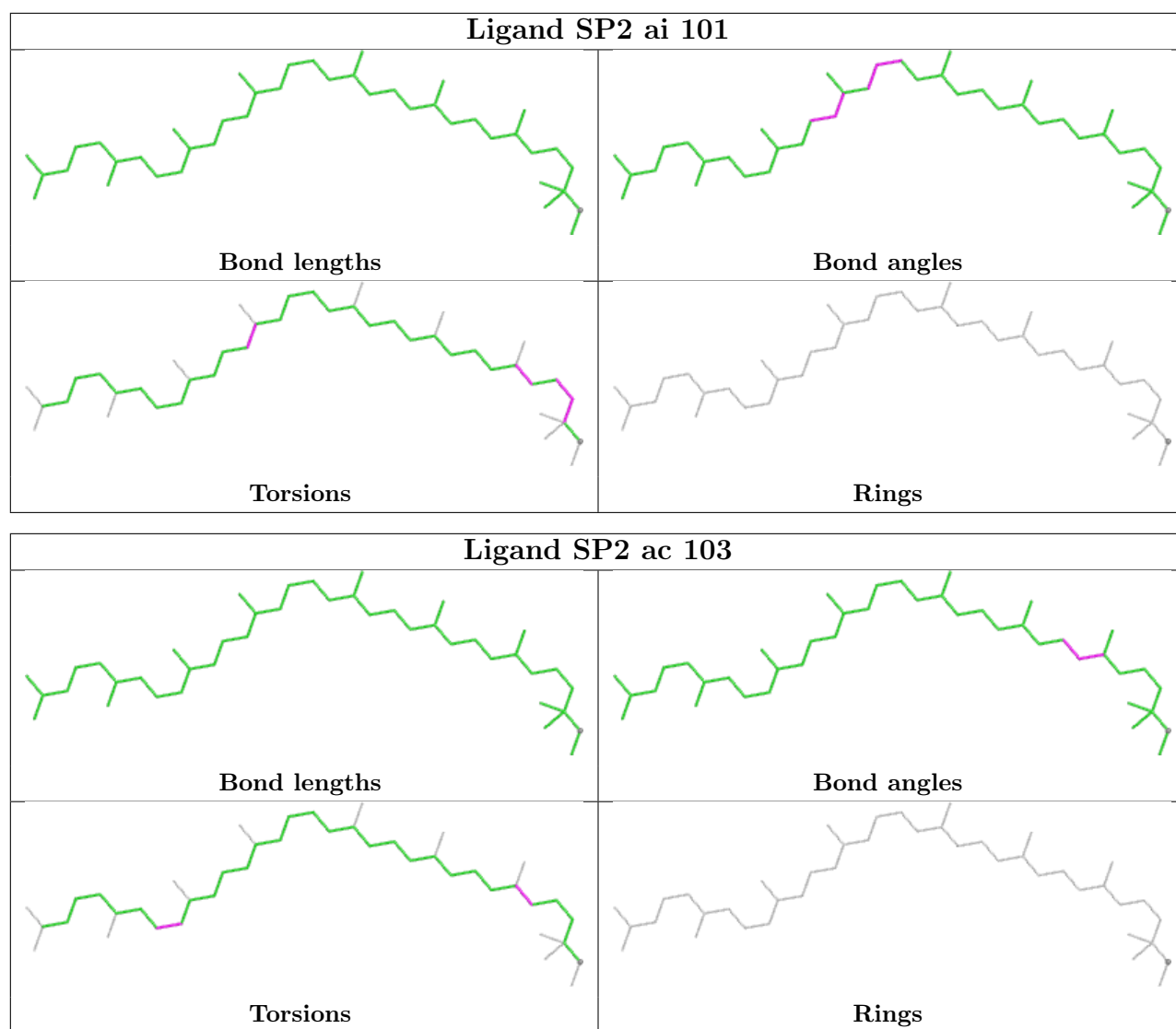


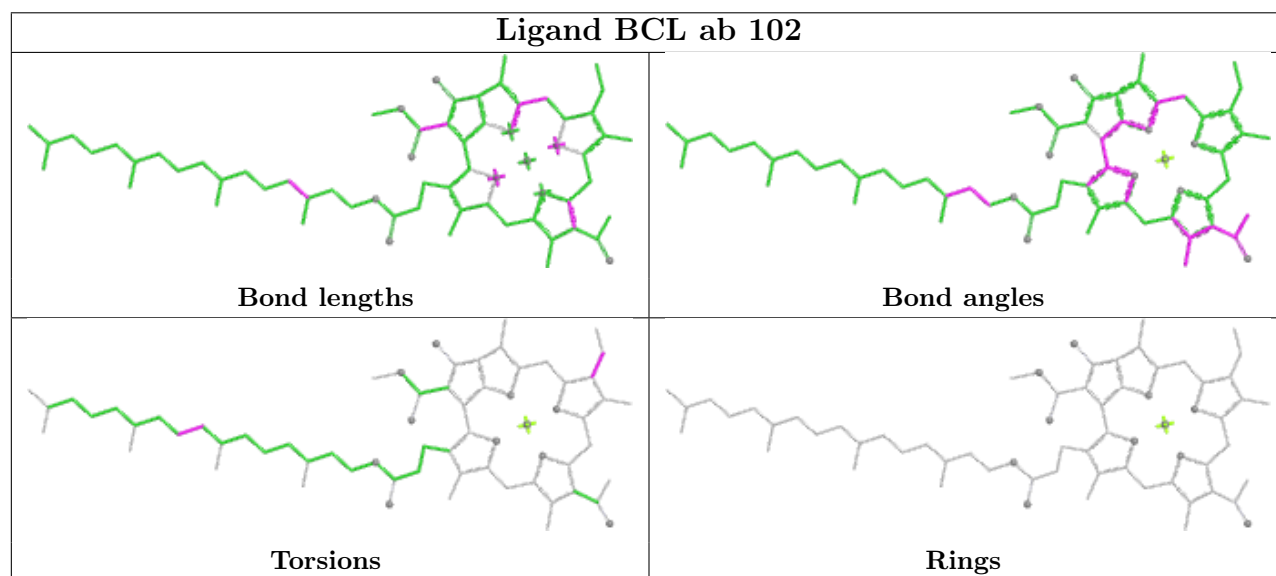
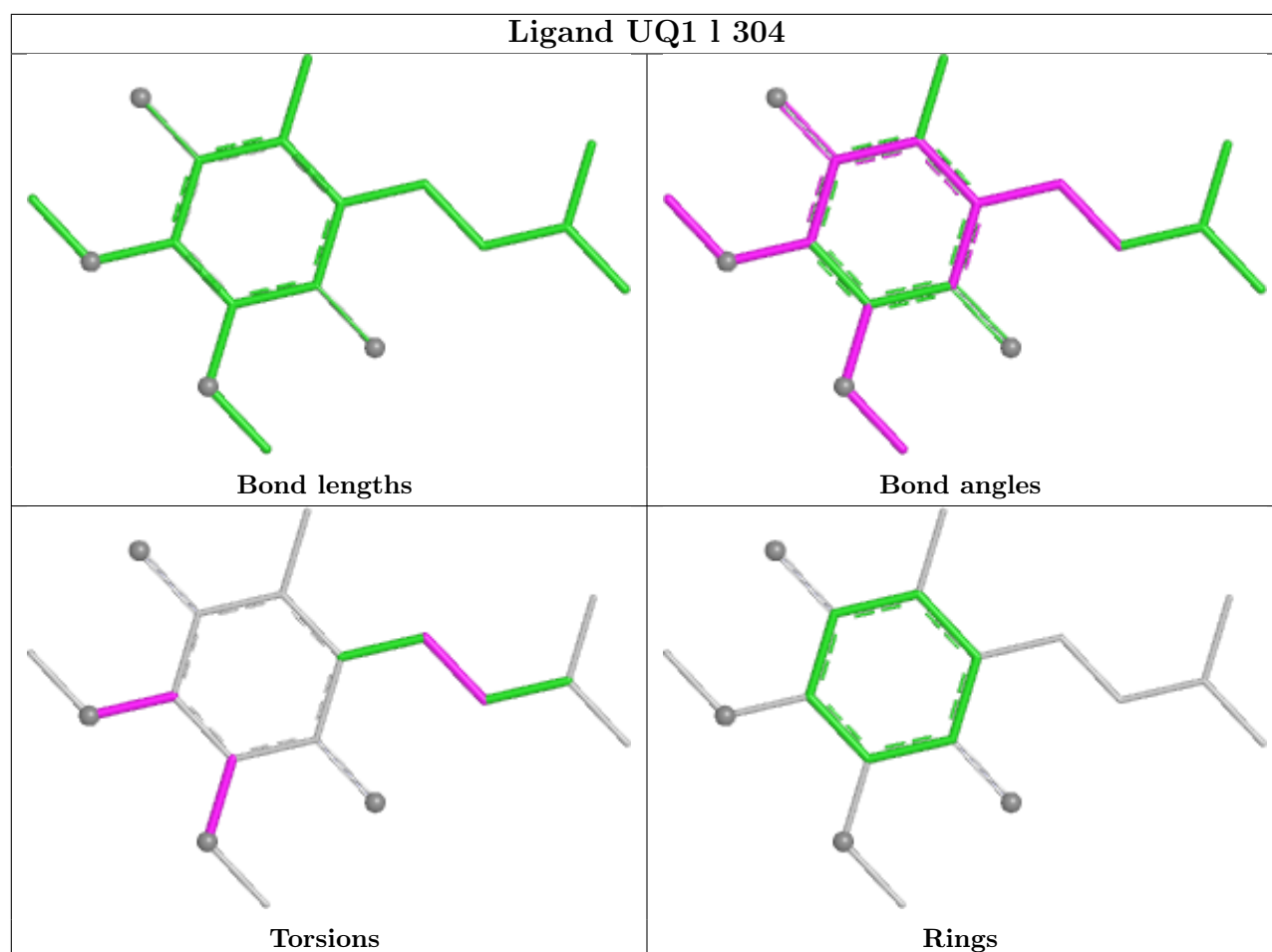


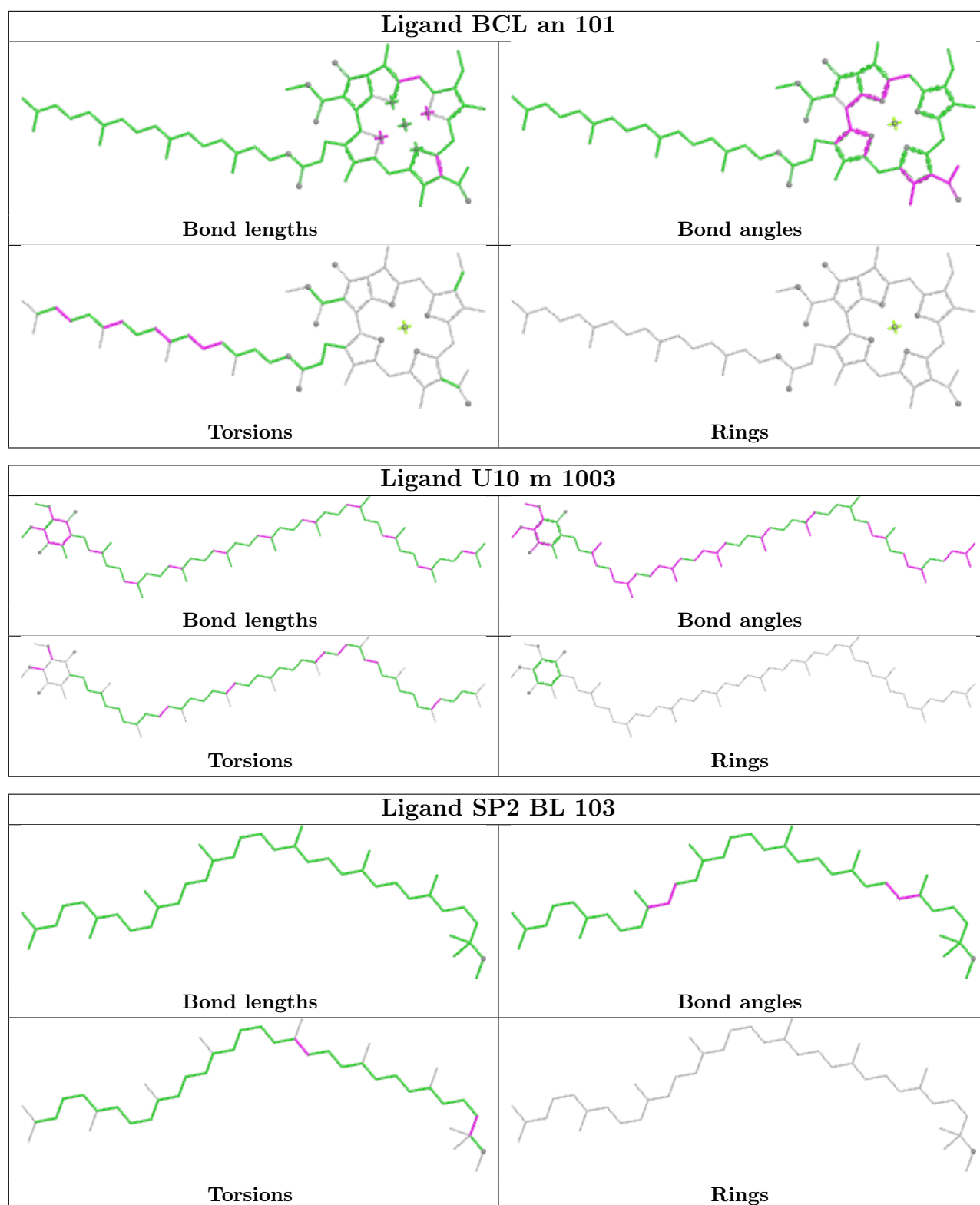


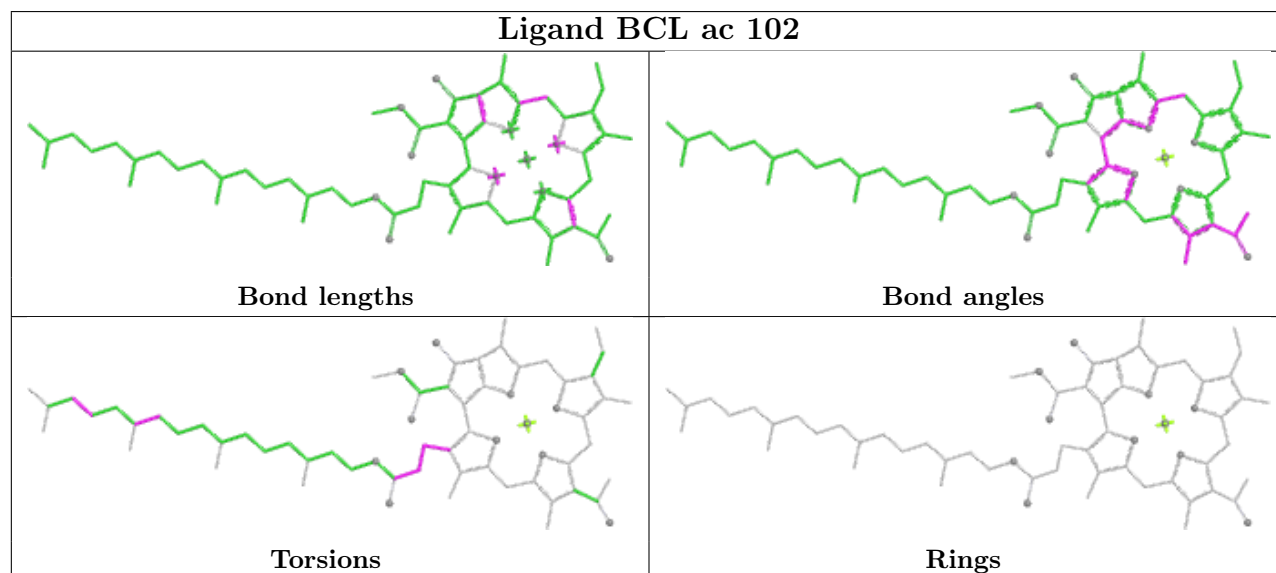
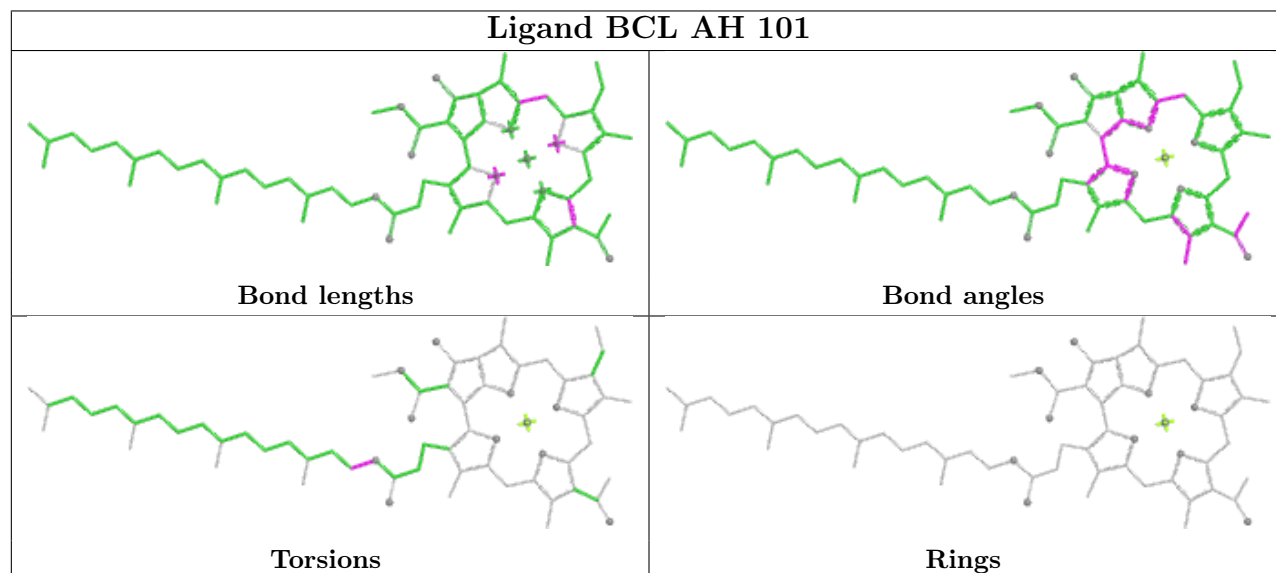
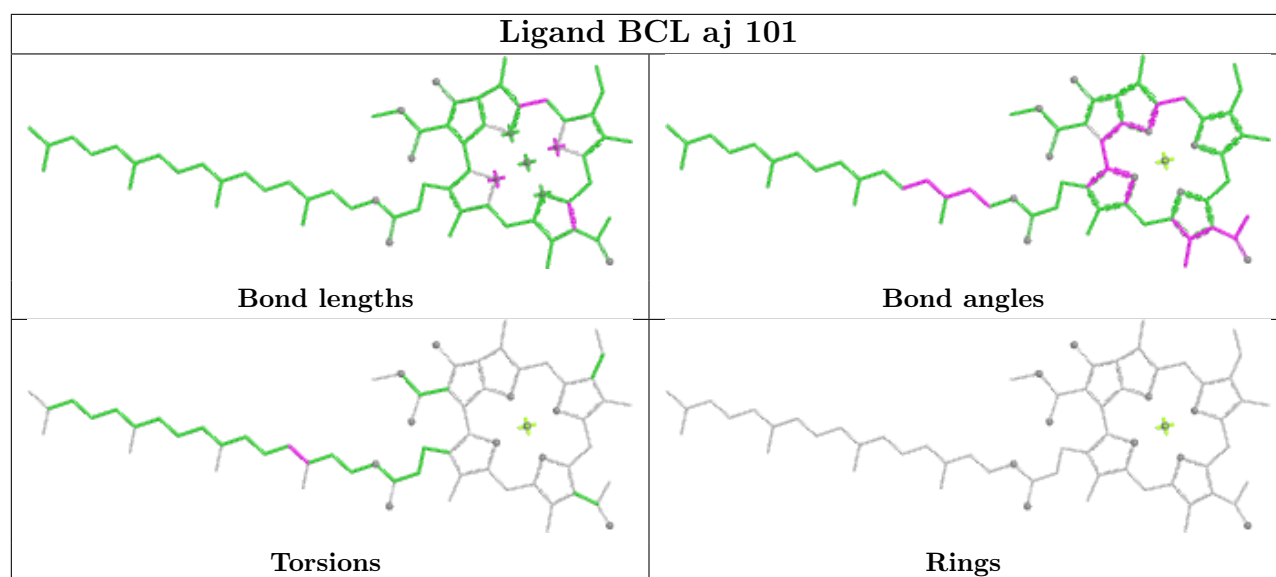


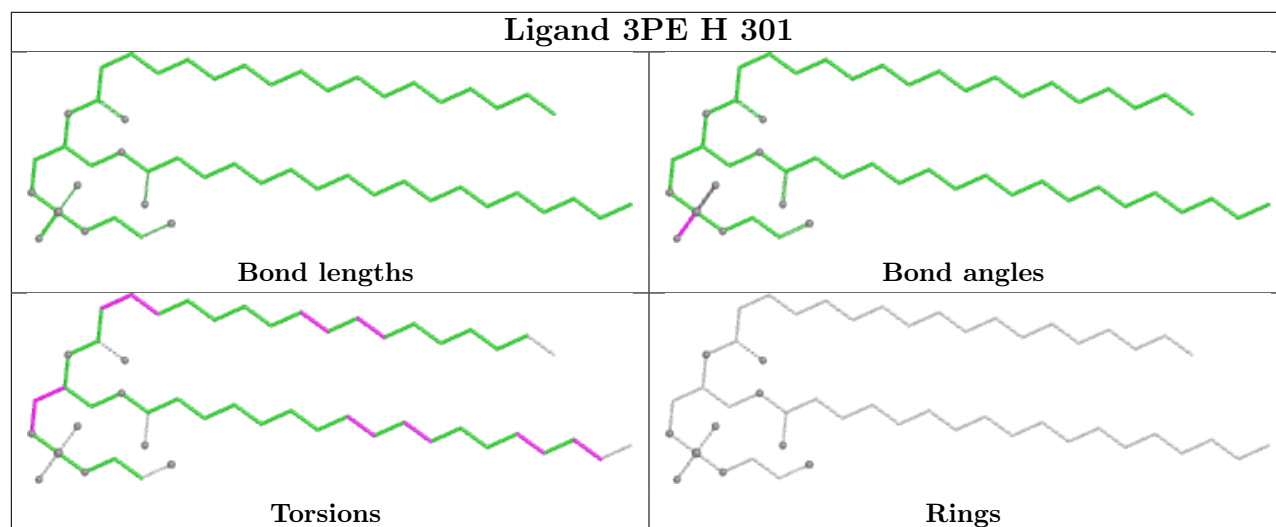
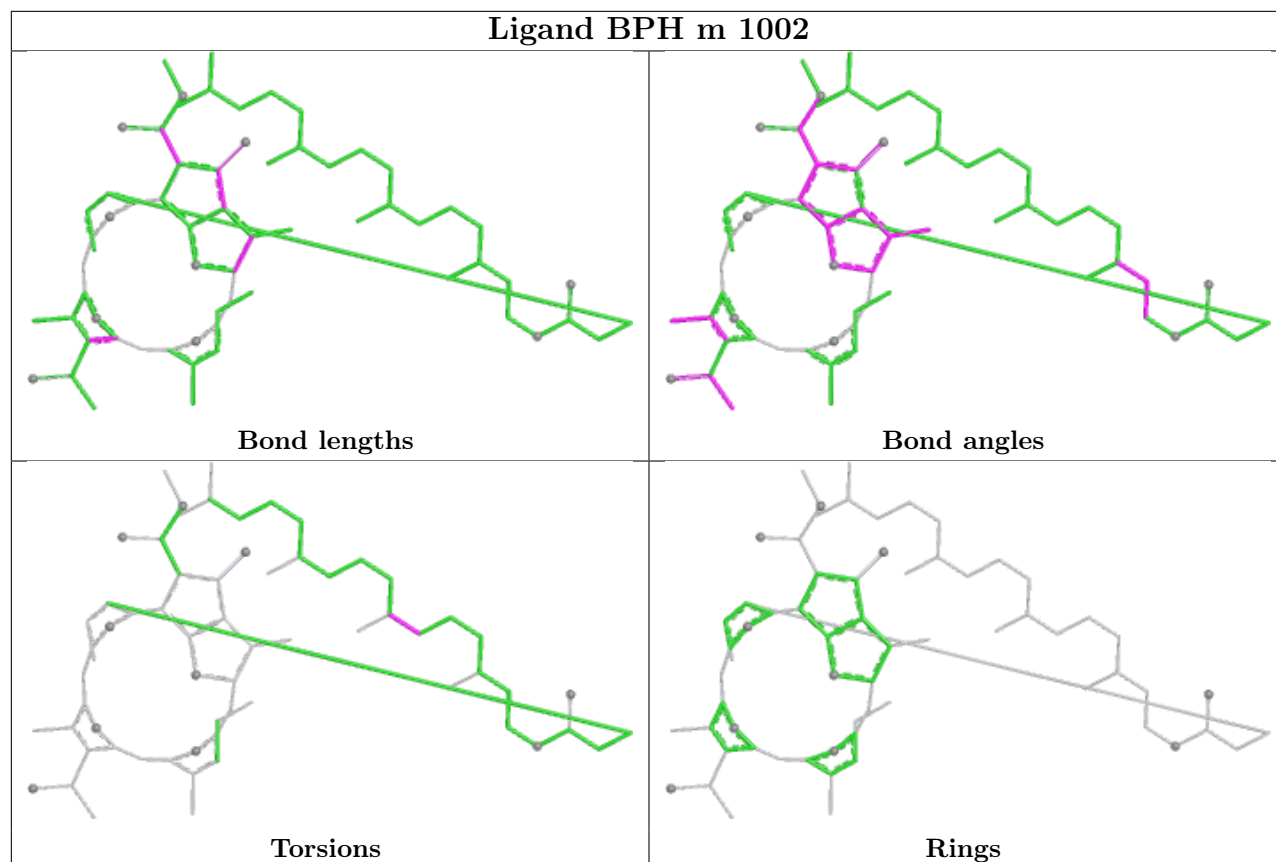


