



wwPDB EM Validation Summary Report ⓘ

Jun 17, 2025 – 12:08 PM JST

PDB ID : 7DDQ / pdb_00007ddq
EMDB ID : EMD-30656
Title : Structure of RC-LH1-PufX from Rhodobacter veldkampii
Authors : Bracun, L.; Yamagata, A.; Shirouzu, M.; Liu, L.N.
Deposited on : 2020-10-29
Resolution : 2.84 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

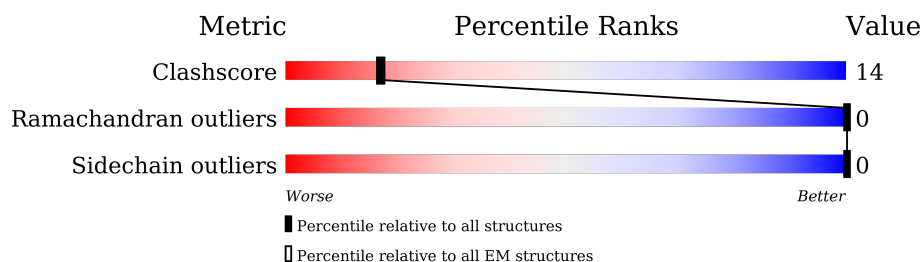
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	a	57	 56% 21% 23%
1	b	57	 60% 33% 7%
1	d	57	 72% 21% 7%
1	e	57	 72% 21% 7%
1	f	57	 67% 26% 7%
1	g	57	 67% 26% 7%
1	i	57	 72% 21% 7%
1	j	57	 63% 30% 7%


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	k	57	
1	n	57	
1	o	57	
1	r	57	
1	s	57	
1	t	57	
1	u	57	
2	A	48	
2	B	48	
2	D	48	
2	E	48	
2	F	48	
2	G	48	
2	I	48	
2	J	48	
2	K	48	
2	N	48	
2	O	48	
2	R	48	
2	S	48	
2	T	48	
2	U	48	
3	X	83	
4	L	276	
5	M	308	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	252	

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
8	SPO	s	201	-	X	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 22571 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 Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	o	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	t	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	r	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	a	44	Total	C	N	O	S	0	0
			373	258	59	54	2		
1	e	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	b	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	k	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	f	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	u	52	Total	C	N	O	S	0	0
			440	302	71	65	2		
1	s	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	n	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	i	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	j	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	g	53	Total	C	N	O	S	0	0
			446	305	72	67	2		
1	d	53	Total	C	N	O	S	0	0
			446	305	72	67	2		

- Molecule 2 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	S	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	O	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	U	43	Total	C	N	O	S	0	0
			354	237	57	59	1		
2	D	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	A	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	J	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	E	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	T	43	Total	C	N	O	S	0	0
			354	237	57	59	1		
2	R	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	K	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	G	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	I	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	F	44	Total	C	N	O	S	0	0
			363	243	58	61	1		
2	B	44	Total	C	N	O	S	0	0
			363	243	58	61	1		

- Molecule 3 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	81	Total	C	N	O	S	0	0
			610	396	100	110	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	275	Total	C	N	O	S	0	0
			2188	1469	350	360	9		

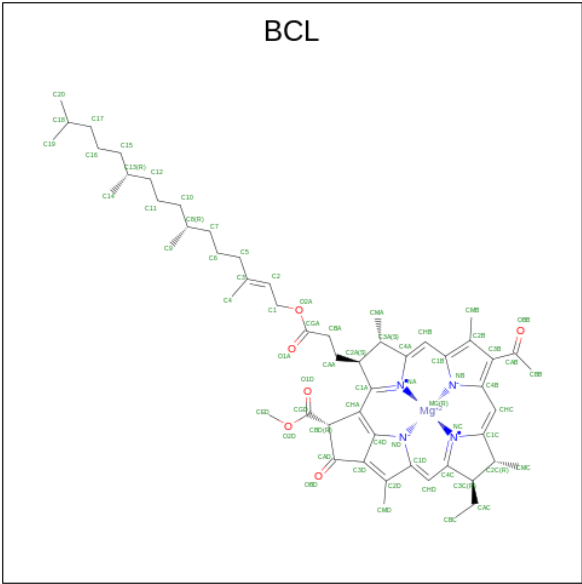
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	305	Total	C	N	O	S	0	0
			2420	1612	393	404	11		

- Molecule 6 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	250	Total	C	N	O	S	0	0
			1907	1223	318	351	15		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
7	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

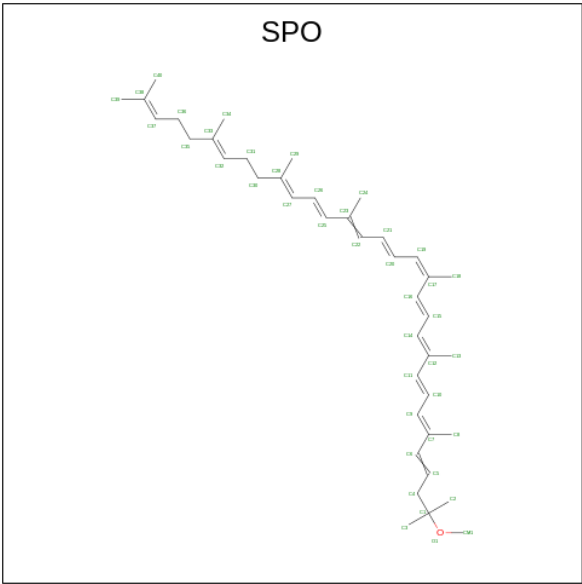
Mol	Chain	Residues	Atoms					AltConf
7	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	u	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	u	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	n	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	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	G	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	j	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	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
7	M	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	F	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	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



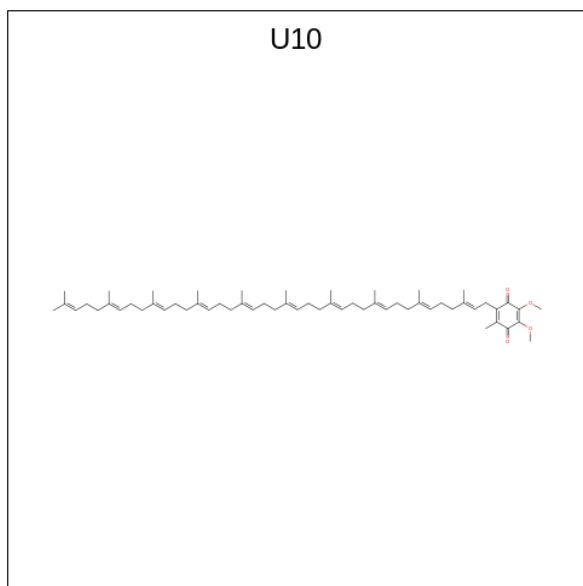
Mol	Chain	Residues	Atoms			AltConf
8	N	1	Total	C	O	0
			42	41	1	
8	t	1	Total	C	O	0
			42	41	1	
8	r	1	Total	C	O	0
			42	41	1	
8	r	1	Total	C	O	0
			42	41	1	
8	D	1	Total	C	O	0
			42	41	1	
8	k	1	Total	C	O	0
			42	41	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
8	E	1	Total	C	O	0
			42	41	1	
8	X	1	Total	C	O	0
			42	41	1	
8	s	1	Total	C	O	0
			42	41	1	
8	j	1	Total	C	O	0
			42	41	1	
8	I	1	Total	C	O	0
			42	41	1	
8	M	1	Total	C	O	0
			42	41	1	
8	g	1	Total	C	O	0
			42	41	1	
8	F	1	Total	C	O	0
			42	41	1	
8	B	1	Total	C	O	0
			42	41	1	

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



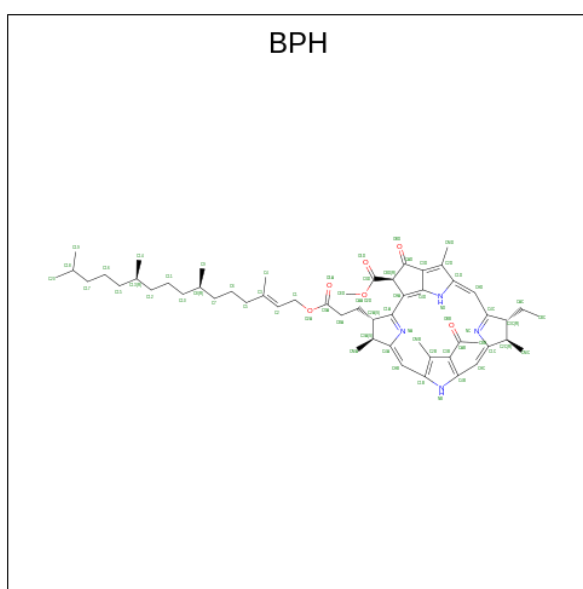
Mol	Chain	Residues	Atoms			AltConf
9	a	1	Total	C	O	0
			48	44	4	
9	L	1	Total	C	O	0
			33	29	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			38	34	4	
9	L	1	Total	C	O	0
			28	24	4	
9	M	1	Total	C	O	0
			48	44	4	
9	M	1	Total	C	O	0
			18	14	4	

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



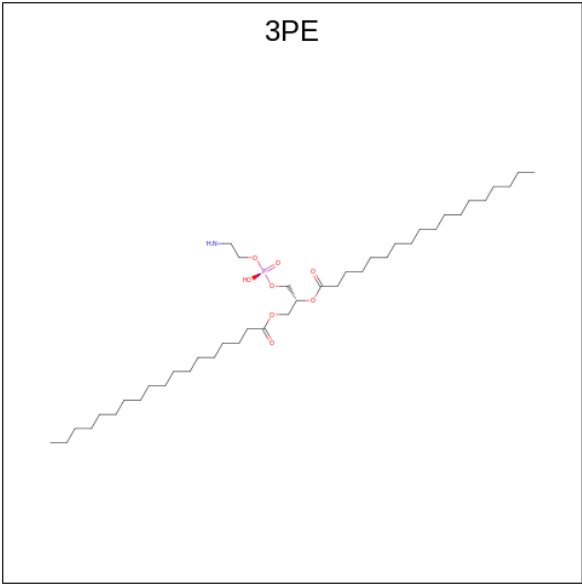
Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	N	O	0
			65	55	4	6	
10	L	1	Total	C	N	O	0
			45	35	4	6	
10	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:

C₄₁H₈₂NO₈P).

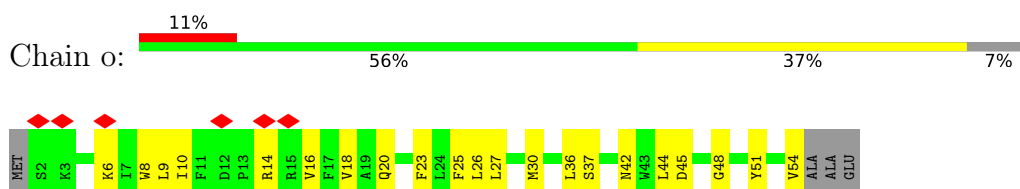


Mol	Chain	Residues	Atoms					AltConf
12	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
12	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
12	d	1	Total	C	N	O	P	0
			43	33	1	8	1	

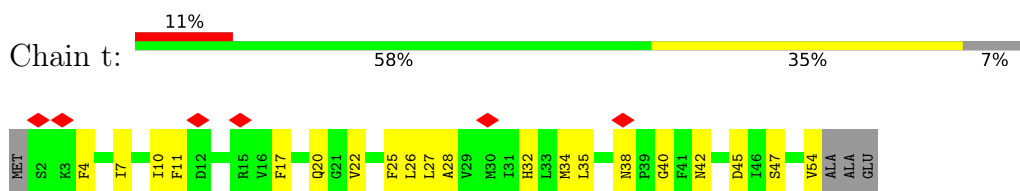
3 Residue-property plots [i](#)

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.

