



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 04:44 AM JST

PDB ID : 9LTI / pdb_00009lti
EMDB ID : EMD-63370
Title : Cryo-EM structure of LH1-RC from Ery. sanguineus
Authors : Yue, X.-Y.; Wang, G.-L.; Yu, L.-J.
Deposited on : 2025-02-06
Resolution : 2.27 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

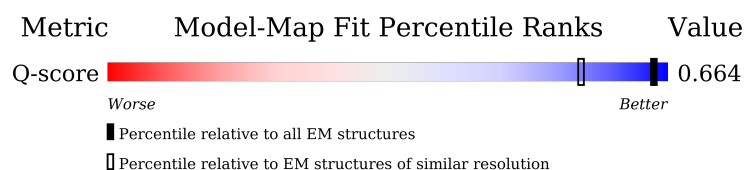
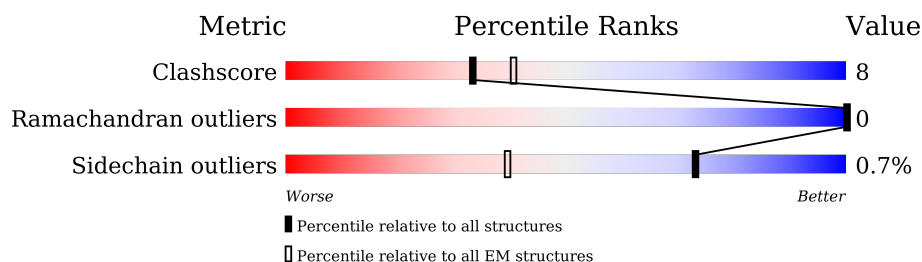
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.27 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.



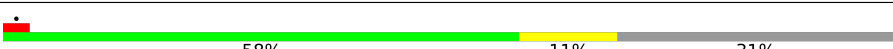
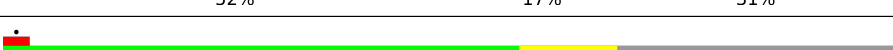
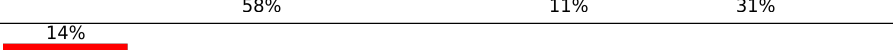
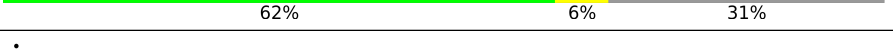
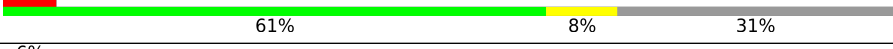
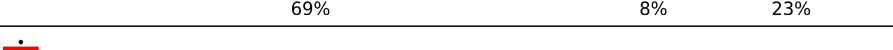
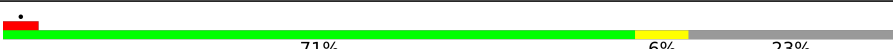
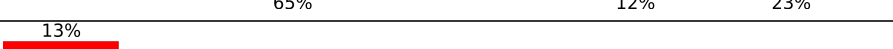
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3593 (1.77 - 2.77)

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

Mol	Chain	Length	Quality of chain
1	A	64	
1	B	64	
1	C	64	
1	D	64	

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Mol	Chain	Length	Quality of chain
1	E	64	
1	F	64	
1	G	64	
1	I	64	
1	J	64	
1	K	64	
1	N	64	
1	O	64	
1	P	64	
1	Q	64	
1	R	64	
1	S	64	
2	a	52	
2	b	52	
2	c	52	
2	d	52	
2	e	52	
2	f	52	
2	g	52	
2	i	52	
2	j	52	
2	k	52	
2	n	52	
2	o	52	
2	p	52	

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Mol	Chain	Length	Quality of chain
2	q	52	
2	r	52	
2	s	52	
3	L	274	
4	H	268	
5	M	323	
6	T	135	

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
9	A1ELD	R	102	-	X	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 22831 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 Light-harvesting complex 1 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	B	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	C	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	D	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	E	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	F	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	G	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	Q	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	I	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	J	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	K	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	R	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	S	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	N	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	O	44	Total	C	N	O	S	0	0
			384	260	67	56	1		
1	P	44	Total	C	N	O	S	0	0
			384	260	67	56	1		

- Molecule 2 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	a	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	p	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	o	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	n	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	s	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	r	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	k	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	j	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	c	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	d	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	e	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	f	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	g	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	q	40	Total	C	N	O	S	0	0
			326	223	49	52	2		
2	i	40	Total	C	N	O	S	0	0
			326	223	49	52	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	273	Total	C	N	O	S	0	0
			2135	1431	340	358	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	265	Total	C	N	O	S	0	0
			2079	1343	347	380	9		

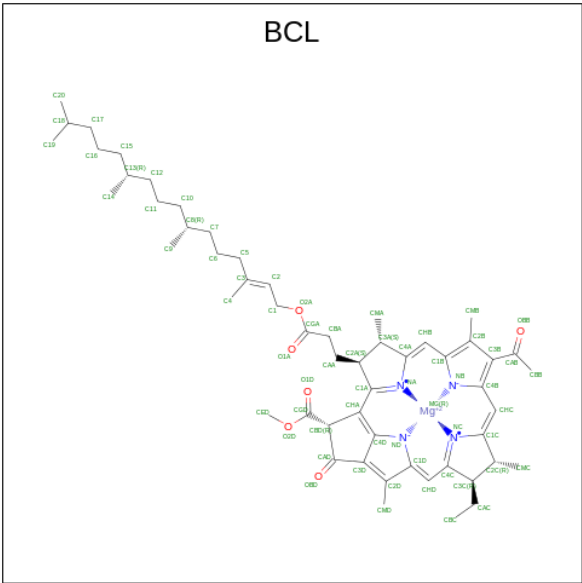
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	320	2543	1689	412	433	9	0	0

- Molecule 6 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	20	120	68	23	28	1	0	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	A	1	66	55	1	4	6	0
7	B	1	66	55	1	4	6	0
7	C	1	66	55	1	4	6	0
7	D	1	66	55	1	4	6	0
7	E	1	66	55	1	4	6	0
7	F	1	66	55	1	4	6	0

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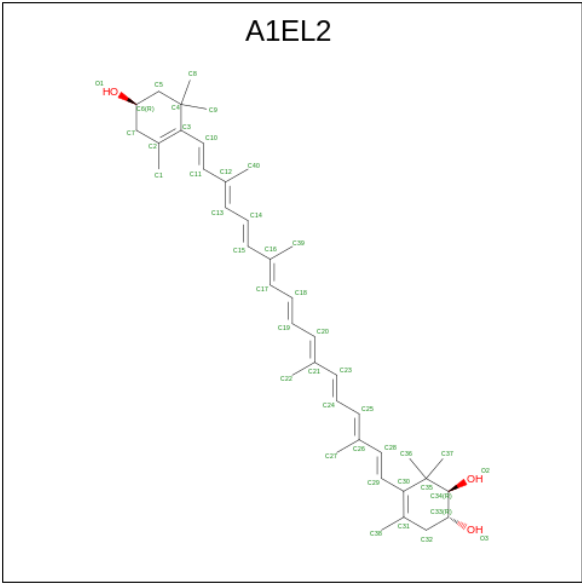
Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	c	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	d	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
7	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is (1 {R},2 {R})-3,3,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-4-ene-1,2-diol (CCD ID: A1EL2) (formula: C₄₀H₅₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	C	O	0
			43	40	3	
8	C	1	Total	C	O	0
			43	40	3	
8	D	1	Total	C	O	0
			43	40	3	
8	E	1	Total	C	O	0
			43	40	3	
8	F	1	Total	C	O	0
			43	40	3	
8	G	1	Total	C	O	0
			43	40	3	
8	Q	1	Total	C	O	0
			43	40	3	
8	I	1	Total	C	O	0
			43	40	3	
8	J	1	Total	C	O	0
			43	40	3	
8	K	1	Total	C	O	0
			43	40	3	
8	N	1	Total	C	O	0
			43	40	3	
8	O	1	Total	C	O	0
			43	40	3	
8	P	1	Total	C	O	0
			43	40	3	
8	r	1	Total	C	O	0
			43	40	3	
8	r	1	Total	C	O	0
			43	40	3	

- Molecule 9 is (2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E},16 {E})-2-[(1 {Z},3 {Z},5 {E})-8-methoxy-4,8-dimethyl-nona-1,3,5-trienyl]-6,11,15-trimethyl-17-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]heptadeca-2,4,6,8,10,12,14,16-octaenal (CCD ID: A1ELD) (formula: C₄₁H₅₆O₃) (labeled as "Ligand of Interest" by depositor).

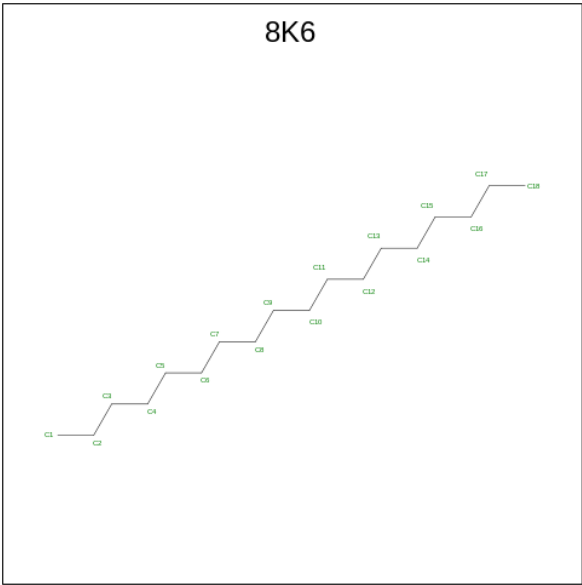


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Mol	Chain	Residues	Atoms			AltConf
9	g	1	Total	C	O	0
			44	41	3	
9	q	1	Total	C	O	0
			44	41	3	

- Molecule 10 is Octadecane (CCD ID: 8K6) (formula: C₁₈H₃₈).



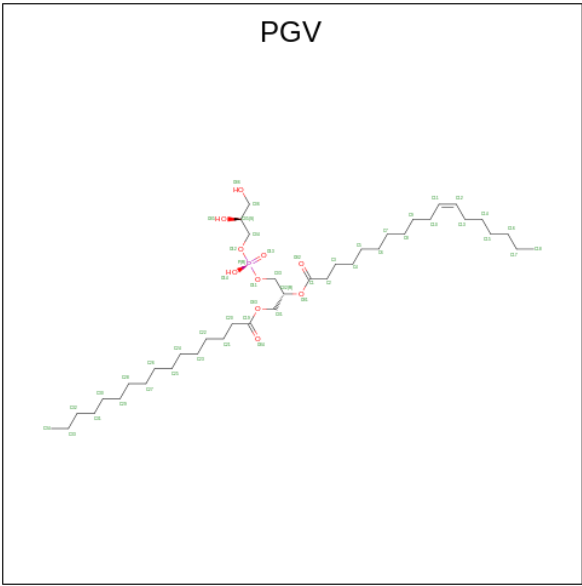
Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	C	0
			9	9	
10	Q	1	Total	C	0
			18	18	
10	Q	1	Total	C	0
			18	18	
10	S	1	Total	C	0
			13	13	
10	f	1	Total	C	0
			14	14	
10	L	1	Total	C	0
			12	12	
10	L	1	Total	C	0
			14	14	
10	L	1	Total	C	0
			10	10	
10	L	1	Total	C	0
			15	15	

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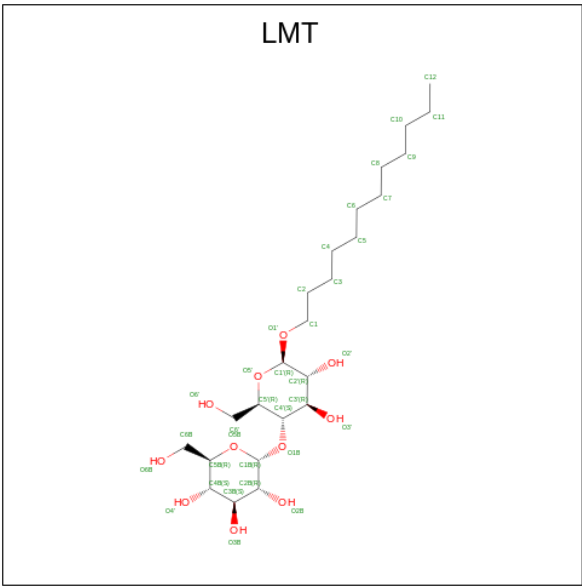
Mol	Chain	Residues	Atoms		AltConf
10	H	1	Total	C	0
			18	18	
10	M	1	Total	C	0
			15	15	

- Molecule 11 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).



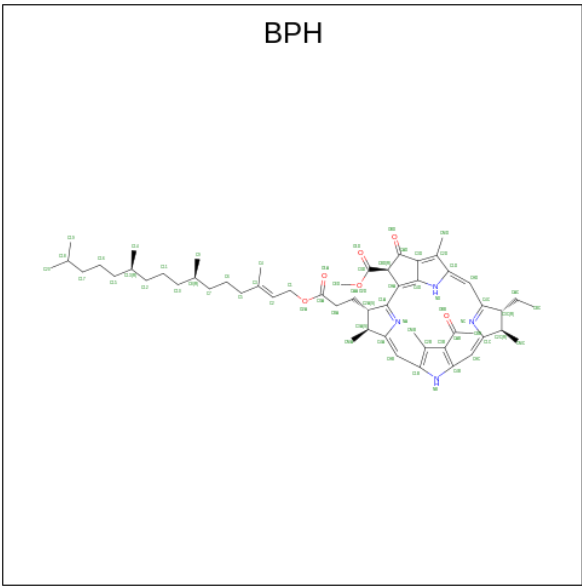
Mol	Chain	Residues	Atoms				AltConf
11	D	1	Total	C	O	P	0
			51	40	10	1	
11	F	1	Total	C	O	P	0
			51	40	10	1	
11	G	1	Total	C	O	P	0
			23	14	8	1	
11	L	1	Total	C	O	P	0
			21	12	8	1	
11	L	1	Total	C	O	P	0
			29	18	10	1	
11	M	1	Total	C	O	P	0
			38	29	8	1	
11	T	1	Total	C	O		0
			20	16	4		
11	T	1	Total	C	O	P	0
			30	21	8	1	

- Molecule 12 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



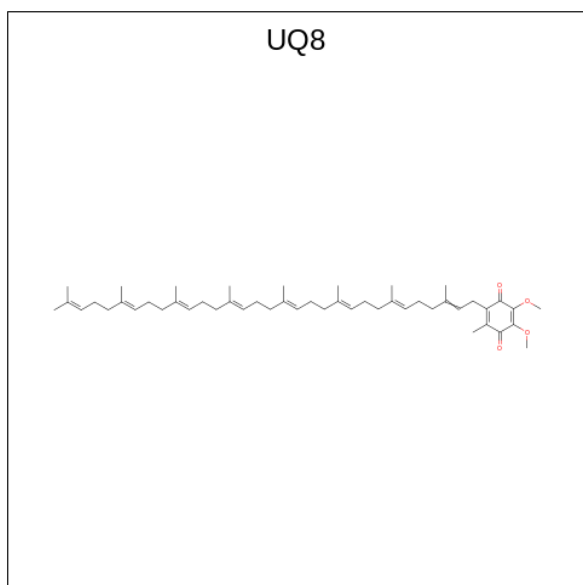
Mol	Chain	Residues	Atoms			AltConf
12	G	1	Total	C	O	0
			30	19	11	
12	N	1	Total	C	O	0
			26	15	11	
12	L	1	Total	C	O	0
			28	17	11	

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄) (labeled as "Ligand of Interest" by depositor).

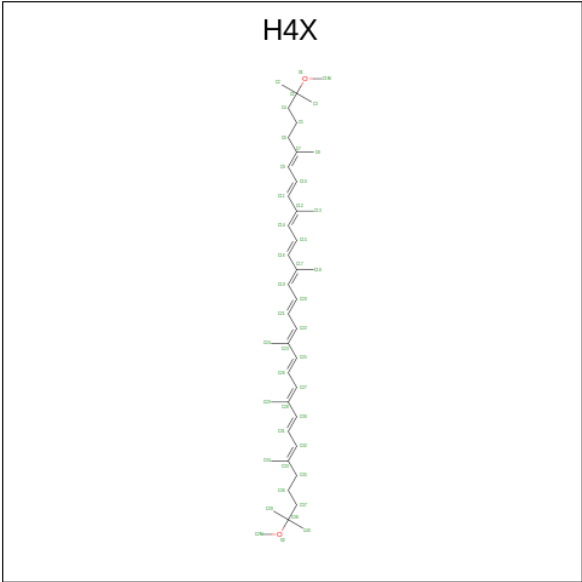


Mol	Chain	Residues	Atoms			AltConf
14	L	1	Total	C	O	0
			19	15	4	
14	L	1	Total	C	O	0
			18	14	4	
14	M	1	Total	C	O	0
			53	49	4	

- Molecule 15 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

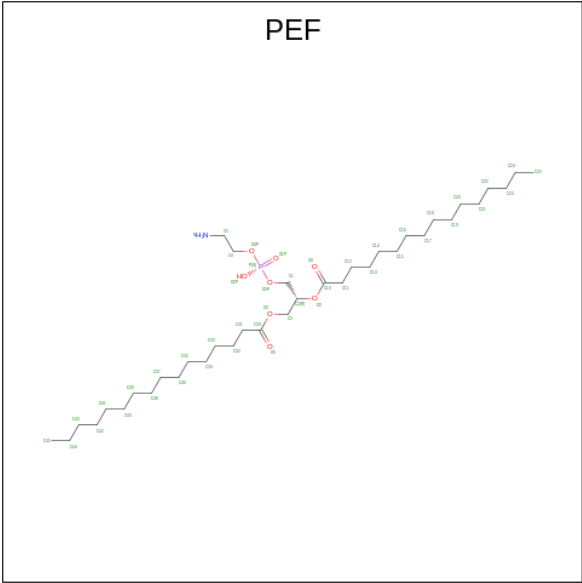
Mol	Chain	Residues	Atoms		AltConf
15	M	1	Total	Fe	0
			1	1	

- Molecule 16 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E},26 {E})-2,31-dimethoxy-2,6,10,14,19,23,27,31-octamethyl-dotriaconta-6,8,10,12,14,16,18,20,22,24,26-undecaene (CCD ID: H4X) (formula: C₄₂H₆₄O₂) (labeled as "Ligand of Interest" by depositor).



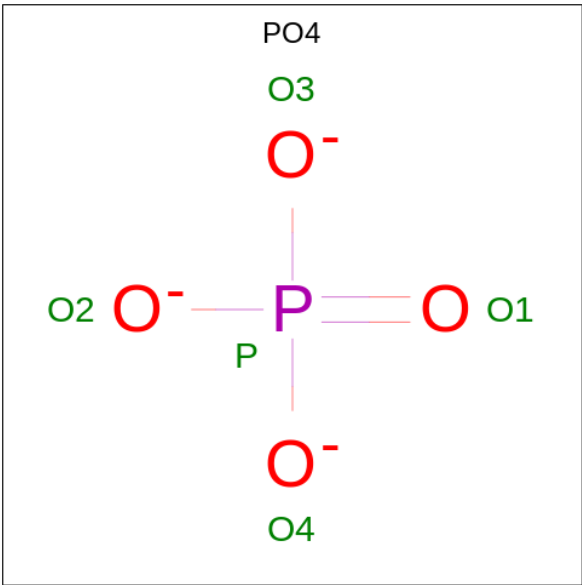
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			44	42	2	

- Molecule 17 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



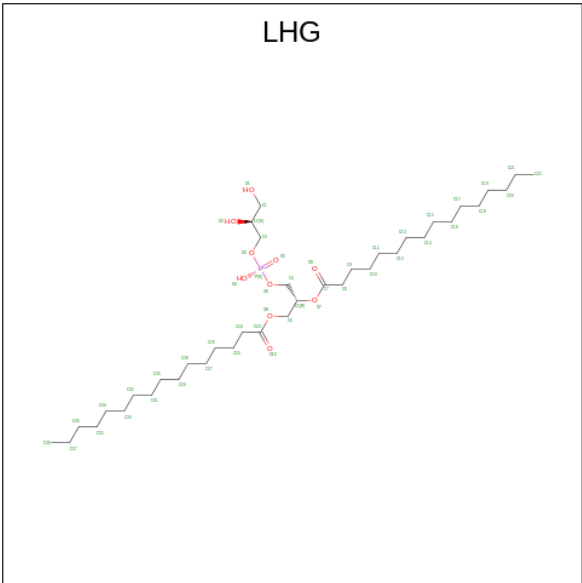
Mol	Chain	Residues	Atoms					AltConf
17	M	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 18 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
18	M	1	Total	O	P	0
			5	4	1	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

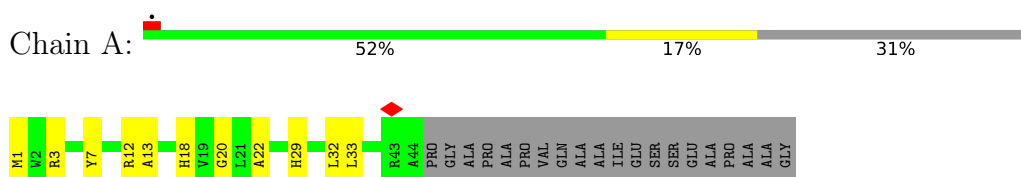


Mol	Chain	Residues	Atoms			AltConf
19	T	1	Total	C	O	0
			10	9	1	

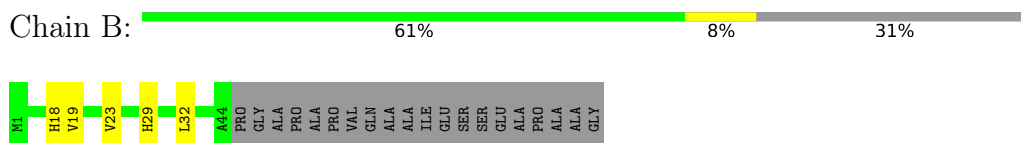
3 Residue-property plots [i](#)

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

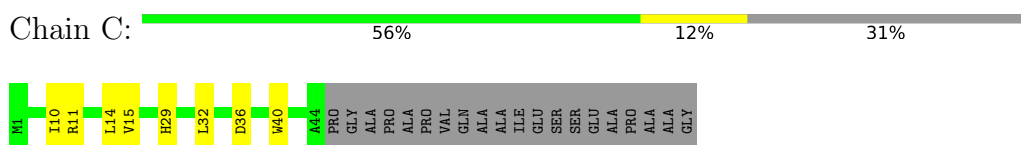
- Molecule 1: Light-harvesting complex 1 alpha chain



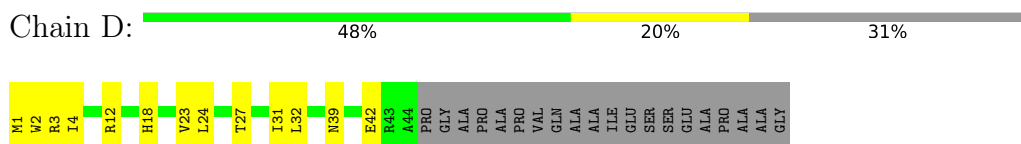
- Molecule 1: Light-harvesting complex 1 alpha chain



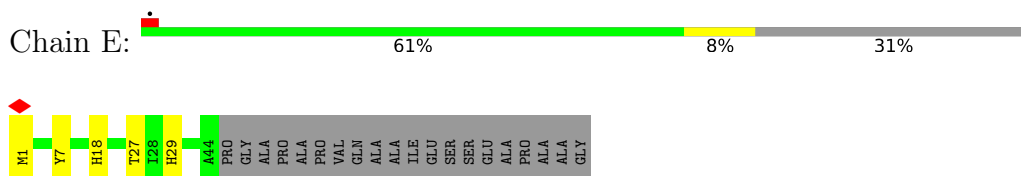
- Molecule 1: Light-harvesting complex 1 alpha chain



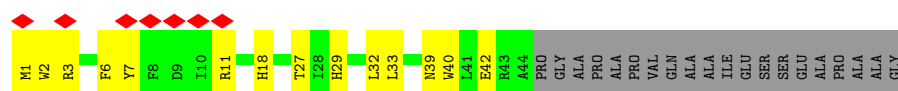
- Molecule 1: Light-harvesting complex 1 alpha chain



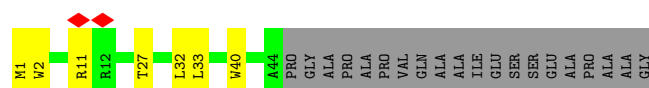
- Molecule 1: Light-harvesting complex 1 alpha chain



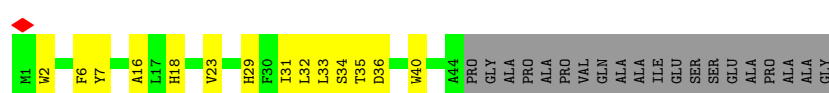
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 1: Light-harvesting complex 1 alpha chain



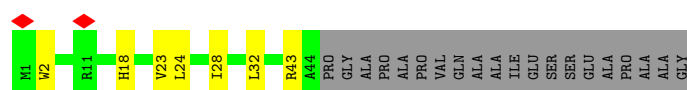
- Molecule 1: Light-harvesting complex 1 alpha chain



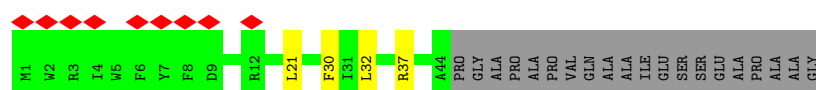
- Molecule 1: Light-harvesting complex 1 alpha chain



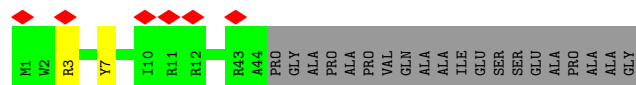
- Molecule 1: Light-harvesting complex 1 alpha chain



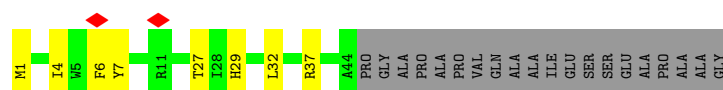
- Molecule 1: Light-harvesting complex 1 alpha chain



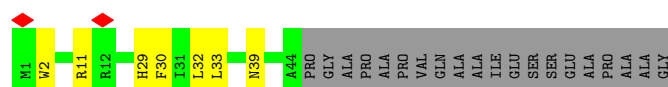
- Molecule 1: Light-harvesting complex 1 alpha chain



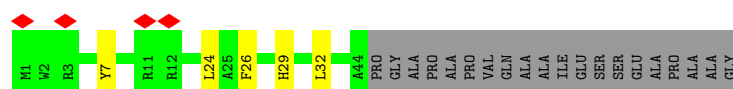
- Molecule 1: Light-harvesting complex 1 alpha chain



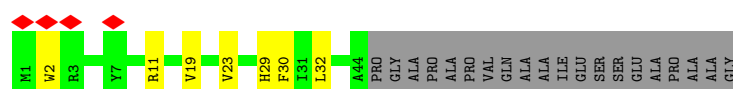
- Molecule 1: Light-harvesting complex 1 alpha chain



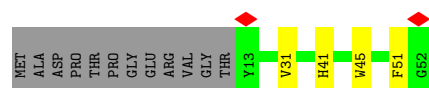
- Molecule 1: Light-harvesting complex 1 alpha chain



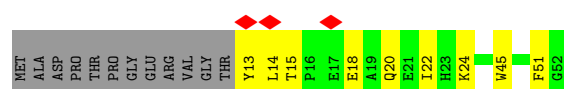
- Molecule 1: Light-harvesting complex 1 alpha chain



- Molecule 2: Antenna complex alpha/beta subunit

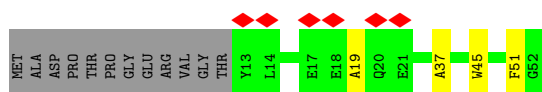


- Molecule 2: Antenna complex alpha/beta subunit

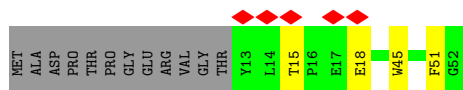


- Molecule 2: Antenna complex alpha/beta subunit

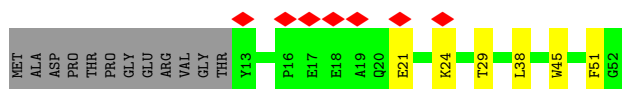




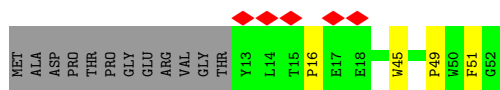
- Molecule 2: Antenna complex alpha/beta subunit



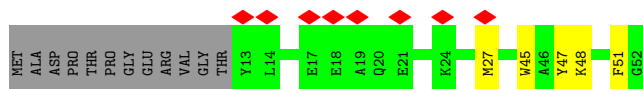
- Molecule 2: Antenna complex alpha/beta subunit



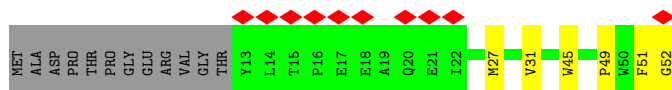
- Molecule 2: Antenna complex alpha/beta subunit



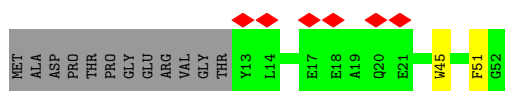
- Molecule 2: Antenna complex alpha/beta subunit



- Molecule 2: Antenna complex alpha/beta subunit



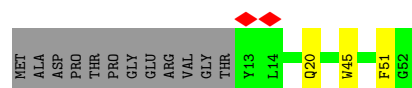
- Molecule 2: Antenna complex alpha/beta subunit



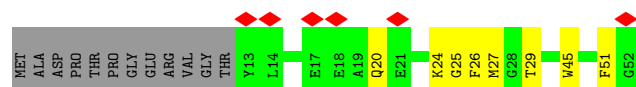
- Molecule 2: Antenna complex alpha/beta subunit



- Molecule 2: Antenna complex alpha/beta subunit



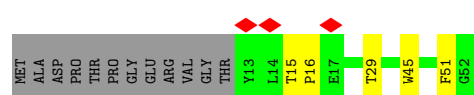
- Molecule 2: Antenna complex alpha/beta subunit



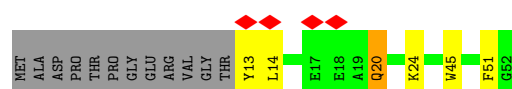
- Molecule 2: Antenna complex alpha/beta subunit



- Molecule 2: Antenna complex alpha/beta subunit

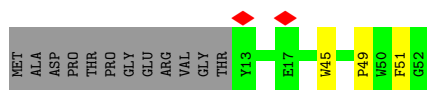


- Molecule 2: Antenna complex alpha/beta subunit



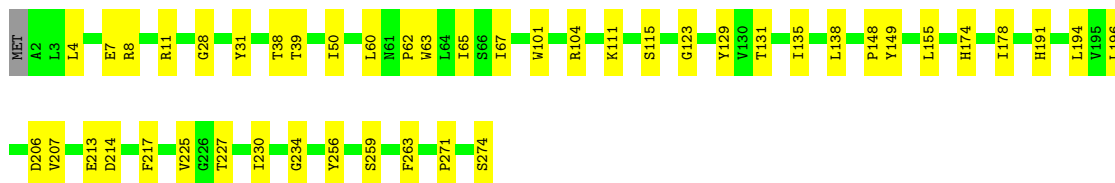
- Molecule 2: Antenna complex alpha/beta subunit





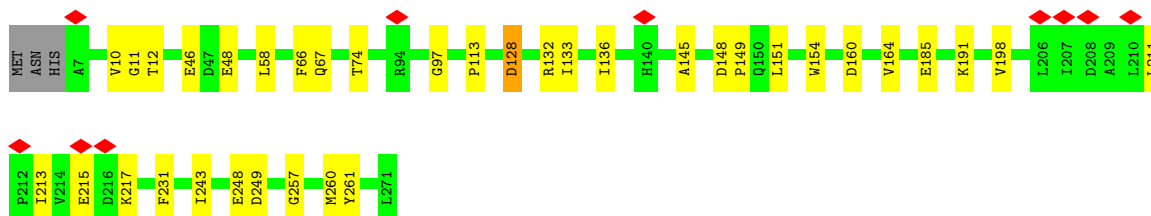
• Molecule 3: Reaction center protein L chain

Chain L: 83% 16%



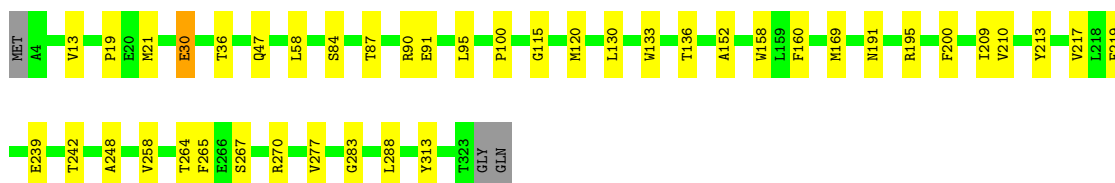
• Molecule 4: Photosynthetic reaction center H subunit

Chain H: 85% 13%



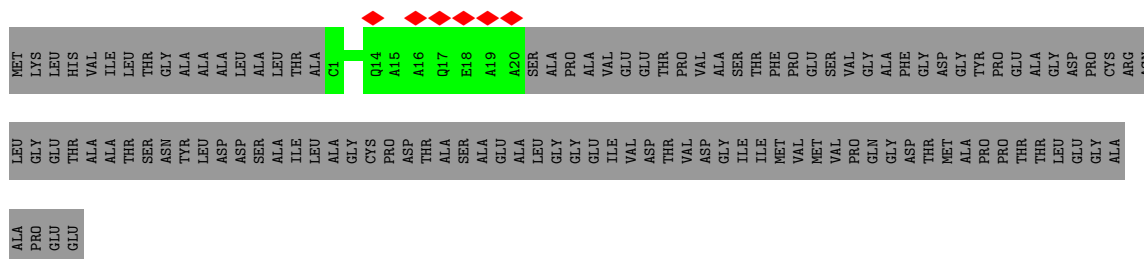
• Molecule 5: Reaction center protein M chain

Chain M: 86% 13%



• Molecule 6: Secreted protein

Chain T: 15% 85%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.532	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0961	Depositor
Map size ($\text{\AA}$)	323.2, 323.2, 323.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, 8K6, FE, A1ELD, BPH, PO4, H4X, BCL, UQ8, PEF, LHG, A1EL2, PGV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/397	0.26	0/540
1	B	0.10	0/397	0.19	0/540
1	C	0.58	0/397	0.87	0/540
1	D	0.09	0/397	0.20	0/540
1	E	0.09	0/397	0.20	0/540
1	F	0.09	0/397	0.25	0/540
1	G	0.09	0/397	0.19	0/540
1	I	0.09	0/397	0.21	0/540
1	J	0.18	0/397	0.27	0/540
1	K	0.54	0/397	0.72	0/540
1	N	0.09	0/397	0.19	0/540
1	O	0.07	0/397	0.18	0/540
1	P	0.19	0/397	0.32	0/540
1	Q	0.09	0/397	0.20	0/540
1	R	0.10	0/397	0.28	0/540
1	S	0.10	0/397	0.28	0/540
2	a	0.14	0/339	0.27	0/462
2	b	0.12	0/339	0.25	0/462
2	c	0.13	0/339	0.26	0/462
2	d	0.11	0/339	0.21	0/462
2	e	0.12	0/339	0.25	0/462
2	f	0.13	0/339	0.28	0/462
2	g	0.13	0/339	0.28	0/462
2	i	0.10	0/339	0.21	0/462
2	j	0.12	0/339	0.24	0/462
2	k	0.11	0/339	0.25	0/462
2	n	0.12	0/339	0.24	0/462
2	o	0.10	0/339	0.21	0/462
2	p	0.11	0/339	0.23	0/462
2	q	0.12	0/339	0.22	0/462
2	r	0.11	0/339	0.26	0/462
2	s	0.11	0/339	0.20	0/462

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	L	0.14	0/2214	0.30	0/3033
4	H	0.23	0/2139	0.36	1/2912 (0.0%)
5	M	0.13	0/2640	0.27	0/3612
6	T	0.06	0/119	0.17	0/161
All	All	0.18	0/18888	0.31	1/25750 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	198	VAL	N-CA-C	-5.57	107.30	112.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	384	0	389	12	0
1	B	384	0	389	5	0
1	C	384	0	389	8	0
1	D	384	0	389	13	0
1	E	384	0	389	10	0
1	F	384	0	389	16	0
1	G	384	0	389	6	0
1	I	384	0	389	12	0
1	J	384	0	389	10	0
1	K	384	0	389	3	0
1	N	384	0	389	11	0
1	O	384	0	389	5	0
1	P	384	0	389	7	0
1	Q	384	0	389	14	0
1	R	384	0	389	12	0
1	S	384	0	389	7	0
2	a	326	0	317	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	326	0	317	3	0
2	c	326	0	317	8	0
2	d	326	0	317	1	0
2	e	326	0	317	8	0
2	f	326	0	317	10	0
2	g	326	0	317	6	0
2	i	326	0	317	2	0
2	j	326	0	317	1	0
2	k	326	0	317	6	0
2	n	326	0	317	4	0
2	o	326	0	317	2	0
2	p	326	0	317	3	0
2	q	326	0	317	3	0
2	r	326	0	317	9	0
2	s	326	0	317	4	0
3	L	2135	0	2086	43	0
4	H	2079	0	2037	25	0
5	M	2543	0	2434	36	0
6	T	120	0	103	0	0
7	A	66	0	74	2	0
7	B	66	0	74	4	0
7	C	66	0	74	5	0
7	D	66	0	74	0	0
7	E	66	0	74	3	0
7	F	66	0	74	3	0
7	G	66	0	74	1	0
7	I	66	0	74	3	0
7	J	66	0	74	1	0
7	K	66	0	74	1	0
7	L	132	0	148	9	0
7	M	132	0	148	4	0
7	N	66	0	74	3	0
7	O	66	0	74	2	0
7	P	66	0	74	3	0
7	Q	66	0	74	1	0
7	R	66	0	74	2	0
7	S	66	0	74	3	0
7	a	66	0	74	4	0
7	b	66	0	74	8	0
7	c	66	0	74	3	0
7	d	66	0	74	4	0
7	e	66	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	f	66	0	74	5	0
7	g	66	0	74	2	0
7	i	66	0	74	0	0
7	j	66	0	74	2	0
7	k	66	0	74	3	0
7	n	66	0	74	5	0
7	o	66	0	74	4	0
7	p	66	0	74	3	0
7	q	66	0	74	3	0
7	r	66	0	74	2	0
7	s	66	0	74	3	0
8	A	43	0	0	1	0
8	B	43	0	0	1	0
8	C	43	0	0	0	0
8	D	43	0	0	1	0
8	E	43	0	0	1	0
8	F	43	0	0	1	0
8	G	43	0	0	0	0
8	I	43	0	0	4	0
8	J	43	0	0	3	0
8	K	43	0	0	1	0
8	N	43	0	0	0	0
8	O	43	0	0	0	0
8	P	43	0	0	1	0
8	Q	43	0	0	1	0
8	r	86	0	0	9	0
9	A	44	0	0	0	0
9	B	44	0	0	1	0
9	C	44	0	0	0	0
9	J	44	0	0	0	0
9	O	44	0	0	1	0
9	R	88	0	0	23	0
9	b	44	0	0	0	0
9	d	44	0	0	1	0
9	e	44	0	0	7	0
9	f	44	0	0	7	0
9	g	44	0	0	3	0
9	j	44	0	0	0	0
9	o	44	0	0	1	0
9	q	44	0	0	0	0
9	r	44	0	0	1	0
10	C	9	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	18	0	38	0	0
10	L	51	0	92	11	0
10	M	15	0	29	1	0
10	Q	36	0	76	8	0
10	S	13	0	25	1	0
10	f	14	0	27	0	0
11	D	51	0	76	8	0
11	F	51	0	76	4	0
11	G	23	0	21	1	0
11	L	50	0	43	4	0
11	M	38	0	50	3	0
11	T	50	0	54	3	0
12	G	30	0	32	0	0
12	L	28	0	29	2	0
12	N	26	0	24	1	0
13	L	130	0	150	6	0
14	L	37	0	32	6	0
14	M	53	0	74	1	0
15	M	1	0	0	0	0
16	M	44	0	0	0	0
17	M	43	0	62	1	0
18	M	5	0	0	0	0
19	T	10	0	14	3	0
All	All	22831	0	21658	370	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 8.