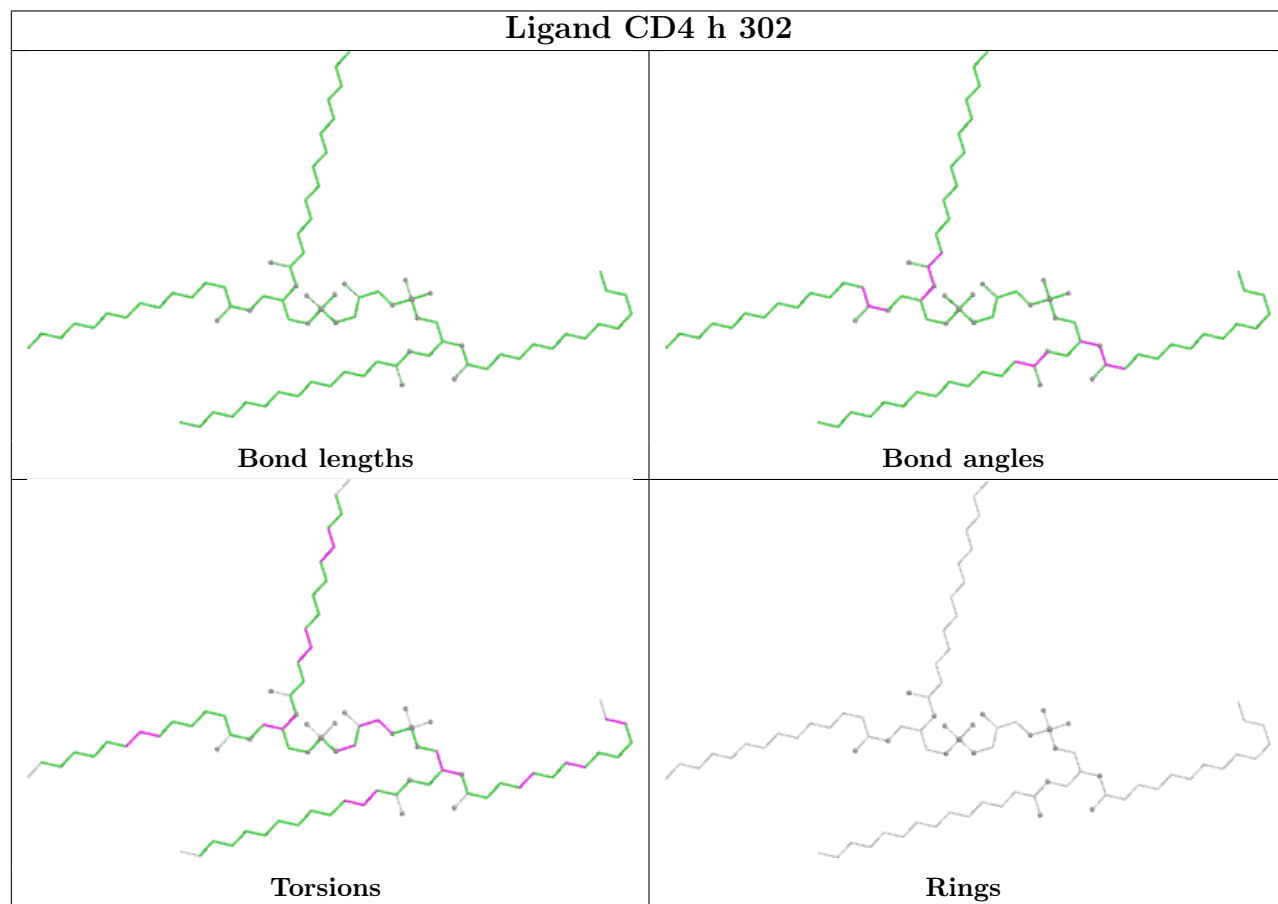
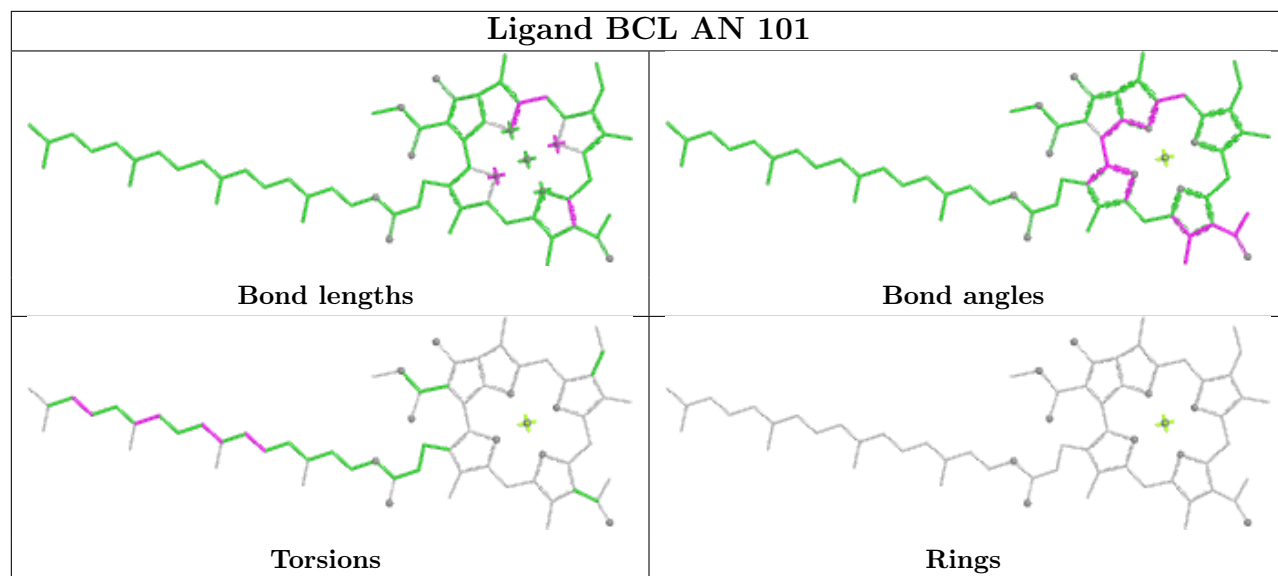


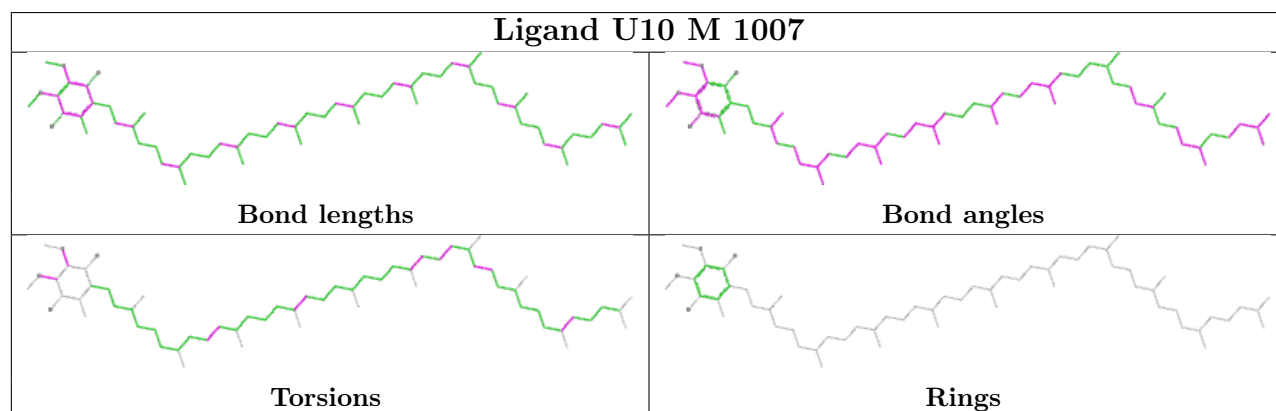
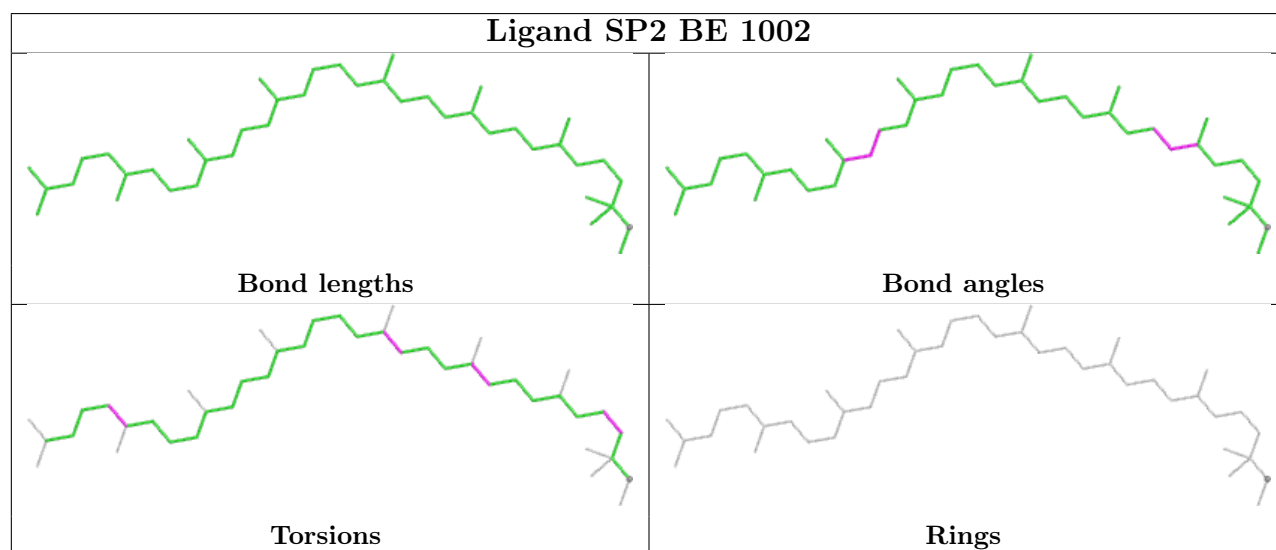
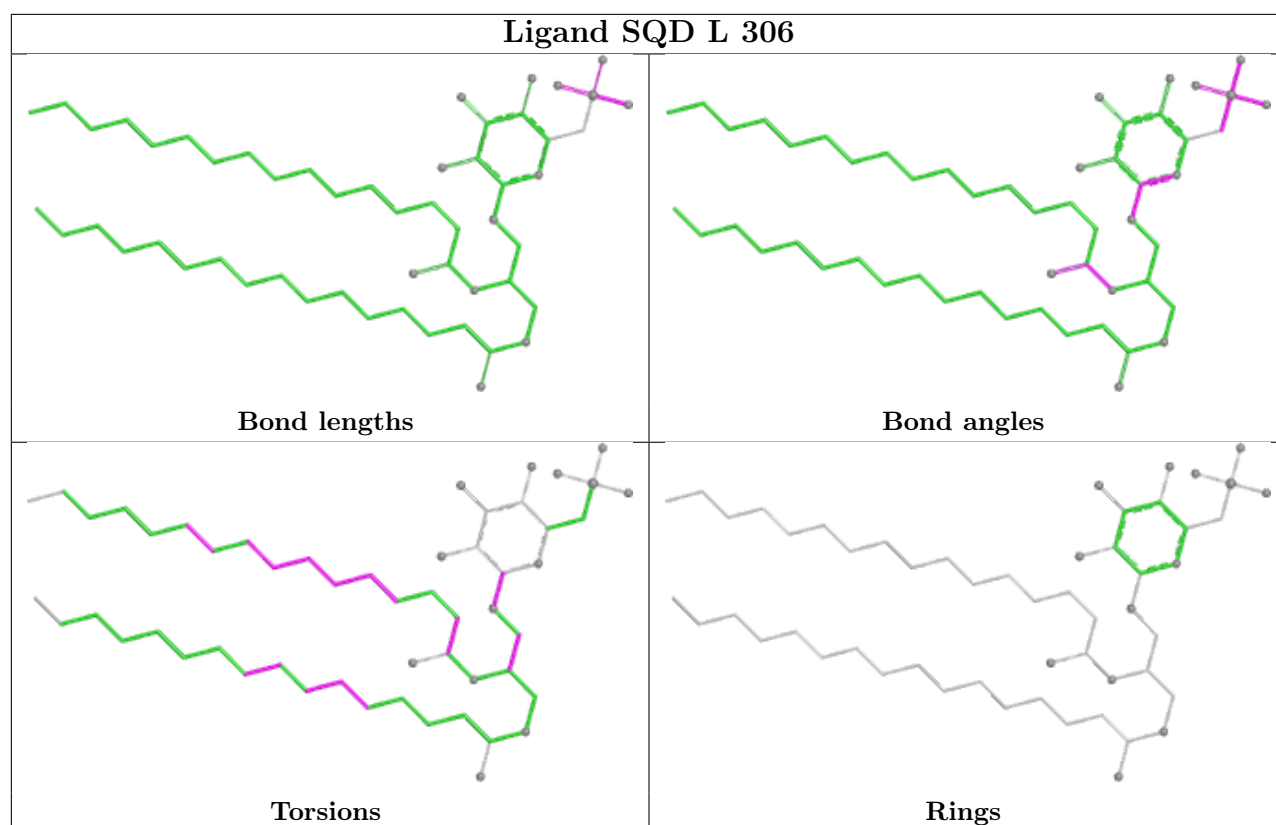


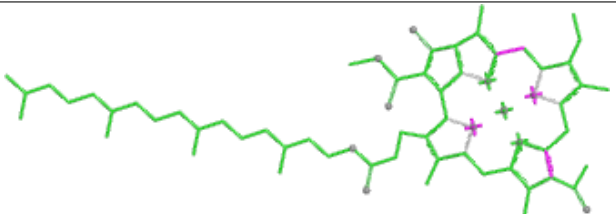
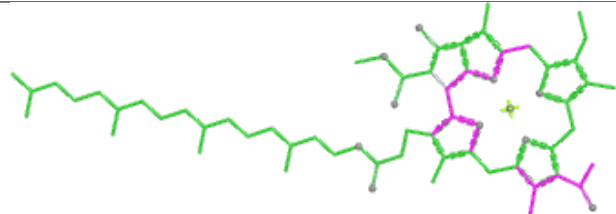
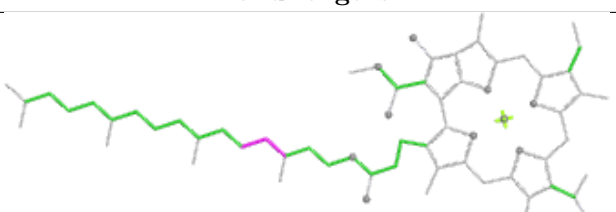
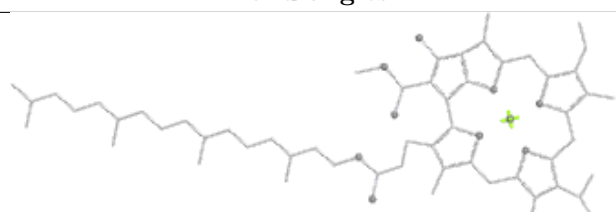


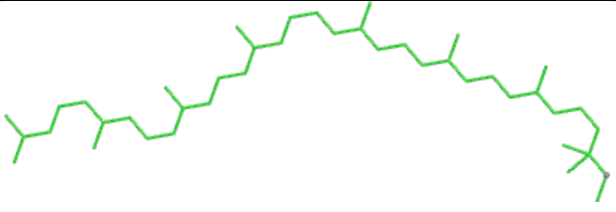
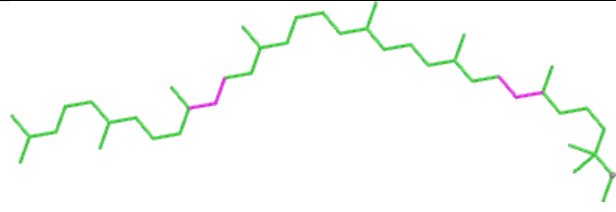
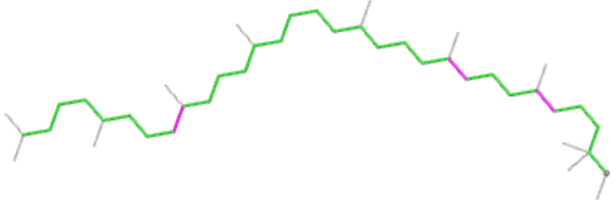
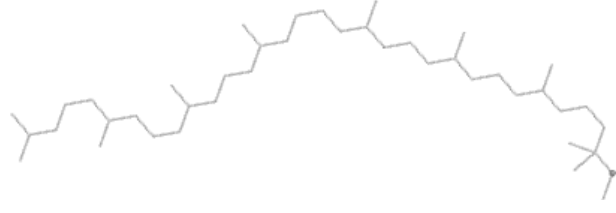


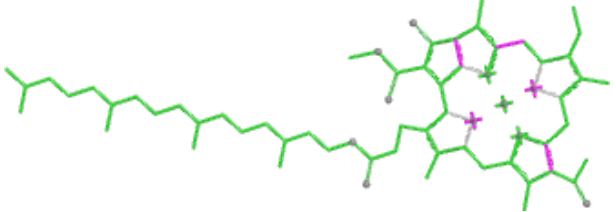
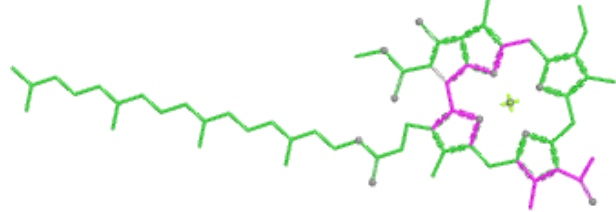
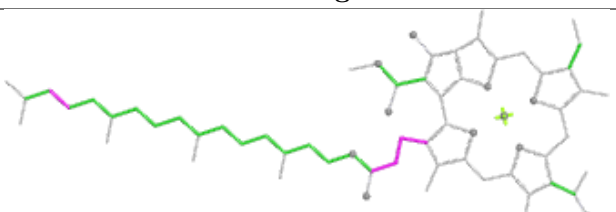
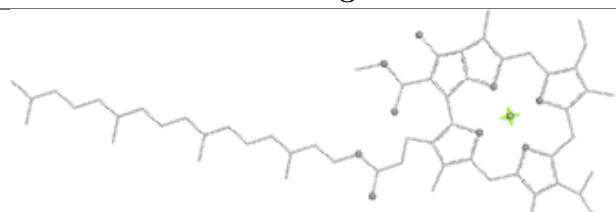