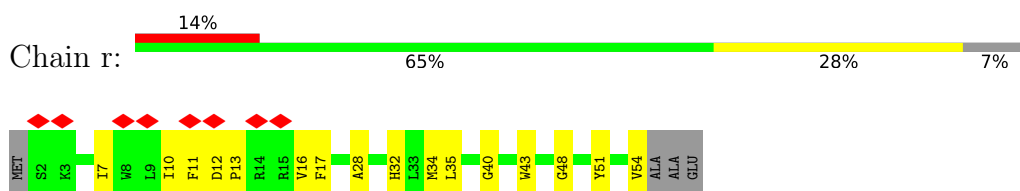
- Molecule 1: Antenna pigment protein alpha chain



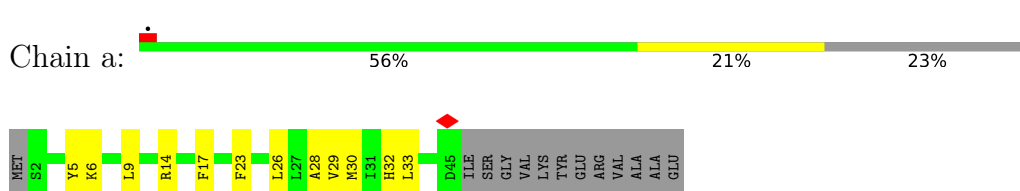
- Molecule 1: Antenna pigment protein alpha chain



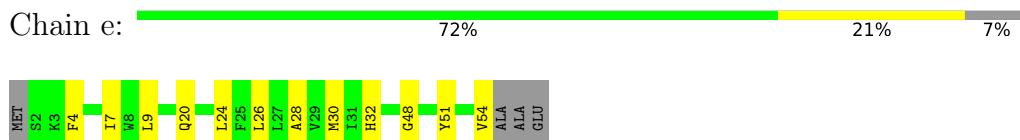
- Molecule 1: Antenna pigment protein alpha chain



- Molecule 1: Antenna pigment protein alpha chain

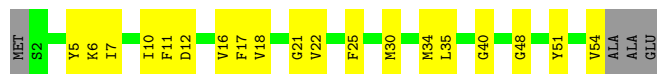


- Molecule 1: Antenna pigment protein alpha chain



- Molecule 1: Antenna pigment protein alpha chain

Chain b:  60% 33% 7%



- Molecule 1: Antenna pigment protein alpha chain

Chain k:  7% 63% 30% 7%



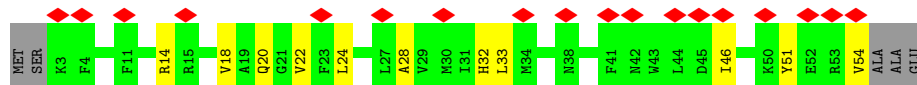
- Molecule 1: Antenna pigment protein alpha chain

Chain f:  67% 26% 7%



- Molecule 1: Antenna pigment protein alpha chain

Chain u:  32% 72% 19% 9%



- Molecule 1: Antenna pigment protein alpha chain

Chain s:  12% 61% 32% 7%



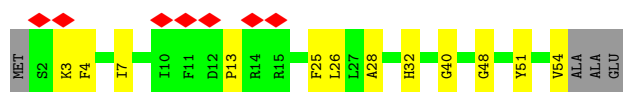
- Molecule 1: Antenna pigment protein alpha chain

Chain n:  9% 65% 28% 7%

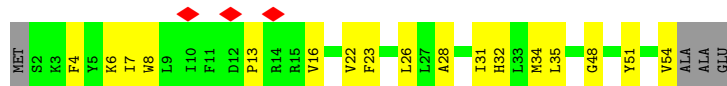


- Molecule 1: Antenna pigment protein alpha chain

Chain i:  12% 72% 21% 7%



- Molecule 1: Antenna pigment protein alpha chain



- Molecule 1: Antenna pigment protein alpha chain



- Molecule 1: Antenna pigment protein alpha chain



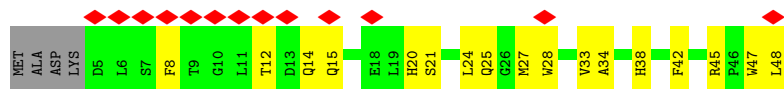
- Molecule 2: Antenna pigment protein beta chain



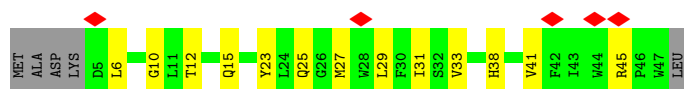
- Molecule 2: Antenna pigment protein beta chain



- Molecule 2: Antenna pigment protein beta chain



- Molecule 2: Antenna pigment protein beta chain



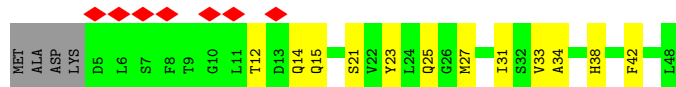
- Molecule 2: Antenna pigment protein beta chain



- Molecule 2: Antenna pigment protein beta chain



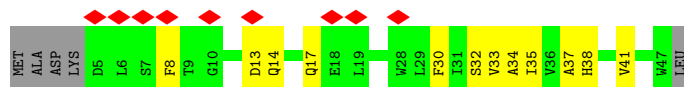
- Molecule 2: Antenna pigment protein beta chain



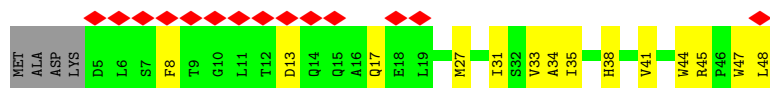
- Molecule 2: Antenna pigment protein beta chain



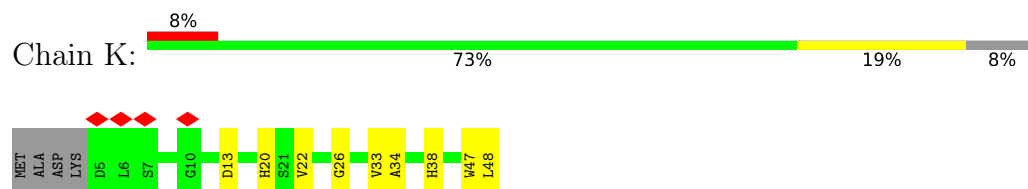
- Molecule 2: Antenna pigment protein beta chain



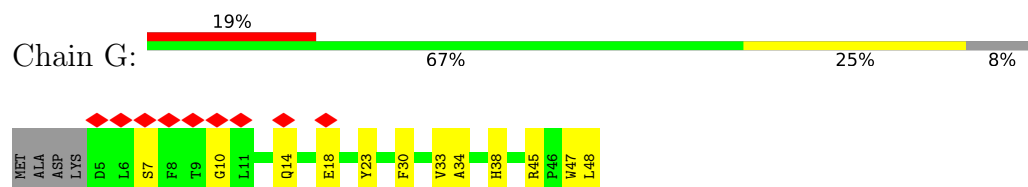
- Molecule 2: Antenna pigment protein beta chain



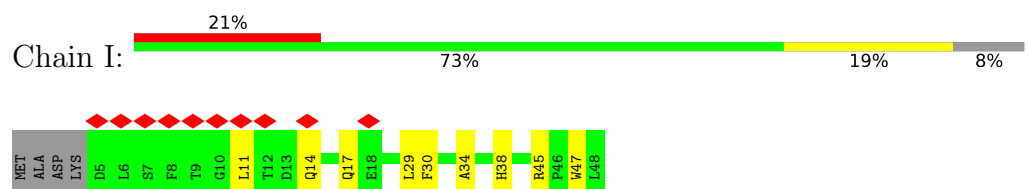
- Molecule 2: Antenna pigment protein beta chain



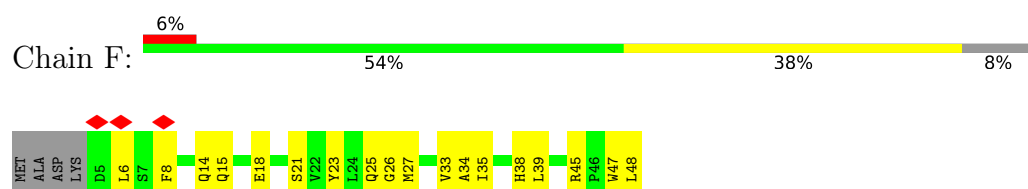
- Molecule 2: Antenna pigment protein beta chain



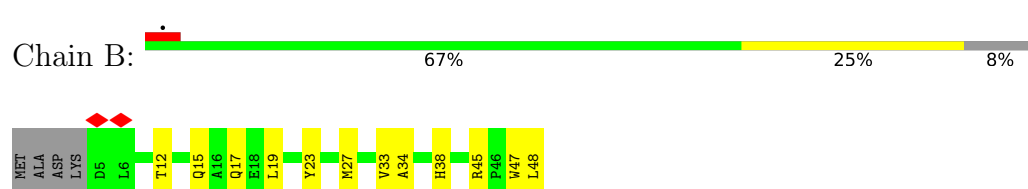
- Molecule 2: Antenna pigment protein beta chain



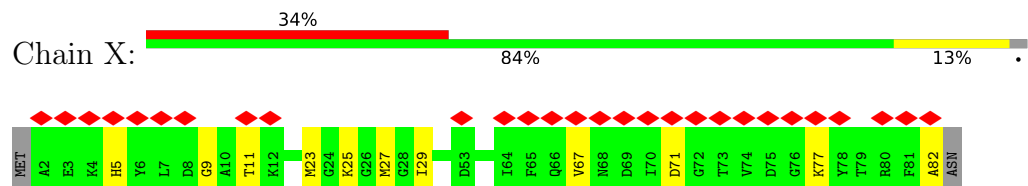
- Molecule 2: Antenna pigment protein beta chain



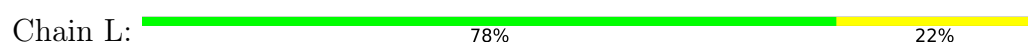
- Molecule 2: Antenna pigment protein beta chain

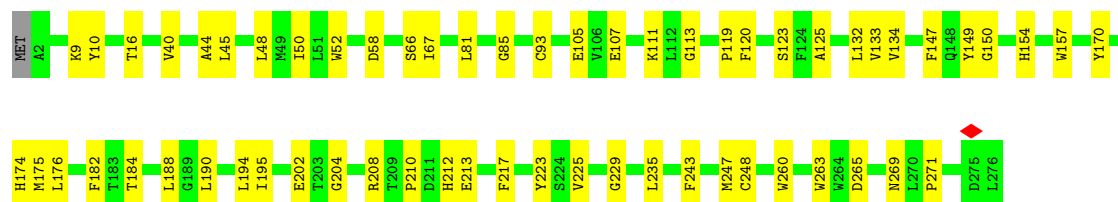


- Molecule 3: PufX

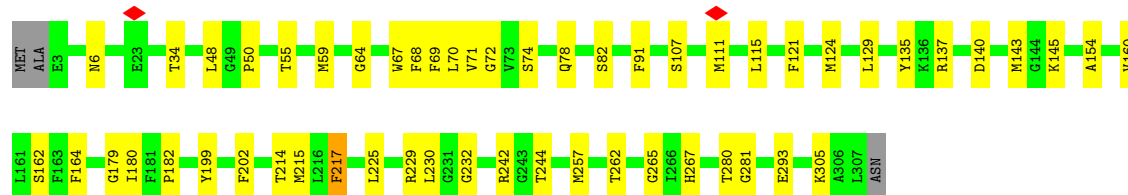
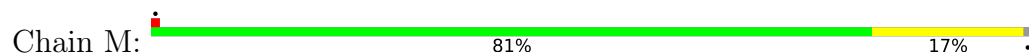


- Molecule 4: Photosynthetic reaction center L subunit

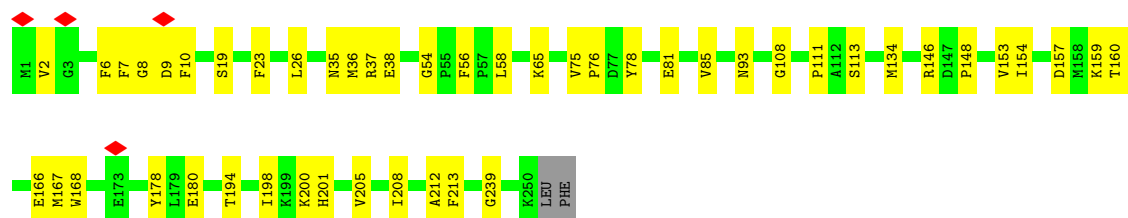
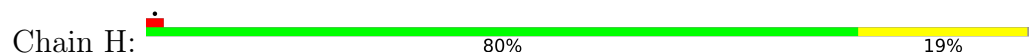




• Molecule 5: Reaction center protein M chain



• Molecule 6: Photosynthetic reaction center subunit H



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0157	Depositor
Map size (Å)	215.8, 215.8, 215.8	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U10, FE, BPH, 3PE, BCL, SPO

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	0.36	0/386	0.60	0/523
1	b	0.31	0/460	0.44	0/622
1	d	0.31	0/460	0.44	0/622
1	e	0.31	0/460	0.43	0/622
1	f	0.29	0/460	0.44	0/622
1	g	0.27	0/460	0.39	0/622
1	i	0.27	0/460	0.46	0/622
1	j	0.27	0/460	0.52	0/622
1	k	0.30	0/460	0.46	0/622
1	n	0.28	0/460	0.38	0/622
1	o	0.28	0/460	0.40	0/622
1	r	0.26	0/460	0.39	0/622
1	s	0.24	0/460	0.38	0/622
1	t	0.23	0/460	0.40	0/622
1	u	0.22	0/454	0.43	0/614
2	A	0.29	0/375	0.41	0/512
2	B	0.31	0/375	0.38	0/512
2	D	0.29	0/375	0.36	0/512
2	E	0.28	0/375	0.37	0/512
2	F	0.26	0/375	0.36	0/512
2	G	0.24	0/375	0.33	0/512
2	I	0.22	0/375	0.33	0/512
2	J	0.25	0/375	0.34	0/512
2	K	0.26	0/375	0.35	0/512
2	N	0.26	0/375	0.36	0/512
2	O	0.24	0/375	0.41	0/512
2	R	0.22	0/375	0.35	0/512
2	S	0.20	0/375	0.36	0/512
2	T	0.21	0/366	0.38	0/501
2	U	0.19	0/366	0.34	0/501
3	X	0.26	0/624	0.50	0/843
4	L	0.35	0/2272	0.48	0/3108

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	M	0.38	0/2507	0.50	0/3421
6	H	0.34	0/1959	0.46	0/2664
All	All	0.30	0/19789	0.44	0/26917