The worst 5 of 370 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:R:102:A1ELD:C35	9:R:102:A1ELD:C36	1.76	1.59
9:R:102:A1ELD:C39	9:R:102:A1ELD:C37	1.80	1.59
9:R:102:A1ELD:C39	1:N:33:LEU:CD1	2.15	1.24
9:R:102:A1ELD:C39	1:N:33:LEU:HD11	1.76	1.14
9:R:102:A1ELD:C39	1:N:33:LEU:HD12	1.80	1.11

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	A	42/64 (66%)	42 (100%)	0	0	100	100
1	B	42/64 (66%)	42 (100%)	0	0	100	100
1	C	42/64 (66%)	42 (100%)	0	0	100	100
1	D	42/64 (66%)	42 (100%)	0	0	100	100
1	E	42/64 (66%)	42 (100%)	0	0	100	100
1	F	42/64 (66%)	42 (100%)	0	0	100	100
1	G	42/64 (66%)	42 (100%)	0	0	100	100
1	I	42/64 (66%)	42 (100%)	0	0	100	100
1	J	42/64 (66%)	42 (100%)	0	0	100	100
1	K	42/64 (66%)	41 (98%)	1 (2%)	0	100	100
1	N	42/64 (66%)	42 (100%)	0	0	100	100
1	O	42/64 (66%)	42 (100%)	0	0	100	100
1	P	42/64 (66%)	42 (100%)	0	0	100	100
1	Q	42/64 (66%)	42 (100%)	0	0	100	100
1	R	42/64 (66%)	42 (100%)	0	0	100	100
1	S	42/64 (66%)	42 (100%)	0	0	100	100
2	a	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	b	38/52 (73%)	38 (100%)	0	0	100	100
2	c	38/52 (73%)	38 (100%)	0	0	100	100
2	d	38/52 (73%)	38 (100%)	0	0	100	100
2	e	38/52 (73%)	38 (100%)	0	0	100	100
2	f	38/52 (73%)	38 (100%)	0	0	100	100
2	g	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	i	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	j	38/52 (73%)	37 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	k	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	n	38/52 (73%)	38 (100%)	0	0	100	100
2	o	38/52 (73%)	38 (100%)	0	0	100	100
2	p	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	q	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
2	r	38/52 (73%)	38 (100%)	0	0	100	100
2	s	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
3	L	271/274 (99%)	268 (99%)	3 (1%)	0	100	100
4	H	263/268 (98%)	258 (98%)	5 (2%)	0	100	100
5	M	318/323 (98%)	314 (99%)	4 (1%)	0	100	100
6	T	18/135 (13%)	18 (100%)	0	0	100	100
All	All	2150/2856 (75%)	2129 (99%)	21 (1%)	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	A	38/49 (78%)	38 (100%)	0	100	100
1	B	38/49 (78%)	38 (100%)	0	100	100
1	C	38/49 (78%)	38 (100%)	0	100	100
1	D	38/49 (78%)	38 (100%)	0	100	100
1	E	38/49 (78%)	38 (100%)	0	100	100
1	F	38/49 (78%)	38 (100%)	0	100	100
1	G	38/49 (78%)	38 (100%)	0	100	100
1	I	38/49 (78%)	38 (100%)	0	100	100
1	J	38/49 (78%)	38 (100%)	0	100	100
1	K	38/49 (78%)	37 (97%)	1 (3%)	40	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	38/49 (78%)	38 (100%)	0	100	100
1	O	38/49 (78%)	38 (100%)	0	100	100
1	P	38/49 (78%)	38 (100%)	0	100	100
1	Q	38/49 (78%)	38 (100%)	0	100	100
1	R	38/49 (78%)	38 (100%)	0	100	100
1	S	38/49 (78%)	38 (100%)	0	100	100
2	a	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	b	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	c	31/40 (78%)	31 (100%)	0	100	100
2	d	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	e	31/40 (78%)	31 (100%)	0	100	100
2	f	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	g	31/40 (78%)	31 (100%)	0	100	100
2	i	31/40 (78%)	31 (100%)	0	100	100
2	j	31/40 (78%)	31 (100%)	0	100	100
2	k	31/40 (78%)	31 (100%)	0	100	100
2	n	31/40 (78%)	31 (100%)	0	100	100
2	o	31/40 (78%)	31 (100%)	0	100	100
2	p	31/40 (78%)	31 (100%)	0	100	100
2	q	31/40 (78%)	30 (97%)	1 (3%)	34	49
2	r	31/40 (78%)	31 (100%)	0	100	100
2	s	31/40 (78%)	31 (100%)	0	100	100
3	L	215/216 (100%)	214 (100%)	1 (0%)	81	89
4	H	216/220 (98%)	212 (98%)	4 (2%)	50	66
5	M	250/252 (99%)	249 (100%)	1 (0%)	84	91
6	T	9/94 (10%)	9 (100%)	0	100	100
All	All	1794/2206 (81%)	1782 (99%)	12 (1%)	73	86

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	128	ASP
4	H	133	ILE

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Mol	Chain	Res	Type
5	M	30	GLU
4	H	136	ILE
2	d	20	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	a	20	GLN
4	H	204	ASN
5	M	302	GLN
5	M	296	ASN
1	P	18	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 1 is monoatomic - leaving 99 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	$\# Z > 2$
7	BCL	b	102	2	69,74,74	1.82	18 (26%)	83,115,115	2.39	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	M	403	5	69,74,74	1.80	18 (26%)	83,115,115	2.61	22 (26%)
10	8K6	C	104	-	8,8,17	0.09	0	7,7,16	0.10	0
10	8K6	f	103	-	13,13,17	0.09	0	12,12,16	0.08	0
8	A1EL2	D	102	-	43,44,44	1.63	8 (18%)	56,62,62	1.53	10 (17%)
9	A1ELD	o	101	-	43,44,44	4.99	31 (72%)	51,58,58	1.86	13 (25%)
7	BCL	B	101	1	69,74,74	1.80	17 (24%)	83,115,115	2.57	26 (31%)
8	A1EL2	B	102	-	43,44,44	1.63	8 (18%)	56,62,62	1.52	10 (17%)
17	PEF	M	407	-	42,42,46	0.28	0	45,47,51	0.32	0
7	BCL	k	101	2	69,74,74	1.78	17 (24%)	83,115,115	2.33	23 (27%)
7	BCL	i	101	2	69,74,74	1.80	17 (24%)	83,115,115	2.52	25 (30%)
8	A1EL2	J	102	-	43,44,44	3.81	29 (67%)	56,62,62	4.38	36 (64%)
10	8K6	M	406	-	14,14,17	0.09	0	13,13,16	0.11	0
14	UQ8	L	304	-	19,19,53	1.01	2 (10%)	23,26,67	0.99	1 (4%)
9	A1ELD	R	103	-	43,44,44	1.74	10 (23%)	51,58,58	1.64	12 (23%)
8	A1EL2	O	103	-	43,44,44	2.90	23 (53%)	56,62,62	1.82	15 (26%)
9	A1ELD	q	101	-	43,44,44	1.70	10 (23%)	51,58,58	1.61	10 (19%)
16	H4X	M	405	-	43,43,43	1.60	8 (18%)	50,54,54	1.27	9 (18%)
11	PGV	M	408	-	37,37,50	1.09	2 (5%)	41,42,56	1.20	4 (9%)
8	A1EL2	K	102	-	43,44,44	1.90	13 (30%)	56,62,62	1.31	7 (12%)
7	BCL	e	102	2	69,74,74	1.81	18 (26%)	83,115,115	2.43	26 (31%)
10	8K6	L	310	-	11,11,17	0.08	0	10,10,16	0.07	0
13	BPH	L	303	-	59,70,70	2.55	15 (25%)	61,101,101	2.17	16 (26%)
7	BCL	c	101	2	69,74,74	1.82	16 (23%)	83,115,115	2.39	22 (26%)
10	8K6	Q	104	-	17,17,17	0.07	0	16,16,16	0.11	0
7	BCL	G	101	1	69,74,74	1.81	19 (27%)	83,115,115	2.61	24 (28%)
11	PGV	D	103	-	50,50,50	0.91	2 (4%)	53,56,56	1.06	4 (7%)
8	A1EL2	C	103	-	43,44,44	1.63	8 (18%)	56,62,62	1.53	9 (16%)
19	LHG	T	302	6	9,9,48	0.28	0	8,8,54	1.12	1 (12%)
12	LMT	L	309	-	29,29,36	1.30	5 (17%)	40,40,47	1.06	1 (2%)
7	BCL	C	101	1	69,74,74	1.80	19 (27%)	83,115,115	2.70	26 (31%)
9	A1ELD	A	103	-	43,44,44	1.66	10 (23%)	51,58,58	1.47	10 (19%)
7	BCL	j	102	2	69,74,74	1.79	16 (23%)	83,115,115	2.44	23 (27%)
7	BCL	R	101	1	69,74,74	1.80	20 (28%)	83,115,115	2.59	22 (26%)
7	BCL	D	101	1	69,74,74	1.82	19 (27%)	83,115,115	2.74	29 (34%)
9	A1ELD	b	101	-	43,44,44	1.83	10 (23%)	51,58,58	1.58	11 (21%)
18	PO4	M	409	-	4,4,4	0.96	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	8K6	H	301	-	17,17,17	0.08	0	16,16,16	0.06	0
12	LMT	N	103	-	27,27,36	1.35	6 (22%)	37,38,47	0.92	1 (2%)
10	8K6	Q	103	-	17,17,17	0.09	0	16,16,16	0.07	0
7	BCL	L	302	3	69,74,74	1.81	17 (24%)	83,115,115	2.32	23 (27%)
8	A1EL2	I	102	-	43,44,44	2.73	22 (51%)	56,62,62	3.18	29 (51%)
7	BCL	o	102	2	69,74,74	1.79	18 (26%)	83,115,115	2.40	27 (32%)
7	BCL	d	102	2	69,74,74	1.81	16 (23%)	83,115,115	2.50	23 (27%)
7	BCL	L	301	3	69,74,74	1.84	17 (24%)	83,115,115	2.62	23 (27%)
7	BCL	f	102	2	69,74,74	1.78	17 (24%)	83,115,115	2.50	27 (32%)
8	A1EL2	A	102	-	43,44,44	1.62	8 (18%)	56,62,62	1.52	10 (17%)
7	BCL	s	101	2	69,74,74	1.80	17 (24%)	83,115,115	2.40	22 (26%)
9	A1ELD	R	102	-	43,44,44	6.22	37 (86%)	51,58,58	4.71	27 (52%)
10	8K6	L	312	-	9,9,17	0.10	0	8,8,16	0.08	0
10	8K6	S	102	-	12,12,17	0.09	0	11,11,16	0.10	0
8	A1EL2	G	102	-	43,44,44	2.26	18 (41%)	56,62,62	1.40	9 (16%)
9	A1ELD	J	103	-	43,44,44	1.87	13 (30%)	51,58,58	1.55	10 (19%)
11	PGV	G	103	-	22,22,50	1.75	3 (13%)	24,26,56	1.48	3 (12%)
7	BCL	I	101	1	69,74,74	1.80	18 (26%)	83,115,115	2.60	27 (32%)
8	A1EL2	r	103	-	43,44,44	4.76	34 (79%)	56,62,62	2.88	30 (53%)
11	PGV	T	301	-	19,19,50	1.52	2 (10%)	21,21,56	1.59	5 (23%)
7	BCL	n	101	2	69,74,74	1.81	17 (24%)	83,115,115	2.44	26 (31%)
9	A1ELD	C	102	-	43,44,44	1.61	6 (13%)	51,58,58	1.76	11 (21%)
10	8K6	L	313	-	14,14,17	0.10	0	13,13,16	0.12	0
7	BCL	F	101	1	69,74,74	1.92	20 (28%)	83,115,115	2.41	23 (27%)
7	BCL	K	101	1	69,74,74	1.81	18 (26%)	83,115,115	2.60	26 (31%)
7	BCL	A	101	1	69,74,74	1.83	20 (28%)	83,115,115	2.67	26 (31%)
7	BCL	r	104	2	69,74,74	1.80	17 (24%)	83,115,115	2.39	20 (24%)
8	A1EL2	Q	102	-	43,44,44	3.24	25 (58%)	56,62,62	1.43	7 (12%)
13	BPH	L	305	-	59,70,70	0.83	4 (6%)	61,101,101	1.27	4 (6%)
8	A1EL2	r	102	-	43,44,44	2.38	14 (32%)	56,62,62	1.67	13 (23%)
9	A1ELD	e	101	-	43,44,44	2.62	22 (51%)	51,58,58	1.53	10 (19%)
9	A1ELD	B	103	-	43,44,44	2.37	19 (44%)	51,58,58	2.06	16 (31%)
8	A1EL2	P	102	-	43,44,44	3.45	21 (48%)	56,62,62	2.23	26 (46%)
9	A1ELD	r	101	-	43,44,44	1.71	10 (23%)	51,58,58	1.59	12 (23%)
7	BCL	g	102	2	69,74,74	1.80	17 (24%)	83,115,115	2.41	25 (30%)
9	A1ELD	j	101	-	43,44,44	1.32	6 (13%)	51,58,58	1.75	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LMT	G	104	-	31,31,36	1.27	5 (16%)	42,42,47	0.93	2 (4%)
7	BCL	Q	101	1	69,74,74	1.80	19 (27%)	83,115,115	2.56	23 (27%)
8	A1EL2	E	102	-	43,44,44	1.63	8 (18%)	56,62,62	1.53	10 (17%)
7	BCL	q	102	2	69,74,74	1.81	17 (24%)	83,115,115	2.47	25 (30%)
14	UQ8	L	306	-	18,18,53	1.07	2 (11%)	22,25,67	0.74	0
7	BCL	S	101	1	69,74,74	1.83	17 (24%)	83,115,115	2.65	25 (30%)
7	BCL	p	101	2	69,74,74	1.80	17 (24%)	83,115,115	2.38	23 (27%)
11	PGV	L	307	-	20,20,50	1.25	2 (10%)	24,25,56	1.38	3 (12%)
7	BCL	O	101	1	69,74,74	1.83	19 (27%)	83,115,115	2.64	23 (27%)
10	8K6	L	311	-	13,13,17	0.08	0	12,12,16	0.11	0
8	A1EL2	F	102	-	43,44,44	1.62	8 (18%)	56,62,62	1.52	10 (17%)
11	PGV	F	103	-	50,50,50	0.90	2 (4%)	53,56,56	1.08	4 (7%)
9	A1ELD	g	101	-	43,44,44	1.69	9 (20%)	51,58,58	1.72	11 (21%)
7	BCL	N	101	1	69,74,74	1.82	20 (28%)	83,115,115	2.61	25 (30%)
7	BCL	E	101	1	69,74,74	1.81	18 (26%)	83,115,115	2.55	25 (30%)
9	A1ELD	d	101	-	43,44,44	1.91	14 (32%)	51,58,58	1.46	9 (17%)
7	BCL	M	401	5	69,74,74	1.89	19 (27%)	83,115,115	2.73	27 (32%)
14	UQ8	M	402	-	53,53,53	0.65	2 (3%)	64,67,67	0.56	0
7	BCL	a	101	2	69,74,74	1.77	17 (24%)	83,115,115	2.35	25 (30%)
9	A1ELD	f	101	-	43,44,44	1.67	9 (20%)	51,58,58	1.52	11 (21%)
7	BCL	P	101	1	69,74,74	1.83	19 (27%)	83,115,115	2.64	25 (30%)
8	A1EL2	N	102	-	43,44,44	1.61	8 (18%)	56,62,62	1.49	10 (17%)
11	PGV	T	303	-	29,29,50	1.22	2 (6%)	33,34,56	1.31	4 (12%)
11	PGV	L	308	-	28,28,50	1.23	2 (7%)	31,34,56	1.28	4 (12%)
7	BCL	J	101	1	69,74,74	1.83	18 (26%)	83,115,115	2.65	23 (27%)
9	A1ELD	O	102	-	43,44,44	3.36	21 (48%)	51,58,58	2.74	17 (33%)

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
7	BCL	b	102	2	-	15/41/137/137	-
7	BCL	M	403	5	-	17/41/137/137	-
10	8K6	C	104	-	-	3/6/6/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	8K6	f	103	-	-	0/11/11/15	-
8	A1EL2	D	102	-	-	4/29/72/72	0/2/2/2
9	A1ELD	o	101	-	-	3/42/61/61	0/1/1/1
7	BCL	B	101	1	-	22/41/137/137	-
8	A1EL2	B	102	-	-	4/29/72/72	0/2/2/2
17	PEF	M	407	-	-	4/46/46/50	-
7	BCL	k	101	2	-	17/41/137/137	-
7	BCL	i	101	2	-	17/41/137/137	-
8	A1EL2	J	102	-	-	4/29/72/72	0/2/2/2
10	8K6	M	406	-	-	2/12/12/15	-
14	UQ8	L	304	-	-	7/11/35/75	0/1/1/1
9	A1ELD	R	103	-	-	5/42/61/61	0/1/1/1
8	A1EL2	O	103	-	-	3/29/72/72	0/2/2/2
9	A1ELD	q	101	-	-	5/42/61/61	0/1/1/1
16	H4X	M	405	-	-	2/51/51/51	-
11	PGV	M	408	-	-	12/39/39/55	-
8	A1EL2	K	102	-	-	4/29/72/72	0/2/2/2
7	BCL	e	102	2	-	14/41/137/137	-
10	8K6	L	310	-	-	0/9/9/15	-
13	BPH	L	303	-	-	11/37/105/105	0/5/6/6
7	BCL	c	101	2	-	26/41/137/137	-
10	8K6	Q	104	-	-	4/15/15/15	-
7	BCL	G	101	1	-	19/41/137/137	-
11	PGV	D	103	-	-	12/55/55/55	-
8	A1EL2	C	103	-	-	4/29/72/72	0/2/2/2
19	LHG	T	302	6	-	3/6/7/53	-
12	LMT	L	309	-	-	7/14/54/61	0/2/2/2
7	BCL	C	101	1	-	16/41/137/137	-
9	A1ELD	A	103	-	-	3/42/61/61	0/1/1/1
7	BCL	j	102	2	-	13/41/137/137	-
7	BCL	R	101	1	-	17/41/137/137	-
7	BCL	D	101	1	-	22/41/137/137	-
9	A1ELD	b	101	-	-	3/42/61/61	0/1/1/1
10	8K6	H	301	-	-	1/15/15/15	-
12	LMT	N	103	-	-	3/12/52/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	8K6	Q	103	-	-	2/15/15/15	-
7	BCL	L	302	3	-	17/41/137/137	-
8	A1EL2	I	102	-	-	4/29/72/72	0/2/2/2
7	BCL	o	102	2	-	19/41/137/137	-
7	BCL	d	102	2	-	16/41/137/137	-
7	BCL	L	301	3	-	9/41/137/137	-
7	BCL	f	102	2	-	17/41/137/137	-
8	A1EL2	A	102	-	-	4/29/72/72	0/2/2/2
7	BCL	s	101	2	-	19/41/137/137	-
9	A1ELD	R	102	-	-	3/42/61/61	0/1/1/1
10	8K6	L	312	-	-	0/7/7/15	-
10	8K6	S	102	-	-	2/10/10/15	-
8	A1EL2	G	102	-	-	4/29/72/72	0/2/2/2
9	A1ELD	J	103	-	-	3/42/61/61	0/1/1/1
11	PGV	G	103	-	-	6/23/23/55	-
7	BCL	I	101	1	-	16/41/137/137	-
8	A1EL2	r	103	-	-	2/29/72/72	0/2/2/2
11	PGV	T	301	-	-	6/20/20/55	-
7	BCL	n	101	2	-	19/41/137/137	-
9	A1ELD	C	102	-	-	3/42/61/61	0/1/1/1
10	8K6	L	313	-	-	0/12/12/15	-
7	BCL	F	101	1	-	16/41/137/137	-
7	BCL	K	101	1	-	16/41/137/137	-
7	BCL	A	101	1	-	11/41/137/137	-
7	BCL	r	104	2	-	18/41/137/137	-
8	A1EL2	Q	102	-	-	4/29/72/72	0/2/2/2
13	BPH	L	305	-	-	16/37/105/105	0/5/6/6
8	A1EL2	r	102	-	-	9/29/72/72	0/2/2/2
9	A1ELD	e	101	-	-	3/42/61/61	0/1/1/1
9	A1ELD	B	103	-	-	3/42/61/61	0/1/1/1
8	A1EL2	P	102	-	-	4/29/72/72	0/2/2/2
9	A1ELD	r	101	-	-	0/42/61/61	0/1/1/1
7	BCL	g	102	2	-	17/41/137/137	-
9	A1ELD	j	101	-	-	3/42/61/61	0/1/1/1
12	LMT	G	104	-	-	4/16/56/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	Q	101	1	-	18/41/137/137	-
8	A1EL2	E	102	-	-	4/29/72/72	0/2/2/2
7	BCL	q	102	2	-	17/41/137/137	-
14	UQ8	L	306	-	-	2/9/33/75	0/1/1/1
7	BCL	S	101	1	-	24/41/137/137	-
7	BCL	p	101	2	-	23/41/137/137	-
11	PGV	L	307	-	-	4/21/21/55	-
7	BCL	O	101	1	-	18/41/137/137	-
10	8K6	L	311	-	-	0/11/11/15	-
8	A1EL2	F	102	-	-	4/29/72/72	0/2/2/2
11	PGV	F	103	-	-	9/55/55/55	-
9	A1ELD	g	101	-	-	3/42/61/61	0/1/1/1
7	BCL	N	101	1	-	13/41/137/137	-
7	BCL	E	101	1	-	17/41/137/137	-
9	A1ELD	d	101	-	-	3/42/61/61	0/1/1/1
7	BCL	M	401	5	-	9/41/137/137	-
14	UQ8	M	402	-	-	8/51/75/75	0/1/1/1
7	BCL	a	101	2	-	18/41/137/137	-
9	A1ELD	f	101	-	-	3/42/61/61	0/1/1/1
7	BCL	P	101	1	-	16/41/137/137	-
8	A1EL2	N	102	-	-	2/29/72/72	0/2/2/2
11	PGV	T	303	-	-	9/31/31/55	-
11	PGV	L	308	-	-	12/33/33/55	-
7	BCL	J	101	1	-	14/41/137/137	-
9	A1ELD	O	102	-	-	3/42/61/61	0/1/1/1

The worst 5 of 1201 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	102	A1ELD	C36-C35	16.77	1.76	1.50
9	R	102	A1ELD	C39-C37	12.20	1.80	1.52
9	R	102	A1ELD	C5-C4	11.91	1.69	1.51
8	r	103	A1EL2	C33-C34	11.72	1.69	1.52
9	o	101	A1ELD	C13-C10	11.63	1.51	1.35

The worst 5 of 1389 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	102	A1EL2	C40-C12-C13	-11.90	106.26	122.92
9	R	102	A1ELD	C11-C10-C13	-11.77	106.44	122.92
7	P	101	BCL	C2B-C1B-NB	11.76	118.12	110.23
9	R	102	A1ELD	C33-C32-C31	-11.50	106.82	122.92
7	J	101	BCL	C2B-C1B-NB	11.49	117.93	110.23

There are no chirality outliers.

5 of 876 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	101	BCL	C1A-C2A-CAA-CBA
7	C	101	BCL	C4B-C3B-CAB-CBB
7	D	101	BCL	C1A-C2A-CAA-CBA
7	D	101	BCL	C2B-C3B-CAB-OB
7	D	101	BCL	C2B-C3B-CAB-CBB

There are no ring outliers.

79 monomers are involved in 220 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	b	102	BCL	8	0
7	M	403	BCL	3	0
10	C	104	8K6	1	0
8	D	102	A1EL2	1	0
9	o	101	A1ELD	1	0
7	B	101	BCL	4	0
8	B	102	A1EL2	1	0
17	M	407	PEF	1	0
7	k	101	BCL	3	0
8	J	102	A1EL2	3	0
10	M	406	8K6	1	0
14	L	304	UQ8	6	0
11	M	408	PGV	3	0
8	K	102	A1EL2	1	0
7	e	102	BCL	2	0
10	L	310	8K6	1	0
13	L	303	BPH	5	0
7	c	101	BCL	3	0
10	Q	104	8K6	4	0
7	G	101	BCL	1	0
11	D	103	PGV	8	0
19	T	302	LHG	3	0

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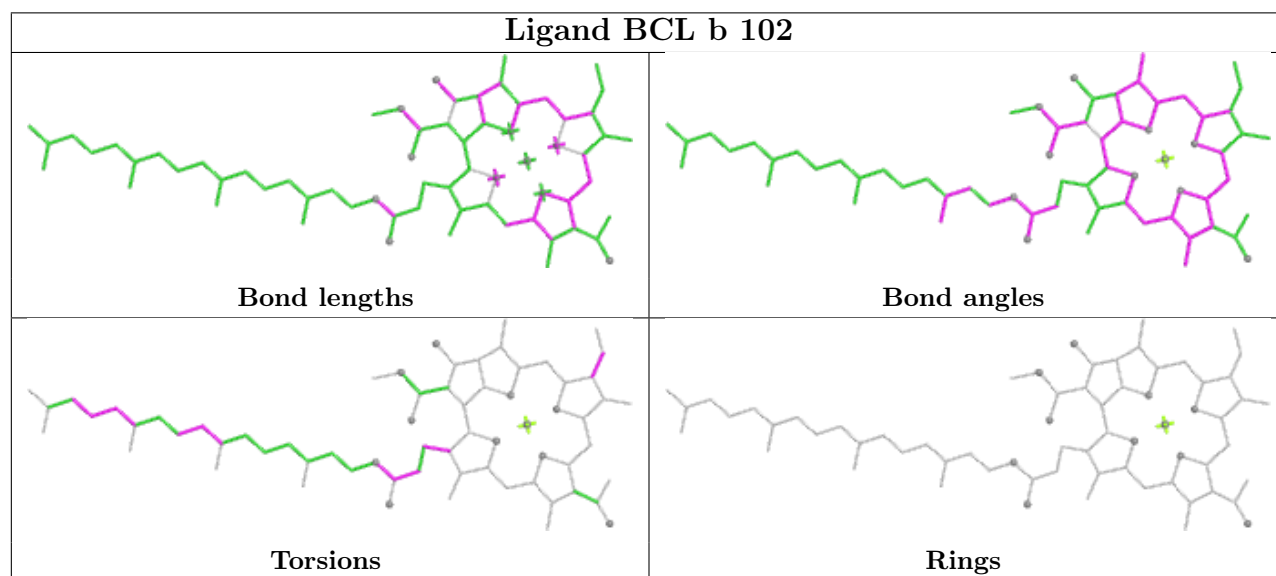
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	309	LMT	2	0
7	C	101	BCL	5	0
7	j	102	BCL	2	0
7	R	101	BCL	2	0
12	N	103	LMT	1	0
10	Q	103	8K6	4	0
7	L	302	BCL	7	0
8	I	102	A1EL2	4	0
7	o	102	BCL	4	0
7	d	102	BCL	4	0
7	L	301	BCL	2	0
7	f	102	BCL	5	0
8	A	102	A1EL2	1	0
7	s	101	BCL	3	0
9	R	102	A1ELD	23	0
10	L	312	8K6	1	0
10	S	102	8K6	1	0
11	G	103	PGV	1	0
7	I	101	BCL	3	0
8	r	103	A1EL2	1	0
7	n	101	BCL	5	0
10	L	313	8K6	7	0
7	F	101	BCL	3	0
7	K	101	BCL	1	0
7	A	101	BCL	2	0
7	r	104	BCL	2	0
8	Q	102	A1EL2	1	0
13	L	305	BPH	1	0
8	r	102	A1EL2	8	0
9	e	101	A1ELD	7	0
9	B	103	A1ELD	1	0
8	P	102	A1EL2	1	0
9	r	101	A1ELD	1	0
7	g	102	BCL	2	0
7	Q	101	BCL	1	0
8	E	102	A1EL2	1	0
7	q	102	BCL	3	0
7	S	101	BCL	3	0
7	p	101	BCL	3	0
11	L	307	PGV	1	0
7	O	101	BCL	2	0
10	L	311	8K6	2	0

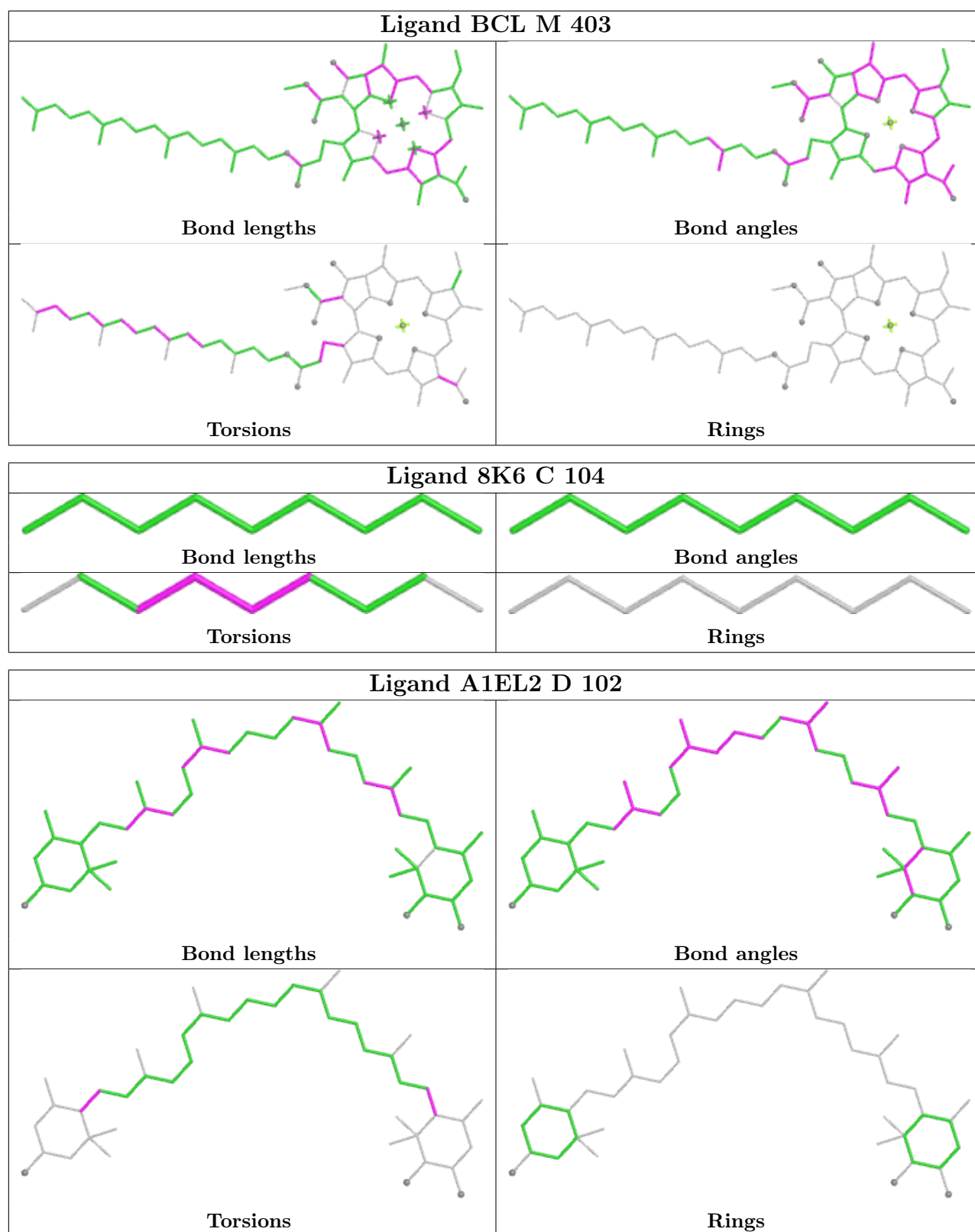
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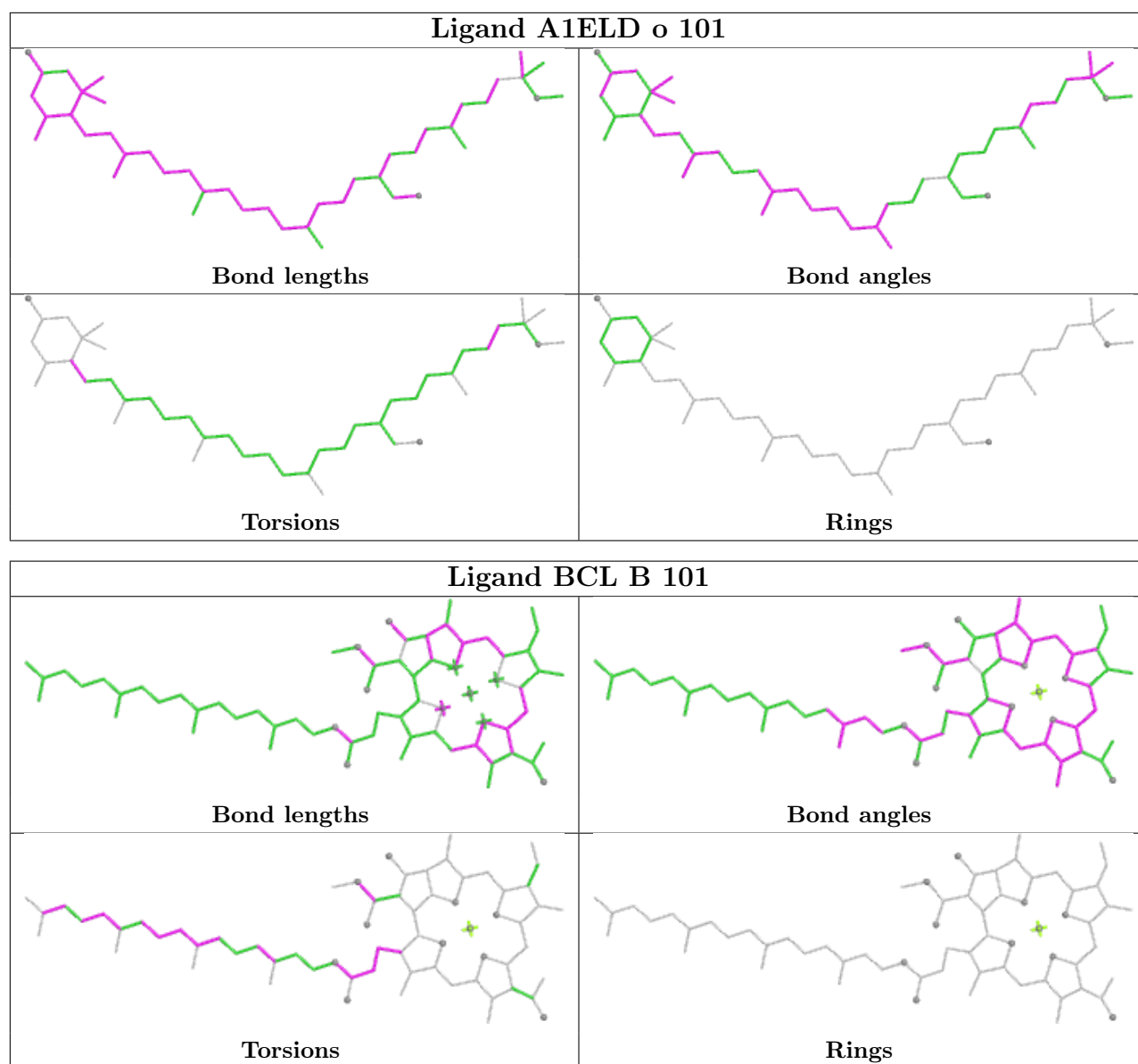
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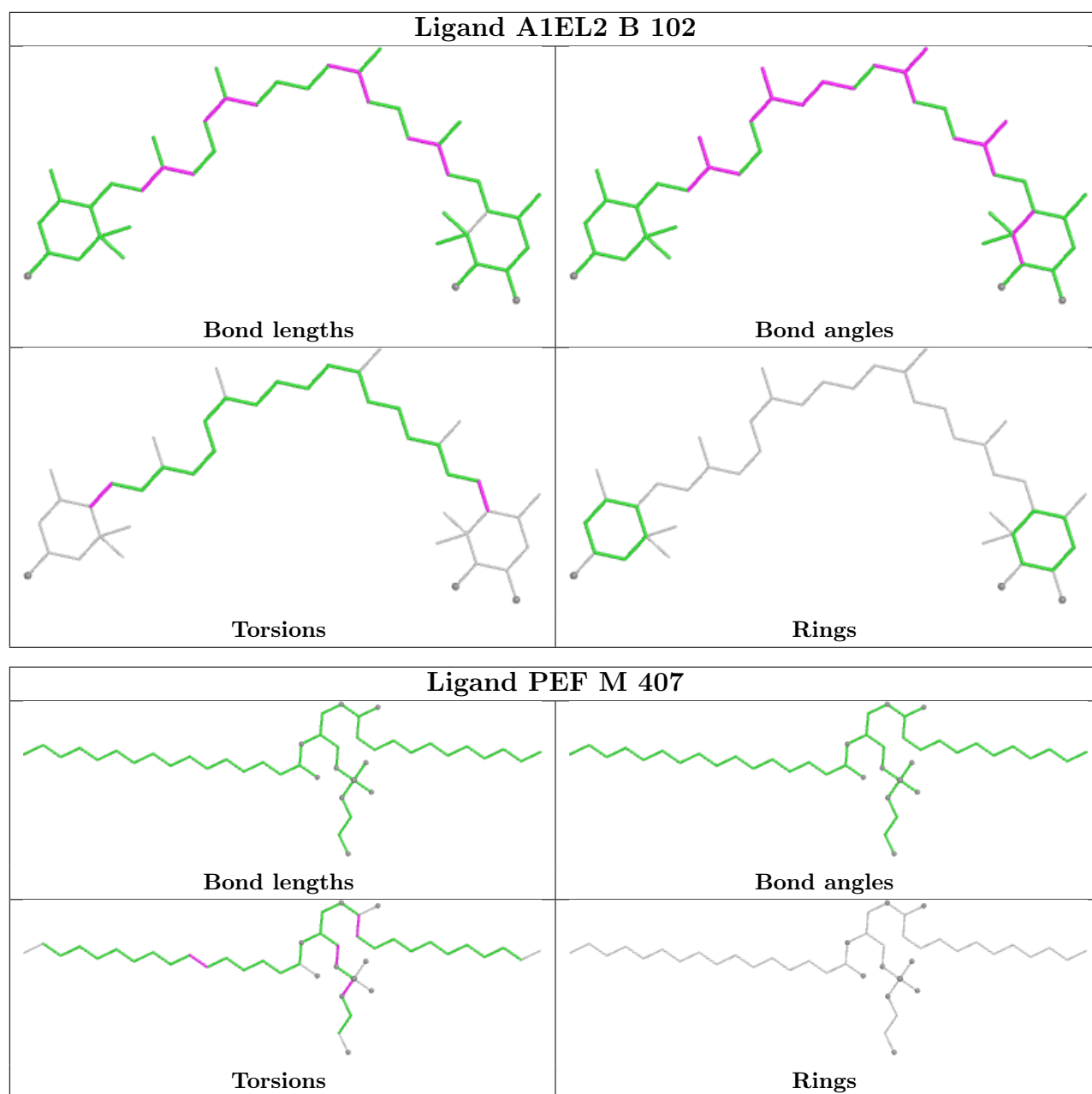
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	102	A1EL2	1	0
11	F	103	PGV	4	0
9	g	101	A1ELD	3	0
7	N	101	BCL	3	0
7	E	101	BCL	3	0
9	d	101	A1ELD	1	0
7	M	401	BCL	1	0
14	M	402	UQ8	1	0
7	a	101	BCL	4	0
9	f	101	A1ELD	7	0
7	P	101	BCL	3	0
11	T	303	PGV	3	0
11	L	308	PGV	3	0
7	J	101	BCL	1	0
9	O	102	A1ELD	1	0