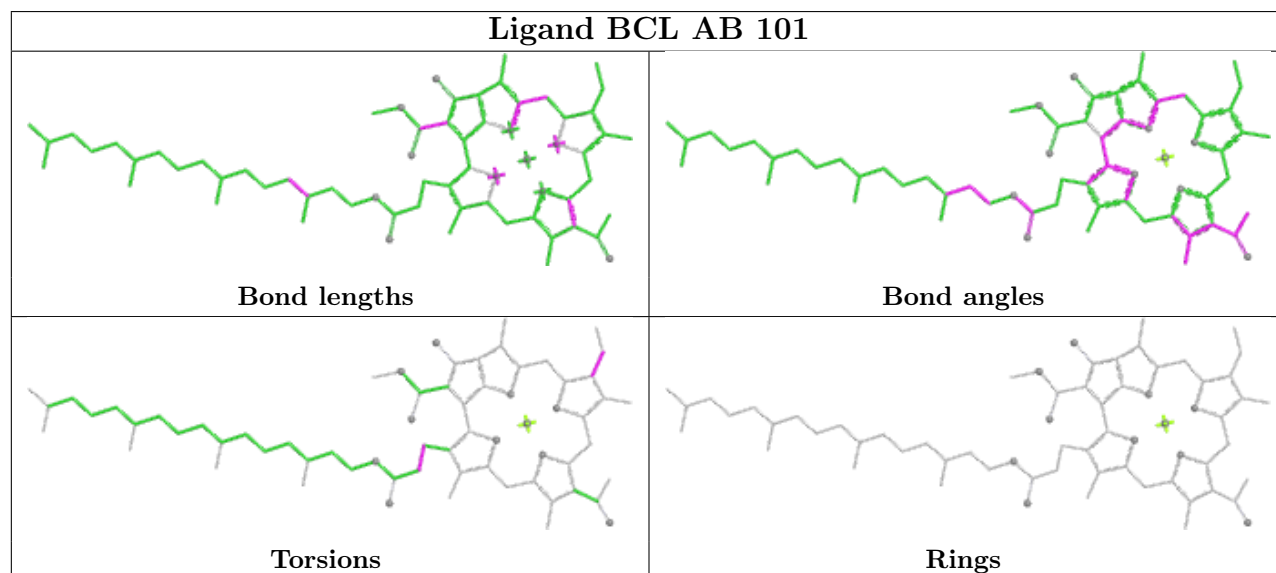
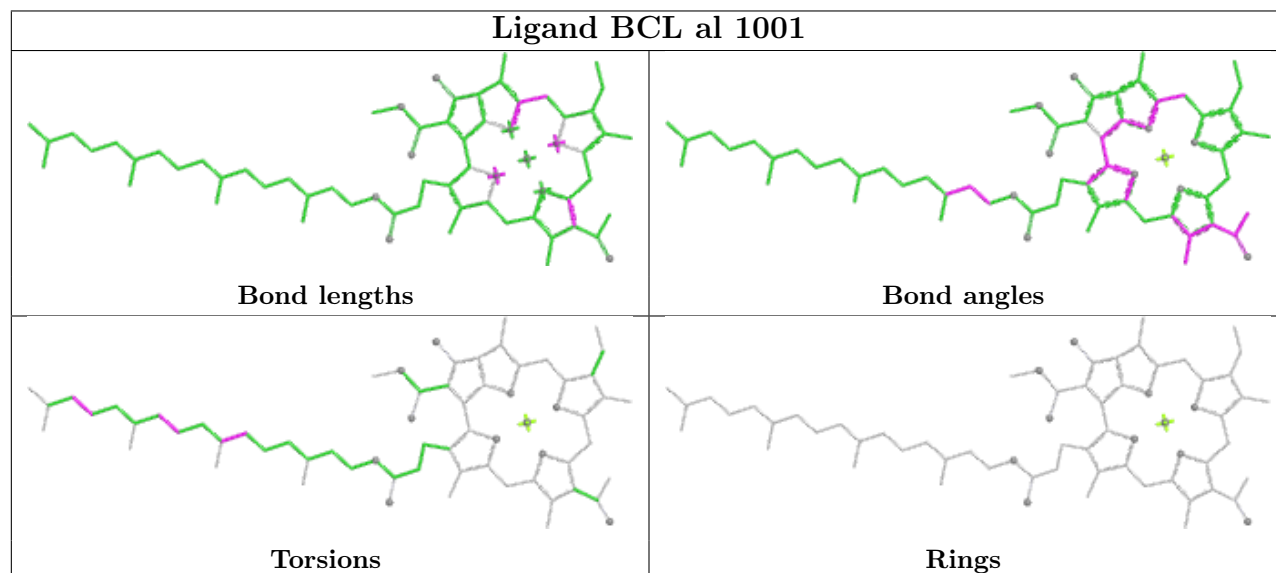
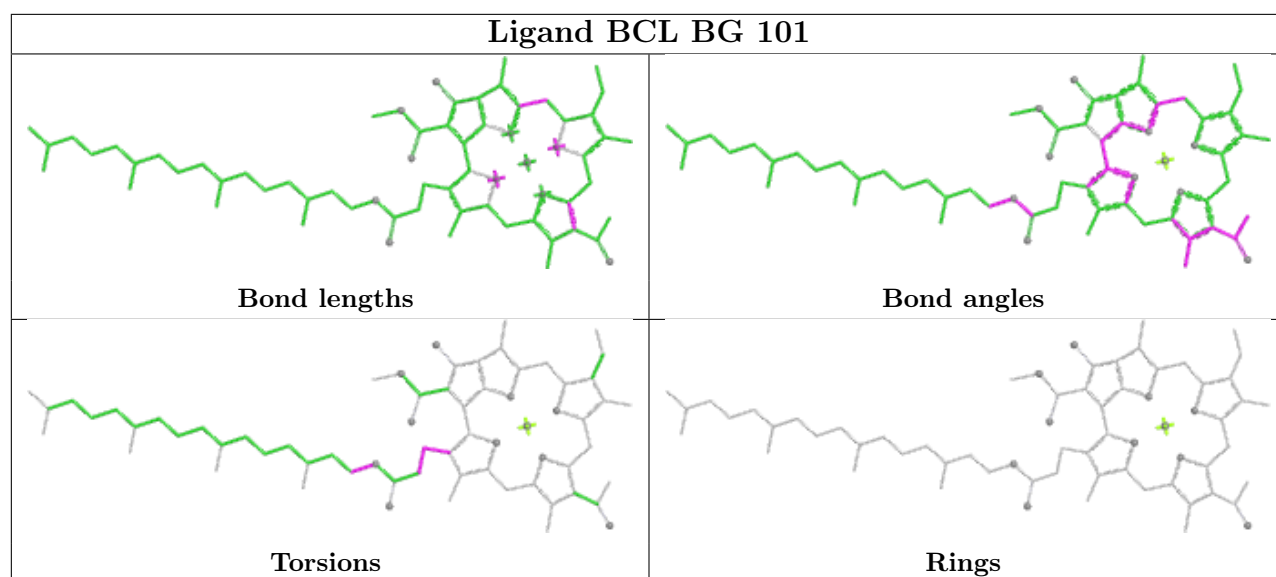


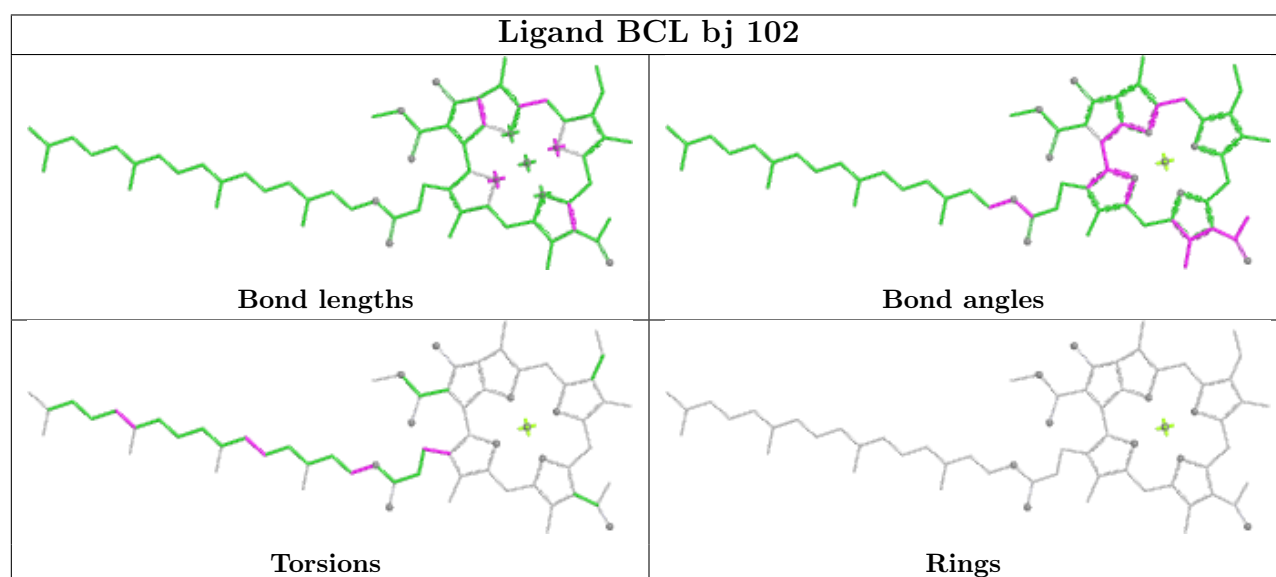
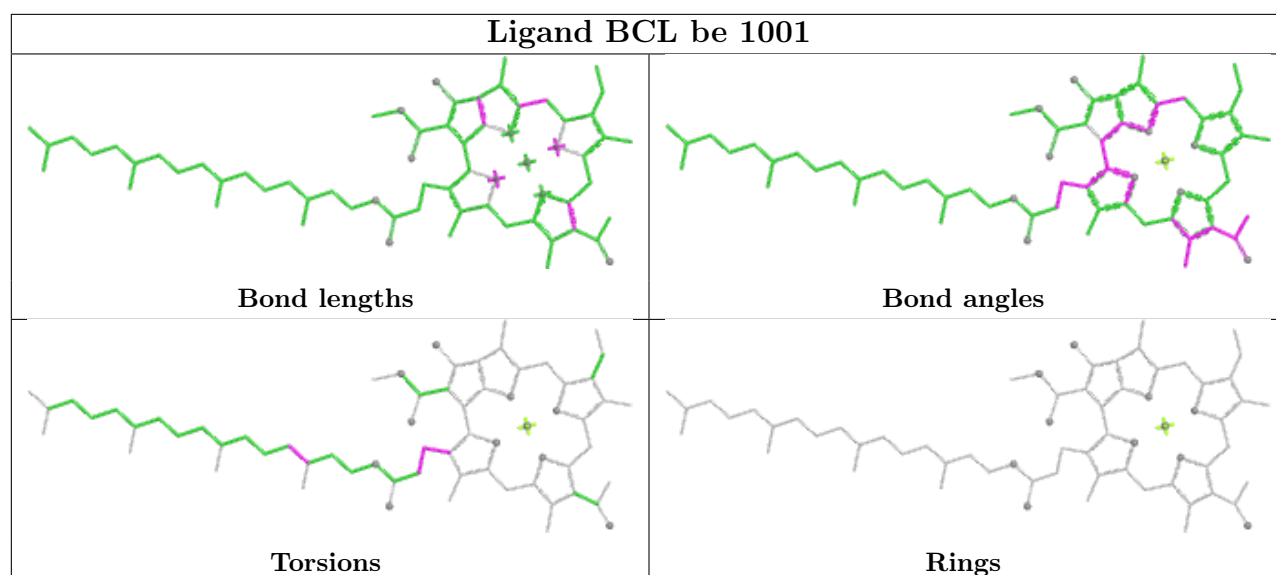
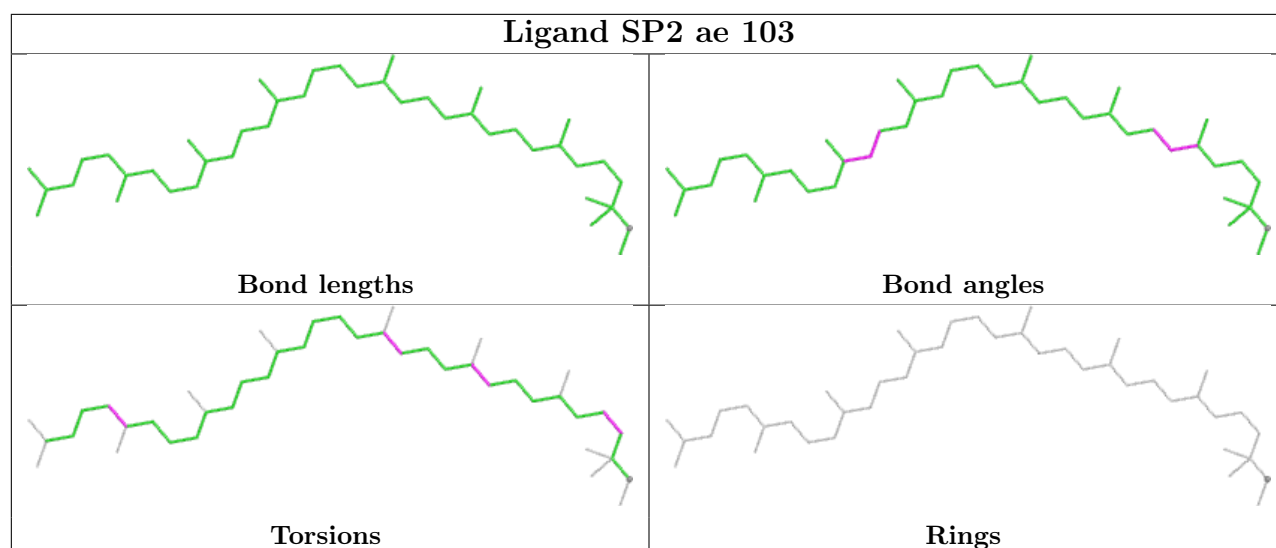


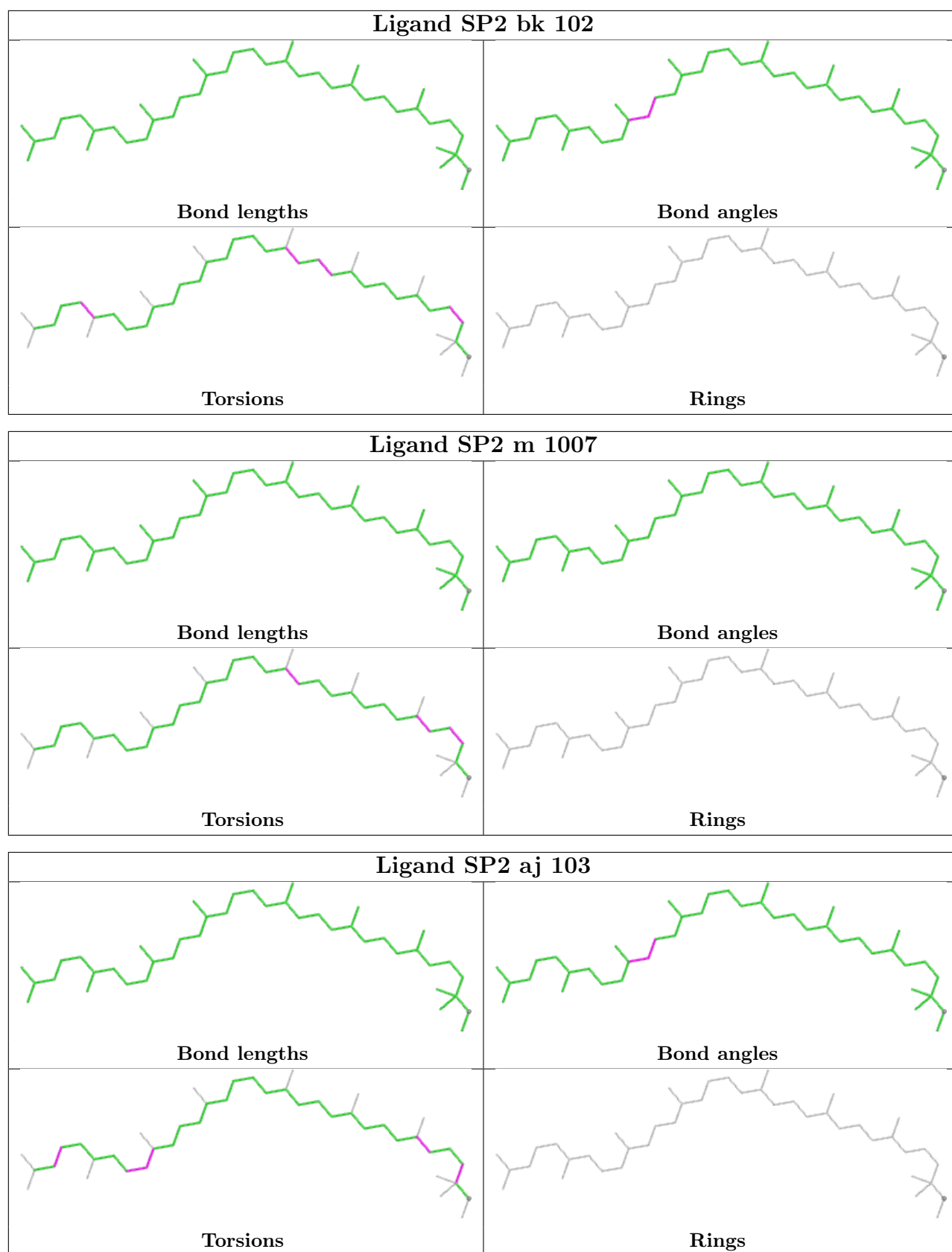
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Bond lengths	Bond angles
	
Torsions	Rings

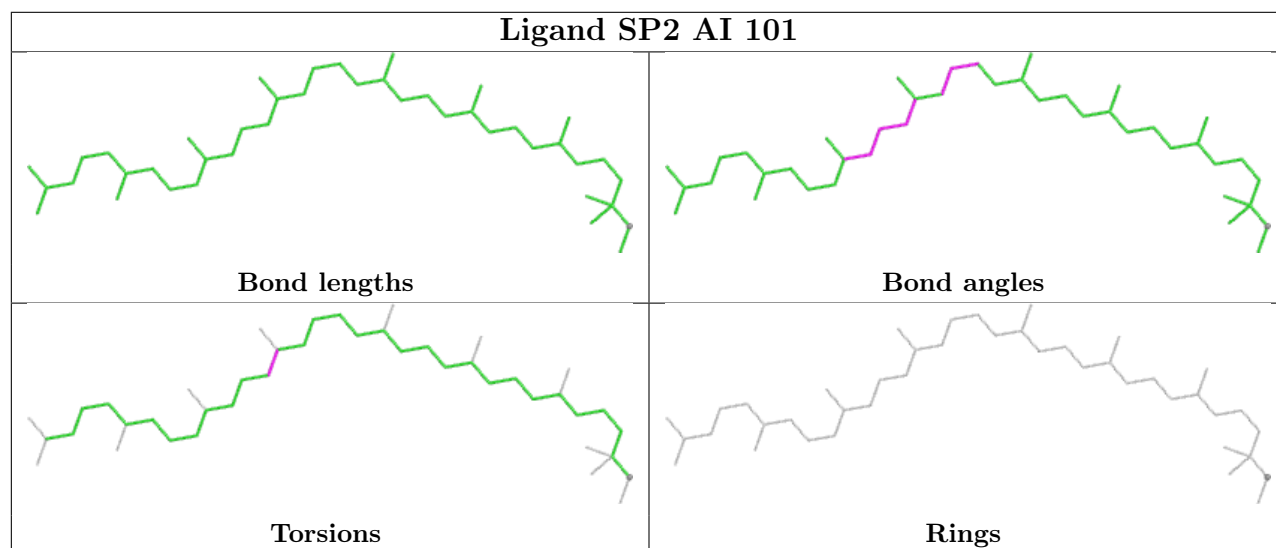
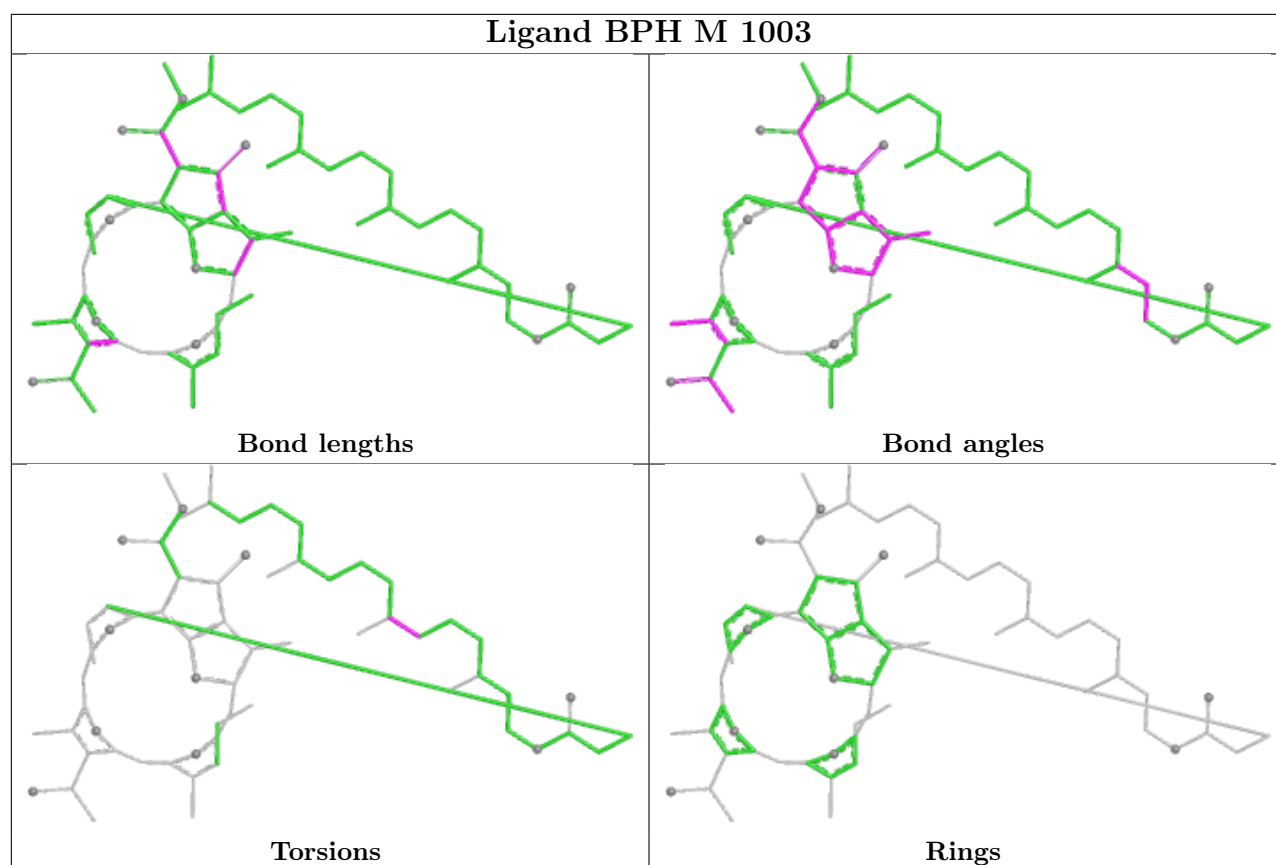
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Bond lengths	Bond angles
	
Torsions	Rings

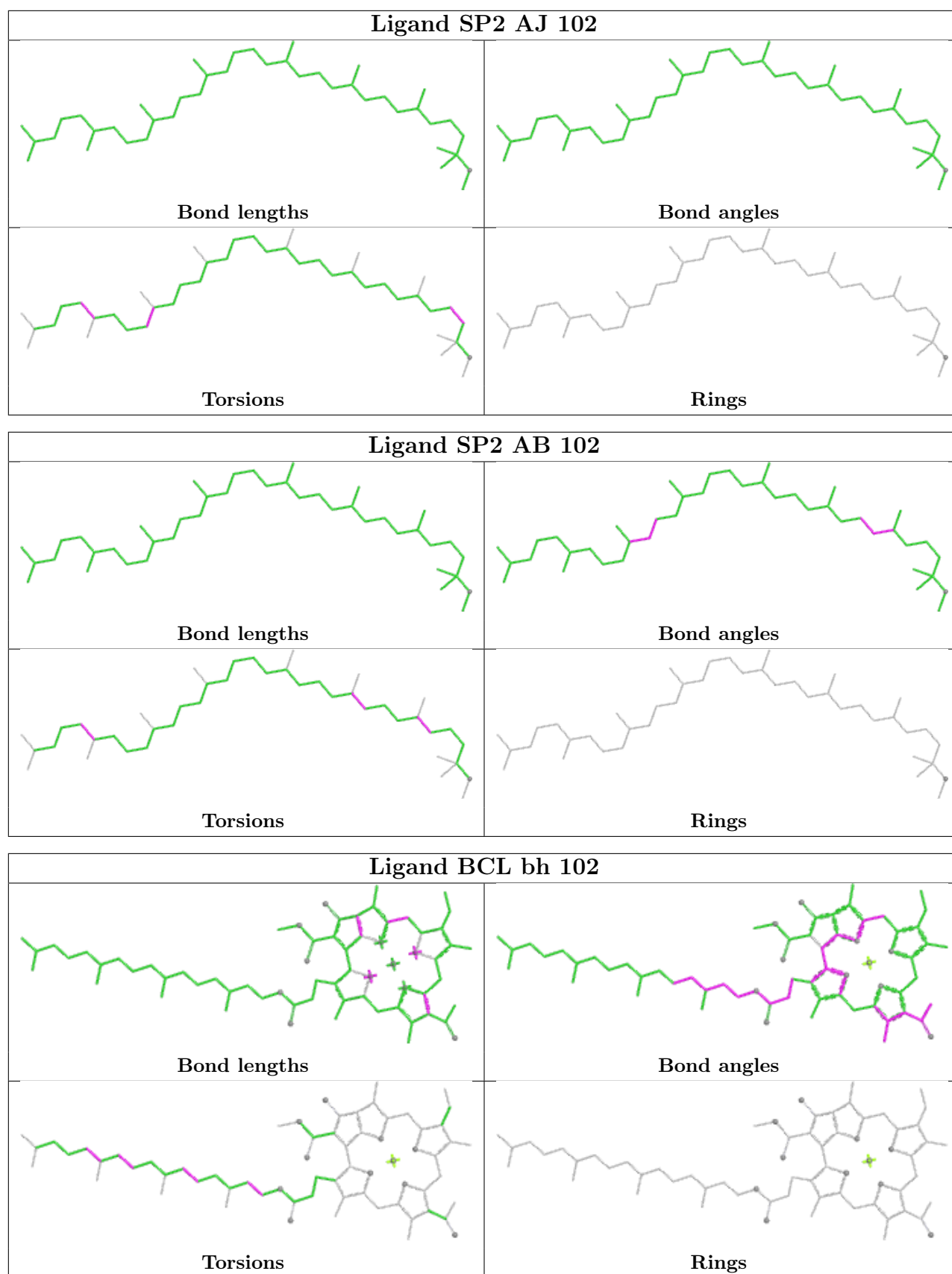
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Bond lengths	Bond angles
	