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	M	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	M	217	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	373	0	384	9	0
1	b	446	0	462	24	0
1	d	446	0	462	13	0
1	e	446	0	462	10	0
1	f	446	0	462	15	0
1	g	446	0	462	10	0
1	i	446	0	462	9	0
1	j	446	0	462	13	0
1	k	446	0	462	15	0
1	n	446	0	462	14	0
1	o	446	0	462	19	0
1	r	446	0	462	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	s	446	0	462	18	0
1	t	446	0	462	21	0
1	u	440	0	457	9	0
2	A	363	0	355	9	0
2	B	363	0	355	10	0
2	D	363	0	355	9	0
2	E	363	0	355	16	0
2	F	363	0	355	15	0
2	G	363	0	355	9	0
2	I	363	0	355	9	0
2	J	363	0	355	9	0
2	K	363	0	355	8	0
2	N	363	0	355	16	0
2	O	363	0	355	13	0
2	R	363	0	355	14	0
2	S	363	0	355	25	0
2	T	354	0	344	9	0
2	U	354	0	344	14	0
3	X	610	0	601	9	0
4	L	2188	0	2126	46	0
5	M	2420	0	2363	55	0
6	H	1907	0	1880	45	0
7	A	66	0	74	3	0
7	D	66	0	74	2	0
7	E	66	0	74	3	0
7	F	132	0	148	9	0
7	G	66	0	74	2	0
7	I	66	0	74	2	0
7	K	66	0	74	3	0
7	L	66	0	74	3	0
7	M	198	0	222	11	0
7	N	66	0	74	5	0
7	O	66	0	74	3	0
7	R	66	0	74	7	0
7	S	66	0	74	2	0
7	a	66	0	74	2	0
7	b	132	0	148	9	0
7	d	66	0	74	9	0
7	e	66	0	74	5	0
7	g	66	0	74	8	0
7	i	66	0	74	0	0
7	j	132	0	148	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	k	66	0	74	3	0
7	n	66	0	74	5	0
7	o	66	0	74	5	0
7	r	66	0	74	8	0
7	s	66	0	74	5	0
7	t	132	0	148	12	0
7	u	132	0	148	11	0
8	B	42	0	60	11	0
8	D	42	0	60	11	0
8	E	42	0	60	17	0
8	F	42	0	60	12	0
8	I	42	0	60	6	0
8	M	42	0	60	13	0
8	N	42	0	60	12	0
8	X	42	0	60	4	0
8	g	42	0	60	8	0
8	j	42	0	60	7	0
8	k	42	0	60	10	0
8	r	84	0	120	20	0
8	s	42	0	60	16	0
8	t	42	0	60	7	0
9	L	99	0	117	5	0
9	M	66	0	78	6	0
9	a	48	0	63	7	0
10	L	110	0	113	9	0
10	M	65	0	76	12	0
11	M	1	0	0	0	0
12	H	102	0	164	10	0
12	d	43	0	63	2	0
All	All	22571	0	23210	625	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 14.

The worst 5 of 625 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)
8:r:102:SPO:H21	7:O:101:BCL:H11	1.53	0.89
8:t:102:SPO:H19	7:t:103:BCL:H11	1.58	0.85
8:t:102:SPO:H37	8:t:102:SPO:H301	1.59	0.84
1:s:24:LEU:HD11	8:s:201:SPO:H27	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:124:MET:HE3	8:M:406:SPO:H351	1.62	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	42/57 (74%)	41 (98%)	1 (2%)	0	100	100
1	b	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	d	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
1	e	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	f	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	g	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
1	i	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	j	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	k	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	n	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	o	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	r	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
1	s	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	t	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
1	u	50/57 (88%)	45 (90%)	5 (10%)	0	100	100
2	A	42/48 (88%)	42 (100%)	0	0	100	100
2	B	42/48 (88%)	42 (100%)	0	0	100	100
2	D	42/48 (88%)	42 (100%)	0	0	100	100
2	E	42/48 (88%)	42 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	42/48 (88%)	42 (100%)	0	0	100	100
2	G	42/48 (88%)	42 (100%)	0	0	100	100
2	I	42/48 (88%)	42 (100%)	0	0	100	100
2	J	42/48 (88%)	42 (100%)	0	0	100	100
2	K	42/48 (88%)	42 (100%)	0	0	100	100
2	N	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
2	O	42/48 (88%)	42 (100%)	0	0	100	100
2	R	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
2	S	42/48 (88%)	42 (100%)	0	0	100	100
2	T	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
2	U	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
3	X	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
4	L	273/276 (99%)	265 (97%)	8 (3%)	0	100	100
5	M	303/308 (98%)	291 (96%)	12 (4%)	0	100	100
6	H	248/252 (98%)	233 (94%)	15 (6%)	0	100	100
All	All	2286/2494 (92%)	2179 (95%)	107 (5%)	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	40/50 (80%)	40 (100%)	0	100	100
1	b	48/50 (96%)	48 (100%)	0	100	100
1	d	48/50 (96%)	48 (100%)	0	100	100
1	e	48/50 (96%)	48 (100%)	0	100	100
1	f	48/50 (96%)	48 (100%)	0	100	100
1	g	48/50 (96%)	48 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	48/50 (96%)	48 (100%)	0	100	100
1	j	48/50 (96%)	48 (100%)	0	100	100
1	k	48/50 (96%)	48 (100%)	0	100	100
1	n	48/50 (96%)	48 (100%)	0	100	100
1	o	48/50 (96%)	48 (100%)	0	100	100
1	r	48/50 (96%)	48 (100%)	0	100	100
1	s	48/50 (96%)	48 (100%)	0	100	100
1	t	48/50 (96%)	48 (100%)	0	100	100
1	u	47/50 (94%)	47 (100%)	0	100	100
2	A	38/41 (93%)	38 (100%)	0	100	100
2	B	38/41 (93%)	38 (100%)	0	100	100
2	D	38/41 (93%)	38 (100%)	0	100	100
2	E	38/41 (93%)	38 (100%)	0	100	100
2	F	38/41 (93%)	38 (100%)	0	100	100
2	G	38/41 (93%)	38 (100%)	0	100	100
2	I	38/41 (93%)	38 (100%)	0	100	100
2	J	38/41 (93%)	38 (100%)	0	100	100
2	K	38/41 (93%)	38 (100%)	0	100	100
2	N	38/41 (93%)	38 (100%)	0	100	100
2	O	38/41 (93%)	38 (100%)	0	100	100
2	R	38/41 (93%)	38 (100%)	0	100	100
2	S	38/41 (93%)	38 (100%)	0	100	100
2	T	37/41 (90%)	37 (100%)	0	100	100
2	U	37/41 (90%)	37 (100%)	0	100	100
3	X	60/62 (97%)	60 (100%)	0	100	100
4	L	219/220 (100%)	219 (100%)	0	100	100
5	M	241/243 (99%)	241 (100%)	0	100	100
6	H	202/204 (99%)	202 (100%)	0	100	100
All	All	2001/2094 (96%)	2001 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30

such sidechains are listed below:

Mol	Chain	Res	Type
2	R	14	GLN
6	H	93	ASN
2	I	14	GLN
2	F	17	GLN
6	H	32	GLN

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 62 ligands modelled in this entry, 1 is monoatomic - leaving 61 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	$\# Z > 2$
8	SPO	X	201	-	40,41,41	2.23	12 (30%)	47,50,50	3.47	17 (36%)
7	BCL	I	101	-	64,74,74	1.19	5 (7%)	78,115,115	1.54	12 (15%)
9	U10	a	102	-	48,48,63	2.70	13 (27%)	58,61,79	1.71	16 (27%)
7	BCL	F	101	-	64,74,74	1.30	9 (14%)	78,115,115	1.72	15 (19%)
7	BCL	N	202	-	64,74,74	1.21	5 (7%)	78,115,115	1.77	15 (19%)
7	BCL	u	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.74	11 (14%)
7	BCL	K	101	-	64,74,74	1.21	6 (9%)	78,115,115	1.56	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	F	103	-	64,74,74	1.20	7 (10%)	78,115,115	1.71	15 (19%)
8	SPO	g	102	-	40,41,41	2.40	12 (30%)	47,50,50	5.01	24 (51%)
8	SPO	s	201	-	40,41,41	2.31	12 (30%)	47,50,50	5.51	25 (53%)
8	SPO	I	102	-	40,41,41	2.33	12 (30%)	47,50,50	4.92	19 (40%)
12	3PE	H	302	-	50,50,50	0.95	2 (4%)	53,55,55	1.16	3 (5%)
7	BCL	e	100	-	64,74,74	1.29	8 (12%)	78,115,115	1.80	16 (20%)
7	BCL	n	100	-	64,74,74	1.22	7 (10%)	78,115,115	1.70	16 (20%)
7	BCL	d	101	-	64,74,74	1.25	8 (12%)	78,115,115	1.70	14 (17%)
7	BCL	g	101	-	64,74,74	1.25	7 (10%)	78,115,115	1.64	14 (17%)
9	U10	L	304	-	38,38,63	2.69	12 (31%)	46,49,79	1.71	13 (28%)
7	BCL	t	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.64	14 (17%)
7	BCL	u	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.62	15 (19%)
7	BCL	o	100	-	64,74,74	1.30	8 (12%)	78,115,115	1.71	11 (14%)
8	SPO	M	406	-	40,41,41	2.26	13 (32%)	47,50,50	4.07	20 (42%)
7	BCL	i	100	-	64,74,74	1.26	8 (12%)	78,115,115	1.62	14 (17%)
7	BCL	j	303	-	64,74,74	1.23	6 (9%)	78,115,115	1.58	13 (16%)
8	SPO	E	201	-	40,41,41	2.24	10 (25%)	47,50,50	5.37	24 (51%)
8	SPO	r	103	-	40,41,41	2.35	12 (30%)	47,50,50	5.14	16 (34%)
9	U10	L	305	-	28,28,63	2.68	10 (35%)	34,37,79	1.45	5 (14%)
7	BCL	j	302	-	64,74,74	1.21	7 (10%)	78,115,115	1.66	15 (19%)
7	BCL	A	101	-	64,74,74	1.27	7 (10%)	78,115,115	1.58	12 (15%)
7	BCL	L	301	-	64,74,74	1.24	7 (10%)	78,115,115	1.55	12 (15%)
9	U10	L	303	-	33,33,63	2.76	10 (30%)	40,43,79	1.64	9 (22%)
7	BCL	G	101	-	64,74,74	1.17	6 (9%)	78,115,115	1.54	13 (16%)
7	BCL	M	407	-	64,74,74	1.30	8 (12%)	78,115,115	1.49	11 (14%)
8	SPO	B	101	-	40,41,41	2.20	11 (27%)	47,50,50	3.96	21 (44%)
12	3PE	d	102	-	42,42,50	1.00	2 (4%)	45,47,55	2.33	7 (15%)
8	SPO	N	201	-	40,41,41	2.21	12 (30%)	47,50,50	5.19	22 (46%)
7	BCL	M	402	-	64,74,74	1.19	5 (7%)	78,115,115	1.82	15 (19%)
10	BPH	M	403	-	51,70,70	1.05	3 (5%)	52,101,101	1.32	4 (7%)
7	BCL	r	101	-	64,74,74	1.24	6 (9%)	78,115,115	1.65	14 (17%)
12	3PE	H	301	-	50,50,50	0.93	3 (6%)	53,55,55	1.15	2 (3%)
8	SPO	t	102	-	40,41,41	2.37	12 (30%)	47,50,50	4.36	24 (51%)
8	SPO	F	102	-	40,41,41	2.26	12 (30%)	47,50,50	3.91	18 (38%)
8	SPO	D	201	-	40,41,41	2.19	11 (27%)	47,50,50	5.18	18 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	b	102	-	64,74,74	1.18	7 (10%)	78,115,115	1.56	12 (15%)
7	BCL	k	101	-	64,74,74	1.22	8 (12%)	78,115,115	1.64	15 (19%)
7	BCL	b	101	-	64,74,74	1.27	6 (9%)	78,115,115	1.88	19 (24%)
8	SPO	j	301	-	40,41,41	2.21	12 (30%)	47,50,50	4.04	18 (38%)
7	BCL	t	103	-	64,74,74	1.25	6 (9%)	78,115,115	1.47	11 (14%)
7	BCL	s	202	-	64,74,74	1.22	6 (9%)	78,115,115	1.60	12 (15%)
7	BCL	M	401	-	64,74,74	1.21	7 (10%)	78,115,115	1.58	12 (15%)
10	BPH	L	302	-	51,70,70	0.91	3 (5%)	52,101,101	1.12	6 (11%)
7	BCL	a	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.67	13 (16%)
7	BCL	D	202	-	64,74,74	1.22	7 (10%)	78,115,115	1.57	13 (16%)
7	BCL	R	101	-	64,74,74	1.19	6 (9%)	78,115,115	1.47	11 (14%)
9	U10	M	408	-	18,18,63	2.86	8 (44%)	22,25,79	1.49	3 (13%)
10	BPH	L	306	-	31,50,70	1.02	1 (3%)	28,77,101	1.37	5 (17%)
8	SPO	r	102	-	40,41,41	2.29	12 (30%)	47,50,50	5.28	24 (51%)
9	U10	M	405	-	48,48,63	2.70	14 (29%)	58,61,79	1.72	14 (24%)
7	BCL	O	101	-	64,74,74	1.18	5 (7%)	78,115,115	1.55	11 (14%)
8	SPO	k	102	-	40,41,41	2.24	12 (30%)	47,50,50	5.30	21 (44%)
7	BCL	S	101	-	64,74,74	1.20	6 (9%)	78,115,115	1.55	11 (14%)
7	BCL	E	202	-	64,74,74	1.18	7 (10%)	78,115,115	1.65	12 (15%)