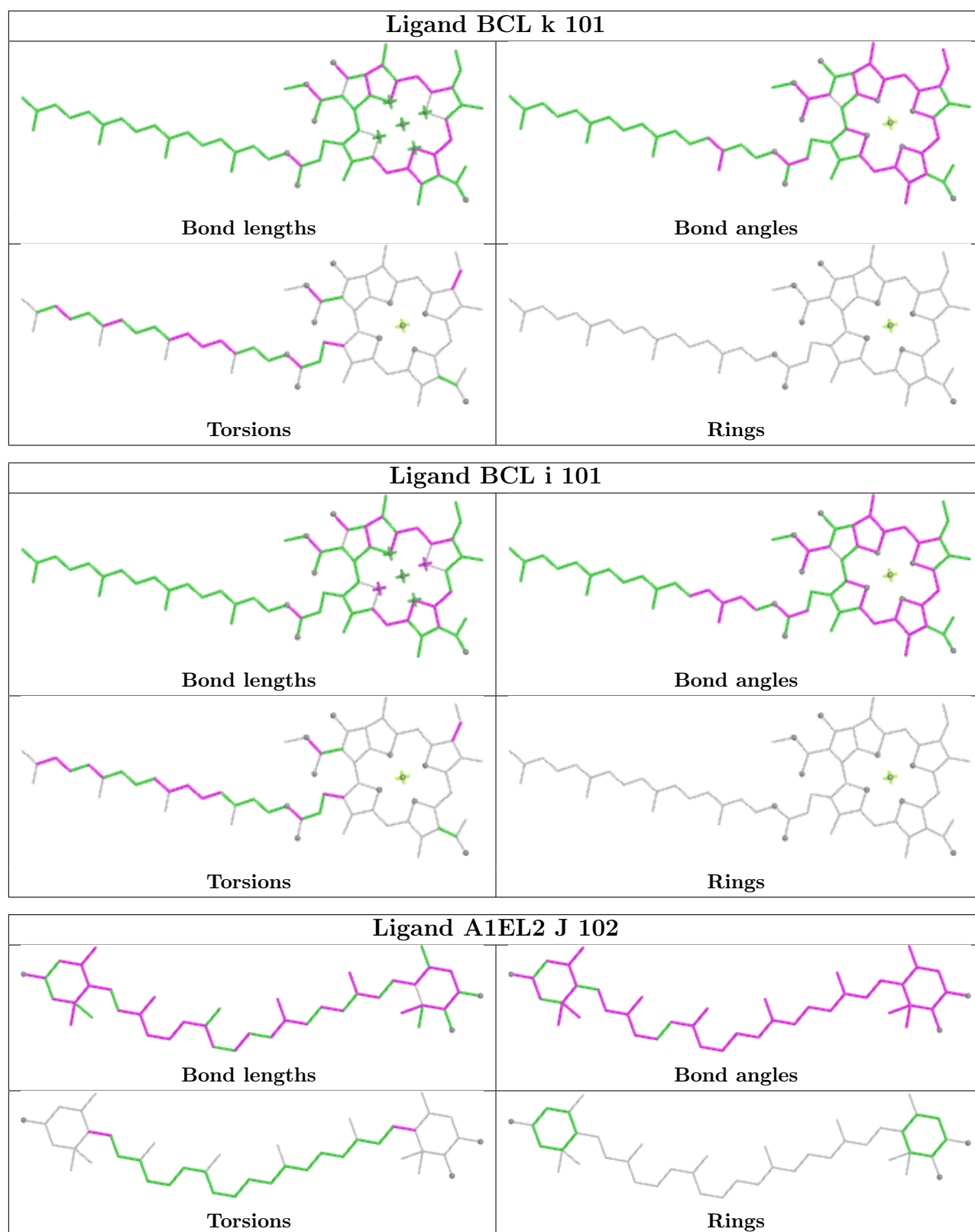
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

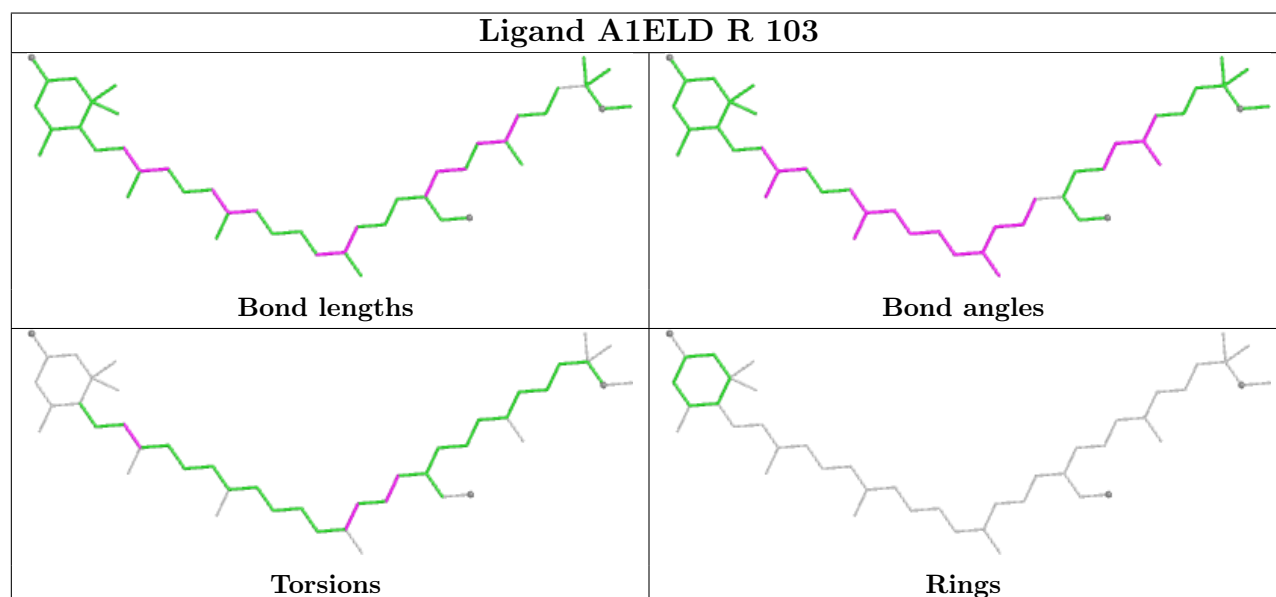
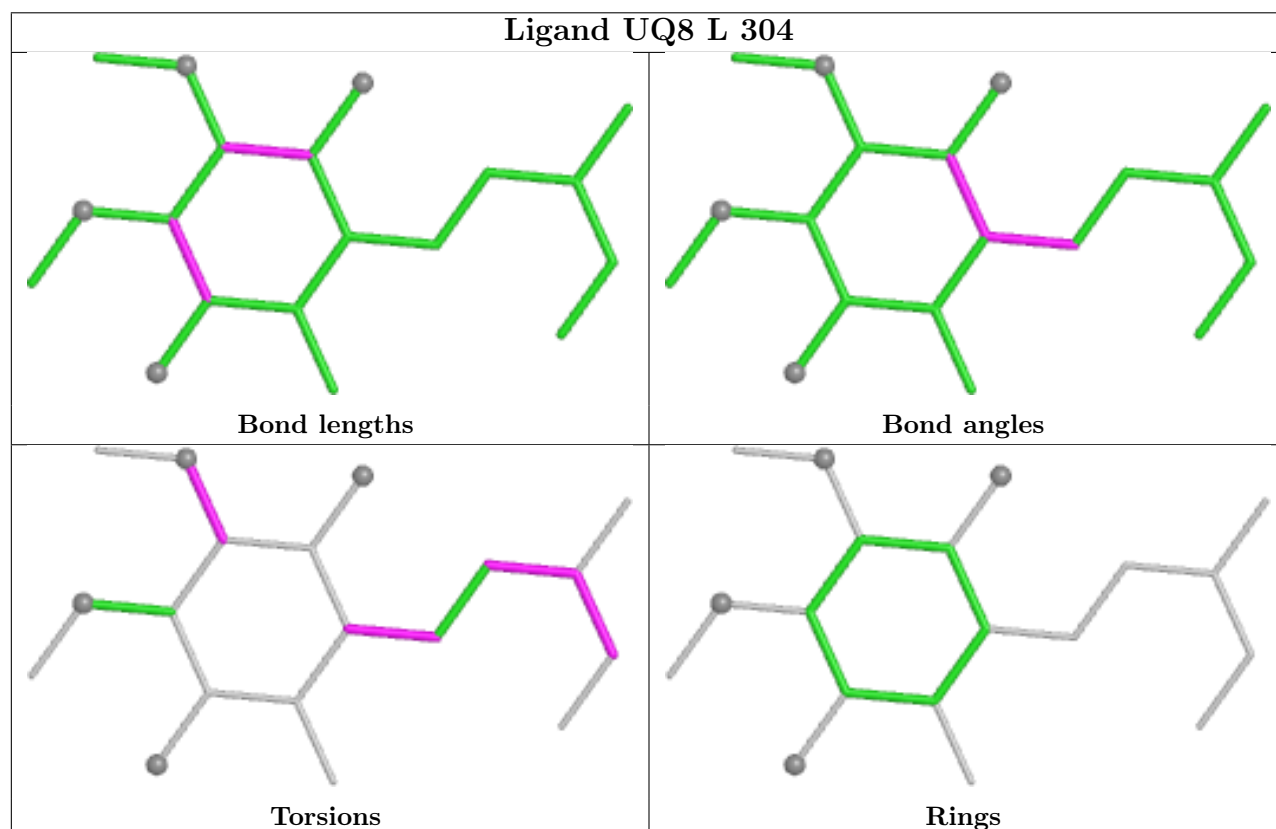
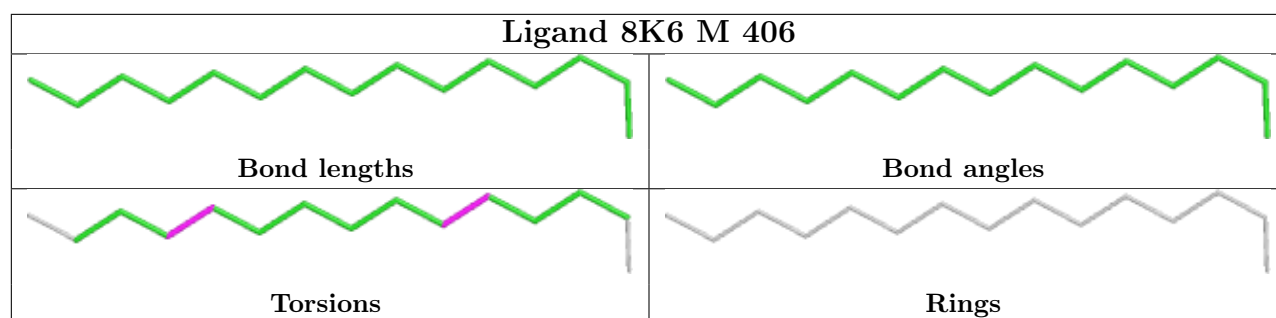


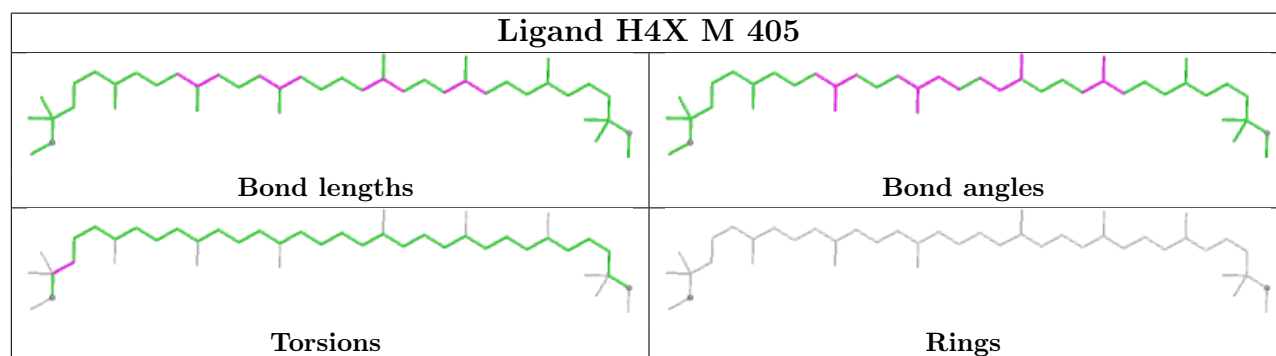
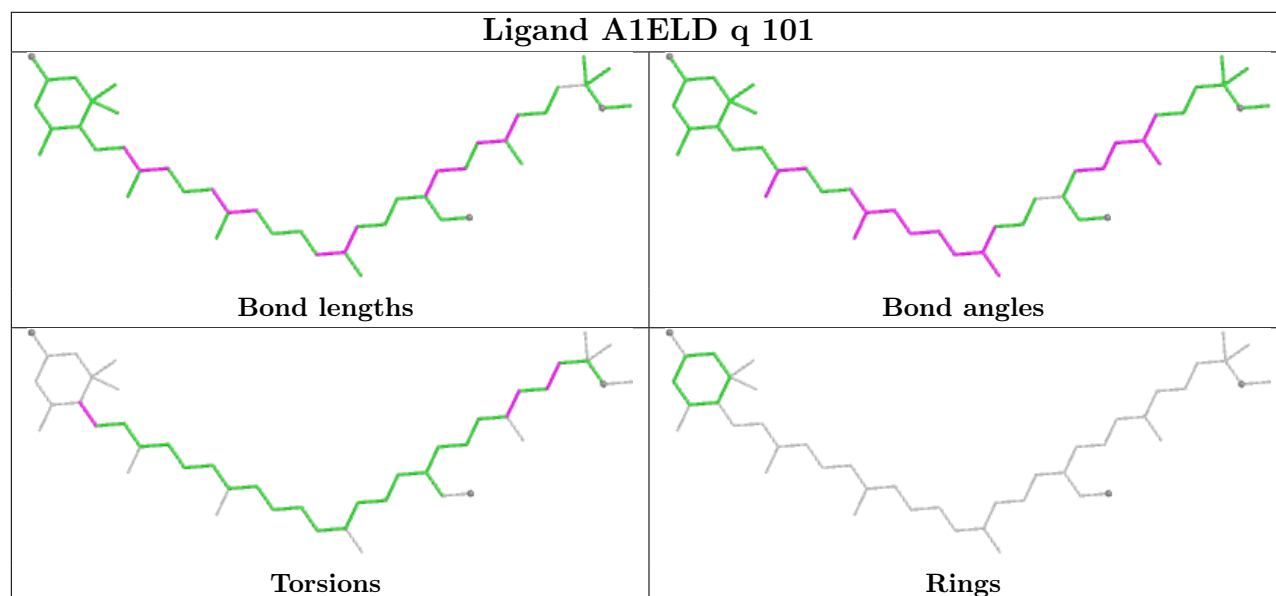
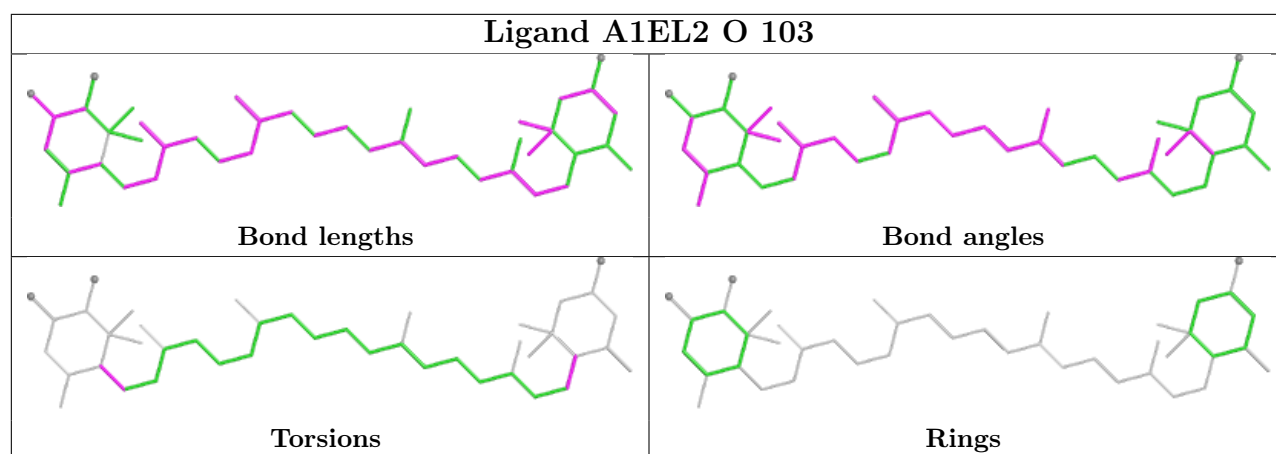


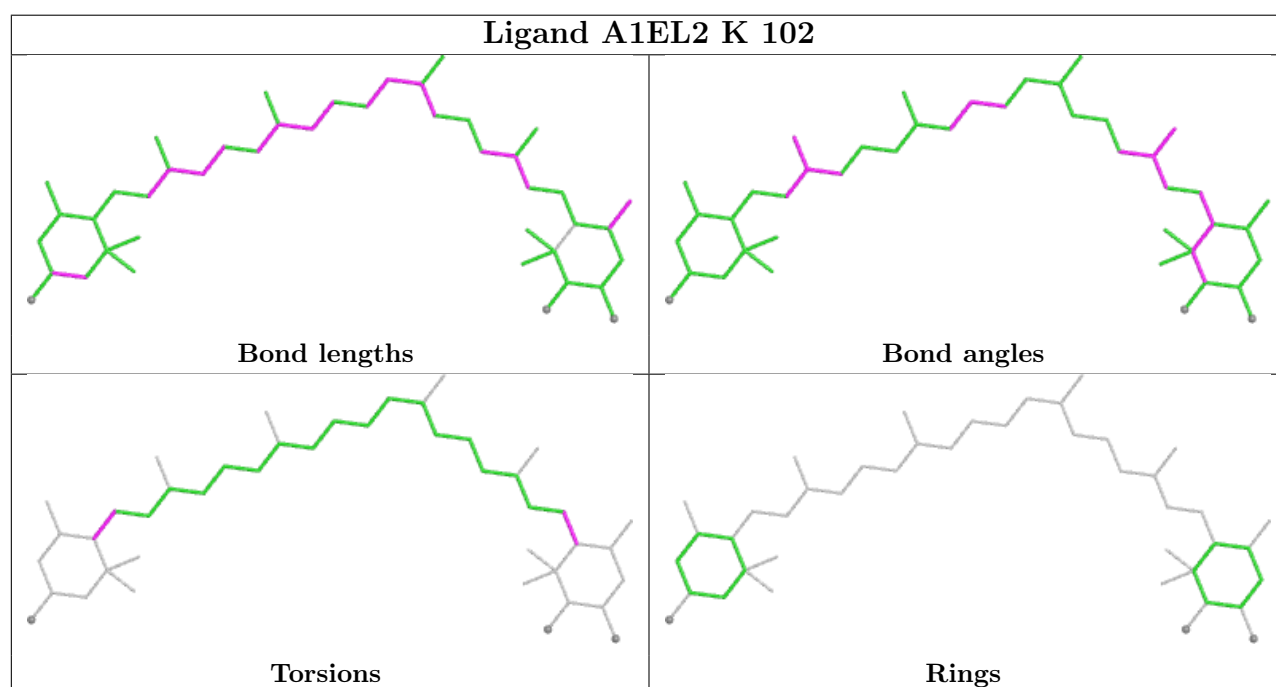
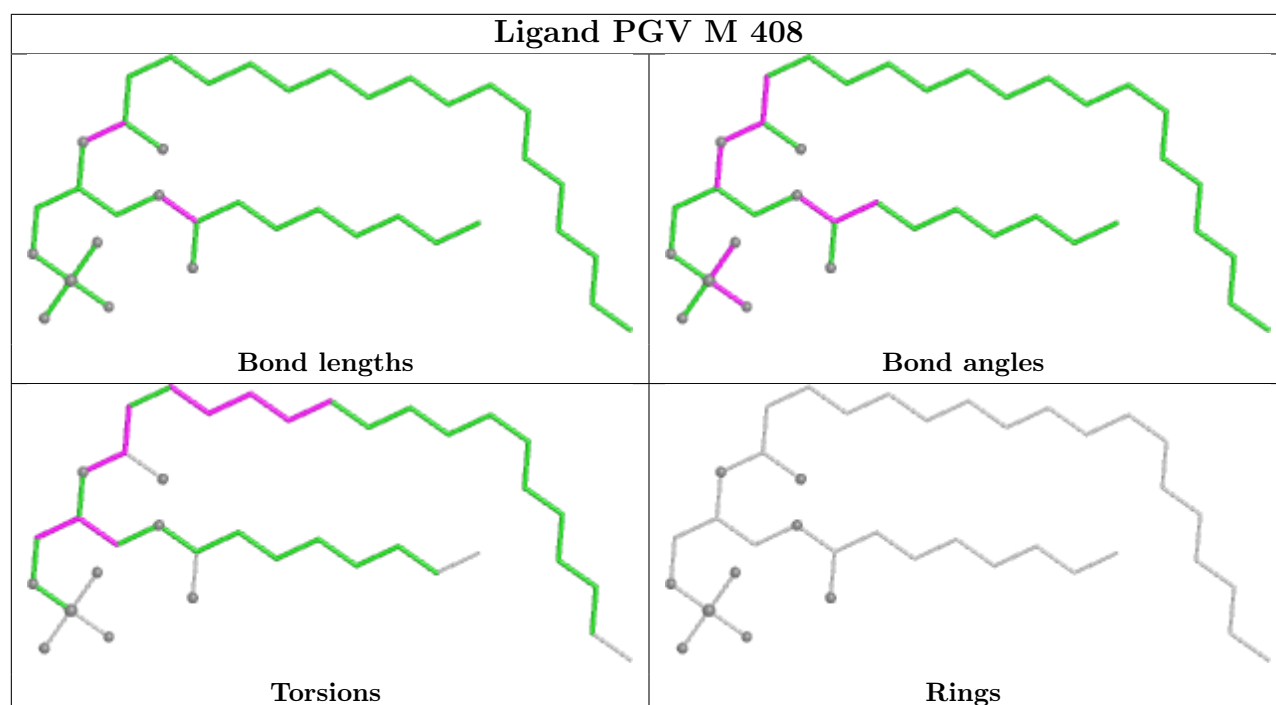


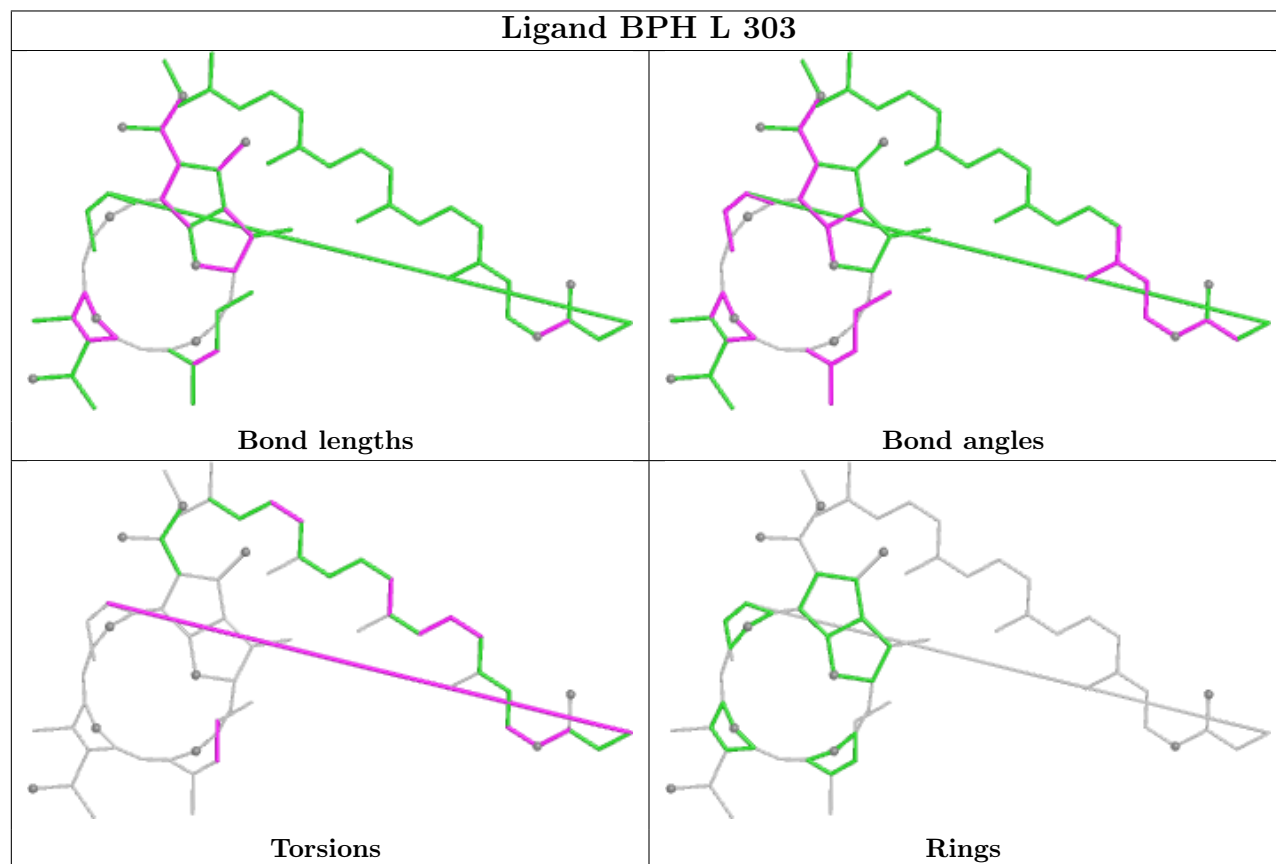
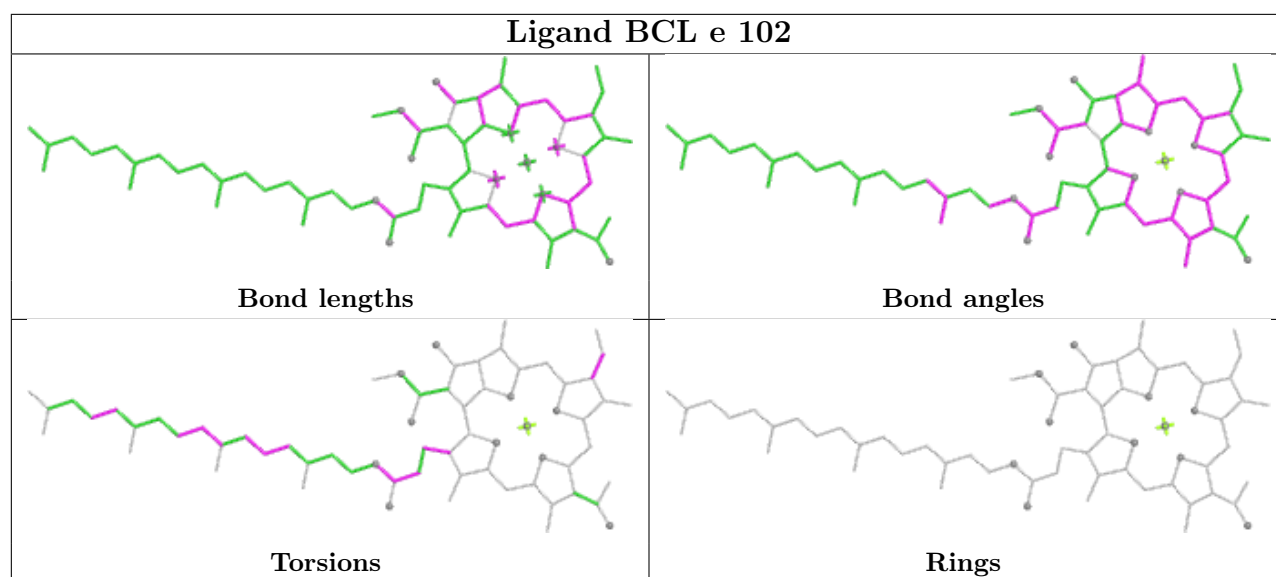


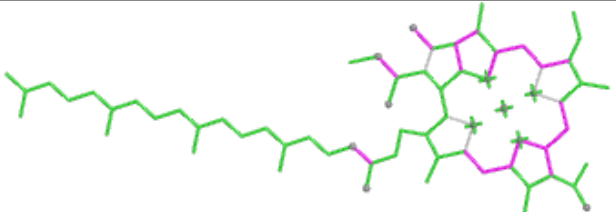
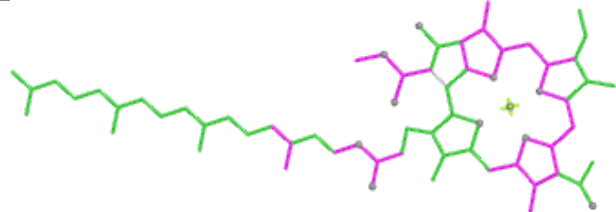
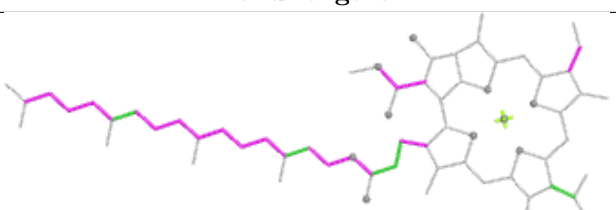
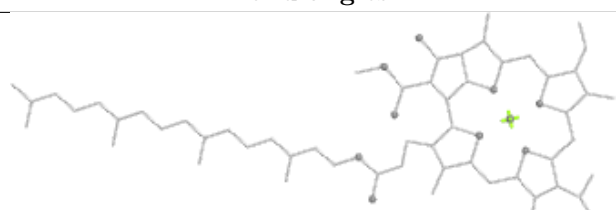




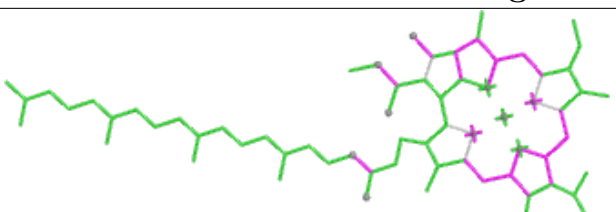
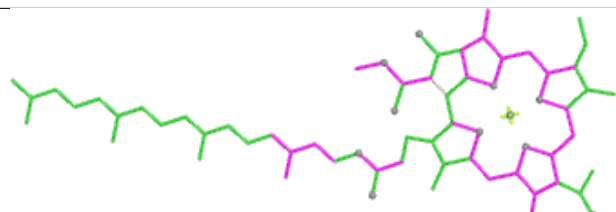
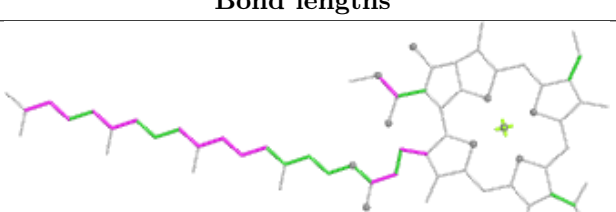
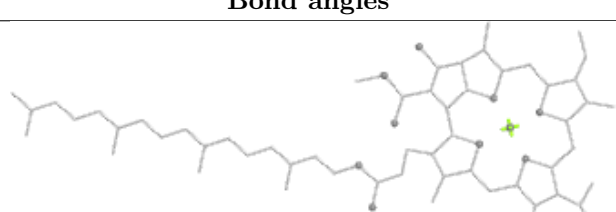


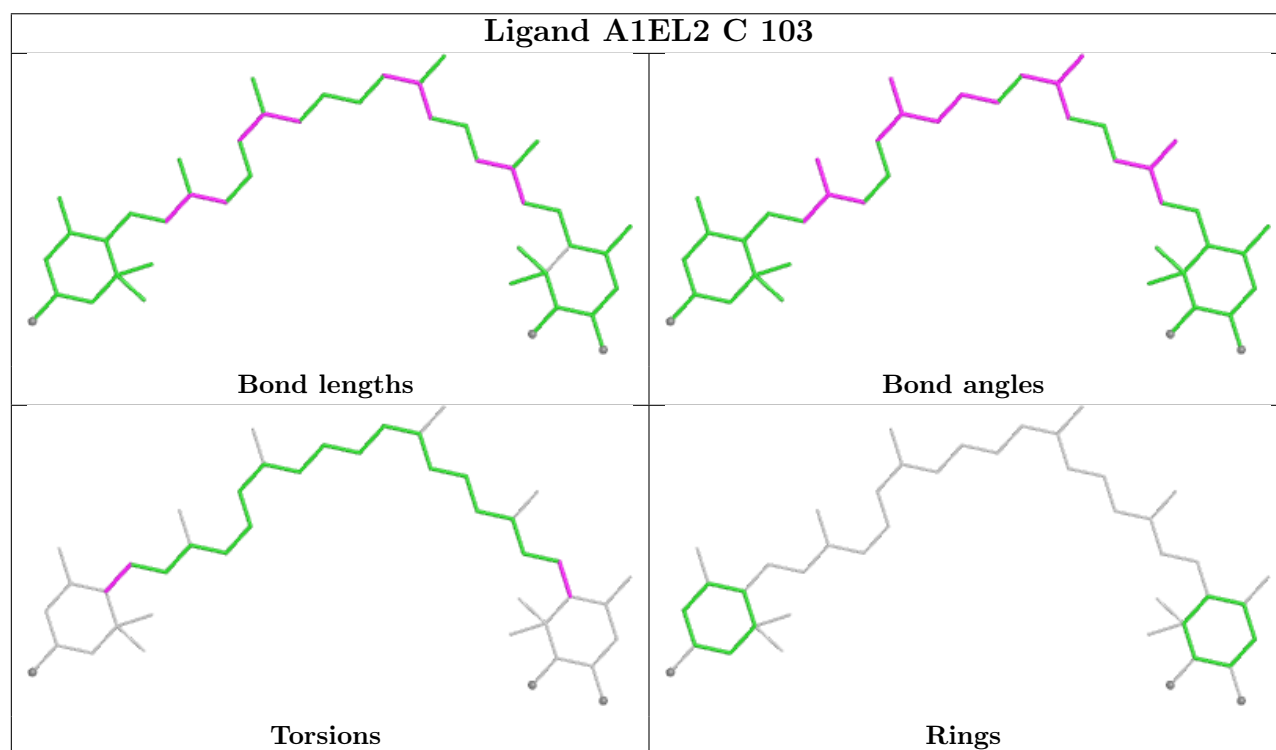
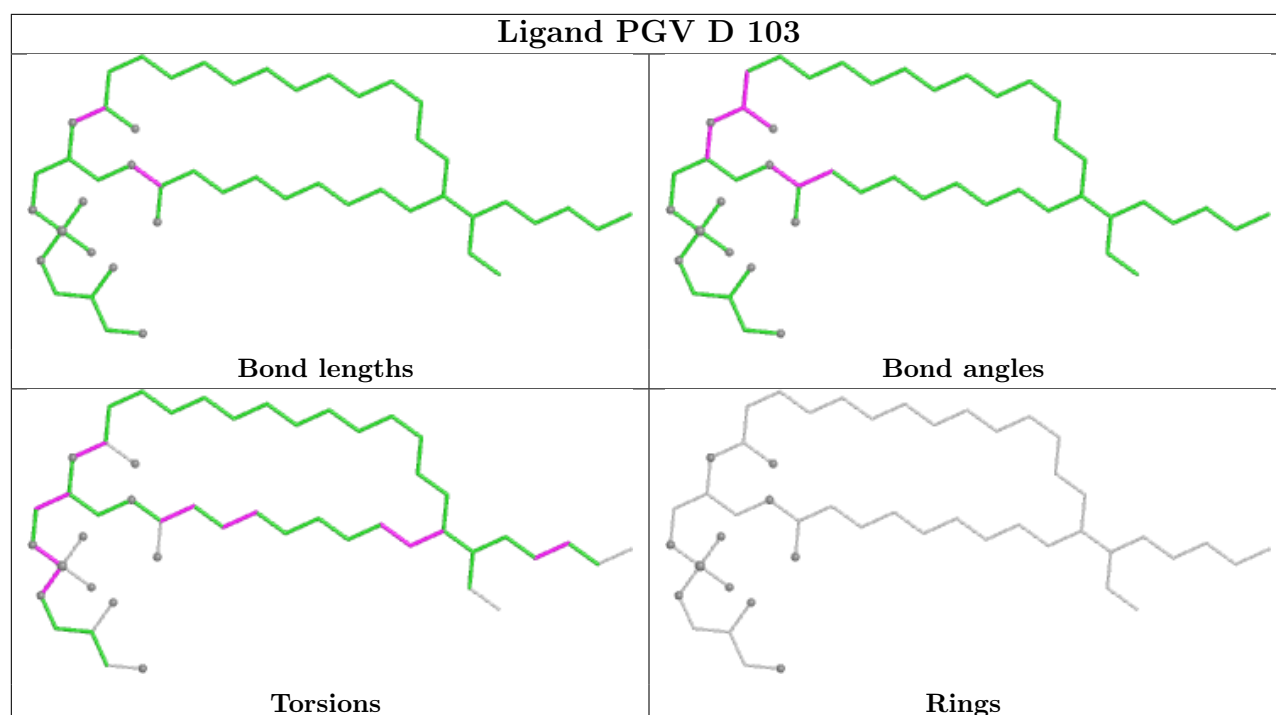


