



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 07:08 AM UTC

PDB ID : 9J2F / pdb_00009j2f
EMDB ID : EMD-61095
Title : Structure of photosynthetic LH1-RC complex from the purple bacterium *Blas-tochloris tepida*
Authors : Kimura, Y.; Kanno, R.; Mori, K.; Matsuda, Y.; Seto, R.; Takenaka, S.; Mino, H.; Ohkubo, T.; Honda, M.; Sasaki, Y.C.; Kishikawa, J.; Mitsuoka, K.; Mio, K.; Hall, M.; Purba, E.R.; Mochizuki, T.; Mizoguchi, A.; Humbel, B.M.; Madigan, M.T.; Wang-Otomo, Z.-Y.; Tani, K.
Deposited on : 2024-08-06
Resolution : 2.20 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)

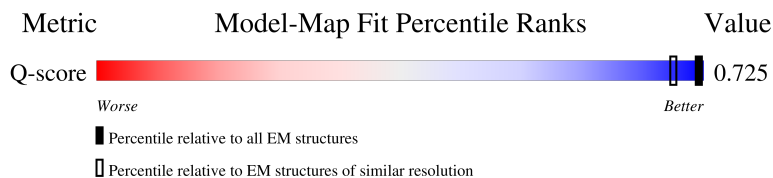
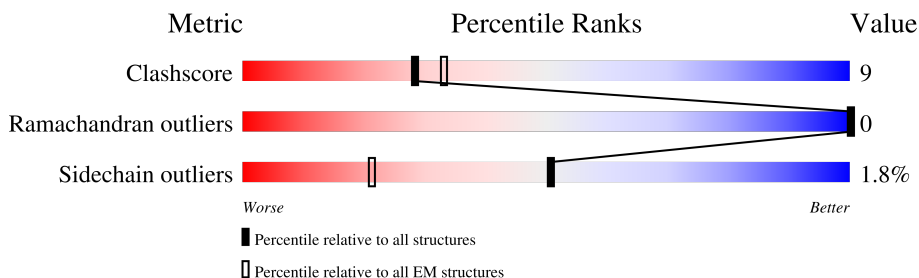
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

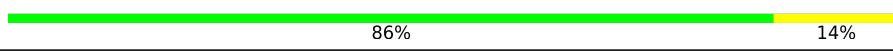
The reported resolution of this entry is 2.20 Å.

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	3184 (1.71 - 2.70)

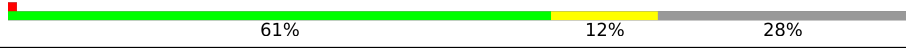
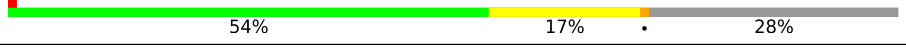
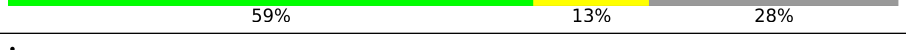
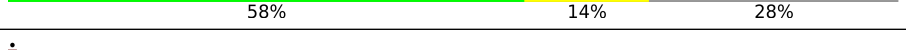
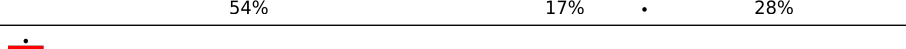
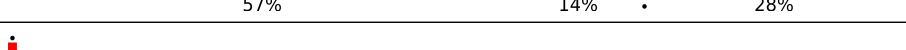
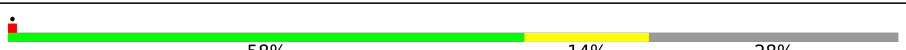
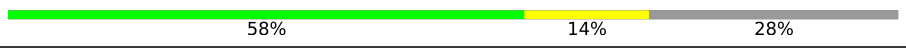
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	C	354	
2	L	274	
3	M	332	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
4	H	260	
5	3	69	
5	6	69	
5	9	69	
5	A	69	
5	D	69	
5	I	69	
5	N	69	
5	Q	69	
5	T	69	
5	W	69	
5	Z	69	
5	b	69	
5	e	69	
5	h	69	
5	k	69	
5	n	69	
5	q	69	
6	0	69	
6	1	69	
6	4	69	
6	7	69	
6	B	69	
6	E	69	
6	J	69	

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Mol	Chain	Length	Quality of chain
6	O	69	
6	R	69	
6	U	69	
6	X	69	
6	c	69	
6	f	69	
6	i	69	
6	l	69	
6	o	69	
6	r	69	
7	G	56	
8	2	57	
8	5	57	
8	8	57	
8	F	57	
8	K	57	
8	P	57	
8	S	57	
8	V	57	
8	Y	57	
8	a	57	
8	d	57	
8	g	57	
8	j	57	
8	m	57	

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Mol	Chain	Length	Quality of chain
8	p	57	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	BCB	0	102	X	-	-	-
13	BCB	1	101	X	-	-	-
13	BCB	3	101	X	-	-	-
13	BCB	4	101	X	-	-	-
13	BCB	6	101	X	-	-	-
13	BCB	7	102	X	-	-	-
13	BCB	9	101	X	-	-	-
13	BCB	A	102	X	-	-	-
13	BCB	B	202	X	-	-	-
13	BCB	D	101	X	-	-	-
13	BCB	E	101	X	-	-	-
13	BCB	I	101	X	-	-	-
13	BCB	J	101	X	-	-	-
13	BCB	L	302	X	-	-	-
13	BCB	L	303	X	-	-	-
13	BCB	M	402	X	-	-	-
13	BCB	M	403	X	-	-	-
13	BCB	N	101	X	-	-	-
13	BCB	O	102	X	-	-	-
13	BCB	Q	402	X	-	-	-
13	BCB	R	102	X	-	-	-
13	BCB	T	101	X	-	-	-
13	BCB	U	102	X	-	-	-
13	BCB	W	302	X	-	-	-
13	BCB	X	102	X	-	-	-
13	BCB	Z	101	X	-	-	-
13	BCB	b	101	X	-	-	-
13	BCB	c	101	X	-	-	-
13	BCB	e	101	X	-	-	-
13	BCB	f	101	X	-	-	-
13	BCB	h	102	X	-	-	-
13	BCB	i	101	X	-	-	-
13	BCB	k	102	X	-	-	-
13	BCB	l	102	X	-	-	-
13	BCB	n	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	BCB	o	102	X	-	-	-
13	BCB	q	101	X	-	-	-
13	BCB	r	101	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 32918 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	331	Total	C	N	O	S	0	0
			2585	1637	455	471	22		

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	273	Total	C	N	O	S	0	0
			2159	1454	347	352	6		

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	331	Total	C	N	O	S	0	0
			2621	1746	433	427	15		

- Molecule 4 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	260	Total	C	N	O	S	0	0
			2041	1313	343	382	3		

- Molecule 5 is a protein called Antenna complex alpha/beta subunit domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	50	Total	C	N	O	0	0
			424	288	72	64		
5	D	50	Total	C	N	O	0	0
			424	288	72	64		
5	I	50	Total	C	N	O	0	0
			424	288	72	64		
5	N	50	Total	C	N	O	0	0
			424	288	72	64		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	50	Total	C	N	O	0	0
			424	288	72	64		
5	T	50	Total	C	N	O	0	0
			424	288	72	64		
5	W	50	Total	C	N	O	0	0
			424	288	72	64		
5	Z	50	Total	C	N	O	0	0
			424	288	72	64		
5	3	50	Total	C	N	O	0	0
			424	288	72	64		
5	6	50	Total	C	N	O	0	0
			424	288	72	64		
5	9	50	Total	C	N	O	0	0
			424	288	72	64		
5	b	50	Total	C	N	O	0	0
			424	288	72	64		
5	e	50	Total	C	N	O	0	0
			424	288	72	64		
5	h	50	Total	C	N	O	0	0
			424	288	72	64		
5	k	50	Total	C	N	O	0	0
			424	288	72	64		
5	n	50	Total	C	N	O	0	0
			424	288	72	64		
5	q	50	Total	C	N	O	0	0
			424	288	72	64		

- Molecule 6 is a protein called Antenna complex alpha/beta subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	51	Total	C	N	O	S	0	0
			407	274	63	69	1		
6	E	51	Total	C	N	O	S	0	0
			407	274	63	69	1		
6	J	48	Total	C	N	O	S	0	0
			386	260	60	65	1		
6	O	51	Total	C	N	O	S	0	0
			407	274	63	69	1		
6	R	50	Total	C	N	O	S	0	0
			400	269	62	68	1		
6	U	50	Total	C	N	O	S	0	0
			400	269	62	68	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	1	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	4	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	7	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	0	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	c	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	f	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	i	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	l	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	o	50	Total 400	C 269	N 62	O 68	S 1	0	0
6	r	50	Total 400	C 269	N 62	O 68	S 1	0	0

- Molecule 7 is a protein called Light-harvesting protein gamma1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	28	Total 232	C 159	N 36	O 37	0	0

- Molecule 8 is a protein called Light-harvesting protein B-1015 gamma chain.

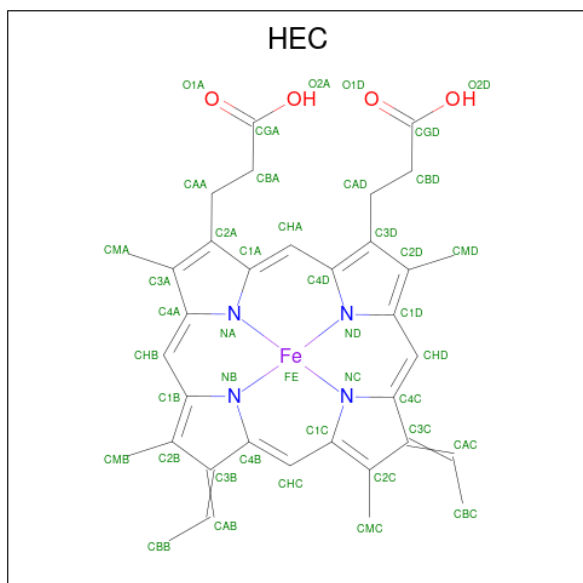
Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	36	Total 279	C 189	N 42	O 48	0	0
8	K	36	Total 279	C 189	N 42	O 48	0	0
8	P	36	Total 279	C 189	N 42	O 48	0	0
8	S	36	Total 279	C 189	N 42	O 48	0	0
8	V	36	Total 279	C 189	N 42	O 48	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	36	Total	C	N	O	0	0
			279	189	42	48		
8	2	36	Total	C	N	O	0	0
			279	189	42	48		
8	5	36	Total	C	N	O	0	0
			279	189	42	48		
8	8	36	Total	C	N	O	0	0
			279	189	42	48		
8	a	36	Total	C	N	O	0	0
			279	189	42	48		
8	d	36	Total	C	N	O	0	0
			279	189	42	48		
8	g	36	Total	C	N	O	0	0
			279	189	42	48		
8	j	36	Total	C	N	O	0	0
			279	189	42	48		
8	m	36	Total	C	N	O	0	0
			279	189	42	48		
8	p	36	Total	C	N	O	0	0
			279	189	42	48		

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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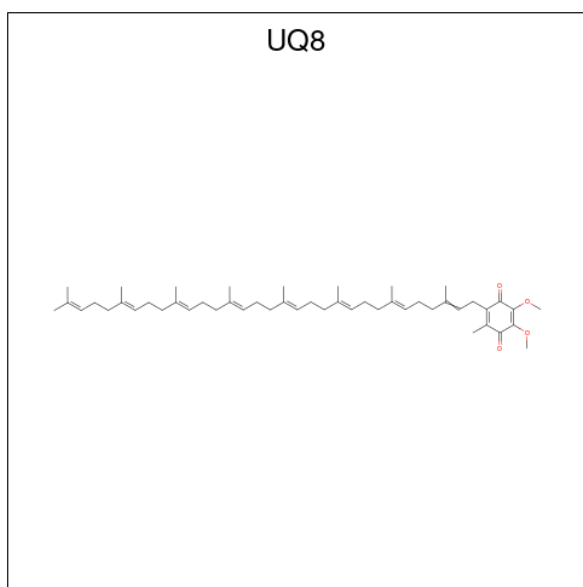
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Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

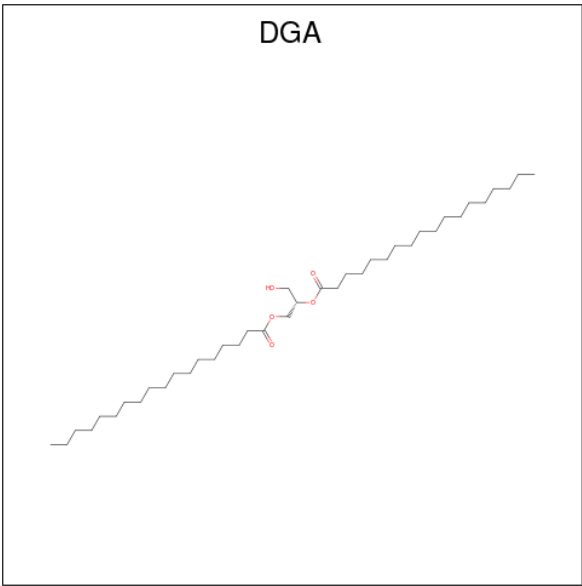
Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Mg	0
			1	1	

- Molecule 11 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



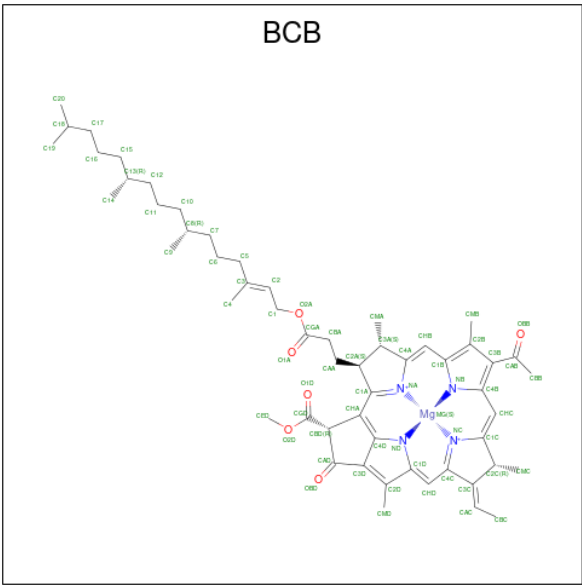
Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	C	O	0
			15	11	4	
11	L	1	Total	C	O	0
			31	27	4	
11	M	1	Total	C	O	0
			25	21	4	
11	M	1	Total	C	O	0
			53	49	4	
11	A	1	Total	C	O	0
			53	49	4	

- Molecule 12 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			23	19	4	

- Molecule 13 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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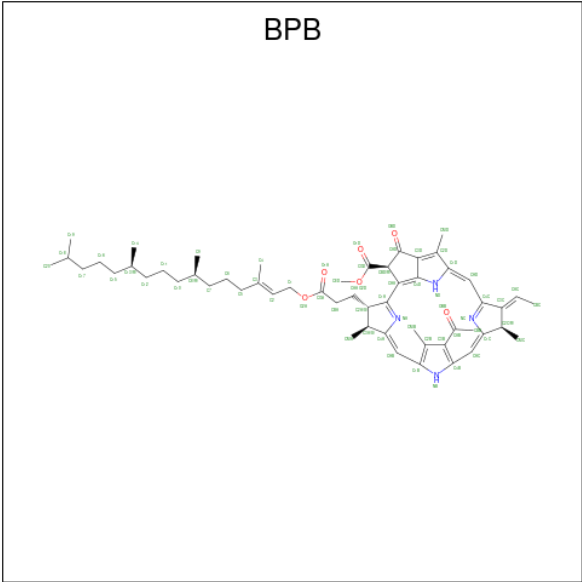
Mol	Chain	Residues	Atoms					AltConf
13	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	4	1	Total 66	C 55	Mg 1	N 4	O 6	0

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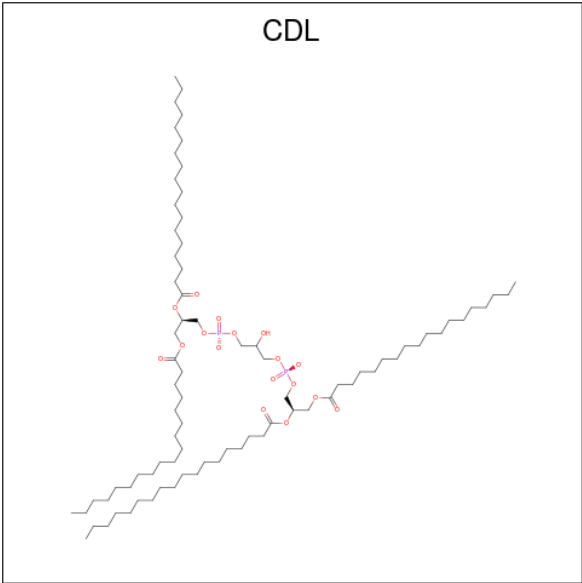
Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	h	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	k	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	l	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
13	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 14 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: C₅₅H₇₄N₄O₆).



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

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total	C	O	P	0
			75	56	17	2	
15	M	1	Total	C	O	P	0
			85	66	17	2	

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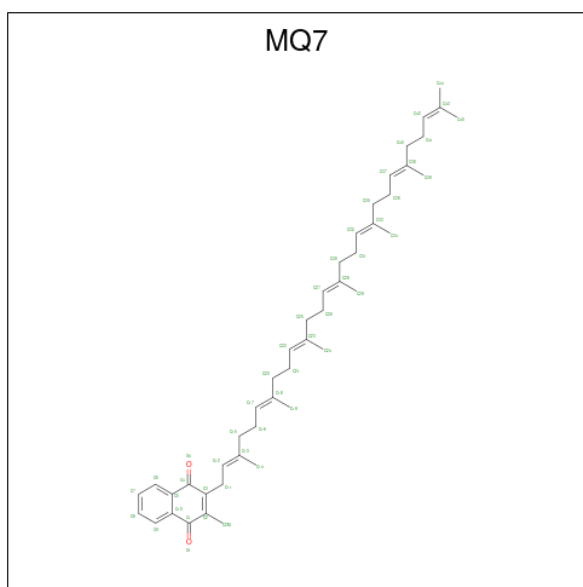
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Mol	Chain	Residues	Atoms				AltConf
15	H	1	Total	C	O	P	0
			98	79	17	2	
15	H	1	Total	C	O	P	0
			72	53	17	2	
15	r	1	Total	C	O	P	0
			68	49	17	2	

- Molecule 16 is FE (III) ION (CCD ID: FE) (formula: Fe).

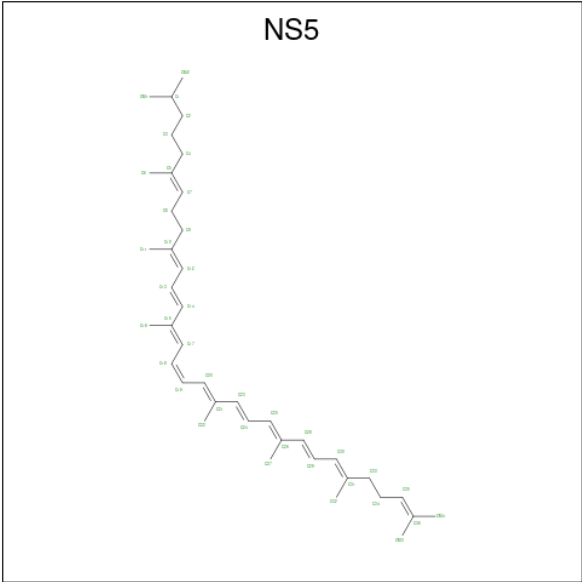
Mol	Chain	Residues	Atoms		AltConf
16	M	1	Total	Fe	0
			1	1	

- Molecule 17 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂).



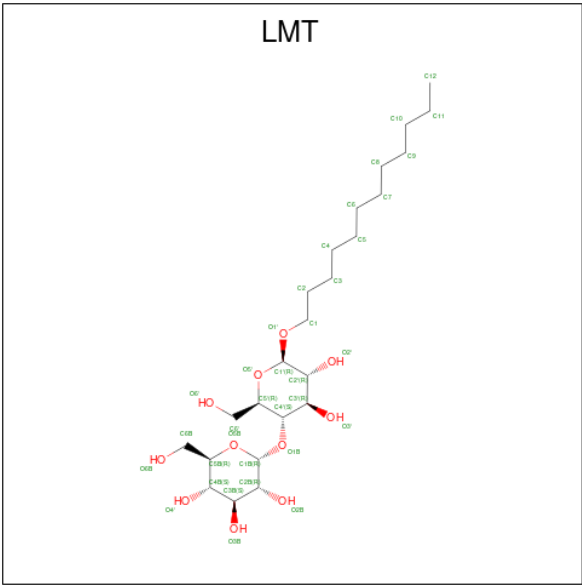
Mol	Chain	Residues	Atoms			AltConf
17	M	1	Total	C	O	0
			48	46	2	

- Molecule 18 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	C		0
			40	40		

- Molecule 19 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



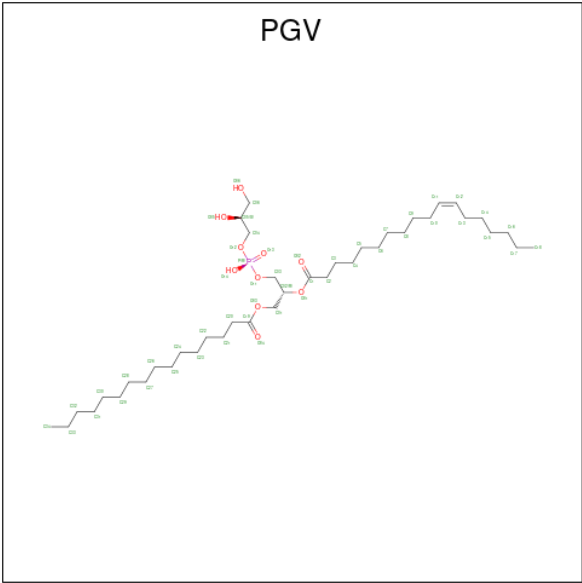
Mol	Chain	Residues	Atoms			AltConf
19	M	1	Total	C	O	0
			25	19	6	
19	B	1	Total	C	O	0
			15	13	2	
19	T	1	Total	C	O	0
			26	19	7	

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Mol	Chain	Residues	Atoms			AltConf
19	b	1	Total	C	O	0
			35	24	11	
19	b	1	Total	C	O	0
			35	24	11	
19	h	1	Total	C	O	0
			35	24	11	
19	k	1	Total	C	O	0
			35	24	11	
19	n	1	Total	C	O	0
			35	24	11	

- Molecule 20 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



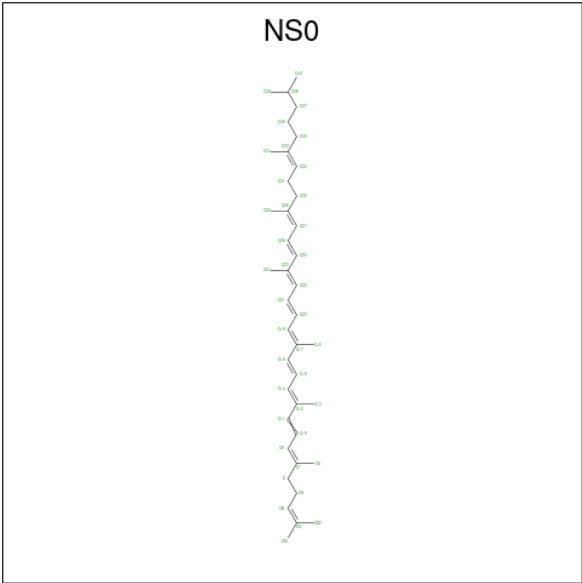
Mol	Chain	Residues	Atoms				AltConf
20	M	1	Total	C	O	P	0
			45	34	10	1	
20	D	1	Total	C	O	P	0
			47	36	10	1	
20	I	1	Total	C	O	P	0
			51	40	10	1	
20	N	1	Total	C	O	P	0
			38	27	10	1	
20	Q	1	Total	C	O	P	0
			49	39	9	1	

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Mol	Chain	Residues	Atoms				AltConf
20	W	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 21 is all-trans-1,2-dihydroneurosporene (CCD ID: NS0) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	D	1	Total	C	0
			40	40	
21	O	1	Total	C	0
			40	40	
21	R	1	Total	C	0
			40	40	
21	U	1	Total	C	0
			40	40	
21	W	1	Total	C	0
			40	40	
21	X	1	Total	C	0
			40	40	
21	2	1	Total	C	0
			40	40	
21	7	1	Total	C	0
			40	40	
21	9	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
21	0	1	Total C 40 40	0
21	h	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	o	1	Total C 40 40	0
21	q	1	Total C 40 40	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	C	98	Total O 98 98	0
22	L	59	Total O 59 59	0
22	M	75	Total O 75 75	0
22	H	22	Total O 22 22	0
22	A	6	Total O 6 6	0
22	B	2	Total O 2 2	0
22	D	6	Total O 6 6	0
22	E	3	Total O 3 3	0
22	I	7	Total O 7 7	0
22	J	3	Total O 3 3	0
22	K	2	Total O 2 2	0
22	N	6	Total O 6 6	0
22	O	3	Total O 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
22	Q	6	Total O 6 6	0
22	R	5	Total O 5 5	0
22	S	1	Total O 1 1	0
22	T	6	Total O 6 6	0
22	U	5	Total O 5 5	0
22	V	2	Total O 2 2	0
22	W	3	Total O 3 3	0
22	X	5	Total O 5 5	0
22	Y	2	Total O 2 2	0
22	Z	4	Total O 4 4	0
22	1	3	Total O 3 3	0
22	2	3	Total O 3 3	0
22	3	5	Total O 5 5	0
22	4	7	Total O 7 7	0
22	5	5	Total O 5 5	0
22	6	10	Total O 10 10	0
22	7	4	Total O 4 4	0
22	8	1	Total O 1 1	0
22	9	6	Total O 6 6	0
22	0	1	Total O 1 1	0
22	b	10	Total O 10 10	0

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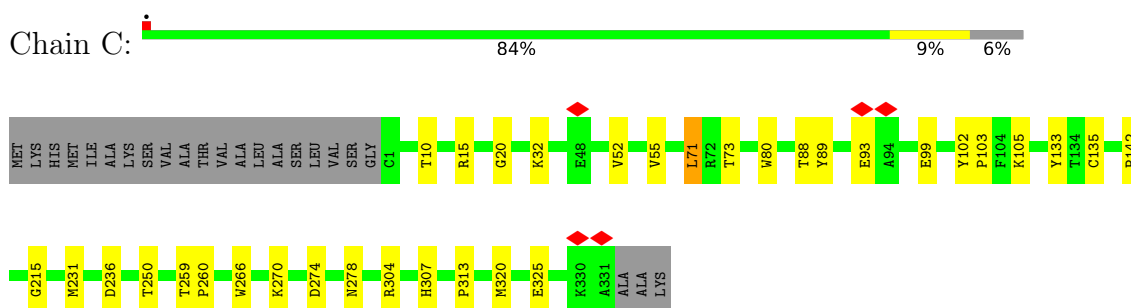
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
22	c	4	Total 4	O 4	0
22	e	9	Total 9	O 9	0
22	f	2	Total 2	O 2	0
22	g	1	Total 1	O 1	0
22	h	4	Total 4	O 4	0
22	i	1	Total 1	O 1	0
22	j	2	Total 2	O 2	0
22	k	5	Total 5	O 5	0
22	l	1	Total 1	O 1	0
22	n	4	Total 4	O 4	0
22	o	1	Total 1	O 1	0
22	p	1	Total 1	O 1	0
22	q	2	Total 2	O 2	0

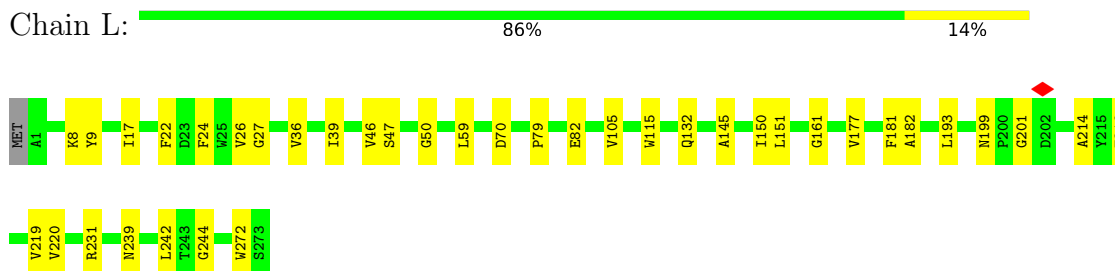
3 Residue-property plots

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

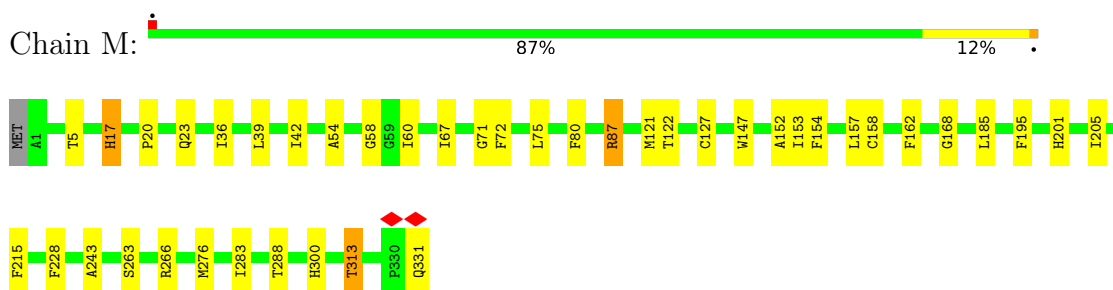
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



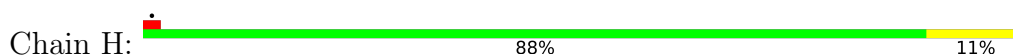
- Molecule 2: Reaction center protein L chain

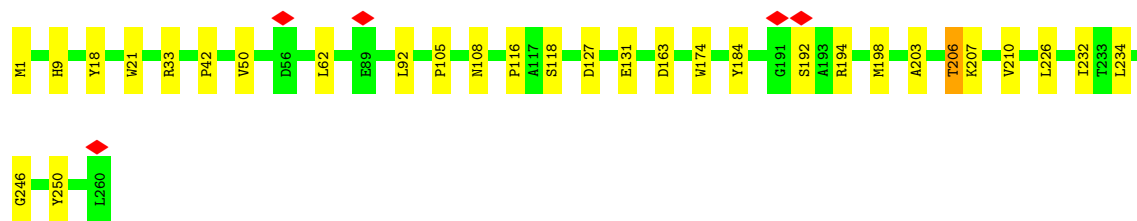


- Molecule 3: Reaction center protein M chain



- Molecule 4: Photosynthetic reaction center subunit H

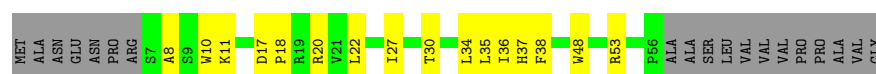




- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



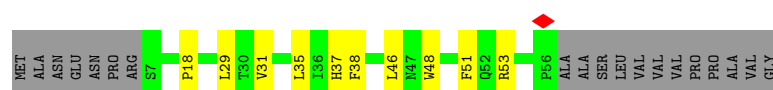
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

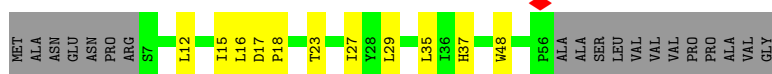


- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein





- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



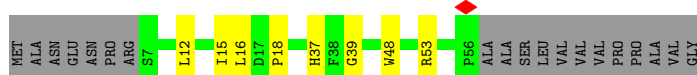
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



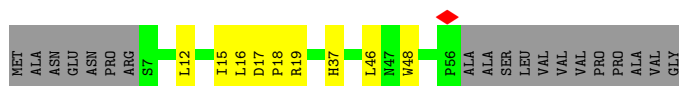
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain e:  64% 9% 28%



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain h:  59% 13% 28%



- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain k:  58% 14% 28%



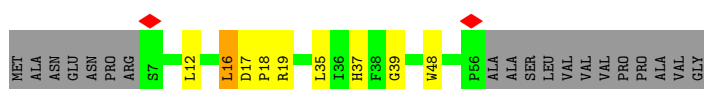
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain n:  59% 13% 28%



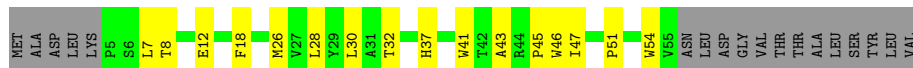
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain q:  59% 12% 28%



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain B:  51% 23% 26%



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain E:  59% 13% 26%



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain J: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain O: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain R: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain U: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain X: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 1: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 4: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 7: 

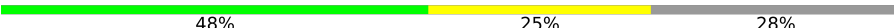


- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain 0: 



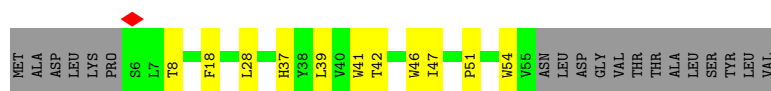
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain c: 



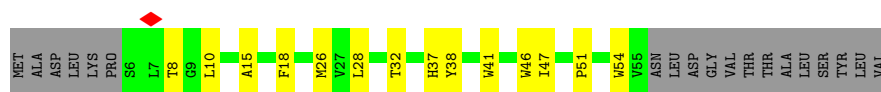
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain f: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain i: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain l: 



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

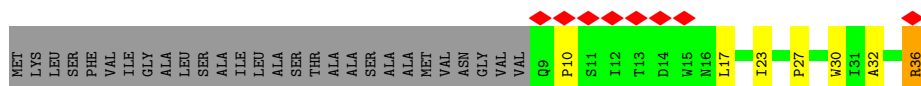
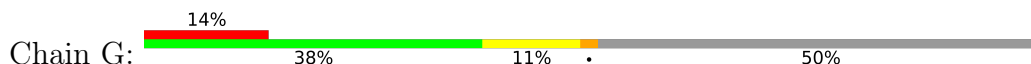
Chain o: 



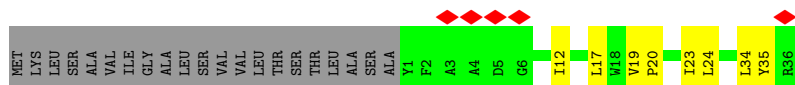
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



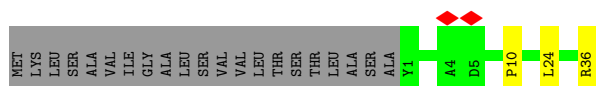
- Molecule 7: Light-harvesting protein gammal