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
8	SPO	X	201	-	-	14/47/47/47	-
7	BCL	I	101	-	-	10/37/137/137	-
9	U10	a	102	-	-	12/45/69/87	0/1/1/1
7	BCL	F	101	-	-	3/37/137/137	-
7	BCL	N	202	-	-	7/37/137/137	-
7	BCL	u	102	-	-	8/37/137/137	-
7	BCL	K	101	-	-	8/37/137/137	-
7	BCL	F	103	-	-	7/37/137/137	-
8	SPO	g	102	-	-	19/47/47/47	-
8	SPO	s	201	-	-	21/47/47/47	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SPO	I	102	-	-	13/47/47/47	-
12	3PE	H	302	-	-	31/54/54/54	-
7	BCL	e	100	-	-	3/37/137/137	-
7	BCL	n	100	-	-	6/37/137/137	-
7	BCL	d	101	-	-	4/37/137/137	-
7	BCL	g	101	-	-	1/37/137/137	-
9	U10	L	304	-	-	15/33/57/87	0/1/1/1
7	BCL	t	101	-	-	4/37/137/137	-
7	BCL	u	101	-	-	3/37/137/137	-
7	BCL	o	100	-	-	10/37/137/137	-
8	SPO	M	406	-	-	21/47/47/47	-
7	BCL	i	100	-	-	3/37/137/137	-
7	BCL	j	303	-	-	9/37/137/137	-
8	SPO	E	201	-	-	17/47/47/47	-
8	SPO	r	103	-	-	18/47/47/47	-
9	U10	L	305	-	-	9/21/45/87	0/1/1/1
7	BCL	j	302	-	-	4/37/137/137	-
7	BCL	A	101	-	-	10/37/137/137	-
7	BCL	L	301	-	-	5/37/137/137	-
9	U10	L	303	-	-	12/27/51/87	0/1/1/1
7	BCL	G	101	-	-	8/37/137/137	-
7	BCL	M	407	-	-	5/37/137/137	-
8	SPO	B	101	-	-	14/47/47/47	-
12	3PE	d	102	-	-	19/46/46/54	-
8	SPO	N	201	-	-	16/47/47/47	-
7	BCL	M	402	-	-	7/37/137/137	-
10	BPH	M	403	-	-	8/37/105/105	0/5/6/6
7	BCL	r	101	-	-	5/37/137/137	-
12	3PE	H	301	-	-	26/54/54/54	-
8	SPO	t	102	-	-	13/47/47/47	-
8	SPO	F	102	-	-	17/47/47/47	-
8	SPO	D	201	-	-	15/47/47/47	-
7	BCL	b	102	-	-	5/37/137/137	-
7	BCL	k	101	-	-	3/37/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	b	101	-	-	10/37/137/137	-
8	SPO	j	301	-	-	19/47/47/47	-
7	BCL	t	103	-	-	6/37/137/137	-
7	BCL	s	202	-	-	4/37/137/137	-
7	BCL	M	401	-	-	2/37/137/137	-
10	BPH	L	302	-	-	4/37/105/105	0/5/6/6
7	BCL	a	101	-	-	5/37/137/137	-
7	BCL	D	202	-	-	6/37/137/137	-
7	BCL	R	101	-	-	10/37/137/137	-
9	U10	M	408	-	-	6/9/33/87	0/1/1/1
10	BPH	L	306	-	-	2/13/81/105	0/5/6/6
8	SPO	r	102	-	-	16/47/47/47	-
9	U10	M	405	-	-	12/45/69/87	0/1/1/1
7	BCL	O	101	-	-	11/37/137/137	-
8	SPO	k	102	-	-	21/47/47/47	-
7	BCL	S	101	-	-	4/37/137/137	-
7	BCL	E	202	-	-	5/37/137/137	-

The worst 5 of 481 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	303	U10	C8-C9	6.23	1.47	1.33
9	L	303	U10	C13-C14	6.17	1.47	1.33
9	L	304	U10	C13-C14	6.14	1.47	1.33
9	M	405	U10	C8-C9	6.05	1.47	1.33
9	L	303	U10	C18-C19	6.02	1.47	1.33

The worst 5 of 850 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	201	SPO	C3-C1-C4	-23.58	74.66	110.86
8	r	102	SPO	C2-C1-C4	-22.57	76.21	110.86
8	g	102	SPO	C2-C1-C4	-22.55	76.24	110.86
8	E	201	SPO	C2-C1-C4	-21.70	77.55	110.86
8	k	102	SPO	C3-C1-C4	-21.57	77.74	110.86

There are no chirality outliers.

5 of 611 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	202	BCL	C2-C1-O2A-CGA
7	O	101	BCL	O2A-C1-C2-C3
7	b	101	BCL	C2-C1-O2A-CGA
7	u	102	BCL	C1A-C2A-CAA-CBA
7	u	102	BCL	O2A-C1-C2-C3

There are no ring outliers.

60 monomers are involved in 316 short contacts:

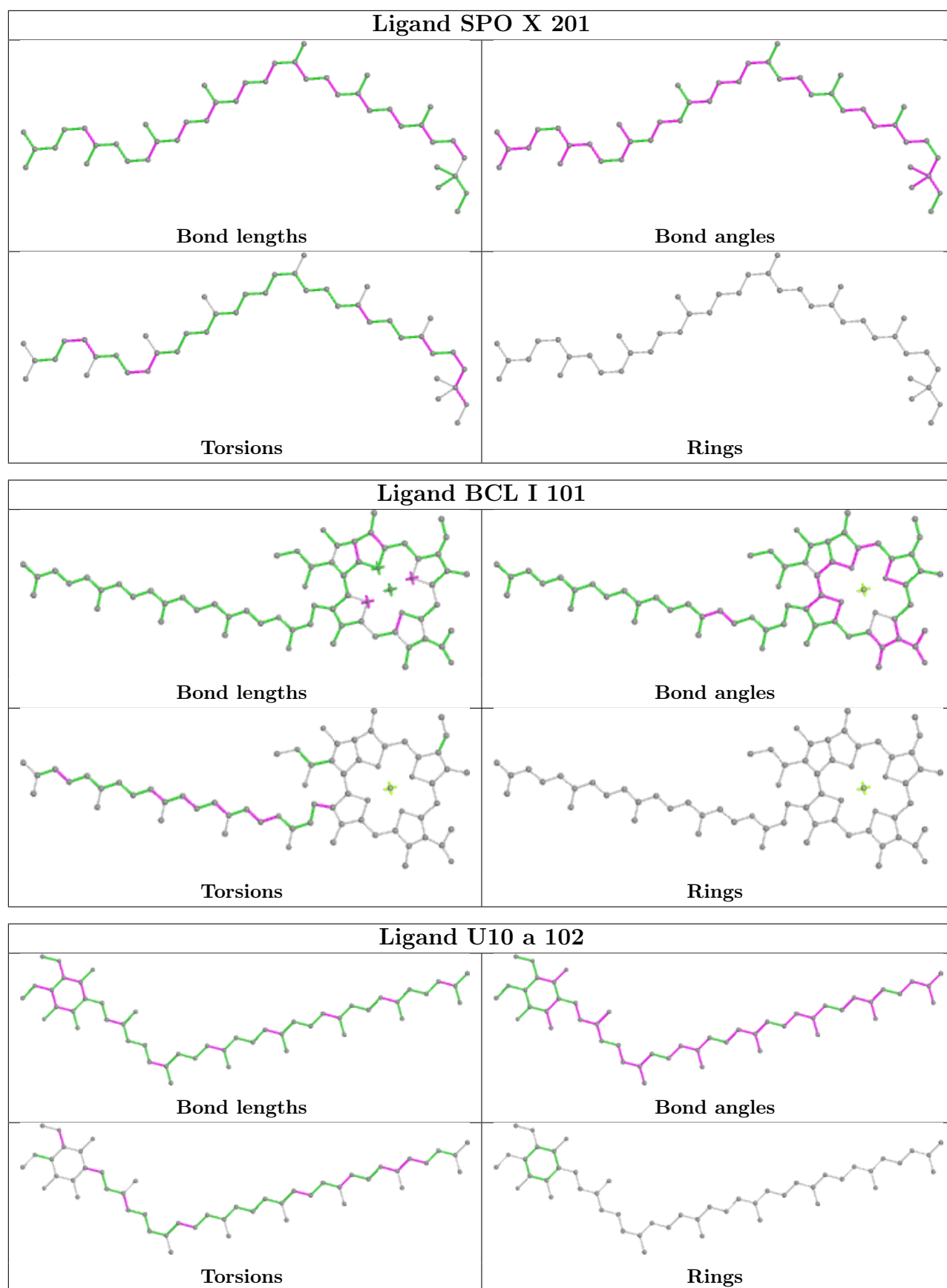
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	X	201	SPO	4	0
7	I	101	BCL	2	0
9	a	102	U10	7	0
7	F	101	BCL	7	0
7	N	202	BCL	5	0
7	u	102	BCL	7	0
7	K	101	BCL	3	0
7	F	103	BCL	2	0
8	g	102	SPO	8	0
8	s	201	SPO	16	0
8	I	102	SPO	6	0
12	H	302	3PE	5	0
7	e	100	BCL	5	0
7	n	100	BCL	5	0
7	d	101	BCL	9	0
7	g	101	BCL	8	0
9	L	304	U10	3	0
7	t	101	BCL	7	0
7	u	101	BCL	4	0
7	o	100	BCL	5	0
8	M	406	SPO	13	0
7	j	303	BCL	4	0
8	E	201	SPO	17	0
8	r	103	SPO	10	0
9	L	305	U10	1	0
7	j	302	BCL	2	0
7	A	101	BCL	3	0
7	L	301	BCL	3	0
9	L	303	U10	1	0
7	G	101	BCL	2	0
7	M	407	BCL	6	0
8	B	101	SPO	11	0
12	d	102	3PE	2	0

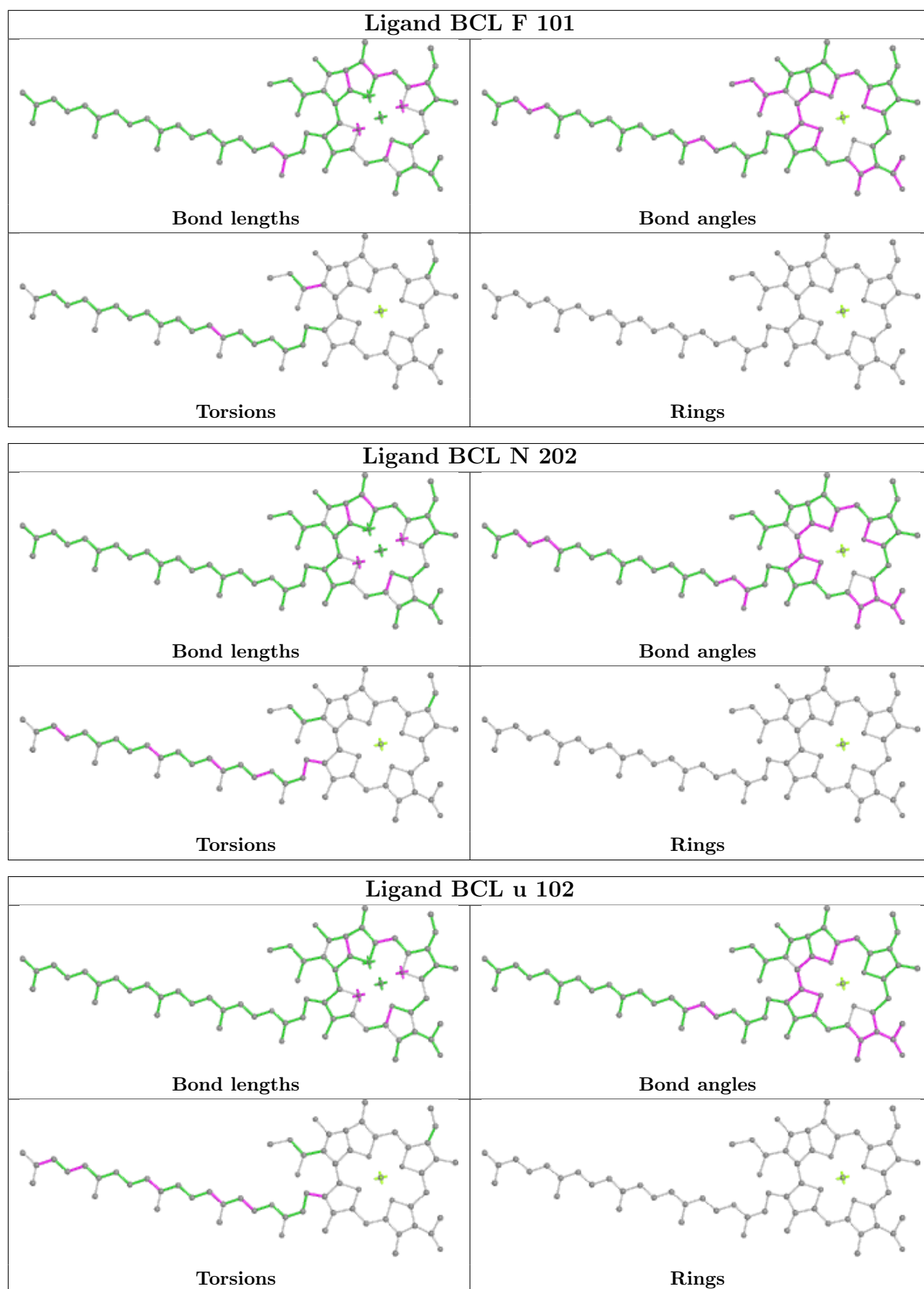
Continued on next page...