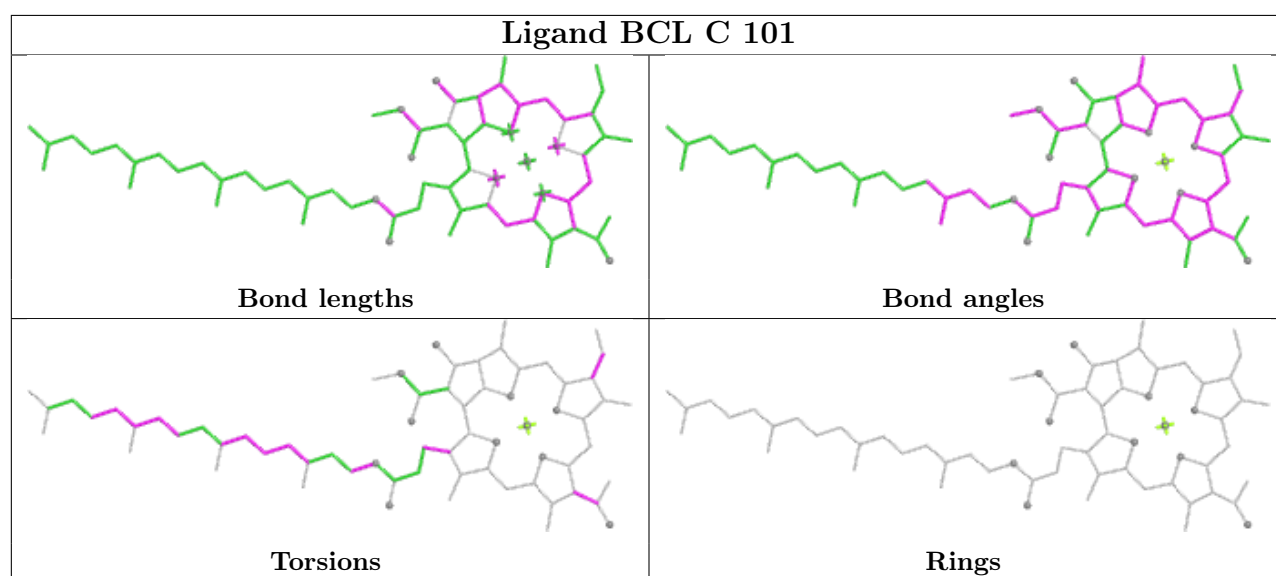
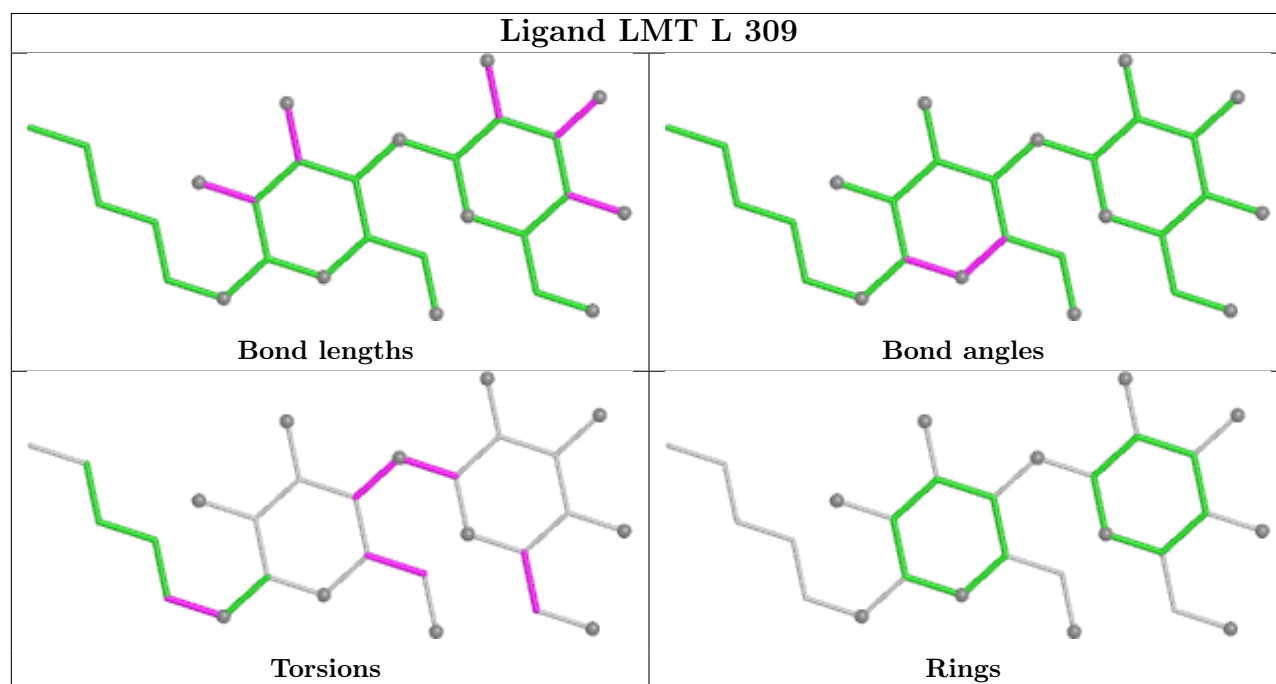
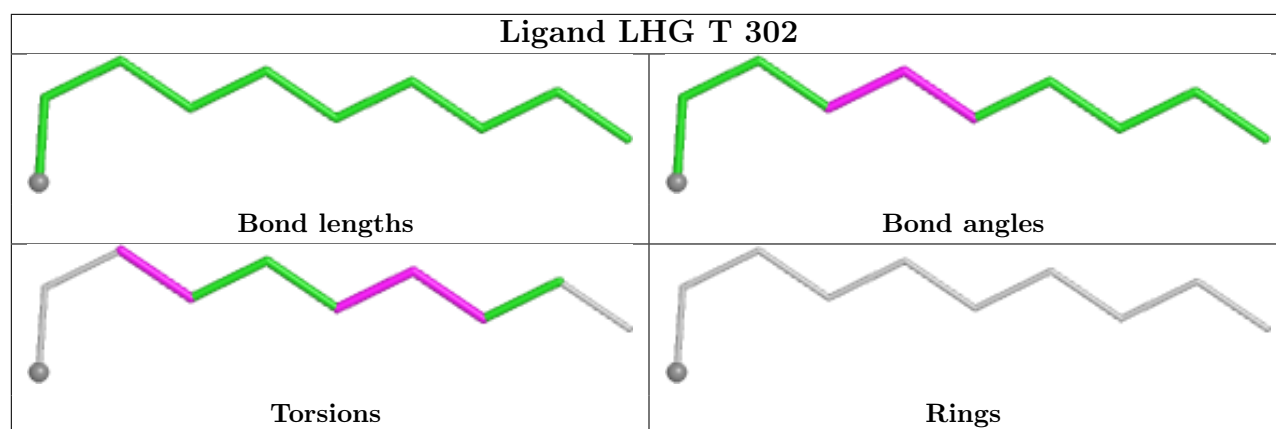


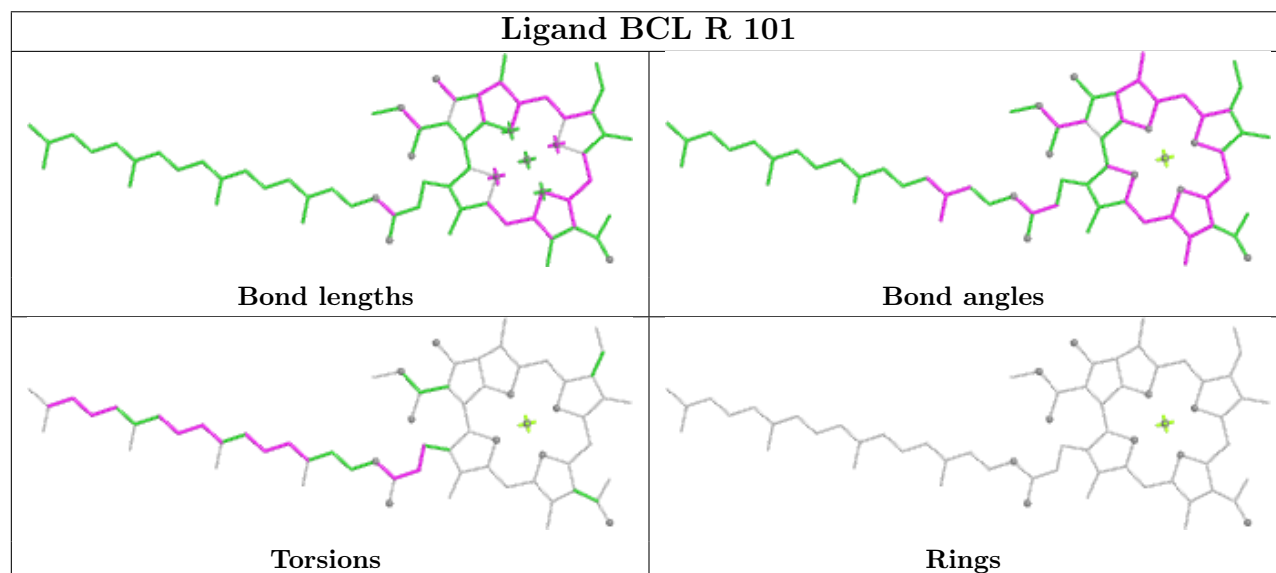
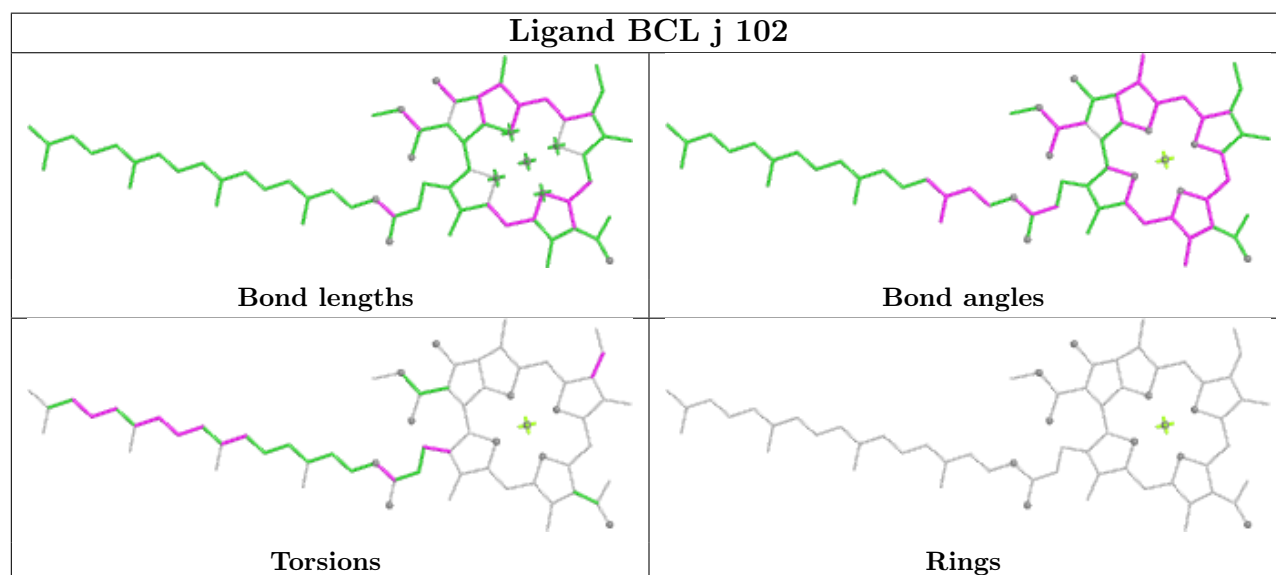
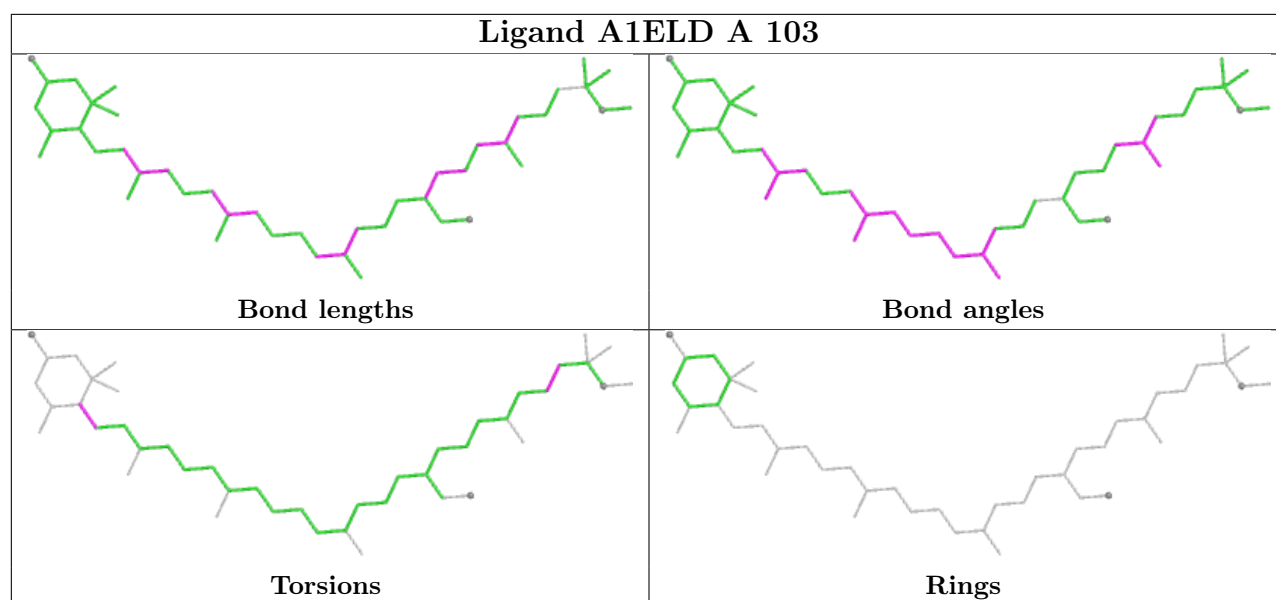
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Bond lengths	Bond angles
	
Torsions	Rings

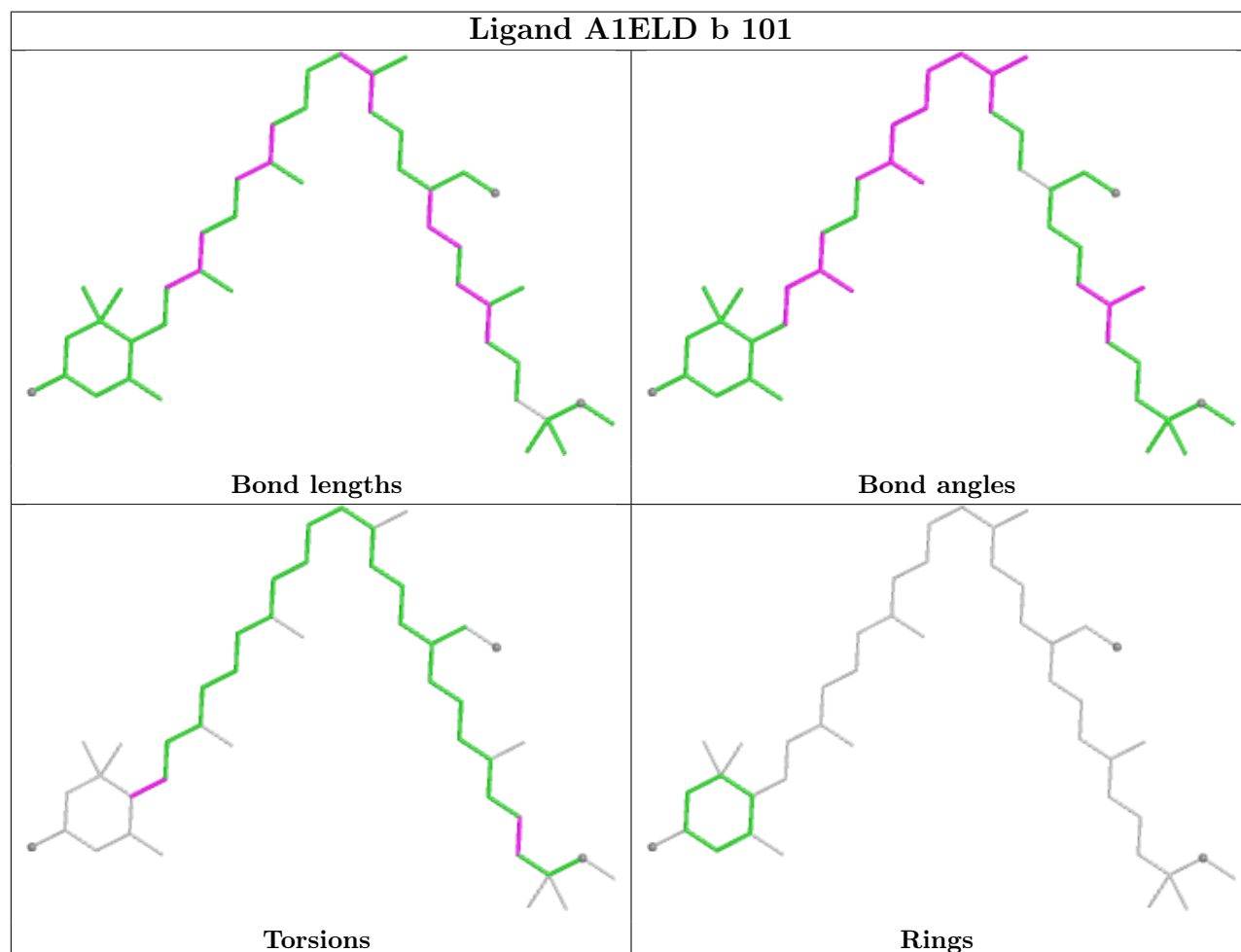
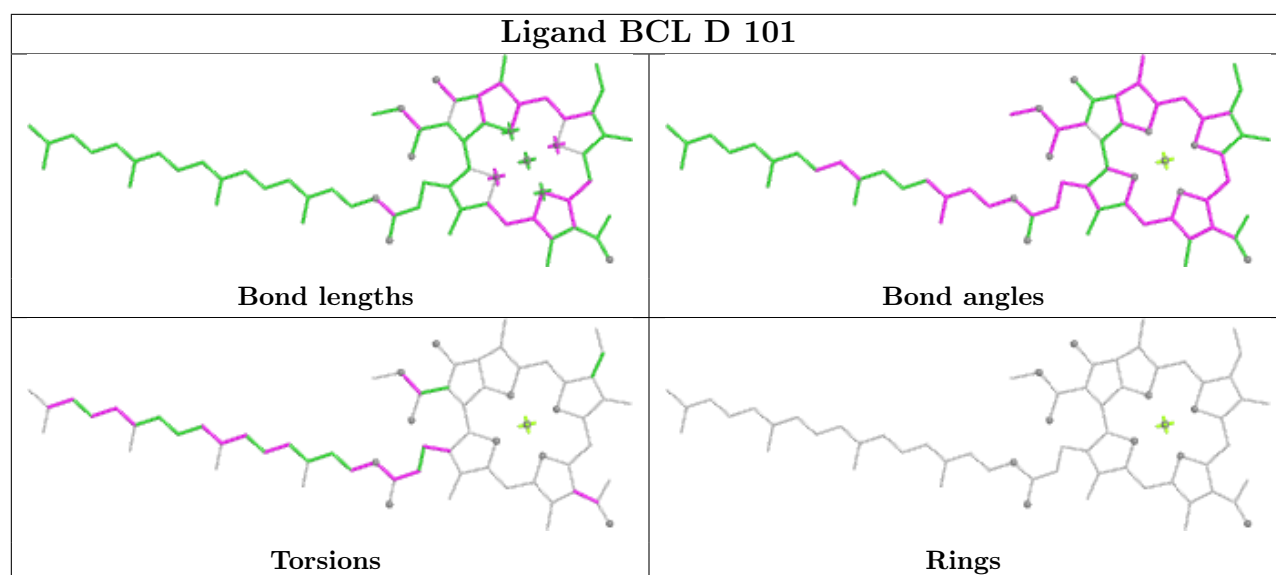
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Bond lengths	Bond angles
	
Torsions	Rings

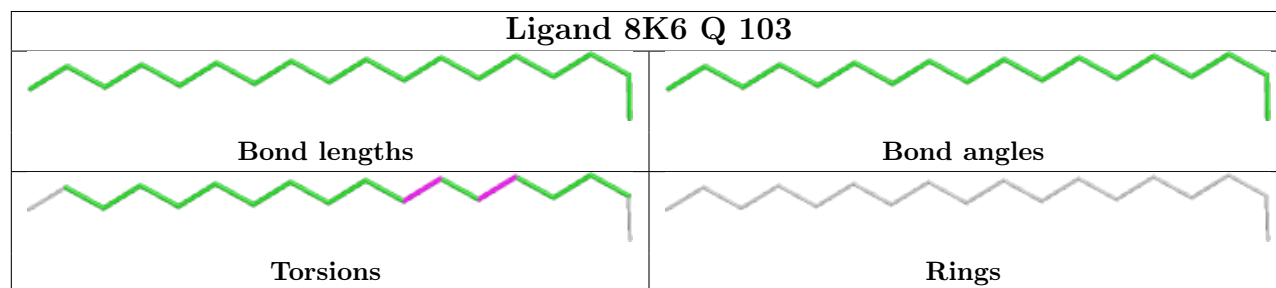
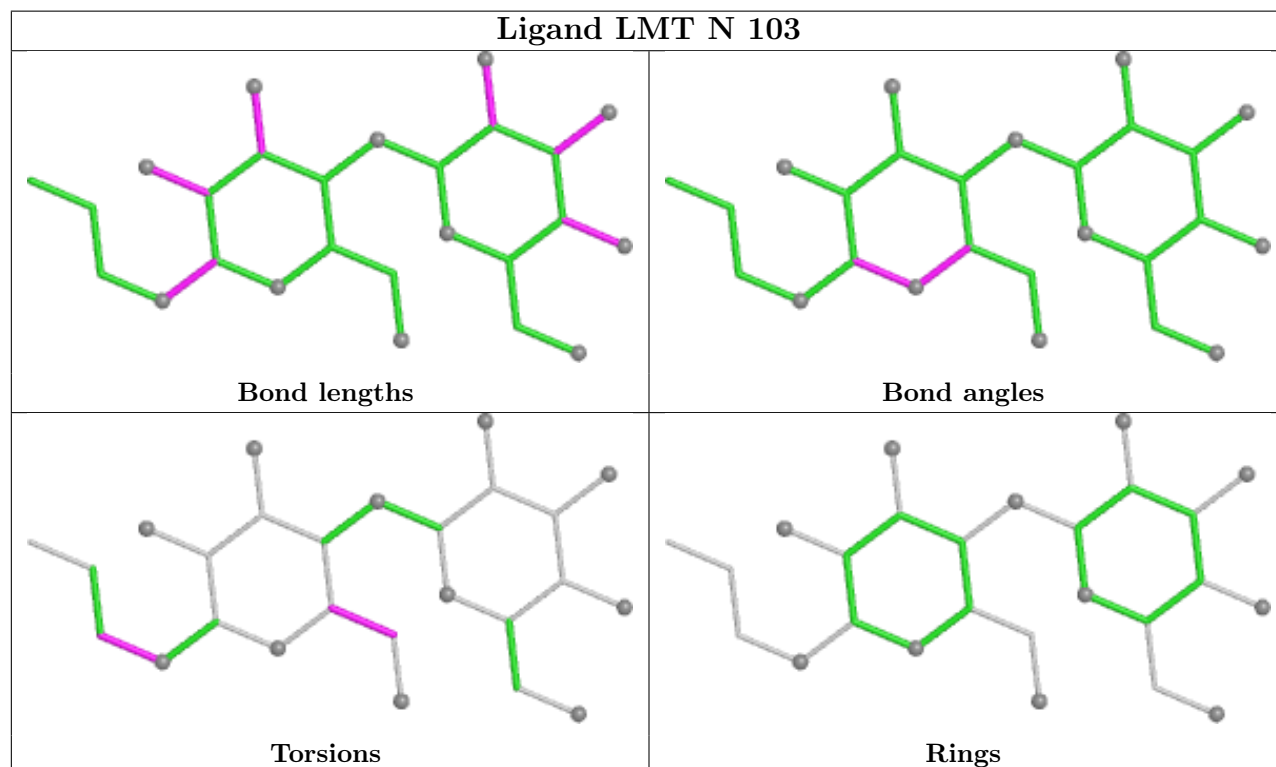
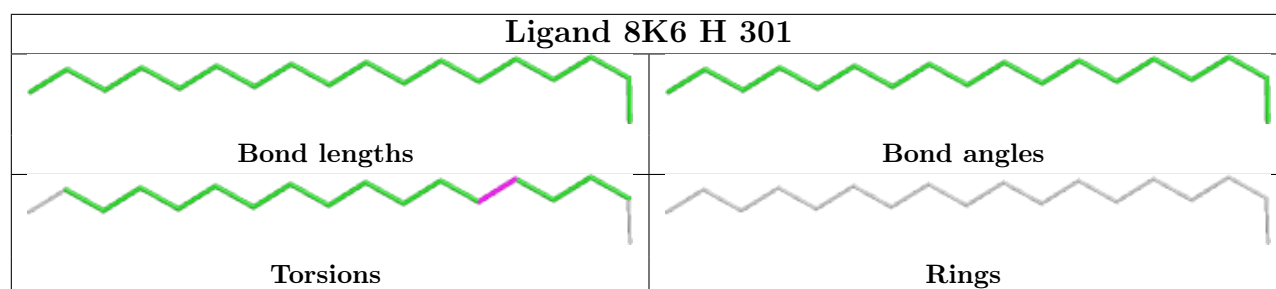
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Bond lengths	Bond angles
	
Torsions	Rings

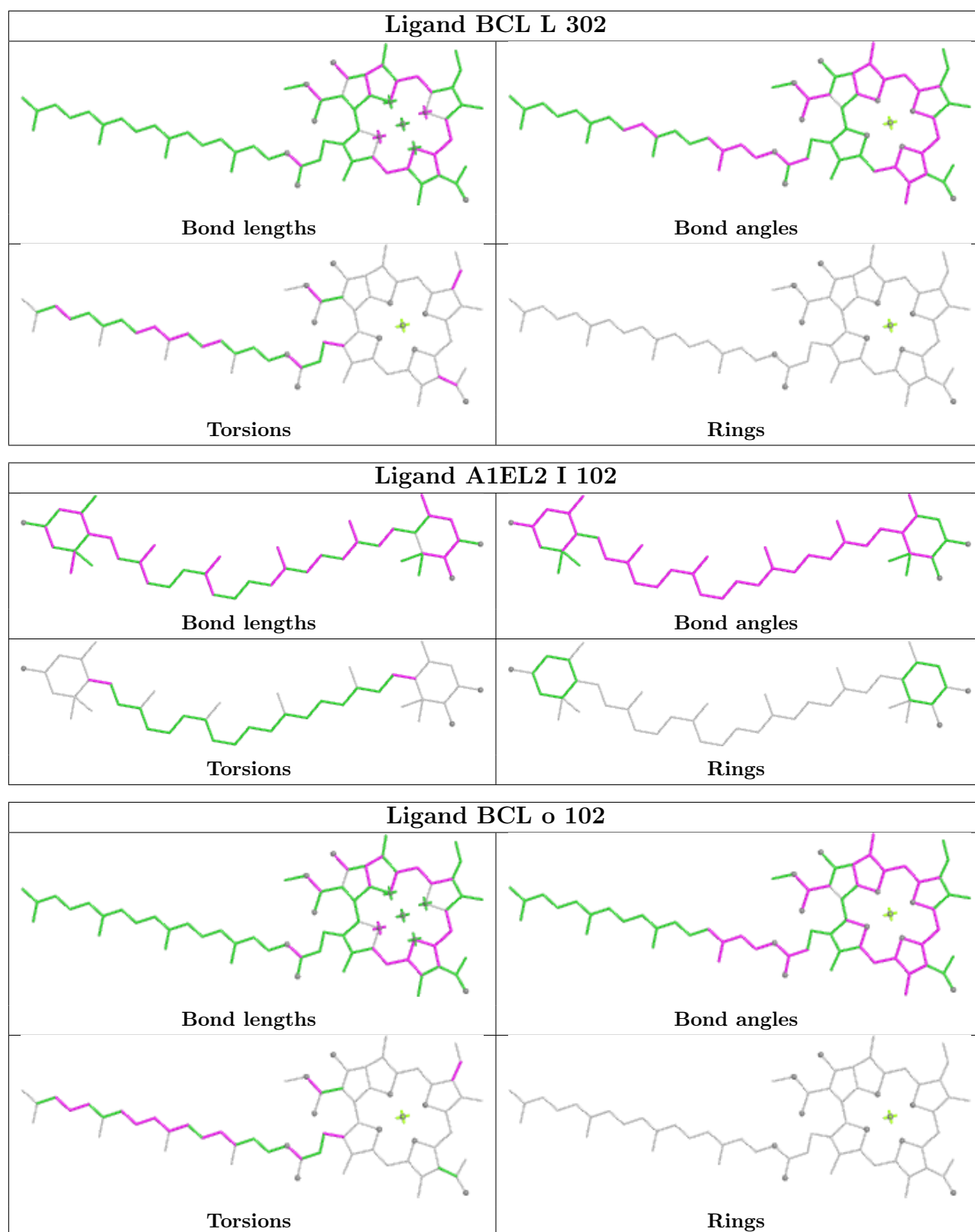


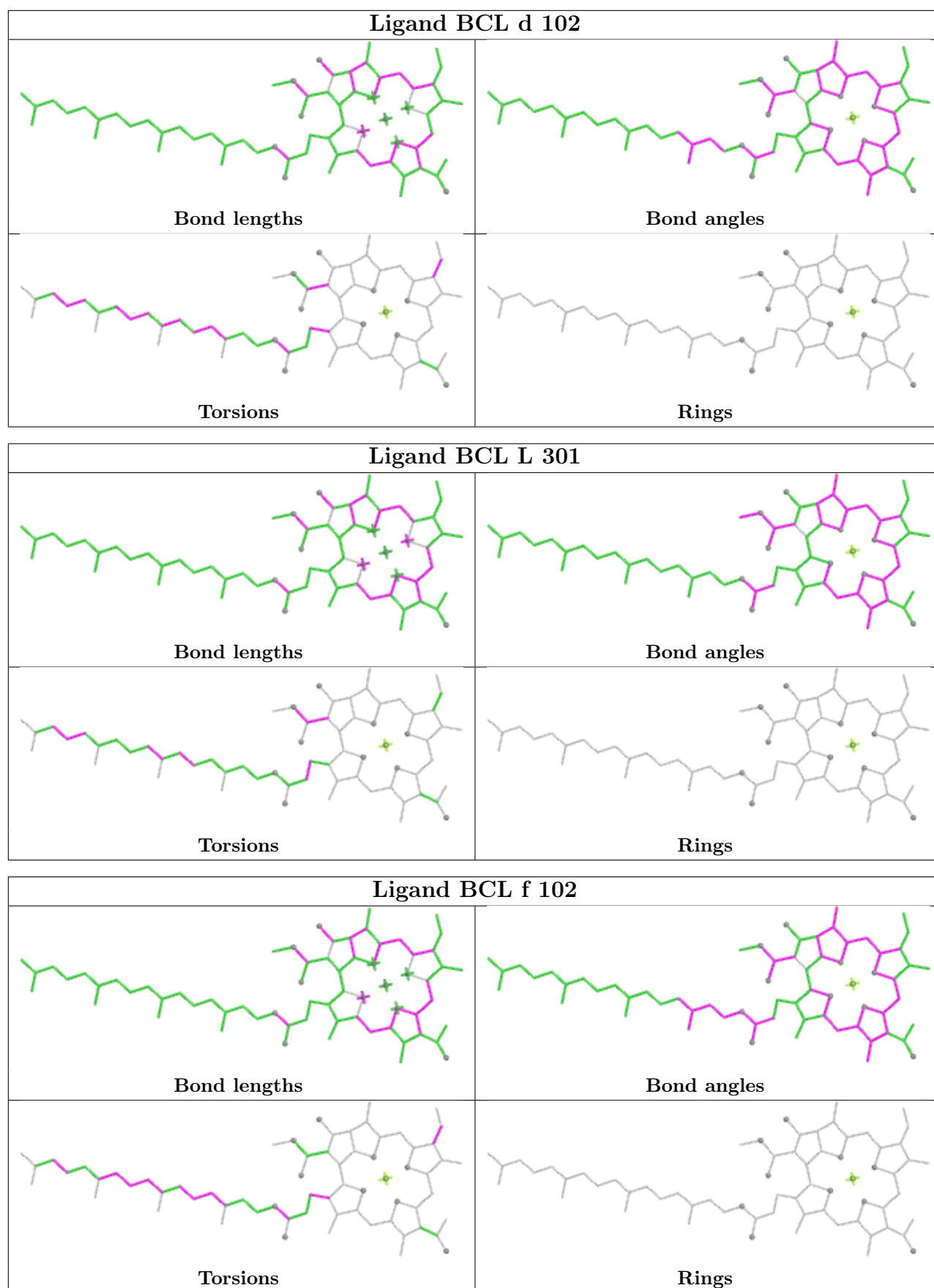


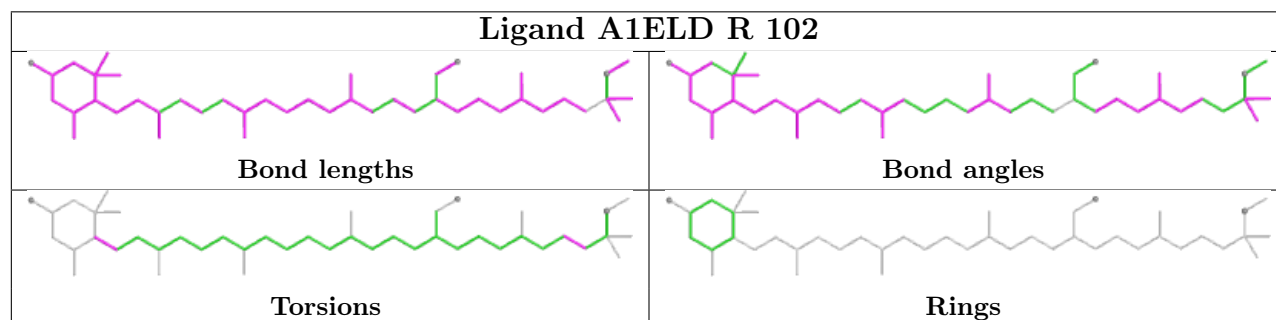
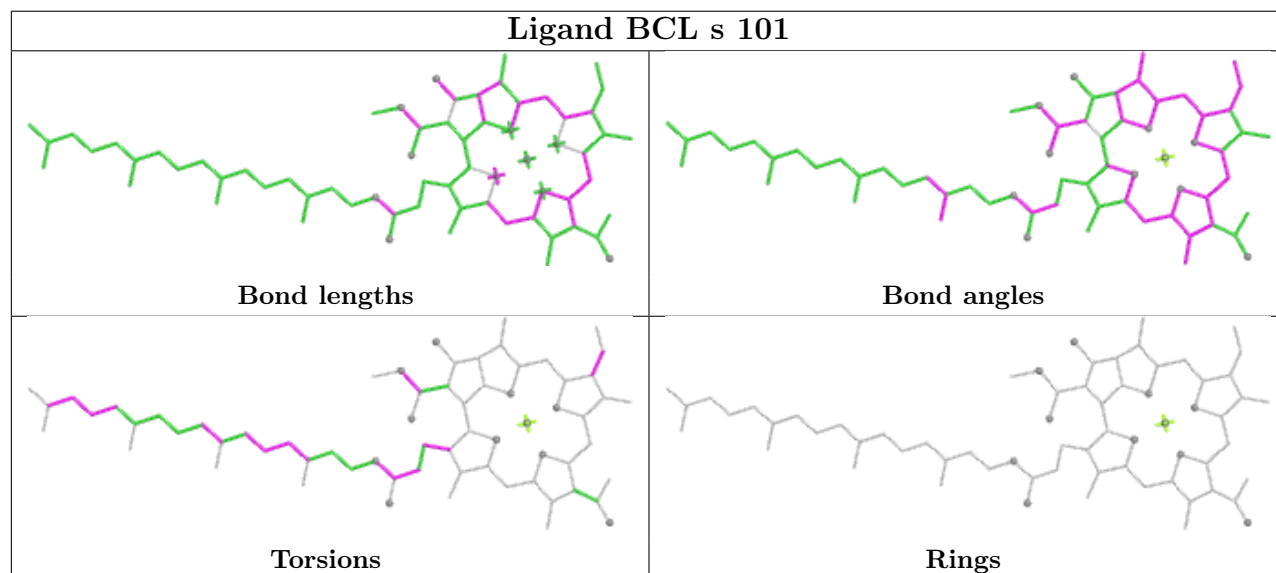
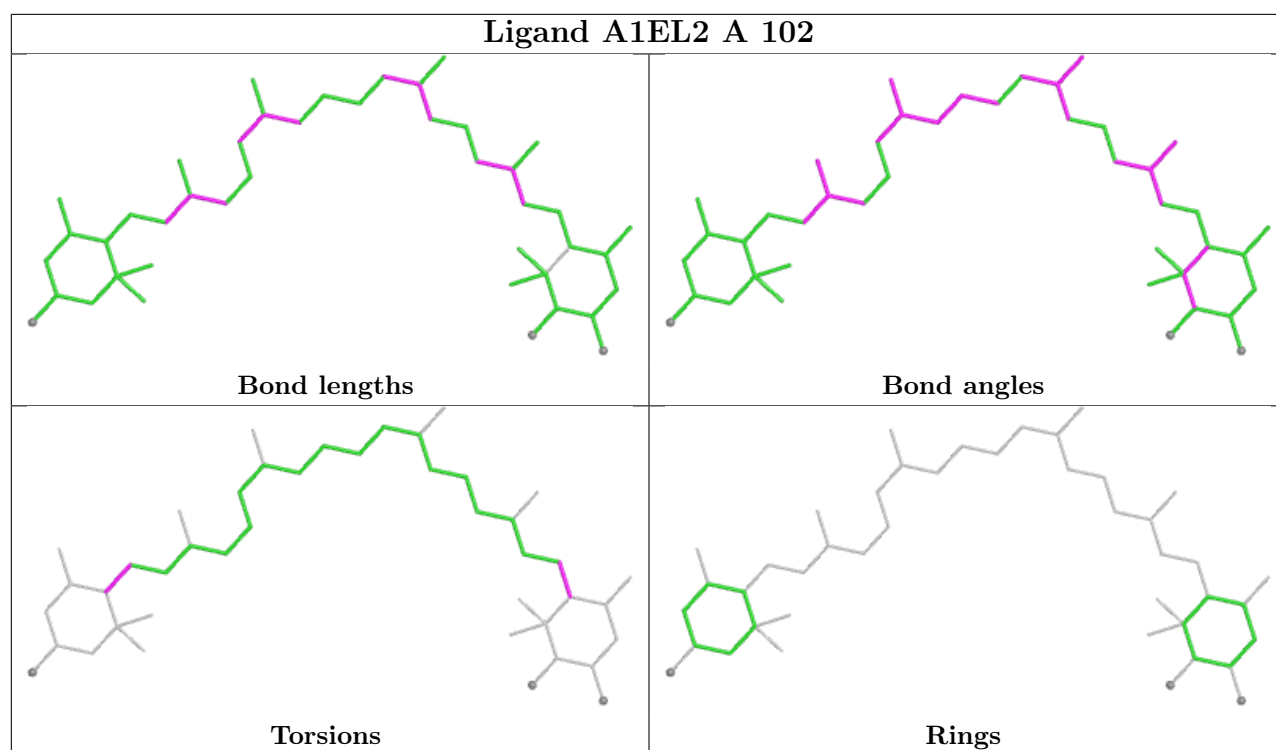