Torsions	Rings

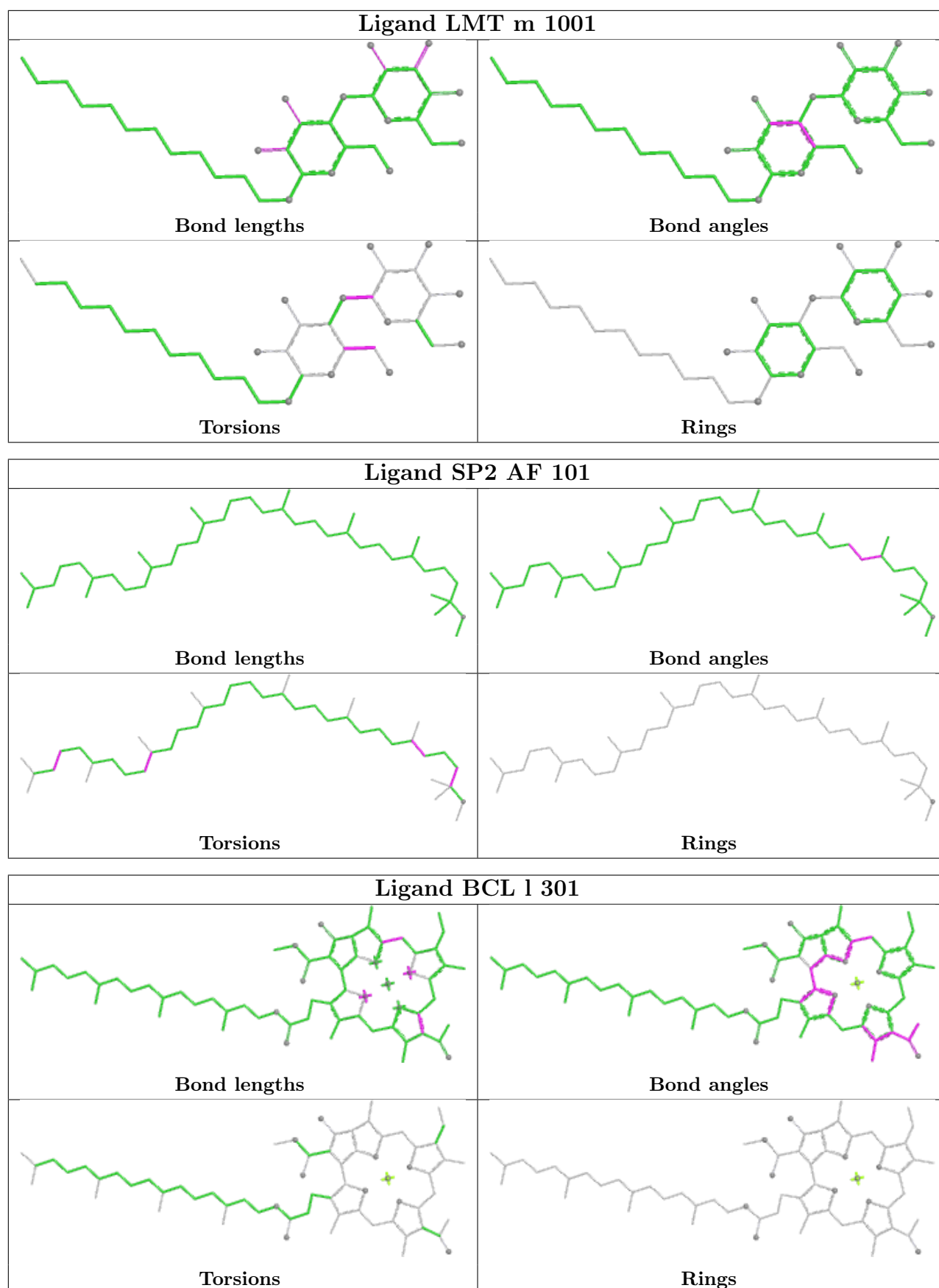


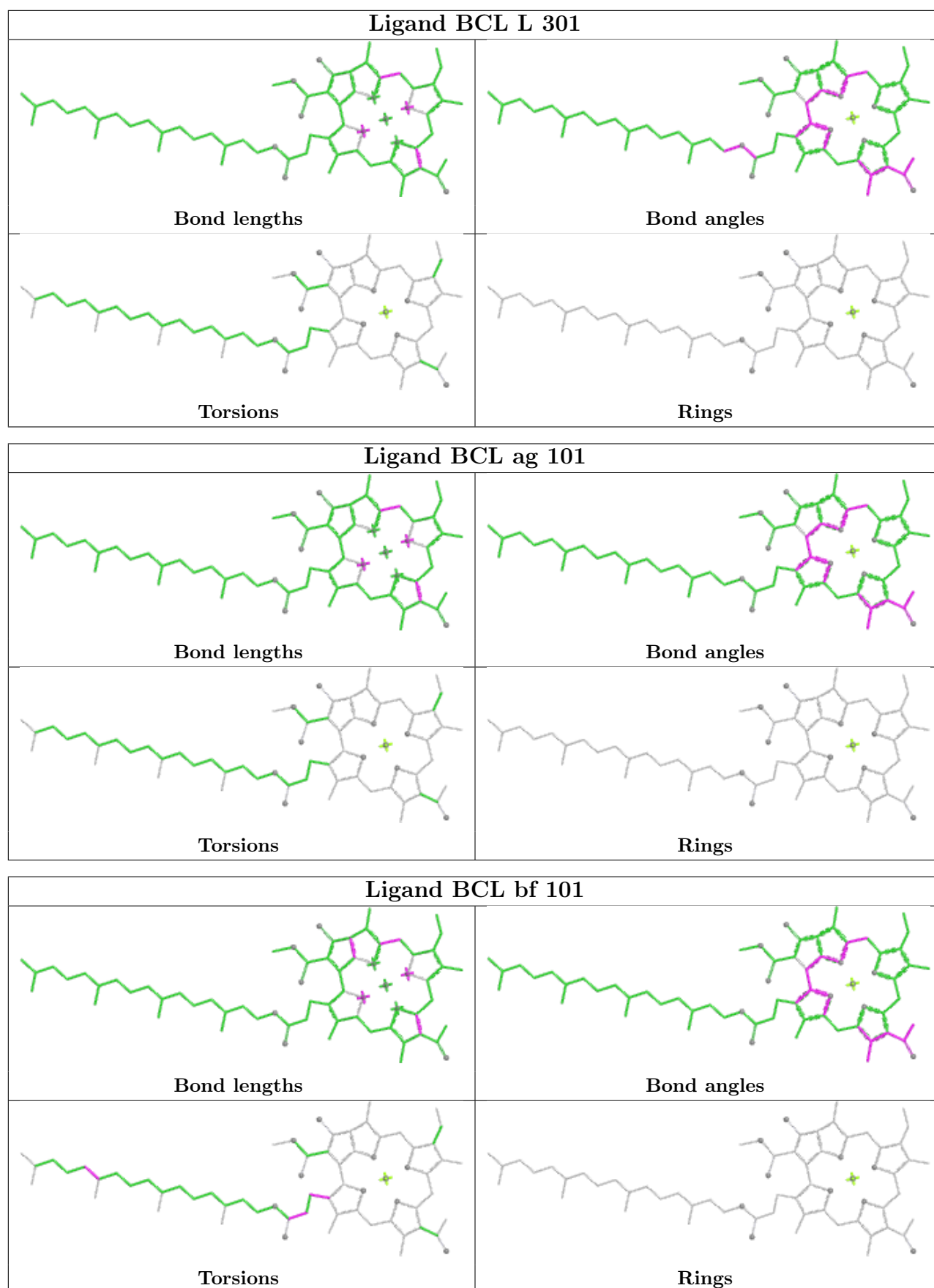


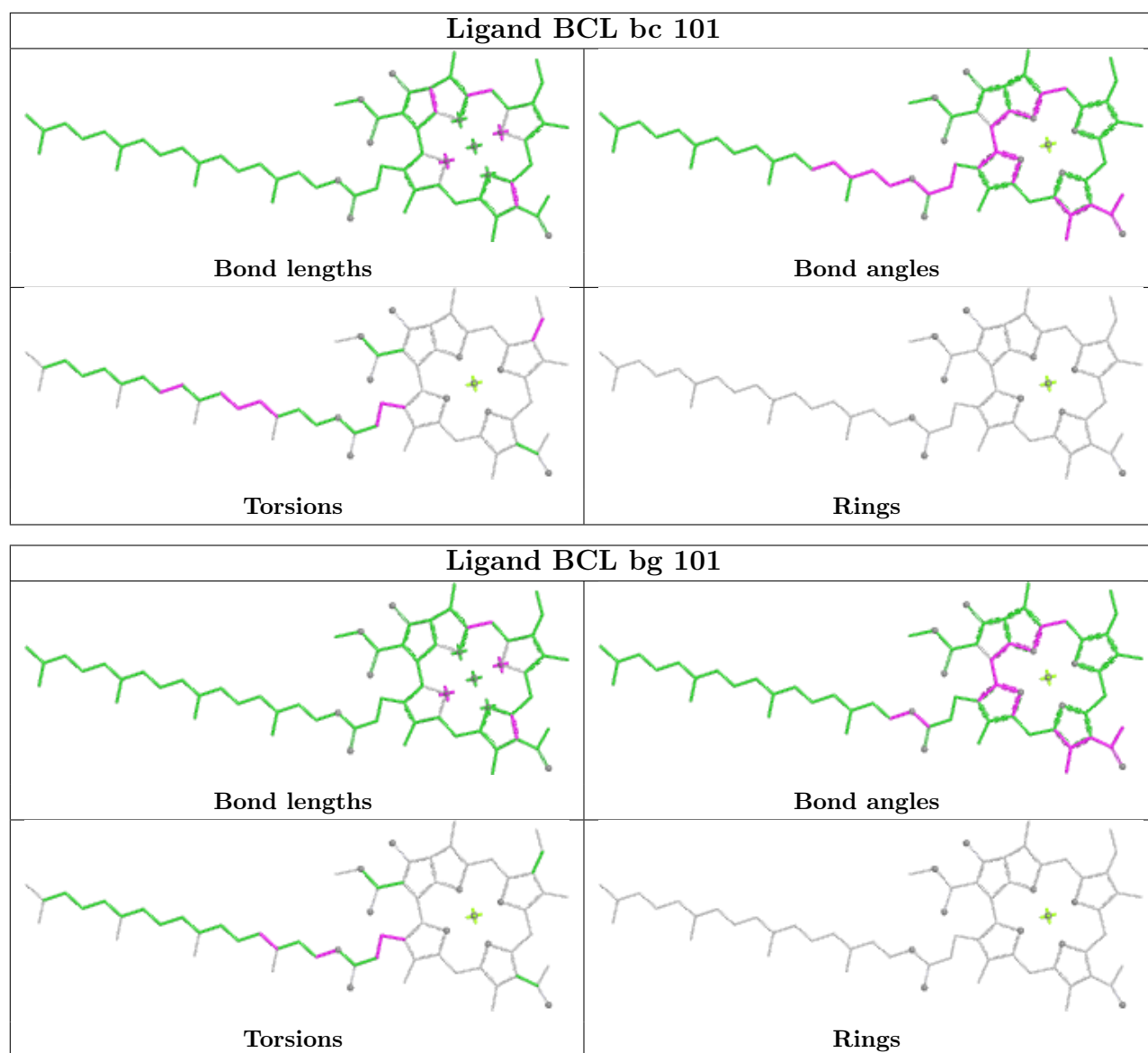


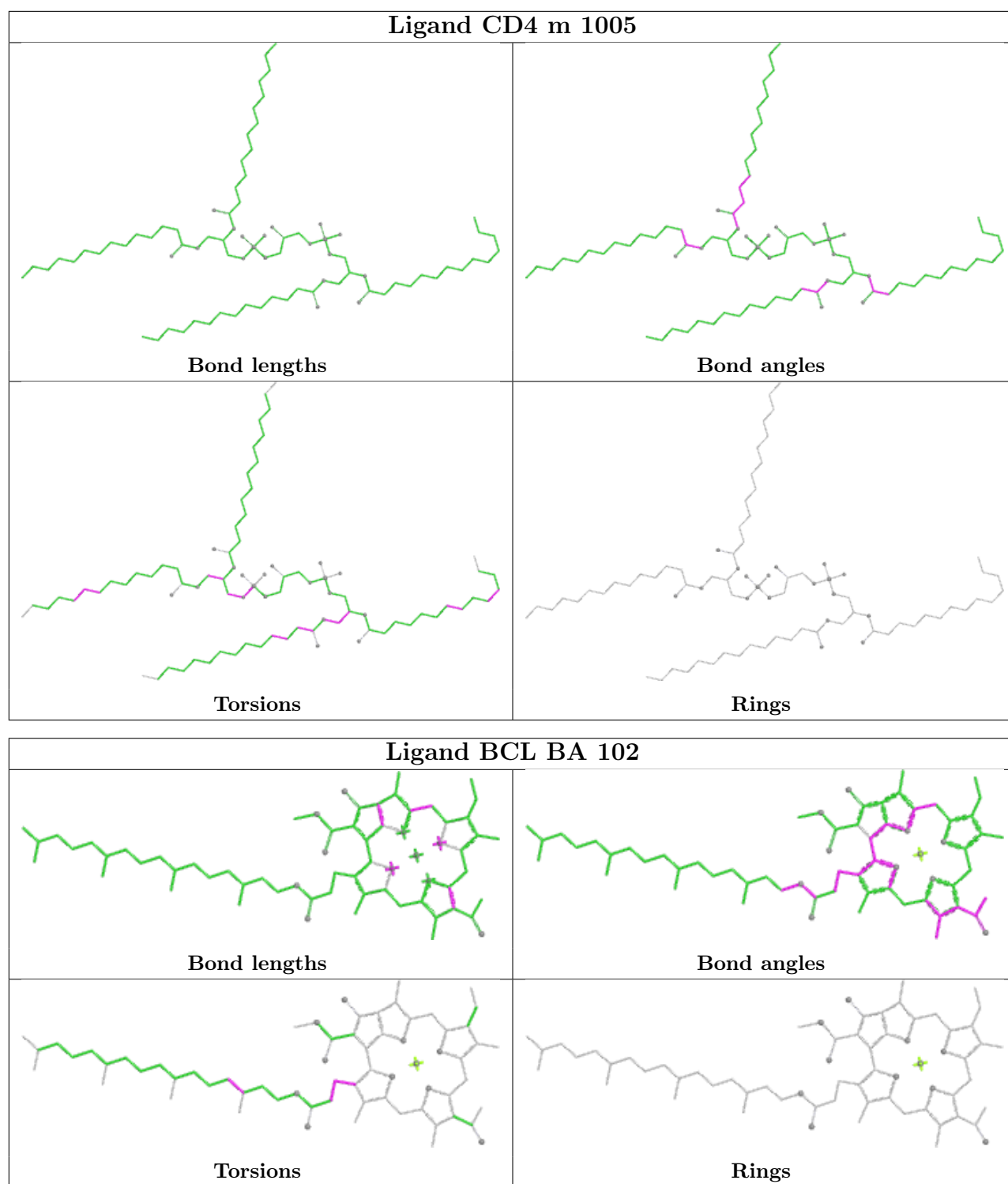


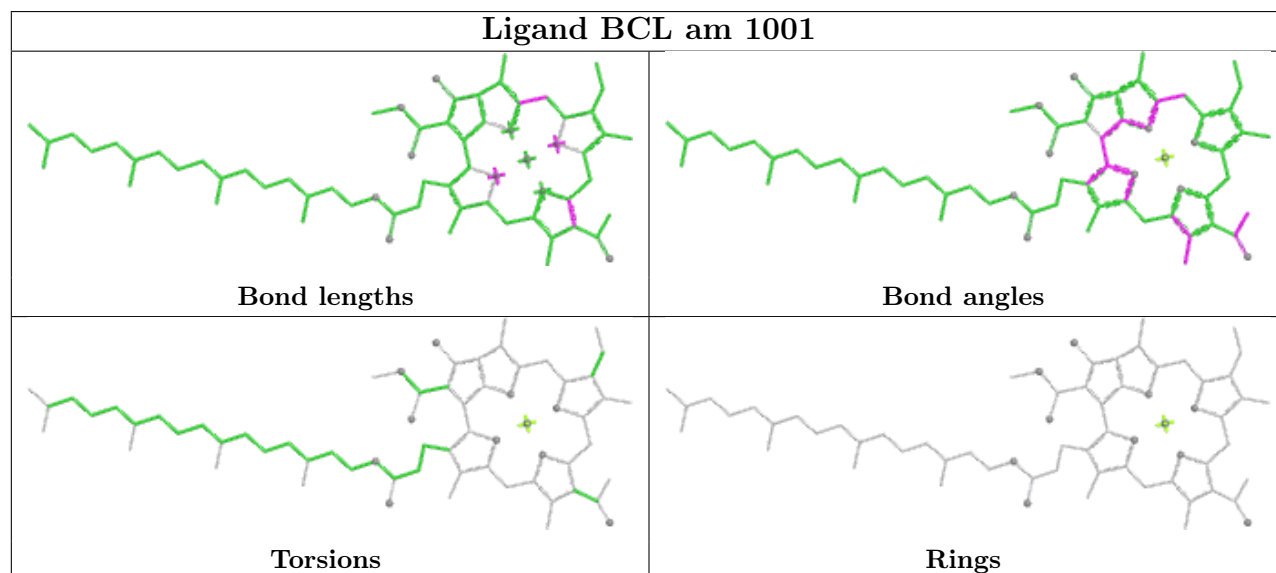
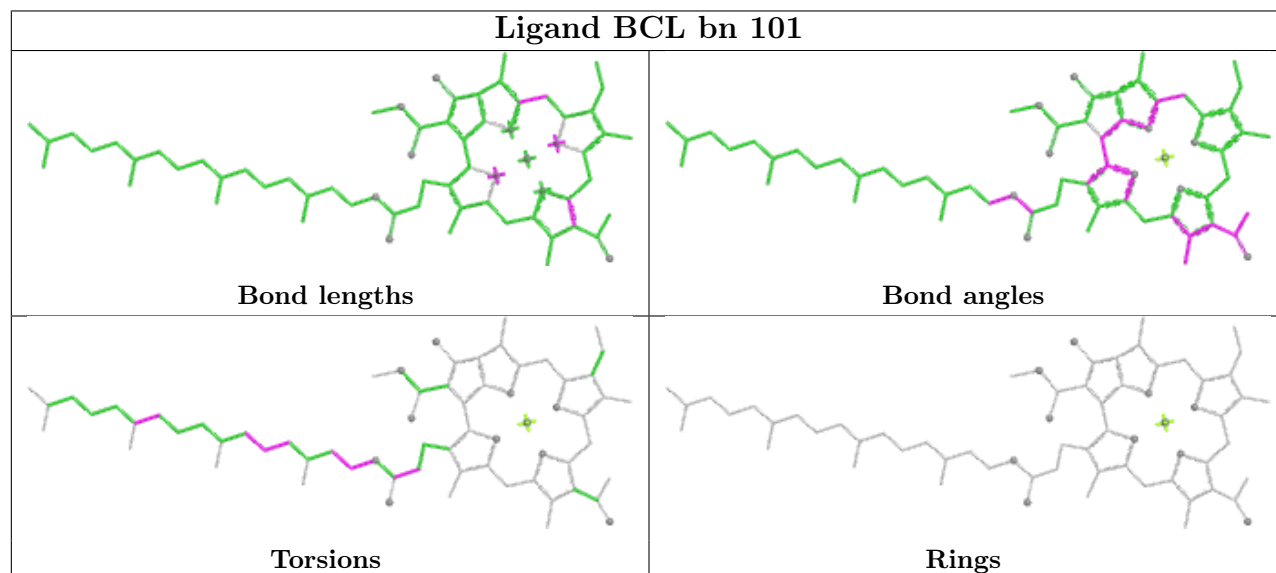
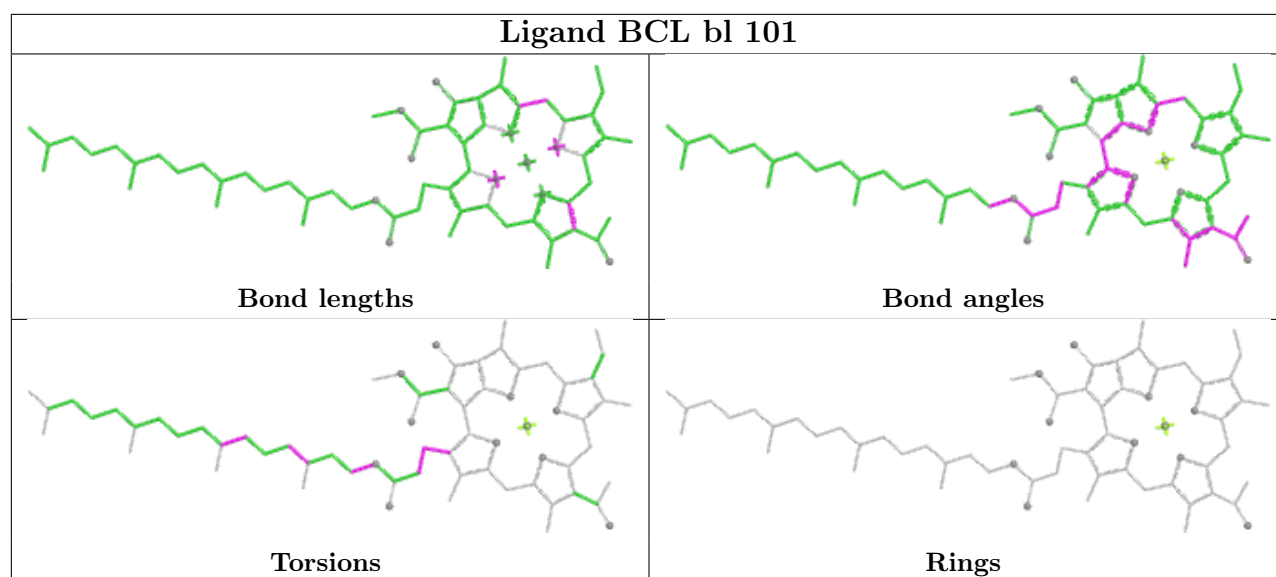