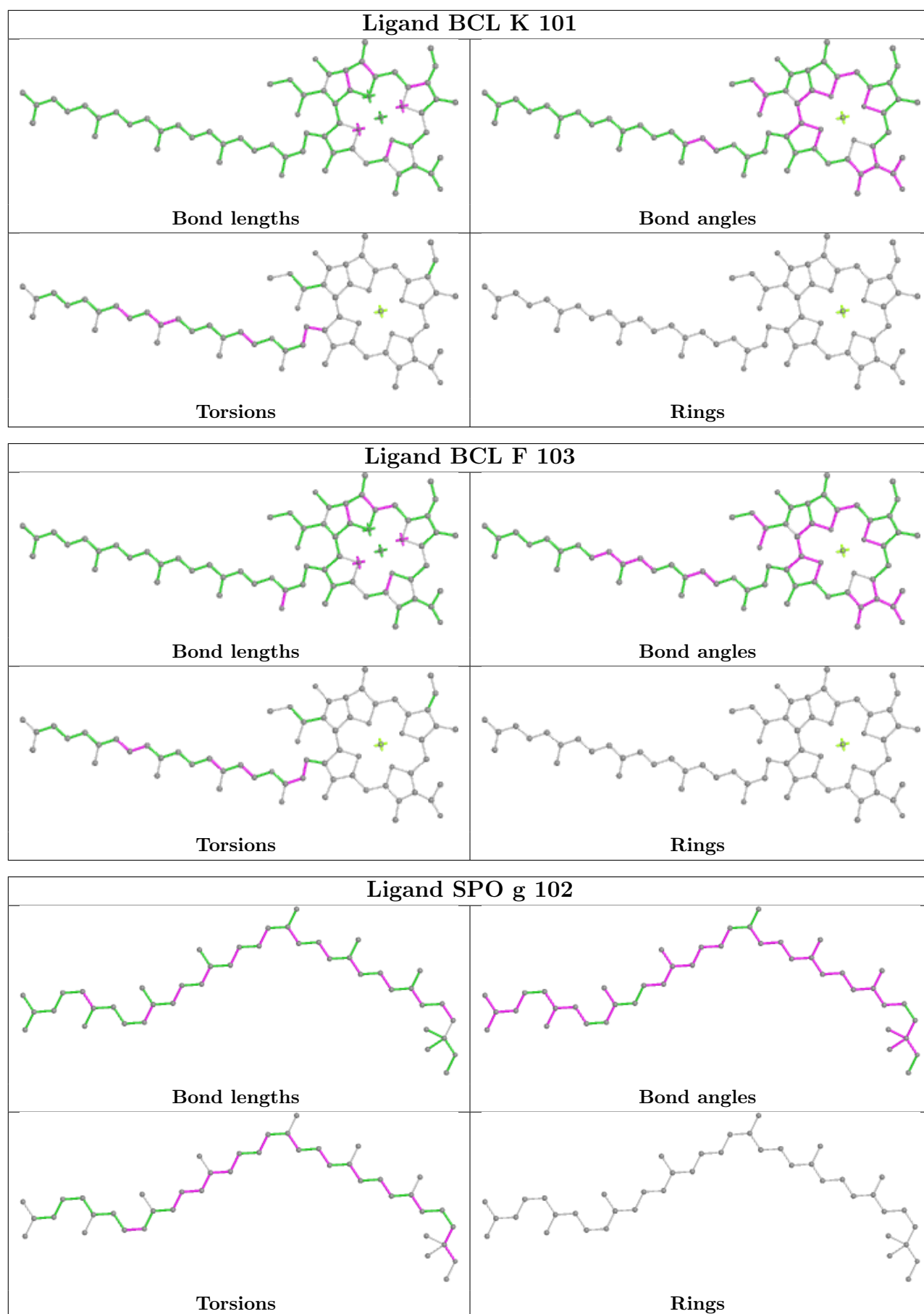
Continued from previous page...

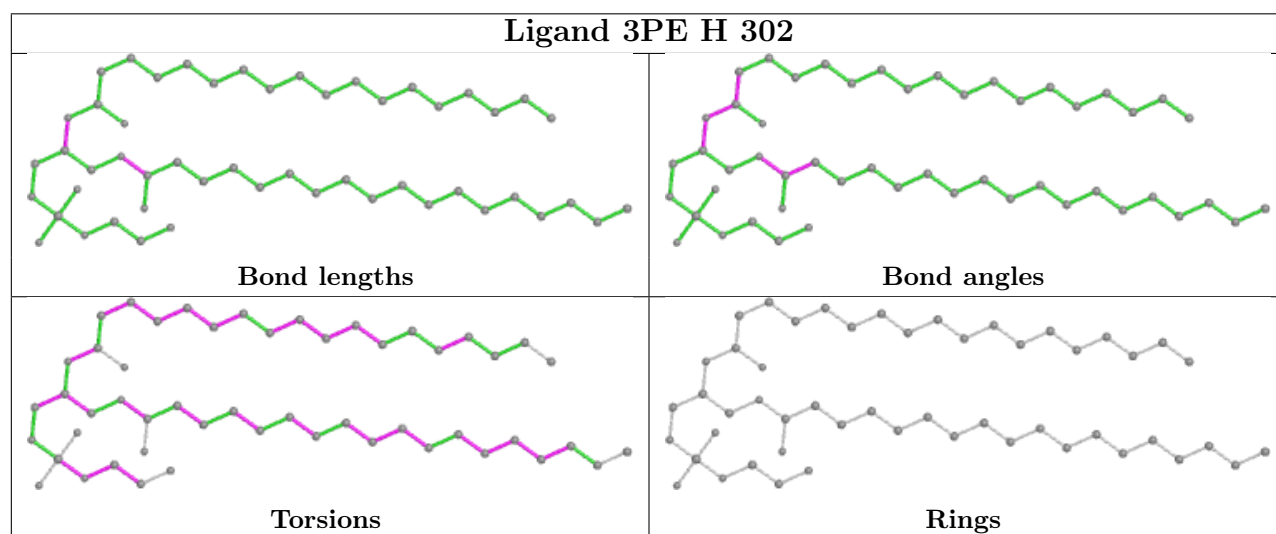
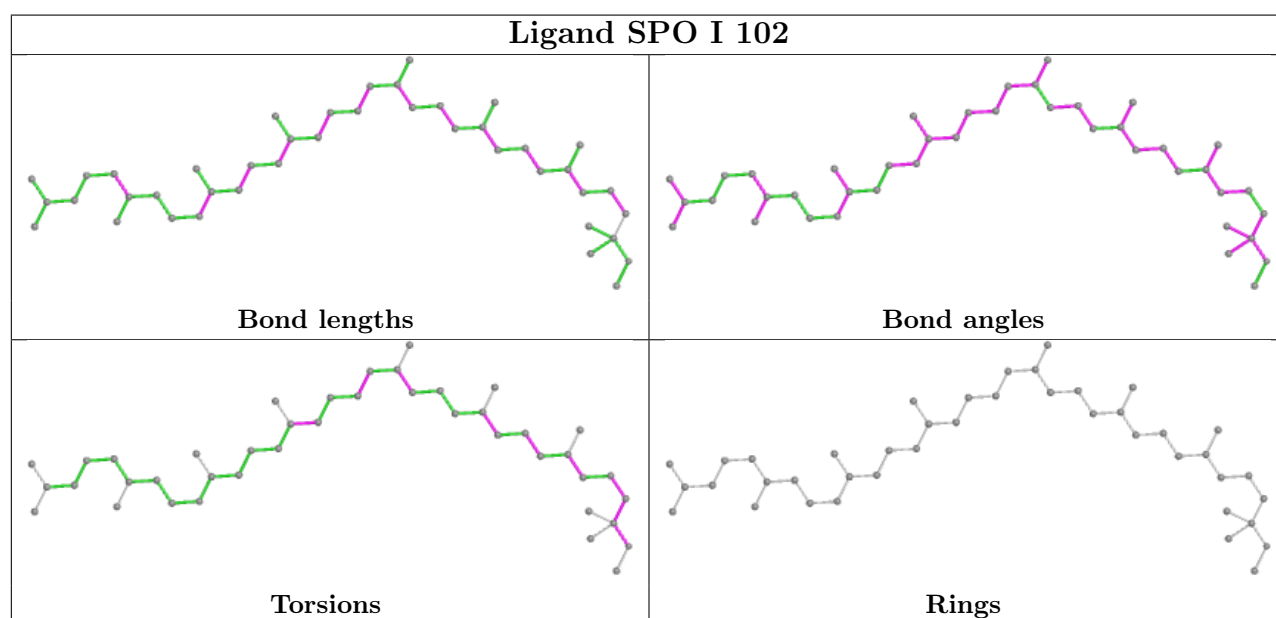
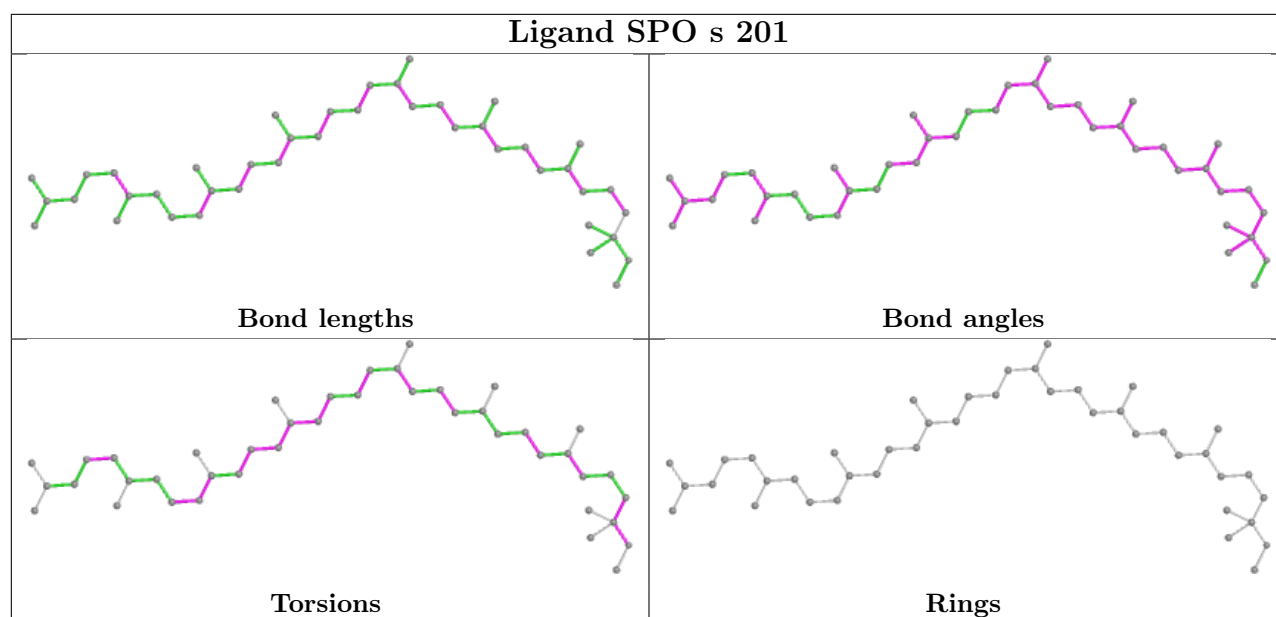
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	201	SPO	12	0
7	M	402	BCL	4	0
10	M	403	BPH	12	0
7	r	101	BCL	8	0
12	H	301	3PE	5	0
8	t	102	SPO	7	0
8	F	102	SPO	12	0
8	D	201	SPO	11	0
7	b	102	BCL	1	0
7	k	101	BCL	3	0
7	b	101	BCL	8	0
8	j	301	SPO	7	0
7	t	103	BCL	5	0
7	s	202	BCL	5	0
7	M	401	BCL	4	0
10	L	302	BPH	6	0
7	a	101	BCL	2	0
7	D	202	BCL	2	0
7	R	101	BCL	7	0
9	M	408	U10	1	0
10	L	306	BPH	3	0
8	r	102	SPO	10	0
9	M	405	U10	5	0
7	O	101	BCL	3	0
8	k	102	SPO	10	0
7	S	101	BCL	2	0
7	E	202	BCL	3	0

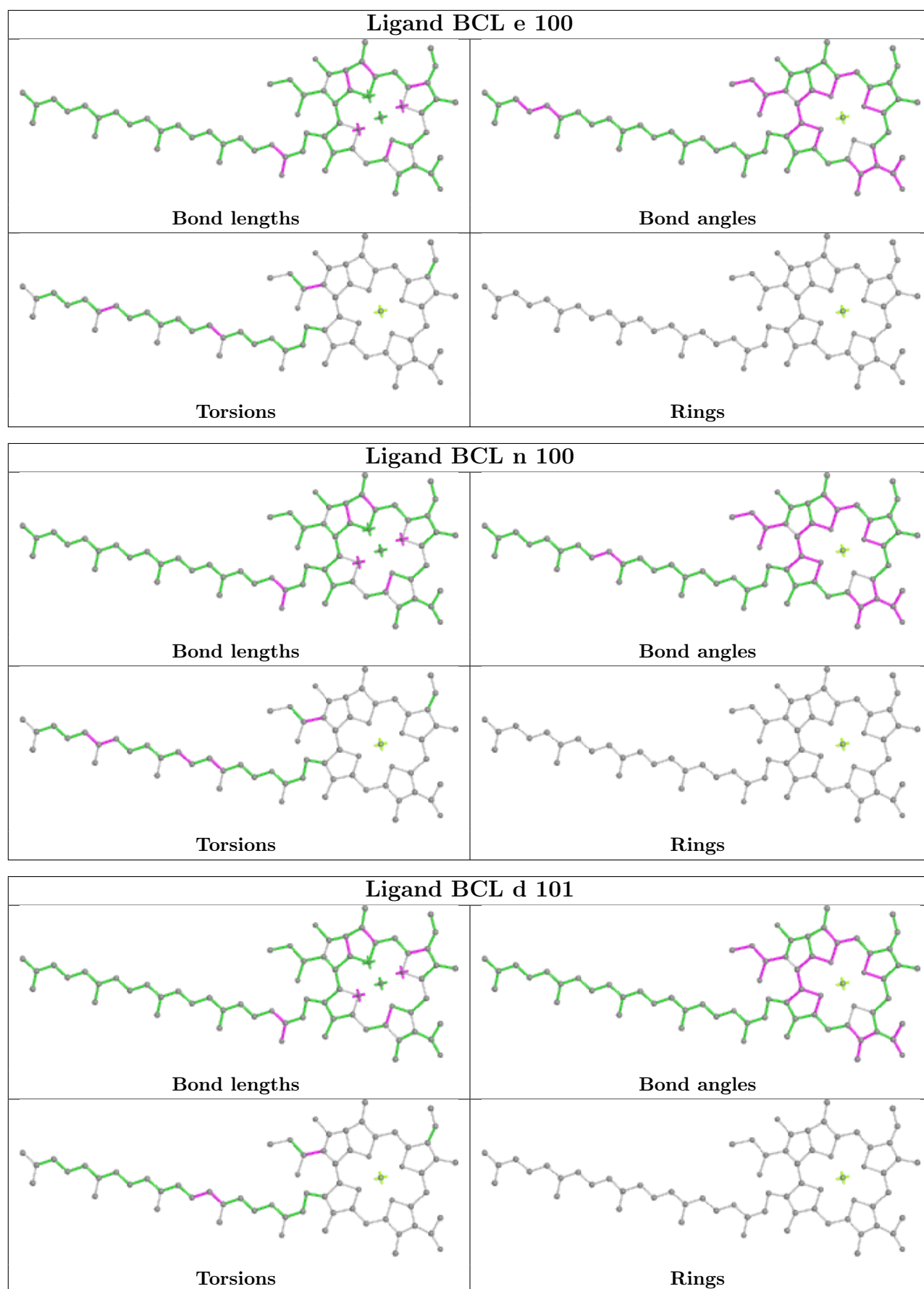
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