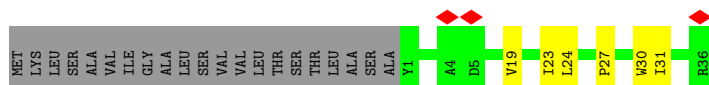
- Molecule 8: Light-harvesting protein B-1015 gamma chain



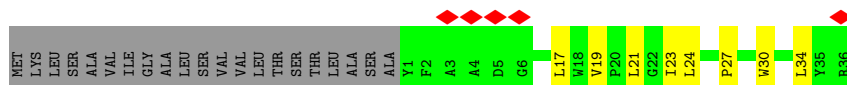
- Molecule 8: Light-harvesting protein B-1015 gamma chain



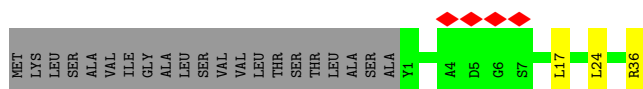
- Molecule 8: Light-harvesting protein B-1015 gamma chain



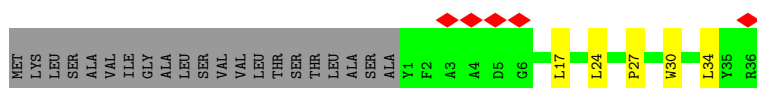
- Molecule 8: Light-harvesting protein B-1015 gamma chain



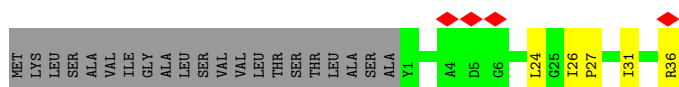
- Molecule 8: Light-harvesting protein B-1015 gamma chain



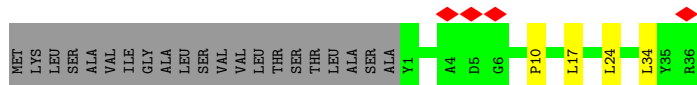
- Molecule 8: Light-harvesting protein B-1015 gamma chain



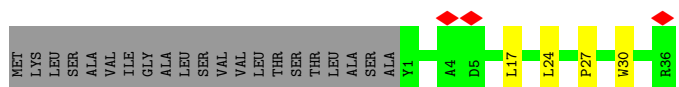
- Molecule 8: Light-harvesting protein B-1015 gamma chain



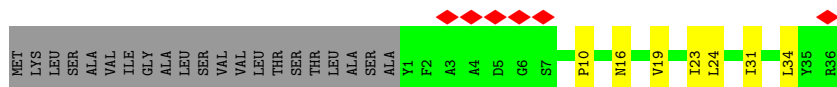
- Molecule 8: Light-harvesting protein B-1015 gamma chain



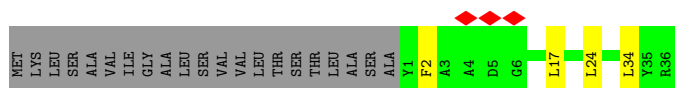
- Molecule 8: Light-harvesting protein B-1015 gamma chain



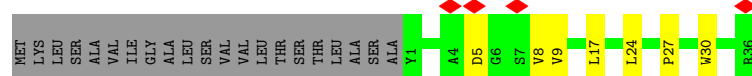
- Molecule 8: Light-harvesting protein B-1015 gamma chain



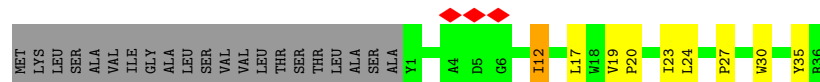
- Molecule 8: Light-harvesting protein B-1015 gamma chain



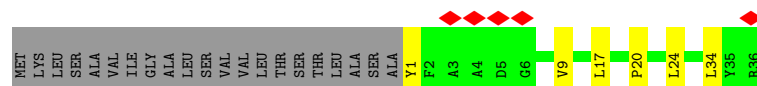
- Molecule 8: Light-harvesting protein B-1015 gamma chain



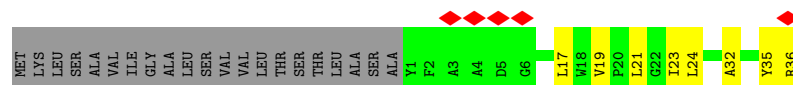
- Molecule 8: Light-harvesting protein B-1015 gamma chain



- Molecule 8: Light-harvesting protein B-1015 gamma chain



- Molecule 8: Light-harvesting protein B-1015 gamma chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	294012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.434	Depositor
Minimum map value	-0.179	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MQ7, NS5, LMT, FME, MG, PGV, DGA, HEC, BPB, FE, UQ8, CDL, BCB, NS0

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	C	0.20	0/2657	0.38	0/3614
2	L	0.21	0/2246	0.40	0/3062
3	M	0.22	0/2725	0.38	0/3718
4	H	0.18	0/2087	0.36	0/2848
5	3	0.22	0/438	0.39	0/599
5	6	0.20	0/438	0.38	0/599
5	9	0.20	0/438	0.35	0/599
5	A	0.20	0/438	0.37	0/599
5	D	0.20	0/438	0.37	0/599
5	I	0.21	0/438	0.37	0/599
5	N	0.18	0/438	0.36	0/599
5	Q	0.19	0/438	0.35	0/599
5	T	0.18	0/438	0.35	0/599
5	W	0.18	0/438	0.37	0/599
5	Z	0.21	0/438	0.39	0/599
5	b	0.19	0/438	0.36	0/599
5	e	0.19	0/438	0.37	0/599
5	h	0.18	0/438	0.34	0/599
5	k	0.20	0/438	0.33	0/599
5	n	0.18	0/438	0.34	0/599
5	q	0.18	0/438	0.36	0/599
6	0	0.20	0/414	0.36	0/569
6	1	0.20	0/414	0.34	0/569
6	4	0.20	0/414	0.35	0/569
6	7	0.20	0/414	0.34	0/569
6	B	0.18	0/422	0.37	0/580
6	E	0.21	0/422	0.34	0/580
6	J	0.20	0/400	0.33	0/550
6	O	0.20	0/422	0.35	0/580
6	R	0.19	0/414	0.34	0/569
6	U	0.22	0/414	0.45	0/569
6	X	0.20	0/414	0.39	0/569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	c	0.20	0/414	0.37	0/569
6	f	0.19	0/414	0.33	0/569
6	i	0.20	0/414	0.41	0/569
6	l	0.19	0/414	0.41	0/569
6	o	0.20	0/414	0.36	0/569
6	r	0.19	0/414	0.36	0/569
7	G	0.18	0/241	0.45	0/333
8	2	0.18	0/288	0.47	0/397
8	5	0.19	0/288	0.43	0/397
8	8	0.19	0/288	0.42	0/397
8	F	0.18	0/288	0.42	0/397
8	K	0.18	0/288	0.41	0/397
8	P	0.17	0/288	0.43	0/397
8	S	0.18	0/288	0.45	0/397
8	V	0.18	0/288	0.47	0/397
8	Y	0.19	0/288	0.46	0/397
8	a	0.17	0/288	0.40	0/397
8	d	0.19	0/288	0.45	0/397
8	g	0.18	0/288	0.41	0/397
8	j	0.20	0/288	0.46	0/397
8	m	0.18	0/288	0.43	0/397
8	p	0.17	0/288	0.40	0/397
All	All	0.20	0/28770	0.38	0/39400

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2585	0	2550	23	0
2	L	2159	0	2087	35	0
3	M	2621	0	2526	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2041	0	2004	20	0
5	3	424	0	442	10	0
5	6	424	0	442	9	0
5	9	424	0	442	14	0
5	A	424	0	442	18	0
5	D	424	0	442	18	0
5	I	424	0	442	13	0
5	N	424	0	442	12	0
5	Q	424	0	442	12	0
5	T	424	0	442	13	0
5	W	424	0	442	12	0
5	Z	424	0	442	15	0
5	b	424	0	442	13	0
5	e	424	0	442	8	0
5	h	424	0	442	11	0
5	k	424	0	442	10	0
5	n	424	0	442	10	0
5	q	424	0	442	10	0
6	0	400	0	402	13	0
6	1	400	0	402	11	0
6	4	400	0	402	15	0
6	7	400	0	402	11	0
6	B	407	0	410	17	0
6	E	407	0	410	12	0
6	J	386	0	386	13	0
6	O	407	0	410	9	0
6	R	400	0	402	11	0
6	U	400	0	402	16	0
6	X	400	0	402	10	0
6	c	400	0	402	17	0
6	f	400	0	402	11	0
6	i	400	0	402	15	0
6	l	400	0	402	10	0
6	o	400	0	402	11	0
6	r	400	0	402	11	0
7	G	232	0	239	7	0
8	2	279	0	287	3	0
8	5	279	0	287	4	0
8	8	279	0	287	4	0
8	F	279	0	287	6	0
8	K	279	0	287	4	0
8	P	279	0	287	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S	279	0	287	7	0
8	V	279	0	287	3	0
8	Y	279	0	287	4	0
8	a	279	0	287	7	0
8	d	279	0	287	6	0
8	g	279	0	287	5	0
8	j	279	0	287	9	0
8	m	279	0	287	5	0
8	p	279	0	287	6	0
9	C	172	0	121	6	0
10	C	1	0	0	0	0
11	A	53	0	74	11	0
11	C	15	0	11	0	0
11	L	31	0	36	2	0
11	M	78	0	101	17	0
12	L	23	0	27	0	0
13	0	66	0	72	11	0
13	1	66	0	72	7	0
13	3	66	0	72	6	0
13	4	66	0	72	8	0
13	6	66	0	72	7	0
13	7	66	0	72	7	0
13	9	66	0	72	7	0
13	A	66	0	72	6	0
13	B	66	0	72	8	0
13	D	66	0	72	9	0
13	E	66	0	72	8	0
13	I	66	0	72	7	0
13	J	66	0	72	7	0
13	L	132	0	144	11	0
13	M	132	0	144	10	0
13	N	66	0	72	5	0
13	O	66	0	72	16	0
13	Q	66	0	72	7	0
13	R	66	0	72	8	0
13	T	66	0	72	5	0
13	U	66	0	72	6	0
13	W	66	0	72	7	0
13	X	66	0	72	7	0
13	Z	66	0	72	8	0
13	b	66	0	72	7	0
13	c	66	0	72	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	e	66	0	72	4	0
13	f	66	0	72	7	0
13	h	66	0	72	6	0
13	i	66	0	72	10	0
13	k	66	0	72	5	0
13	l	66	0	72	7	0
13	n	66	0	72	5	0
13	o	66	0	72	12	0
13	q	66	0	72	4	0
13	r	66	0	72	7	0
14	L	65	0	74	4	0
14	M	65	0	74	5	0
15	H	170	0	237	14	0
15	L	75	0	94	4	0
15	M	85	0	117	10	0
15	r	68	0	80	7	0
16	M	1	0	0	0	0
17	M	48	0	64	1	0
18	M	40	0	60	1	0
19	B	15	0	19	0	0
19	M	25	0	35	3	0
19	T	26	0	35	2	0
19	b	70	0	92	6	0
19	h	35	0	46	2	0
19	k	35	0	46	0	0
19	n	35	0	46	2	0
20	D	47	0	65	6	0
20	I	51	0	76	4	0
20	M	45	0	58	1	0
20	N	38	0	44	2	0
20	Q	49	0	72	5	0
20	W	48	0	67	1	0
21	0	40	0	0	0	0
21	2	40	0	0	0	0
21	7	40	0	0	0	0
21	9	40	0	0	0	0
21	A	40	0	0	0	0
21	D	40	0	0	0	0
21	O	40	0	0	0	0
21	R	40	0	0	0	0
21	U	40	0	0	0	0
21	W	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	X	40	0	0	0	0
21	h	40	0	0	0	0
21	k	40	0	0	0	0
21	l	40	0	0	0	0
21	o	40	0	0	1	0
21	q	40	0	0	0	0
22	0	1	0	0	0	0
22	1	3	0	0	0	0
22	2	3	0	0	0	0
22	3	5	0	0	0	0
22	4	7	0	0	0	0
22	5	5	0	0	0	0
22	6	10	0	0	0	0
22	7	4	0	0	0	0
22	8	1	0	0	0	0
22	9	6	0	0	0	0
22	A	6	0	0	0	0
22	B	2	0	0	0	0
22	C	98	0	0	0	0
22	D	6	0	0	0	0
22	E	3	0	0	0	0
22	H	22	0	0	0	0
22	I	7	0	0	0	0
22	J	3	0	0	0	0
22	K	2	0	0	0	0
22	L	59	0	0	0	0
22	M	75	0	0	0	0
22	N	6	0	0	0	0
22	O	3	0	0	0	0
22	Q	6	0	0	0	0
22	R	5	0	0	0	0
22	S	1	0	0	0	0
22	T	6	0	0	1	0
22	U	5	0	0	0	0
22	V	2	0	0	0	0
22	W	3	0	0	0	0
22	X	5	0	0	0	0
22	Y	2	0	0	0	0
22	Z	4	0	0	0	0
22	b	10	0	0	0	0
22	c	4	0	0	0	0
22	e	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	f	2	0	0	0	0
22	g	1	0	0	0	0
22	h	4	0	0	0	0
22	i	1	0	0	1	0
22	j	2	0	0	0	0
22	k	5	0	0	0	0
22	l	1	0	0	0	0
22	n	4	0	0	0	0
22	o	1	0	0	0	0
22	p	1	0	0	0	0
22	q	2	0	0	0	0
All	All	32918	0	32674	616	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 9.

The worst 5 of 616 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)
1:C:135:CYS:SG	9:C:402:HEC:CAC	2.11	1.38
1:C:135:CYS:SG	9:C:402:HEC:HAC	1.67	1.32
13:L:302:BCB:H2C	13:M:403:BCB:H2C	1.50	0.94
6:r:34:VAL:HG13	15:r:102:CDL:H381	1.57	0.85
6:J:26:MET:HE1	13:J:101:BCB:H172	1.60	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	329/354 (93%)	323 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
3	M	329/332 (99%)	320 (97%)	9 (3%)	0	100	100
4	H	258/260 (99%)	251 (97%)	7 (3%)	0	100	100
5	3	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	6	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
5	9	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	A	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	D	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
5	I	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
5	N	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	Q	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	T	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	W	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	Z	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	b	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	e	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	h	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
5	k	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
5	n	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
5	q	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	0	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	1	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
6	4	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	7	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	B	49/69 (71%)	47 (96%)	2 (4%)	0	100	100
6	E	49/69 (71%)	48 (98%)	1 (2%)	0	100	100
6	J	46/69 (67%)	45 (98%)	1 (2%)	0	100	100
6	O	49/69 (71%)	48 (98%)	1 (2%)	0	100	100
6	R	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
6	U	48/69 (70%)	44 (92%)	4 (8%)	0	100	100
6	X	48/69 (70%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
6	f	48/69 (70%)	47 (98%)	1 (2%)	0	100	100
6	i	48/69 (70%)	45 (94%)	3 (6%)	0	100	100
6	l	48/69 (70%)	43 (90%)	5 (10%)	0	100	100
6	o	48/69 (70%)	46 (96%)	2 (4%)	0	100	100
6	r	48/69 (70%)	44 (92%)	4 (8%)	0	100	100
7	G	26/56 (46%)	26 (100%)	0	0	100	100
8	2	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	5	34/57 (60%)	34 (100%)	0	0	100	100
8	8	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	F	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	K	34/57 (60%)	34 (100%)	0	0	100	100
8	P	34/57 (60%)	34 (100%)	0	0	100	100
8	S	34/57 (60%)	34 (100%)	0	0	100	100
8	V	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	Y	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	a	34/57 (60%)	34 (100%)	0	0	100	100
8	d	34/57 (60%)	34 (100%)	0	0	100	100
8	g	34/57 (60%)	34 (100%)	0	0	100	100
8	j	34/57 (60%)	34 (100%)	0	0	100	100
8	m	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
8	p	34/57 (60%)	34 (100%)	0	0	100	100
All	All	3356/4477 (75%)	3250 (97%)	106 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	279/295 (95%)	273 (98%)	6 (2%)	45	61
2	L	213/214 (100%)	212 (100%)	1 (0%)	81	90
3	M	257/258 (100%)	249 (97%)	8 (3%)	35	48
4	H	209/209 (100%)	203 (97%)	6 (3%)	37	51
5	3	45/59 (76%)	45 (100%)	0	100	100
5	6	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	9	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	A	45/59 (76%)	43 (96%)	2 (4%)	25	34
5	D	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	I	45/59 (76%)	45 (100%)	0	100	100
5	N	45/59 (76%)	45 (100%)	0	100	100
5	Q	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	T	45/59 (76%)	42 (93%)	3 (7%)	15	17
5	W	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	Z	45/59 (76%)	45 (100%)	0	100	100
5	b	45/59 (76%)	45 (100%)	0	100	100
5	e	45/59 (76%)	45 (100%)	0	100	100
5	h	45/59 (76%)	45 (100%)	0	100	100
5	k	45/59 (76%)	45 (100%)	0	100	100
5	n	45/59 (76%)	44 (98%)	1 (2%)	45	61
5	q	45/59 (76%)	43 (96%)	2 (4%)	25	34
6	0	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	1	43/59 (73%)	43 (100%)	0	100	100
6	4	43/59 (73%)	43 (100%)	0	100	100
6	7	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	B	44/59 (75%)	43 (98%)	1 (2%)	44	59
6	E	44/59 (75%)	43 (98%)	1 (2%)	44	59
6	J	41/59 (70%)	41 (100%)	0	100	100
6	O	44/59 (75%)	43 (98%)	1 (2%)	44	59
6	R	43/59 (73%)	43 (100%)	0	100	100
6	U	43/59 (73%)	41 (95%)	2 (5%)	23	31
6	X	43/59 (73%)	42 (98%)	1 (2%)	44	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	c	43/59 (73%)	43 (100%)	0	100	100
6	f	43/59 (73%)	43 (100%)	0	100	100
6	i	43/59 (73%)	43 (100%)	0	100	100
6	l	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	o	43/59 (73%)	42 (98%)	1 (2%)	44	59
6	r	43/59 (73%)	41 (95%)	2 (5%)	23	31
7	G	25/44 (57%)	24 (96%)	1 (4%)	28	38
8	2	29/45 (64%)	28 (97%)	1 (3%)	32	44
8	5	29/45 (64%)	29 (100%)	0	100	100
8	8	29/45 (64%)	29 (100%)	0	100	100
8	F	29/45 (64%)	28 (97%)	1 (3%)	32	44
8	K	29/45 (64%)	29 (100%)	0	100	100
8	P	29/45 (64%)	29 (100%)	0	100	100
8	S	29/45 (64%)	29 (100%)	0	100	100
8	V	29/45 (64%)	29 (100%)	0	100	100
8	Y	29/45 (64%)	29 (100%)	0	100	100
8	a	29/45 (64%)	29 (100%)	0	100	100
8	d	29/45 (64%)	29 (100%)	0	100	100
8	g	29/45 (64%)	27 (93%)	2 (7%)	14	16
8	j	29/45 (64%)	28 (97%)	1 (3%)	32	44
8	m	29/45 (64%)	29 (100%)	0	100	100
8	p	29/45 (64%)	28 (97%)	1 (3%)	32	44
All	All	2915/3701 (79%)	2862 (98%)	53 (2%)	51	68

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	O	30	LEU
5	W	35	LEU
5	q	16	LEU
5	Q	16	LEU
5	T	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
5	W	52	GLN
5	Z	52	GLN
5	b	44	ASN
5	3	44	ASN
2	L	158	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FME	H	1	4	8,9,10	0.50	0	8,9,11	1.18	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	O-C-CA	-2.56	118.19	124.77
4	H	1	FME	CA-N-CN	-2.09	119.61	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA
4	H	1	FME	CB-CA-N-CN
4	H	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 2 are monoatomic - leaving 87 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	$\# Z > 2$
13	BCB	R	102	-	60,74,74	2.98	18 (30%)	59,115,115	2.32	16 (27%)
13	BCB	q	101	-	60,74,74	3.10	18 (30%)	59,115,115	2.27	15 (25%)
12	DGA	L	301	1	22,22,43	1.37	3 (13%)	24,24,45	1.76	5 (20%)
19	LMT	b	102	-	36,36,36	0.45	0	47,47,47	0.79	0
17	MQ7	M	405	-	49,49,49	1.39	2 (4%)	61,63,63	1.47	14 (22%)
11	UQ8	L	305	-	31,31,53	1.62	2 (6%)	39,40,67	1.46	7 (17%)
21	NS0	7	101	-	39,39,39	1.17	3 (7%)	46,46,46	1.26	6 (13%)
13	BCB	B	202	-	60,74,74	3.02	17 (28%)	59,115,115	2.24	14 (23%)
13	BCB	6	101	-	60,74,74	3.11	18 (30%)	59,115,115	2.26	15 (25%)
21	NS0	2	101	-	39,39,39	1.18	3 (7%)	46,46,46	1.16	9 (19%)
15	CDL	H	301	-	97,97,99	0.92	4 (4%)	103,109,111	1.07	6 (5%)
11	UQ8	M	408	-	53,53,53	1.28	2 (3%)	66,67,67	1.56	15 (22%)
9	HEC	C	403	1	46,50,50	1.77	9 (19%)	58,82,82	1.55	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	UQ8	C	406	-	15,15,53	2.23	2 (13%)	20,21,67	1.44	2 (10%)
13	BCB	f	101	-	60,74,74	2.97	18 (30%)	59,115,115	2.20	15 (25%)
20	PGV	W	301	-	47,47,50	0.95	2 (4%)	50,53,56	1.09	4 (8%)
13	BCB	D	101	-	60,74,74	3.08	18 (30%)	59,115,115	2.30	14 (23%)
21	NS0	k	101	-	39,39,39	1.15	4 (10%)	46,46,46	1.29	9 (19%)
13	BCB	c	101	-	60,74,74	2.97	18 (30%)	59,115,115	2.30	15 (25%)
13	BCB	W	302	-	60,74,74	3.07	18 (30%)	59,115,115	2.31	14 (23%)
20	PGV	I	102	-	50,50,50	0.89	2 (4%)	53,56,56	1.04	3 (5%)
21	NS0	o	101	-	39,39,39	1.15	3 (7%)	46,46,46	1.20	6 (13%)
9	HEC	C	402	1	46,50,50	1.77	11 (23%)	58,82,82	1.55	11 (18%)
20	PGV	Q	401	-	48,48,50	0.96	2 (4%)	51,53,56	1.00	2 (3%)
21	NS0	X	101	-	39,39,39	1.15	3 (7%)	46,46,46	1.22	8 (17%)
13	BCB	0	102	-	60,74,74	2.96	17 (28%)	59,115,115	2.28	14 (23%)
13	BCB	k	102	-	60,74,74	3.10	18 (30%)	59,115,115	2.13	15 (25%)
13	BCB	M	403	-	60,74,74	3.12	18 (30%)	59,115,115	2.37	19 (32%)
15	CDL	H	302	-	71,71,99	1.10	4 (5%)	77,83,111	1.10	5 (6%)
13	BCB	b	101	-	60,74,74	3.03	18 (30%)	59,115,115	2.31	18 (30%)
13	BCB	J	101	-	60,74,74	2.98	17 (28%)	59,115,115	2.23	14 (23%)
13	BCB	n	101	-	60,74,74	3.08	18 (30%)	59,115,115	2.23	16 (27%)
15	CDL	M	409	-	84,84,99	0.99	4 (4%)	90,96,111	1.12	9 (10%)
13	BCB	r	101	-	60,74,74	3.00	17 (28%)	59,115,115	2.19	14 (23%)
21	NS0	R	101	-	39,39,39	1.16	3 (7%)	46,46,46	1.26	7 (15%)
13	BCB	h	102	-	60,74,74	3.08	18 (30%)	59,115,115	2.26	16 (27%)
19	LMT	h	103	-	36,36,36	0.36	0	47,47,47	0.71	1 (2%)
11	UQ8	A	101	-	53,53,53	1.25	2 (3%)	66,67,67	1.59	14 (21%)
19	LMT	k	103	-	36,36,36	0.44	0	47,47,47	0.88	1 (2%)
20	PGV	D	102	-	46,46,50	0.95	2 (4%)	49,52,56	1.08	3 (6%)
14	BPB	L	304	-	57,70,70	0.90	6 (10%)	55,101,101	0.94	3 (5%)
13	BCB	O	102	-	60,74,74	2.95	18 (30%)	59,115,115	2.31	13 (22%)
20	PGV	N	102	-	37,37,50	1.08	2 (5%)	40,43,56	1.06	3 (7%)
13	BCB	I	101	-	60,74,74	3.10	18 (30%)	59,115,115	2.26	16 (27%)
19	LMT	M	410	-	25,25,36	0.42	0	30,30,47	0.64	0
15	CDL	r	102	-	67,67,99	1.11	4 (5%)	73,79,111	1.15	5 (6%)
13	BCB	l	102	-	60,74,74	2.98	18 (30%)	59,115,115	2.22	15 (25%)
13	BCB	M	402	-	60,74,74	3.03	18 (30%)	59,115,115	2.41	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCB	o	102	-	60,74,74	2.95	18 (30%)	59,115,115	2.28	14 (23%)
9	HEC	C	401	1	46,50,50	1.74	9 (19%)	58,82,82	1.65	14 (24%)
21	NS0	D	103	-	39,39,39	1.18	3 (7%)	46,46,46	1.15	6 (13%)
11	UQ8	M	407	-	25,25,53	1.76	2 (8%)	31,33,67	1.47	7 (22%)
13	BCB	3	101	-	60,74,74	3.06	18 (30%)	59,115,115	2.35	16 (27%)
13	BCB	1	101	-	60,74,74	2.95	18 (30%)	59,115,115	2.22	15 (25%)
13	BCB	T	101	-	60,74,74	3.11	18 (30%)	59,115,115	2.19	15 (25%)
15	CDL	L	306	-	74,74,99	1.06	4 (5%)	80,86,111	1.19	8 (10%)
21	NS0	A	103	-	39,39,39	1.16	4 (10%)	46,46,46	1.17	8 (17%)
13	BCB	7	102	-	60,74,74	2.97	17 (28%)	59,115,115	2.14	15 (25%)
9	HEC	C	404	1	46,50,50	1.78	11 (23%)	58,82,82	1.59	11 (18%)
13	BCB	9	101	-	60,74,74	3.08	18 (30%)	59,115,115	2.38	16 (27%)
21	NS0	l	101	-	39,39,39	1.14	3 (7%)	46,46,46	1.23	9 (19%)
19	LMT	B	201	-	14,14,36	0.70	0	14,14,47	0.58	0
14	BPB	M	404	-	57,70,70	0.87	3 (5%)	55,101,101	0.93	3 (5%)
21	NS0	W	303	-	39,39,39	1.17	3 (7%)	46,46,46	1.30	7 (15%)
13	BCB	E	101	-	60,74,74	2.98	17 (28%)	59,115,115	2.20	15 (25%)
13	BCB	X	102	-	60,74,74	2.97	17 (28%)	59,115,115	2.18	16 (27%)
13	BCB	i	101	-	60,74,74	2.97	17 (28%)	59,115,115	2.31	15 (25%)
21	NS0	O	101	-	39,39,39	1.14	3 (7%)	46,46,46	1.20	7 (15%)
21	NS0	0	101	-	39,39,39	1.17	3 (7%)	46,46,46	1.16	7 (15%)
13	BCB	L	302	-	60,74,74	3.05	18 (30%)	59,115,115	2.34	15 (25%)
13	BCB	Z	101	-	60,74,74	3.07	18 (30%)	59,115,115	2.28	16 (27%)
21	NS0	9	102	-	39,39,39	1.17	4 (10%)	46,46,46	1.27	8 (17%)
21	NS0	U	101	-	39,39,39	1.15	3 (7%)	46,46,46	1.22	8 (17%)
19	LMT	T	102	-	26,26,36	0.41	0	31,31,47	1.04	2 (6%)
18	NS5	M	406	-	39,39,39	1.14	5 (12%)	46,46,46	1.20	6 (13%)
19	LMT	n	102	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
13	BCB	A	102	-	60,74,74	3.10	18 (30%)	59,115,115	2.38	17 (28%)
13	BCB	e	101	-	60,74,74	3.09	18 (30%)	59,115,115	2.26	16 (27%)
19	LMT	b	103	-	36,36,36	0.41	0	47,47,47	0.94	2 (4%)
13	BCB	Q	402	-	60,74,74	3.10	18 (30%)	59,115,115	2.26	14 (23%)
13	BCB	L	303	-	60,74,74	3.05	18 (30%)	59,115,115	2.51	16 (27%)
20	PGV	M	411	-	44,44,50	0.97	2 (4%)	47,50,56	0.96	3 (6%)
13	BCB	U	102	-	60,74,74	2.96	18 (30%)	59,115,115	2.27	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	NS0	h	101	-	39,39,39	1.16	4 (10%)	46,46,46	1.15	6 (13%)
13	BCB	N	101	-	60,74,74	3.08	18 (30%)	59,115,115	2.24	15 (25%)
21	NS0	q	102	-	39,39,39	1.16	3 (7%)	46,46,46	1.19	7 (15%)
13	BCB	4	101	-	60,74,74	2.91	17 (28%)	59,115,115	2.22	13 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCB	R	102	-	2/2/21/26	6/37/137/137	-
13	BCB	q	101	-	2/2/21/26	16/37/137/137	-
12	DGA	L	301	1	-	12/23/23/45	-
19	LMT	b	102	-	-	11/21/61/61	0/2/2/2
17	MQ7	M	405	-	-	0/41/61/61	0/2/2/2
11	UQ8	L	305	-	-	7/25/49/75	0/1/1/1
21	NS0	7	101	-	-	6/43/43/43	-
13	BCB	B	202	-	2/2/21/26	6/37/137/137	-
13	BCB	6	101	-	2/2/21/26	8/37/137/137	-
21	NS0	2	101	-	-	6/43/43/43	-
15	CDL	H	301	-	-	41/108/108/110	-
11	UQ8	M	408	-	-	11/51/75/75	0/1/1/1
9	HEC	C	403	1	-	4/14/54/54	-
11	UQ8	C	406	-	-	0/6/30/75	0/1/1/1
13	BCB	f	101	-	2/2/21/26	13/37/137/137	-
20	PGV	W	301	-	-	16/52/52/55	-
13	BCB	D	101	-	2/2/21/26	10/37/137/137	-
21	NS0	k	101	-	-	4/43/43/43	-
13	BCB	c	101	-	2/2/21/26	11/37/137/137	-
13	BCB	W	302	-	2/2/21/26	10/37/137/137	-
20	PGV	I	102	-	-	16/55/55/55	-
21	NS0	o	101	-	-	5/43/43/43	-
9	HEC	C	402	1	-	7/14/54/54	-
20	PGV	Q	401	-	-	17/52/52/55	-
21	NS0	X	101	-	-	4/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCB	0	102	-	2/2/21/26	10/37/137/137	-
13	BCB	k	102	-	2/2/21/26	11/37/137/137	-
13	BCB	M	403	-	2/2/21/26	8/37/137/137	-
15	CDL	H	302	-	-	37/82/82/110	-
13	BCB	b	101	-	2/2/21/26	12/37/137/137	-
13	BCB	J	101	-	2/2/21/26	11/37/137/137	-
13	BCB	n	101	-	2/2/21/26	4/37/137/137	-
15	CDL	M	409	-	-	36/95/95/110	-
13	BCB	r	101	-	2/2/21/26	12/37/137/137	-
21	NS0	R	101	-	-	6/43/43/43	-
13	BCB	h	102	-	2/2/21/26	5/37/137/137	-
19	LMT	h	103	-	-	4/21/61/61	0/2/2/2
11	UQ8	A	101	-	-	14/51/75/75	0/1/1/1
19	LMT	k	103	-	-	3/21/61/61	0/2/2/2
20	PGV	D	102	-	-	13/51/51/55	-
14	BPB	L	304	-	-	2/37/105/105	0/5/6/6
13	BCB	O	102	-	2/2/21/26	15/37/137/137	-
20	PGV	N	102	-	-	11/42/42/55	-
13	BCB	I	101	-	2/2/21/26	6/37/137/137	-
19	LMT	M	410	-	-	6/17/37/61	0/1/1/2
15	CDL	r	102	-	-	39/78/78/110	-
13	BCB	l	102	-	2/2/21/26	4/37/137/137	-
13	BCB	M	402	-	2/2/21/26	7/37/137/137	-
13	BCB	o	102	-	2/2/21/26	16/37/137/137	-
9	HEC	C	401	1	-	6/14/54/54	-
21	NS0	D	103	-	-	3/43/43/43	-
11	UQ8	M	407	-	-	0/18/42/75	0/1/1/1
13	BCB	3	101	-	2/2/21/26	14/37/137/137	-
13	BCB	1	101	-	2/2/21/26	12/37/137/137	-
13	BCB	T	101	-	2/2/21/26	11/37/137/137	-
15	CDL	L	306	-	-	27/85/85/110	-
21	NS0	A	103	-	-	2/43/43/43	-
13	BCB	7	102	-	2/2/21/26	18/37/137/137	-
9	HEC	C	404	1	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCB	9	101	-	2/2/21/26	14/37/137/137	-
21	NS0	l	101	-	-	5/43/43/43	-
19	LMT	B	201	-	-	6/13/13/61	-
14	BPB	M	404	-	-	4/37/105/105	0/5/6/6
21	NS0	W	303	-	-	7/43/43/43	-
13	BCB	E	101	-	2/2/21/26	11/37/137/137	-
13	BCB	X	102	-	2/2/21/26	18/37/137/137	-
13	BCB	i	101	-	2/2/21/26	10/37/137/137	-
21	NS0	O	101	-	-	8/43/43/43	-
21	NS0	0	101	-	-	4/43/43/43	-
13	BCB	L	302	-	2/2/21/26	4/37/137/137	-
13	BCB	Z	101	-	2/2/21/26	7/37/137/137	-
21	NS0	9	102	-	-	5/43/43/43	-
21	NS0	U	101	-	-	6/43/43/43	-
19	LMT	T	102	-	-	1/17/38/61	0/1/1/2
18	NS5	M	406	-	-	2/43/43/43	-
19	LMT	n	102	-	-	4/21/61/61	0/2/2/2
13	BCB	A	102	-	2/2/21/26	18/37/137/137	-
13	BCB	e	101	-	2/2/21/26	10/37/137/137	-
19	LMT	b	103	-	-	6/21/61/61	0/2/2/2
13	BCB	Q	402	-	2/2/21/26	8/37/137/137	-
13	BCB	L	303	-	2/2/21/26	3/37/137/137	-
20	PGV	M	411	-	-	13/49/49/55	-
13	BCB	U	102	-	2/2/21/26	7/37/137/137	-
21	NS0	h	101	-	-	1/43/43/43	-
13	BCB	N	101	-	2/2/21/26	16/37/137/137	-
21	NS0	q	102	-	-	6/43/43/43	-
13	BCB	4	101	-	2/2/21/26	8/37/137/137	-

The worst 5 of 828 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402	BCB	C1D-C2D	9.24	1.50	1.39
13	9	101	BCB	C1D-C2D	9.04	1.49	1.39
13	L	303	BCB	C1D-C2D	8.95	1.49	1.39
13	M	403	BCB	C1A-CHA	8.82	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	k	102	BCB	C1A-CHA	8.81	1.50	1.40

The worst 5 of 875 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	303	BCB	O2D-CGD-CBD	9.74	121.65	110.95
13	q	101	BCB	C4B-CHC-C1C	8.87	127.03	121.32
13	M	402	BCB	O2D-CGD-CBD	8.76	120.58	110.95
13	A	102	BCB	C4B-CHC-C1C	8.55	126.82	121.32
13	M	403	BCB	O2D-CGD-CBD	8.48	120.26	110.95

5 of 76 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	L	302	BCB	NA
13	L	302	BCB	NC
13	L	303	BCB	NA
13	L	303	BCB	NC
13	M	402	BCB	NA

5 of 851 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	401	HEC	C2B-C3B-CAB-CBB
9	C	401	HEC	C2C-C3C-CAC-CBC
9	C	401	HEC	C4C-C3C-CAC-CBC
9	C	402	HEC	C2B-C3B-CAB-CBB
9	C	402	HEC	C4B-C3B-CAB-CBB

There are no ring outliers.