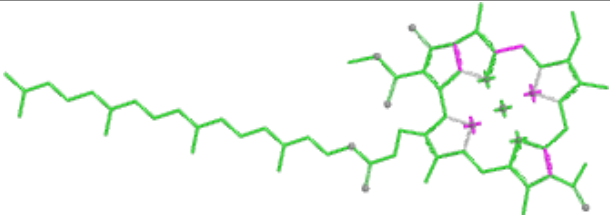
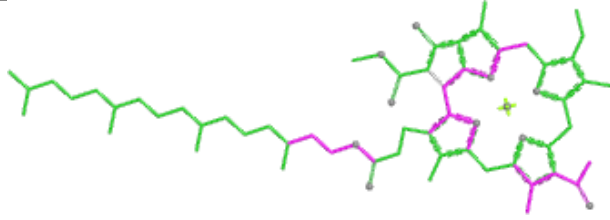
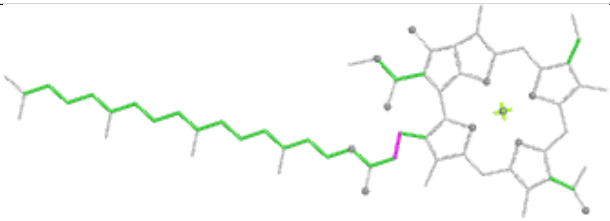
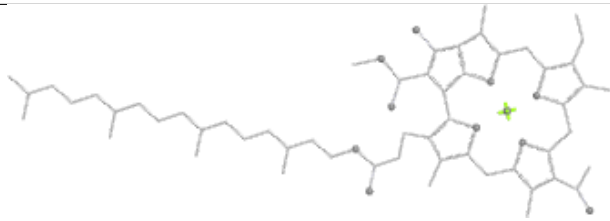
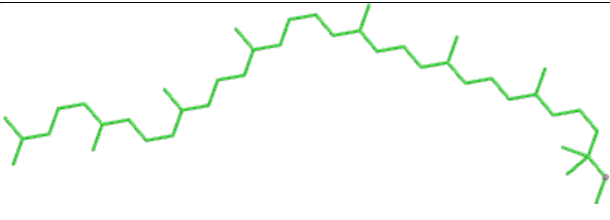
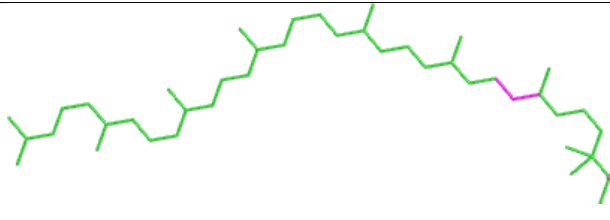
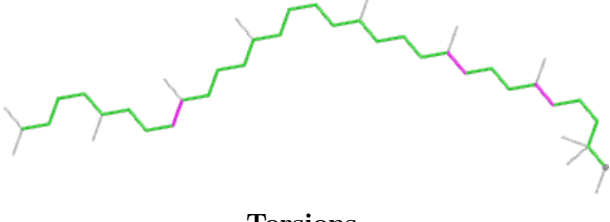
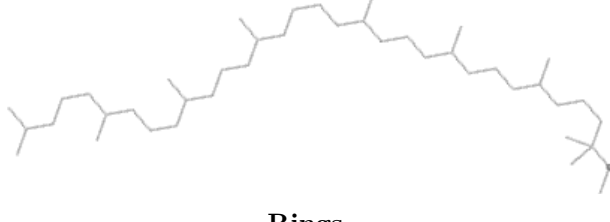
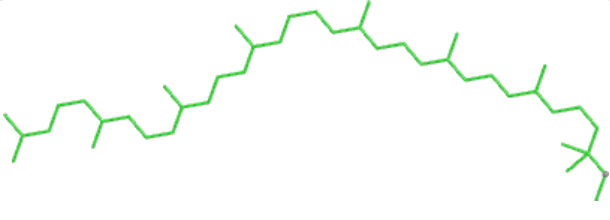
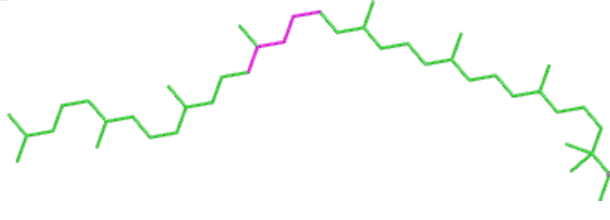
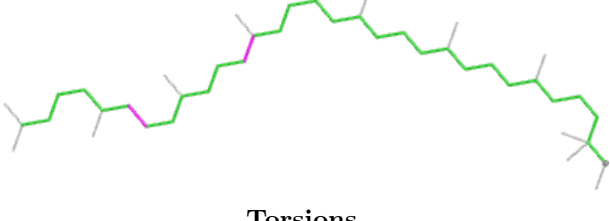
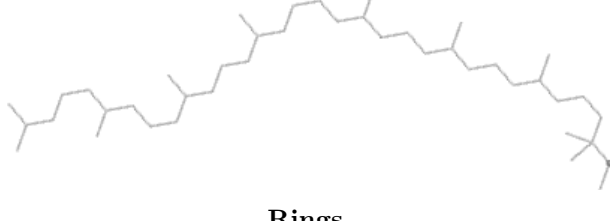


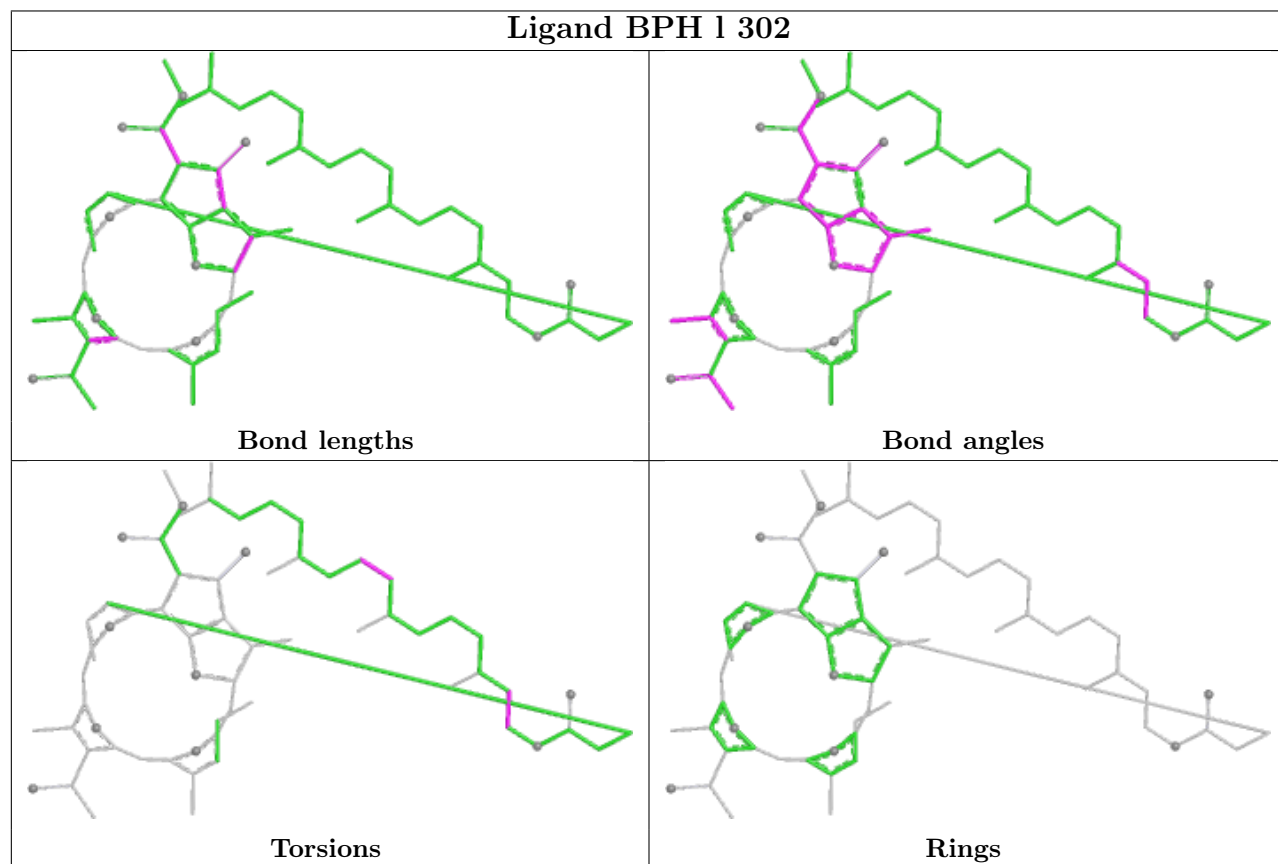
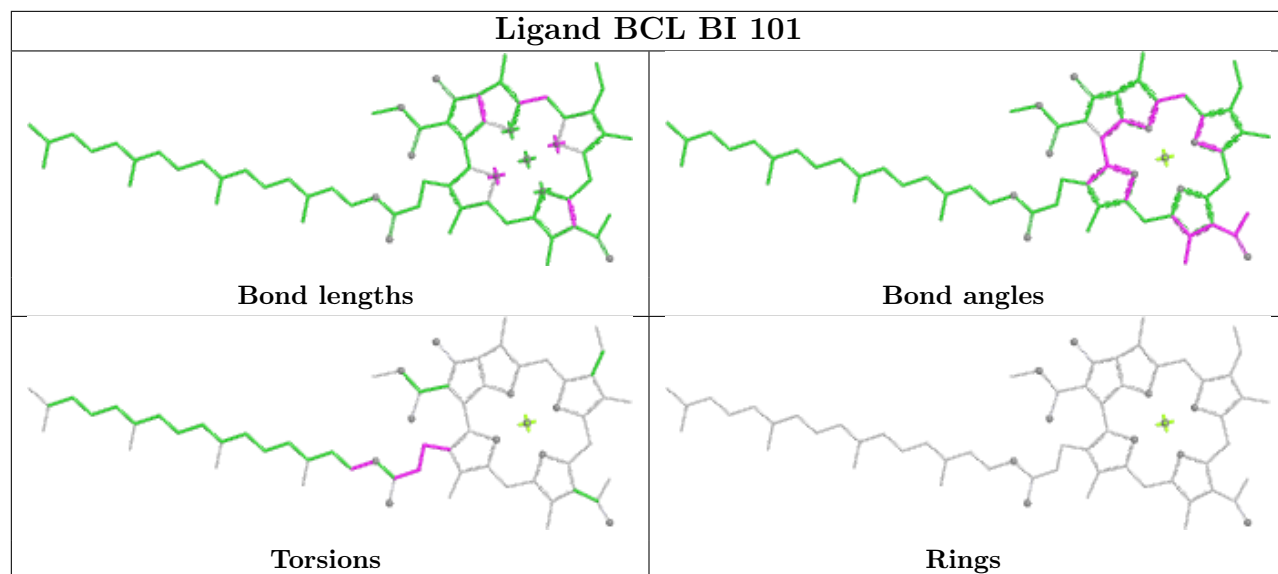


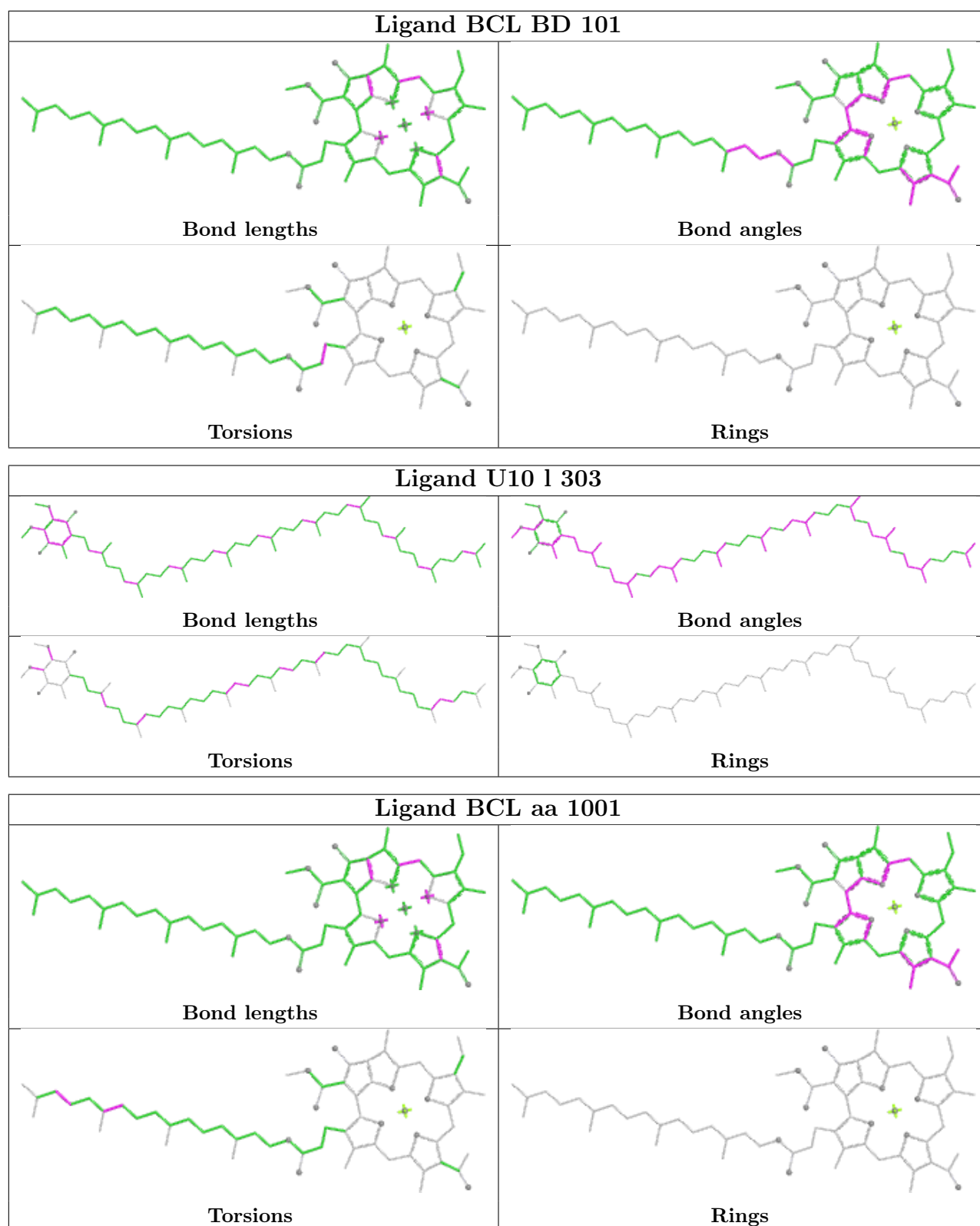


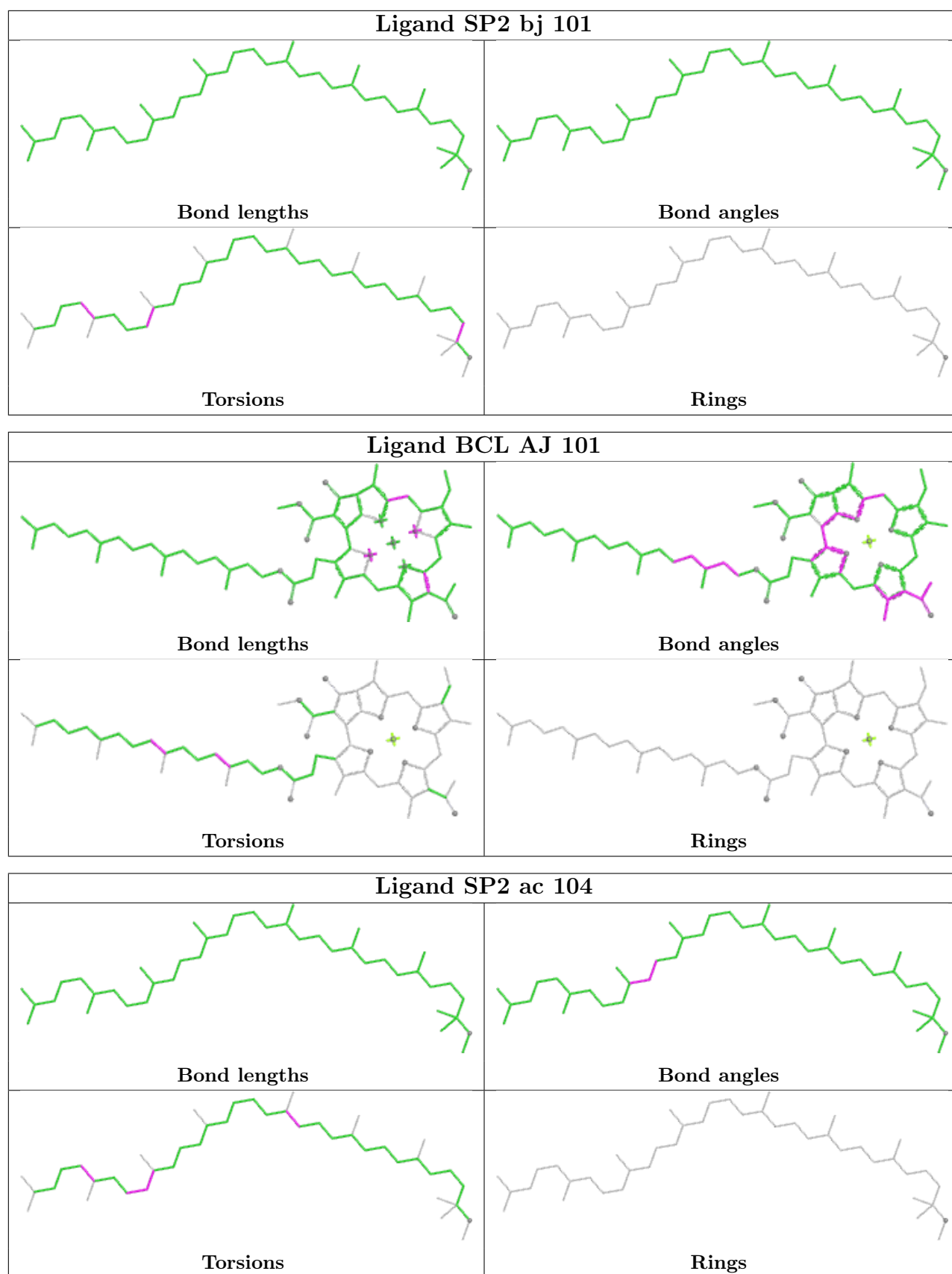


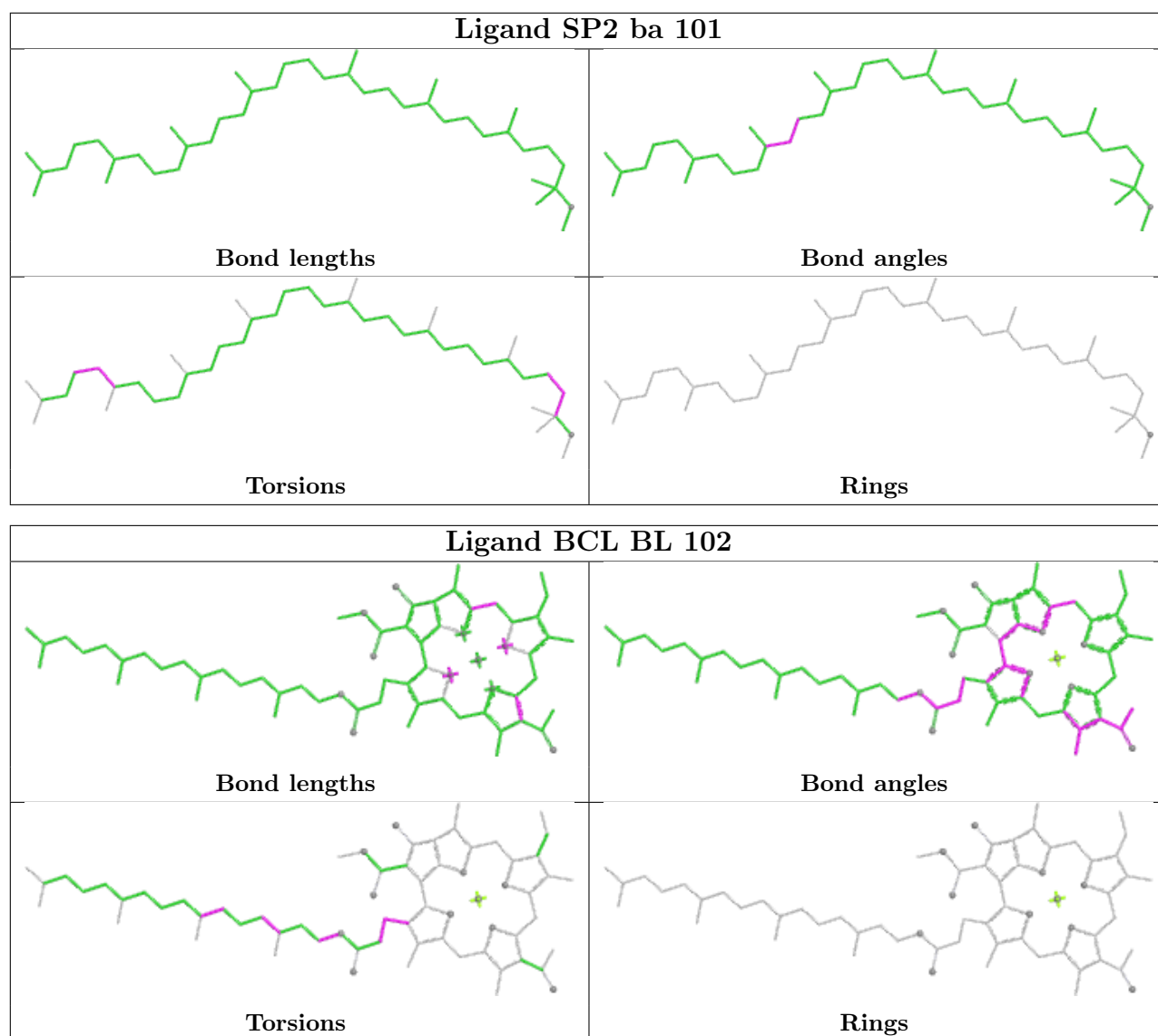


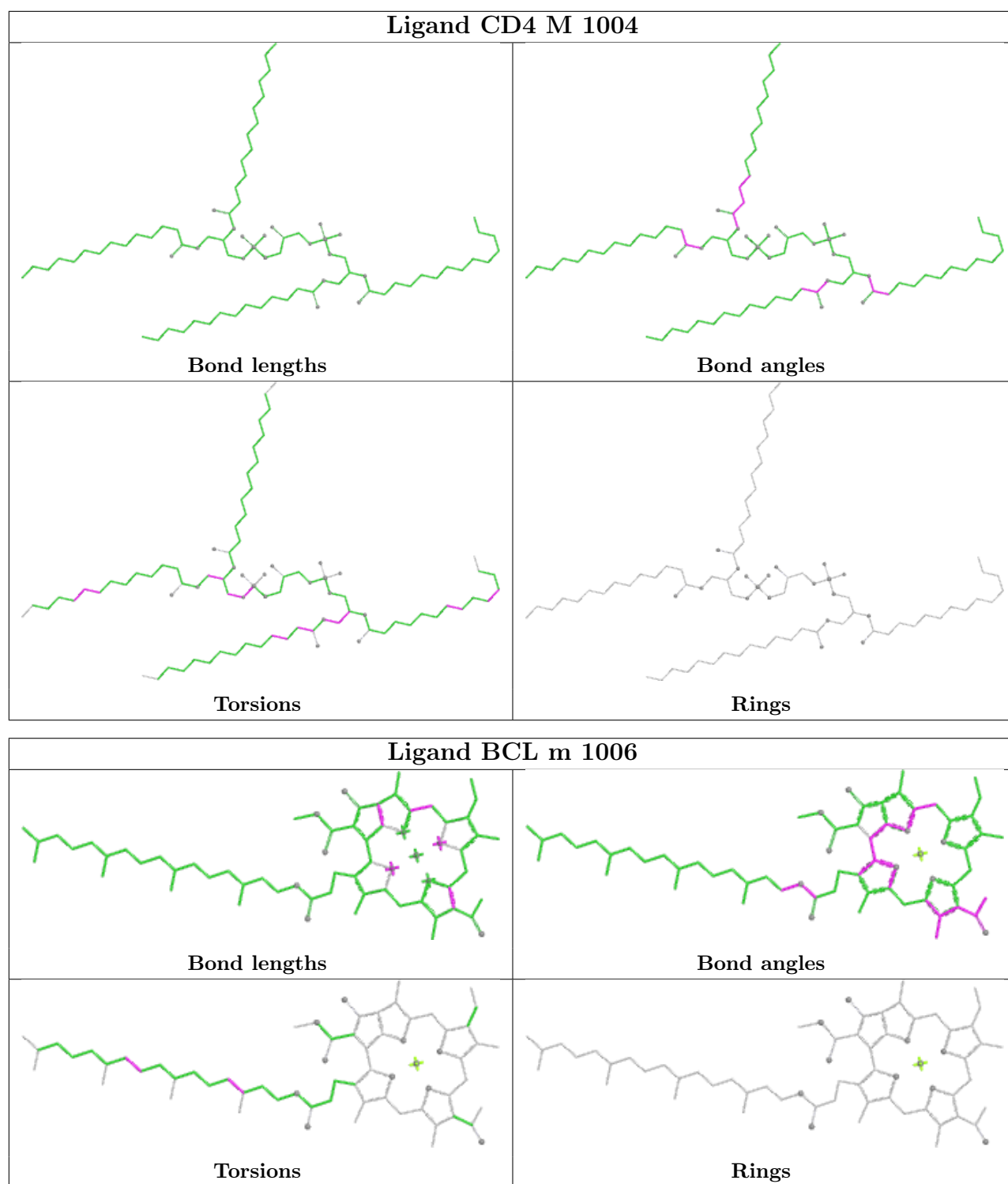
Ligand BCL bd 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SP2 ah 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
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 Bond lengths	 Bond angles
 Torsions	 Rings