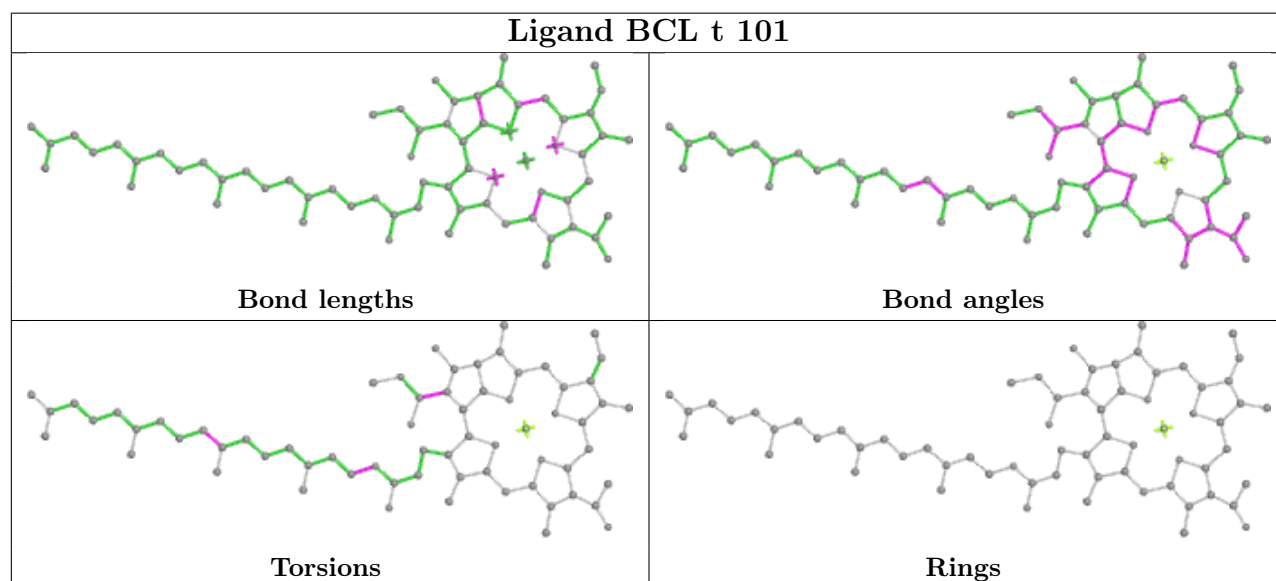
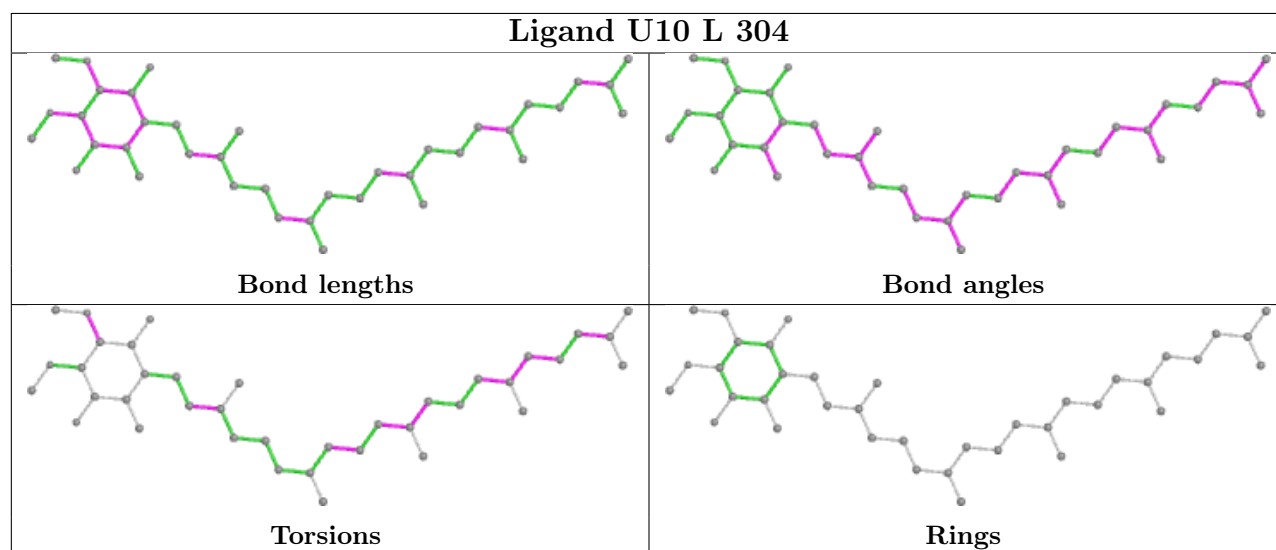
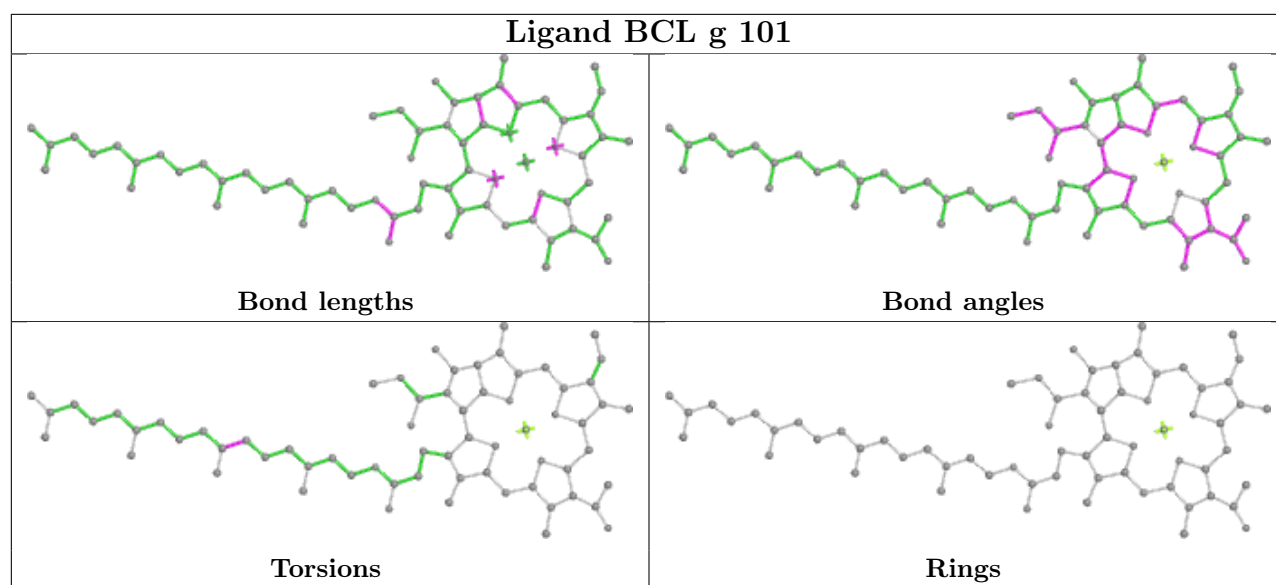


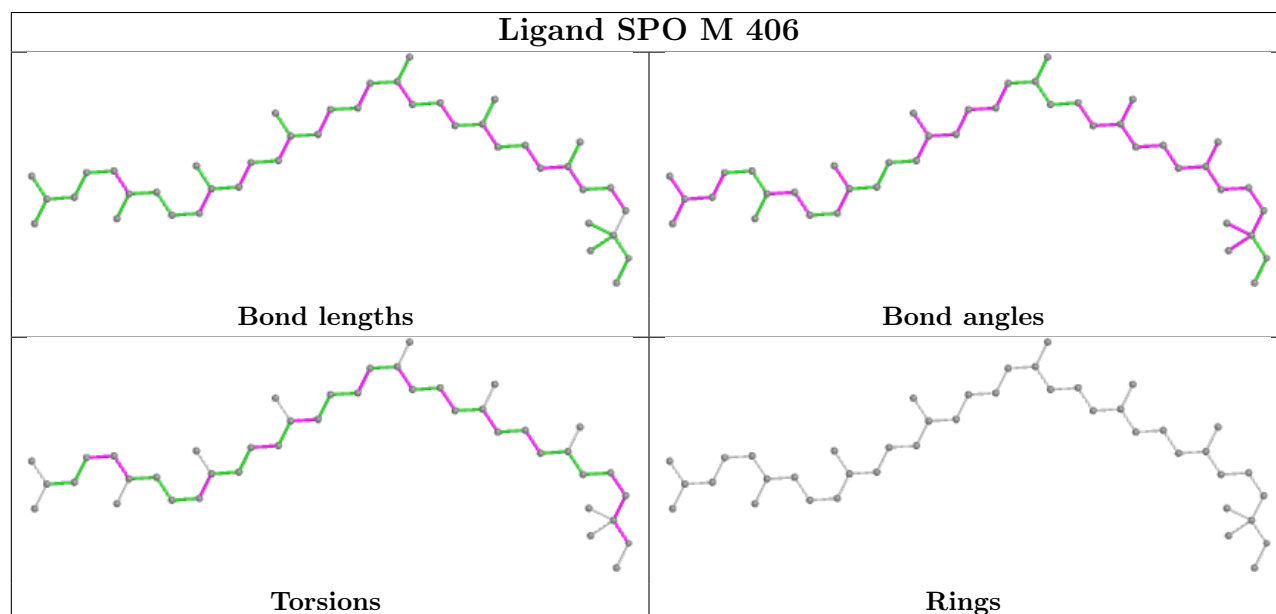
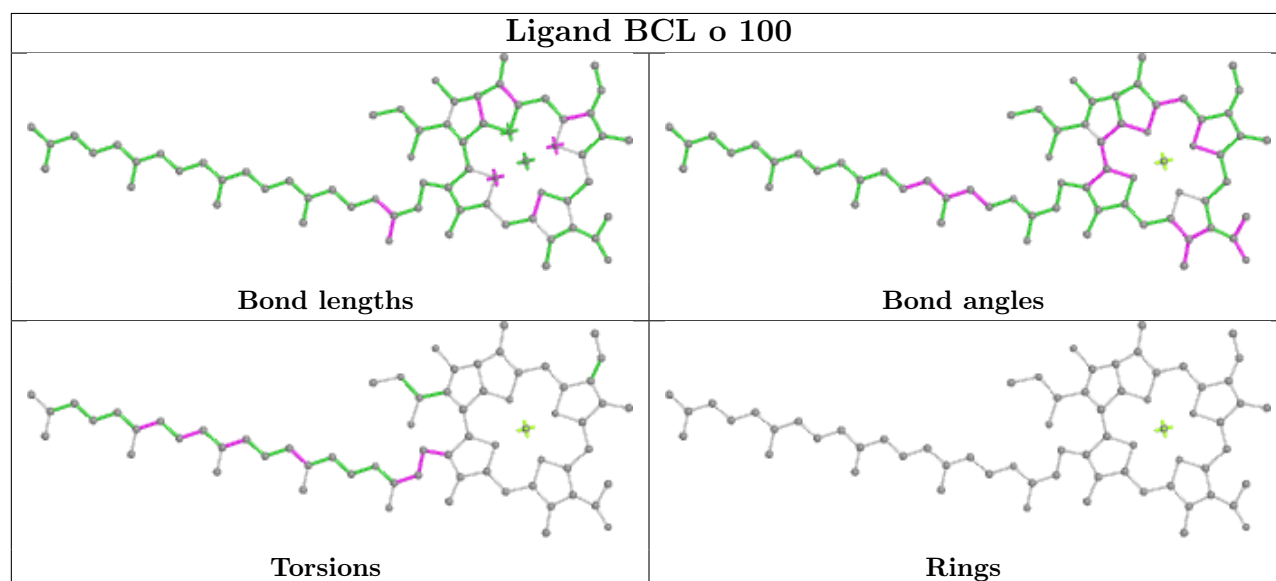
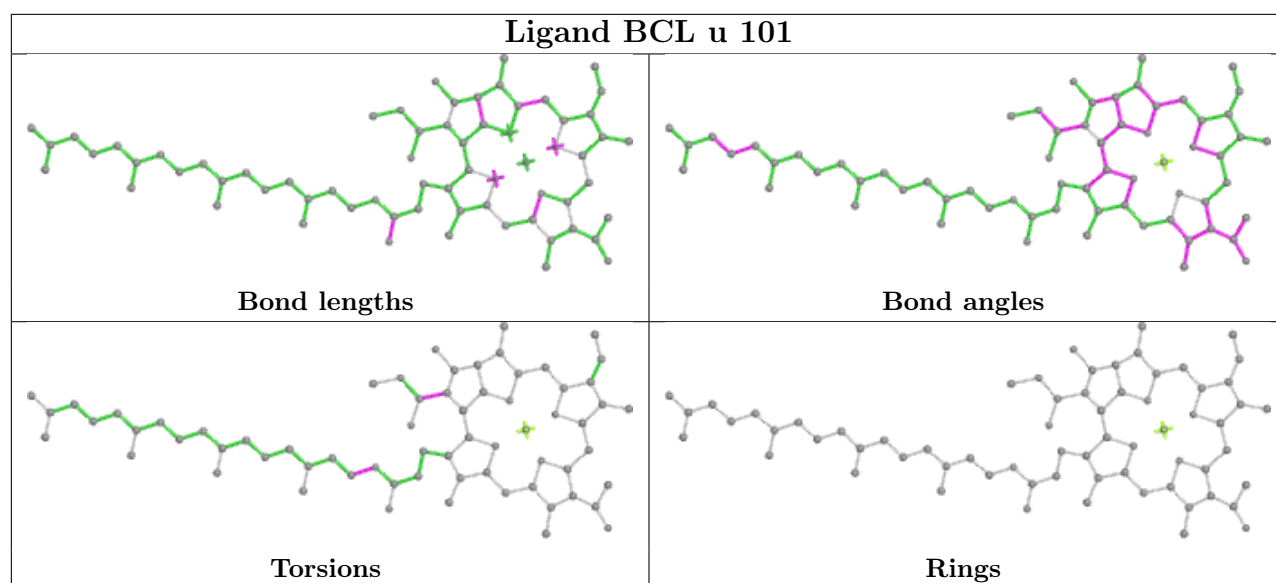