66 monomers are involved in 364 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	R	102	BCB	8	0
13	q	101	BCB	4	0
19	b	102	LMT	3	0
17	M	405	MQ7	1	0
11	L	305	UQ8	2	0
13	B	202	BCB	8	0
13	6	101	BCB	7	0
15	H	301	CDL	12	0

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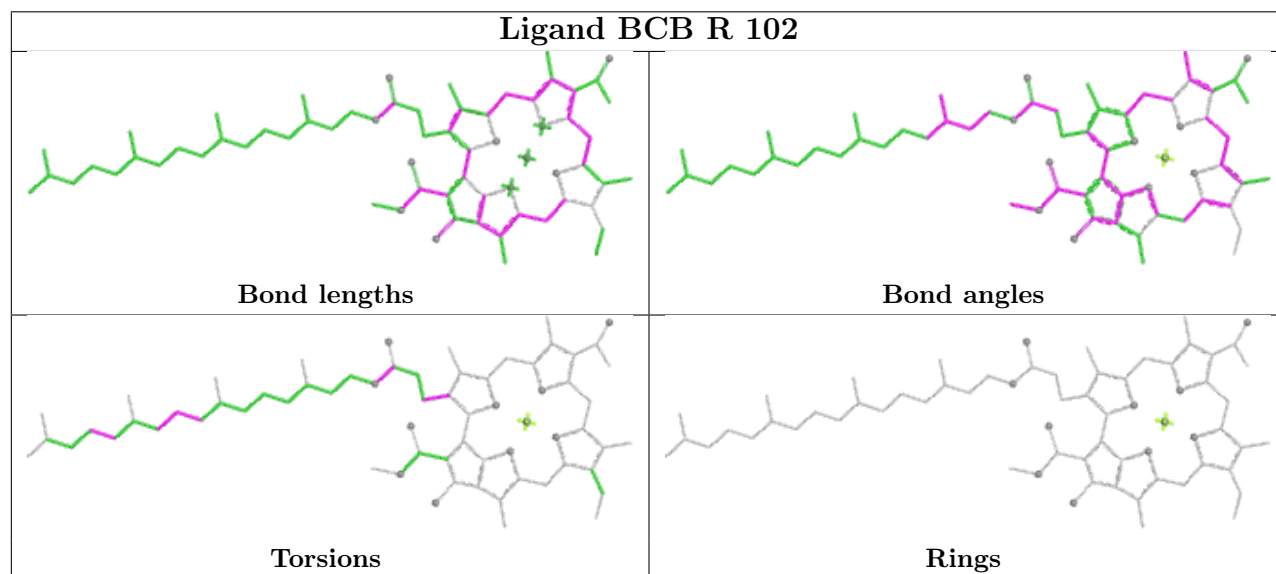
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	408	UQ8	15	0
9	C	403	HEC	1	0
13	f	101	BCB	7	0
20	W	301	PGV	1	0
13	D	101	BCB	9	0
13	c	101	BCB	9	0
13	W	302	BCB	7	0
20	I	102	PGV	4	0
21	o	101	NS0	1	0
9	C	402	HEC	5	0
20	Q	401	PGV	5	0
13	0	102	BCB	11	0
13	k	102	BCB	5	0
13	M	403	BCB	7	0
15	H	302	CDL	2	0
13	b	101	BCB	7	0
13	J	101	BCB	7	0
13	n	101	BCB	5	0
15	M	409	CDL	10	0
13	r	101	BCB	7	0
13	h	102	BCB	6	0
19	h	103	LMT	2	0
11	A	101	UQ8	11	0
20	D	102	PGV	6	0
14	L	304	BPB	4	0
13	O	102	BCB	16	0
20	N	102	PGV	2	0
13	I	101	BCB	7	0
19	M	410	LMT	3	0
15	r	102	CDL	7	0
13	l	102	BCB	7	0
13	M	402	BCB	3	0
13	o	102	BCB	12	0
11	M	407	UQ8	2	0
13	3	101	BCB	6	0
13	1	101	BCB	7	0
13	T	101	BCB	5	0
15	L	306	CDL	4	0
13	7	102	BCB	7	0
13	9	101	BCB	7	0
14	M	404	BPB	5	0
13	E	101	BCB	8	0

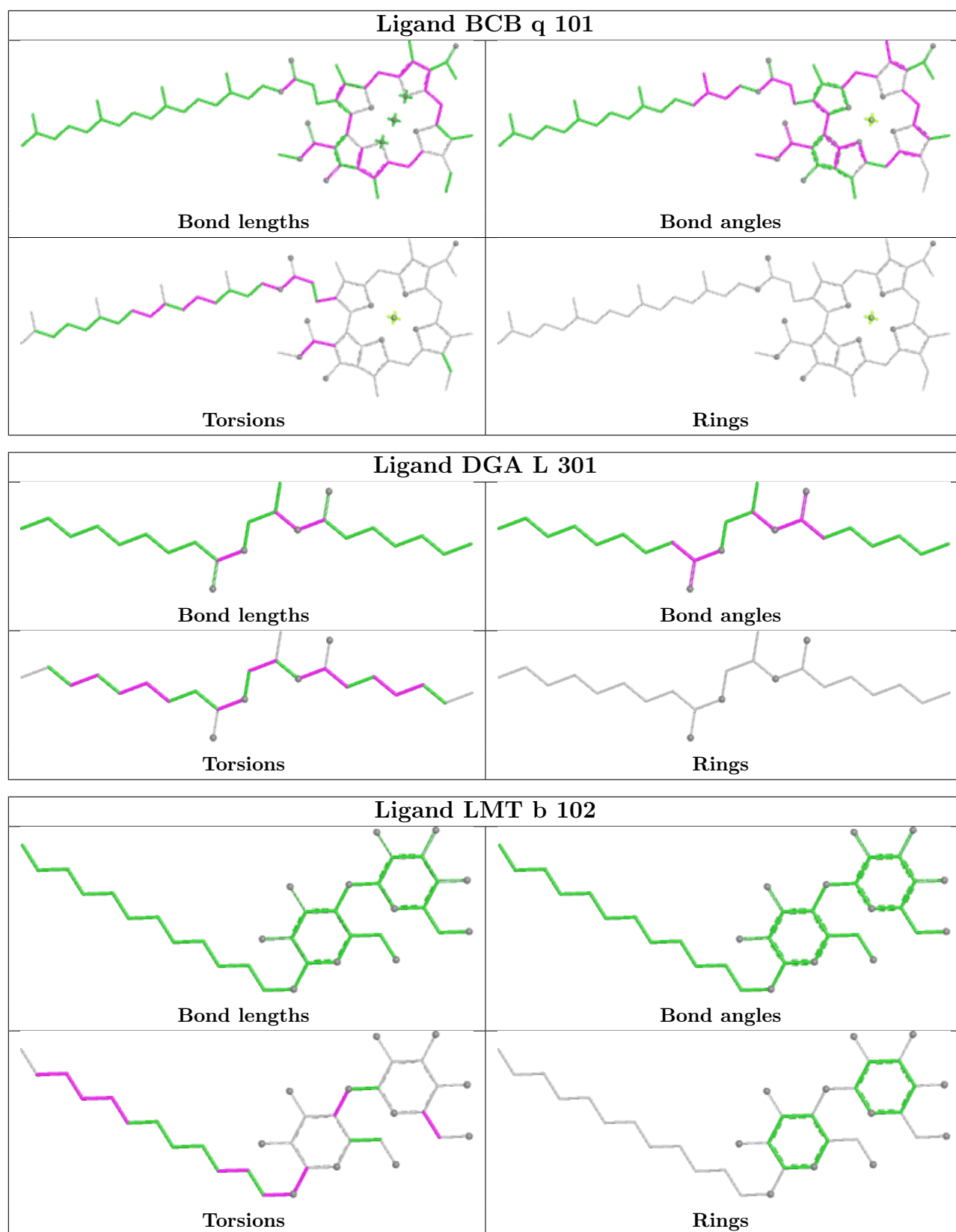
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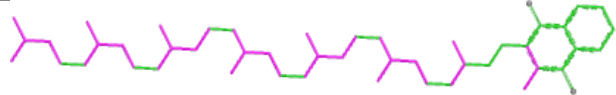
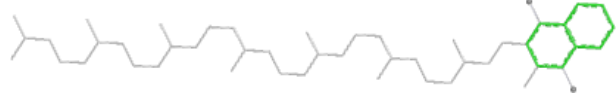
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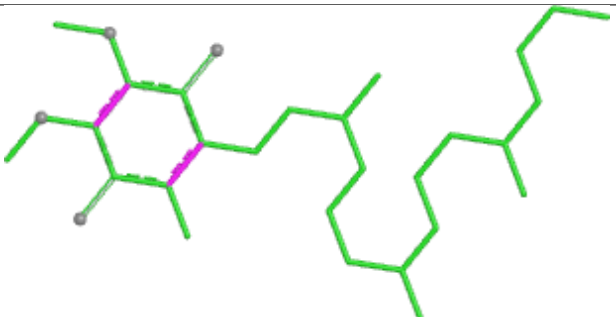
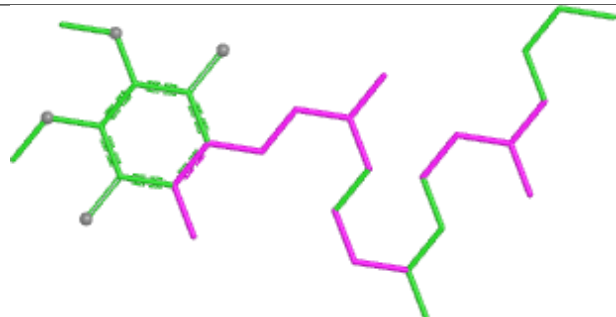
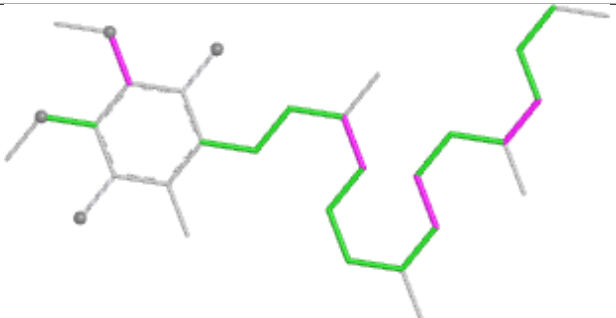
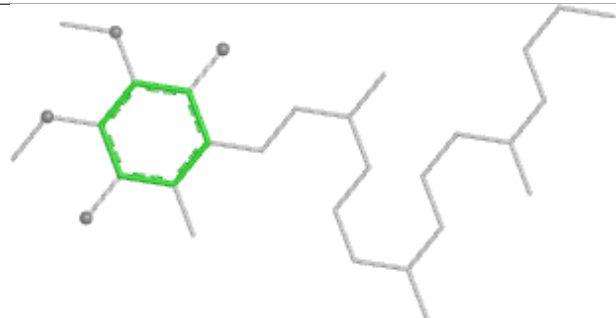
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	X	102	BCB	7	0
13	i	101	BCB	10	0
13	L	302	BCB	7	0
13	Z	101	BCB	8	0
19	T	102	LMT	2	0
18	M	406	NS5	1	0
19	n	102	LMT	2	0
13	A	102	BCB	6	0
13	e	101	BCB	4	0
19	b	103	LMT	3	0
13	Q	402	BCB	7	0
13	L	303	BCB	5	0
20	M	411	PGV	1	0
13	U	102	BCB	6	0
13	N	101	BCB	5	0
13	4	101	BCB	8	0

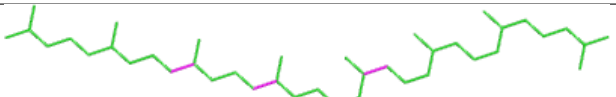
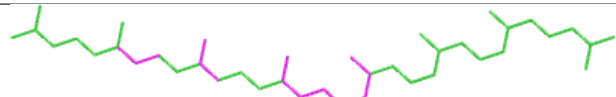
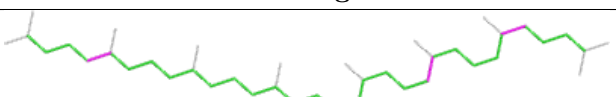
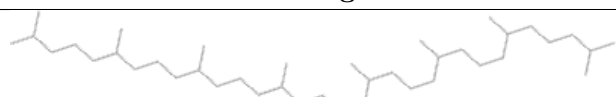
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

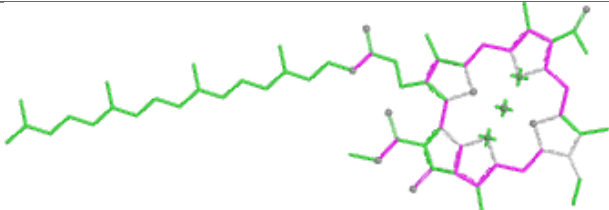
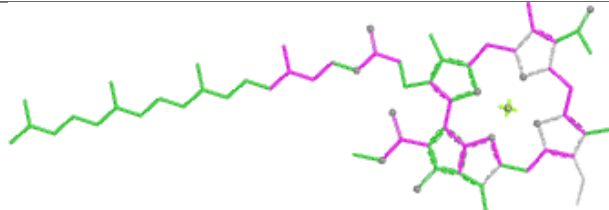
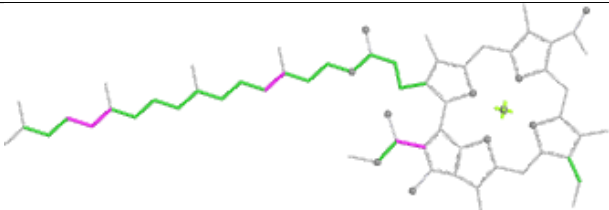
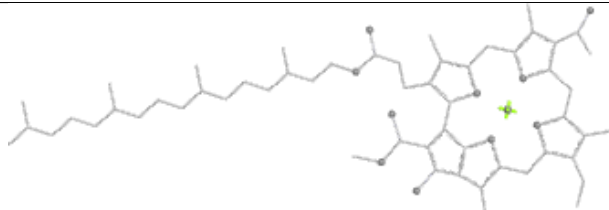


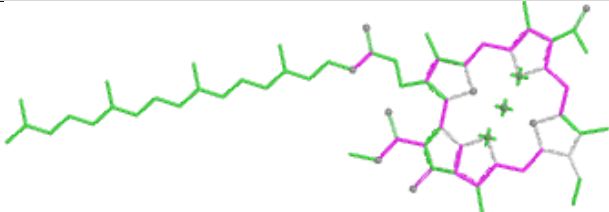
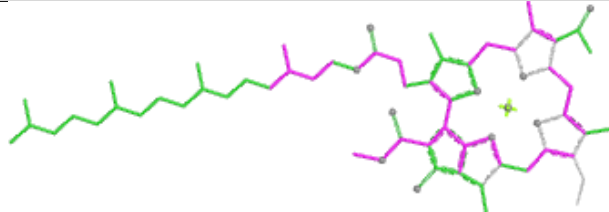
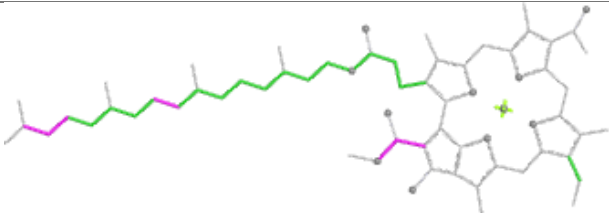
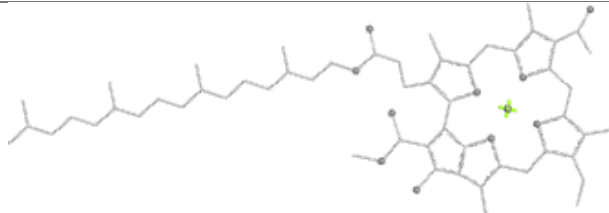


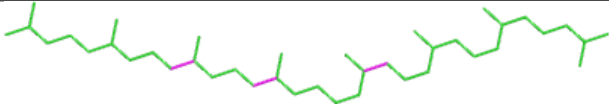
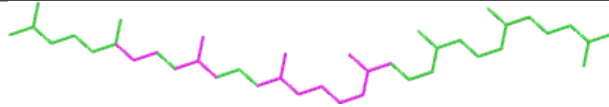
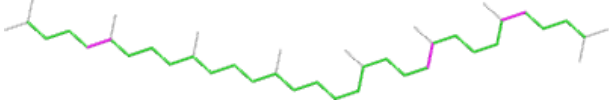
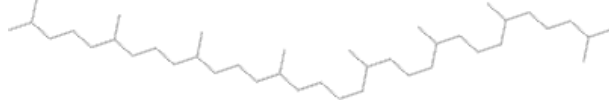
Ligand MQ7 M 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

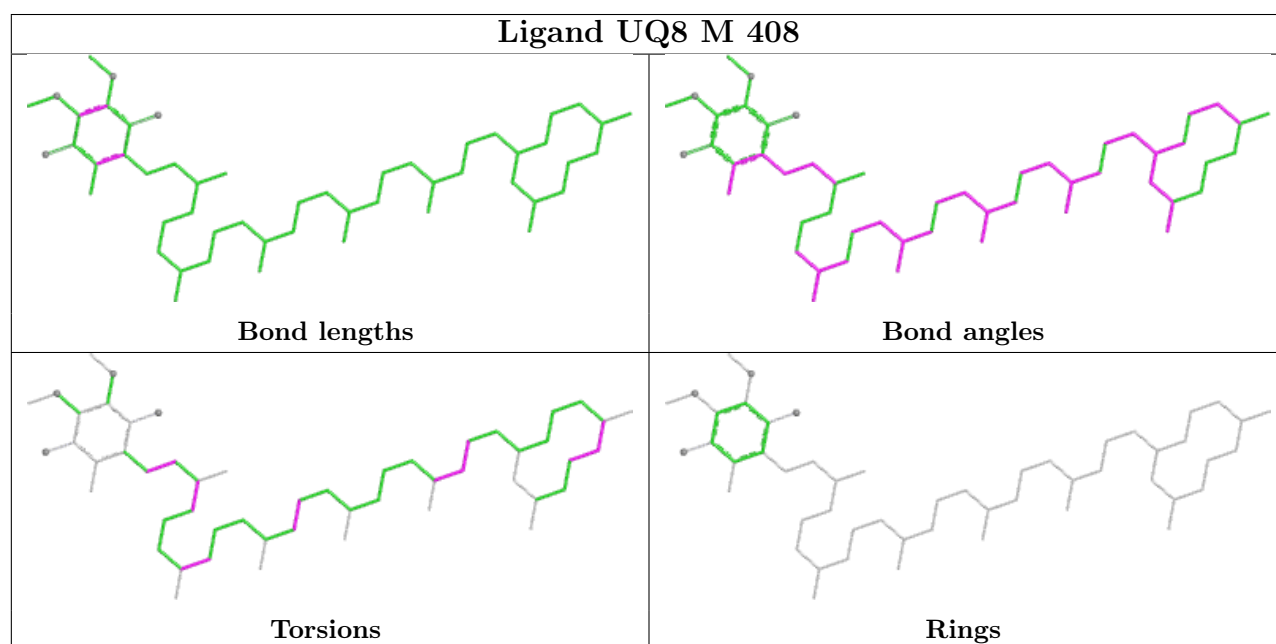
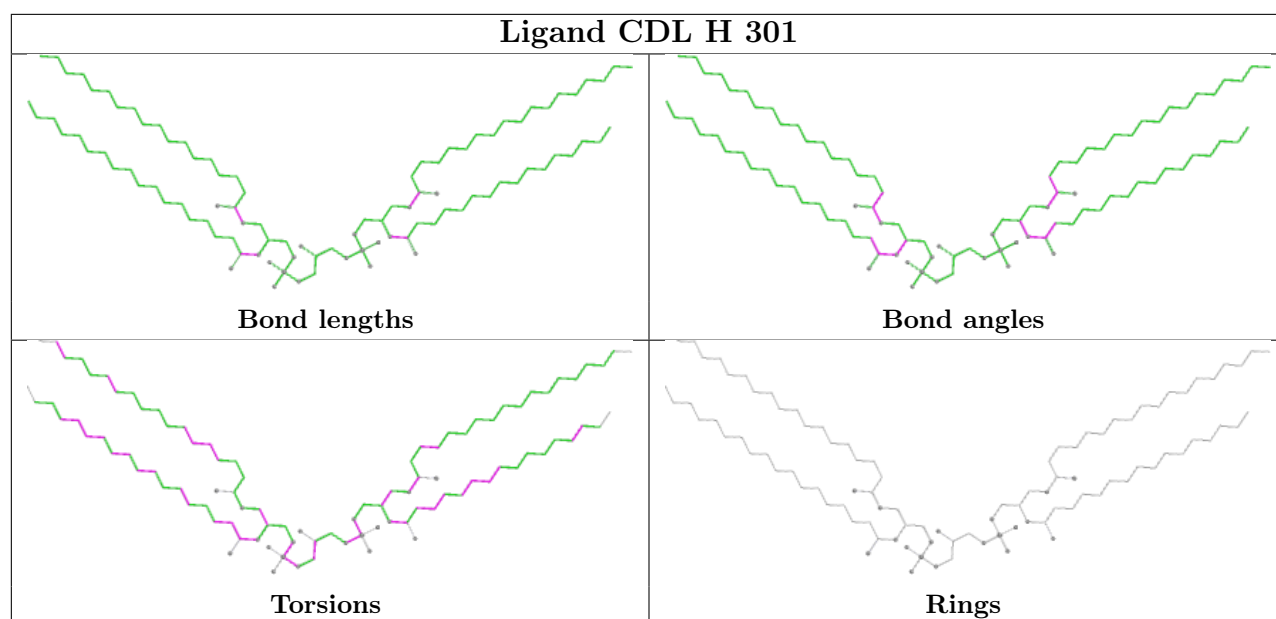
Ligand UQ8 L 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

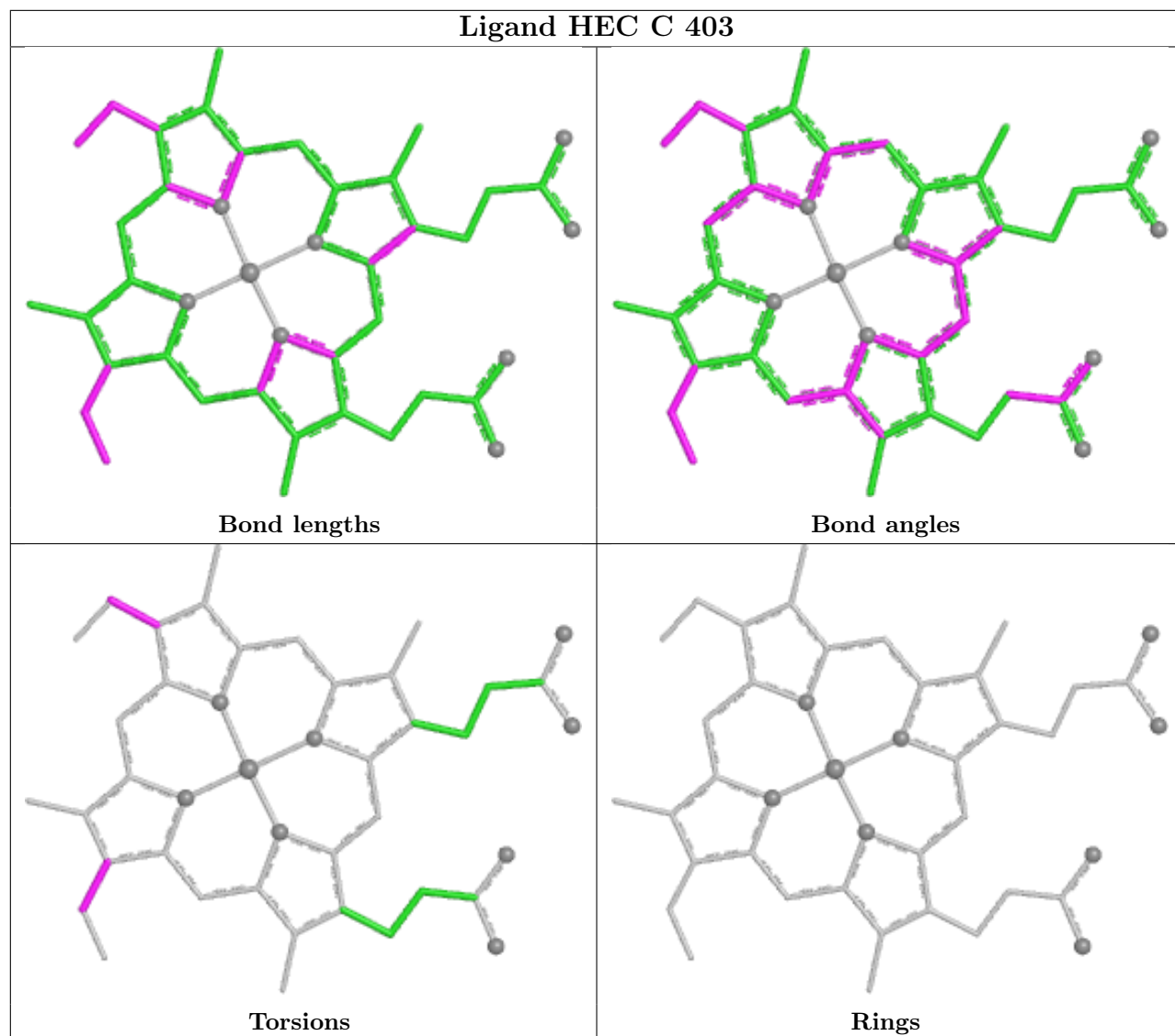
Ligand NS0 7 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

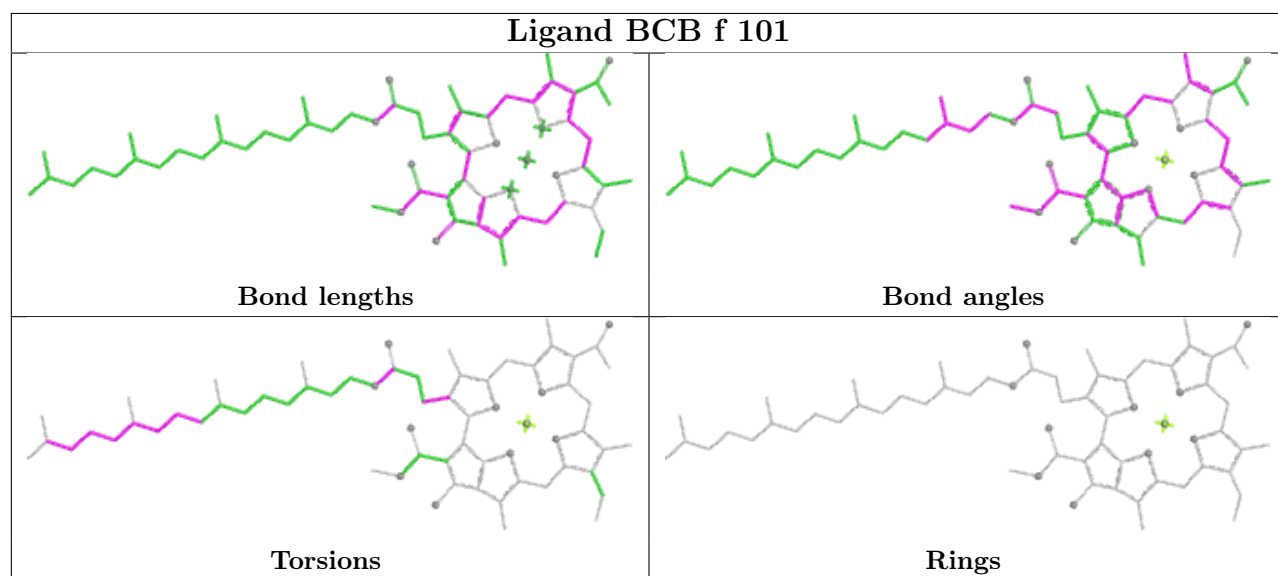
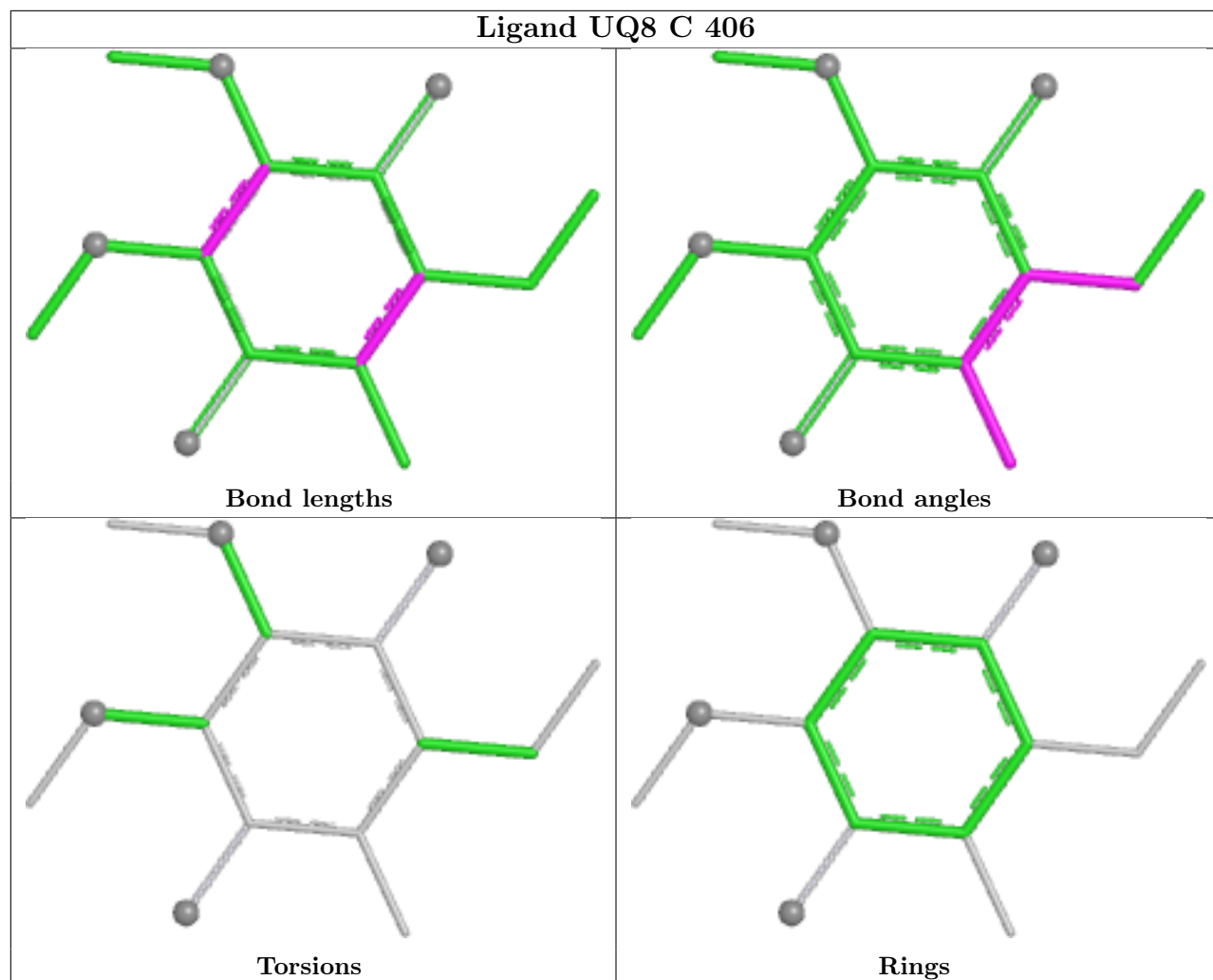
Ligand BCB B 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