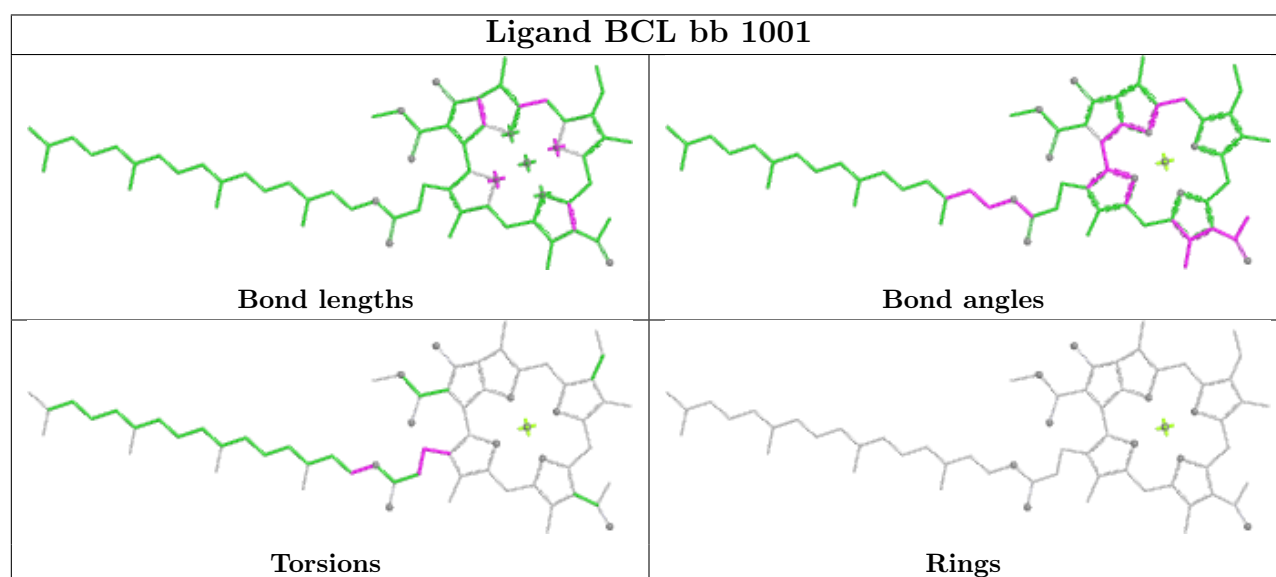
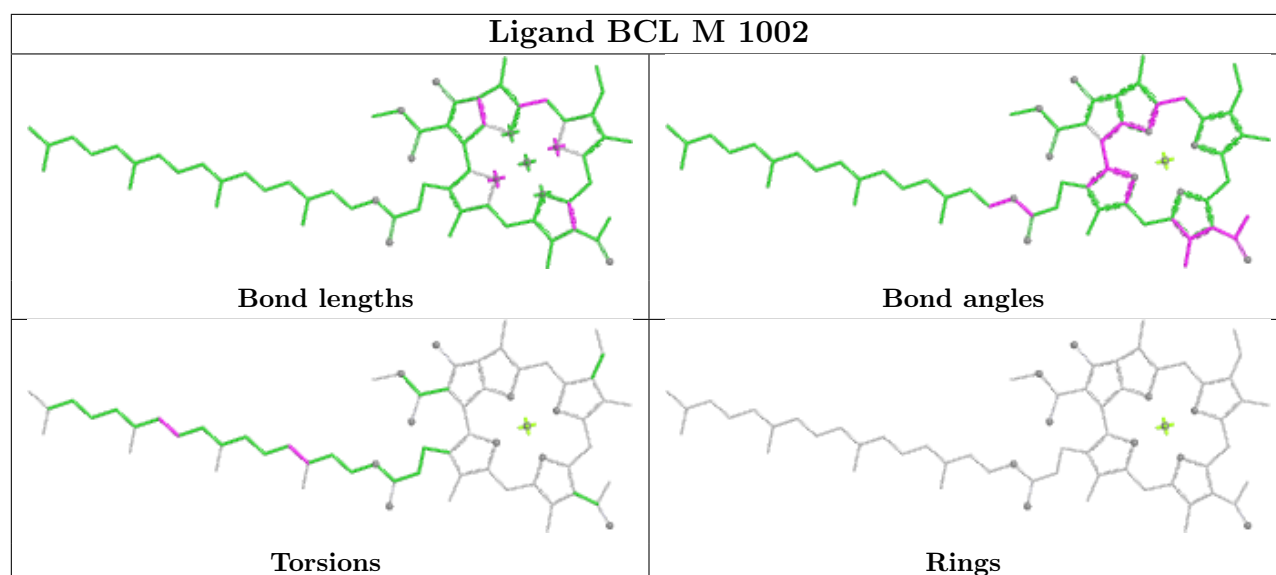
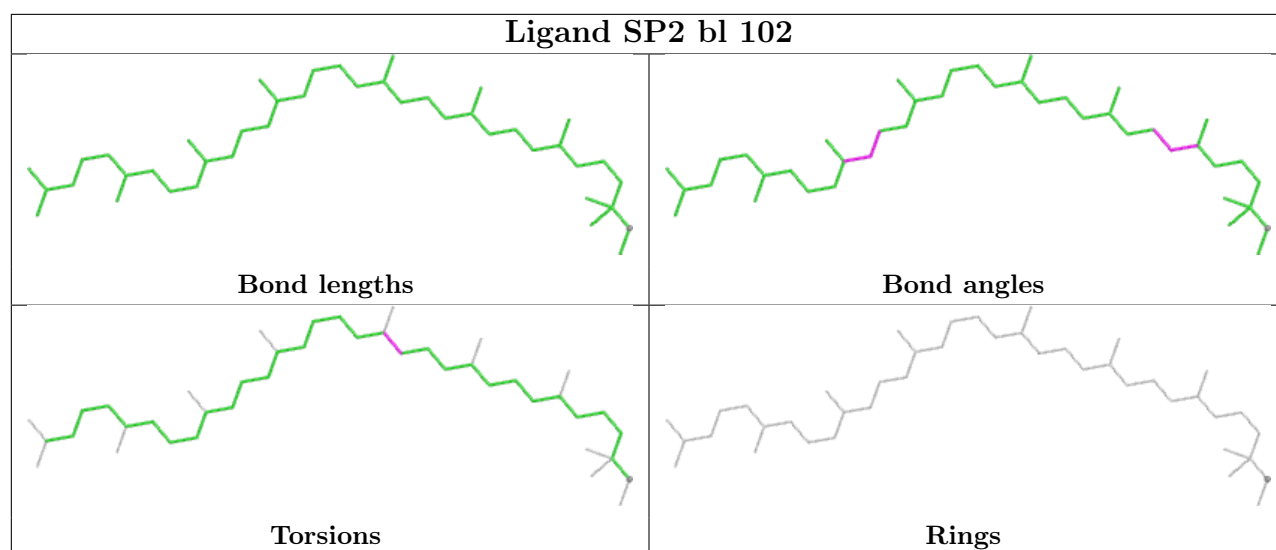


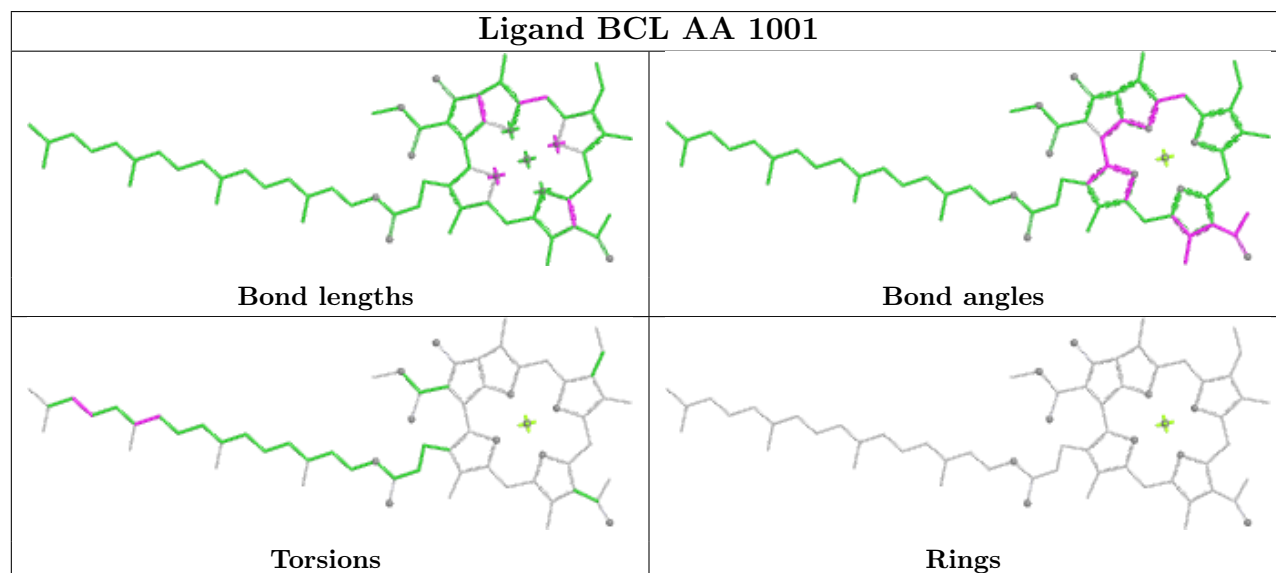
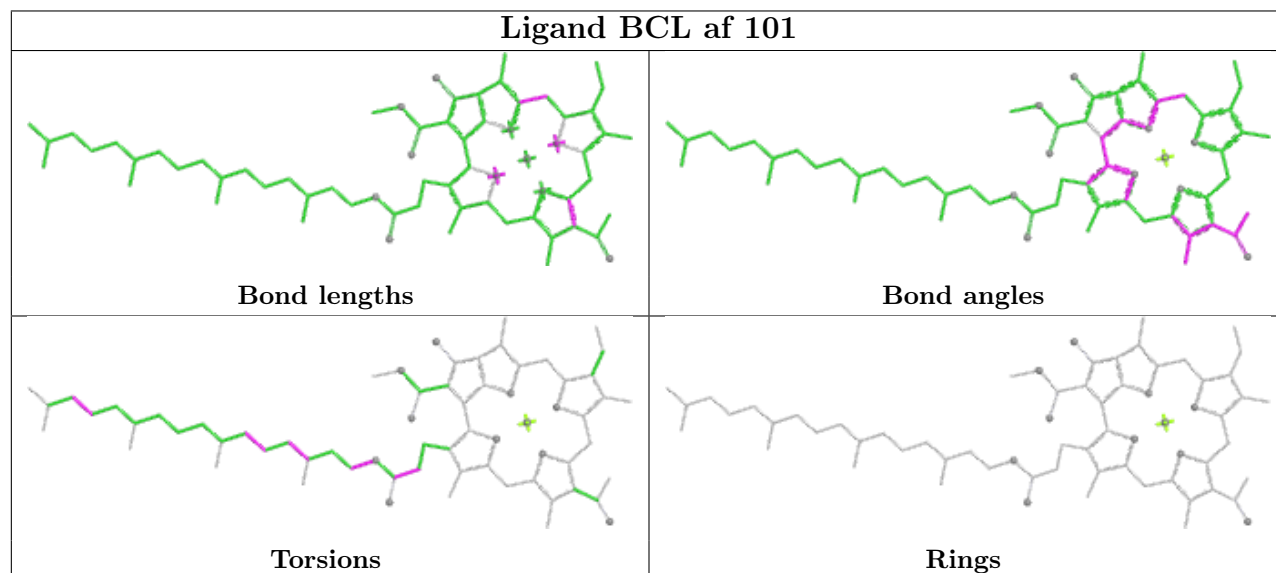
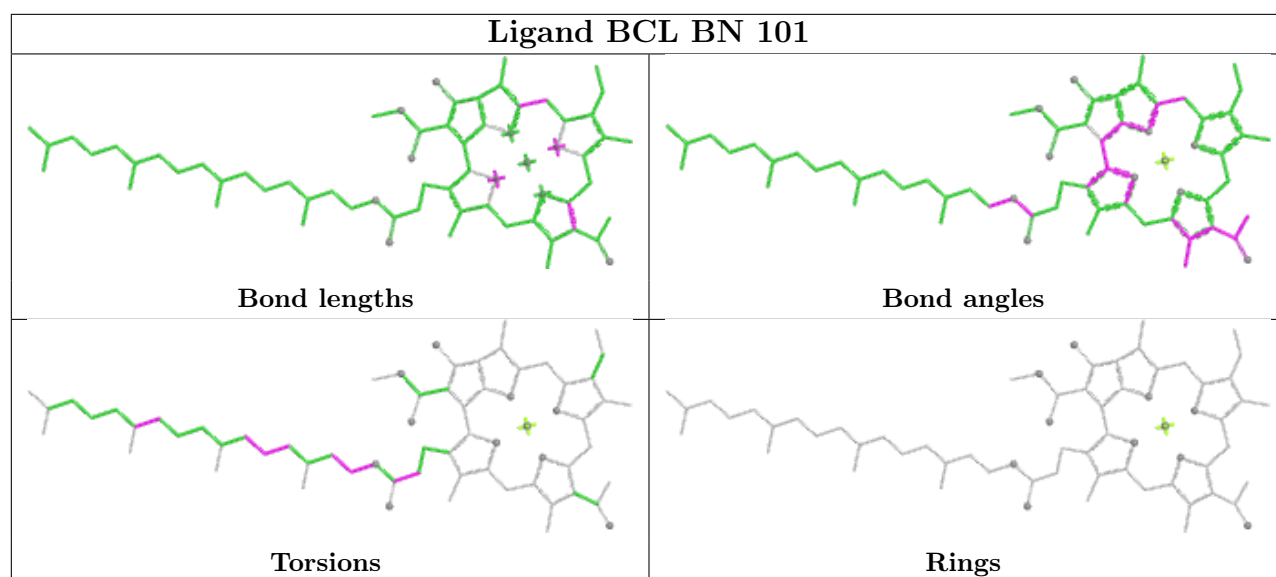


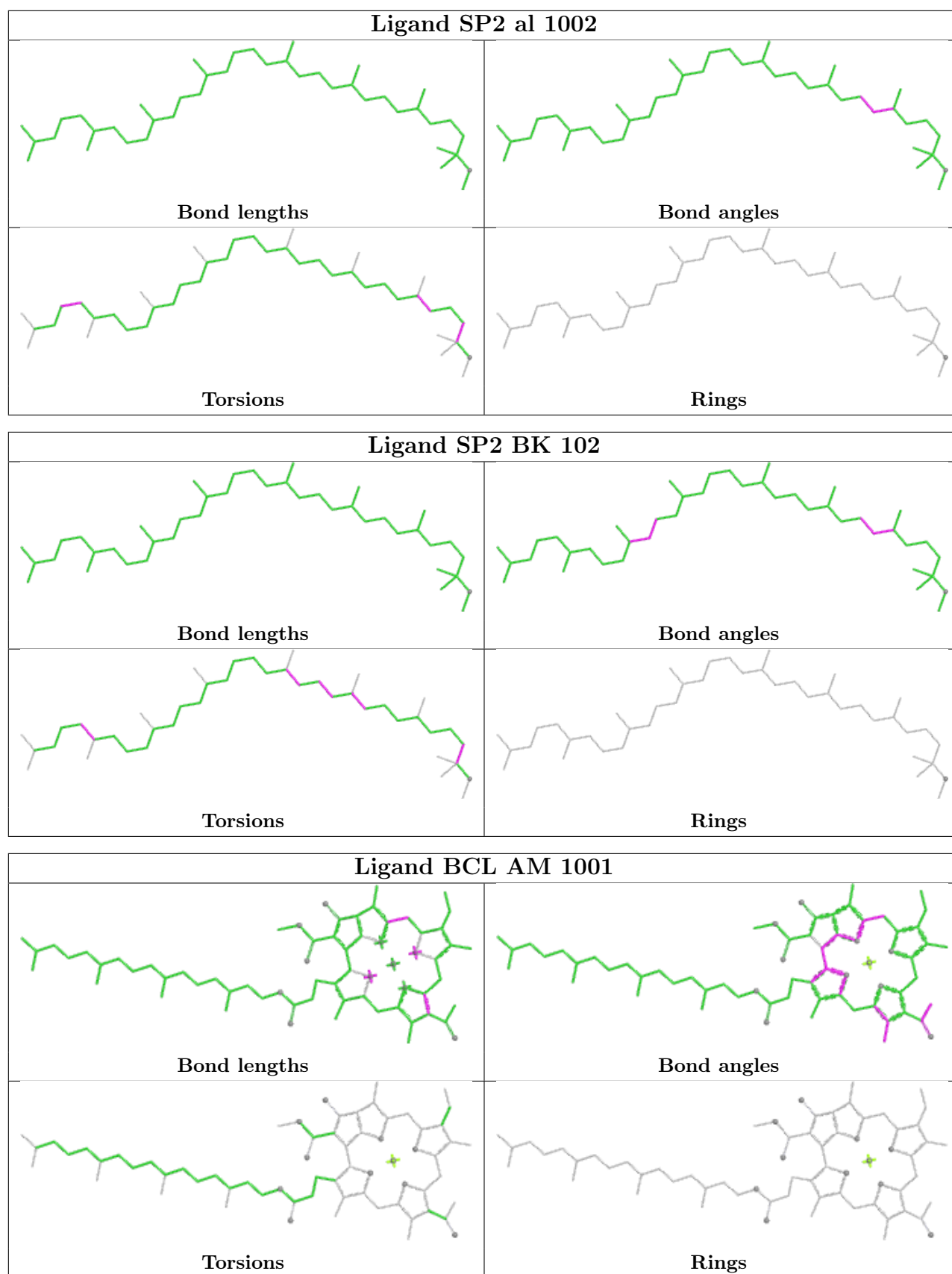


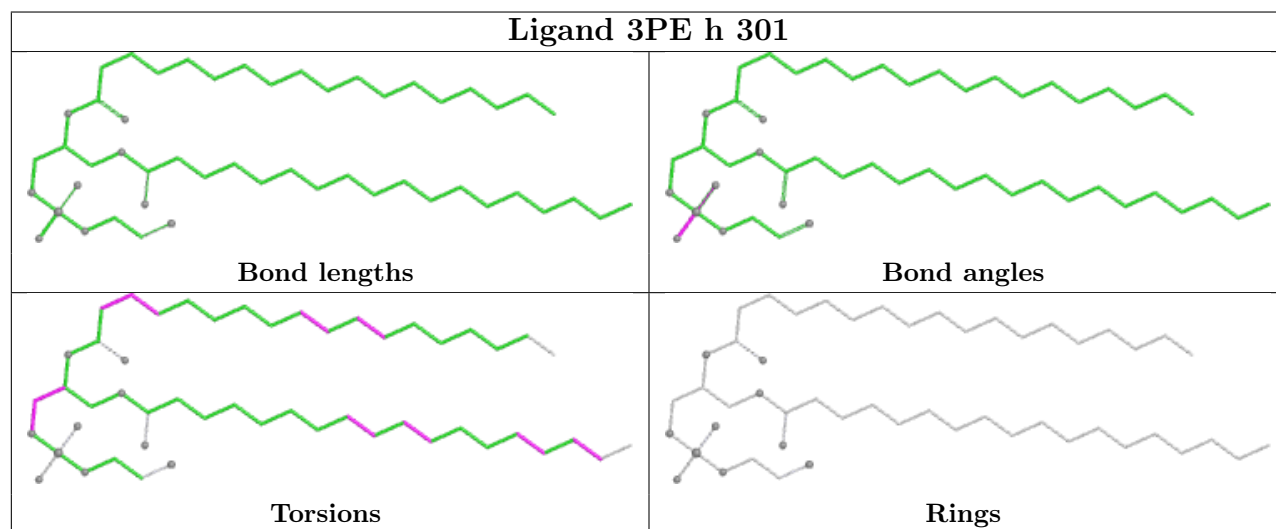
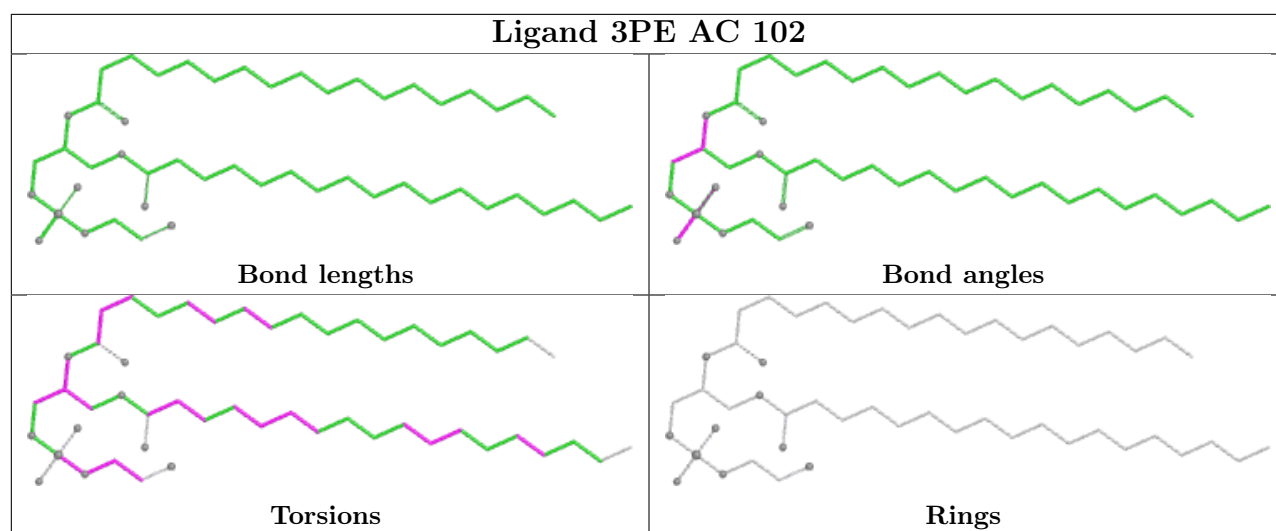
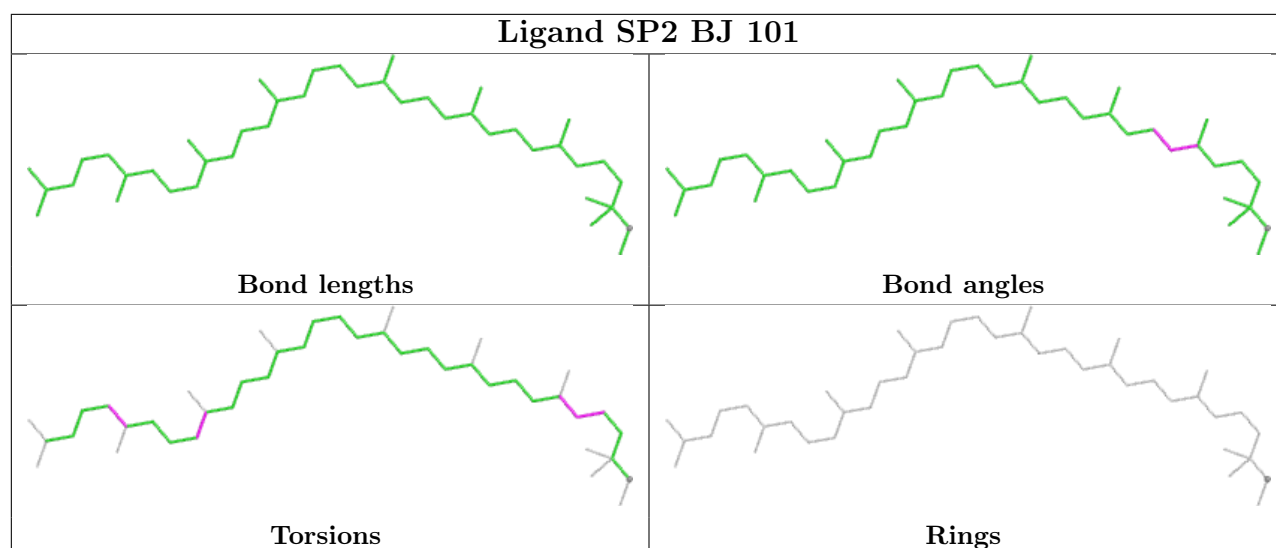