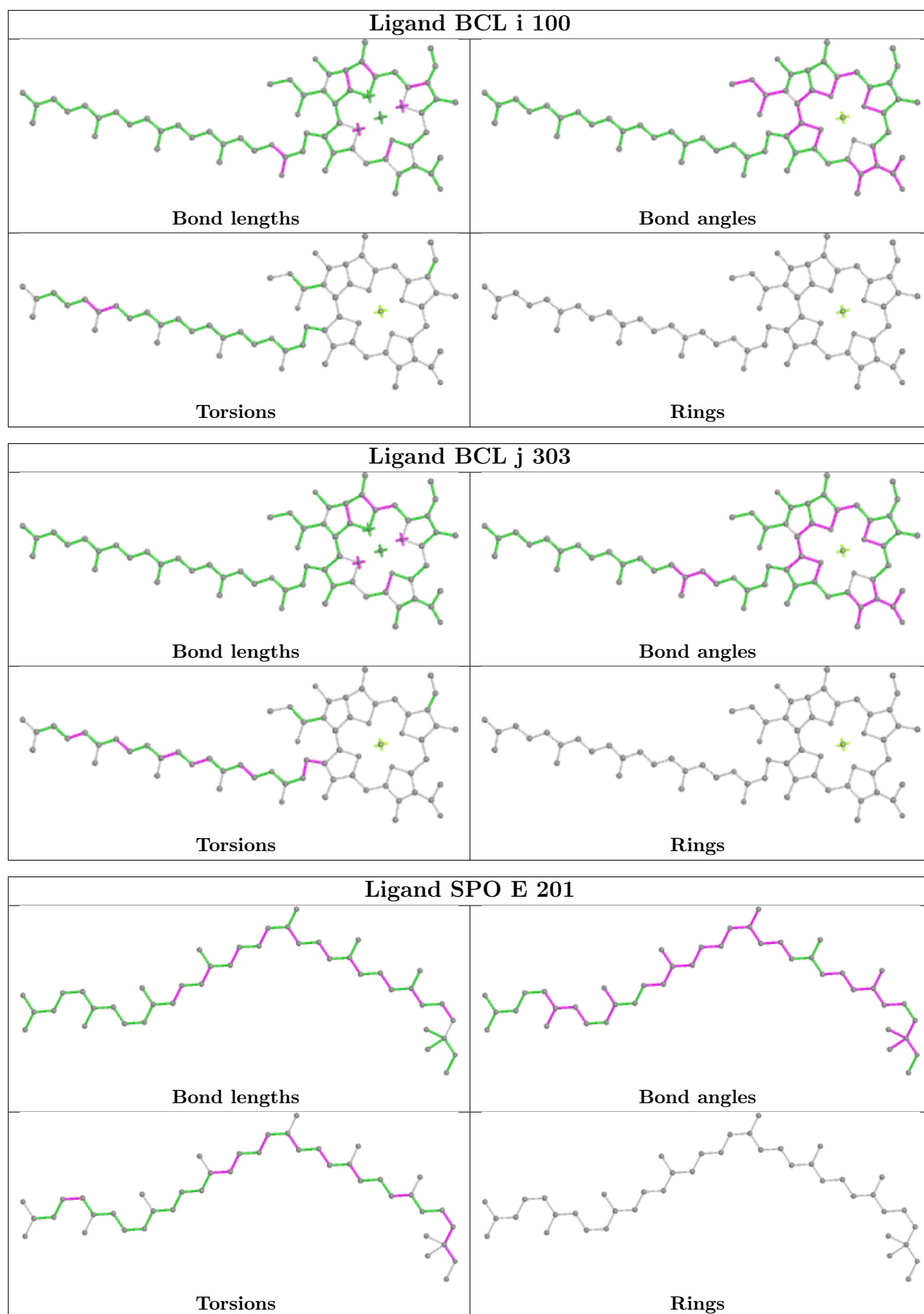


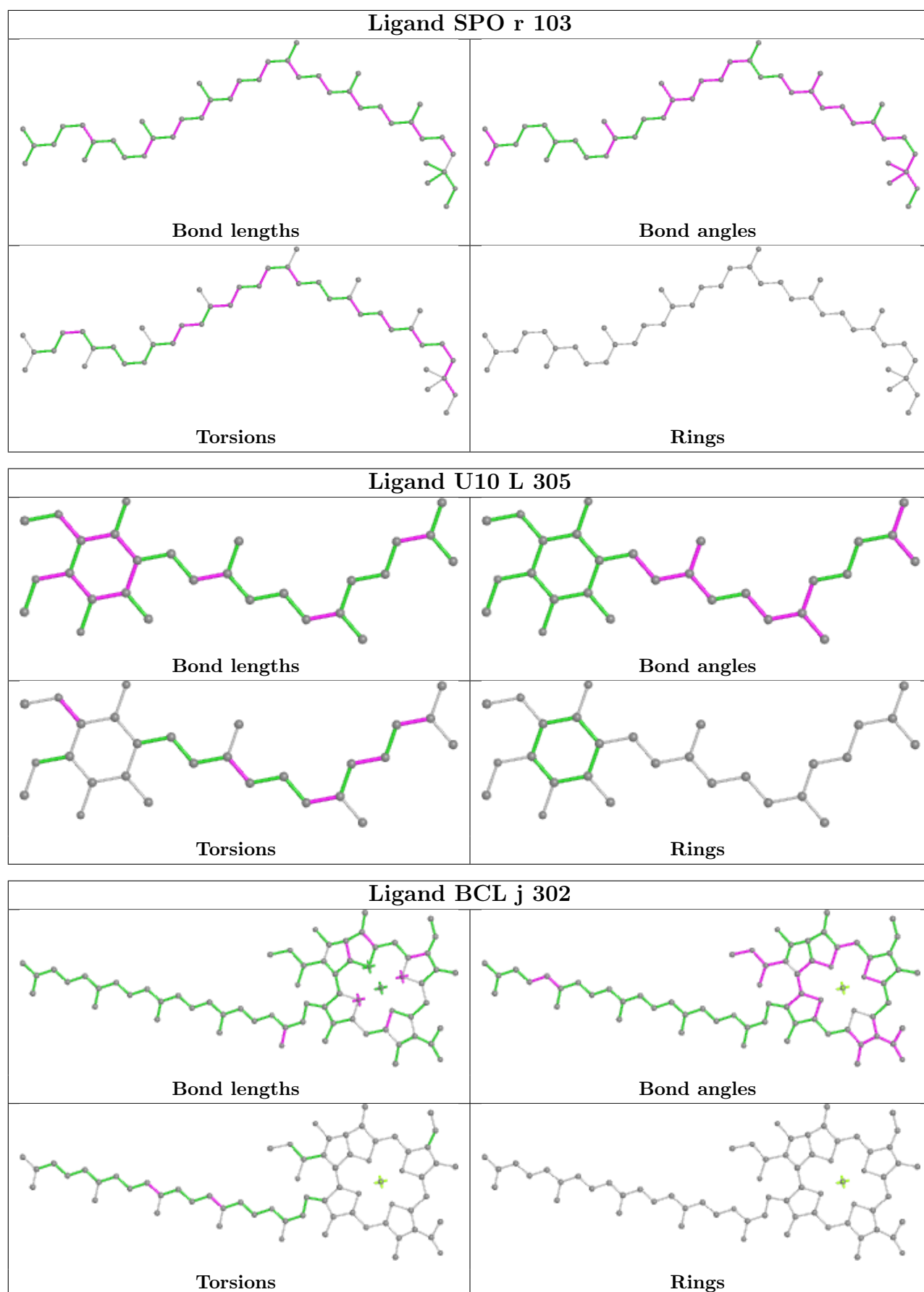


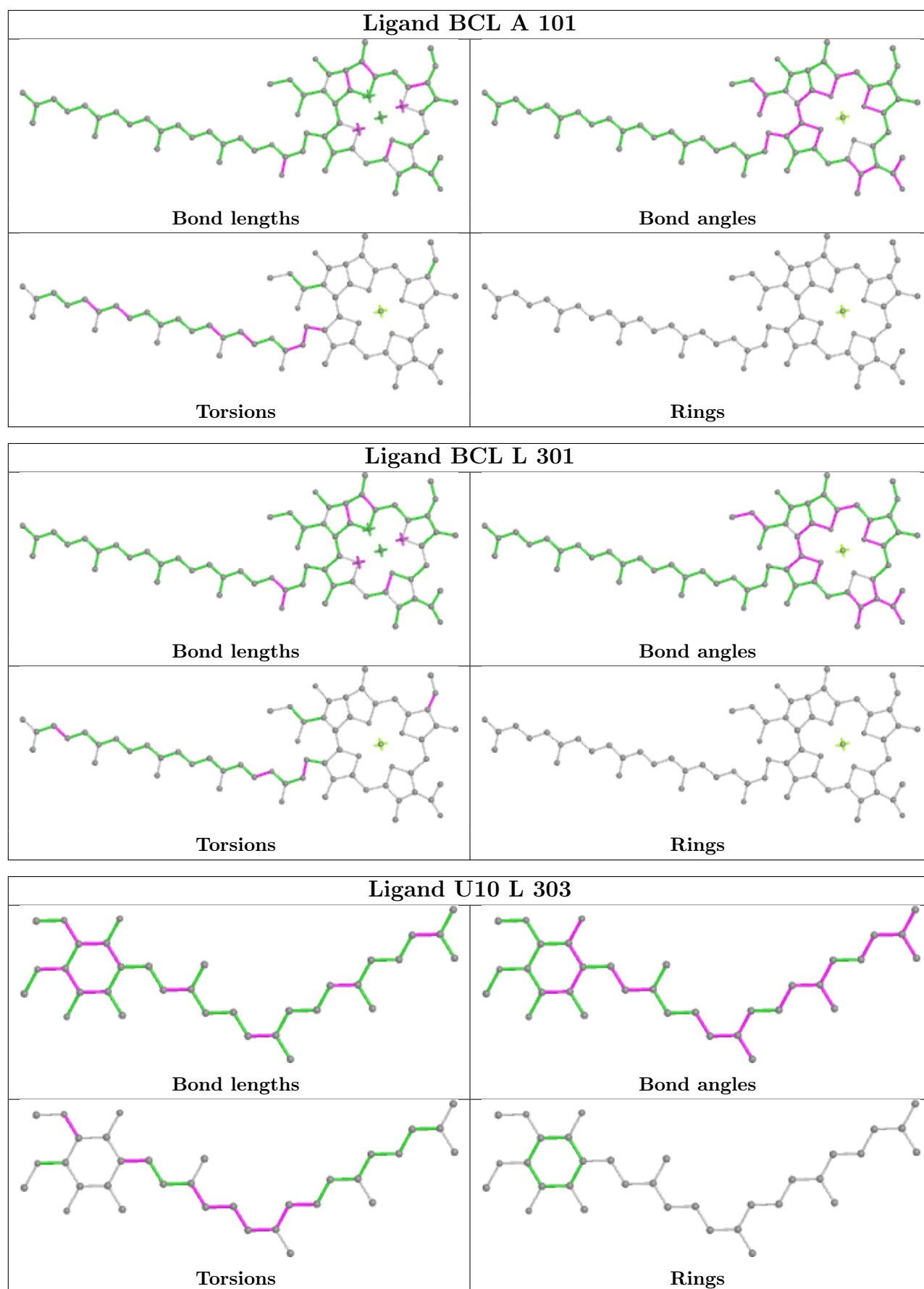