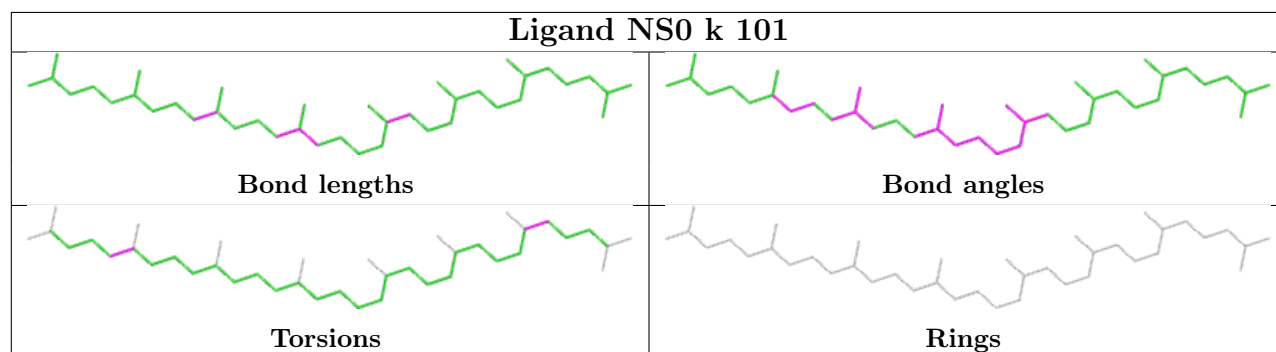
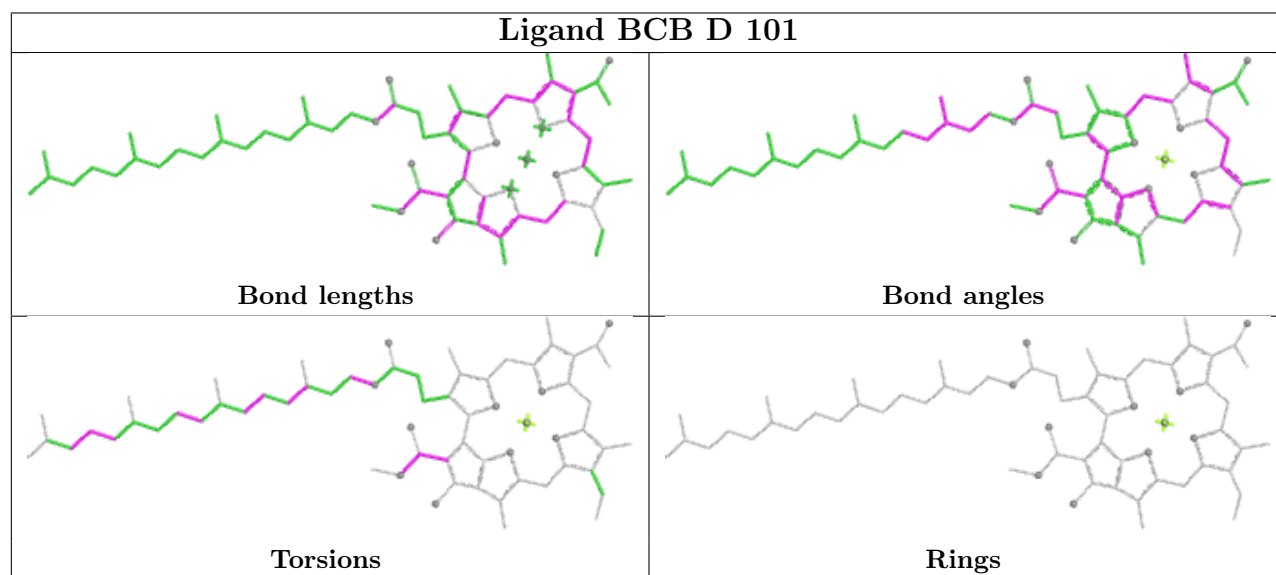
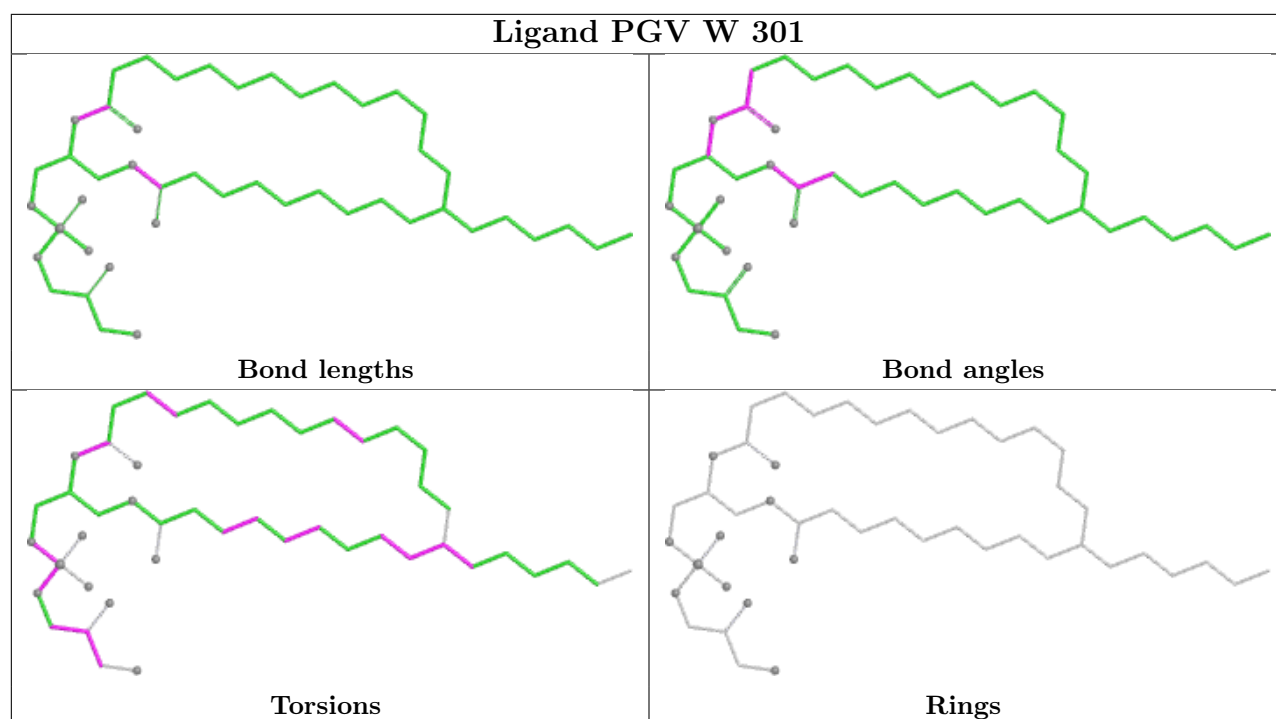
Ligand BCB 6 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

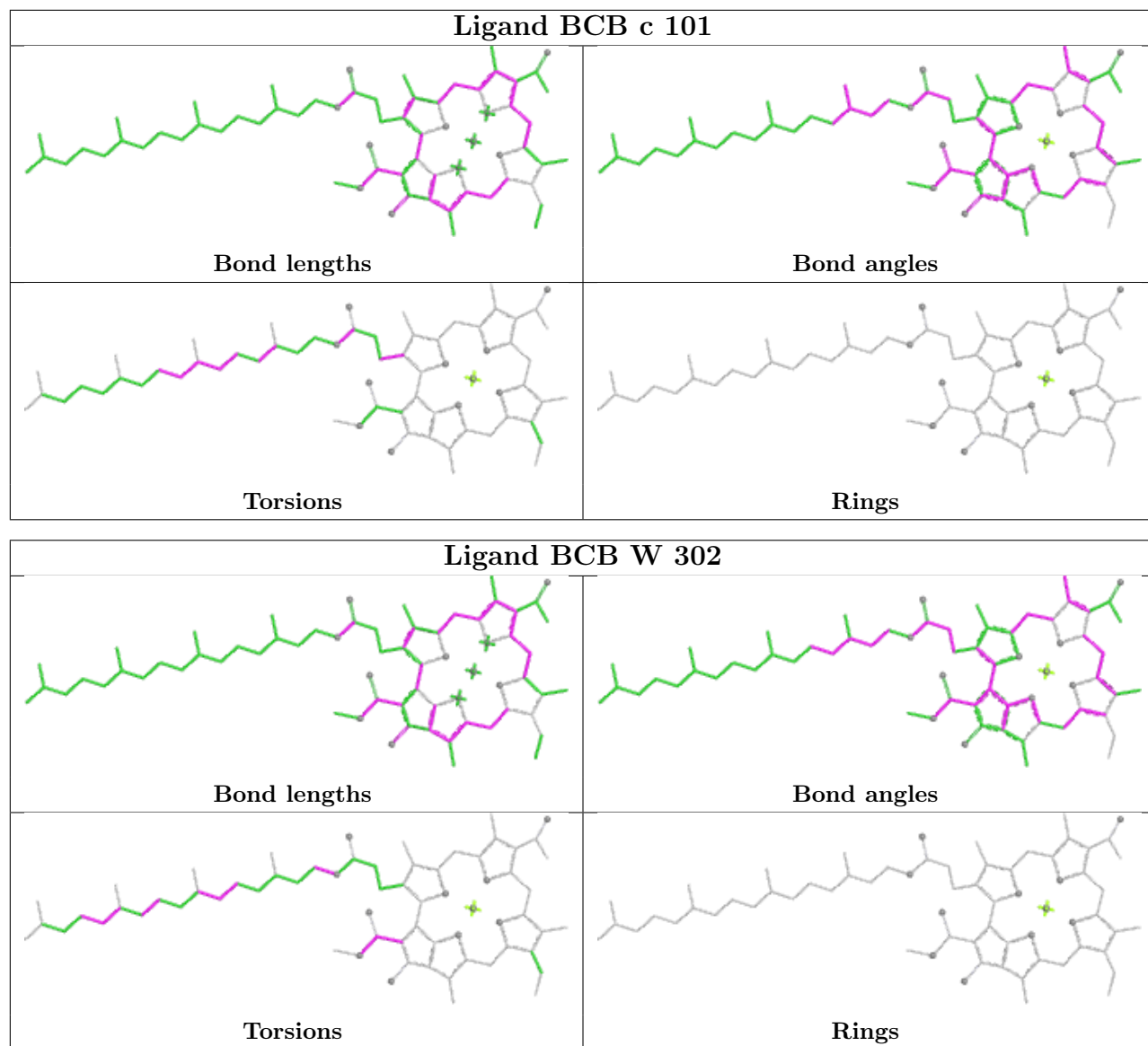
Ligand NS0 2 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

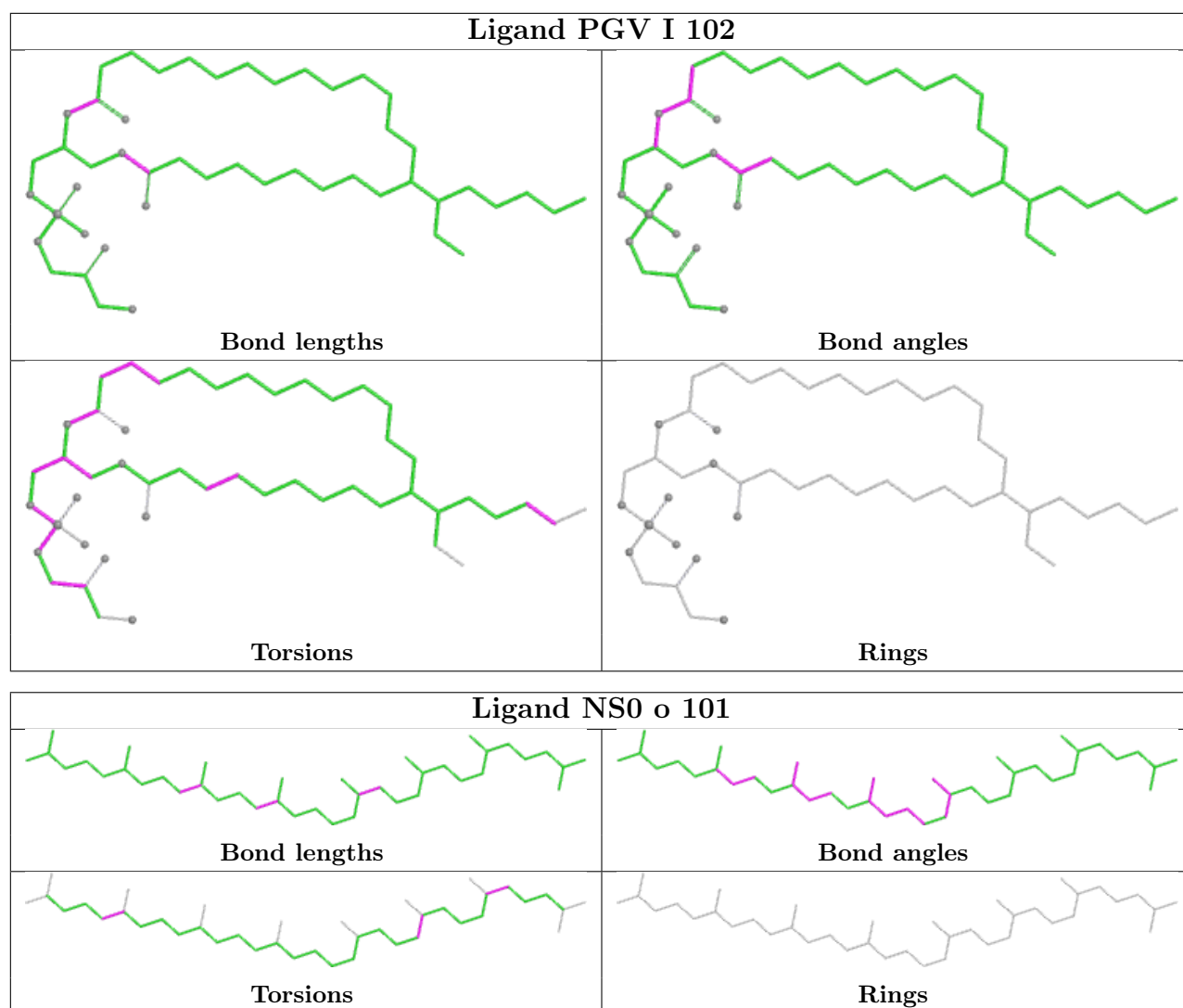


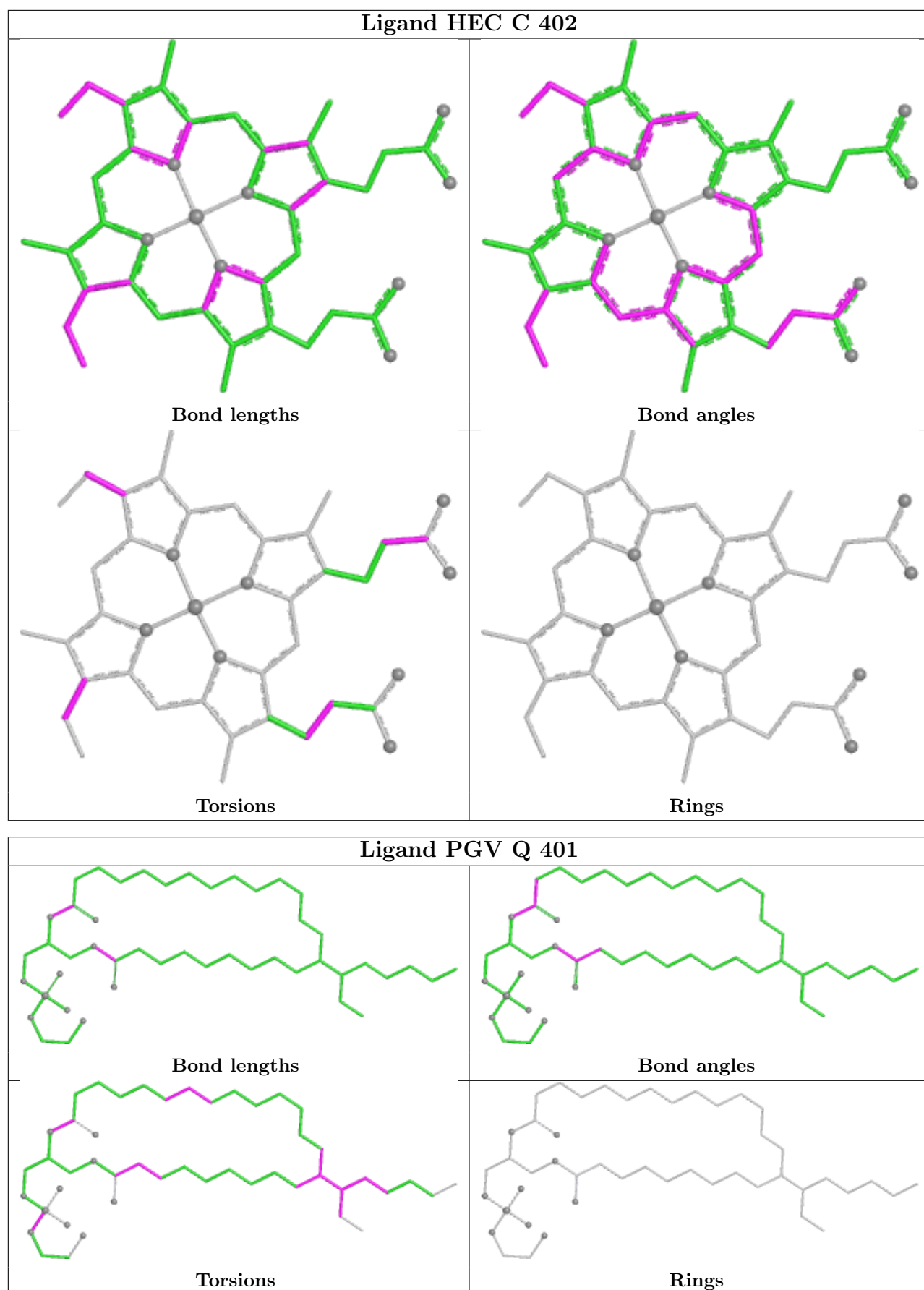


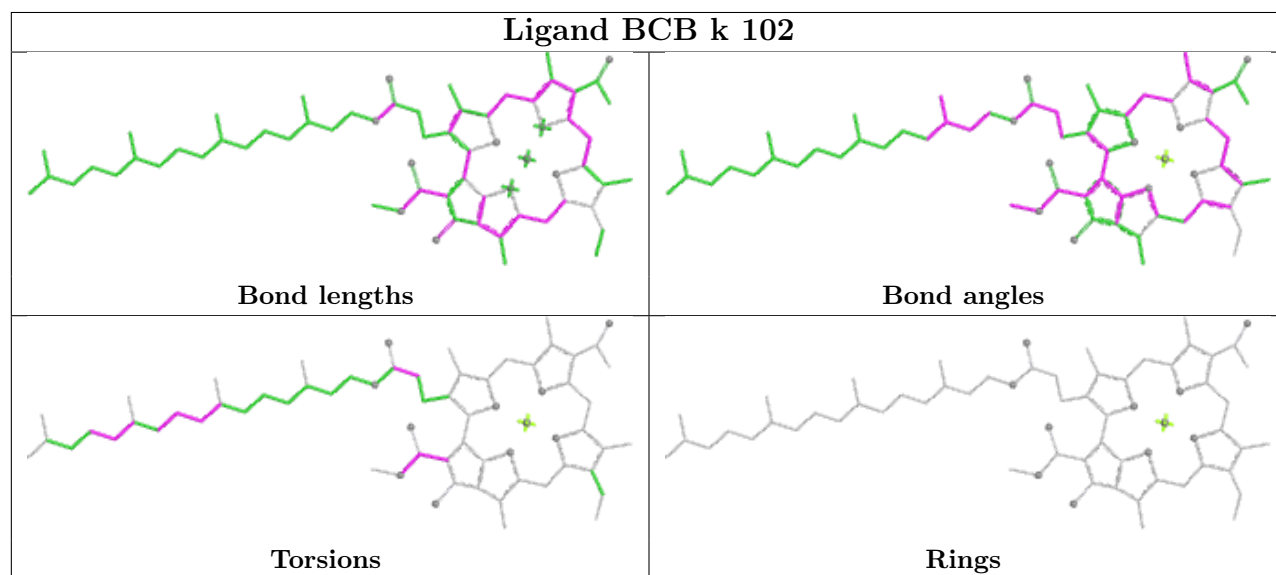
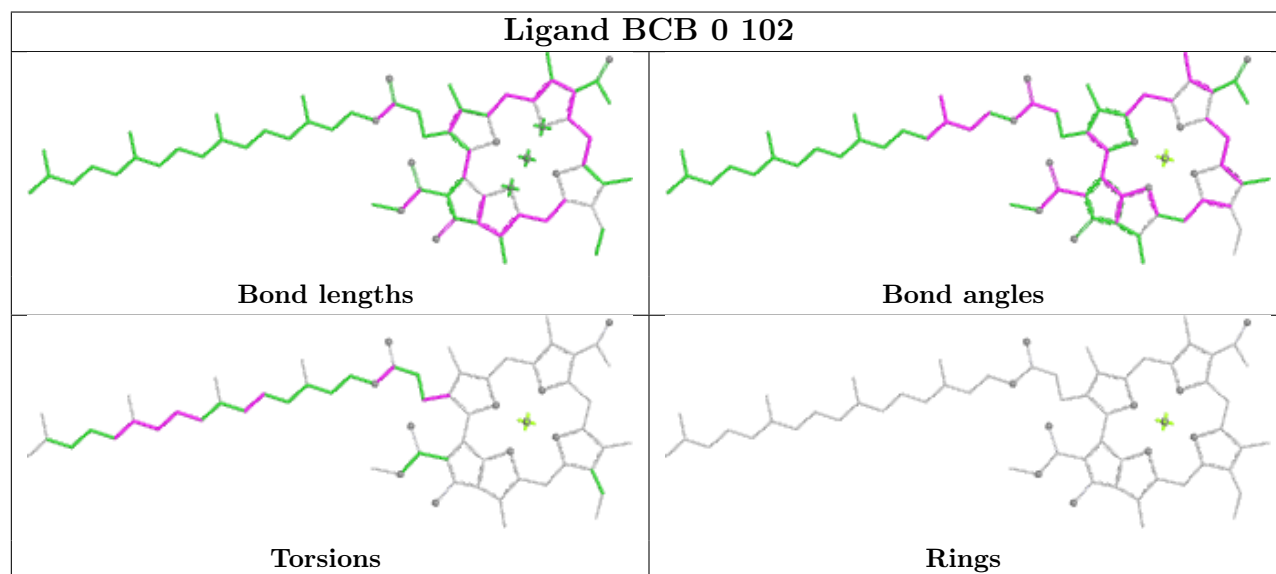
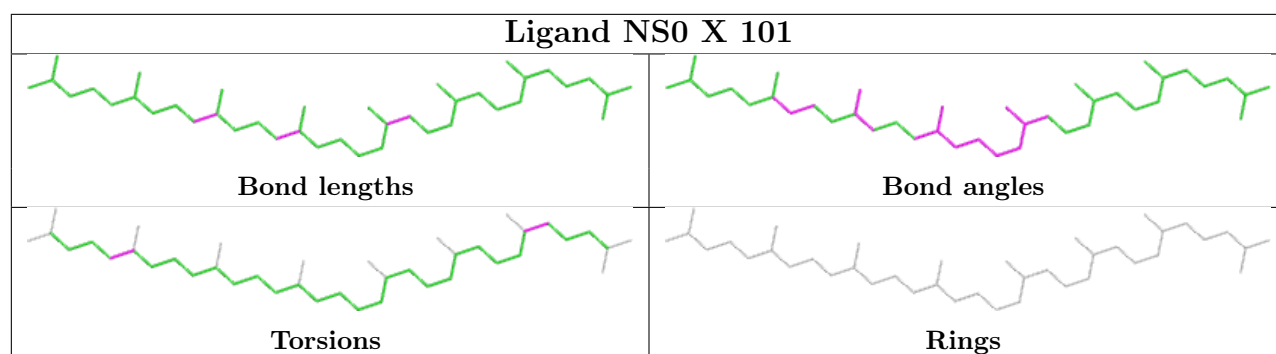


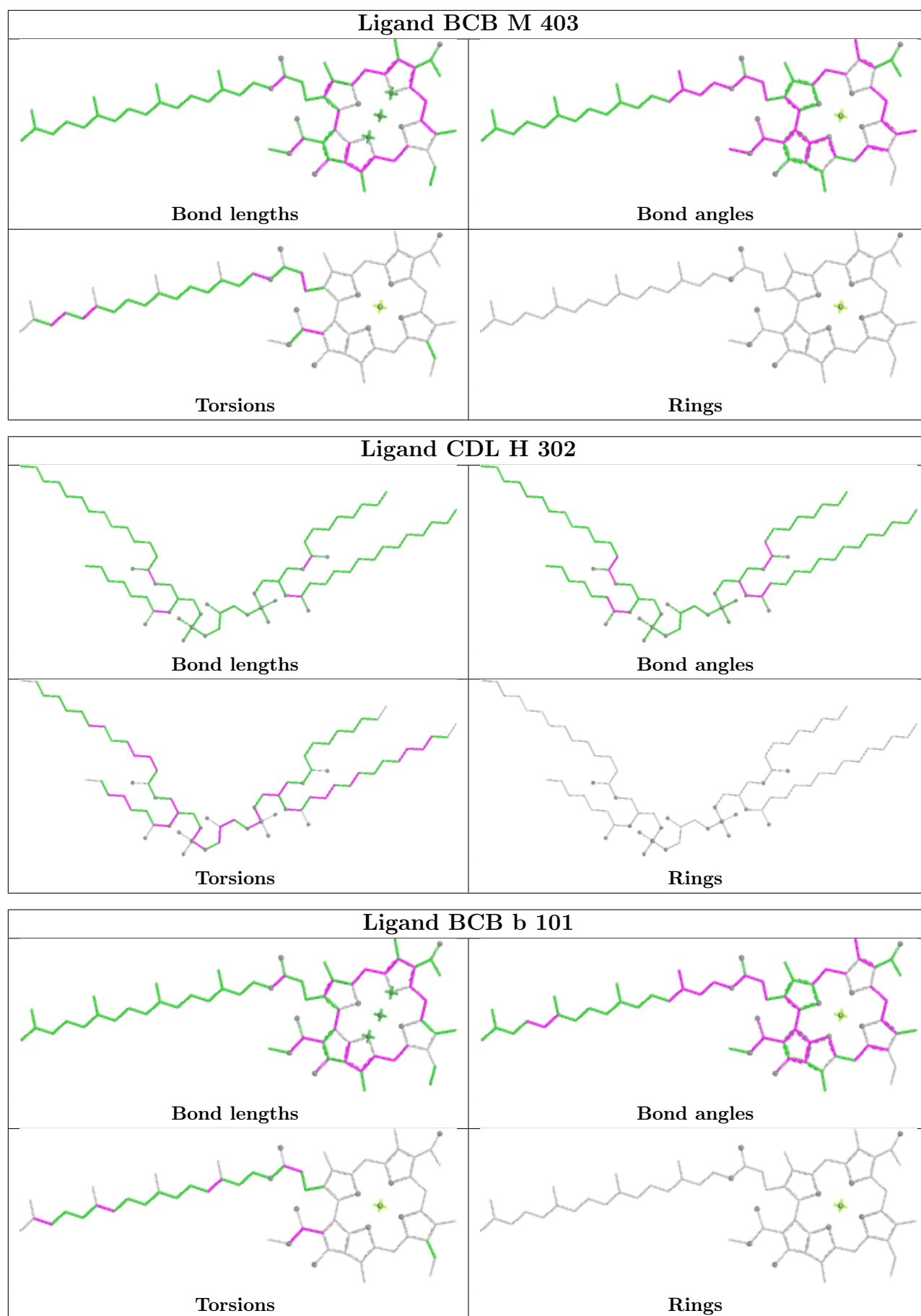


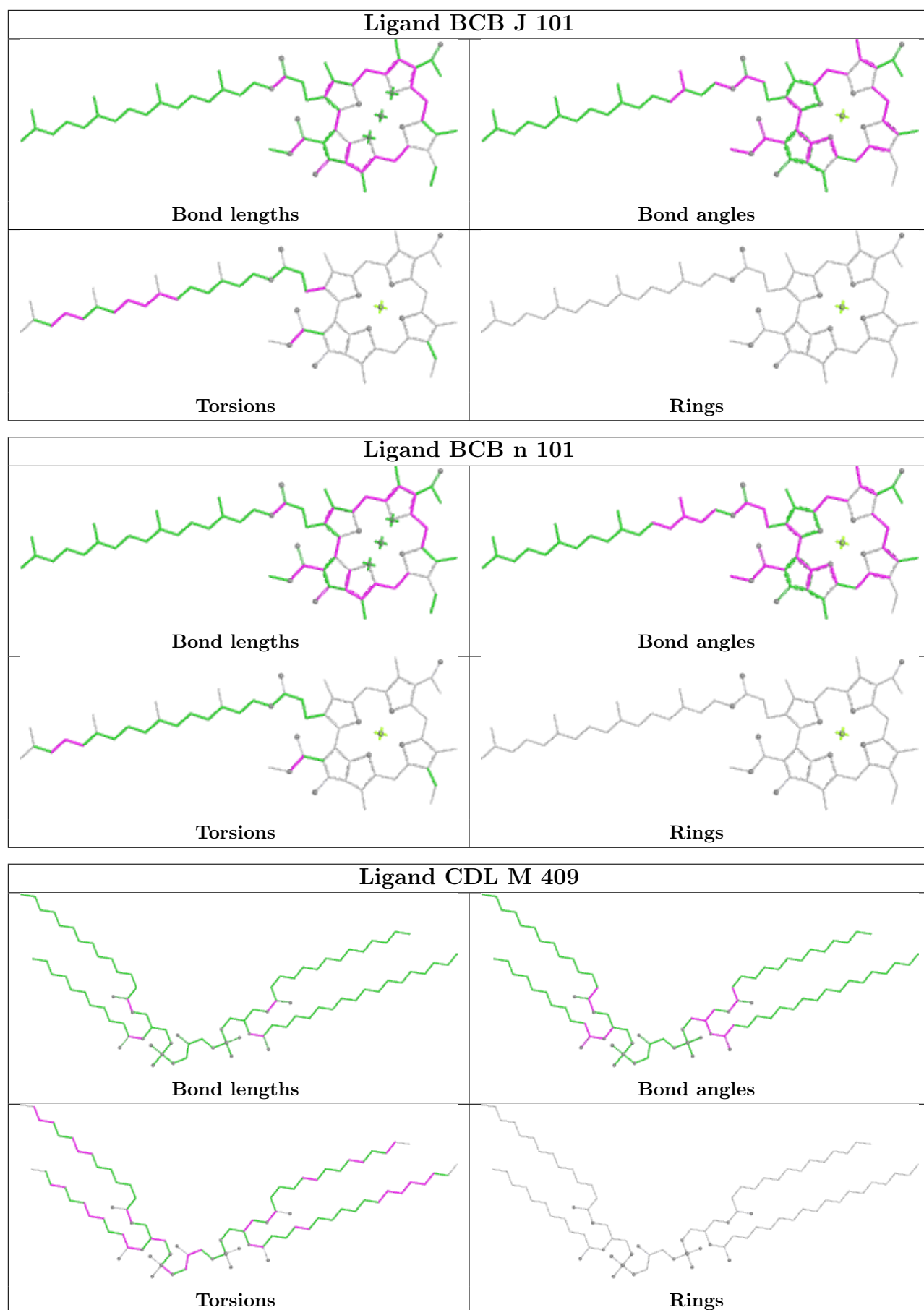


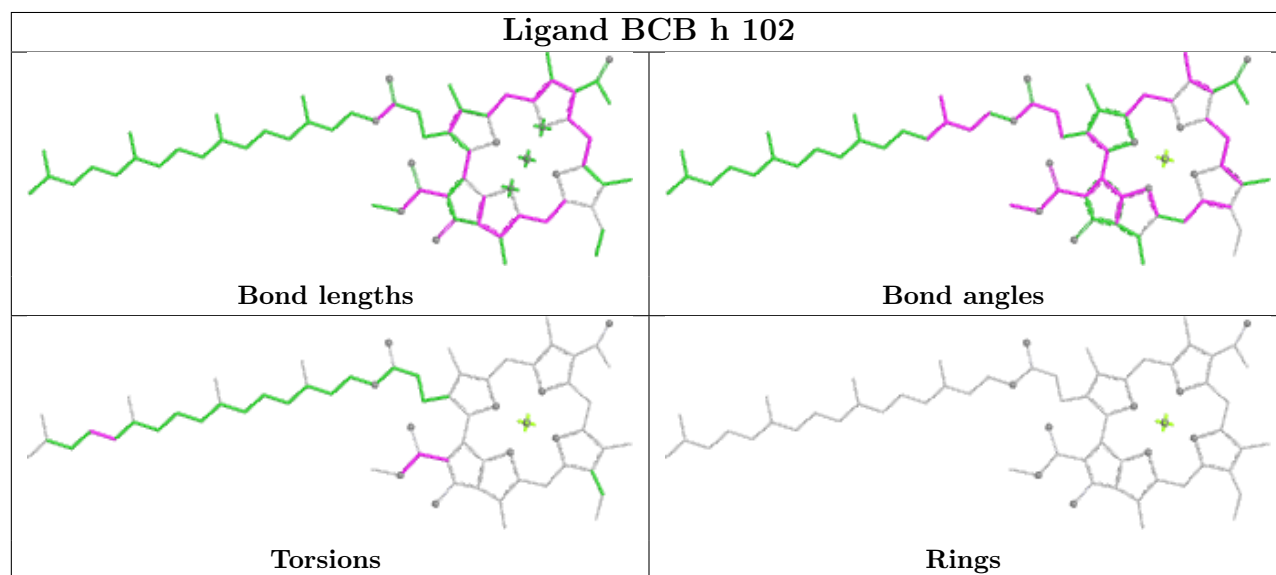
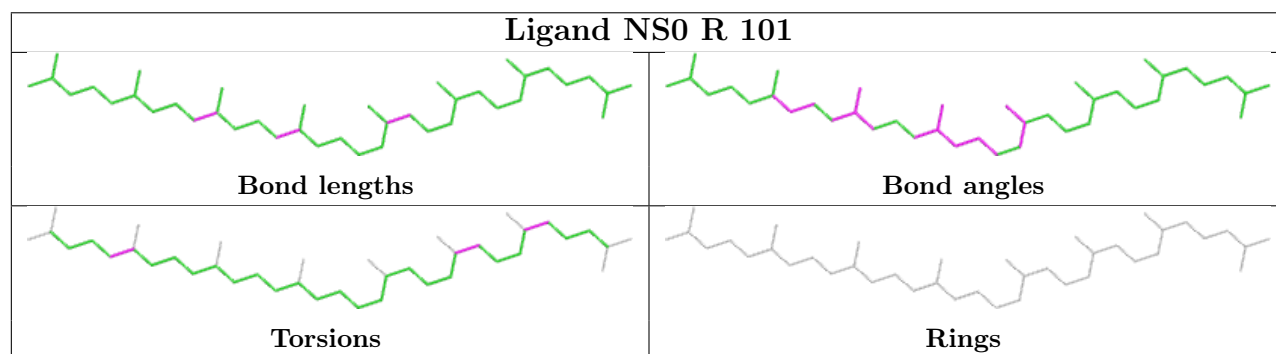
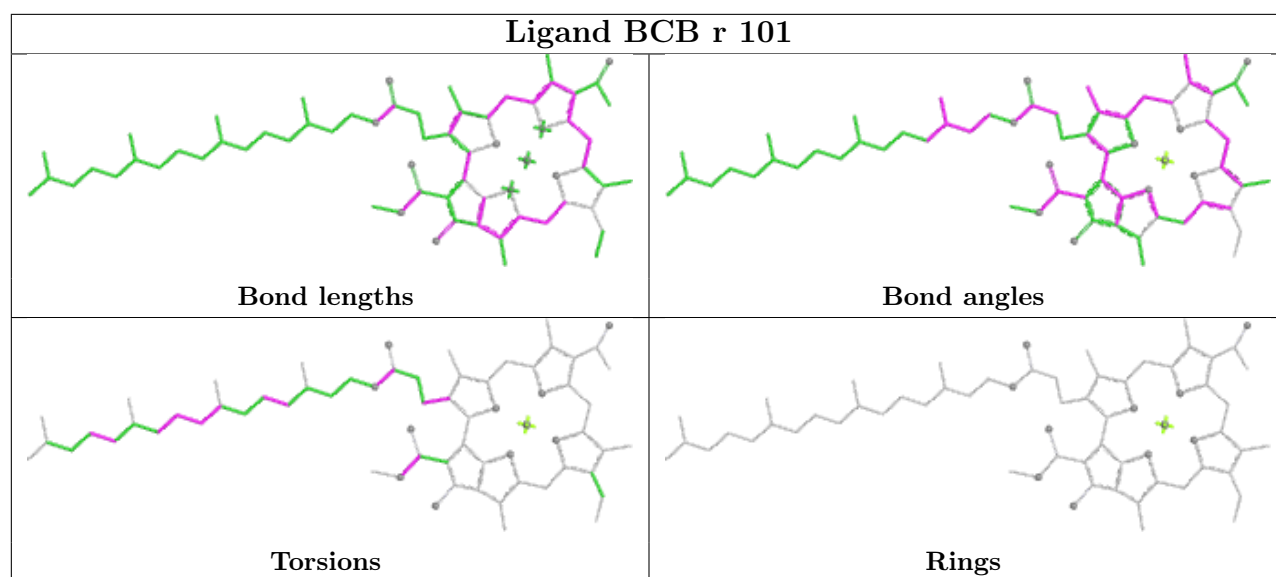