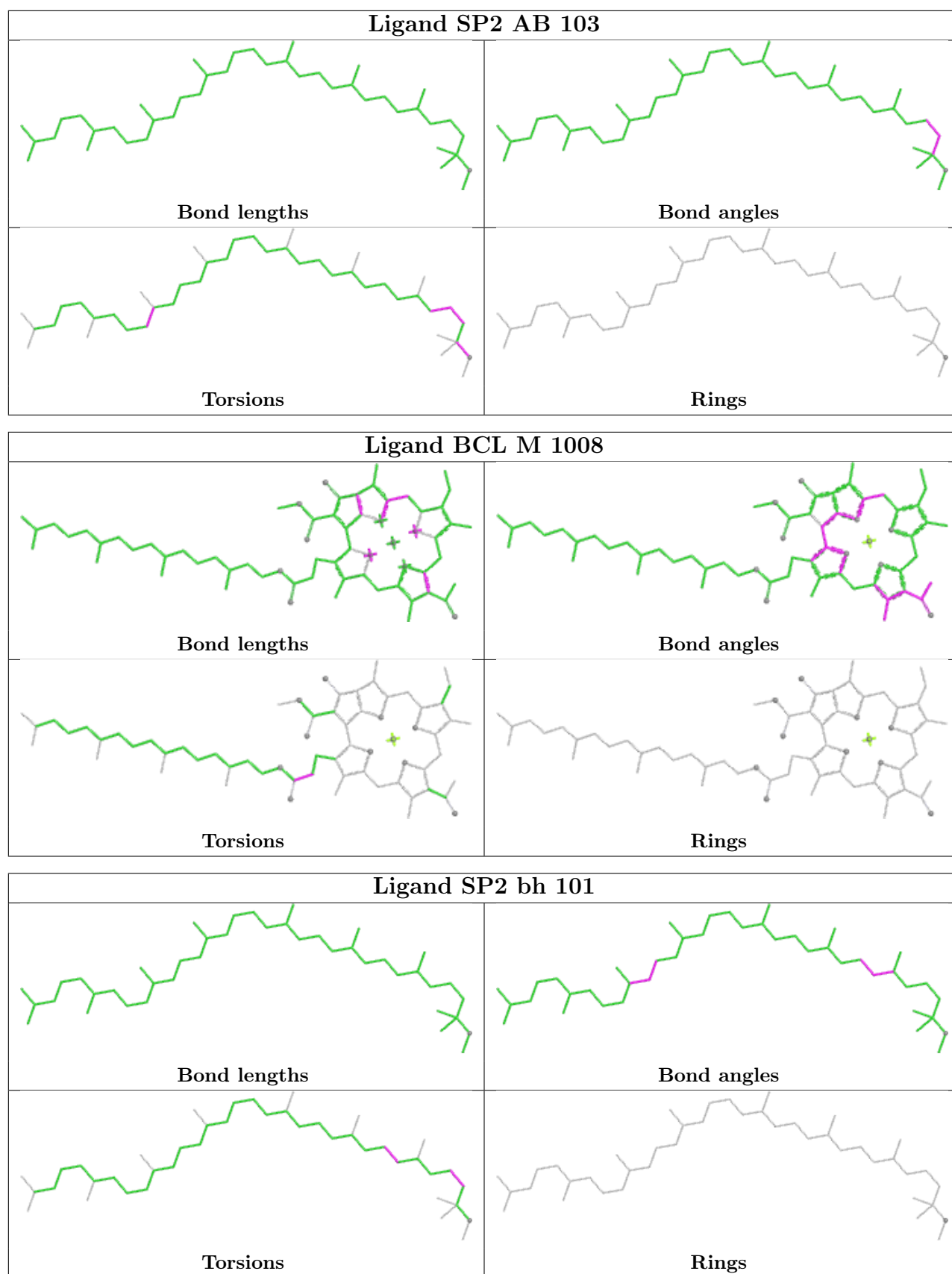


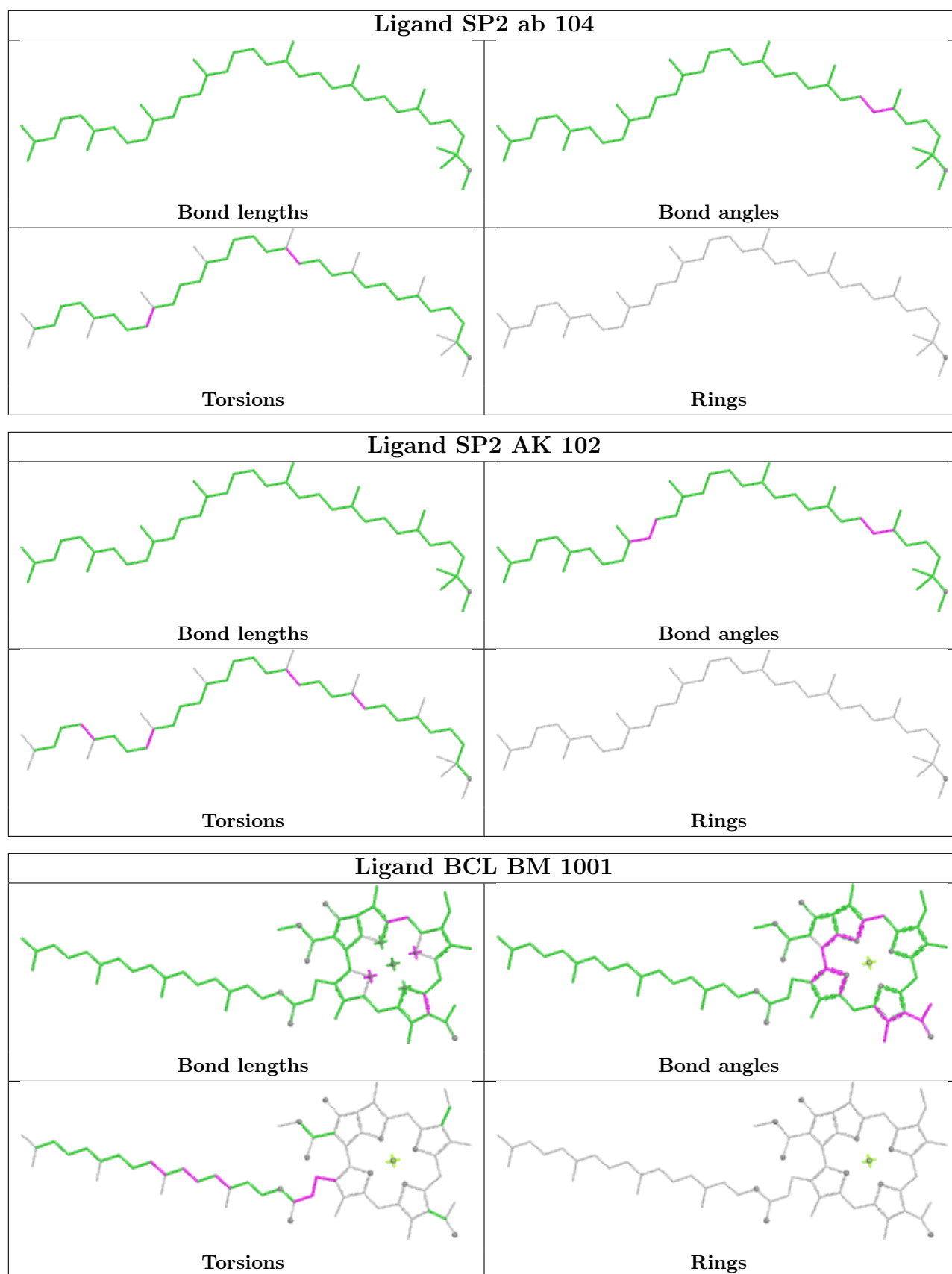


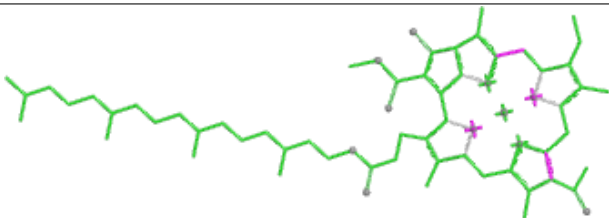
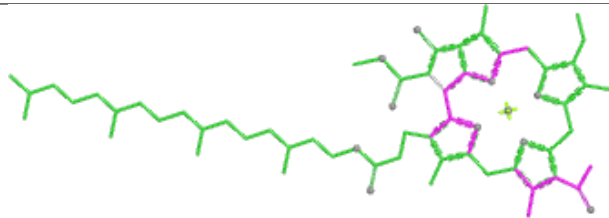
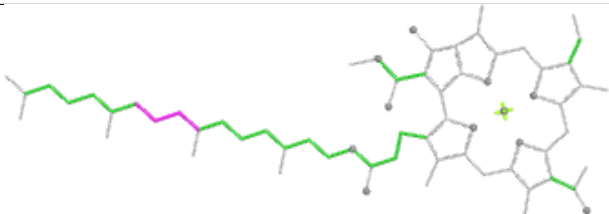
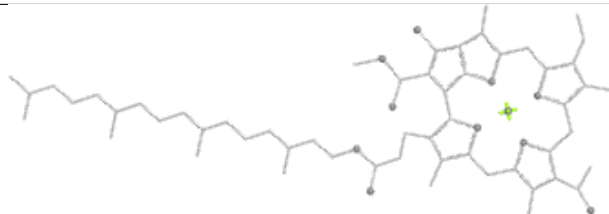


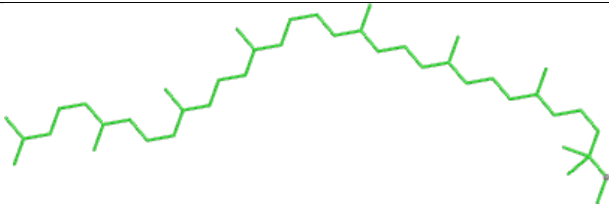
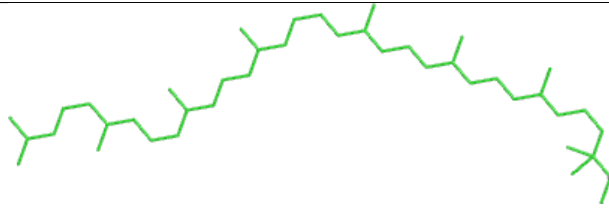
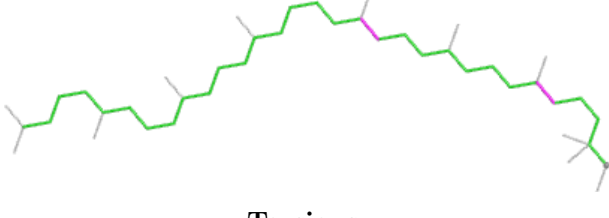
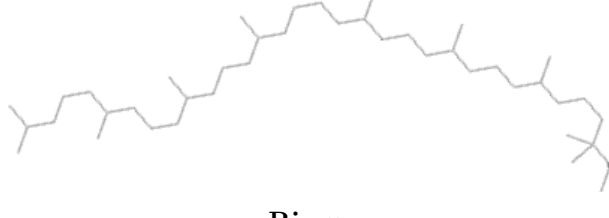


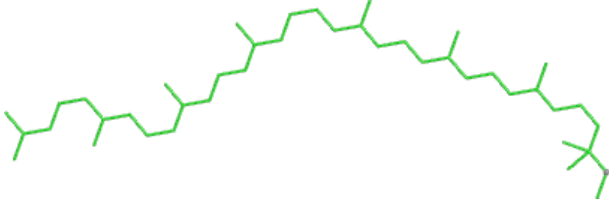
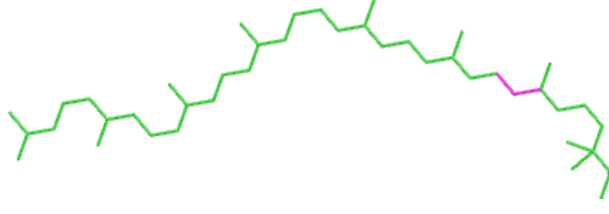
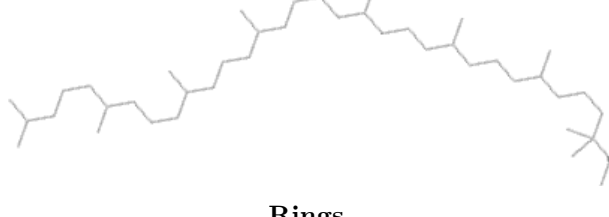






Ligand BCL ae 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SP2 M 1005	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SP2 af 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

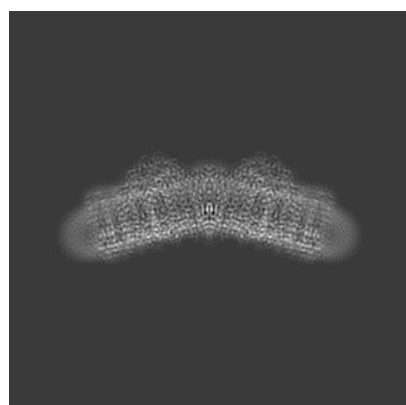
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13590. These allow visual inspection of the internal detail of the map and identification of artifacts.

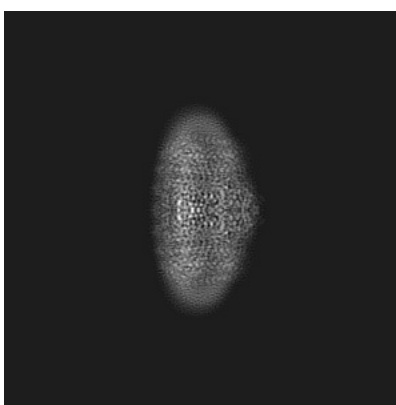
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

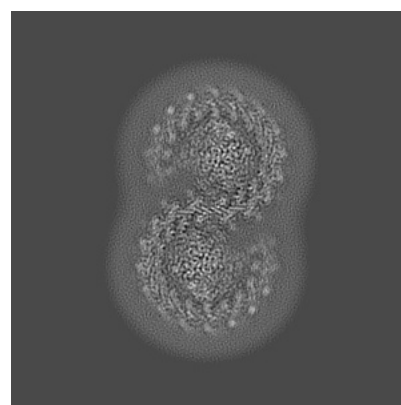
6.1.1 Primary map



X



Y

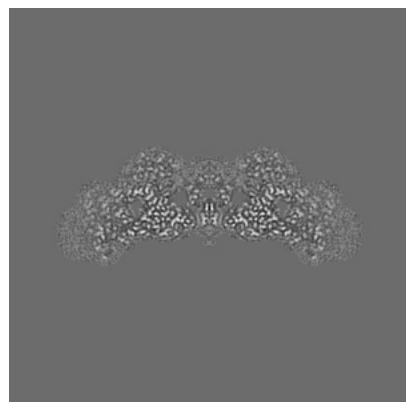


Z

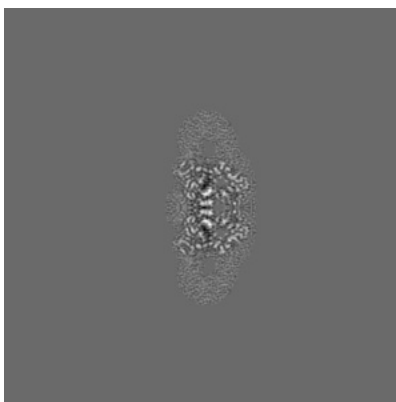
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

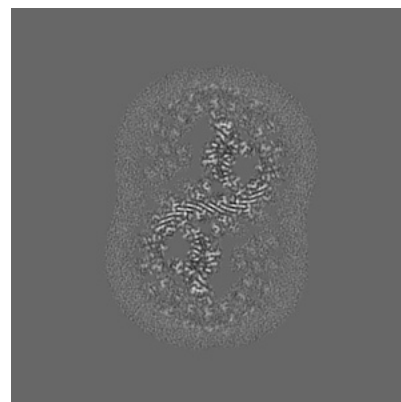
6.2.1 Primary map



X Index: 256



Y Index: 256

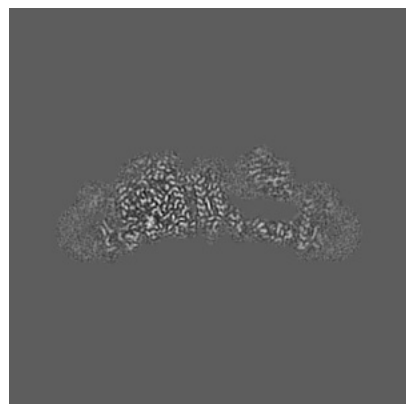


Z Index: 256

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

6.3 Largest variance slices [i](#)

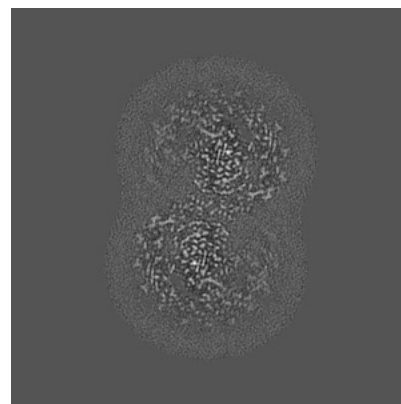
6.3.1 Primary map



X Index: 239



Y Index: 187

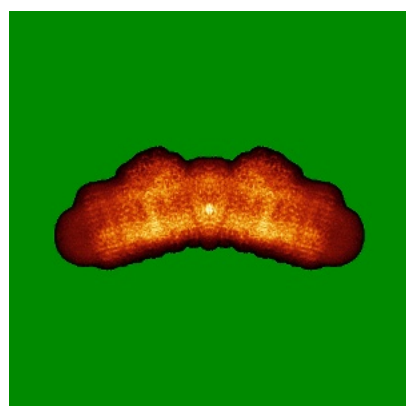


Z Index: 236

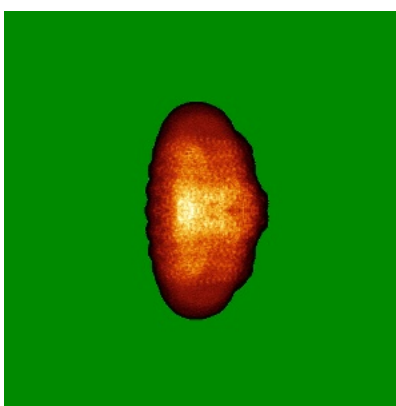
The images above show the largest variance slices of the map in three orthogonal directions.

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

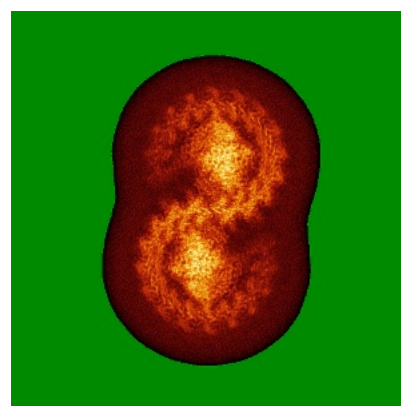
6.4.1 Primary map



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

This section was not generated.