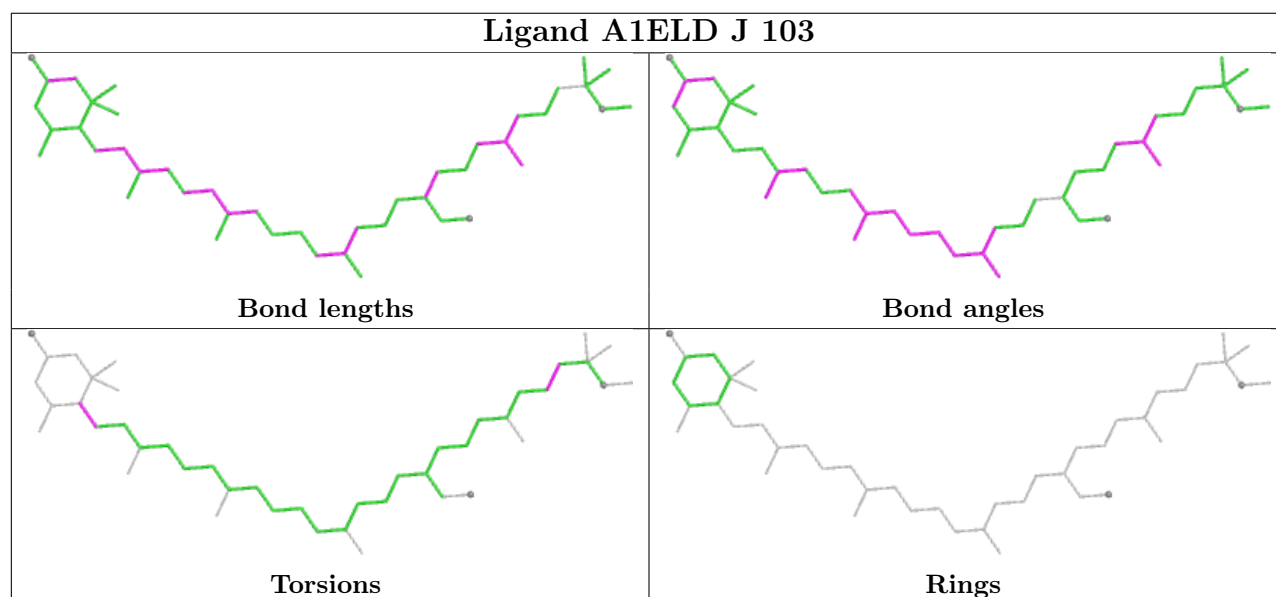
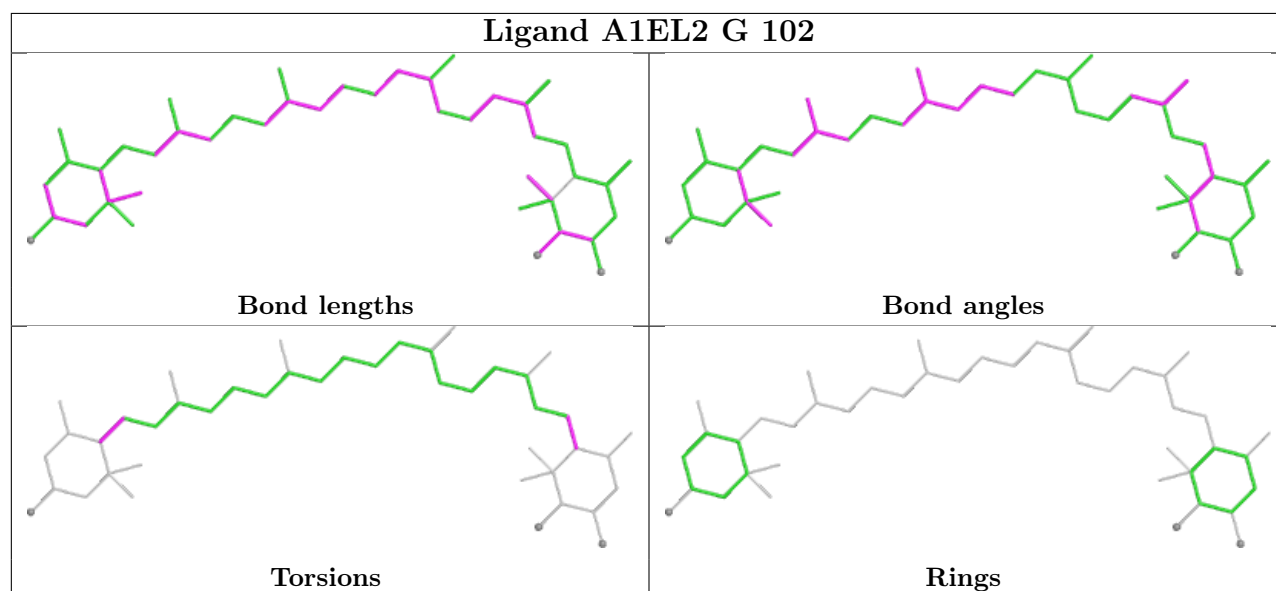
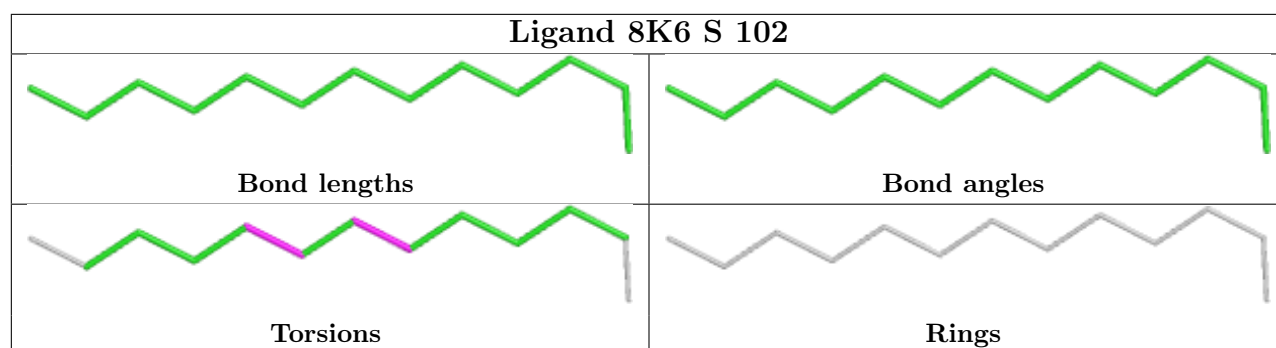


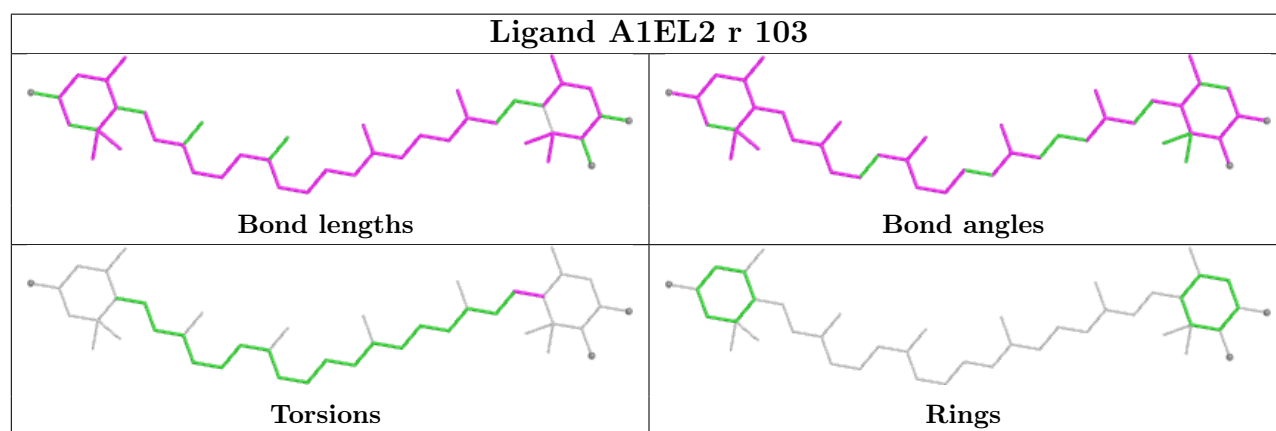
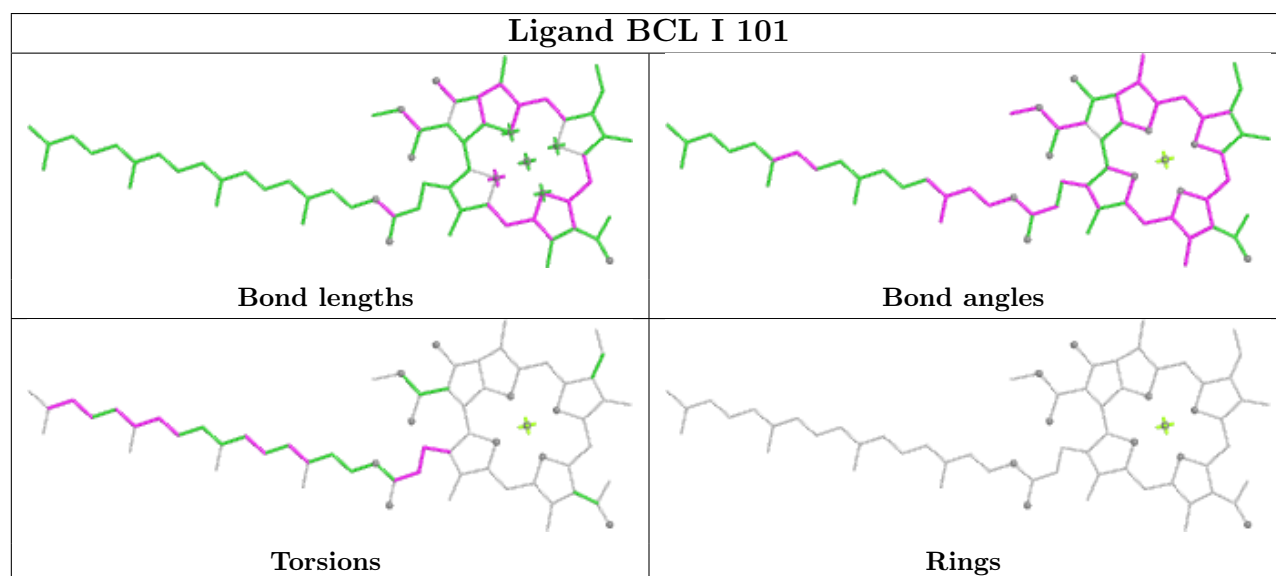
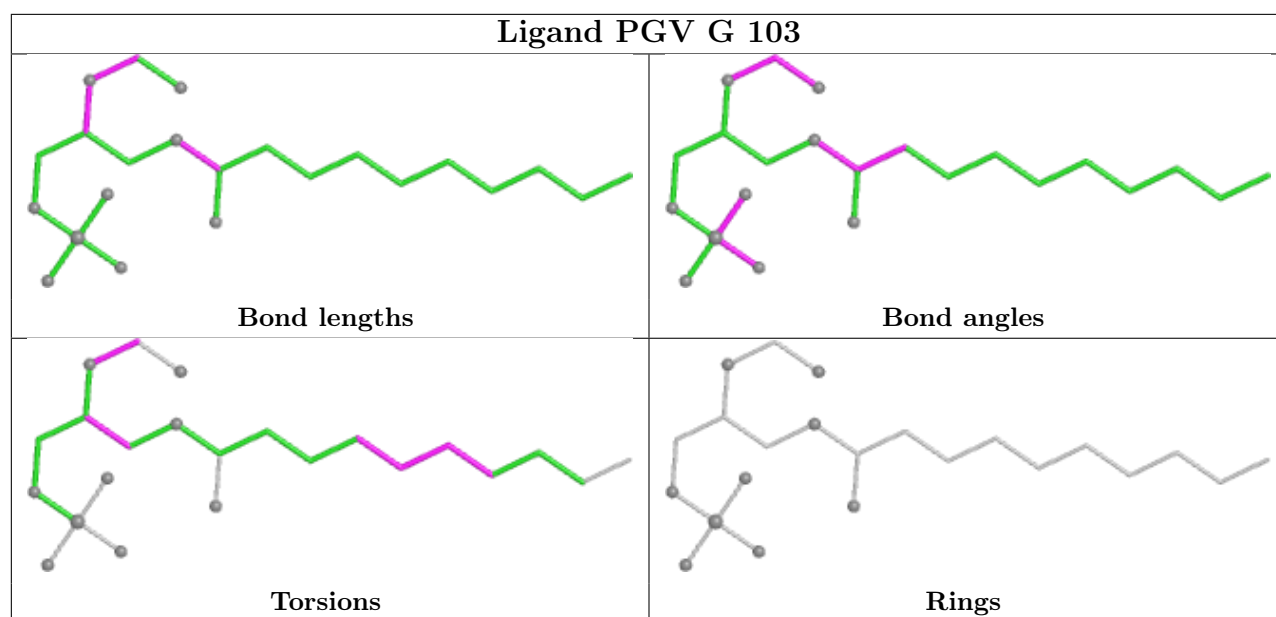


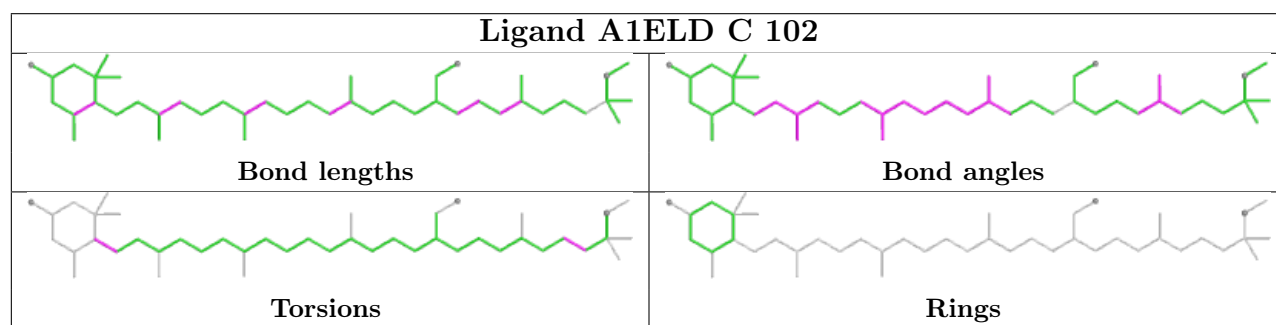
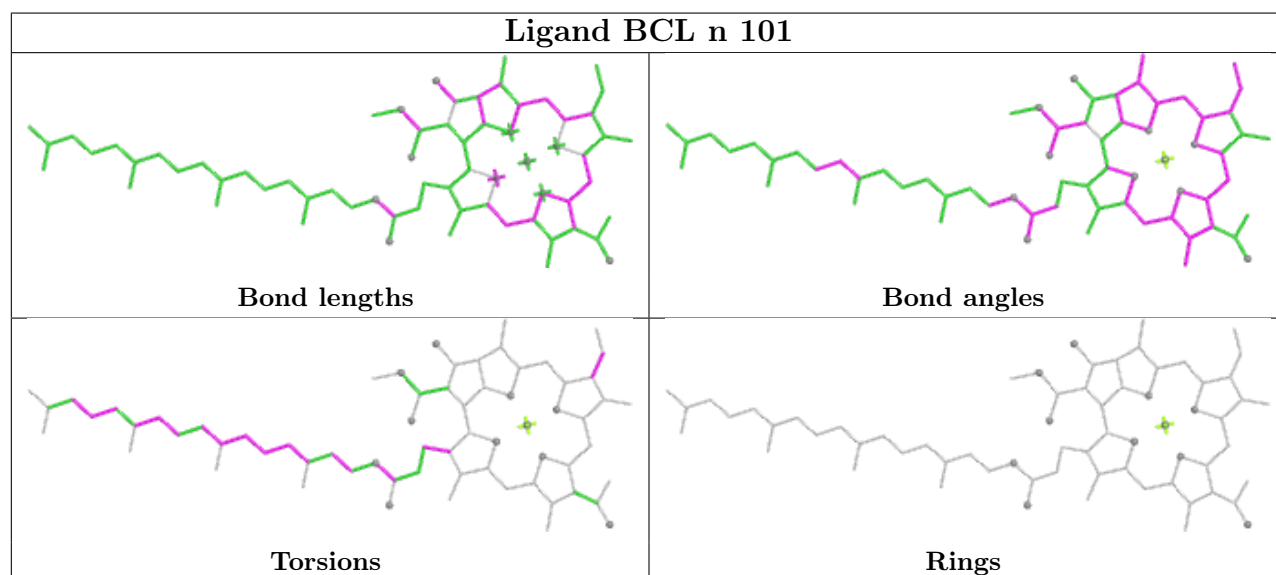
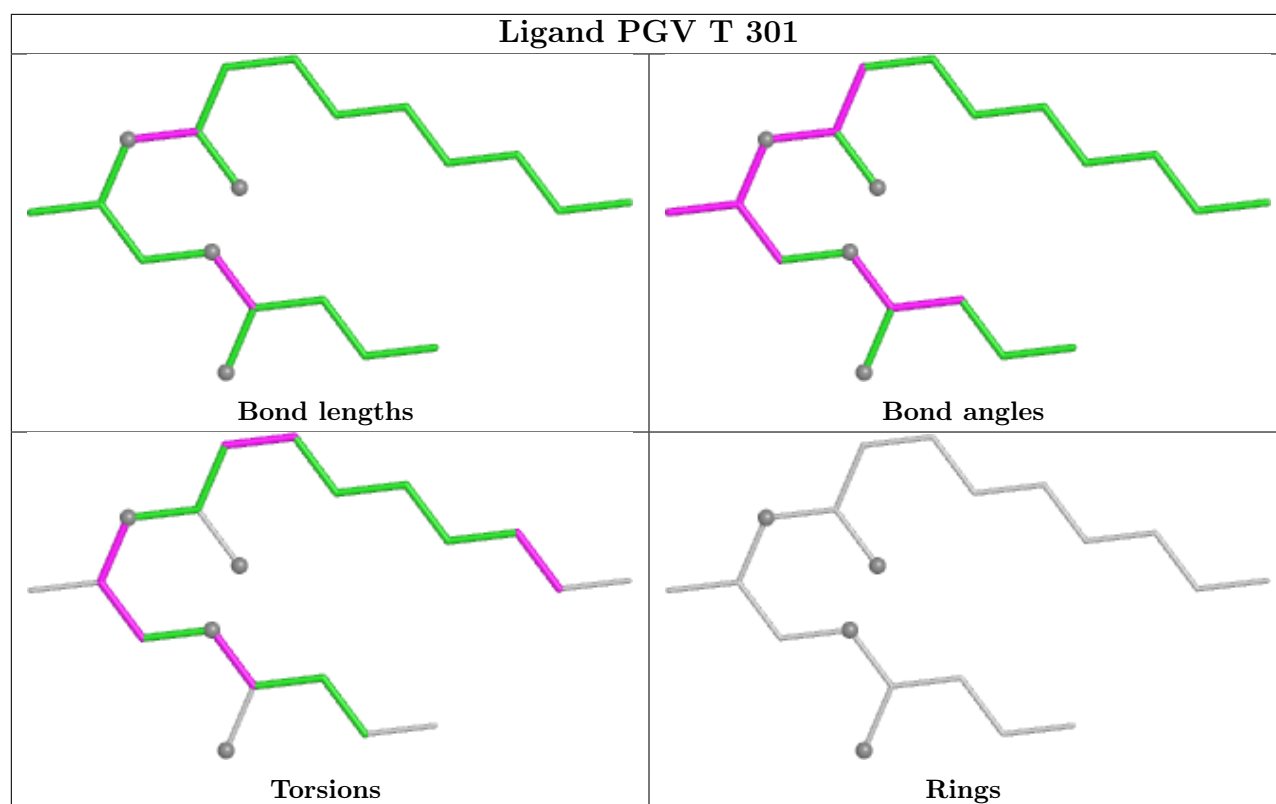


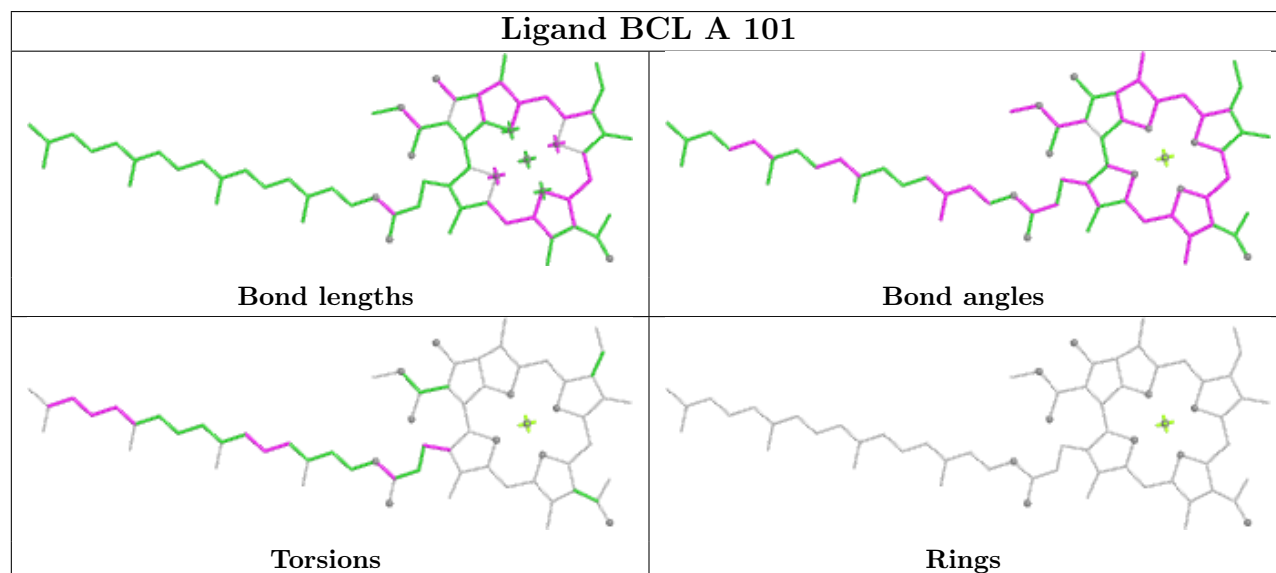
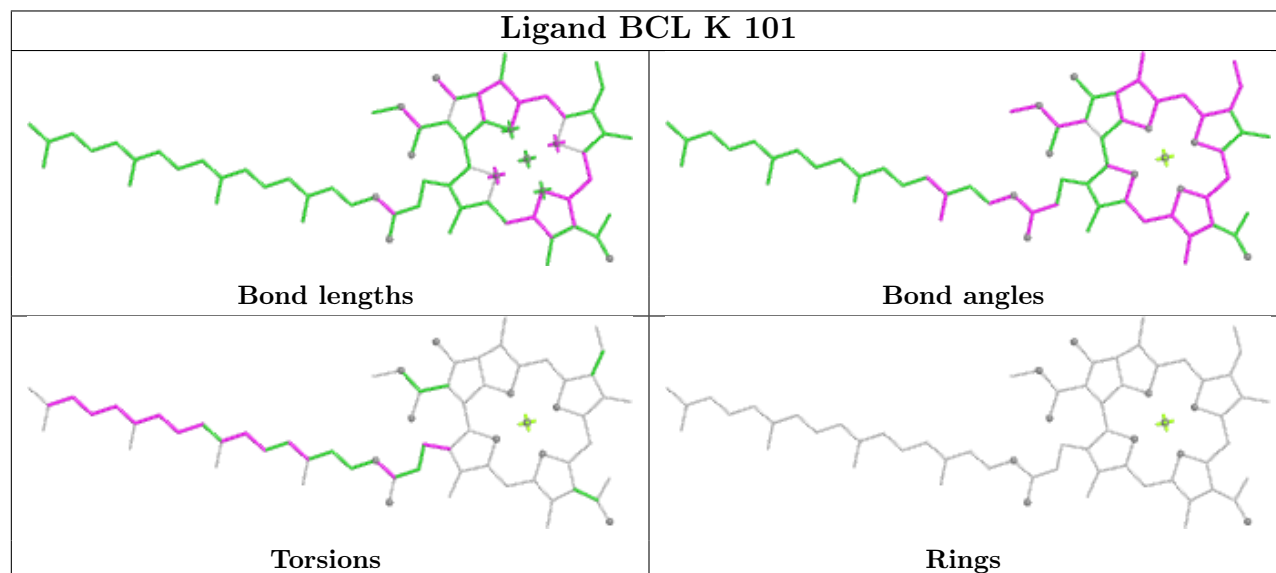
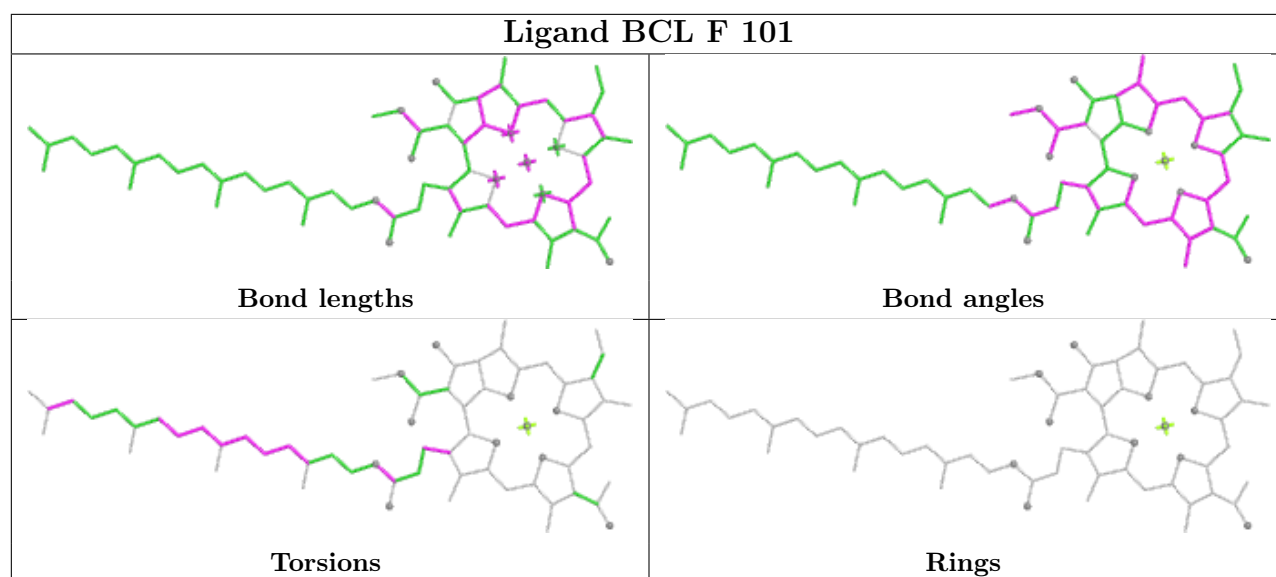


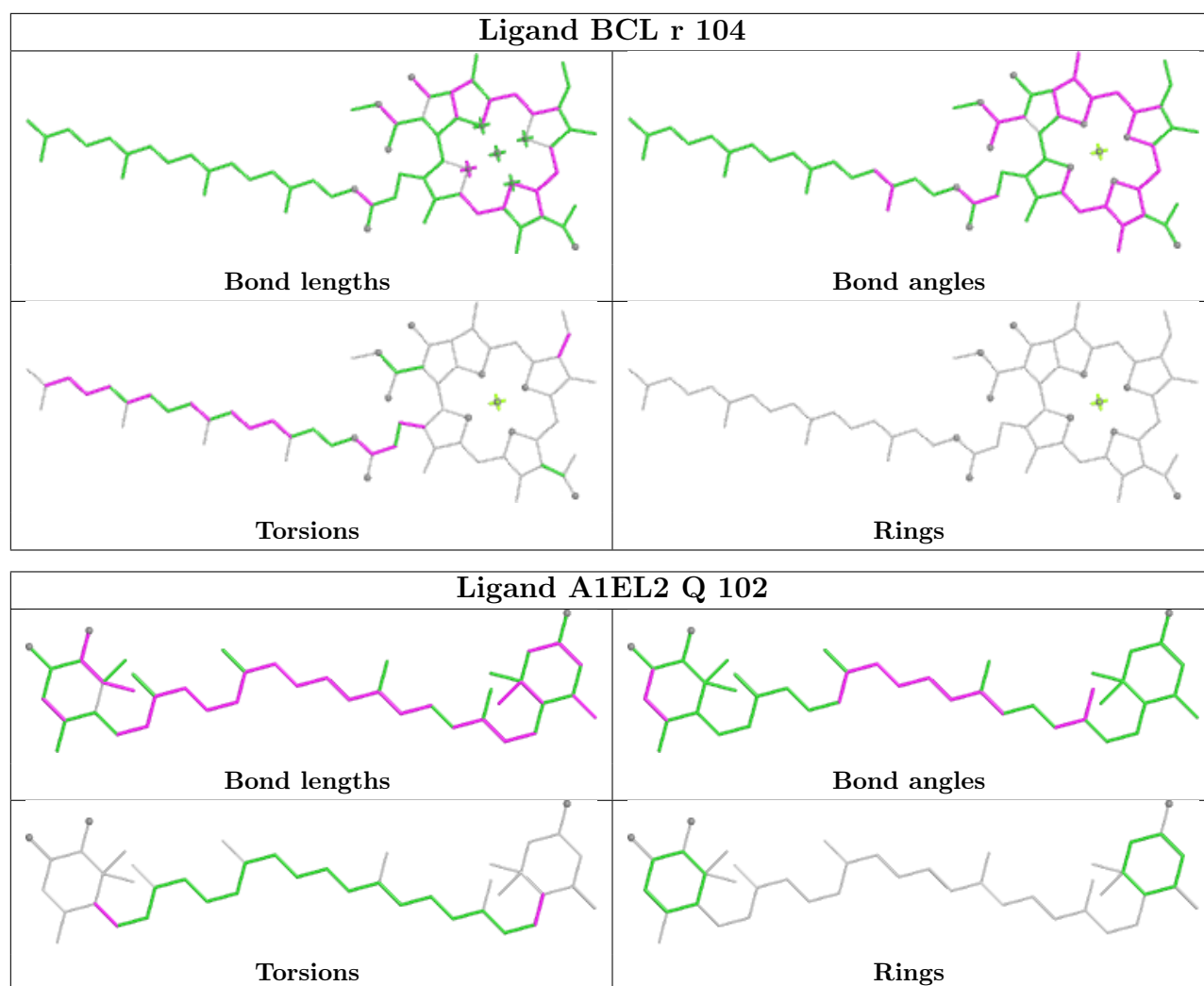


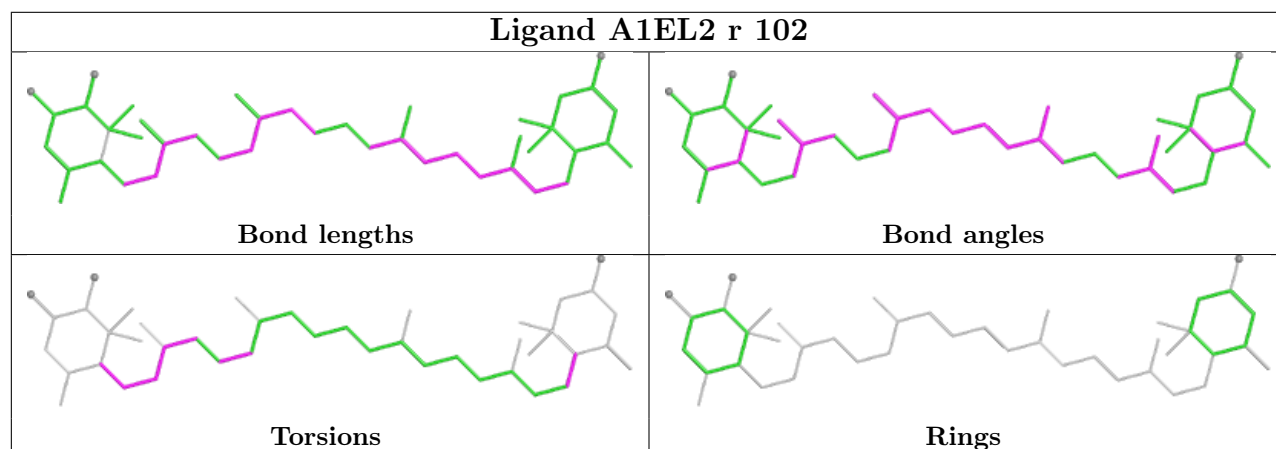
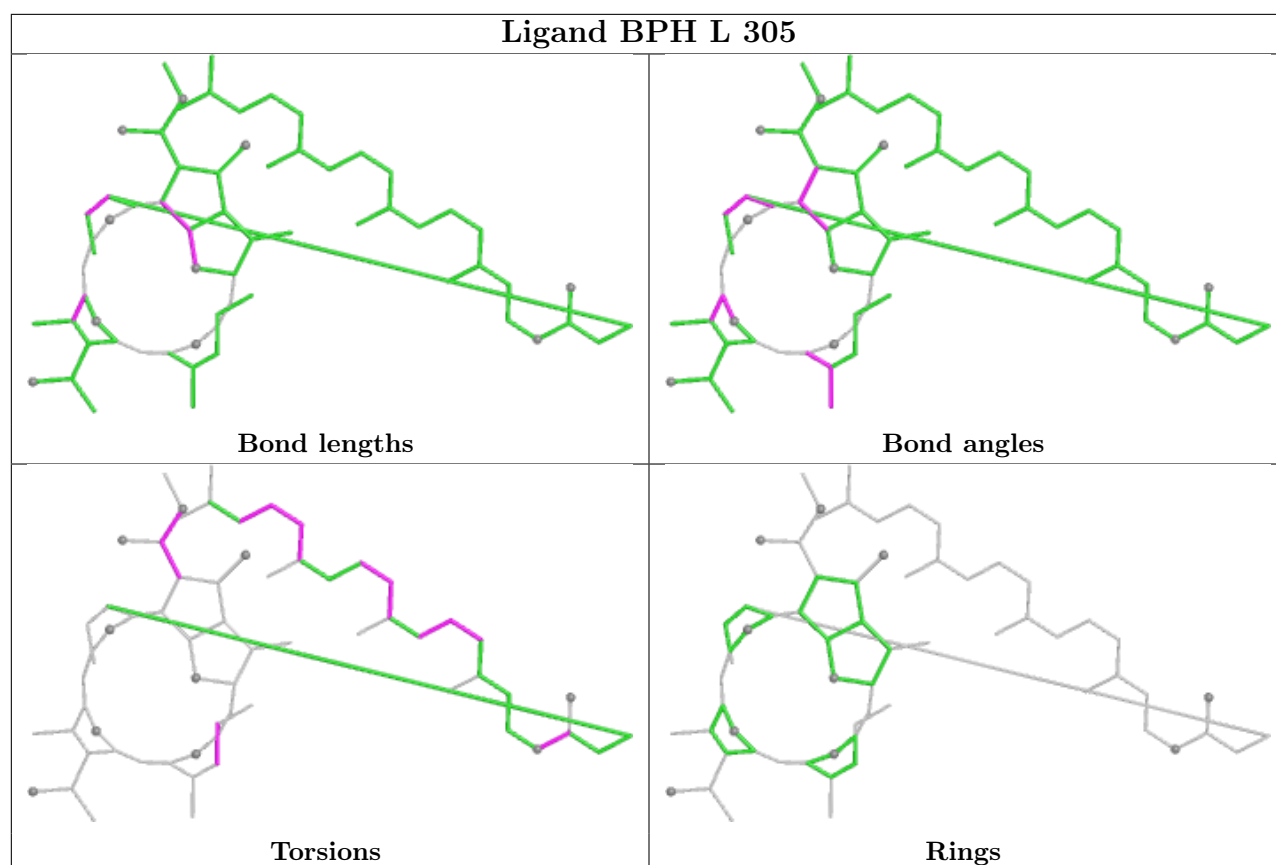