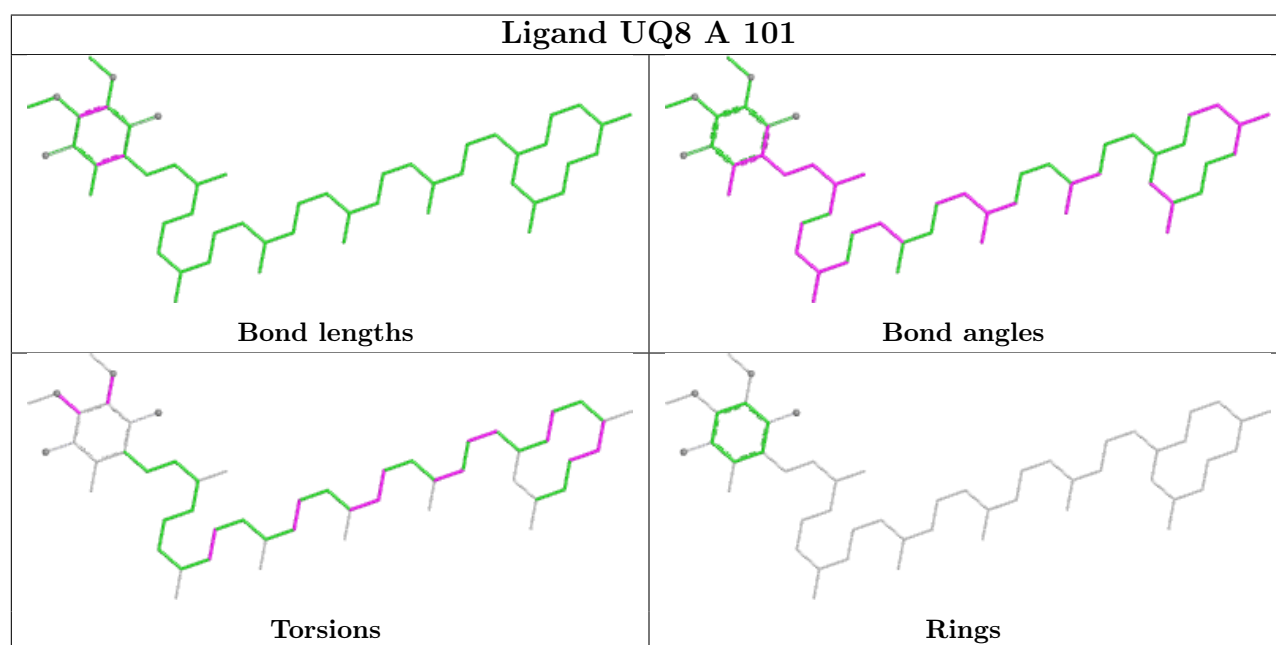
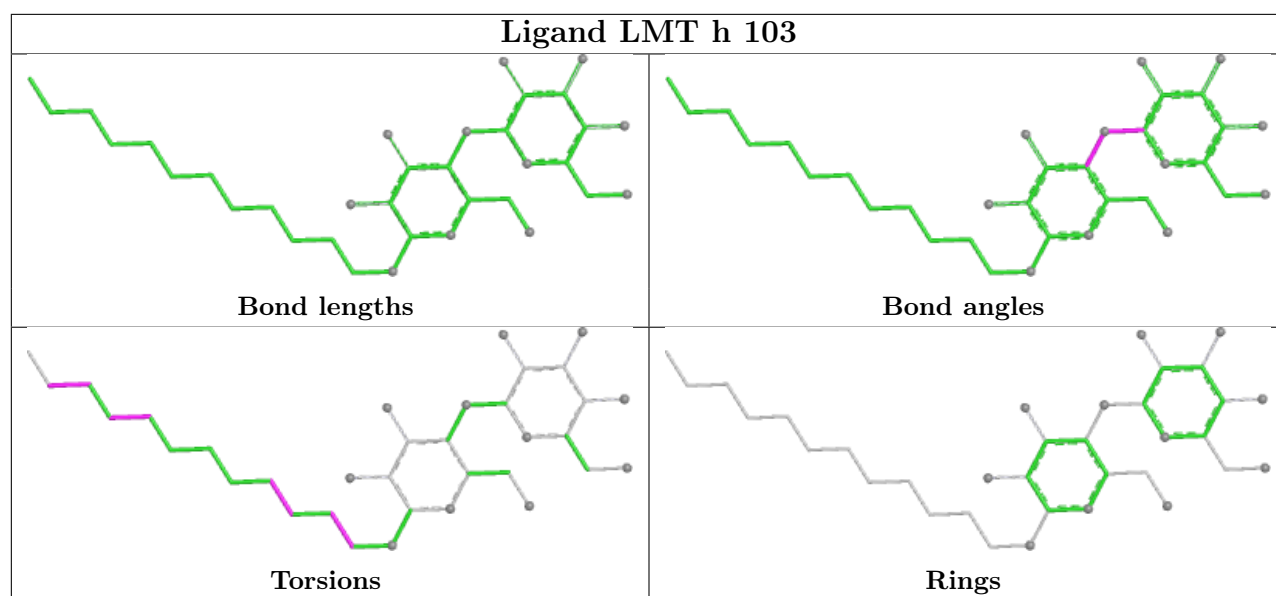


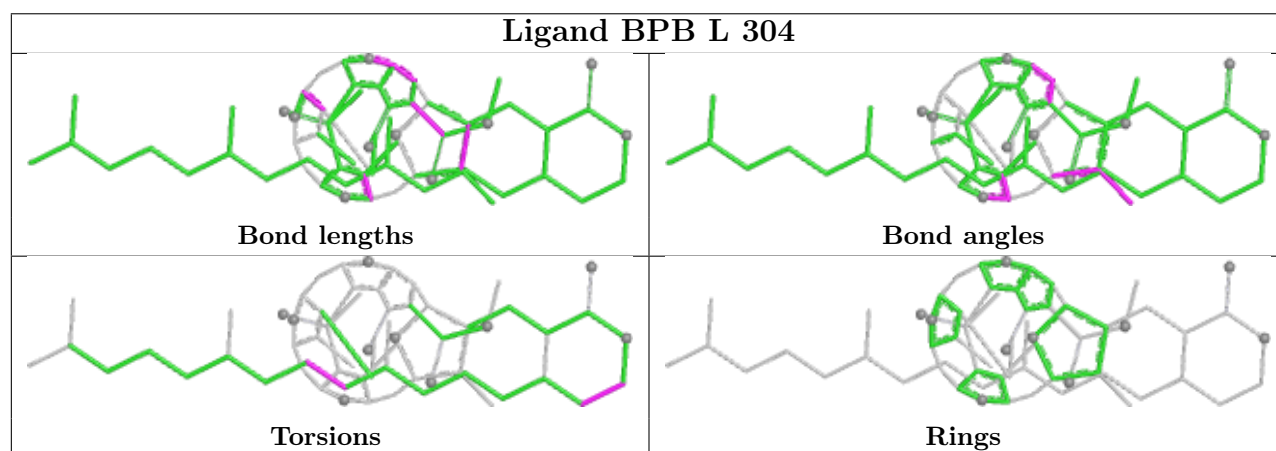
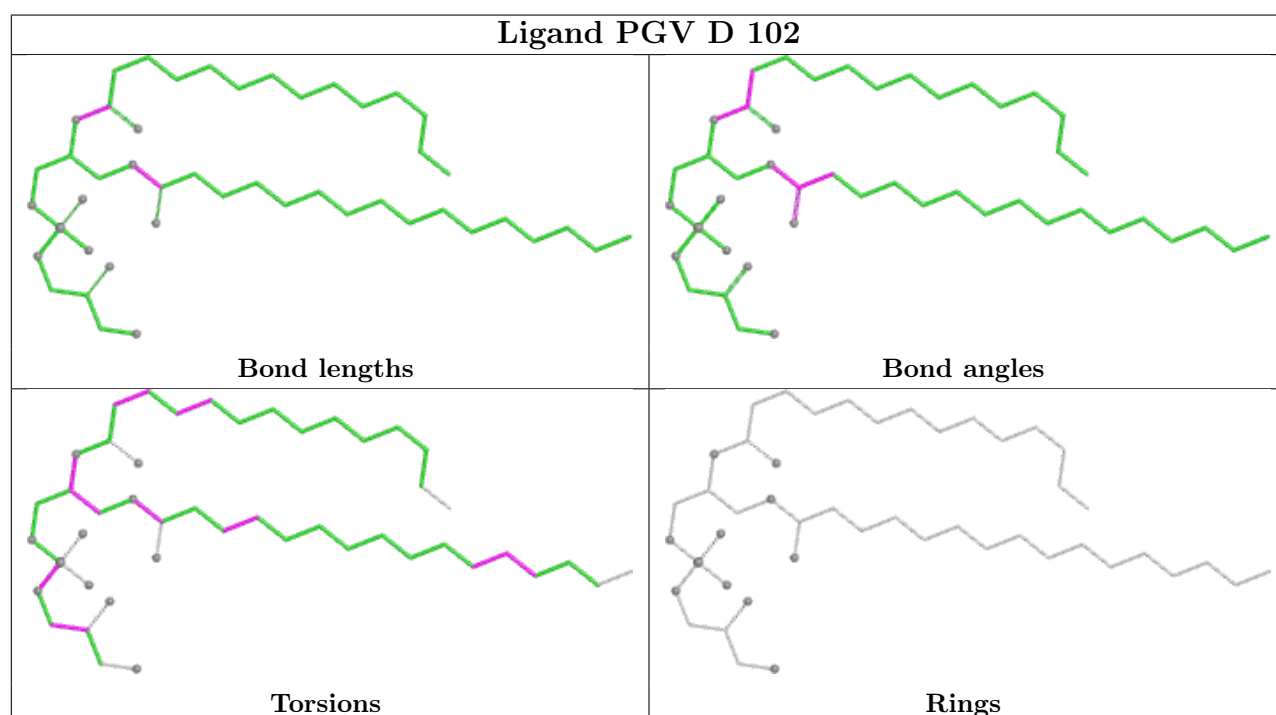
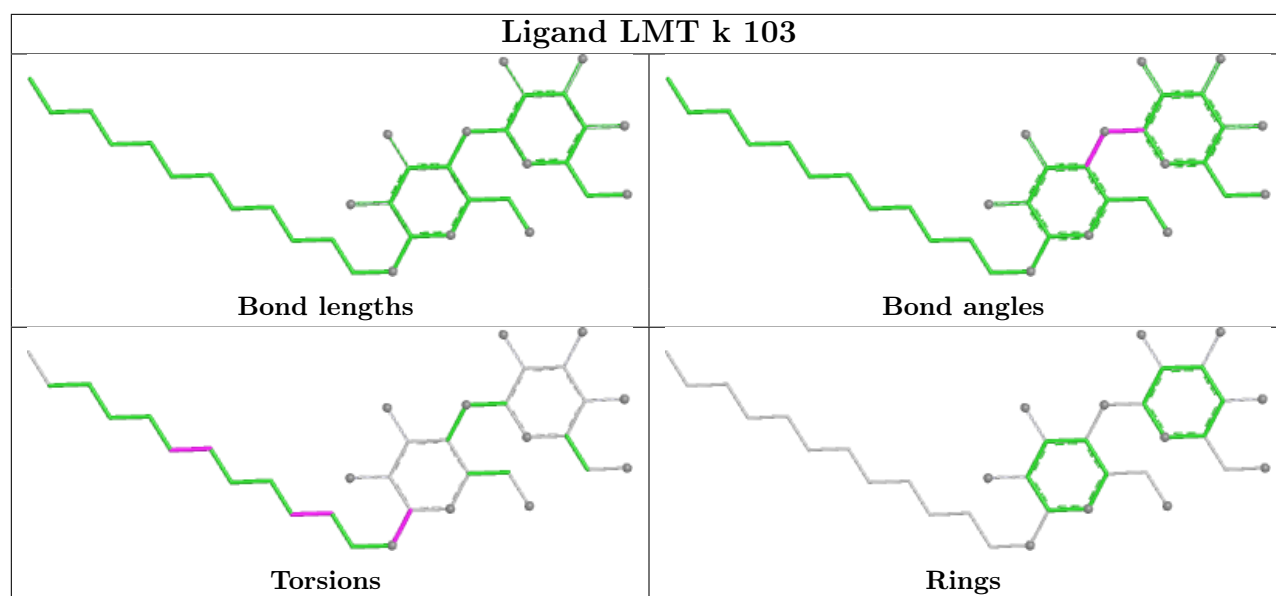


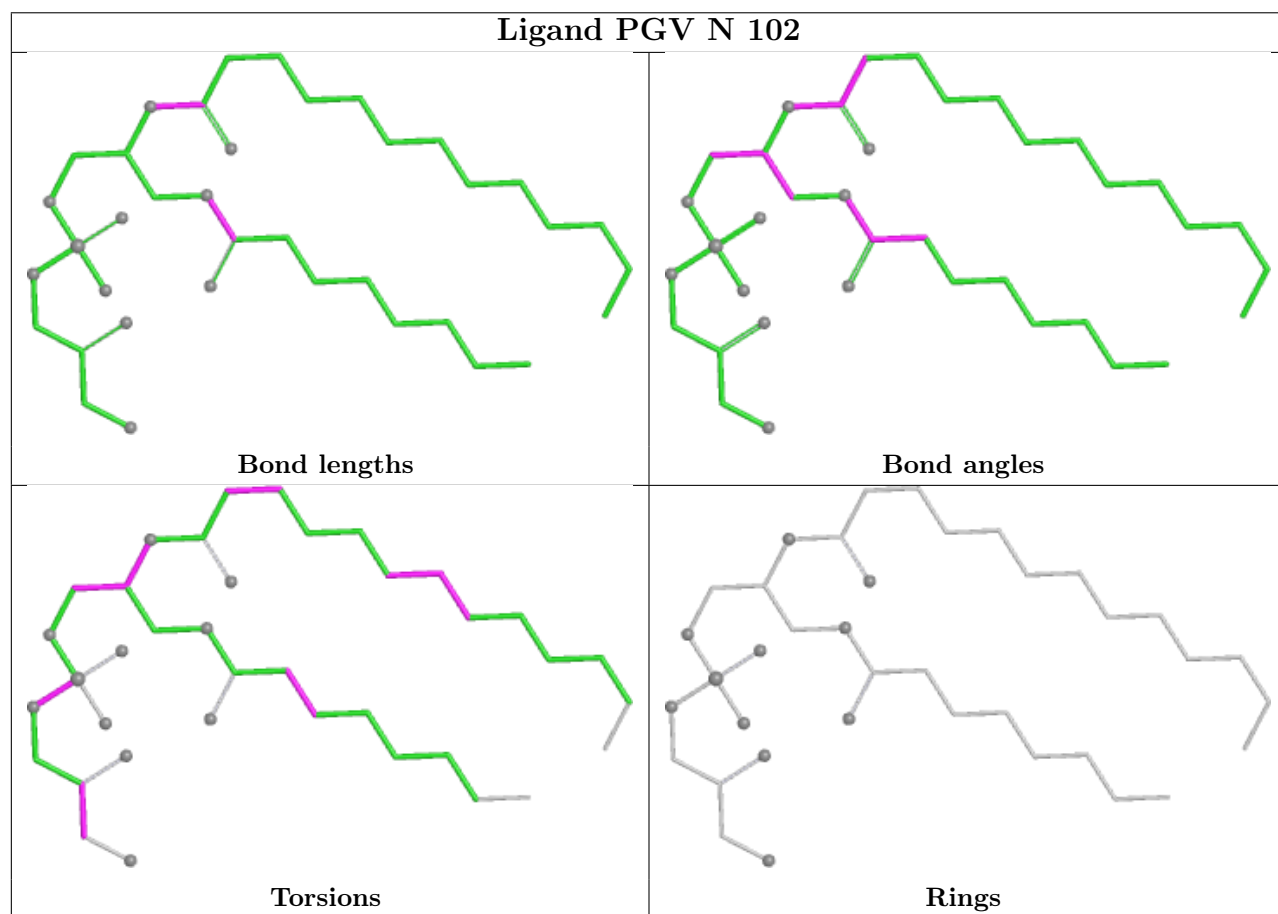
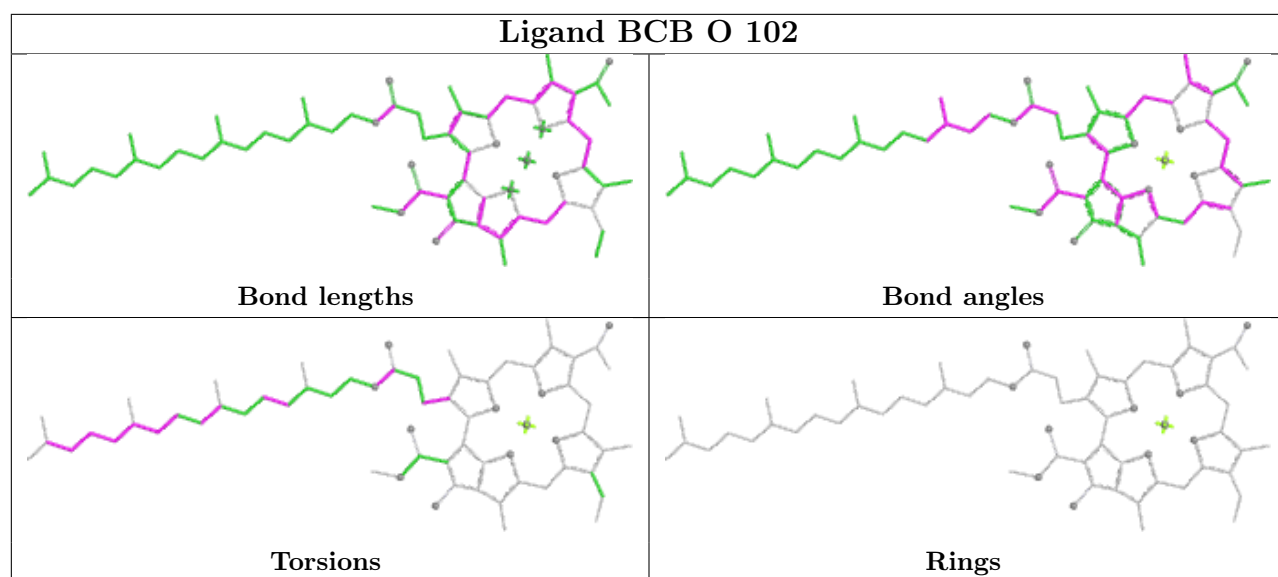


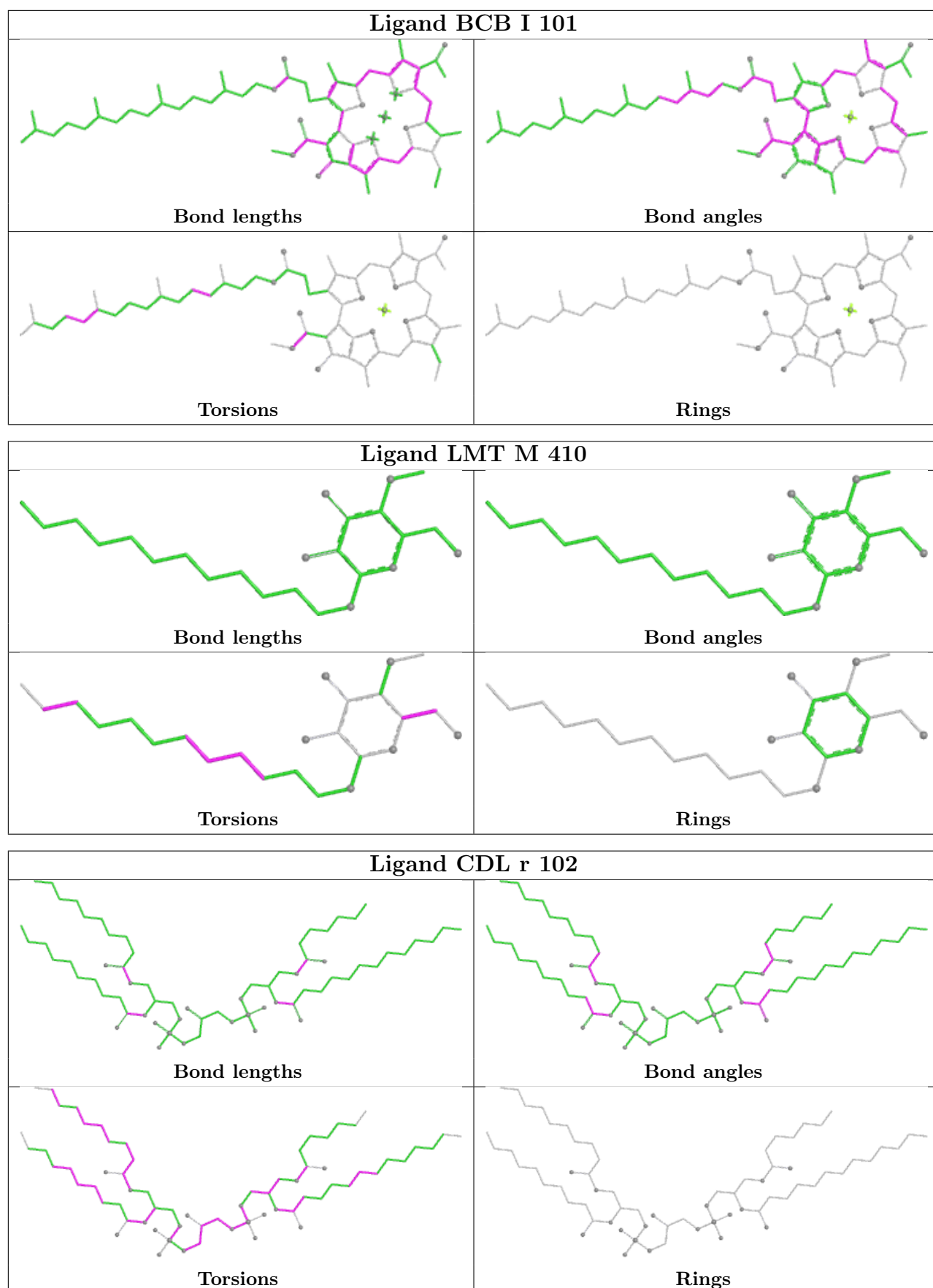


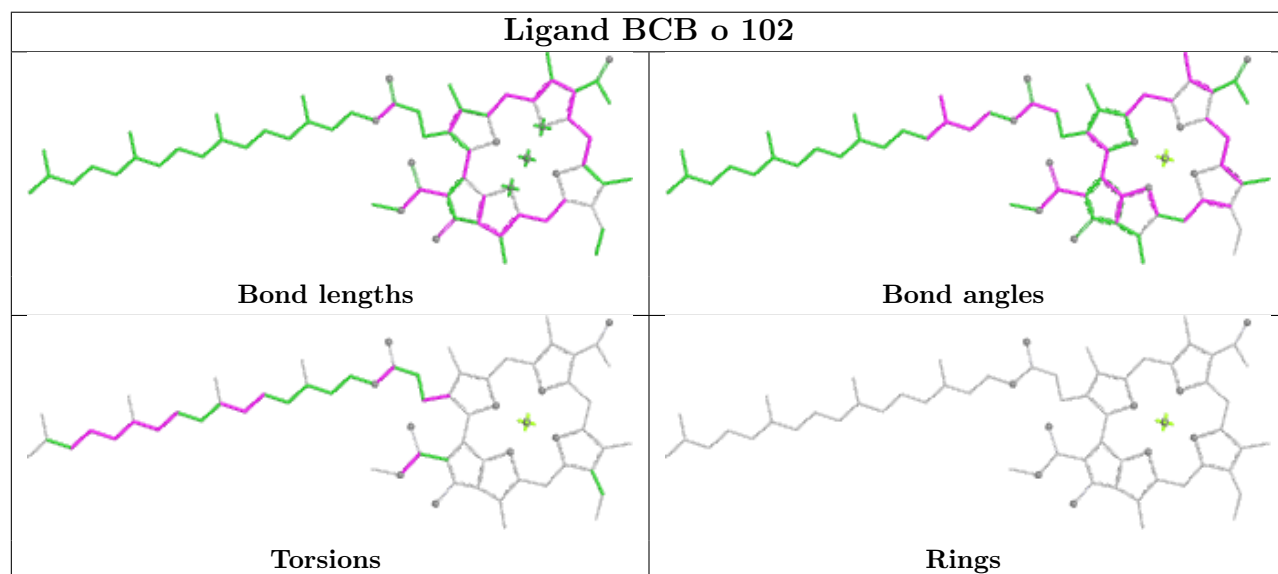
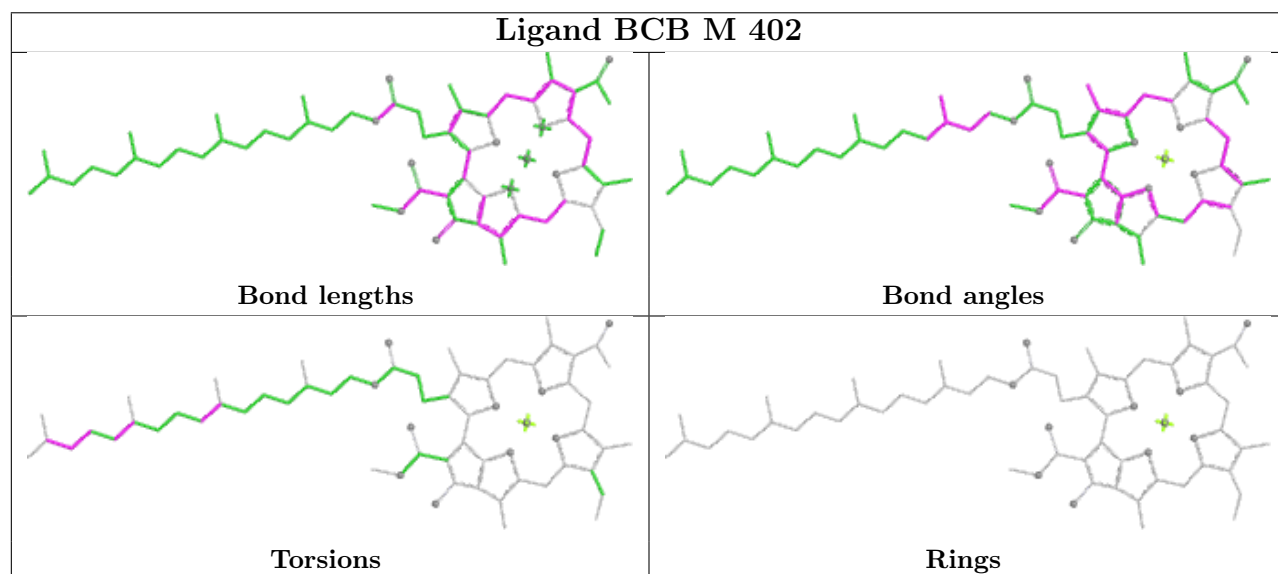
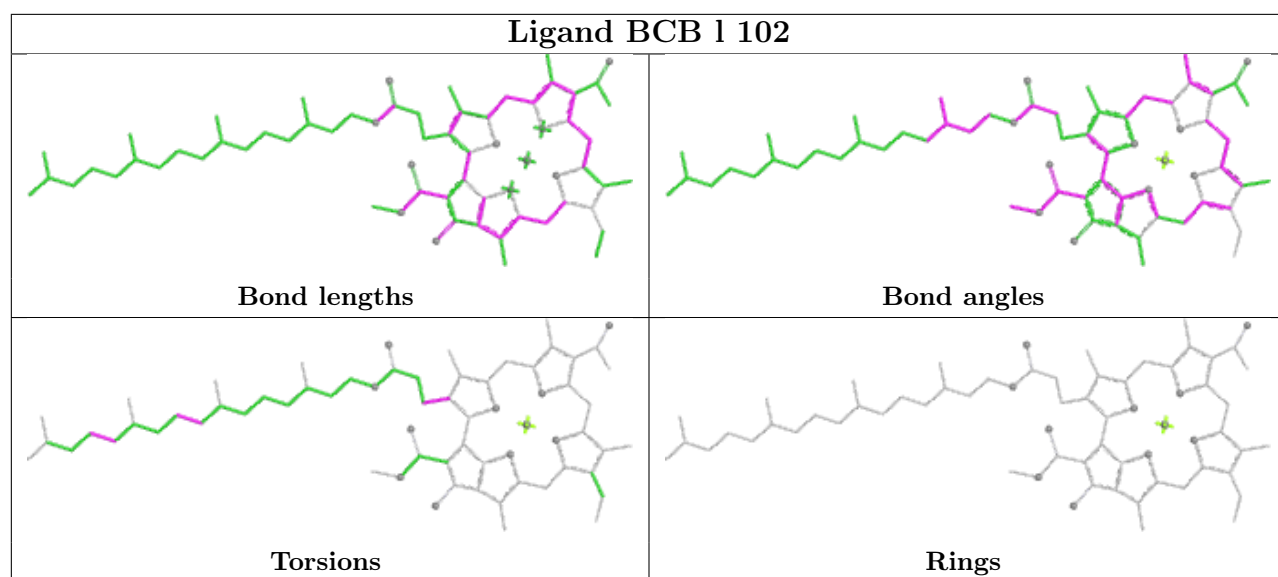


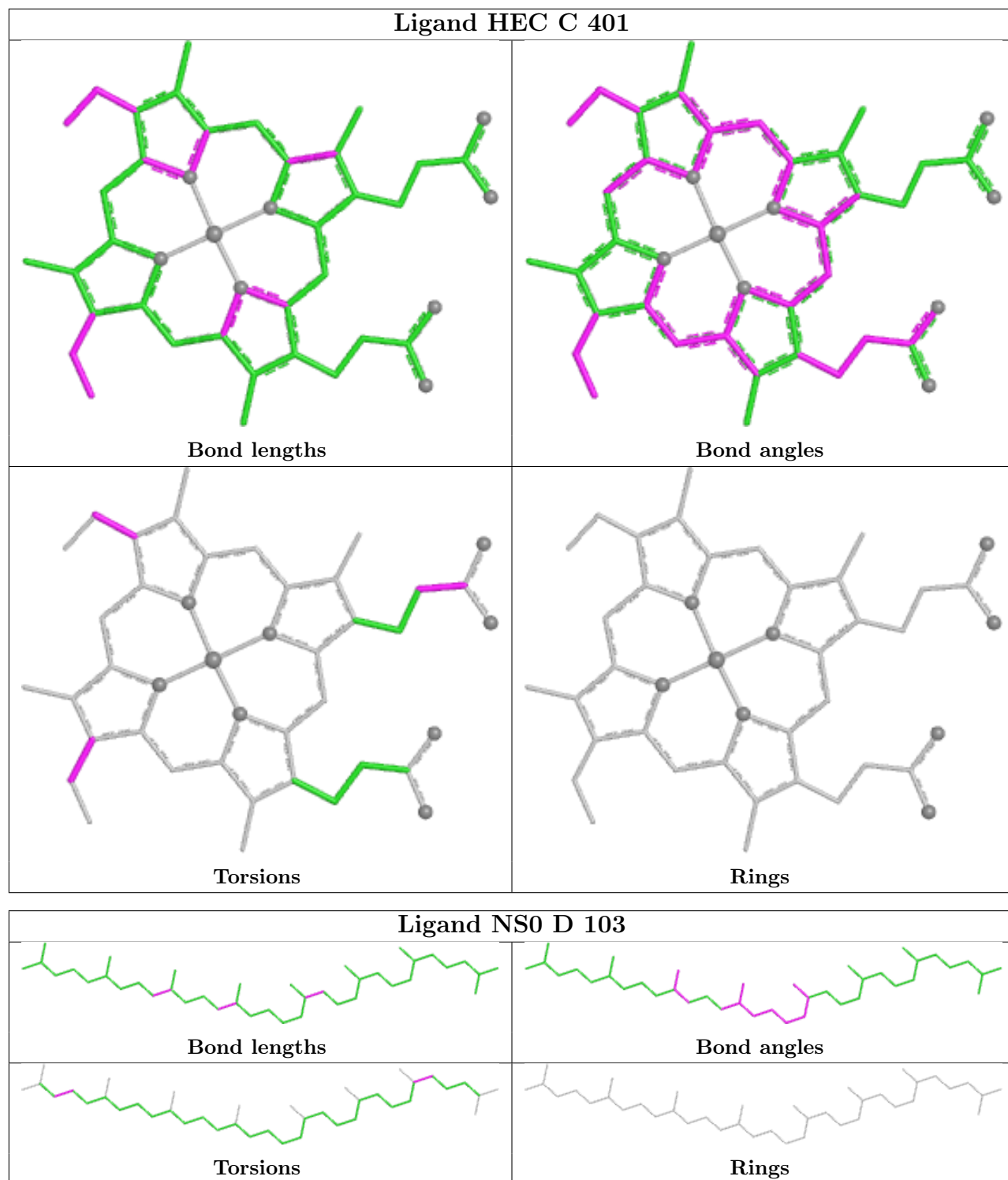


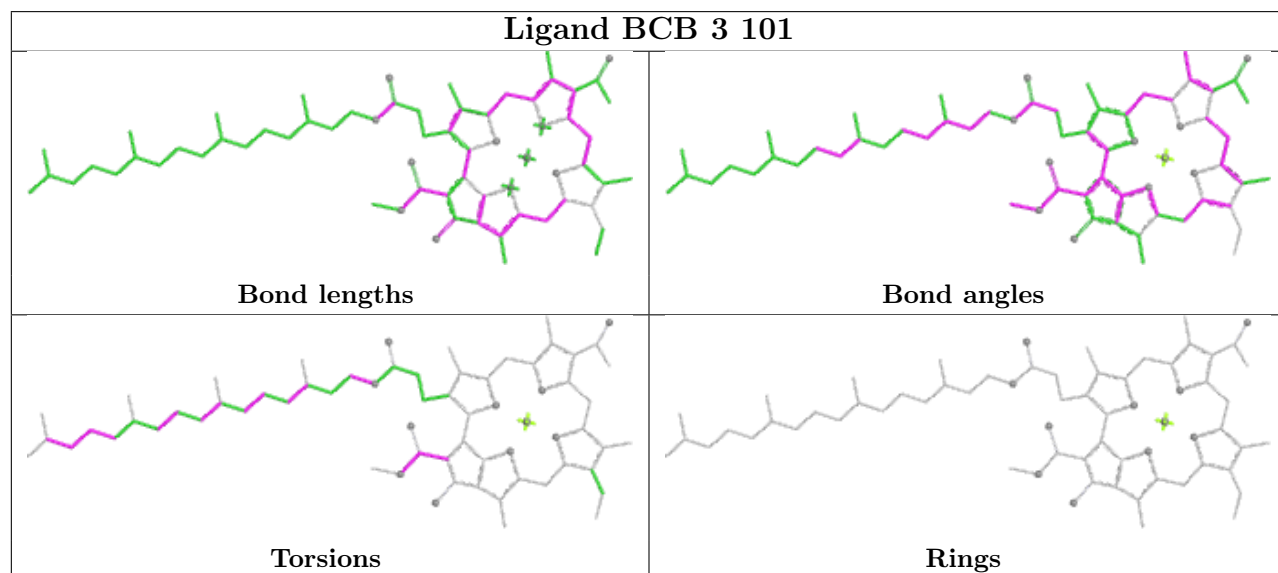
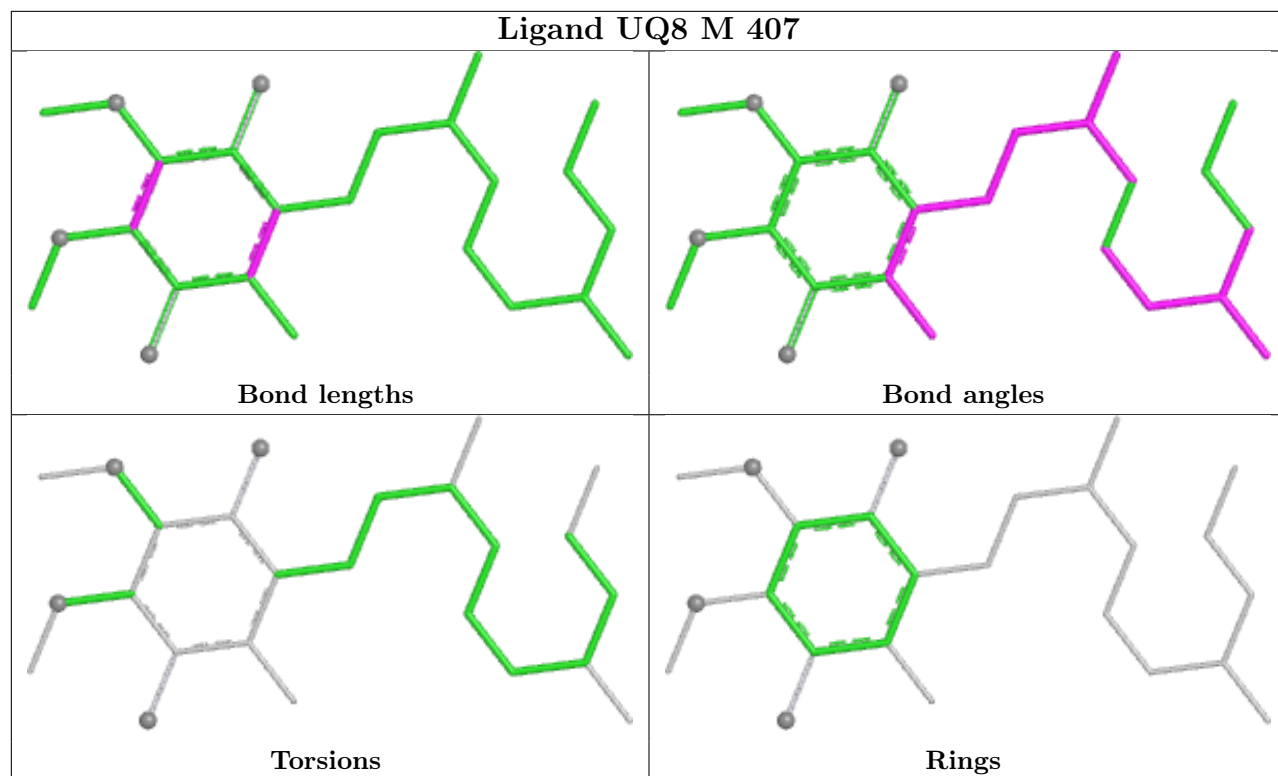