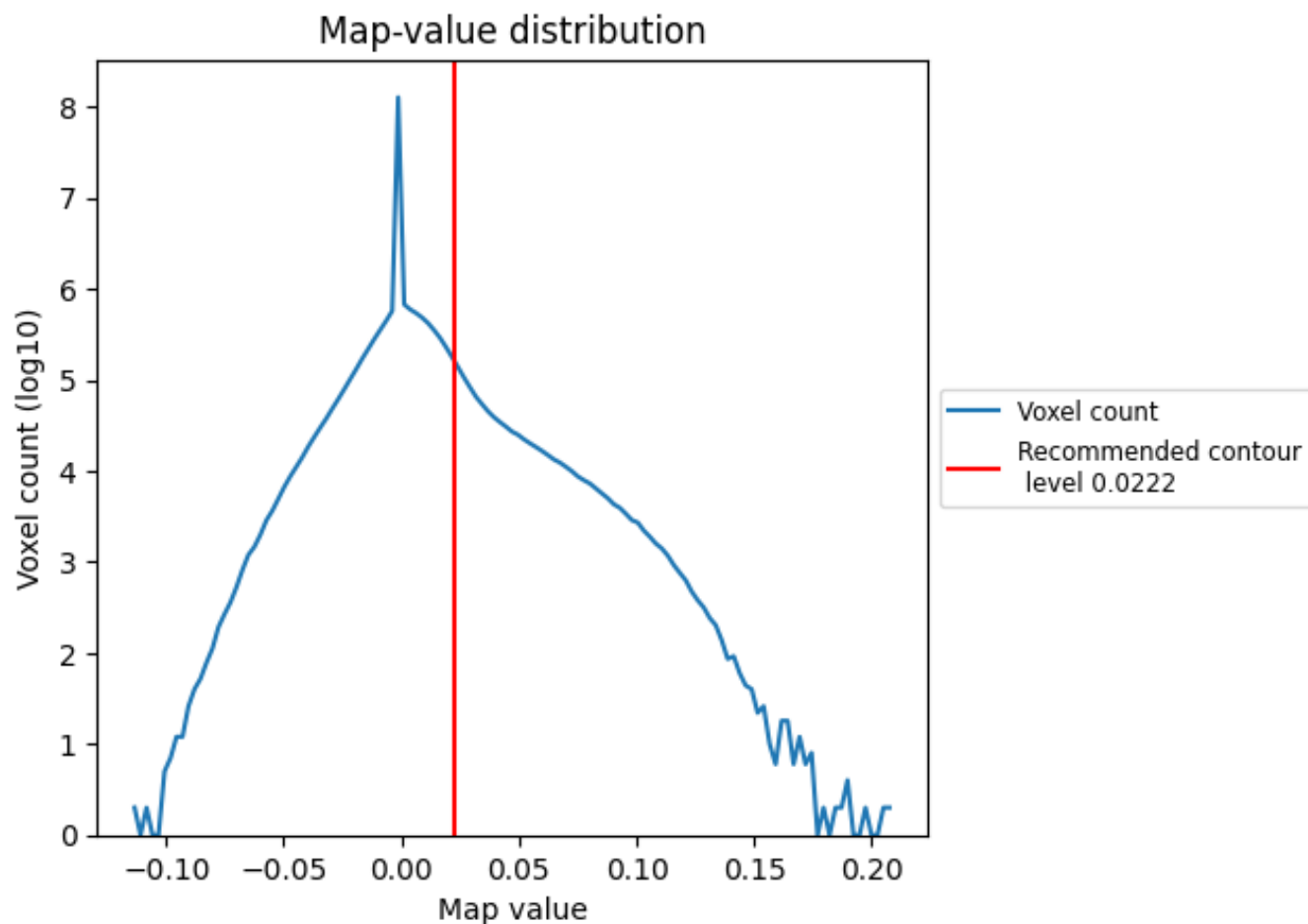
6.6 Mask visualisation

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

7 Map analysis [i](#)

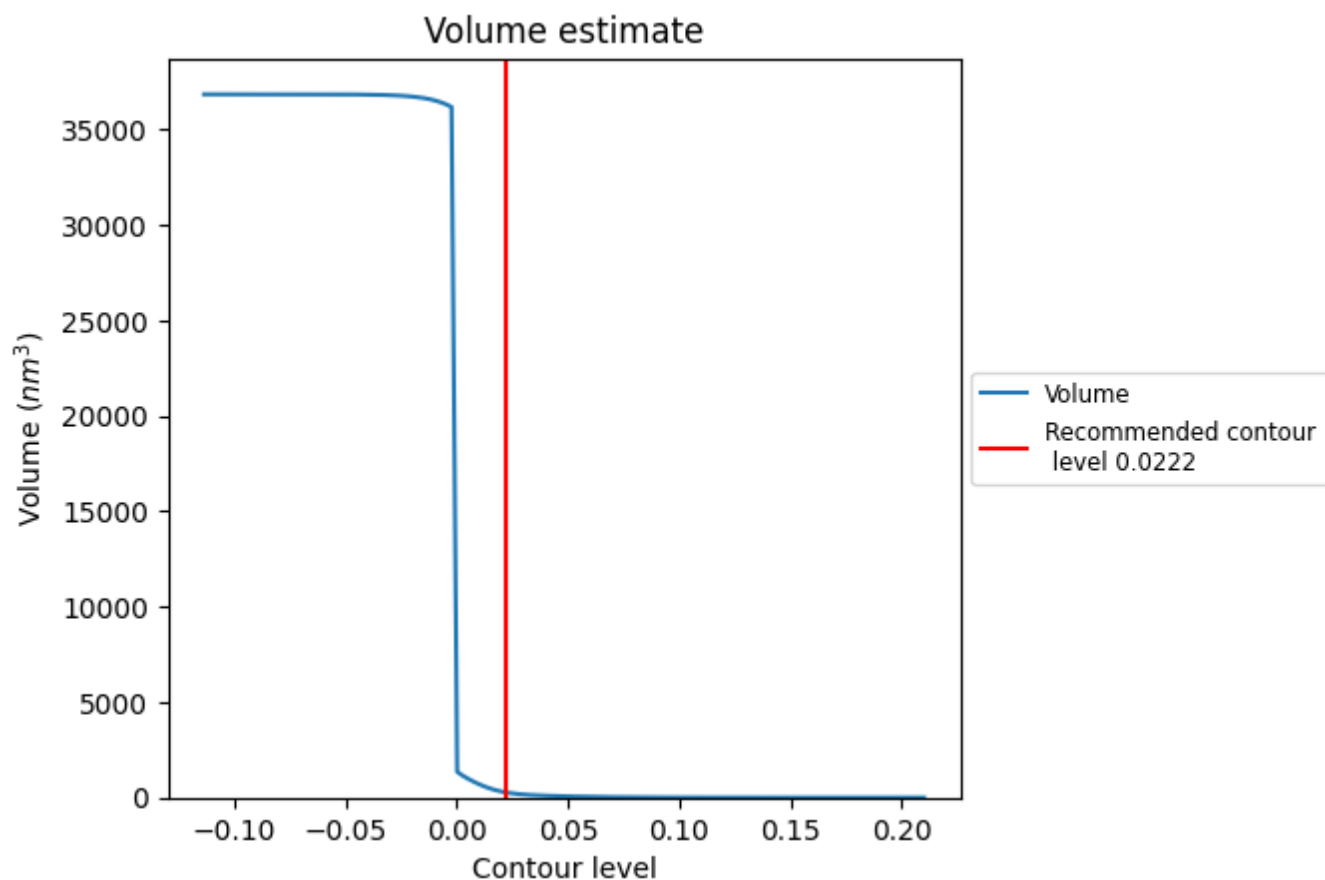
This section contains the results of statistical analysis of the map.

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.

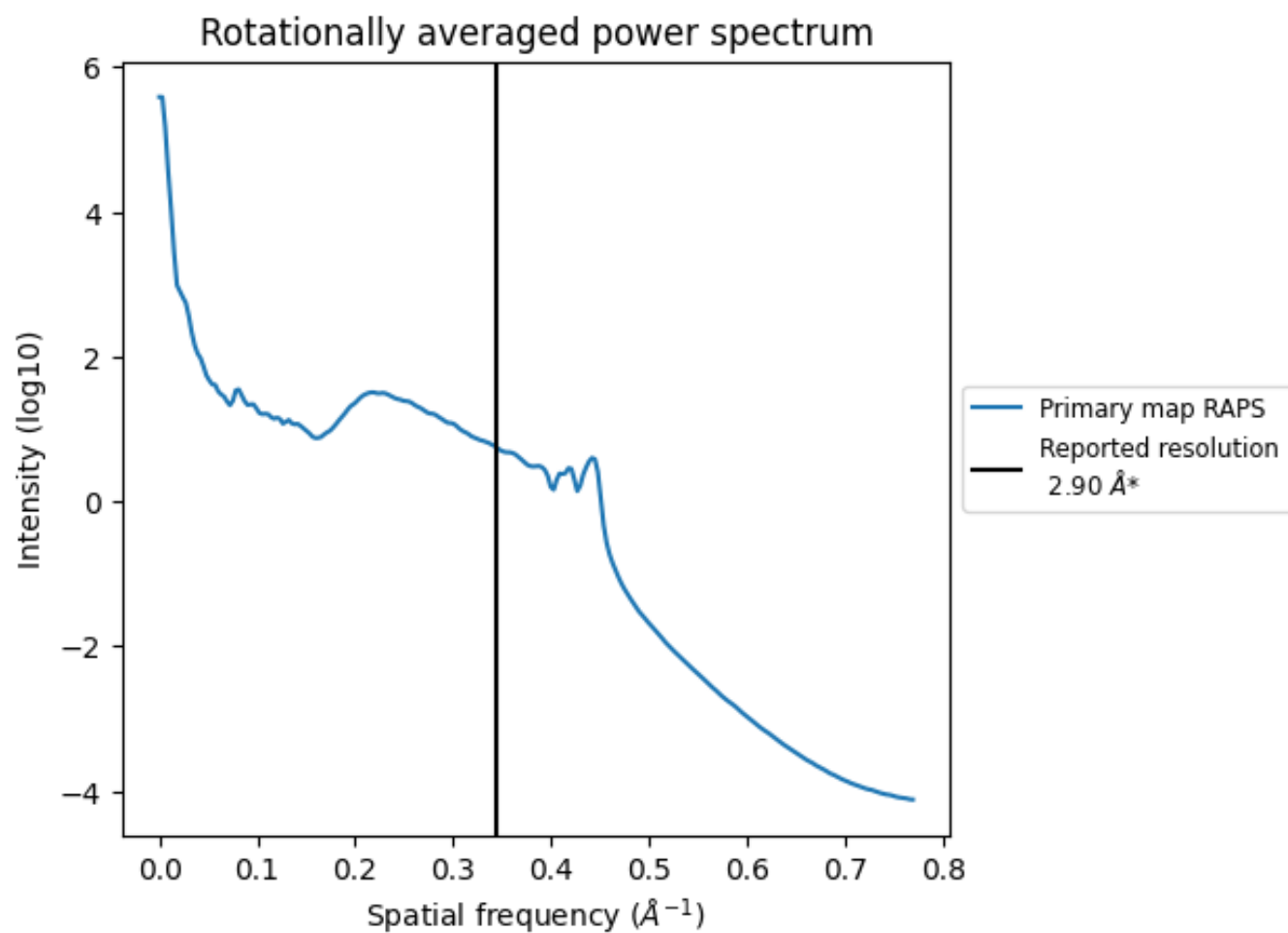
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 271 nm^3 ; this corresponds to an approximate mass of 245 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 ⓘ

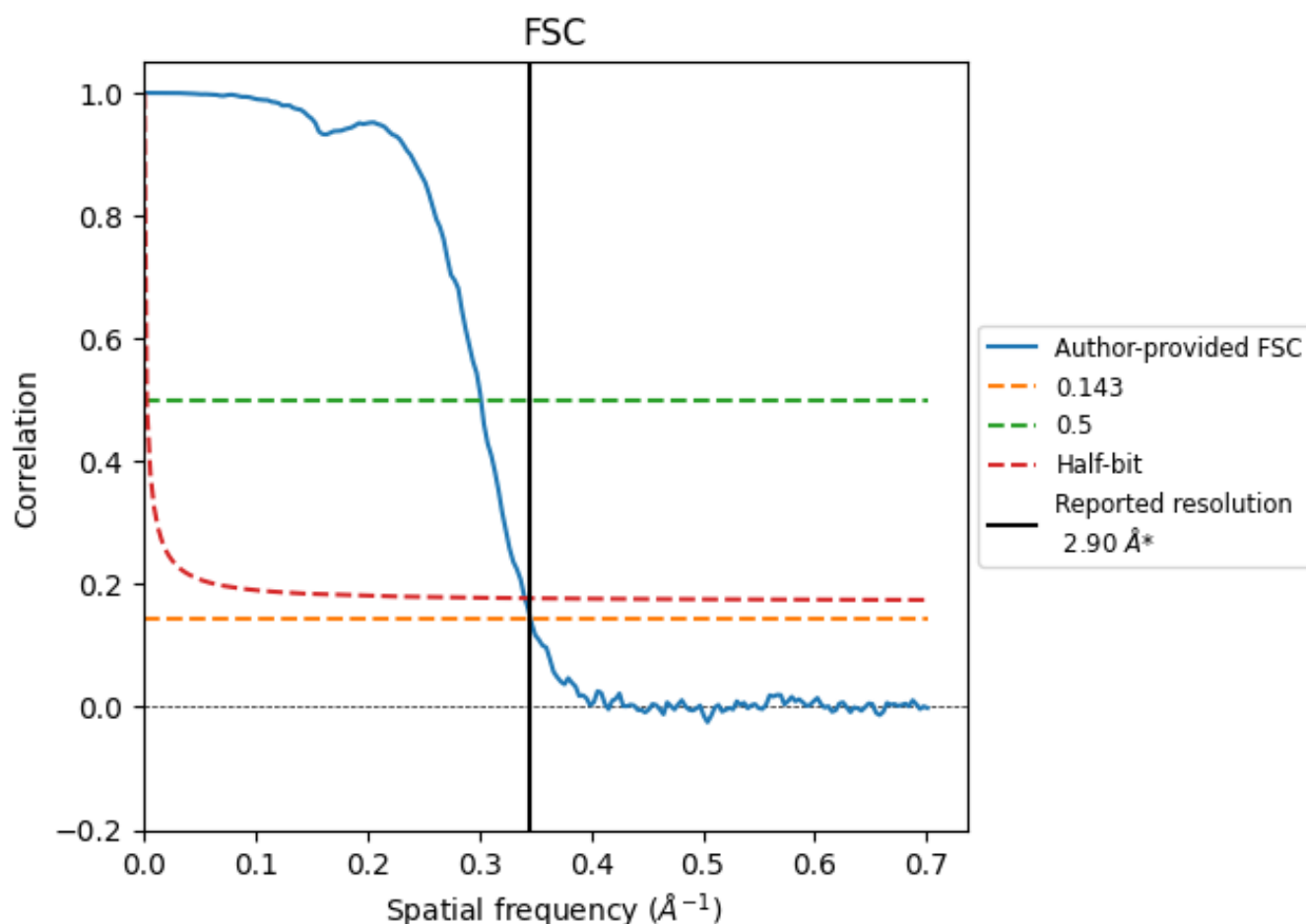


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

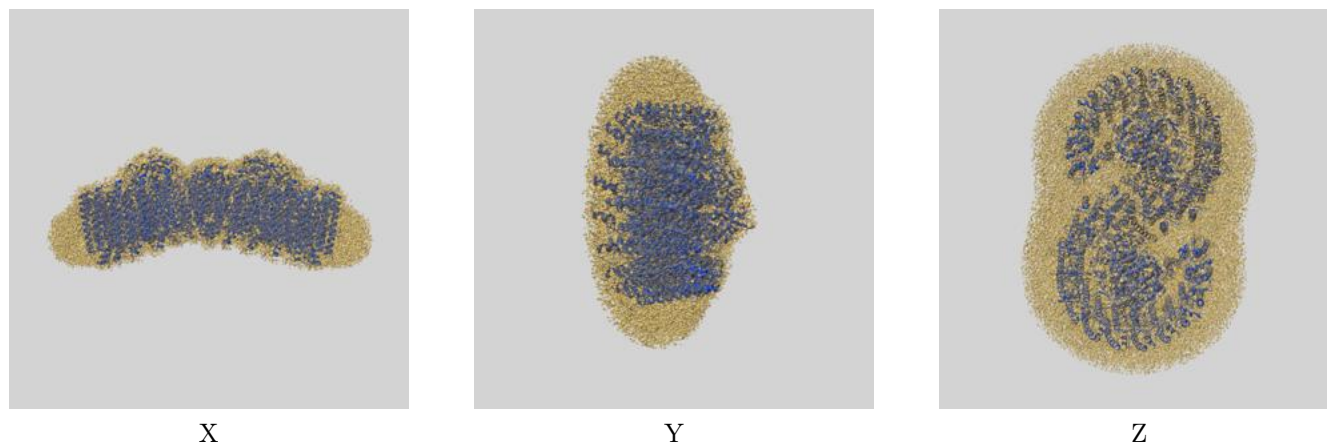
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.31	2.93
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

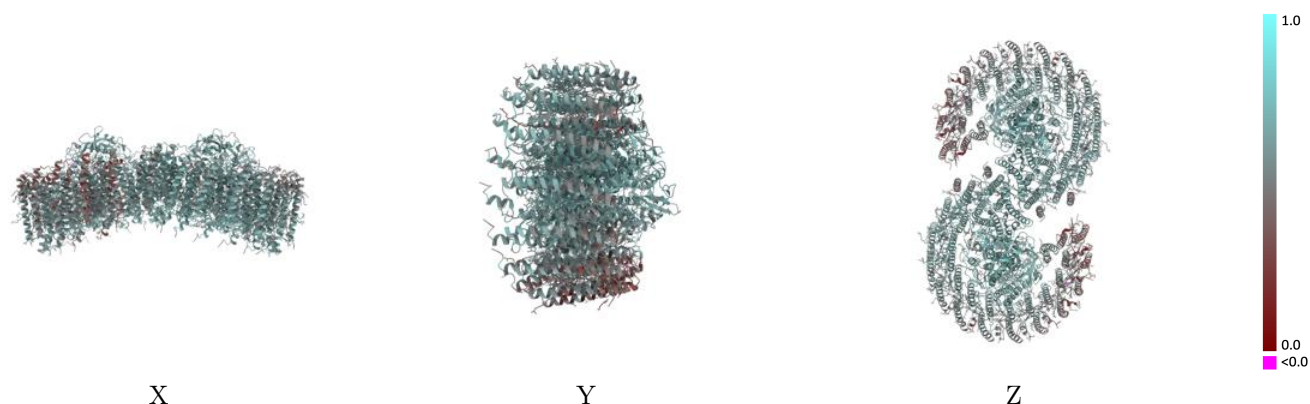
This section contains information regarding the fit between EMDB map EMD-13590 and PDB model 7PQD. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0222 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](#)

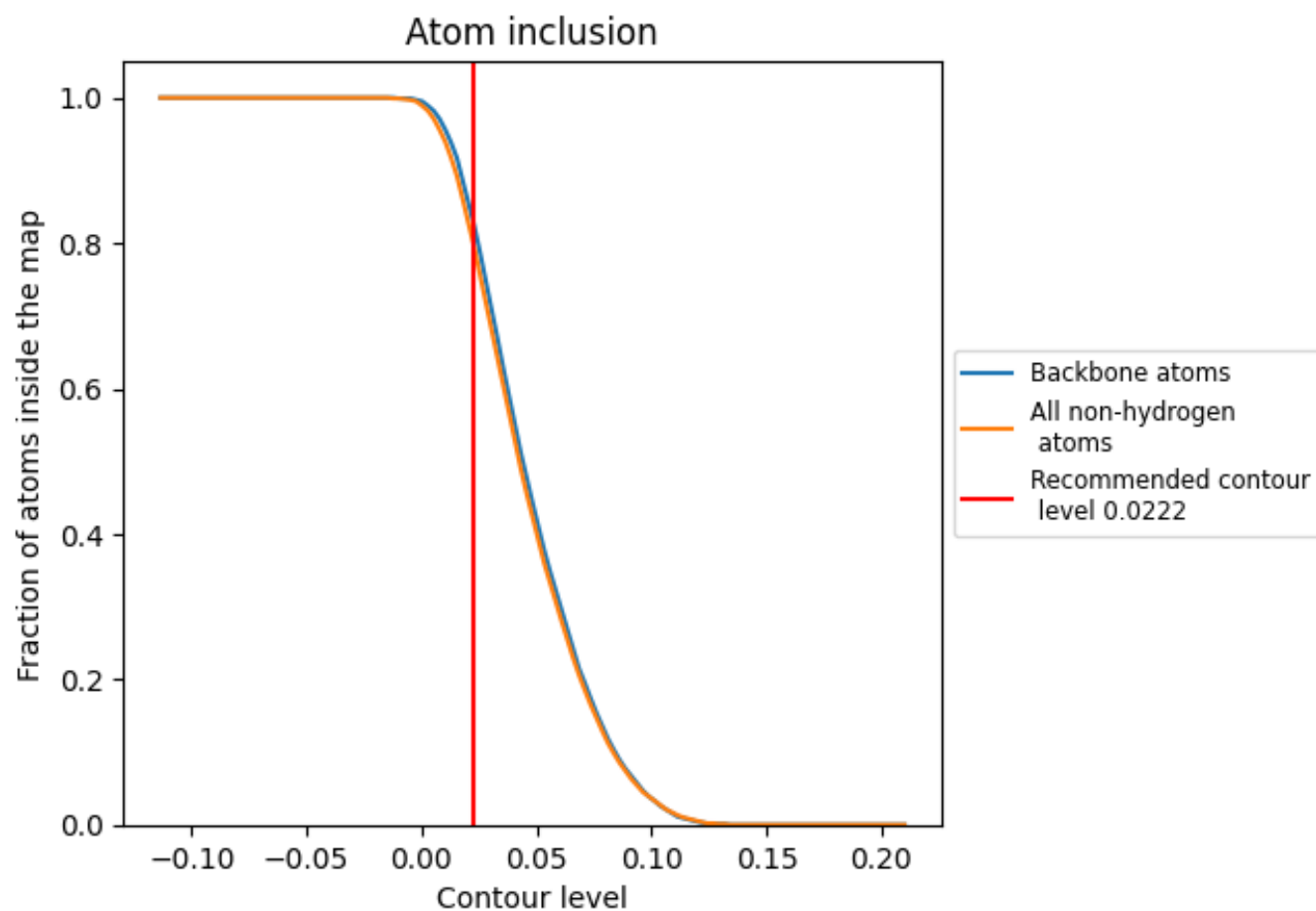


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 80% 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 (0.0222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.5820
AA	 0.9290	 0.6410
AB	 0.9060	 0.6380
AC	 0.8590	 0.6070
AD	 0.8970	 0.6180
AE	 0.8650	 0.6020
AF	 0.7840	 0.5740
AG	 0.7950	 0.5730
AH	 0.8040	 0.5820
AI	 0.7770	 0.5600
AJ	 0.7540	 0.5510
AK	 0.7170	 0.5250
AL	 0.6530	 0.4990
AM	 0.5300	 0.4500
AN	 0.4240	 0.4020
BA	 0.9170	 0.6430
BB	 0.9060	 0.6310
BC	 0.8500	 0.6010
BD	 0.8320	 0.5960
BE	 0.7850	 0.5670
BF	 0.7360	 0.5340
BG	 0.7730	 0.5640
BH	 0.7320	 0.5280
BI	 0.7380	 0.5350
BJ	 0.7110	 0.5300
BK	 0.6220	 0.4780
BL	 0.5450	 0.4430
BM	 0.4760	 0.3910
BN	 0.4130	 0.3840
H	 0.8820	 0.6140
L	 0.9620	 0.6740
M	 0.9420	 0.6590
UA	 0.5290	 0.4460
UB	 0.5760	 0.5110
UU	 0.6660	 0.5290



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Chain	Atom inclusion	Q-score
X	 0.9280	 0.6460
aa	 0.9260	 0.6390
ab	 0.9120	 0.6400
ac	 0.8510	 0.6090
ad	 0.8720	 0.6040
ae	 0.8380	 0.5880
af	 0.7780	 0.5690
ag	 0.8070	 0.5770
ah	 0.7980	 0.5810
ai	 0.7740	 0.5580
aj	 0.7570	 0.5500
ak	 0.7120	 0.5230
al	 0.6380	 0.4960
am	 0.5260	 0.4480
an	 0.4310	 0.4000
ba	 0.9100	 0.6440
bb	 0.8900	 0.6310
bc	 0.8870	 0.6120
bd	 0.8320	 0.5960
be	 0.8170	 0.5830
bf	 0.7340	 0.5340
bg	 0.7750	 0.5620
bh	 0.7290	 0.5270
bi	 0.7310	 0.5360
bj	 0.7070	 0.5290
bk	 0.6220	 0.4850
bl	 0.5440	 0.4400
bm	 0.4760	 0.3890
bn	 0.4080	 0.3840
h	 0.8810	 0.6140
l	 0.9640	 0.6740
m	 0.9430	 0.6600
ua	 0.5250	 0.4480
ub	 0.5760	 0.5080
uu	 0.6660	 0.5310
x	 0.9170	 0.6390