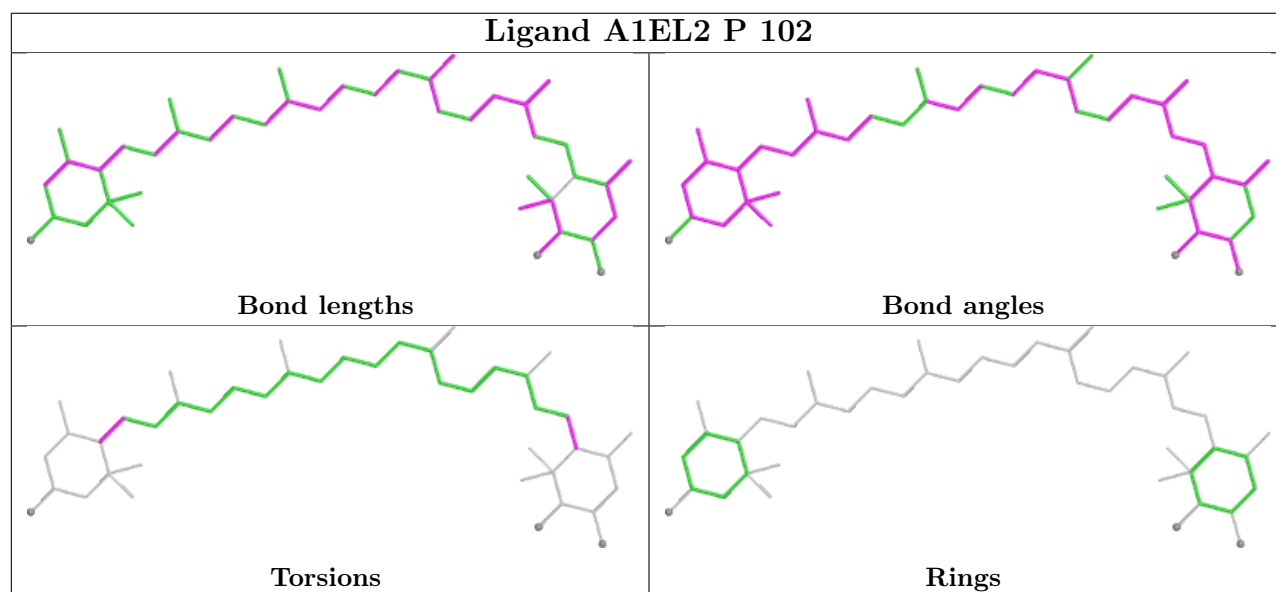
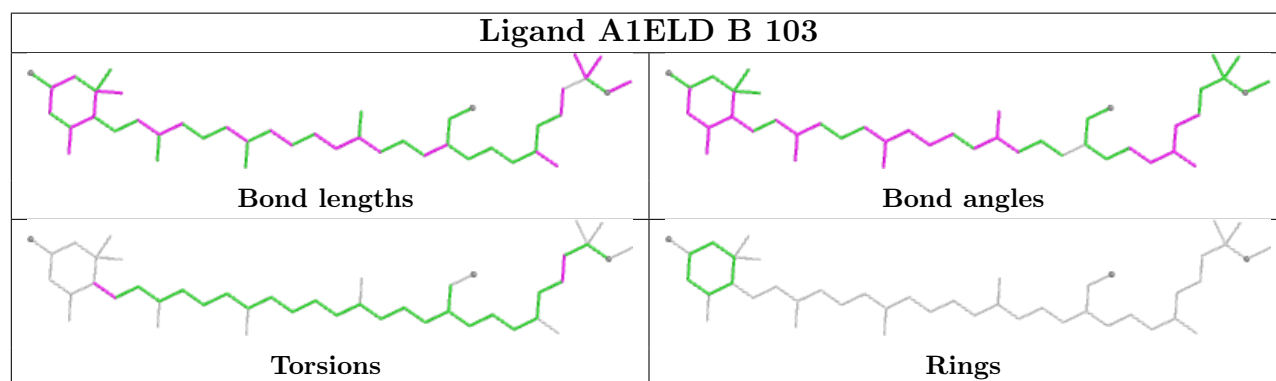
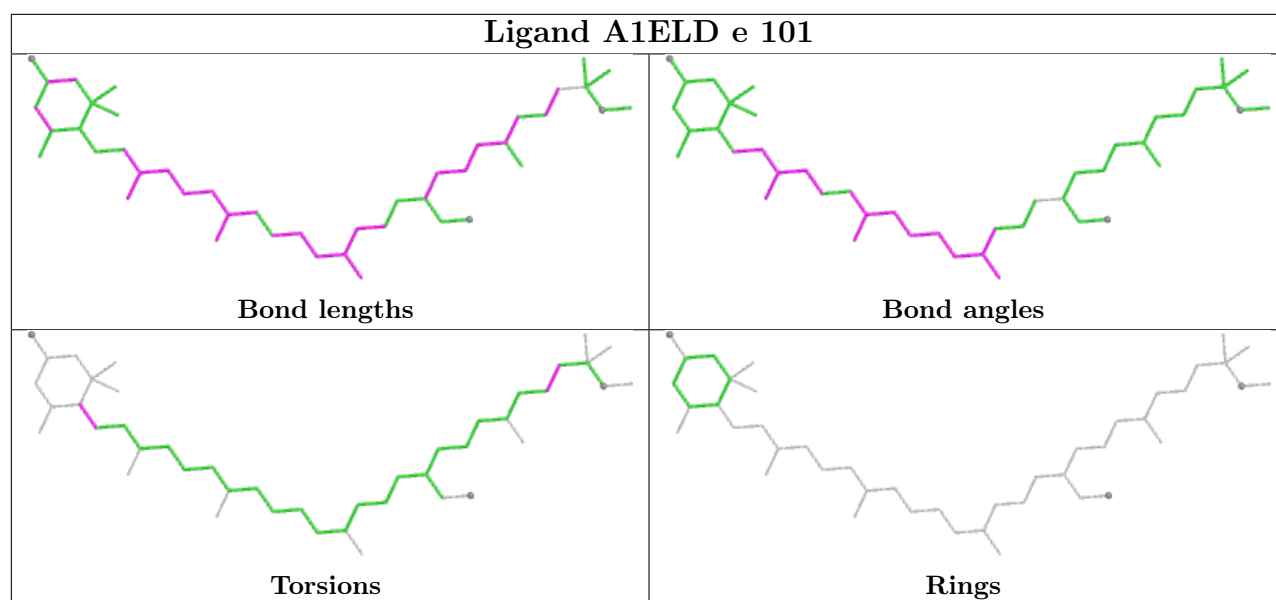


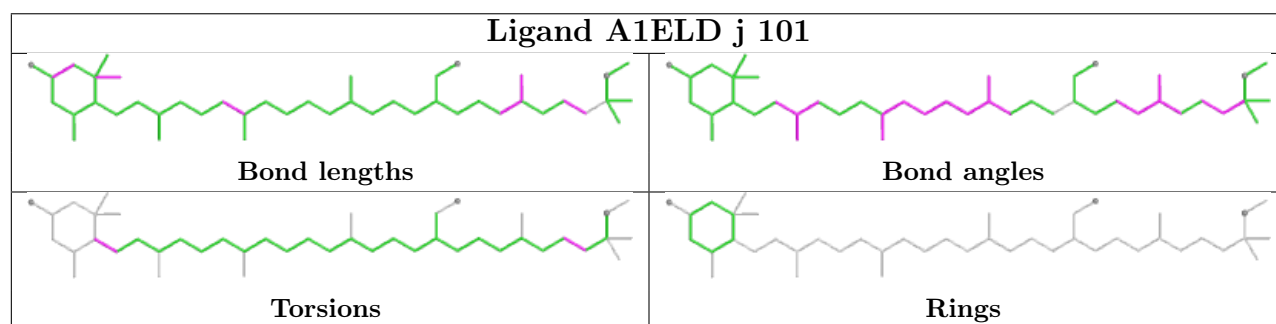
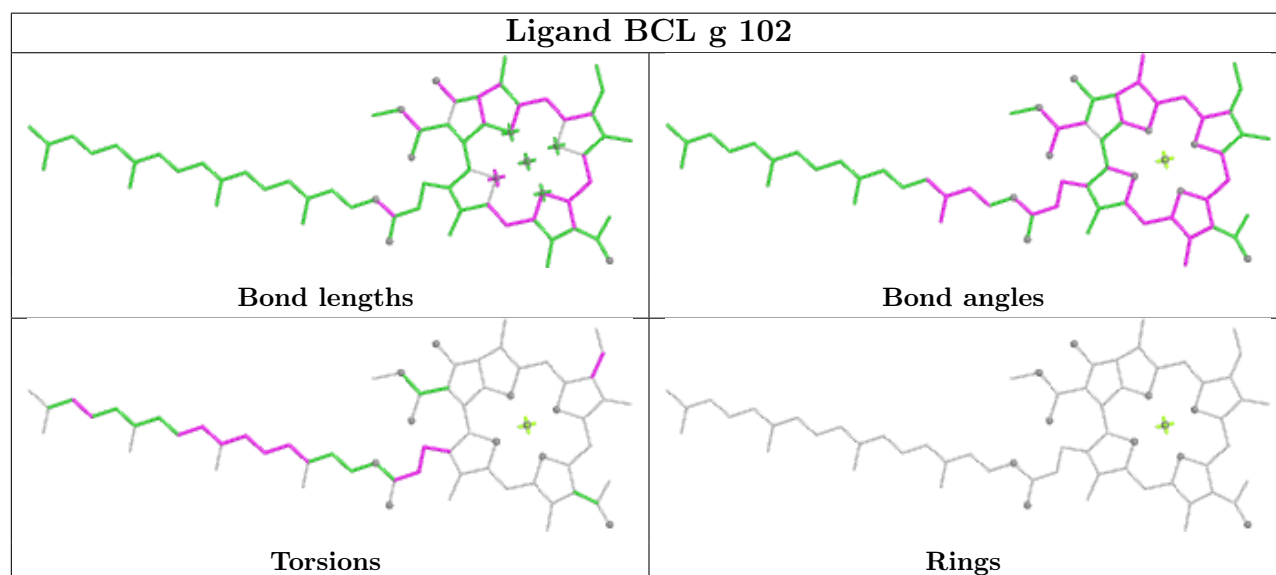
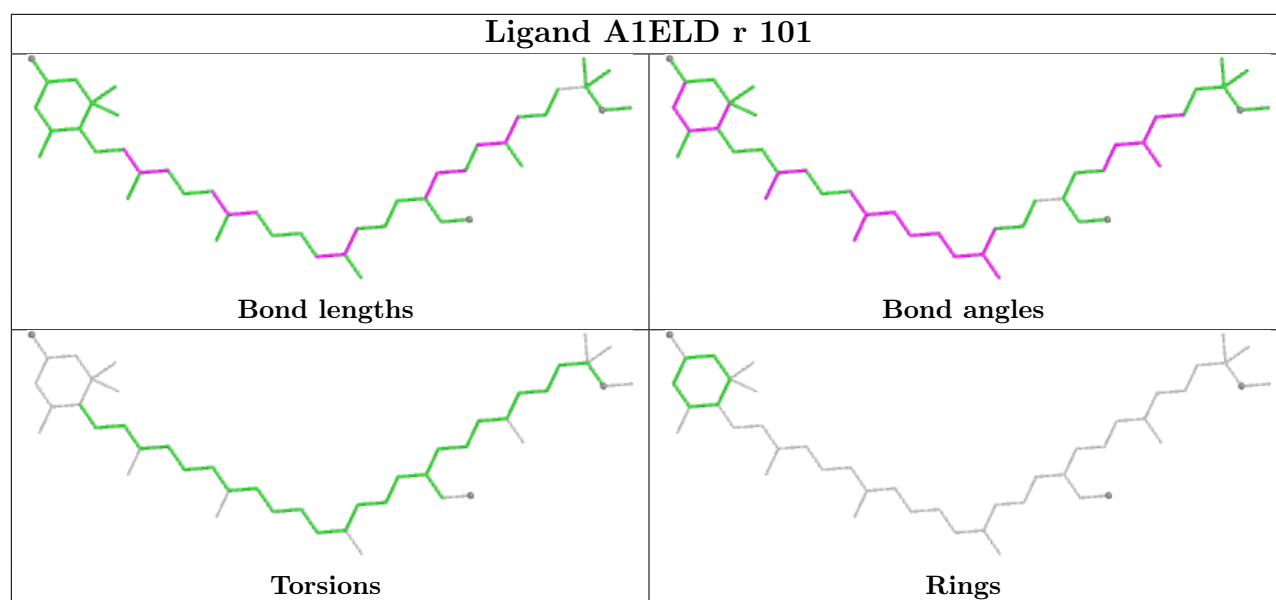


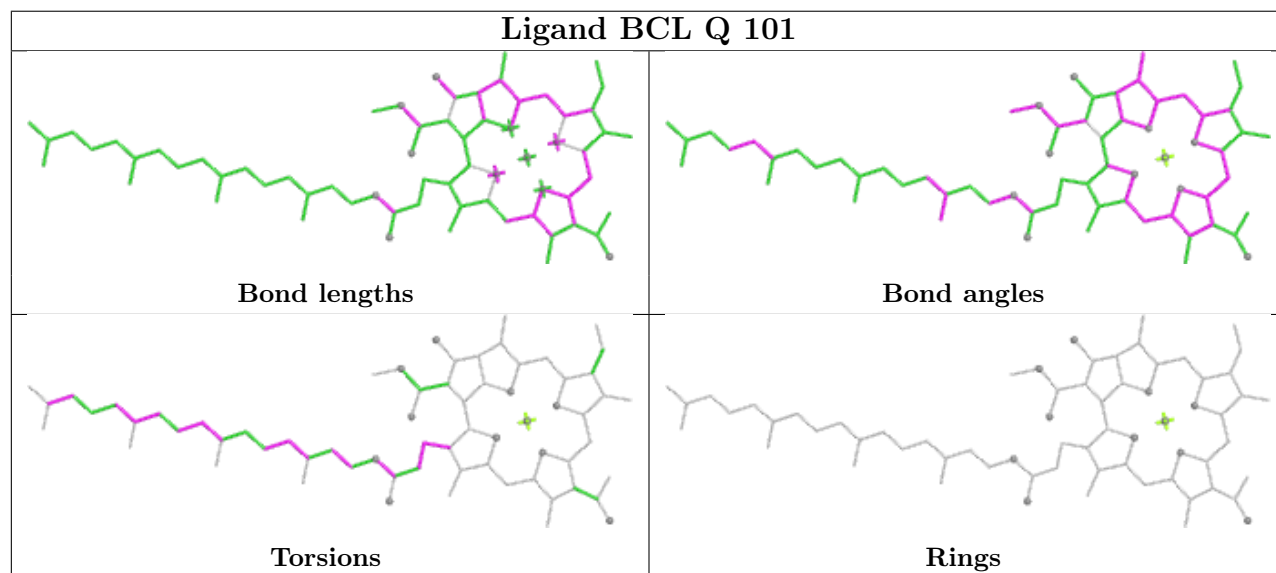
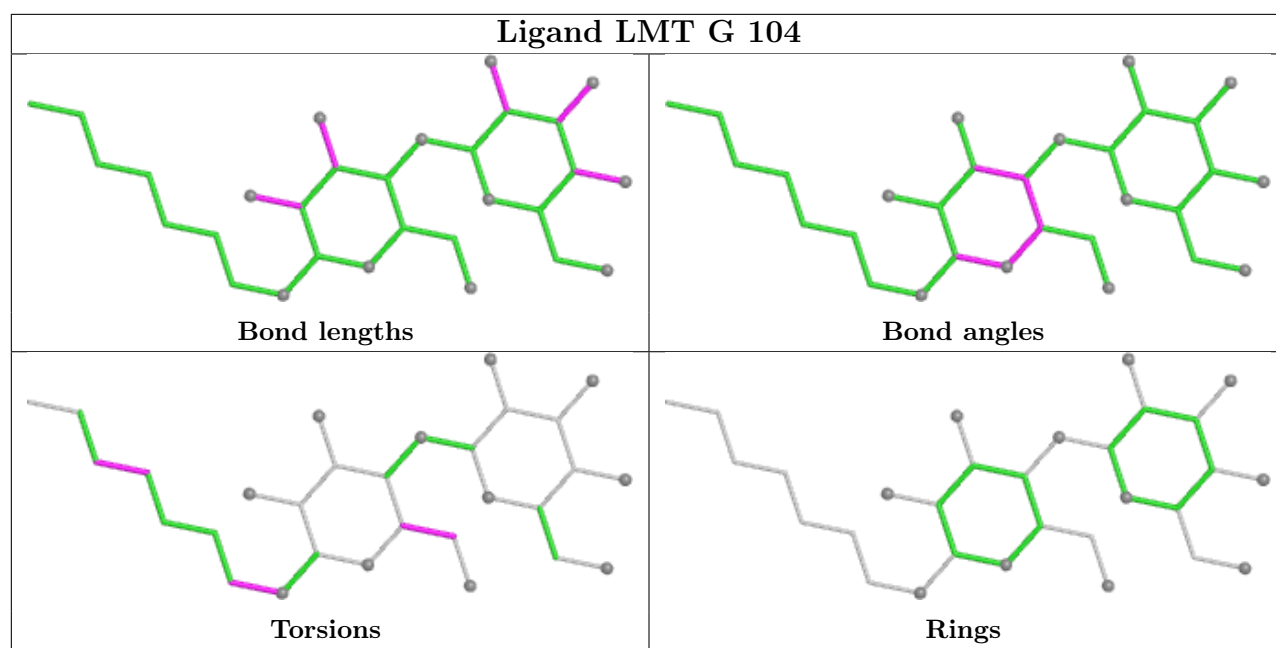


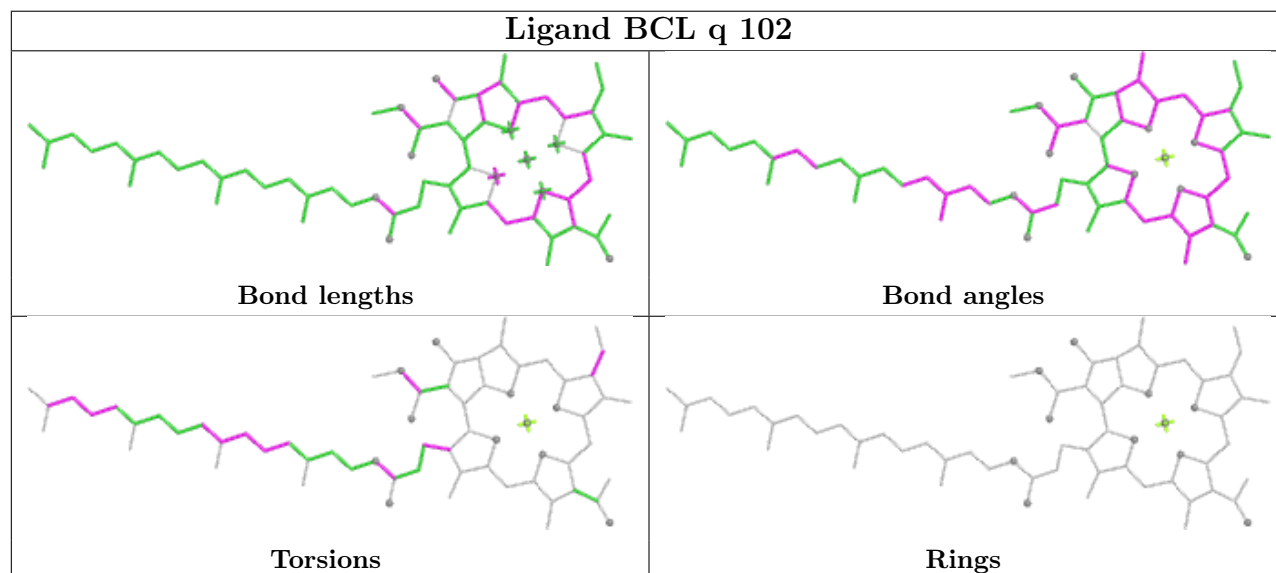
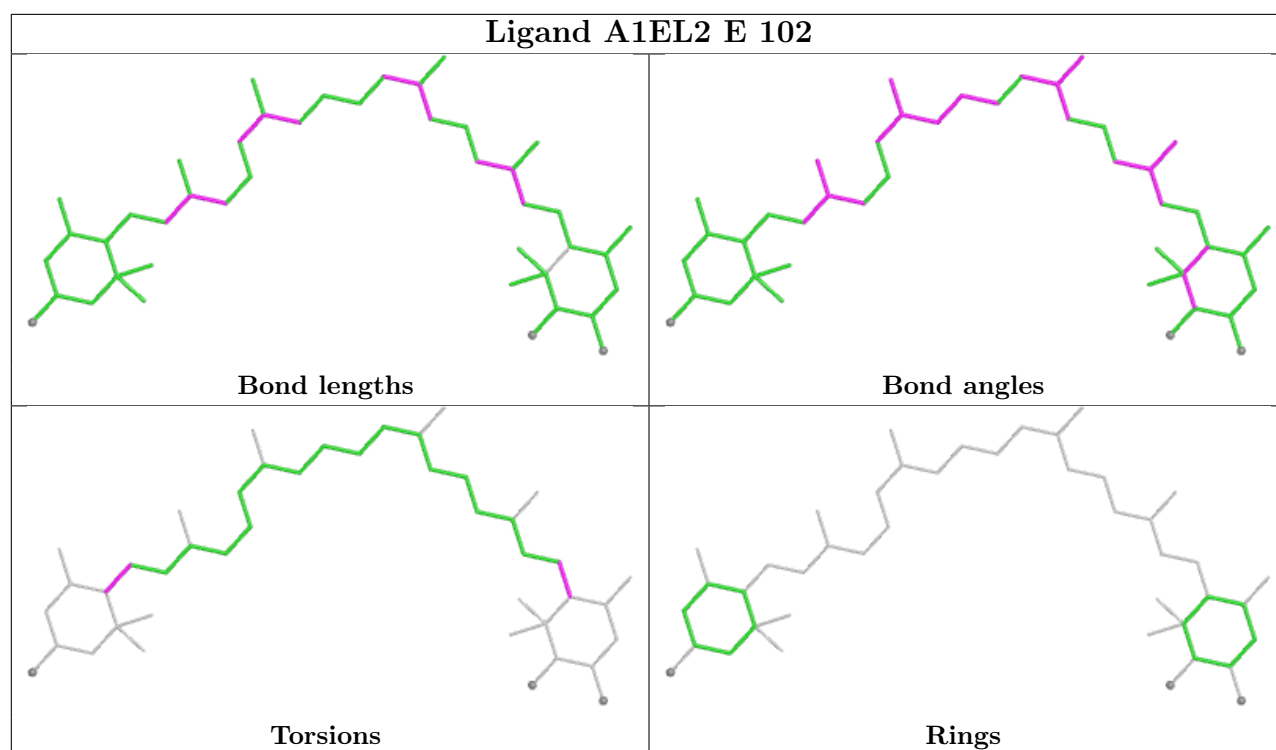


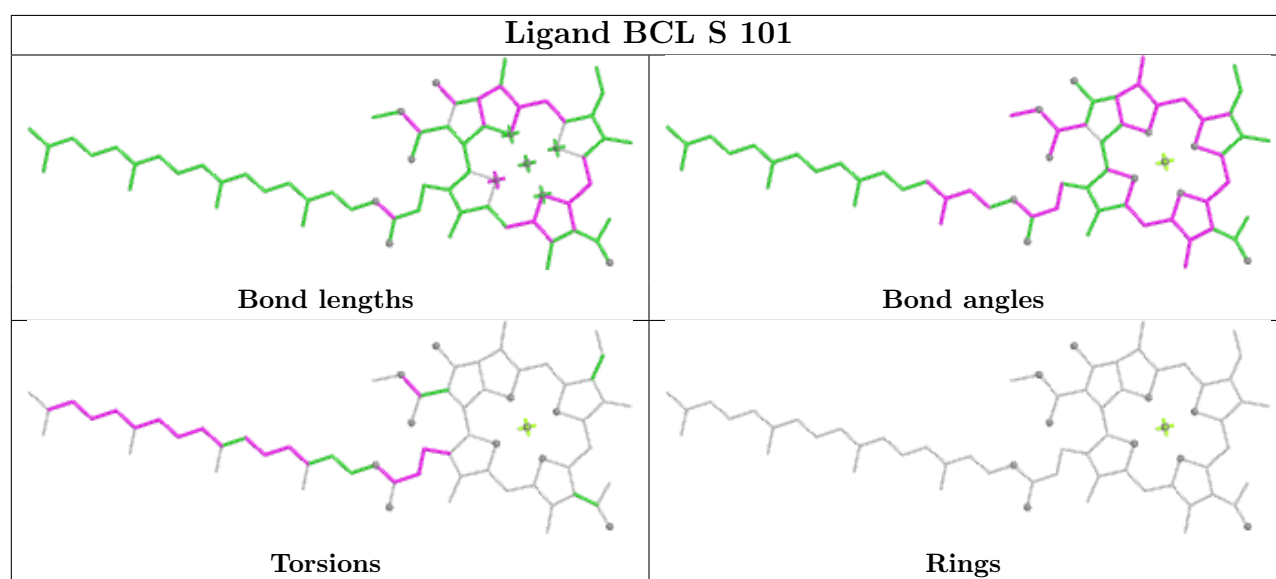
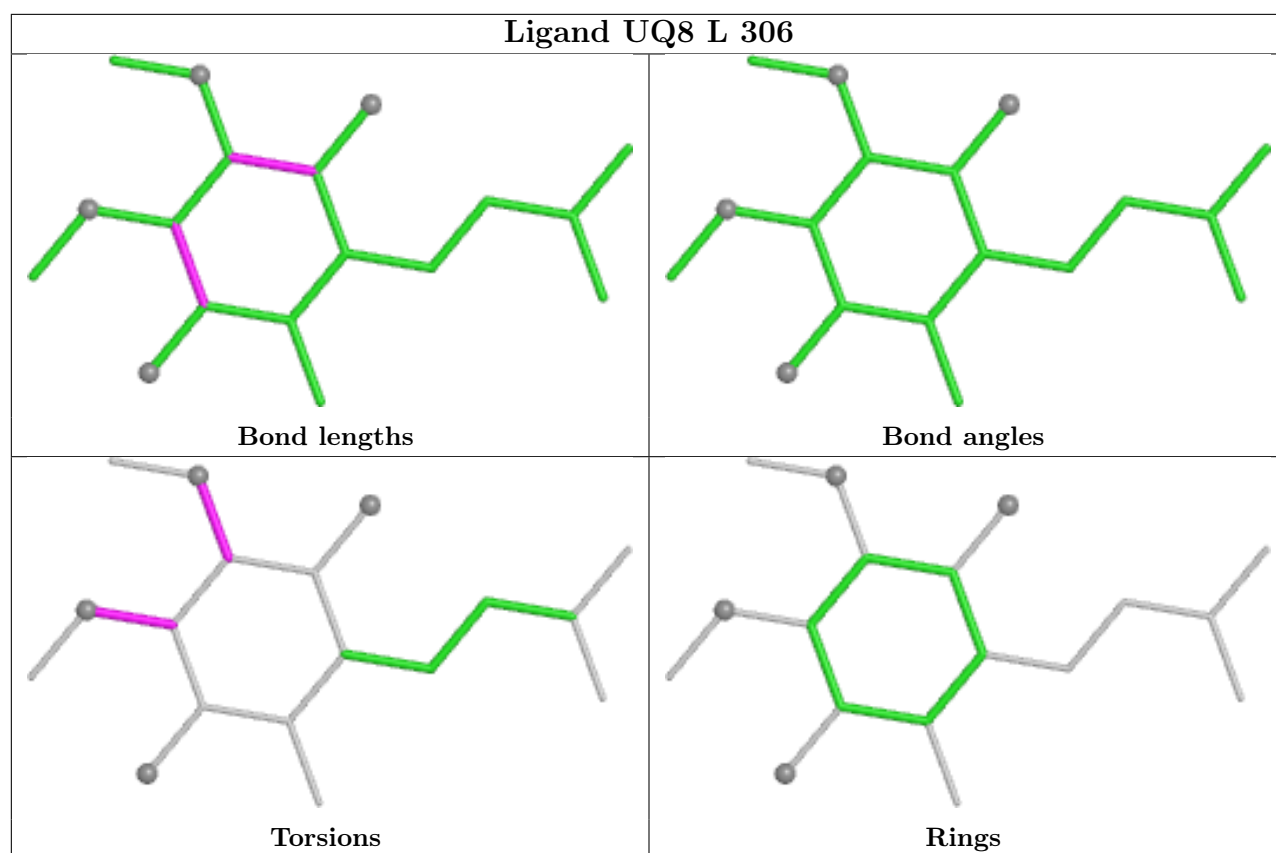


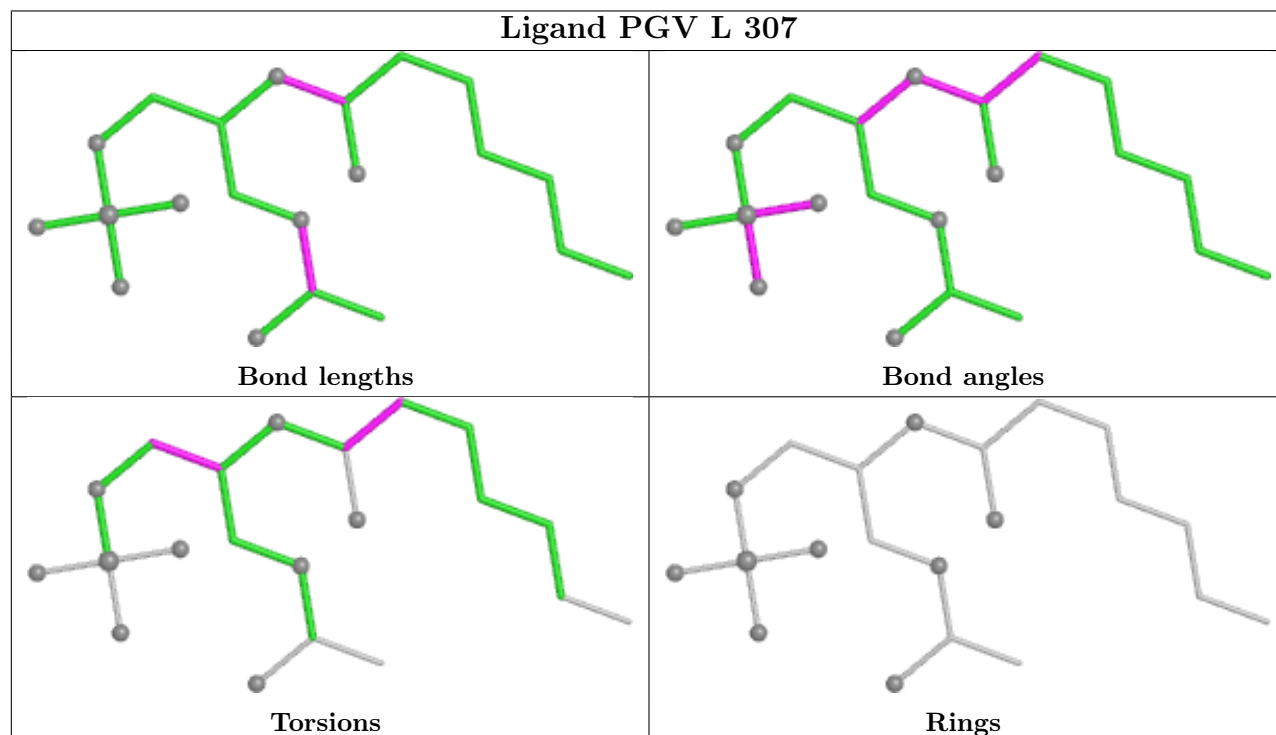
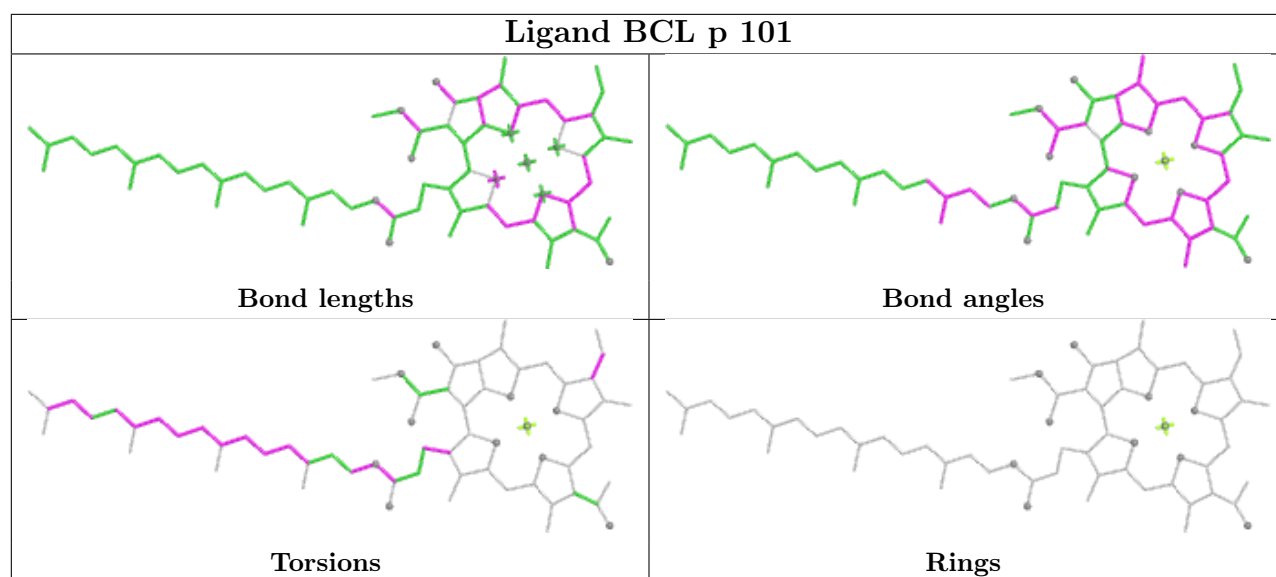


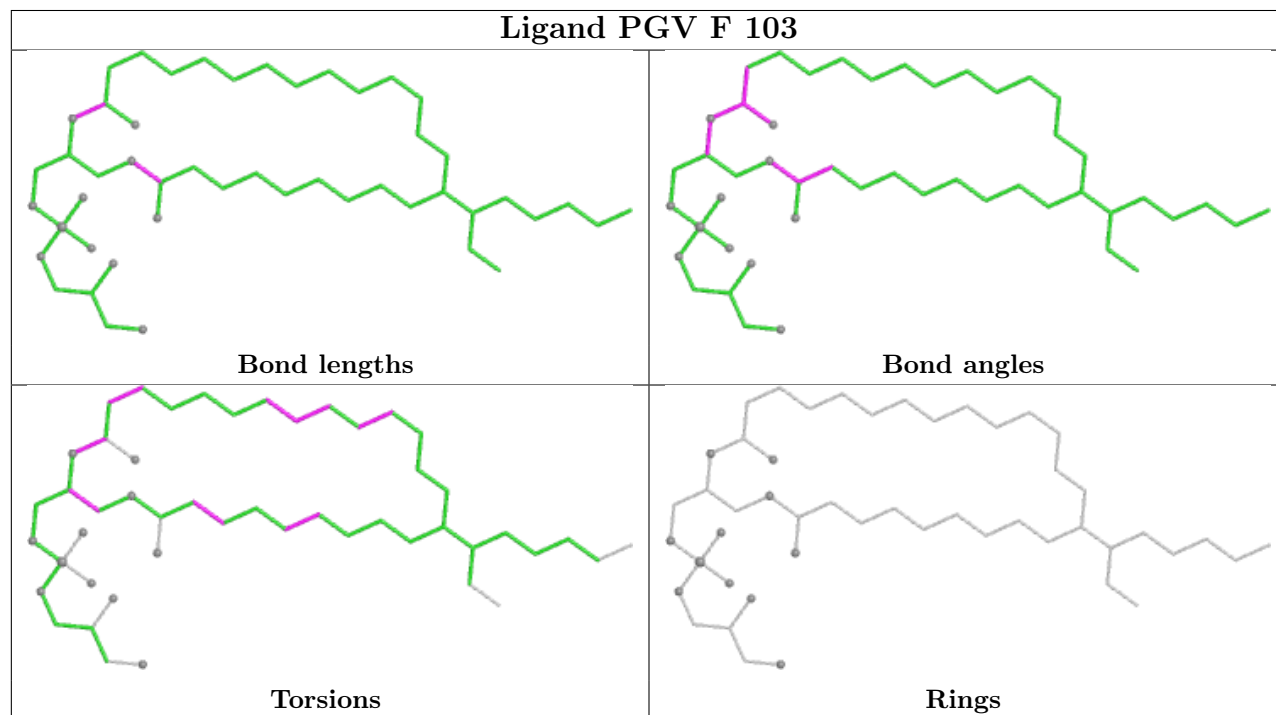
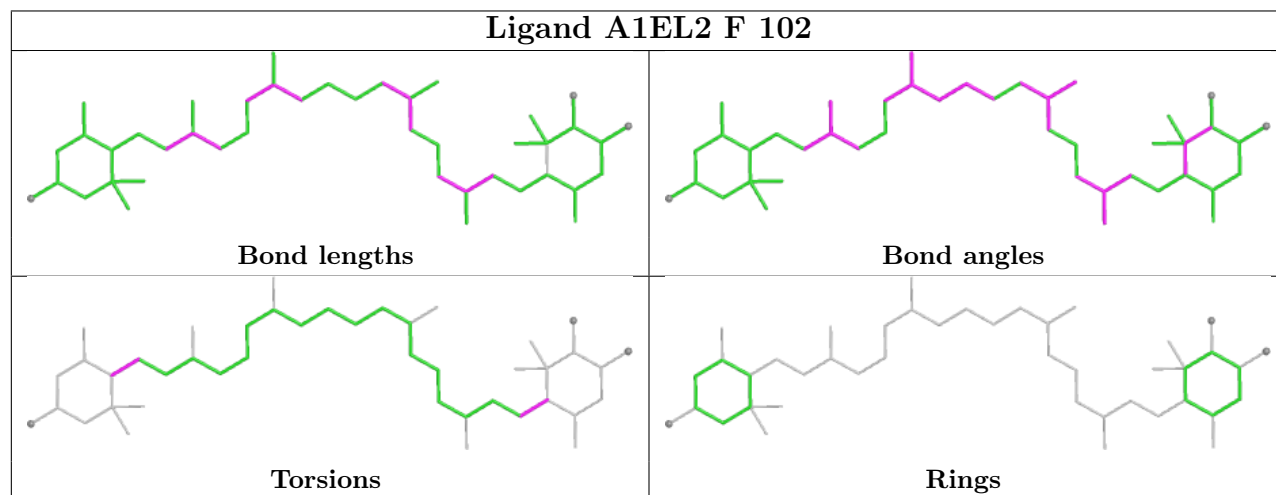
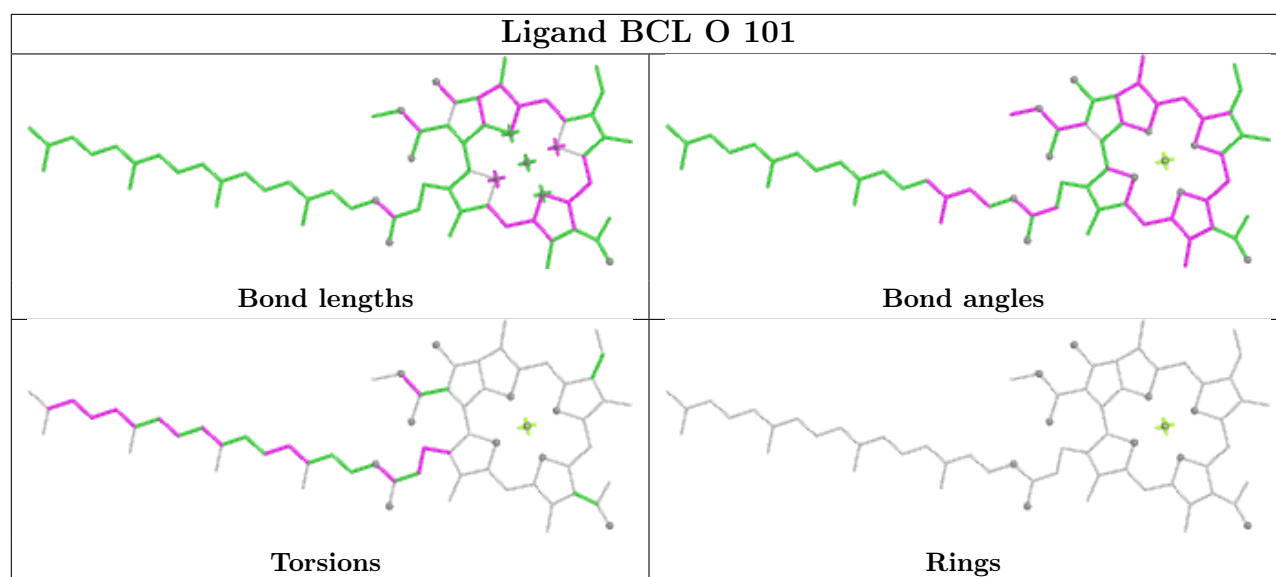