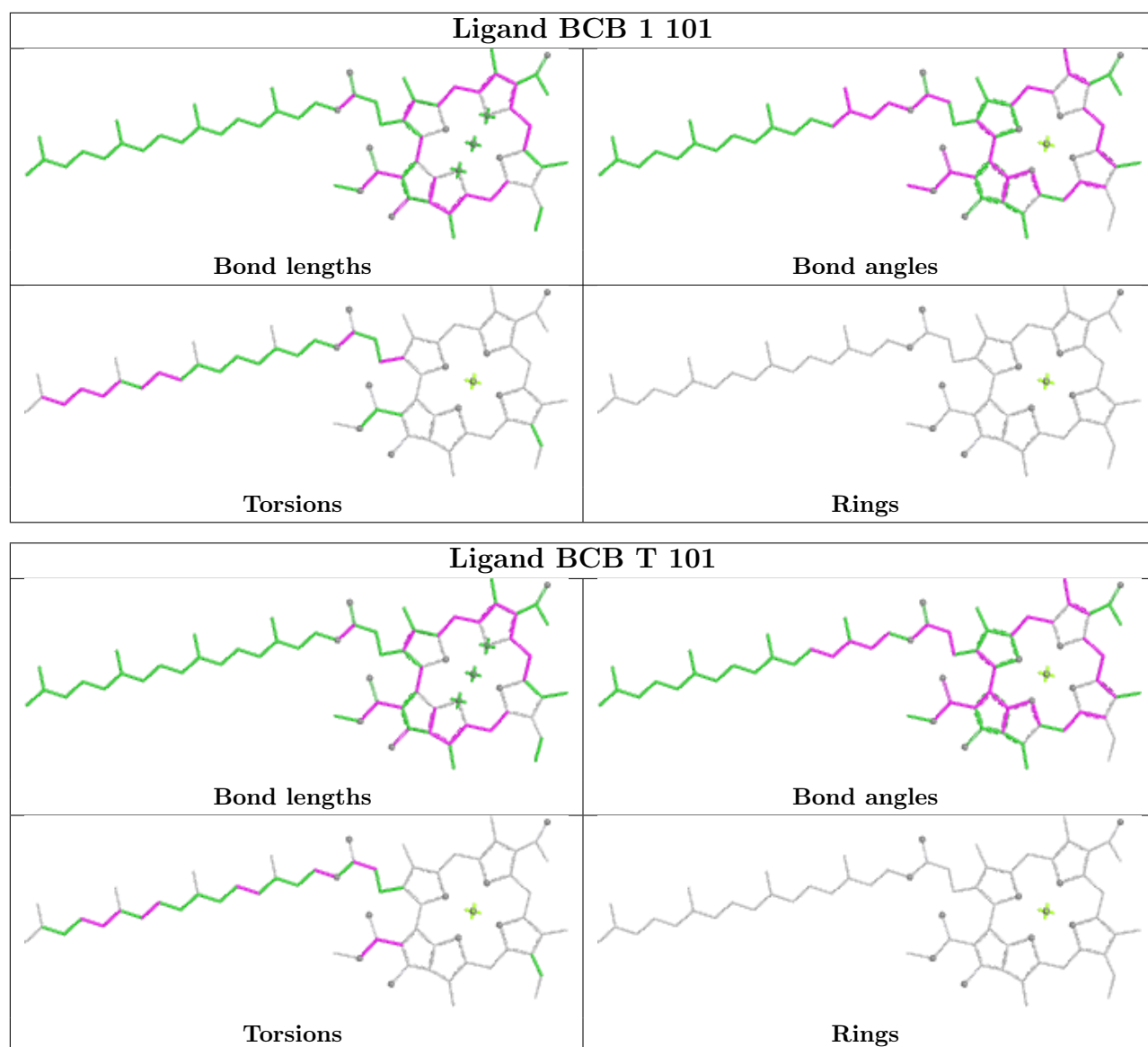


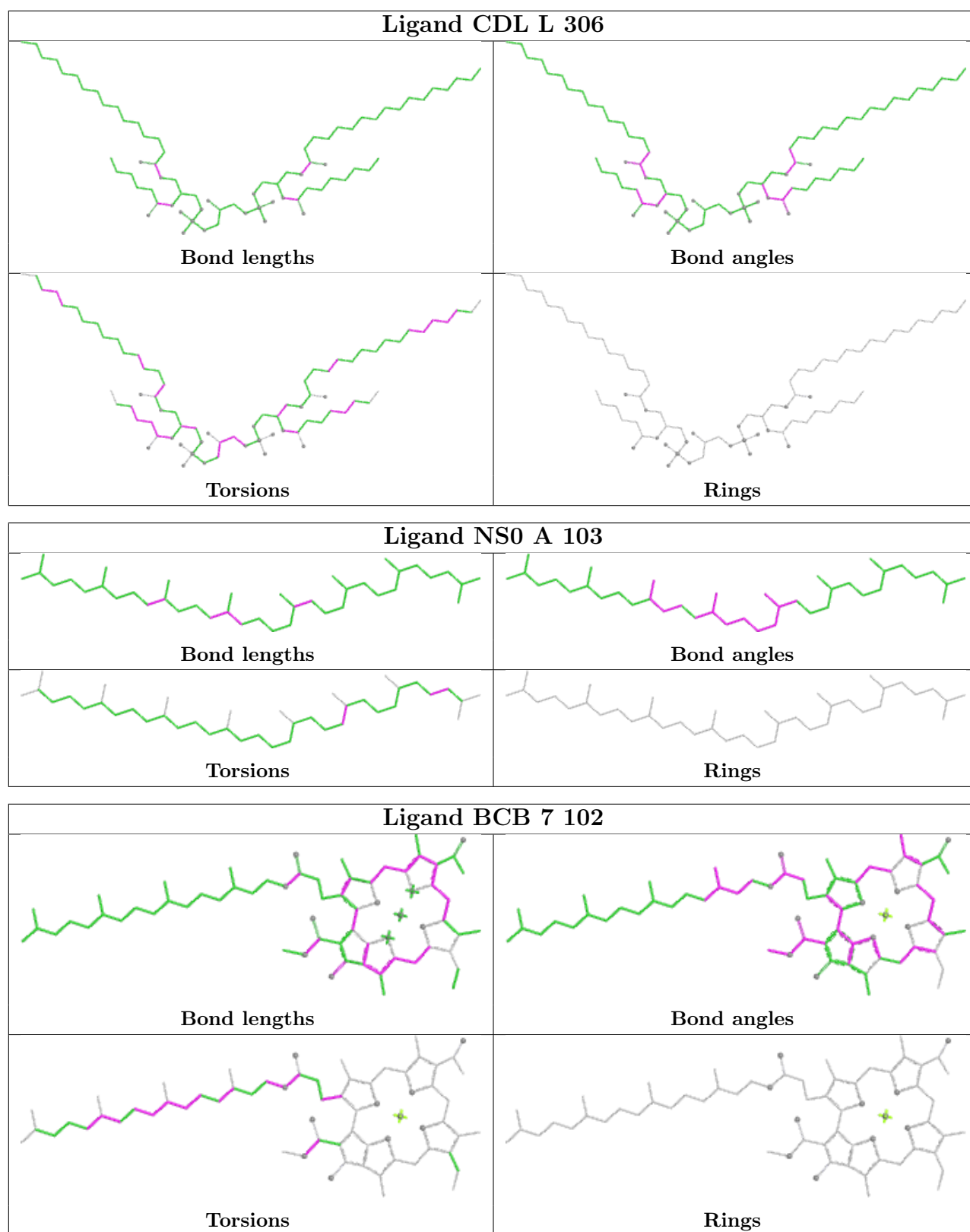


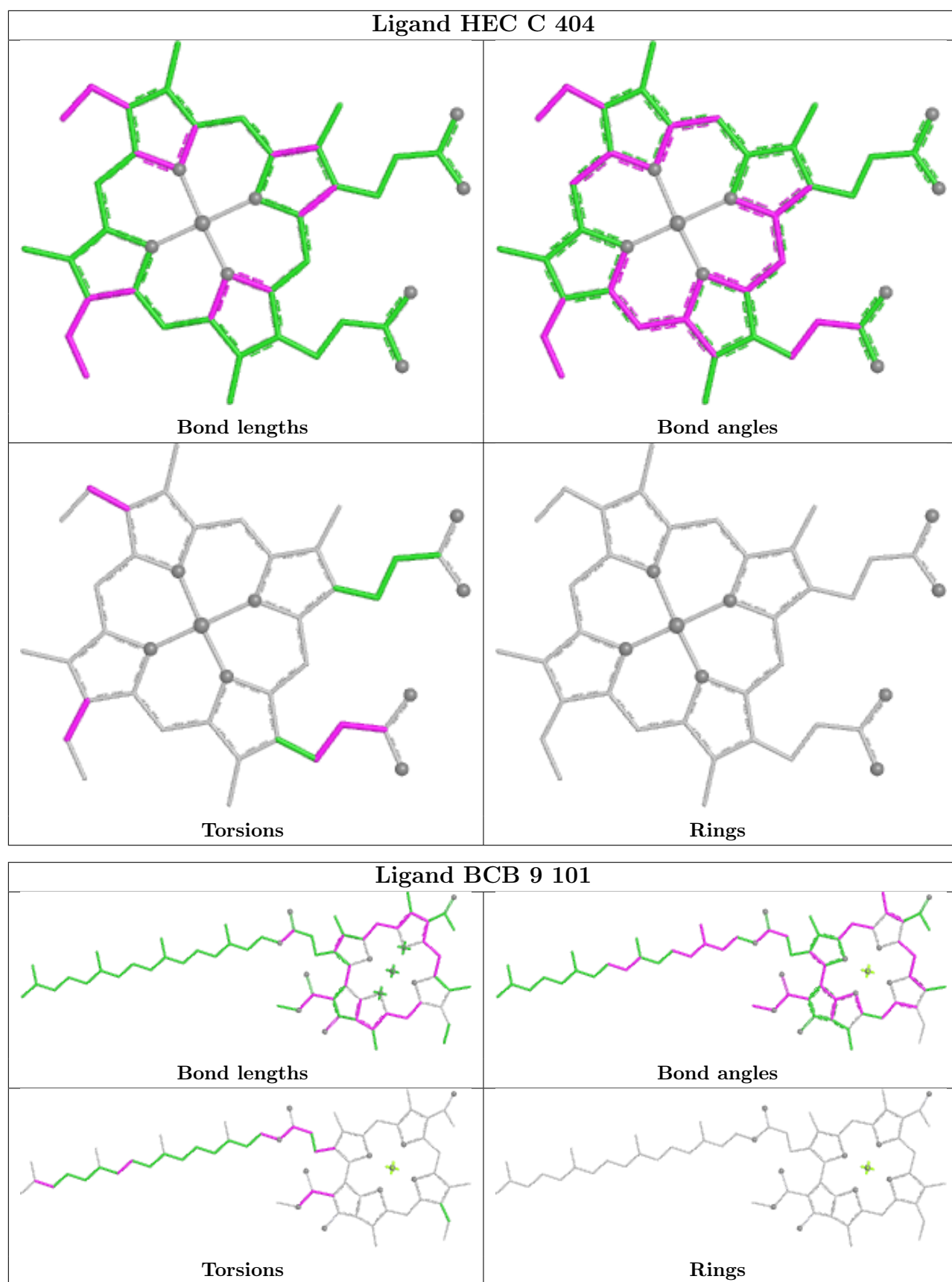


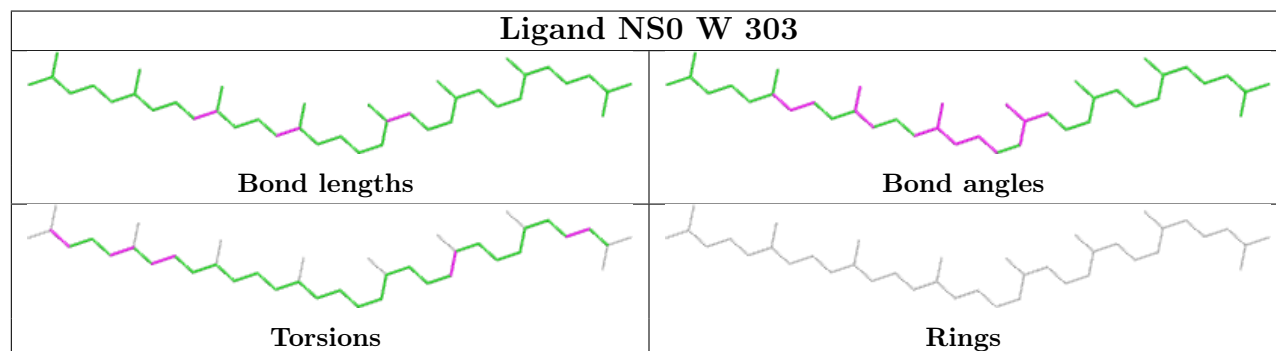
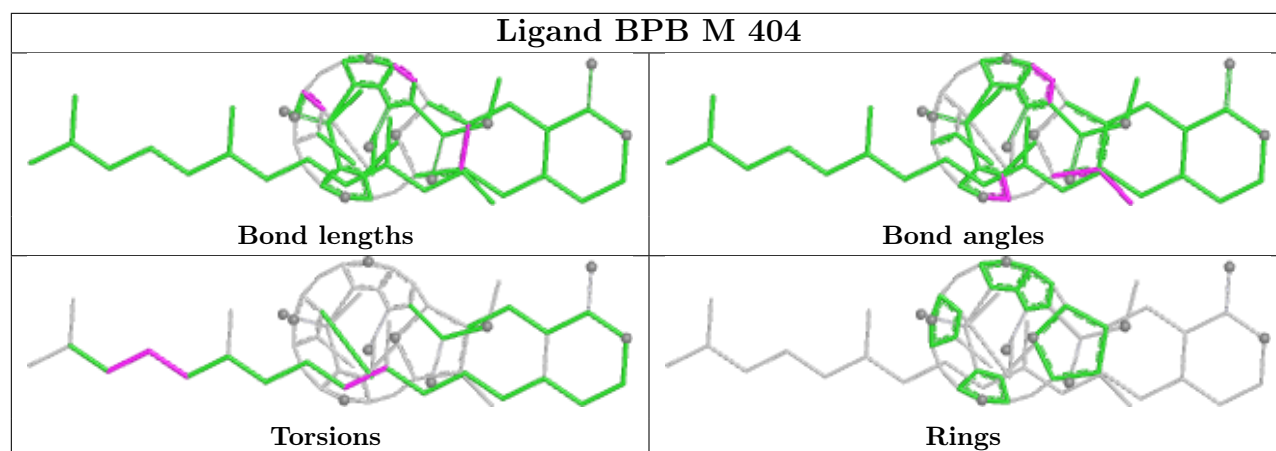
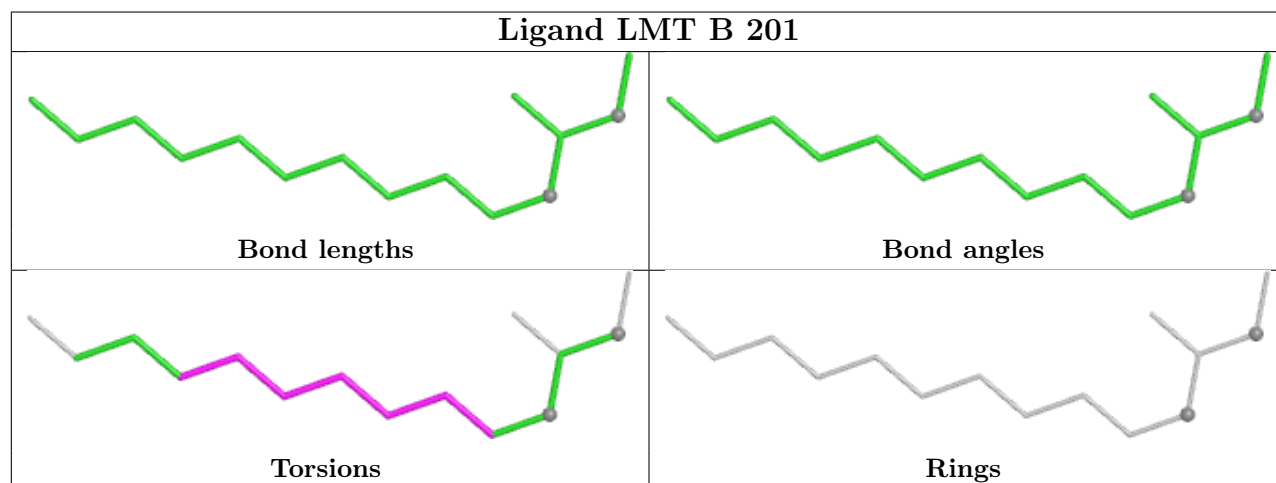
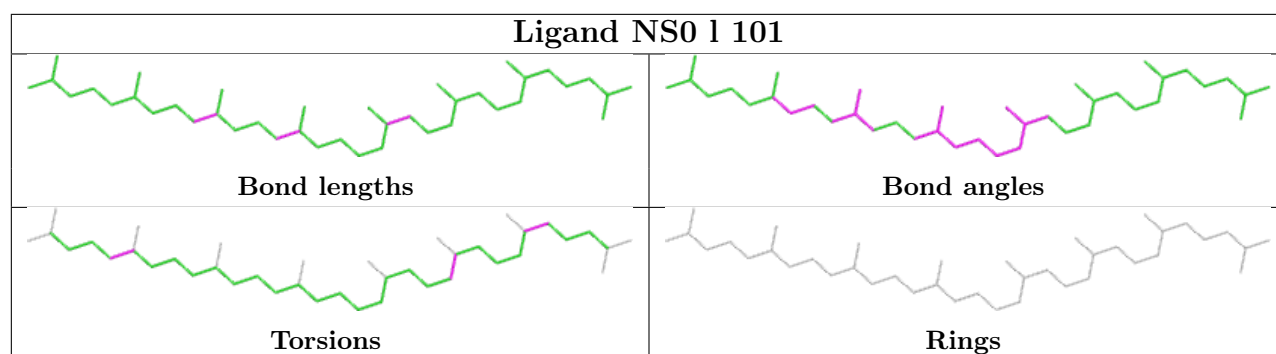


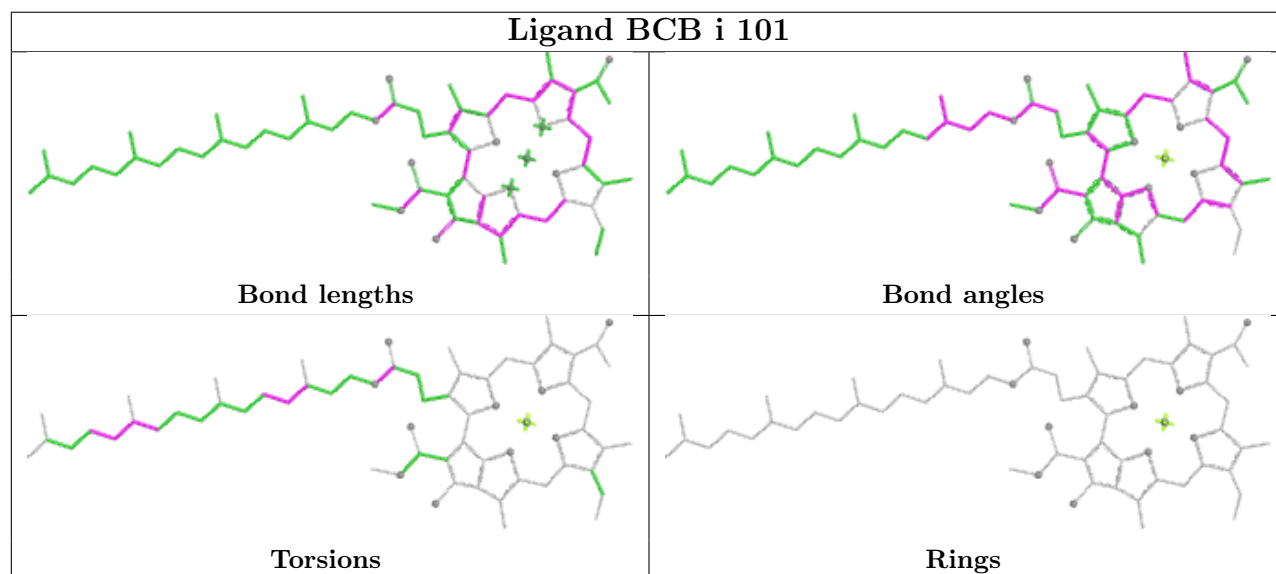
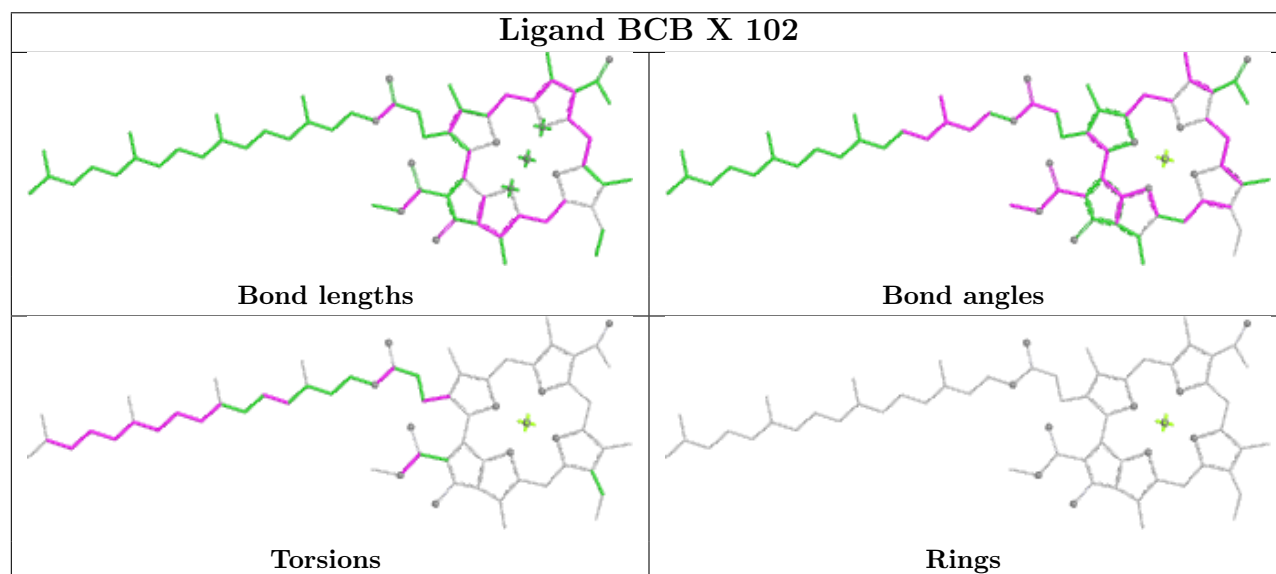
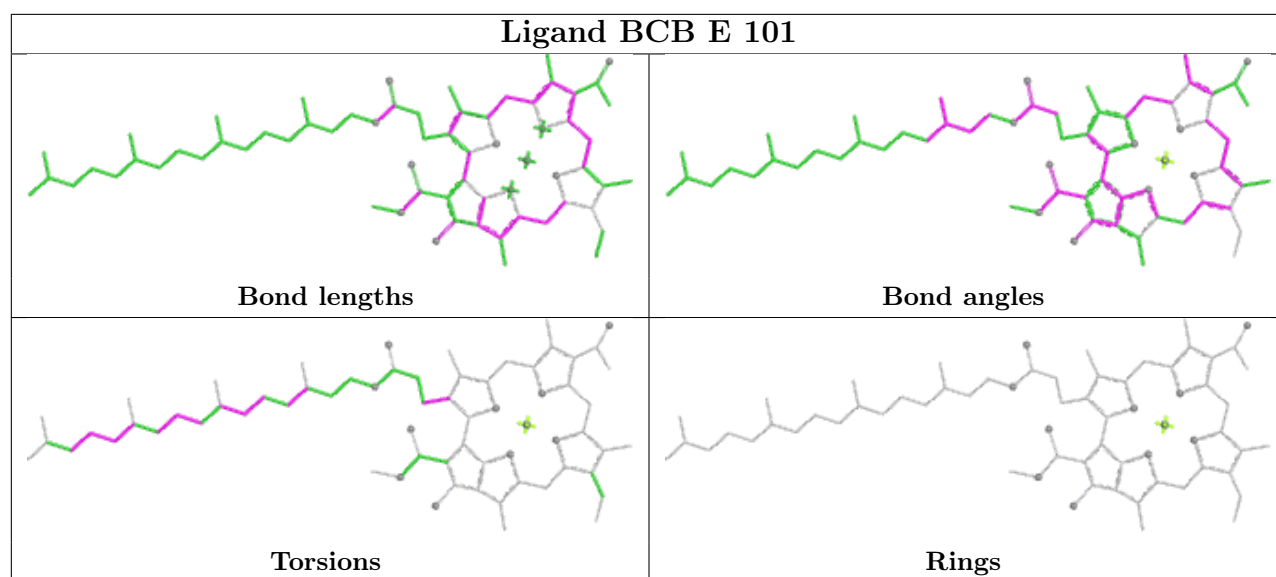


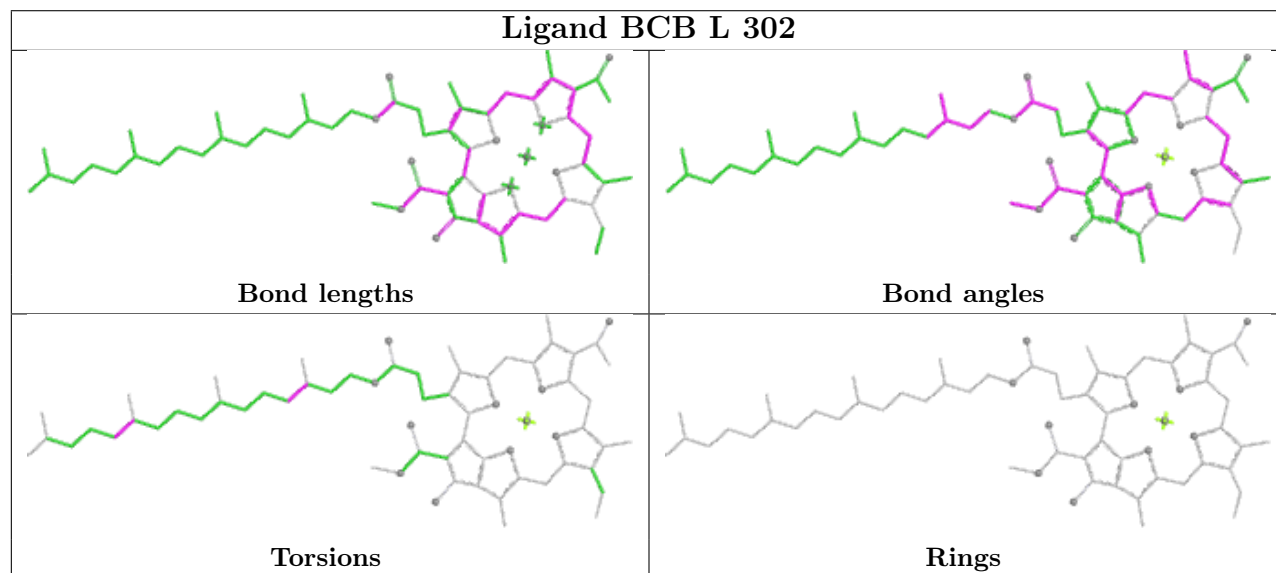
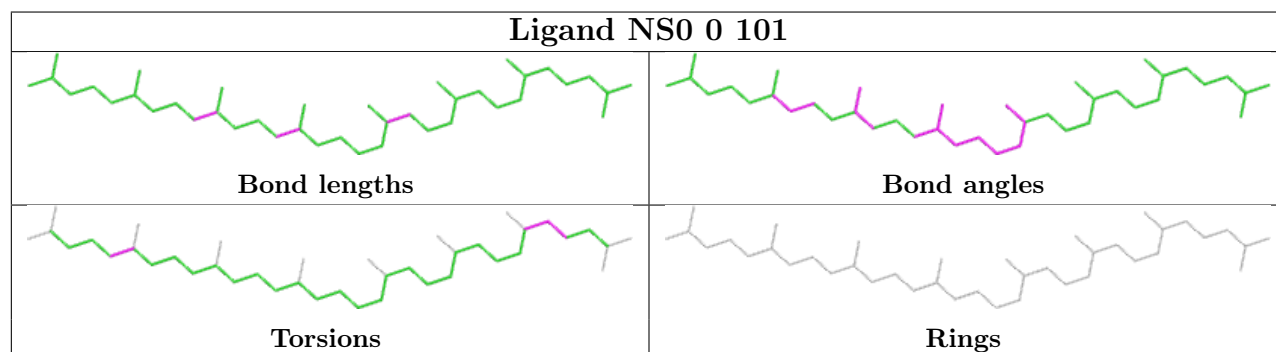
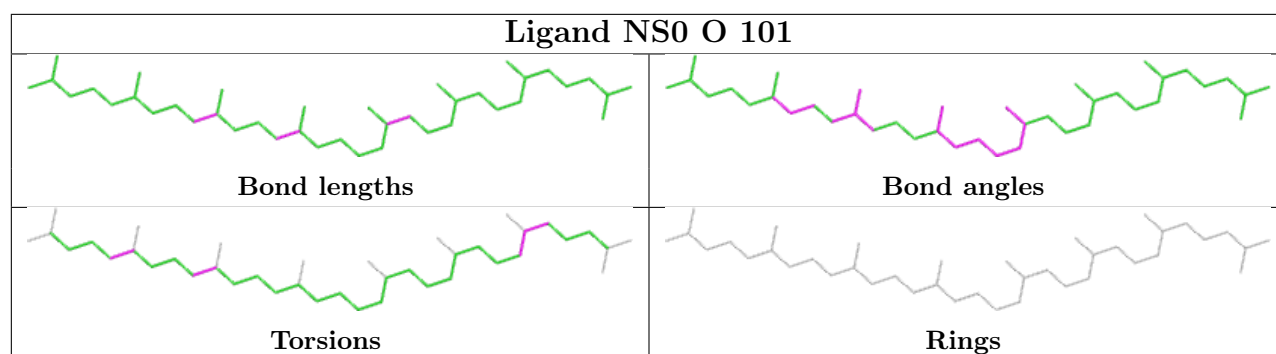


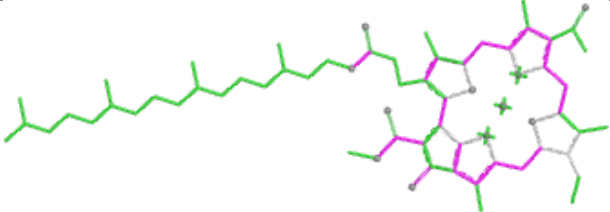
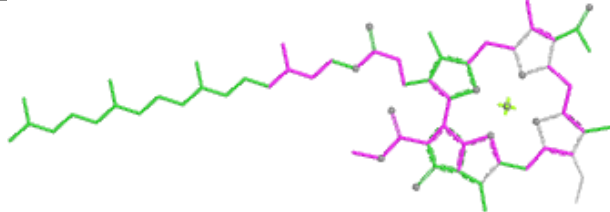
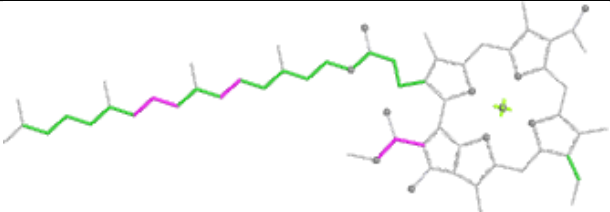
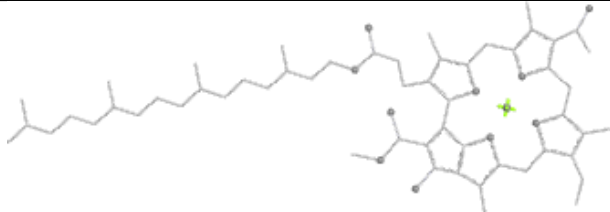
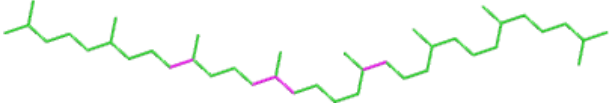
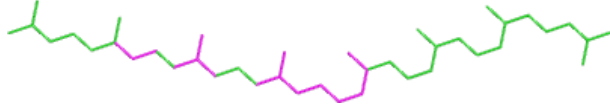
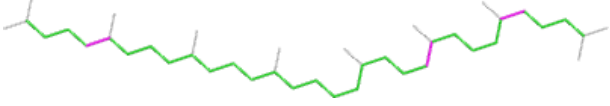
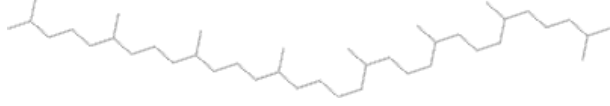
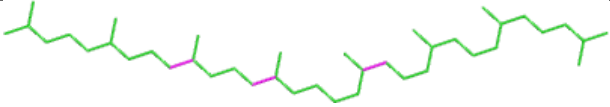
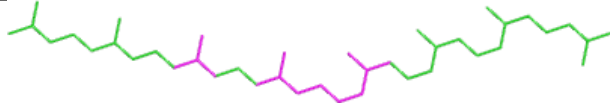
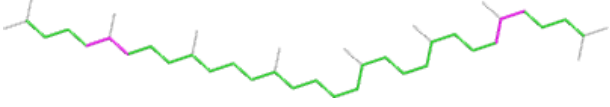
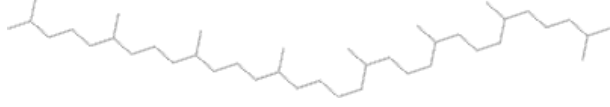


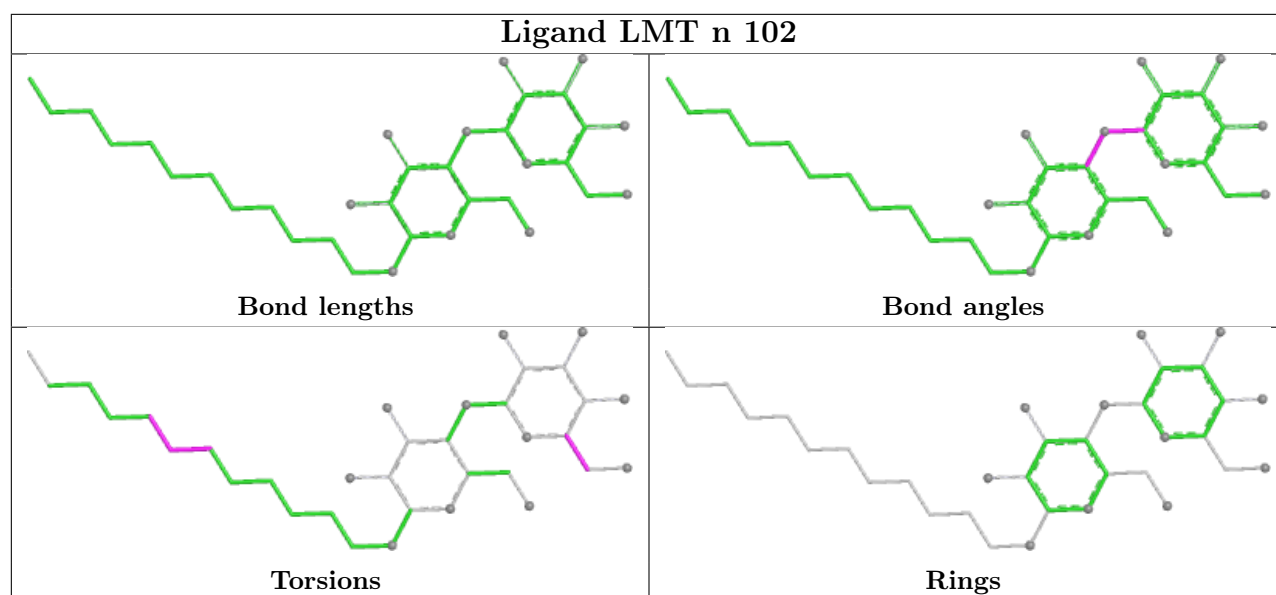
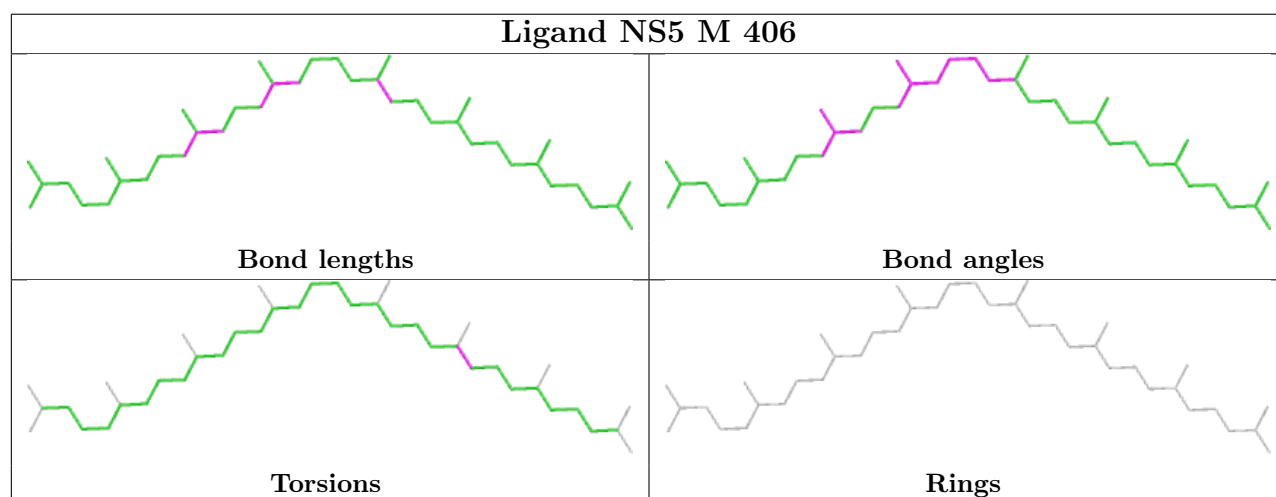
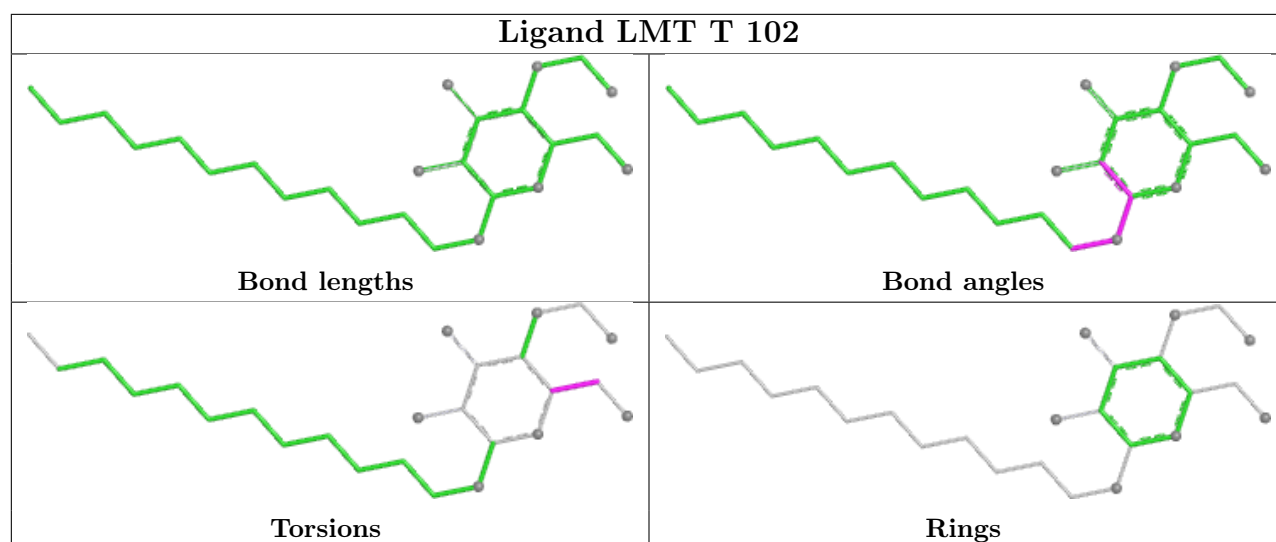


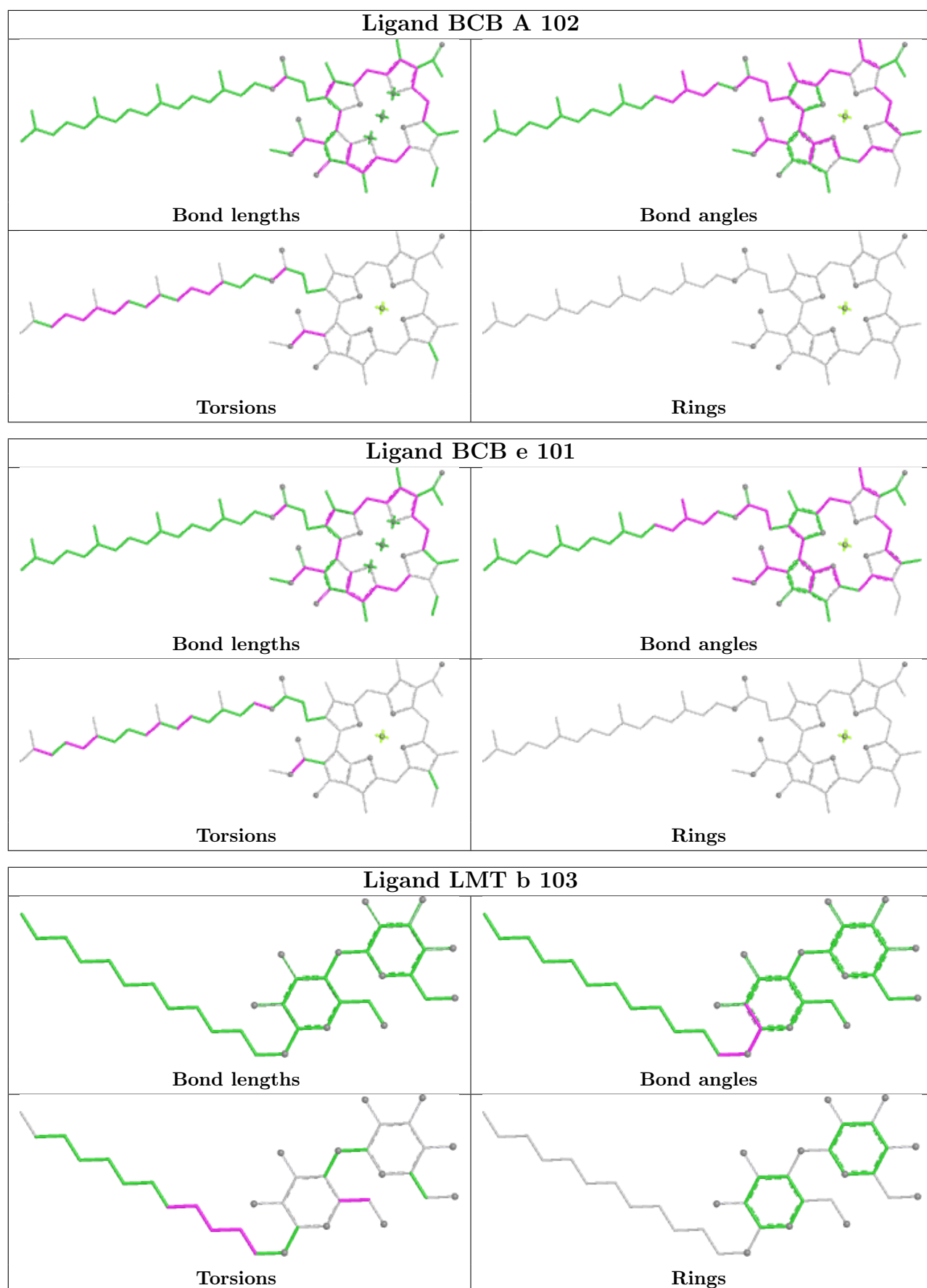


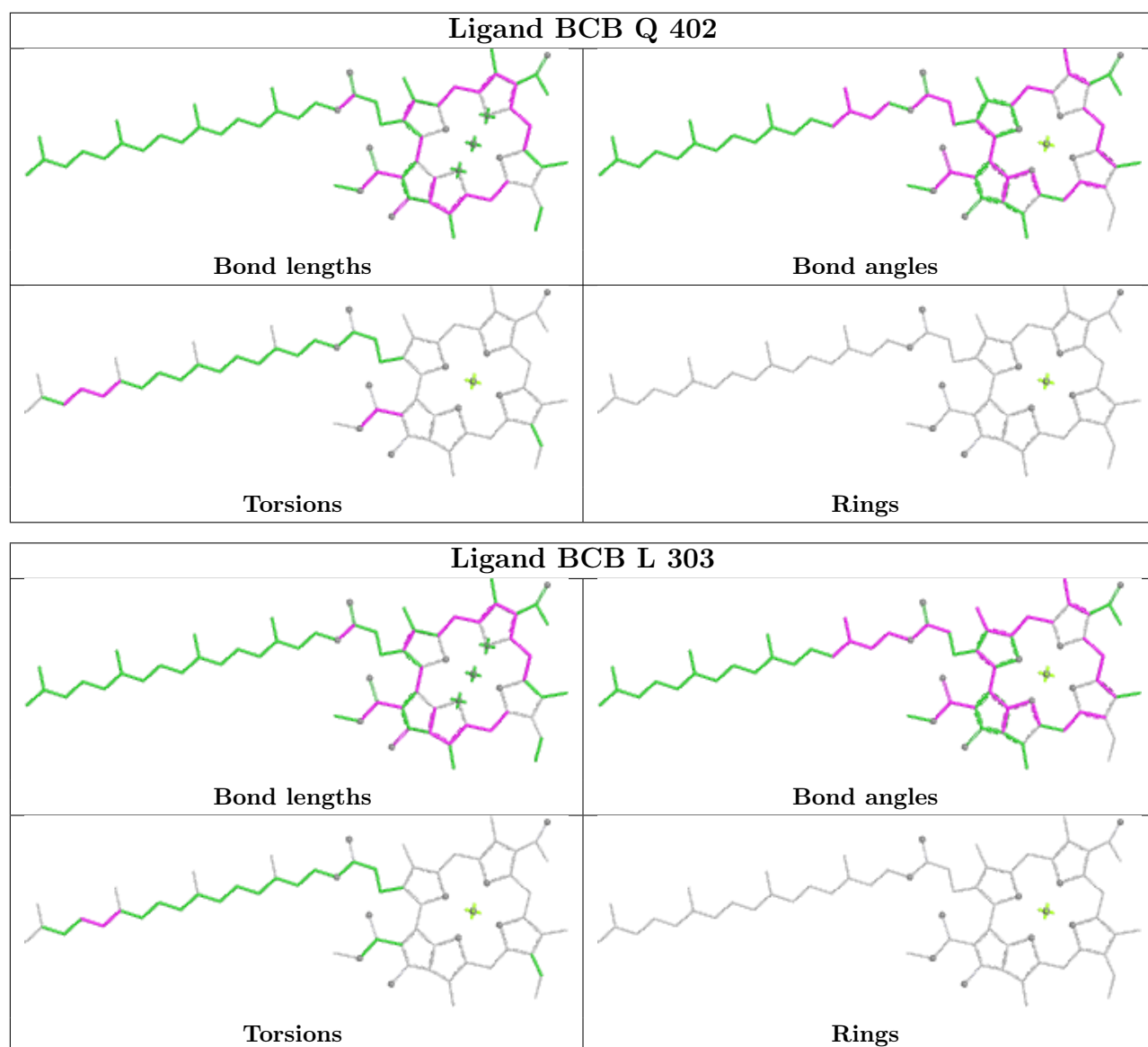


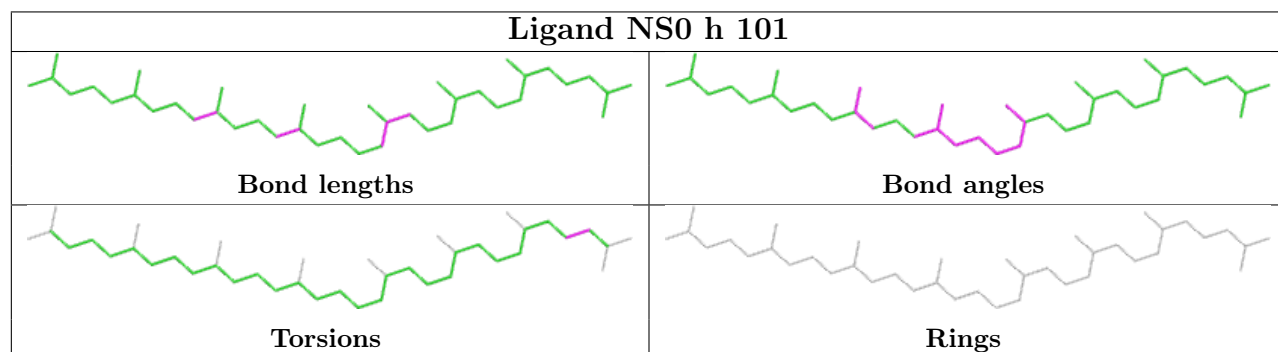
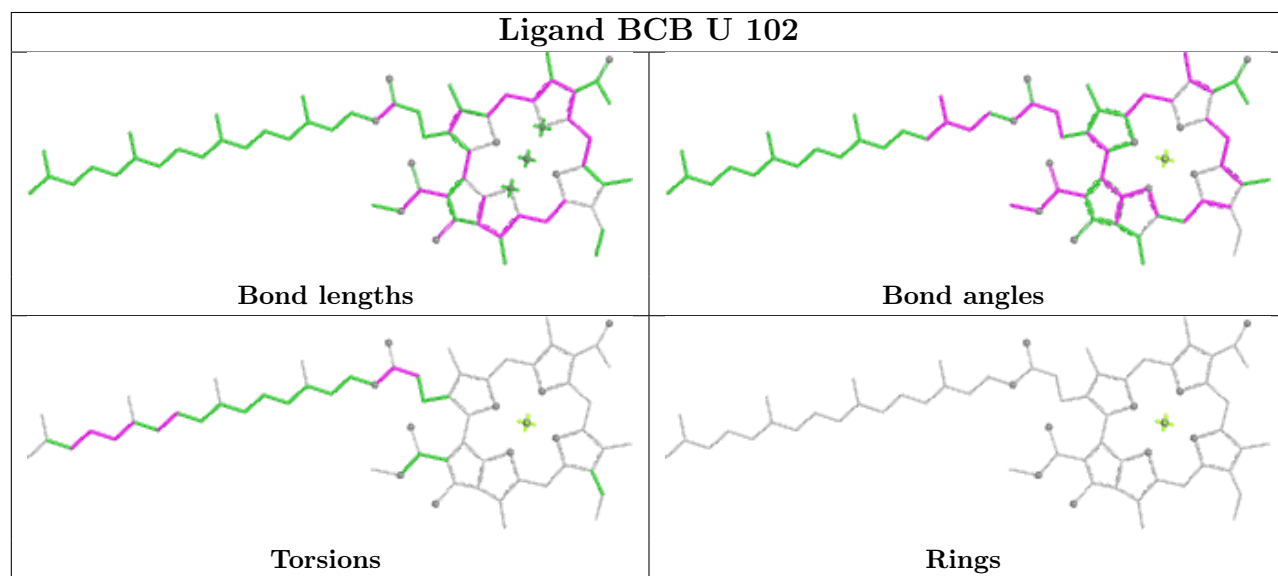
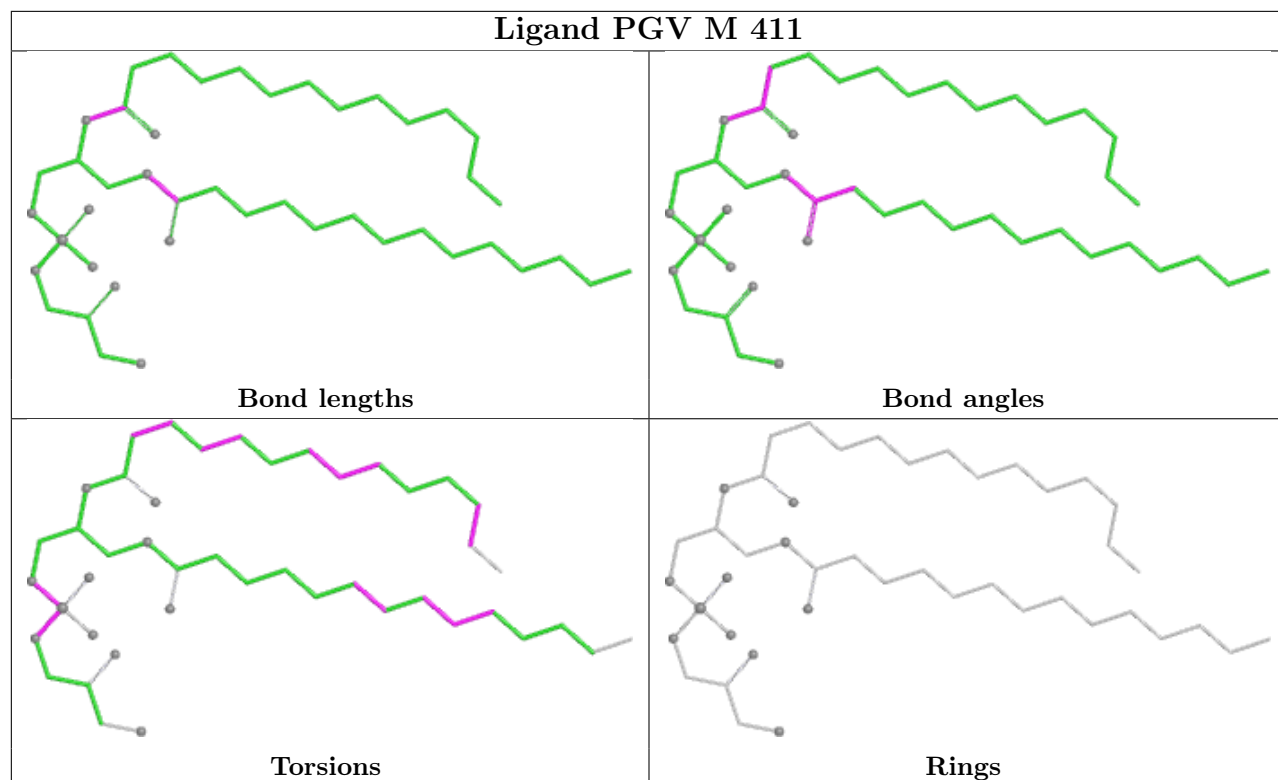


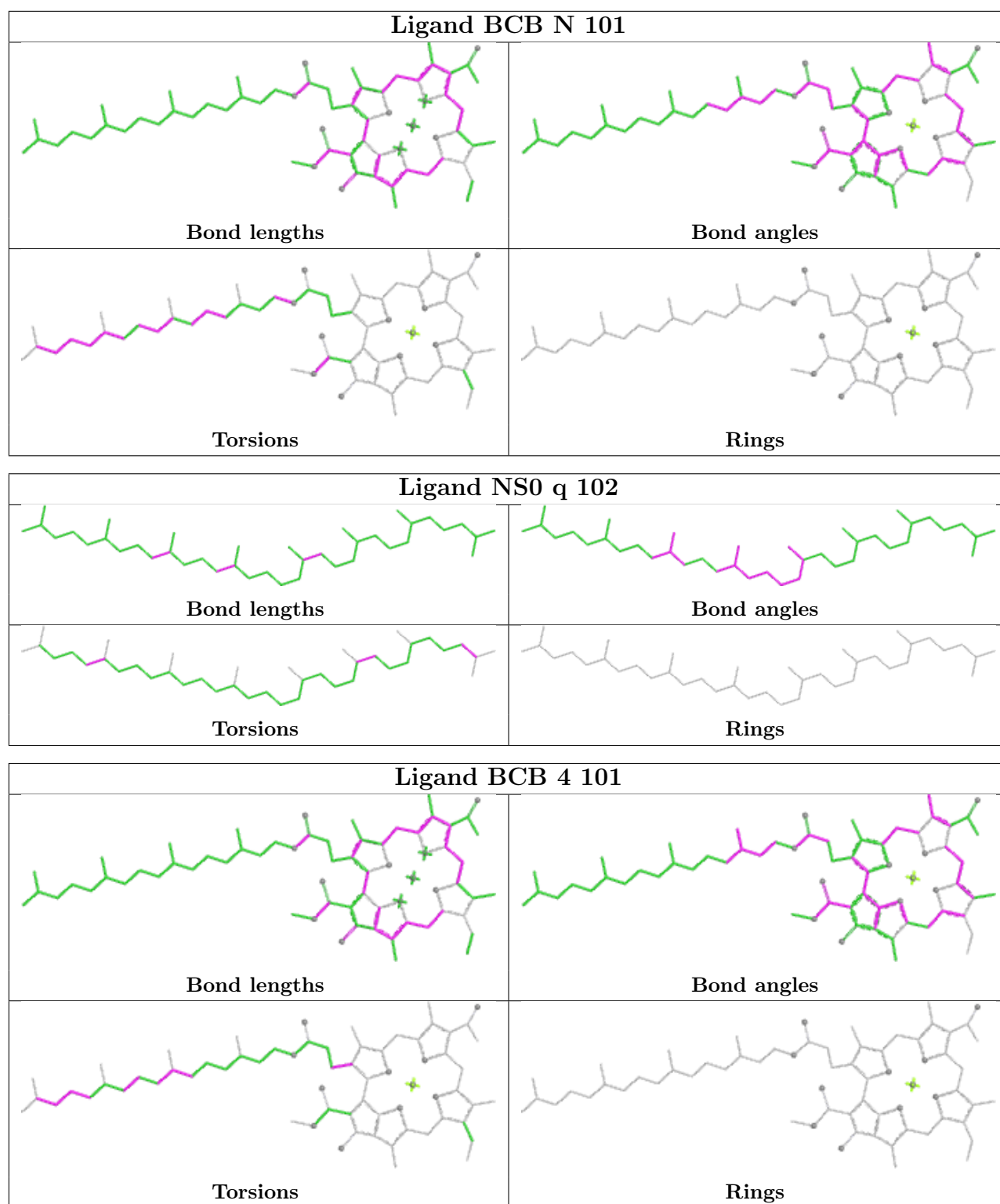
Ligand BCB Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand NS0 9 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand NS0 U 101	
 Bond lengths	 Bond angles
 Torsions	 Rings











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

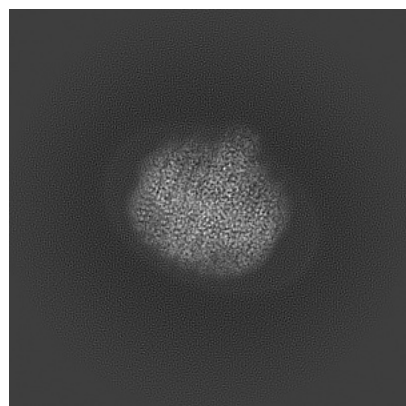
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61095. These allow visual inspection of the internal detail of the map and identification of artifacts.

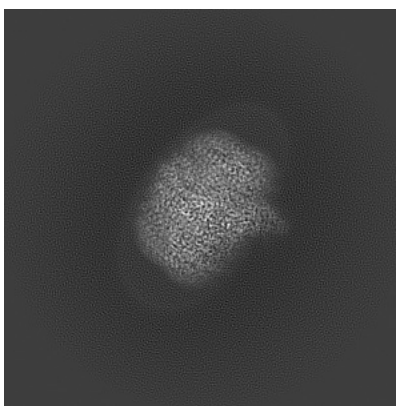
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

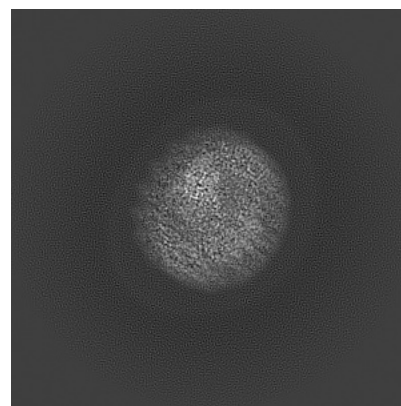
6.1.1 Primary map



X

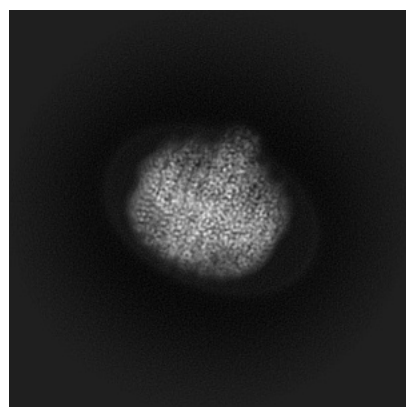


Y

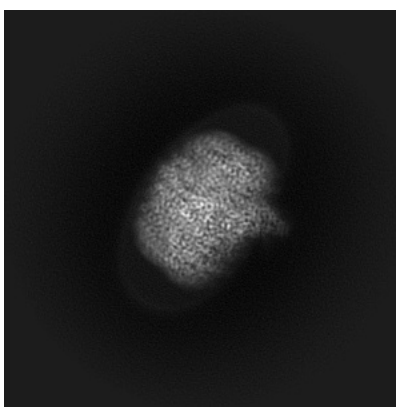


Z

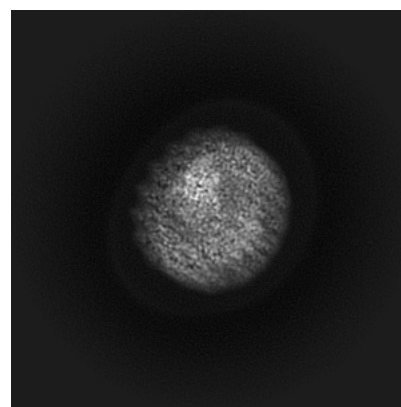
6.1.2 Raw map



X



Y

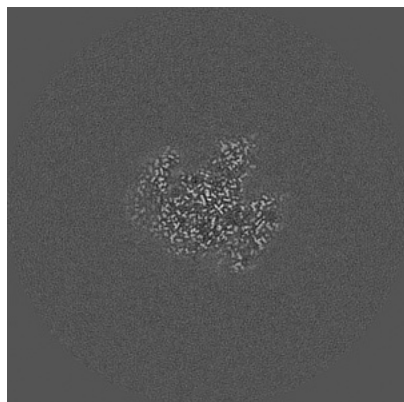


Z

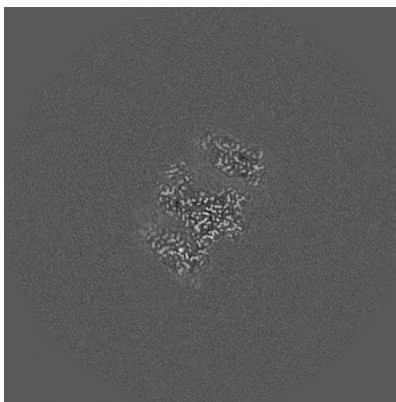
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

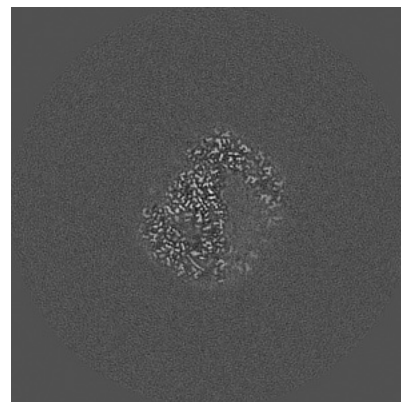
6.2.1 Primary map



X Index: 200

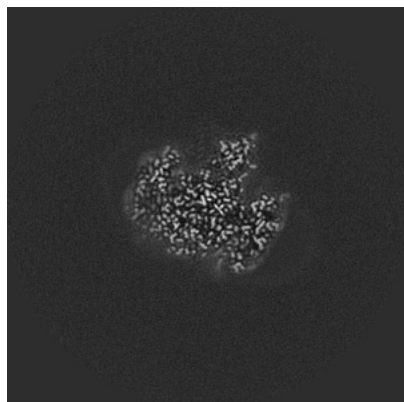


Y Index: 200

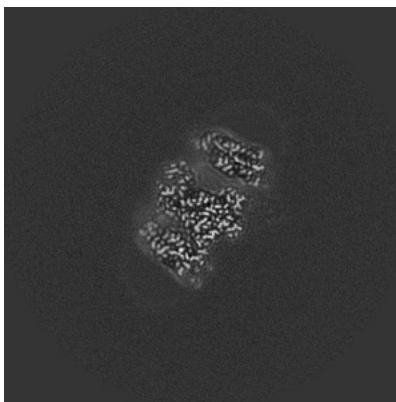


Z Index: 200

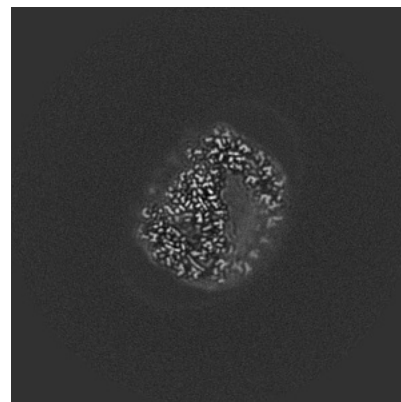
6.2.2 Raw map



X Index: 200



Y Index: 200

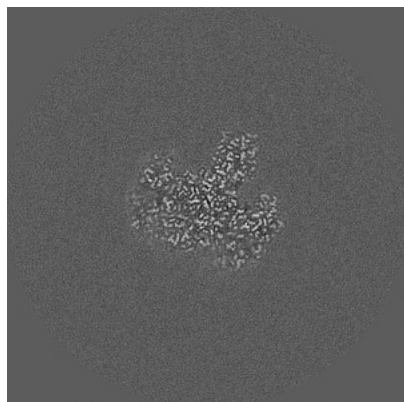


Z Index: 200

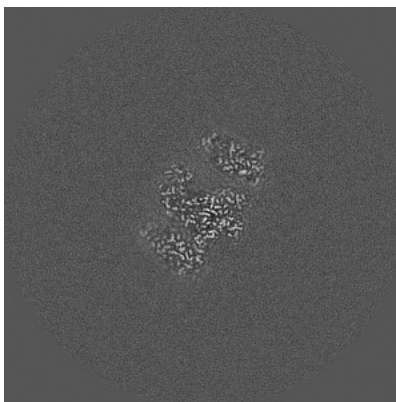
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

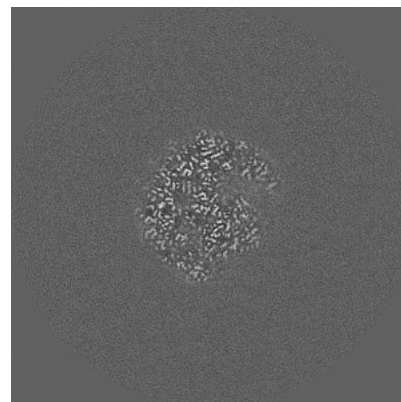
6.3.1 Primary map



X Index: 194

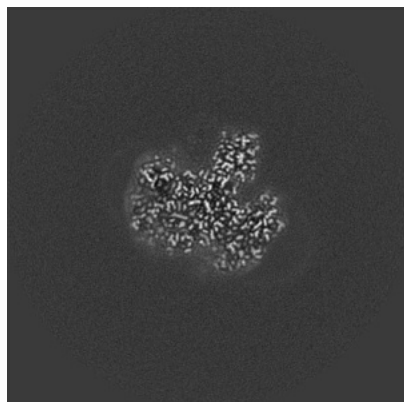


Y Index: 201

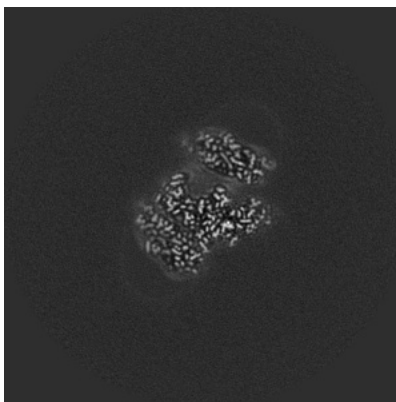


Z Index: 183

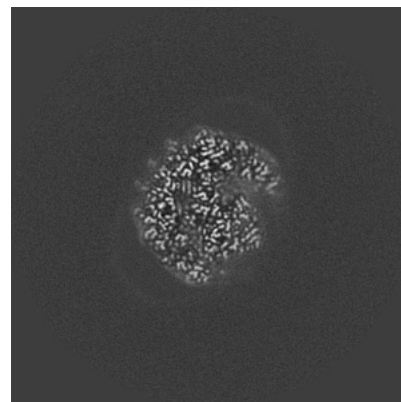
6.3.2 Raw map



X Index: 193



Y Index: 212

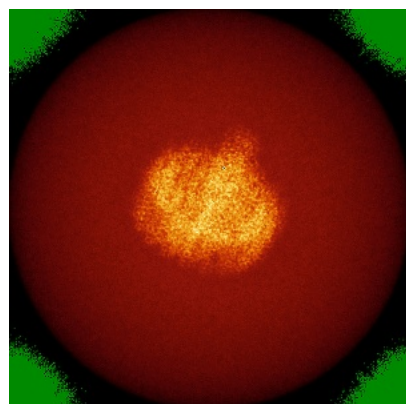


Z Index: 183

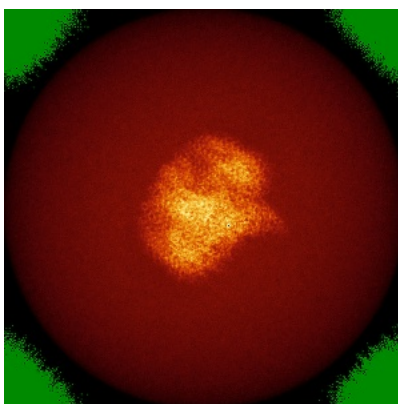
The images above show the largest variance slices of the map in three orthogonal directions.