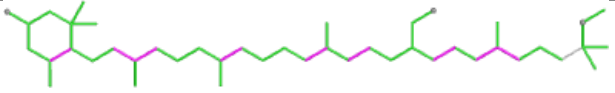
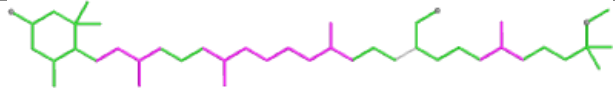
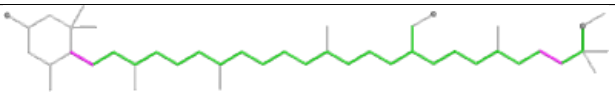
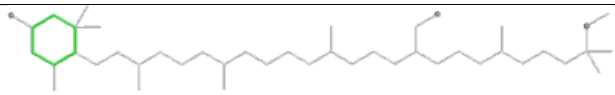
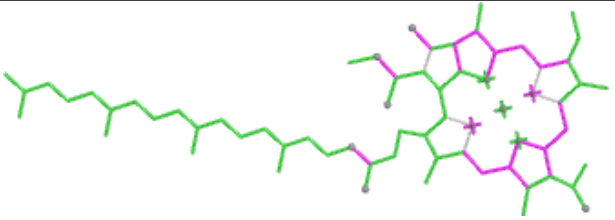
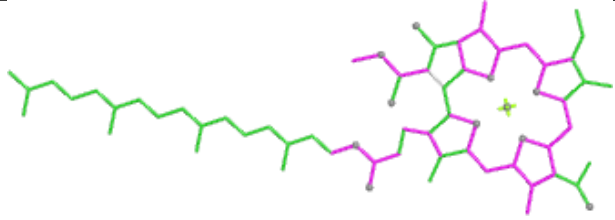
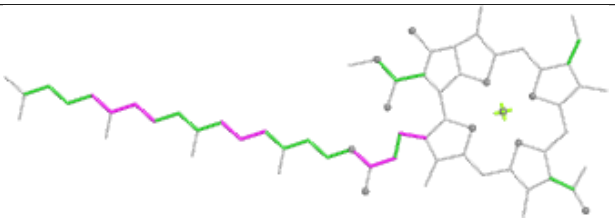
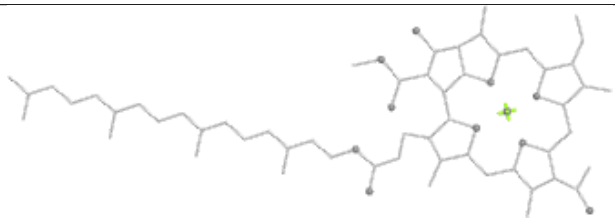
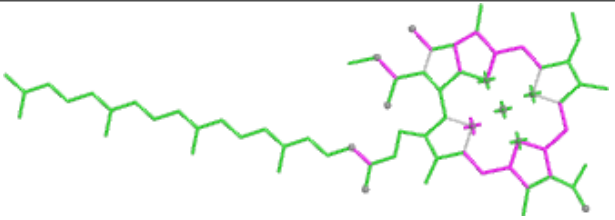
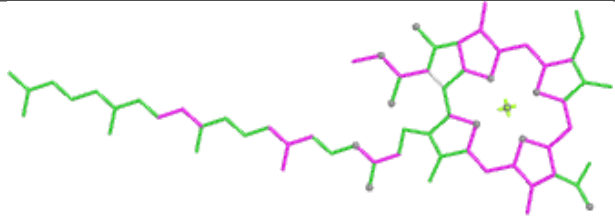
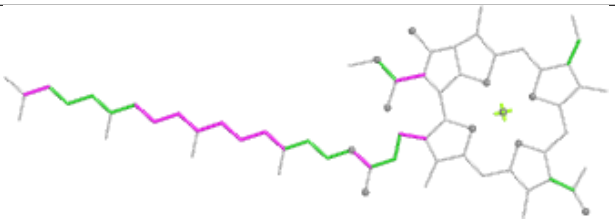
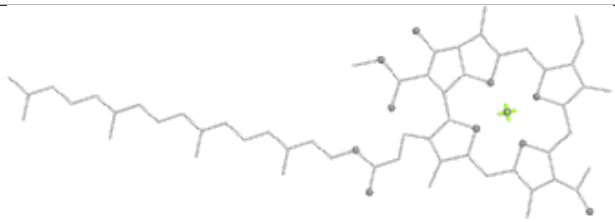


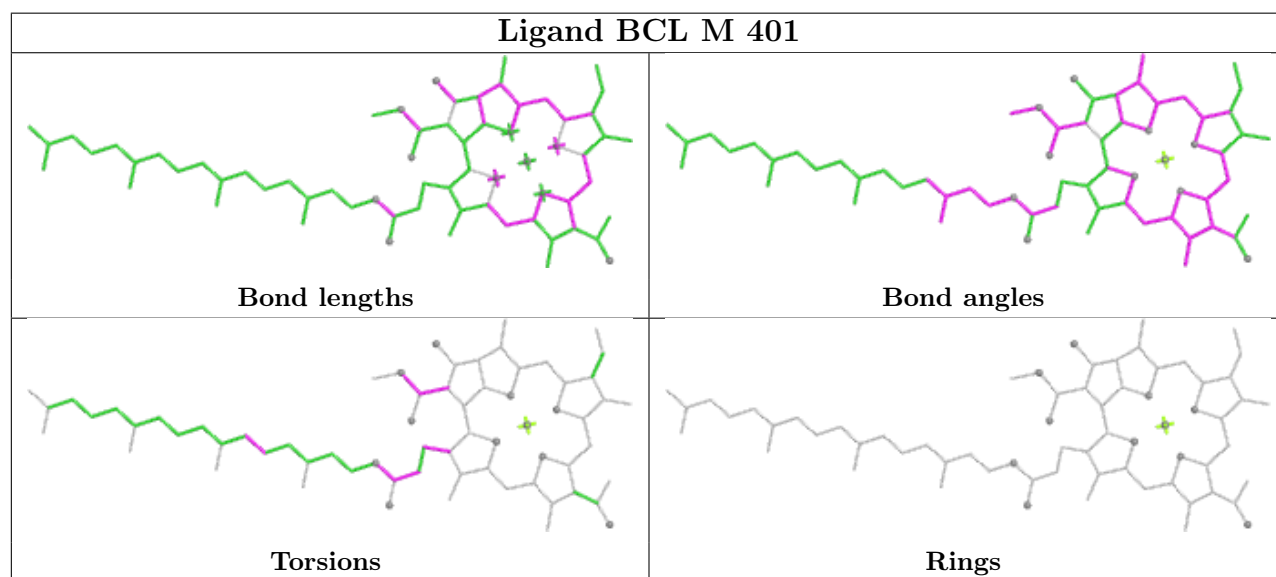
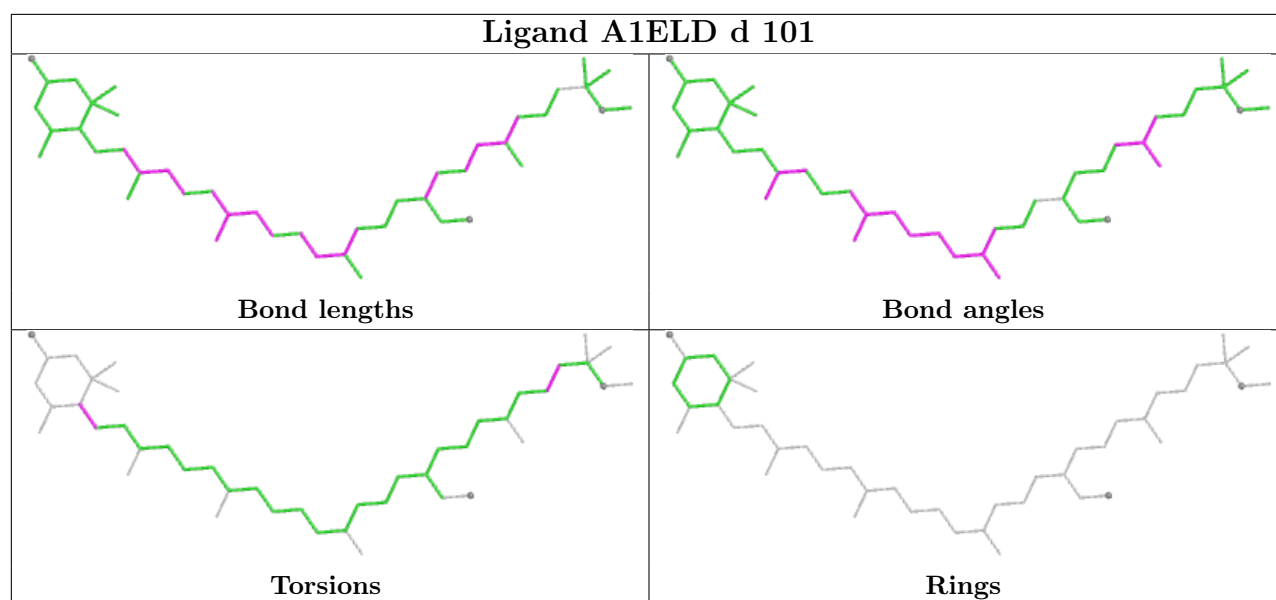


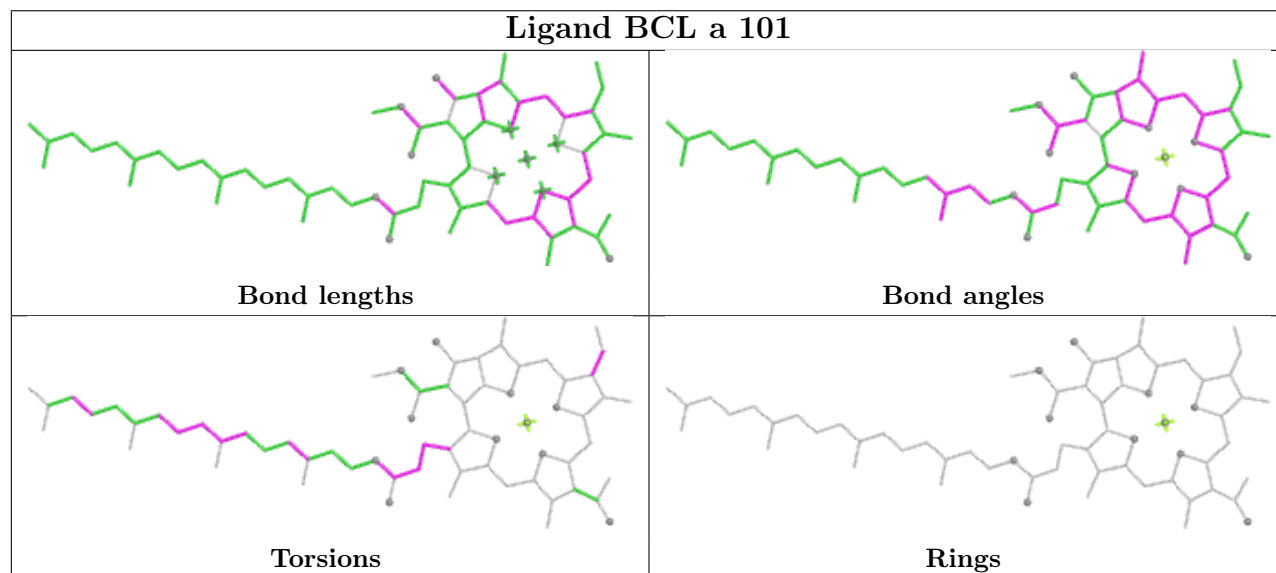
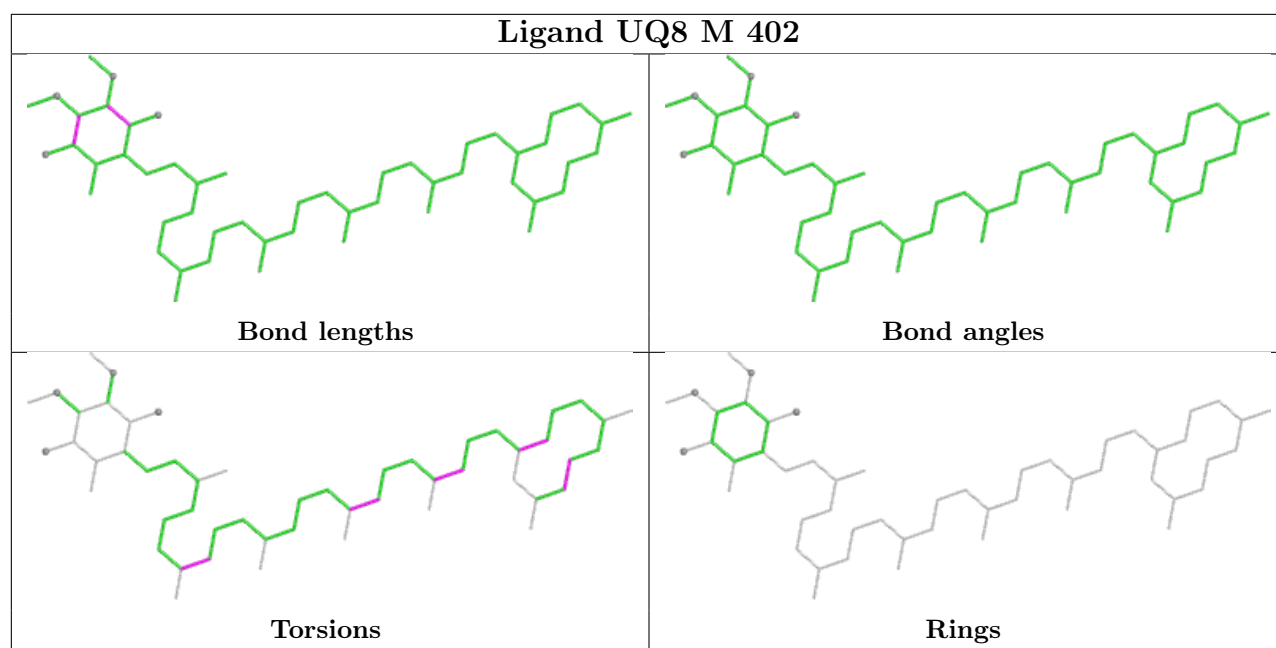


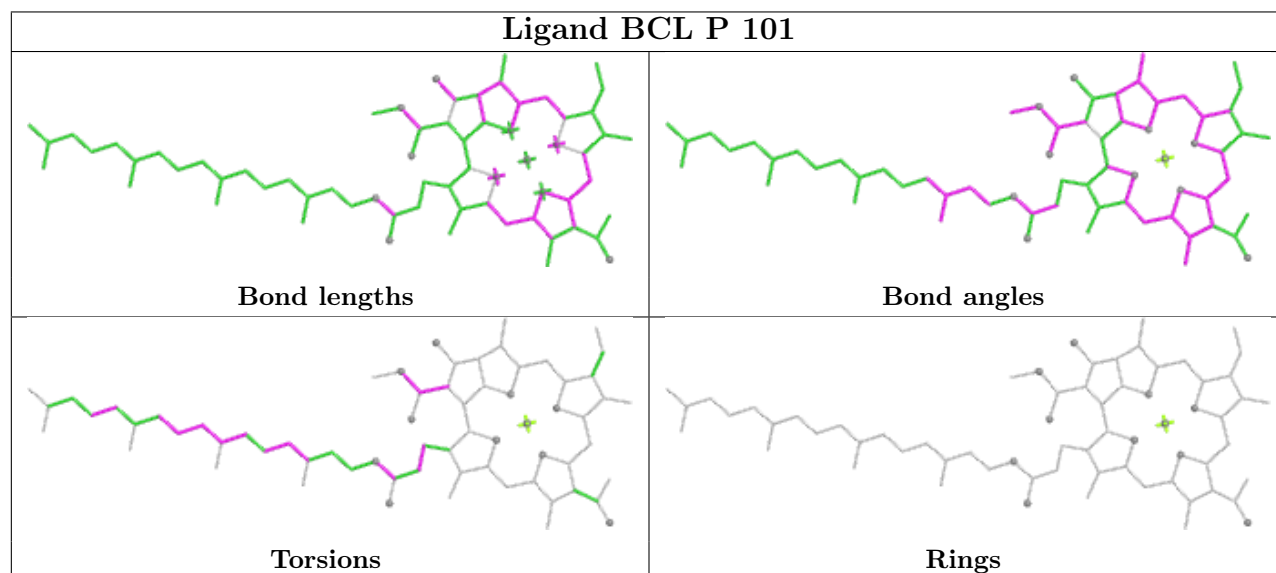
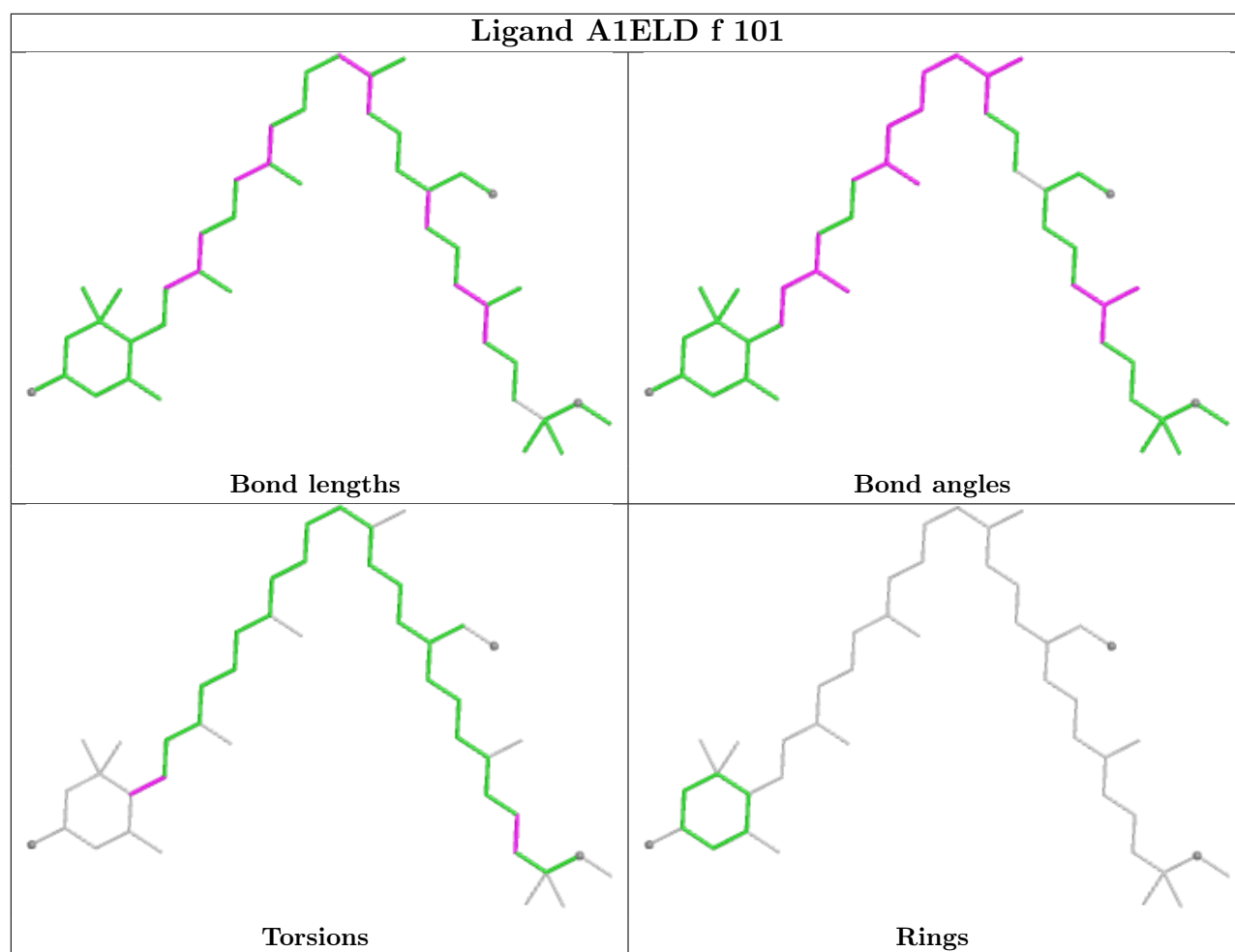


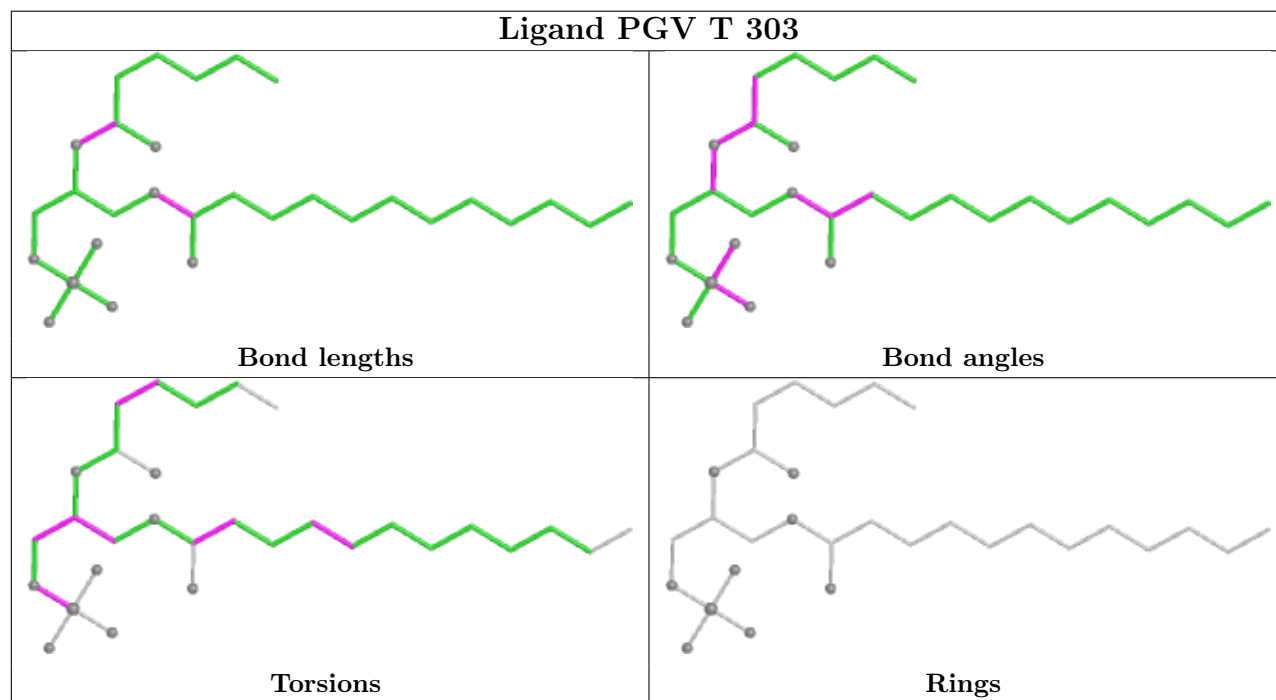
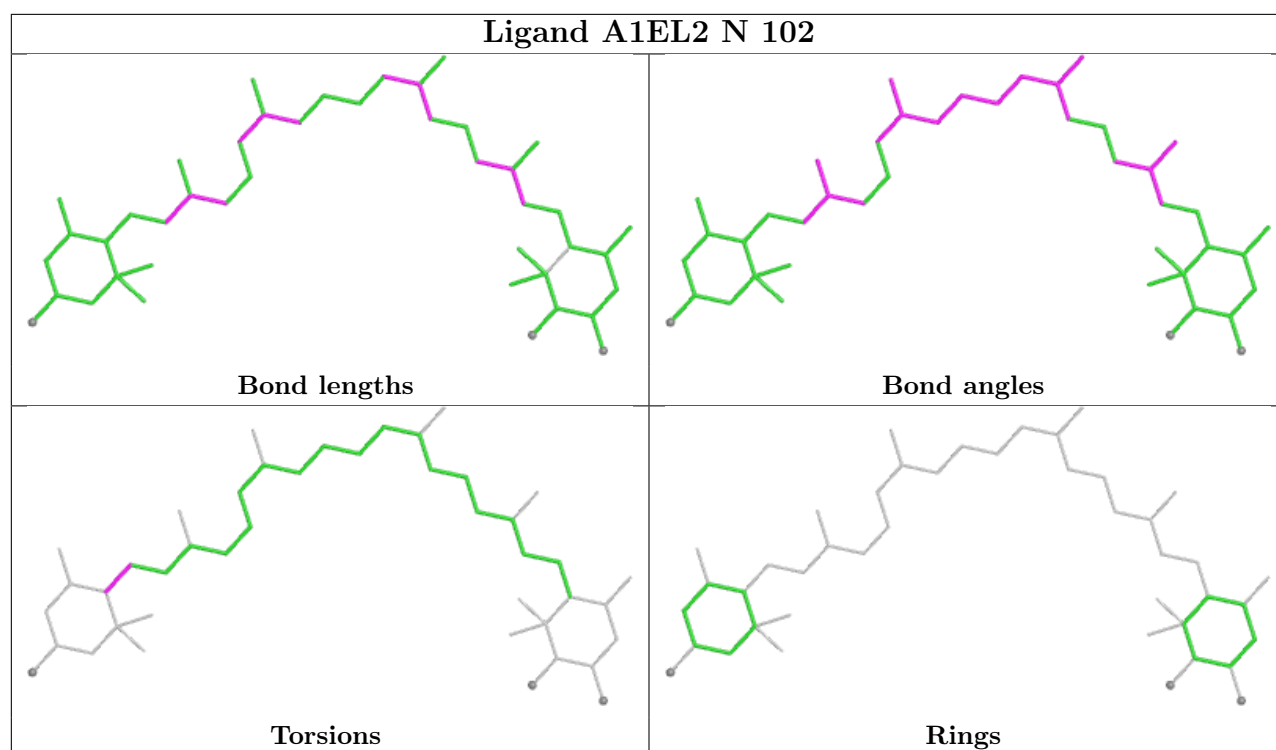


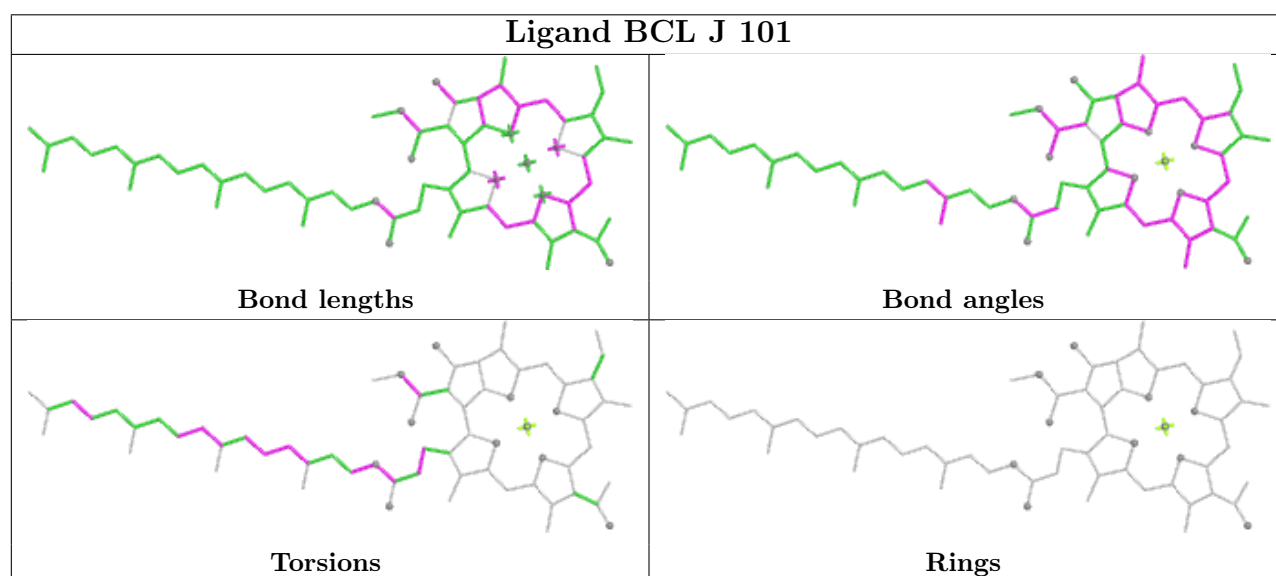
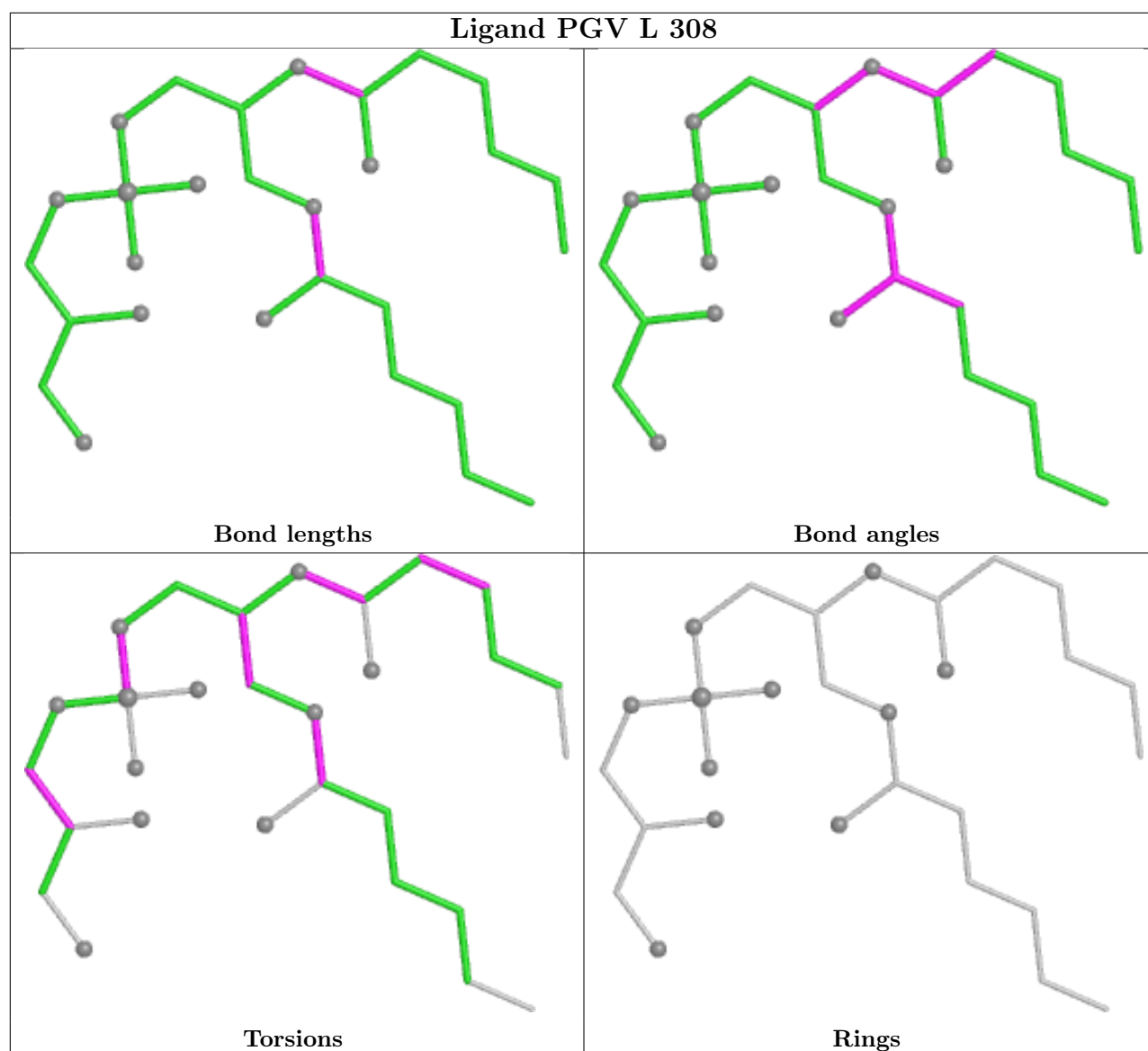
Ligand A1ELD g 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL N 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL E 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

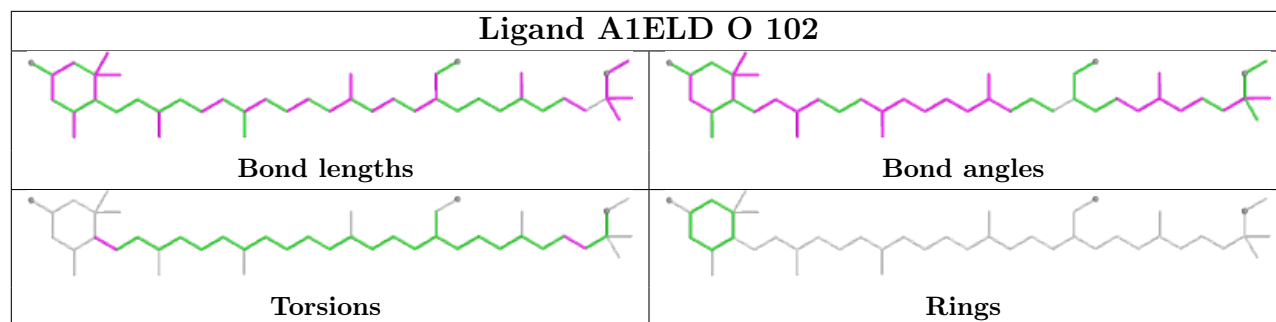












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

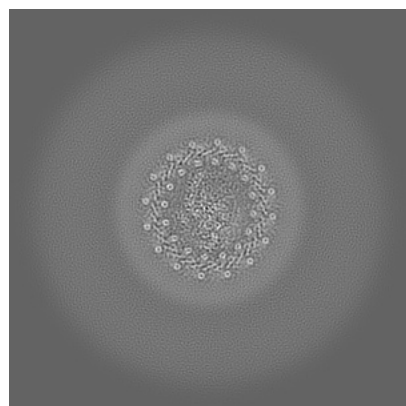
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63370. These allow visual inspection of the internal detail of the map and identification of artifacts.