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

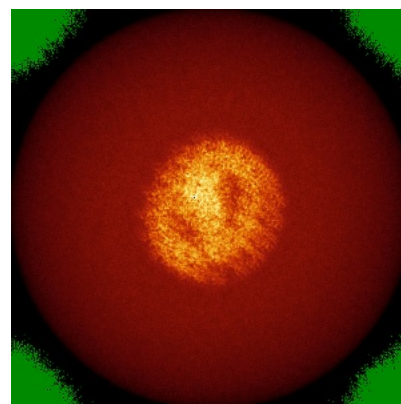
6.4.1 Primary map



X

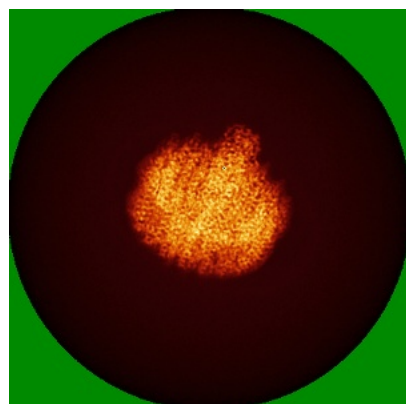


Y

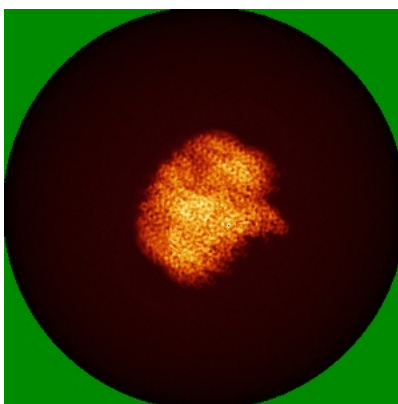


Z

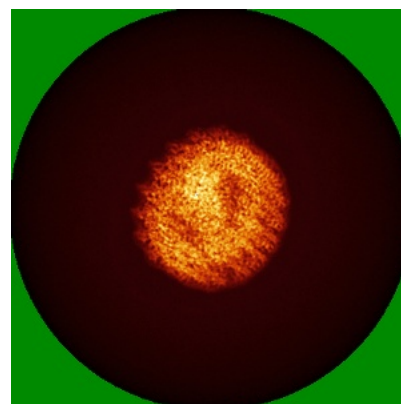
6.4.2 Raw map



X



Y

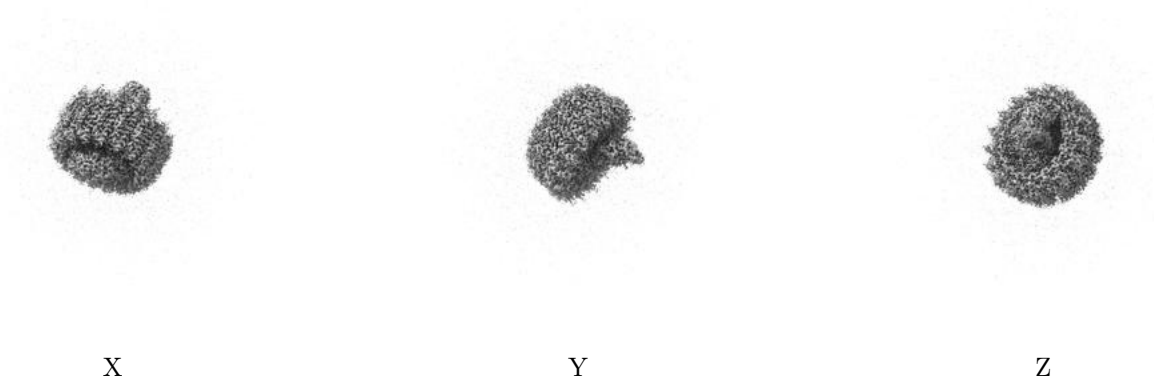


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

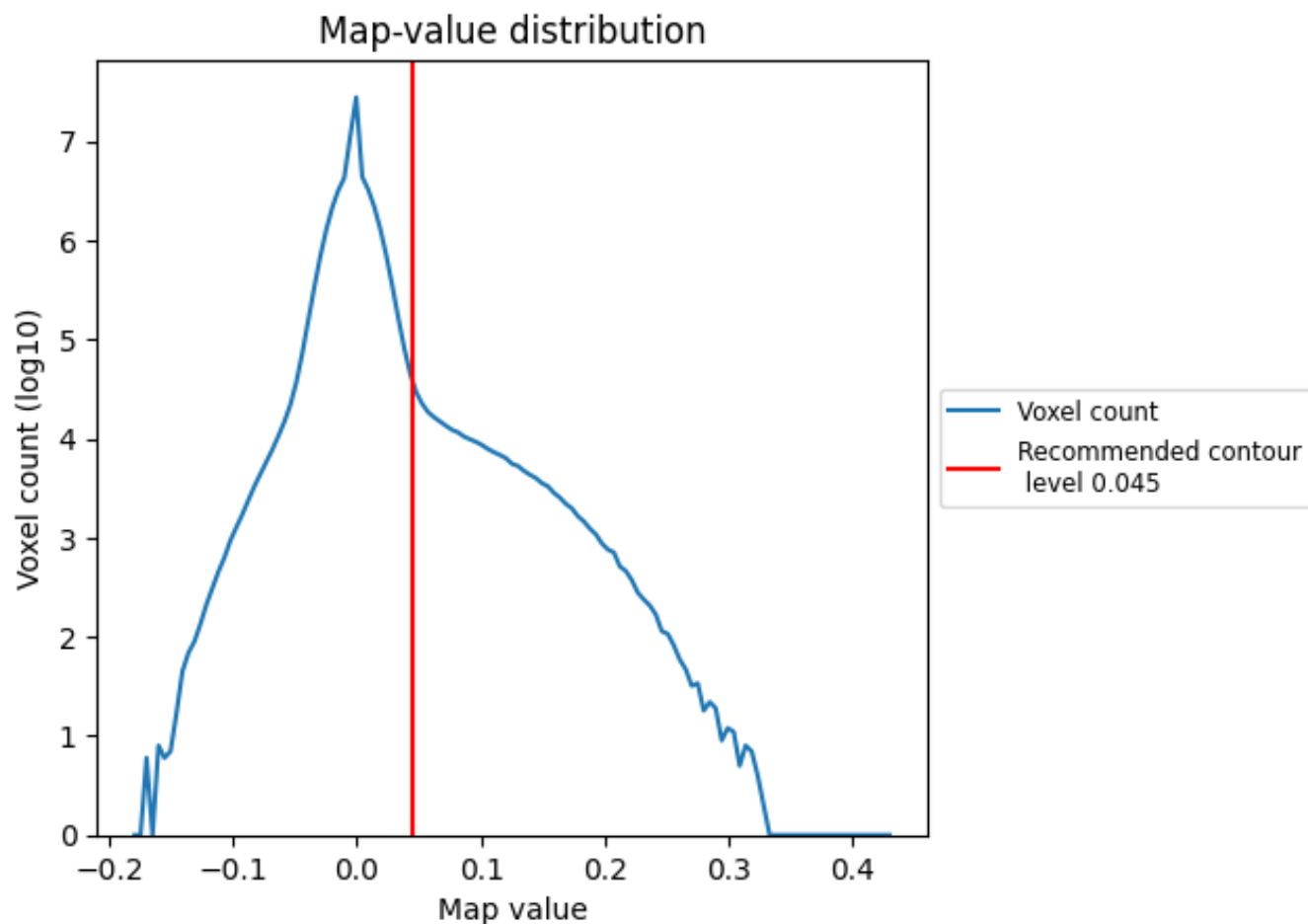
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

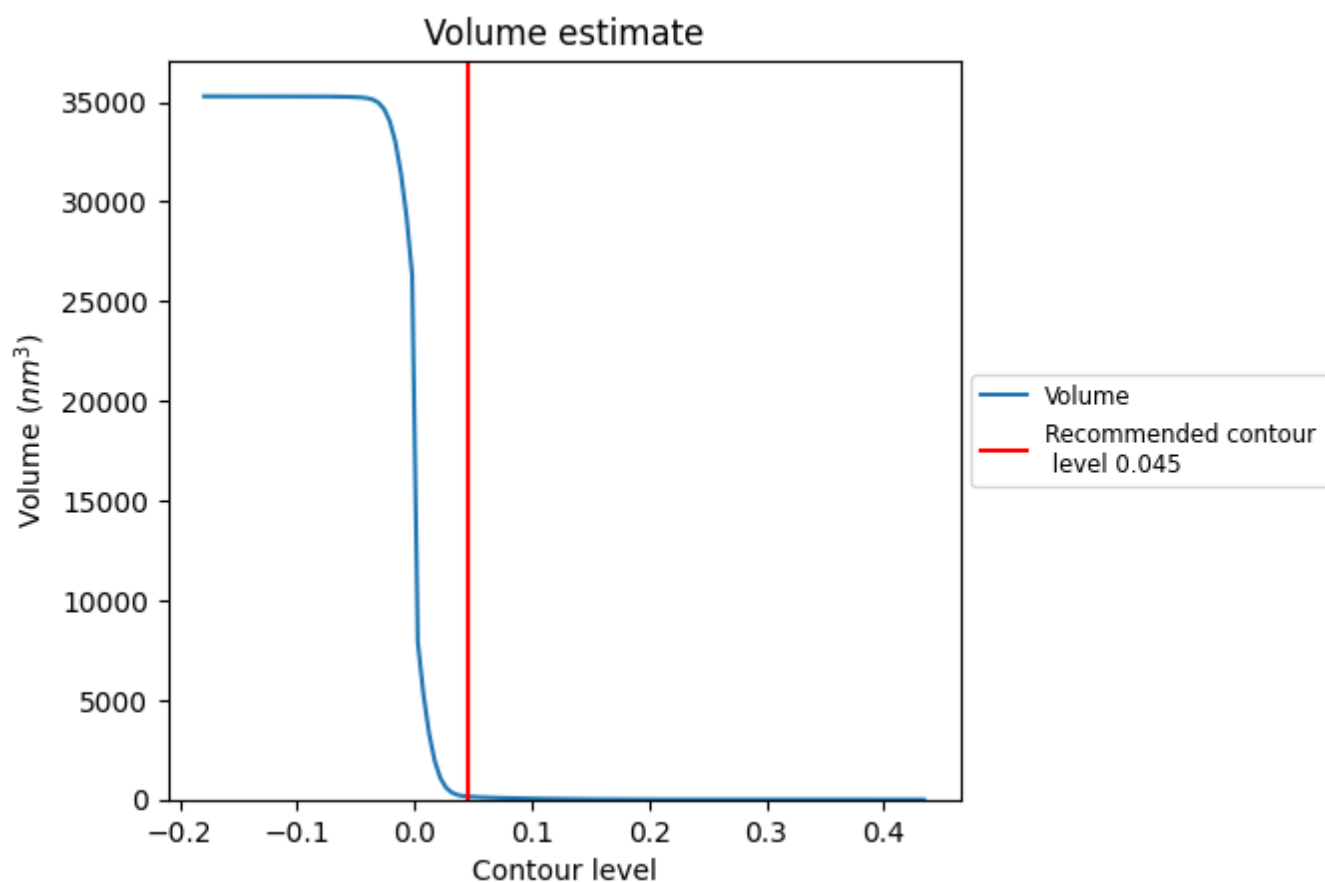
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

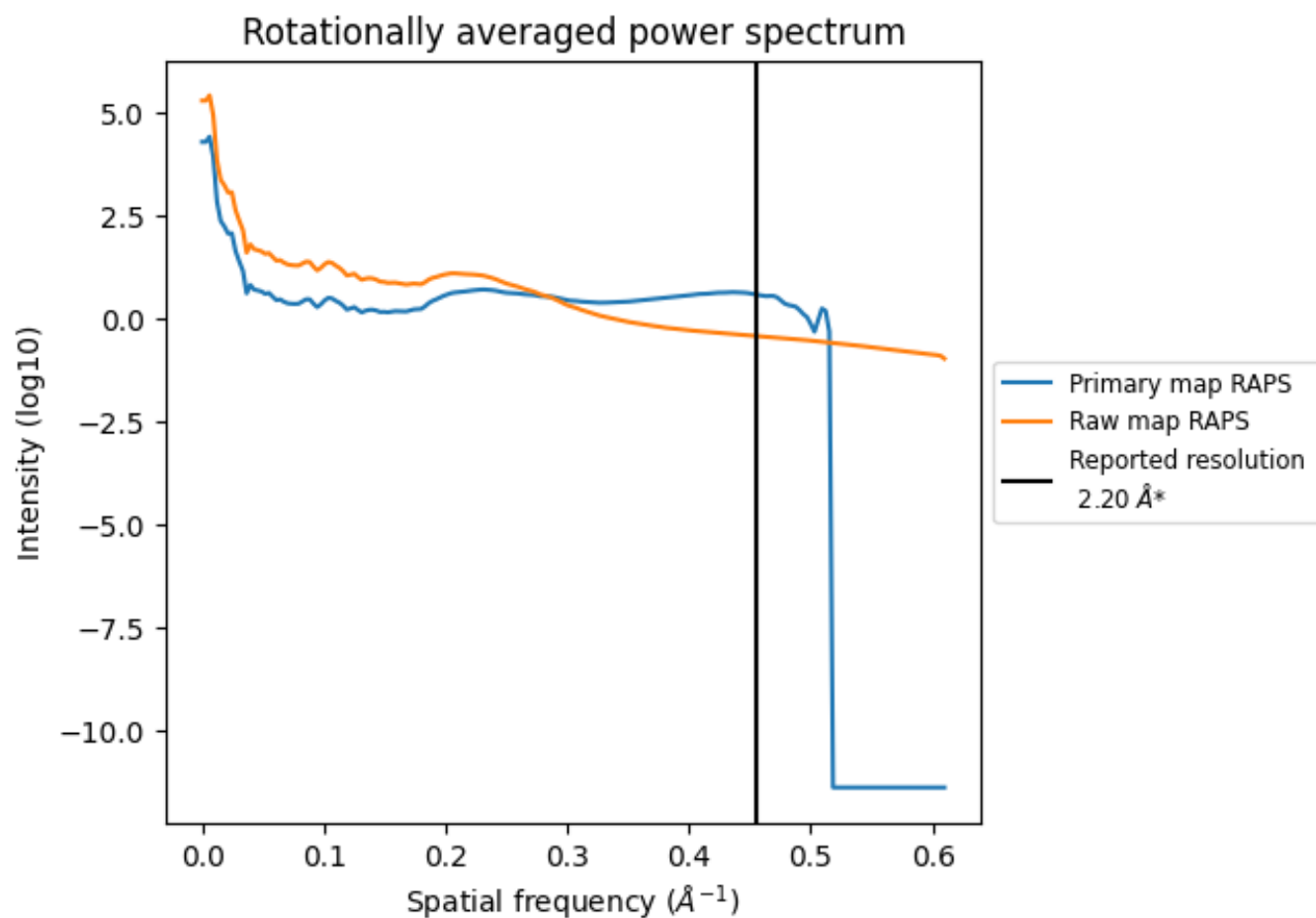
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 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 ⓘ

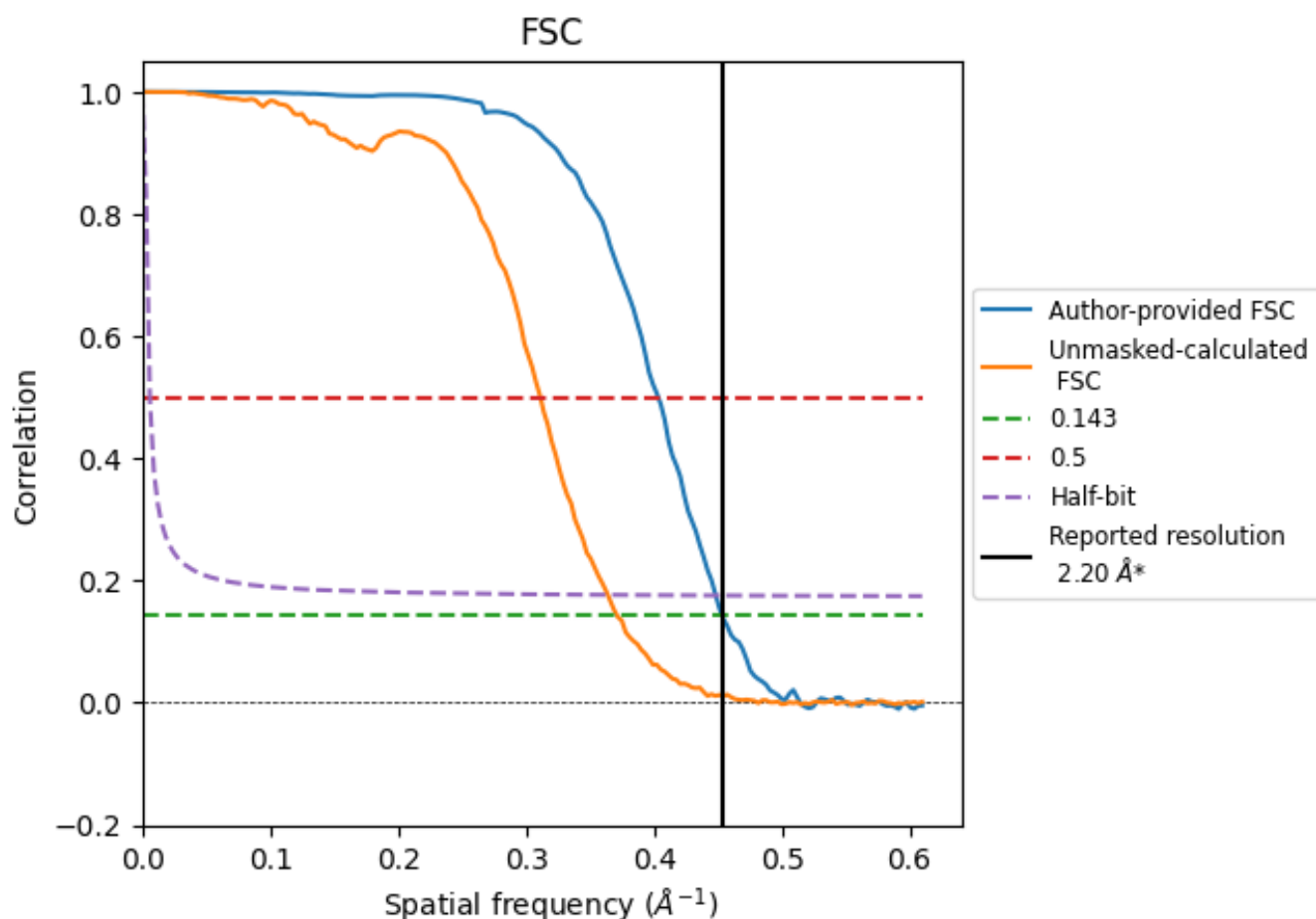


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

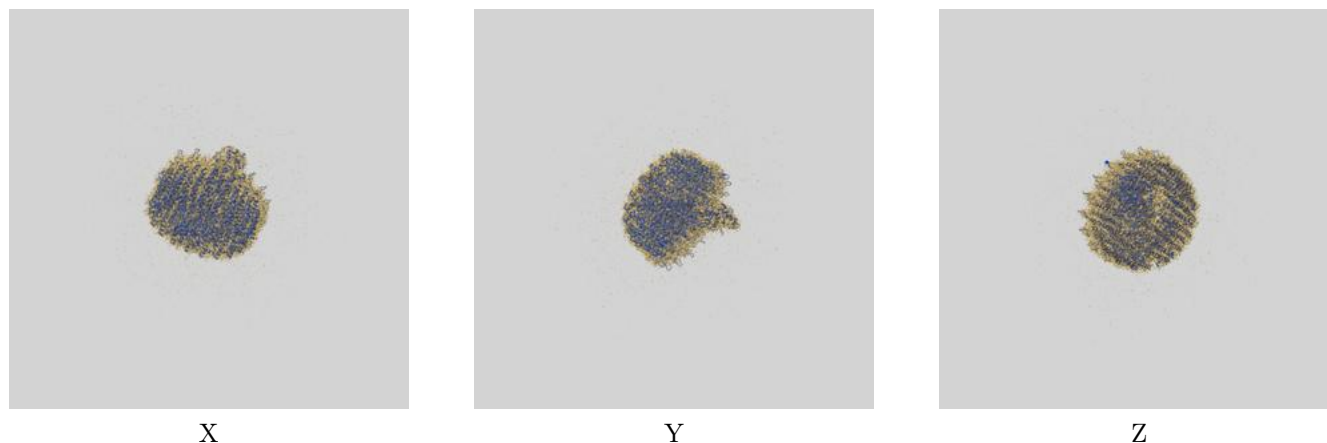
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.21	2.48	2.23
Unmasked-calculated*	2.69	3.21	2.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.69 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

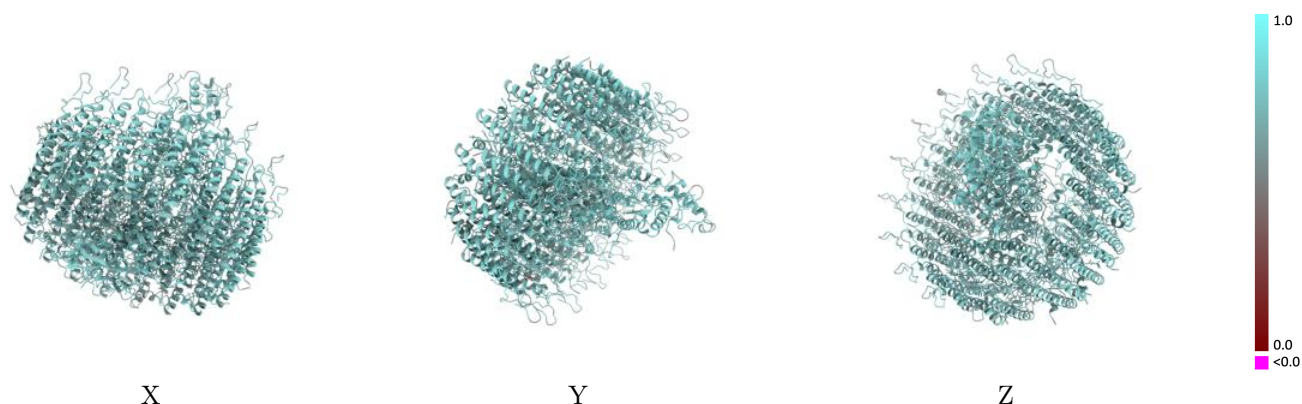
This section contains information regarding the fit between EMDB map EMD-61095 and PDB model 9J2F. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



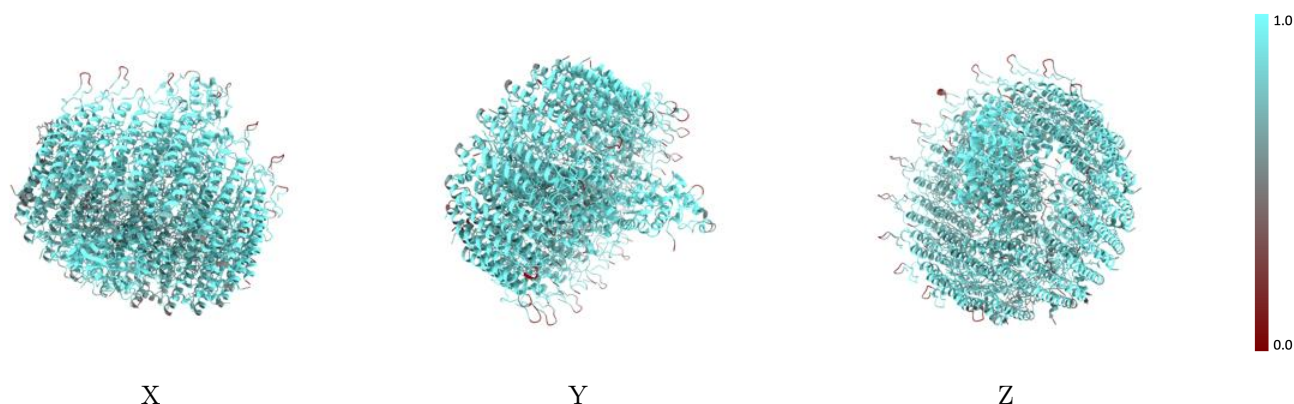
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



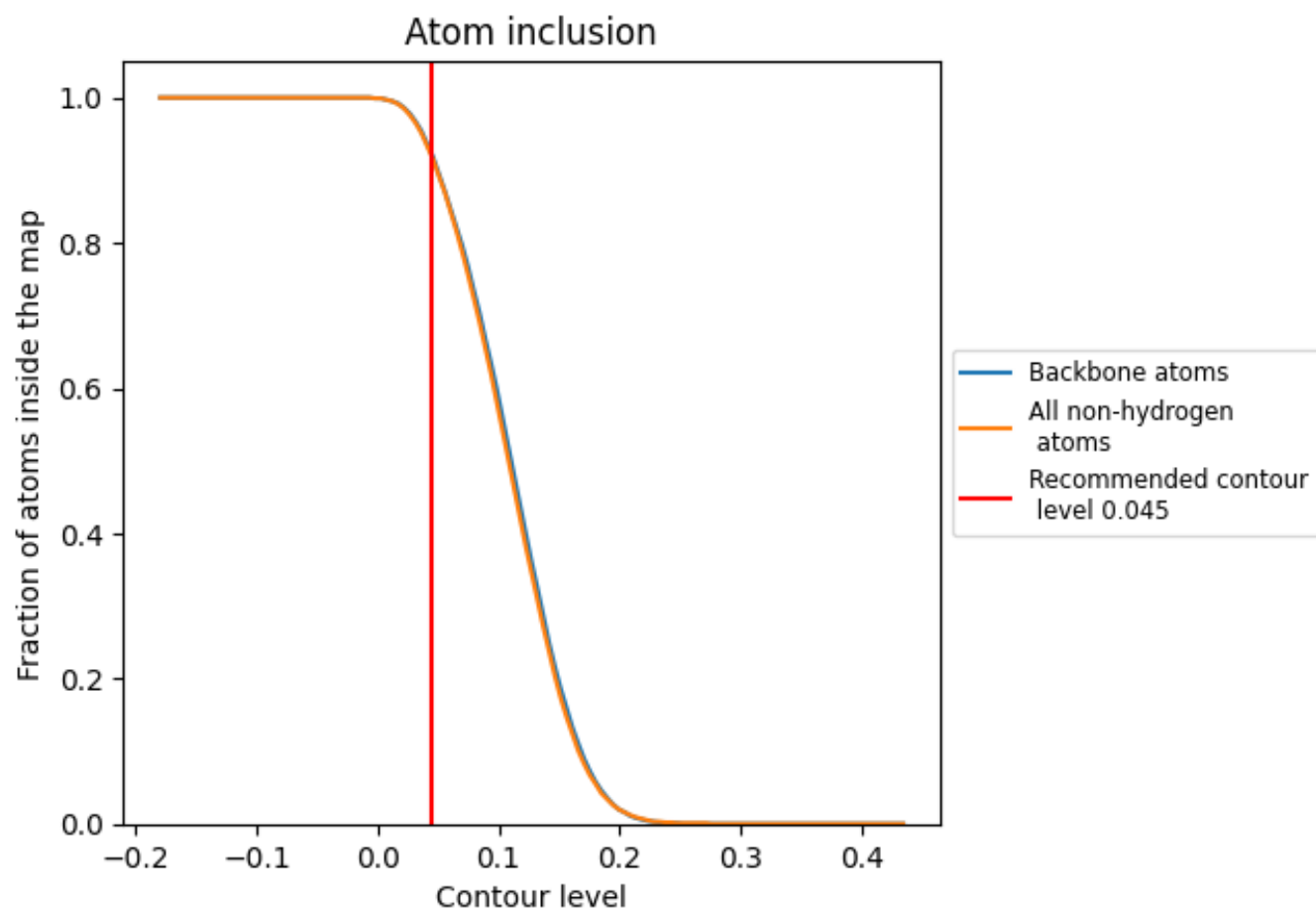
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.7250
0	 0.9210	 0.7210
1	 0.9600	 0.7460
2	 0.9010	 0.7020
3	 0.9640	 0.7430
4	 0.9320	 0.7340
5	 0.8750	 0.7030
6	 0.9470	 0.7320
7	 0.9310	 0.7340
8	 0.8860	 0.7010
9	 0.9490	 0.7350
A	 0.9050	 0.7200
B	 0.8600	 0.6930
C	 0.9540	 0.7460
D	 0.9410	 0.7300
E	 0.9460	 0.7350
F	 0.8320	 0.7000
G	 0.6060	 0.6270
H	 0.9160	 0.7160
I	 0.9370	 0.7240
J	 0.9520	 0.7380
K	 0.9010	 0.7070
L	 0.9720	 0.7600
M	 0.9580	 0.7480
N	 0.9310	 0.7270
O	 0.9460	 0.7270
P	 0.8540	 0.6930
Q	 0.9270	 0.7230
R	 0.9210	 0.7220
S	 0.8460	 0.6950
T	 0.8700	 0.6950
U	 0.8870	 0.7000
V	 0.8170	 0.6830
W	 0.9300	 0.7230
X	 0.9050	 0.7210



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Chain	Atom inclusion	Q-score
Y	 0.8650	 0.6920
Z	 0.9490	 0.7400
a	 0.7870	 0.6870
b	 0.8930	 0.7150
c	 0.9190	 0.7290
d	 0.8320	 0.6880
e	 0.9600	 0.7360
f	 0.9390	 0.7290
g	 0.8860	 0.7030
h	 0.9200	 0.7200
i	 0.9080	 0.7130
j	 0.9010	 0.6970
k	 0.9270	 0.7180
l	 0.9230	 0.7200
m	 0.8830	 0.6970
n	 0.8900	 0.7140
o	 0.9210	 0.7170
p	 0.8390	 0.6920
q	 0.8830	 0.7010
r	 0.7900	 0.6730