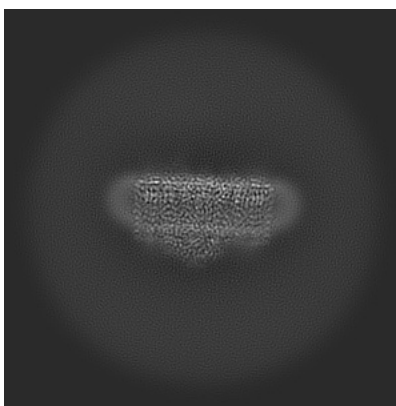
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

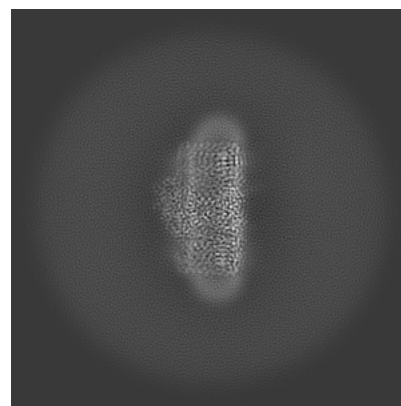
6.1.1 Primary map



X

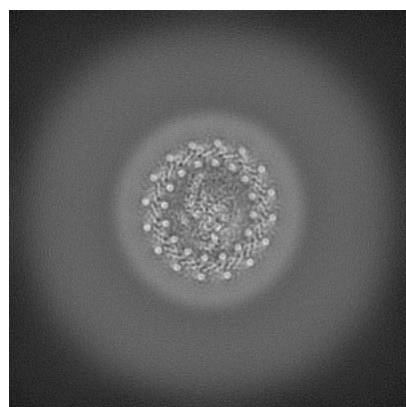


Y

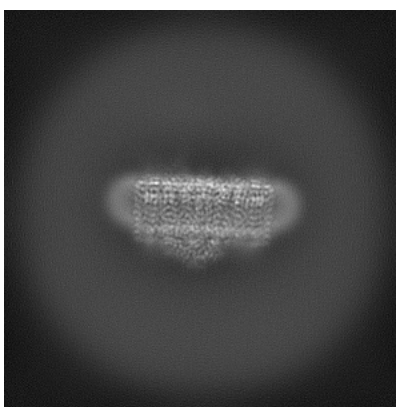


Z

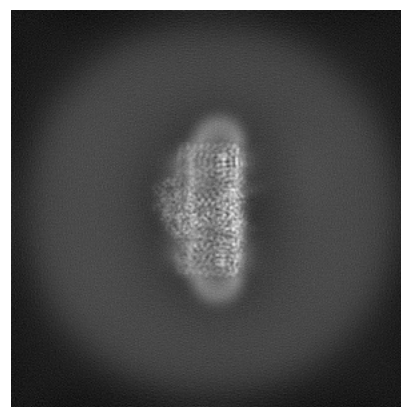
6.1.2 Raw map



X



Y

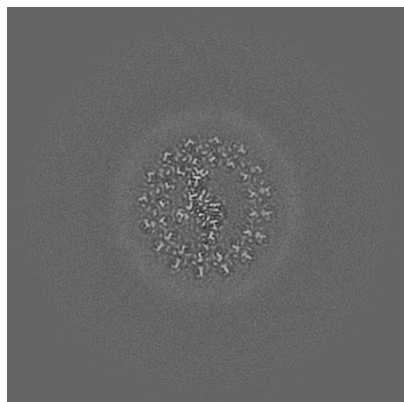


Z

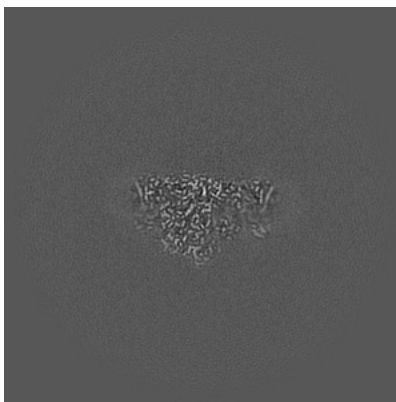
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

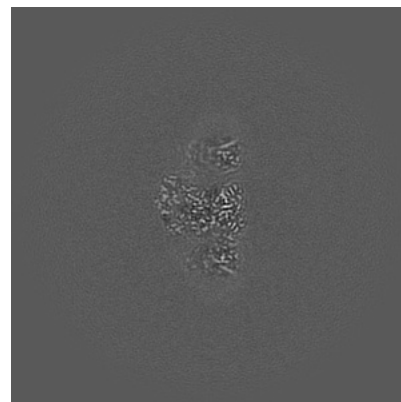
6.2.1 Primary map



X Index: 200

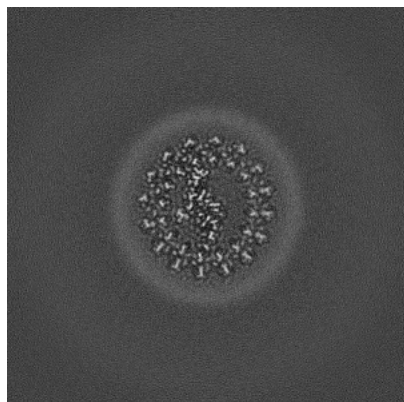


Y Index: 200

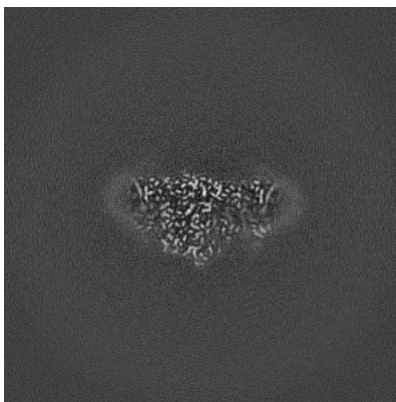


Z Index: 200

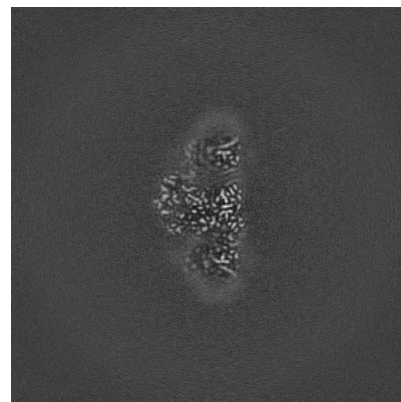
6.2.2 Raw map



X Index: 200



Y Index: 200

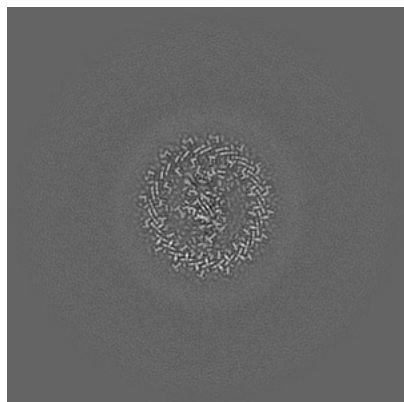


Z Index: 200

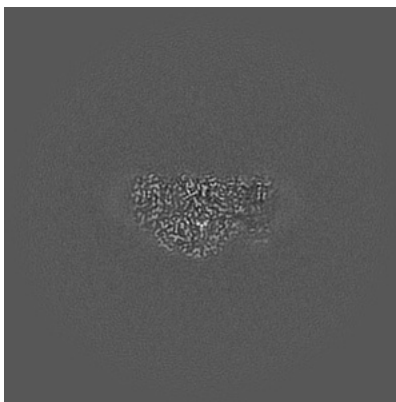
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

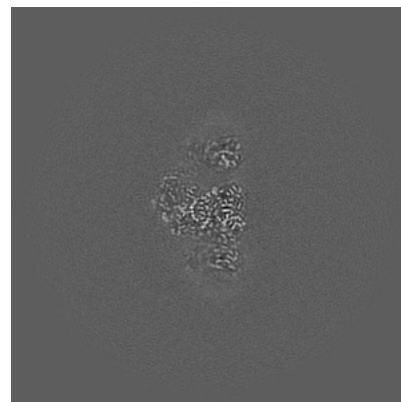
6.3.1 Primary map



X Index: 213

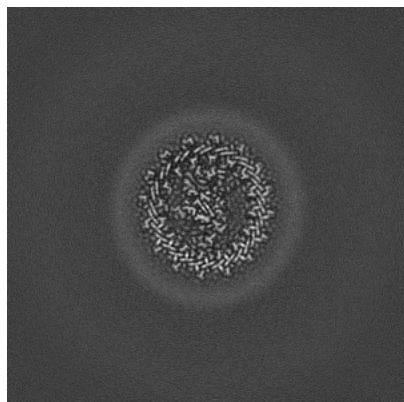


Y Index: 195

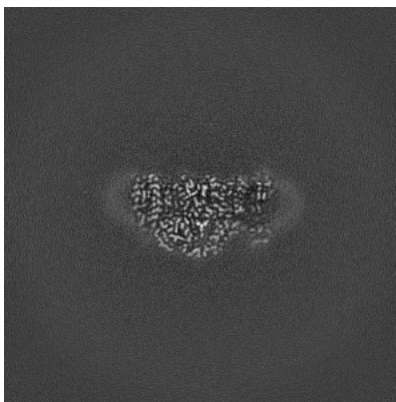


Z Index: 198

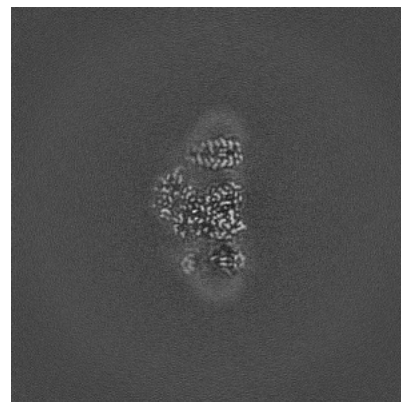
6.3.2 Raw map



X Index: 213



Y Index: 195

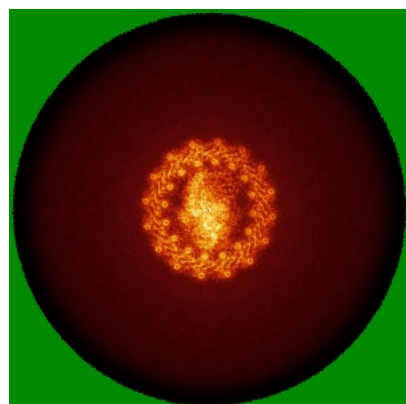


Z Index: 194

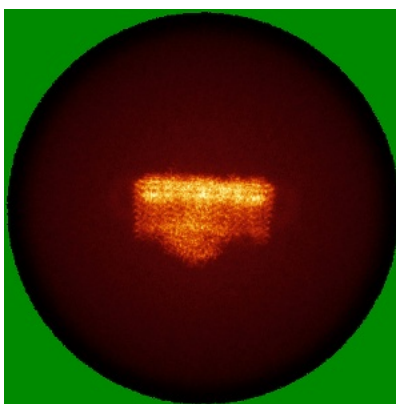
The images above show the largest variance slices of the map in three orthogonal directions.

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

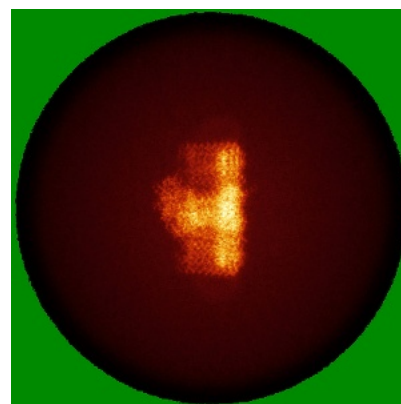
6.4.1 Primary map



X

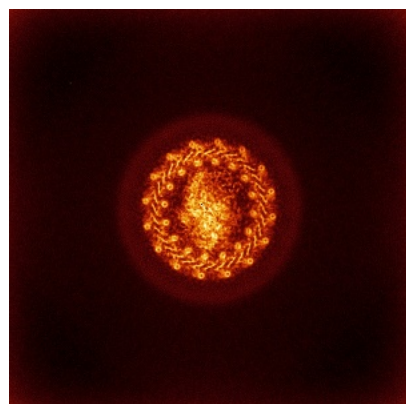


Y

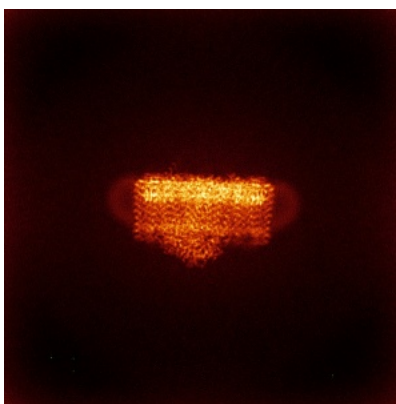


Z

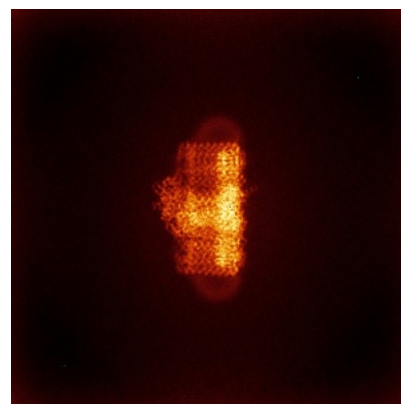
6.4.2 Raw map



X



Y

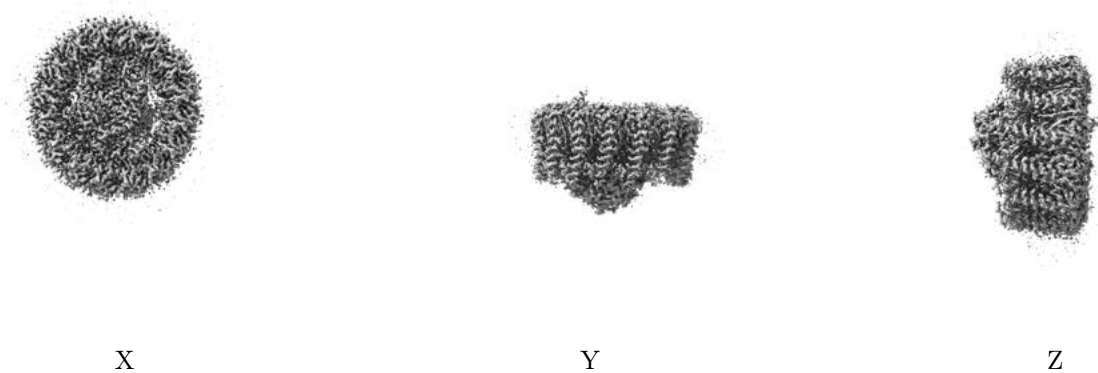


Z

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.

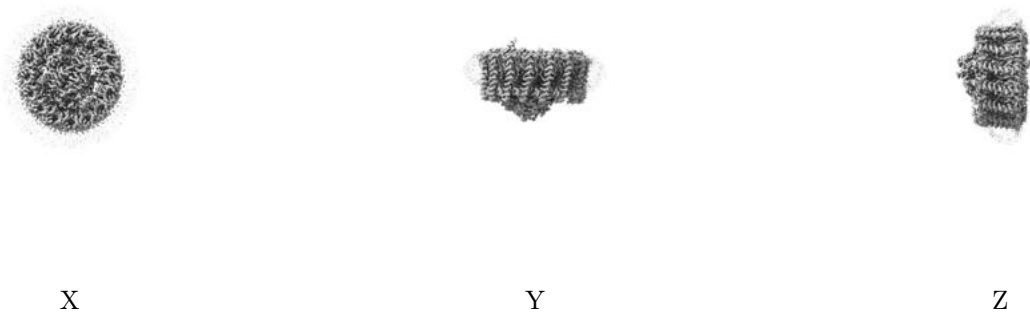
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0961. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

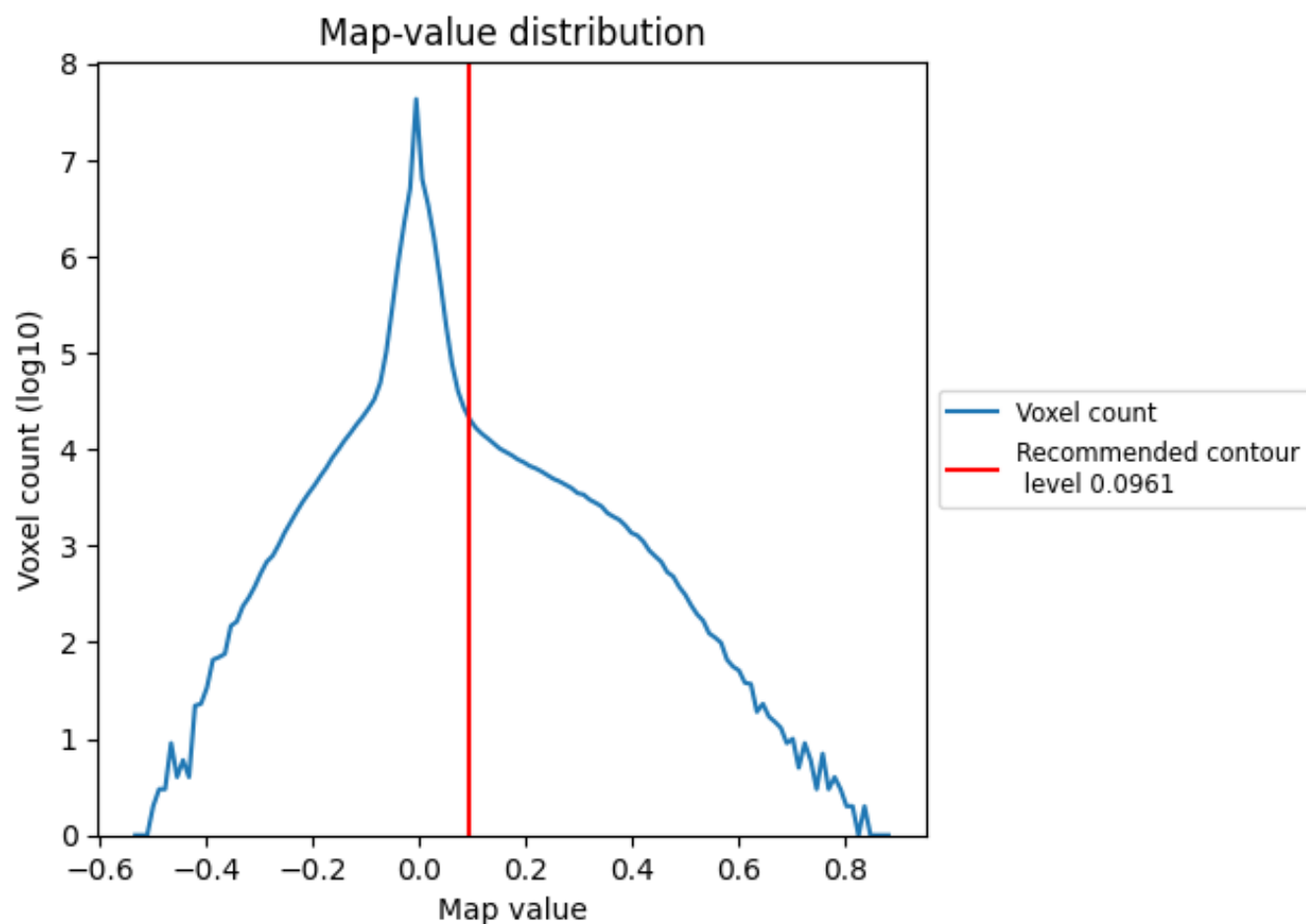
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

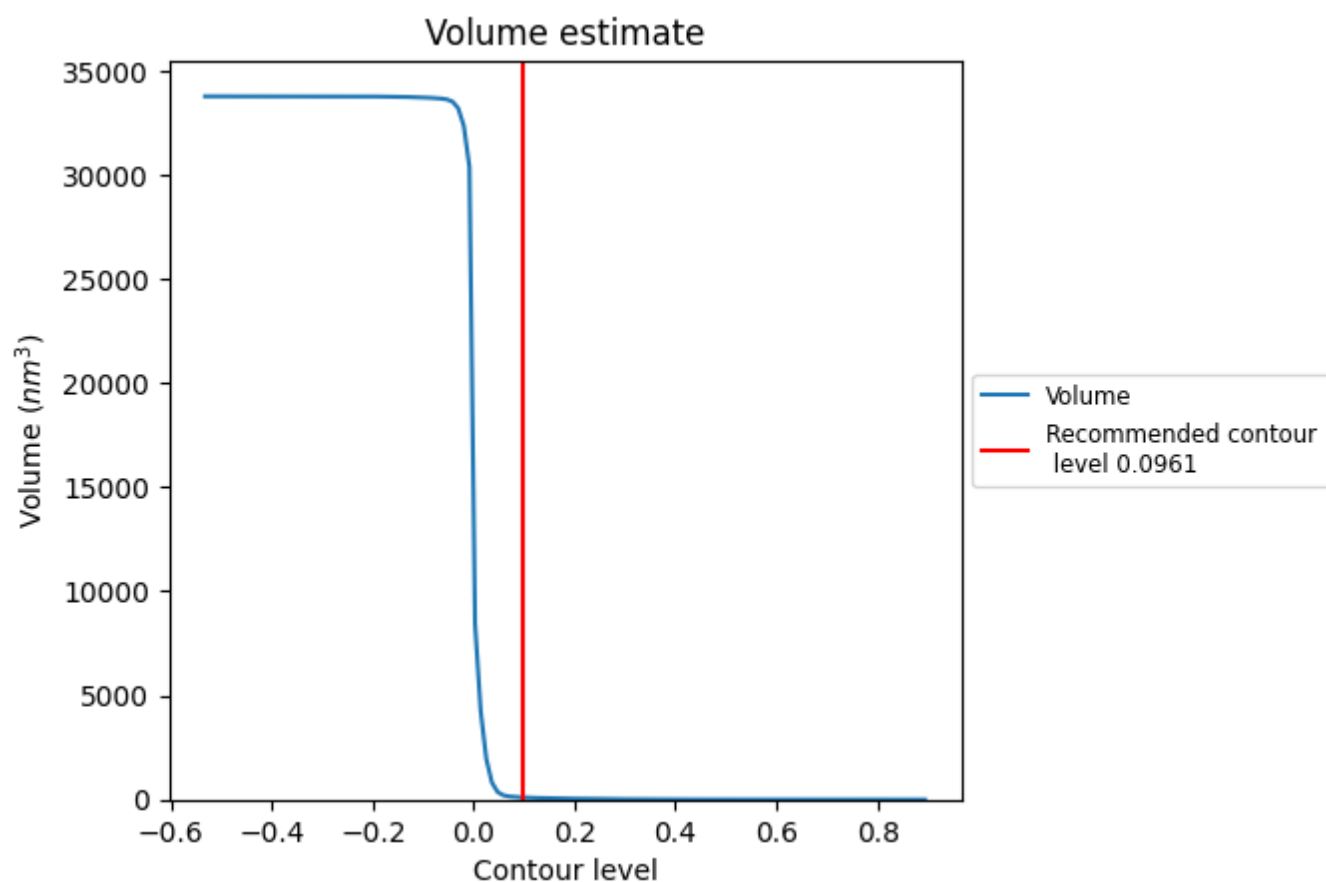
This section contains the results of statistical analysis of the map.

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.

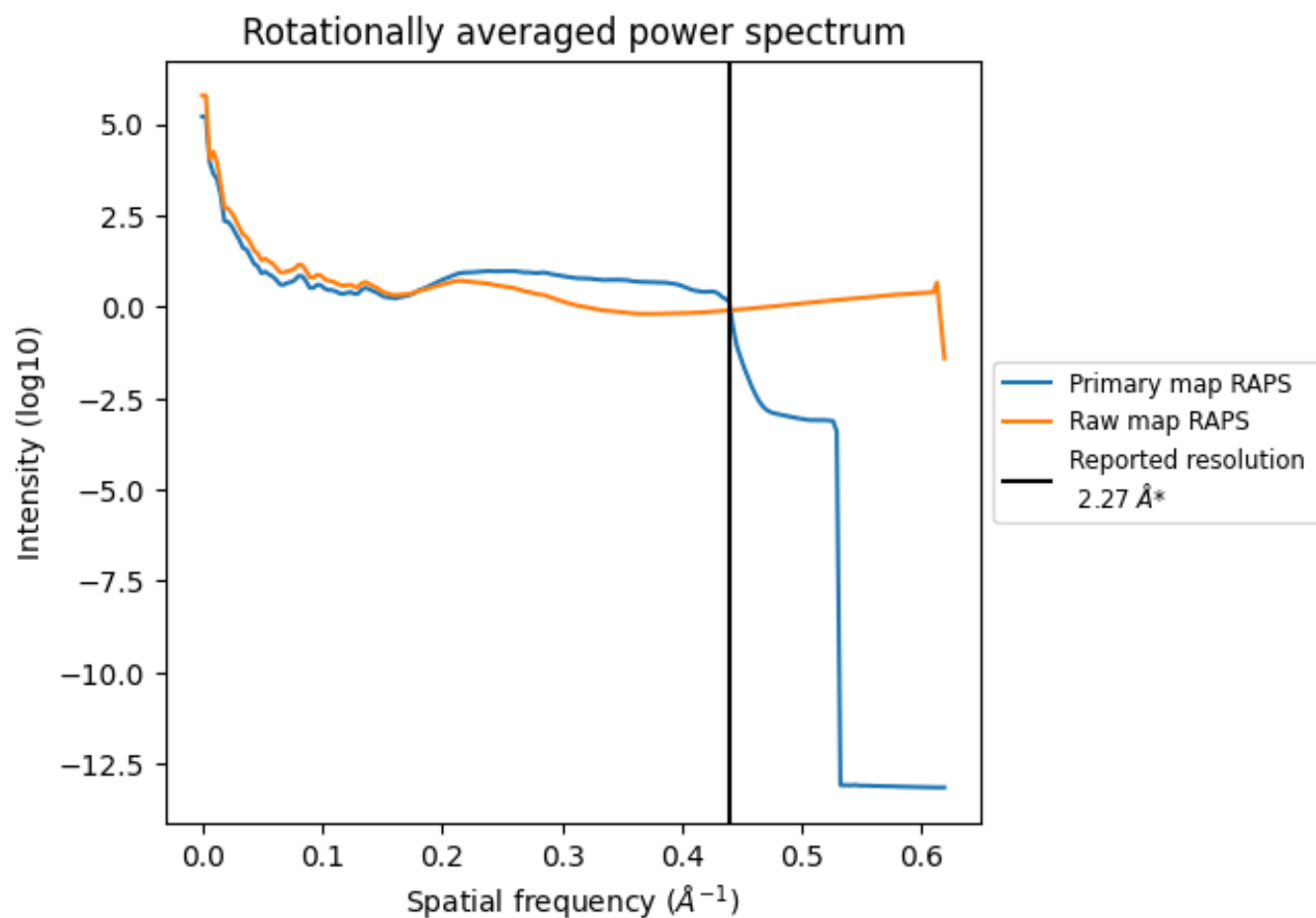
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 ⓘ

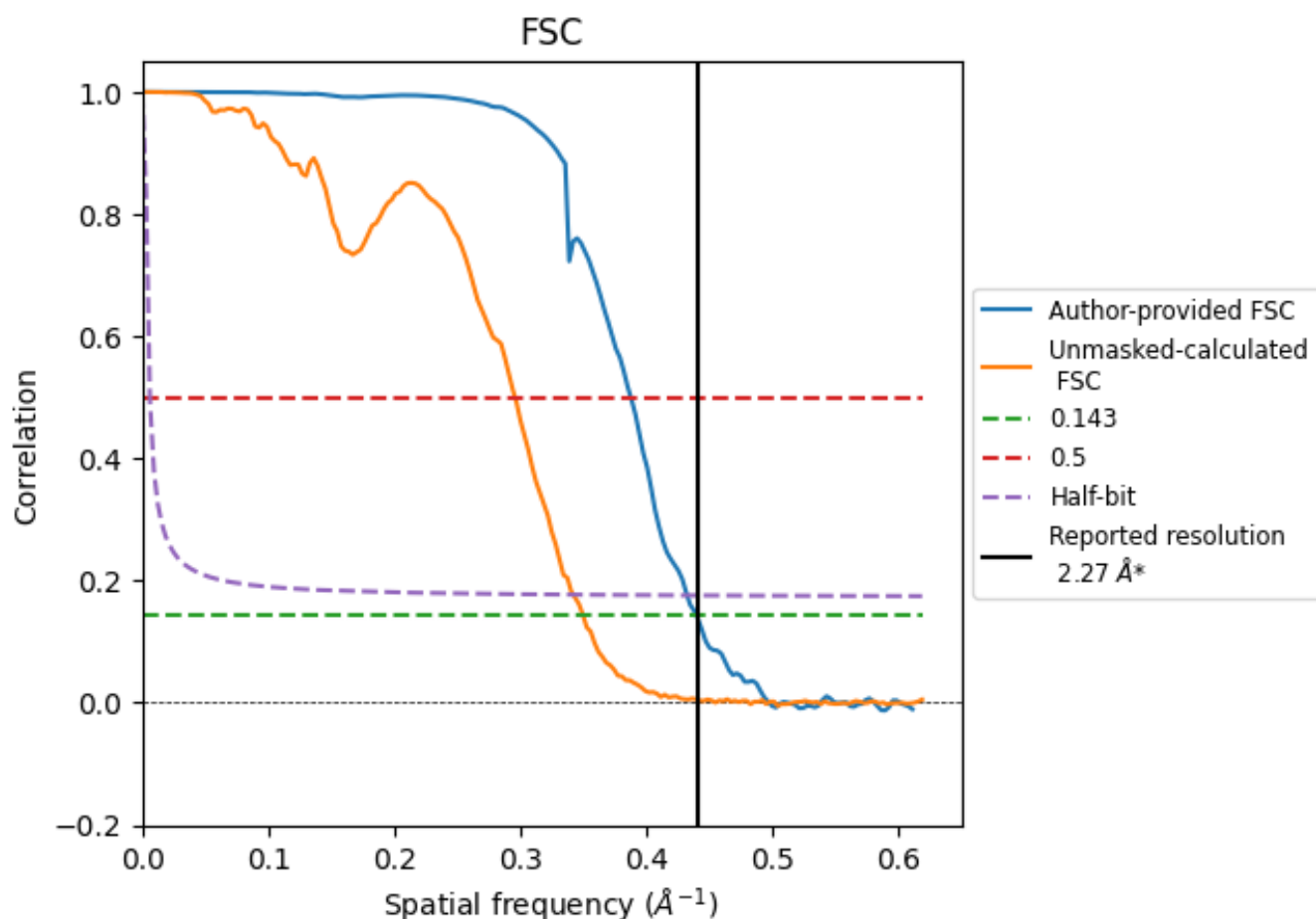


*Reported resolution corresponds to spatial frequency of 0.441 Å⁻¹

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 0.441 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

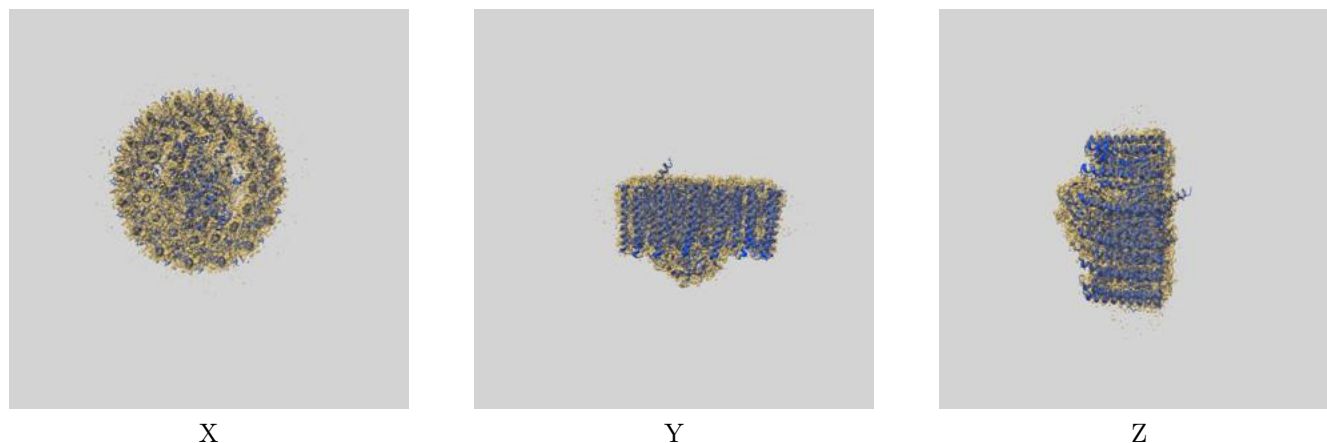
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.27	2.58	2.31
Unmasked-calculated*	2.86	3.38	2.92

*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 2.86 differs from the reported value 2.27 by more than 10 %

9 Map-model fit [i](#)

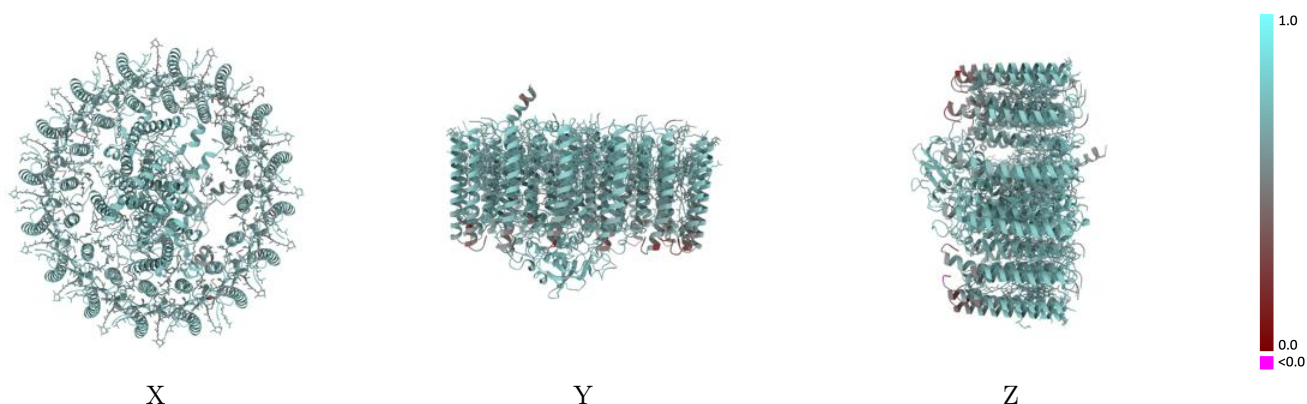
This section contains information regarding the fit between EMDB map EMD-63370 and PDB model 9LTI. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



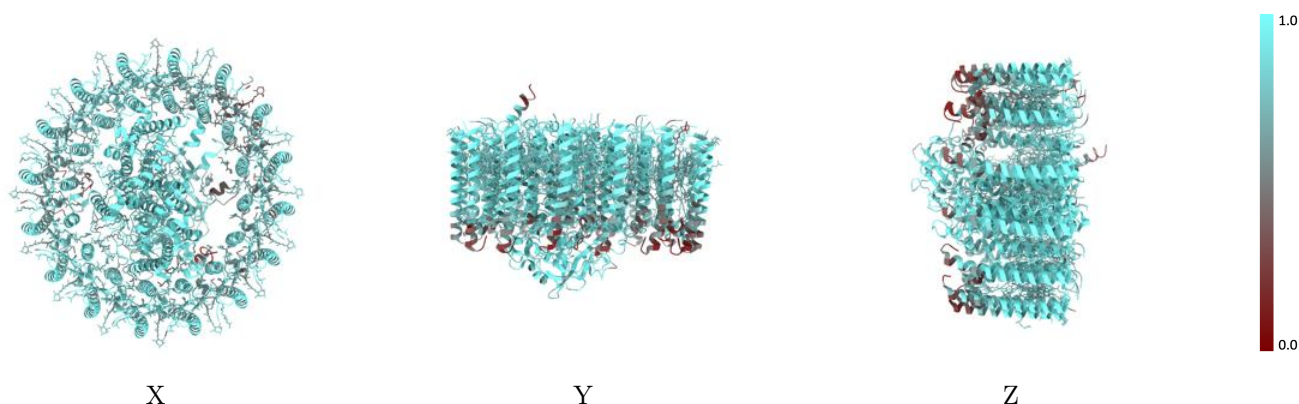
The images above show the 3D surface view of the map at the recommended contour level 0.0961 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



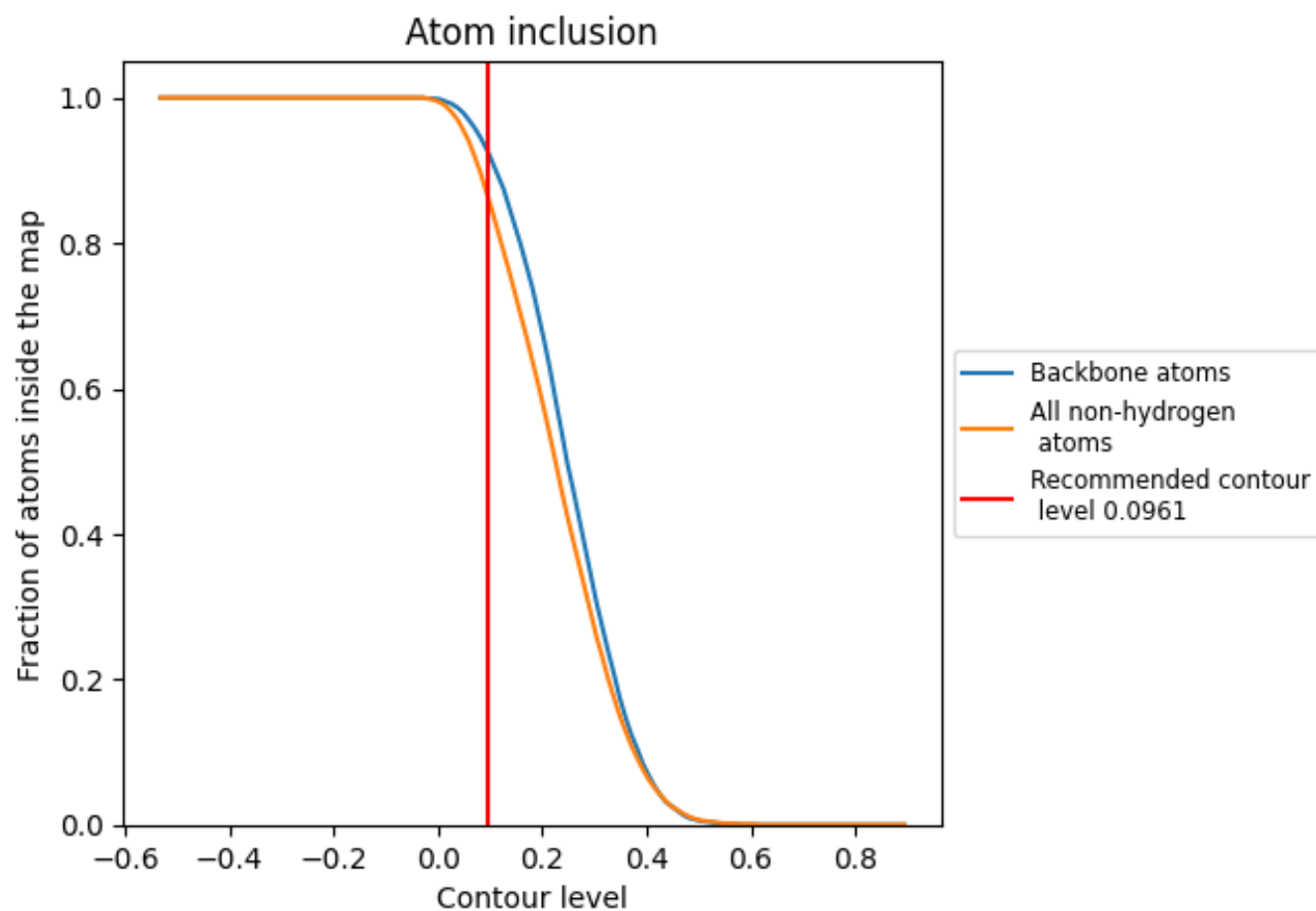
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0961).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.0961) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.6640
A	 0.9270	 0.6780
B	 0.9130	 0.6790
C	 0.9070	 0.6680
D	 0.9100	 0.6810
E	 0.8480	 0.6590
F	 0.7520	 0.6360
G	 0.8710	 0.6620
H	 0.8940	 0.6880
I	 0.9090	 0.6730
J	 0.8420	 0.6580
K	 0.7320	 0.6170
L	 0.9590	 0.7080
M	 0.9540	 0.7100
N	 0.8180	 0.6430
O	 0.7910	 0.6400
P	 0.8230	 0.6310
Q	 0.9040	 0.6670
R	 0.7590	 0.6230
S	 0.8200	 0.6440
T	 0.6500	 0.6150
a	 0.8670	 0.6570
b	 0.8550	 0.6530
c	 0.8720	 0.6620
d	 0.8710	 0.6730
e	 0.7680	 0.6210
f	 0.7730	 0.6240
g	 0.8100	 0.6070
i	 0.8700	 0.6610
j	 0.7680	 0.6350
k	 0.6790	 0.5950
n	 0.7730	 0.6210
o	 0.8080	 0.6320
p	 0.7830	 0.6290
q	 0.8690	 0.6620



Continued on next page...

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Chain	Atom inclusion	Q-score
r	 0.6780	 0.5940
s	 0.8150	 0.6370