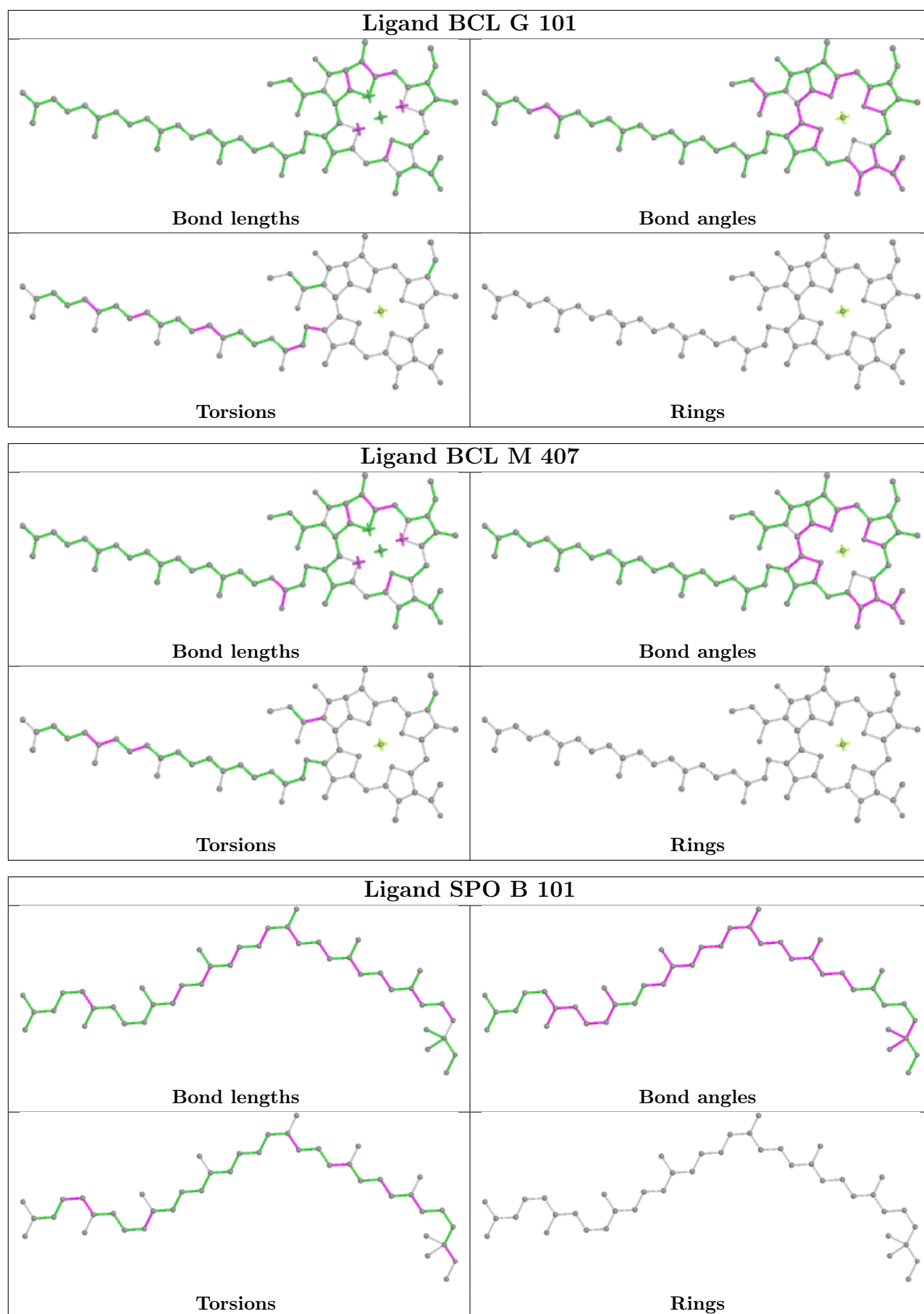


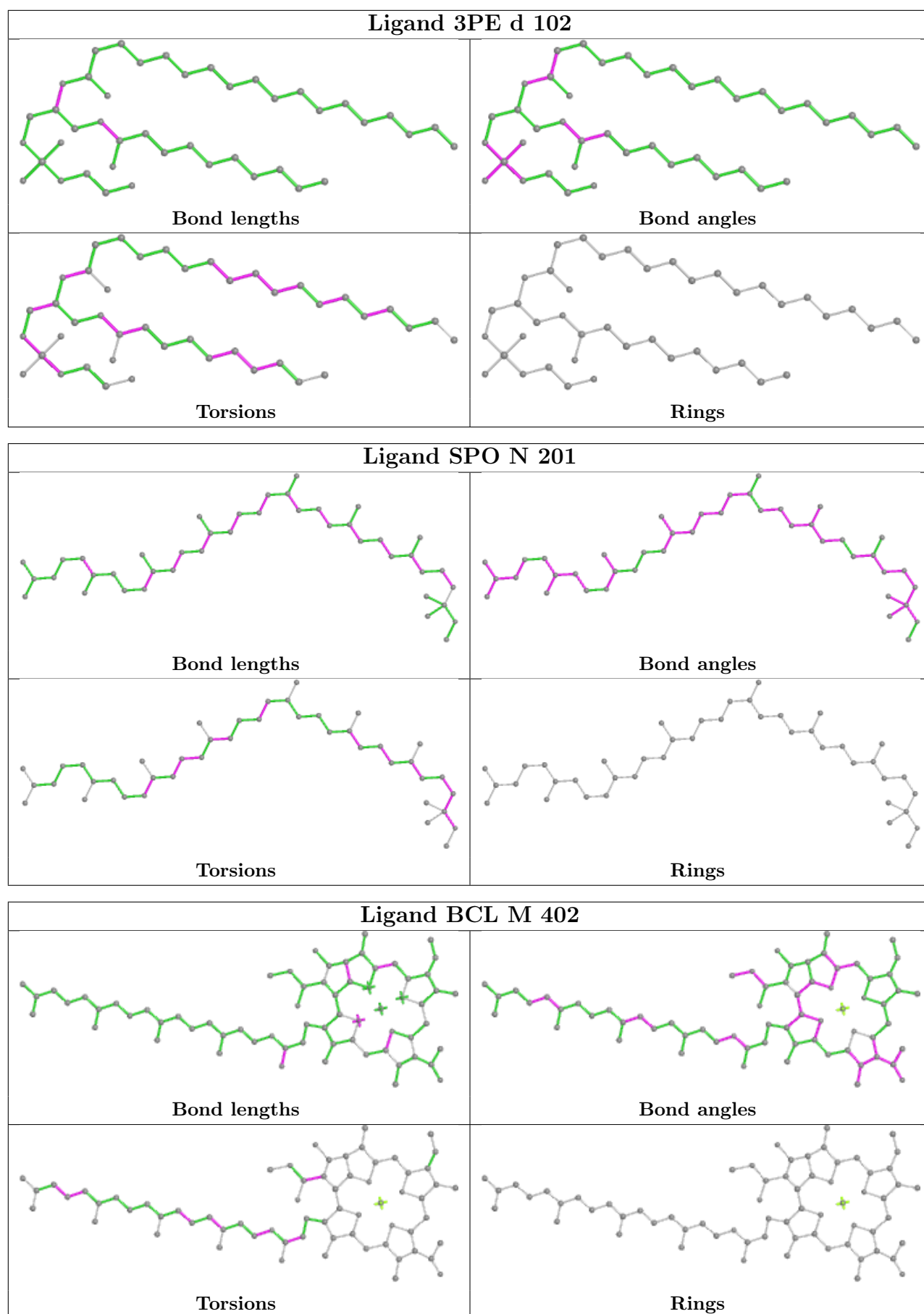


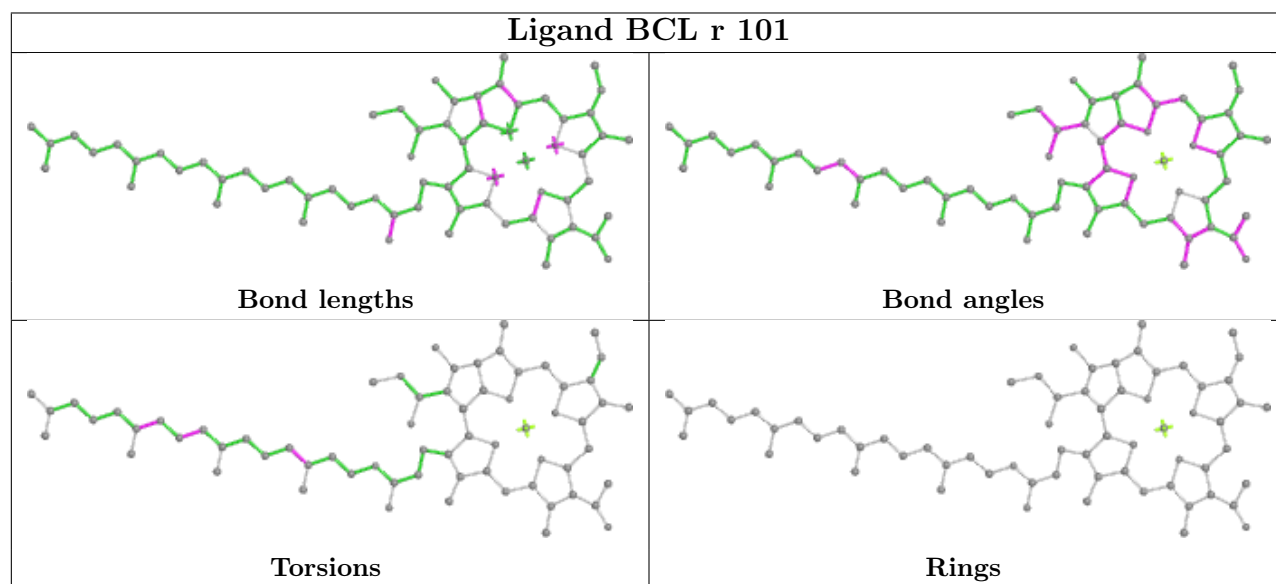
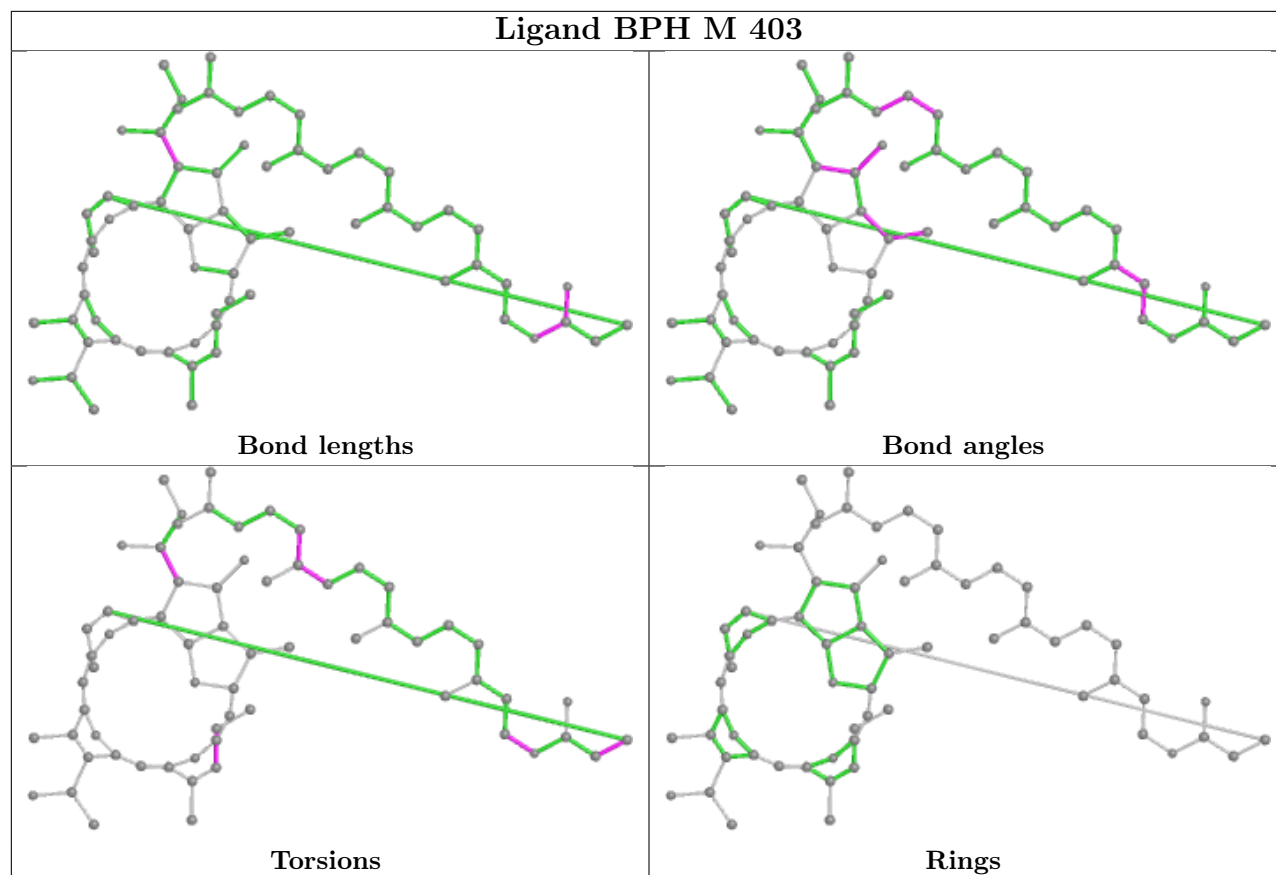


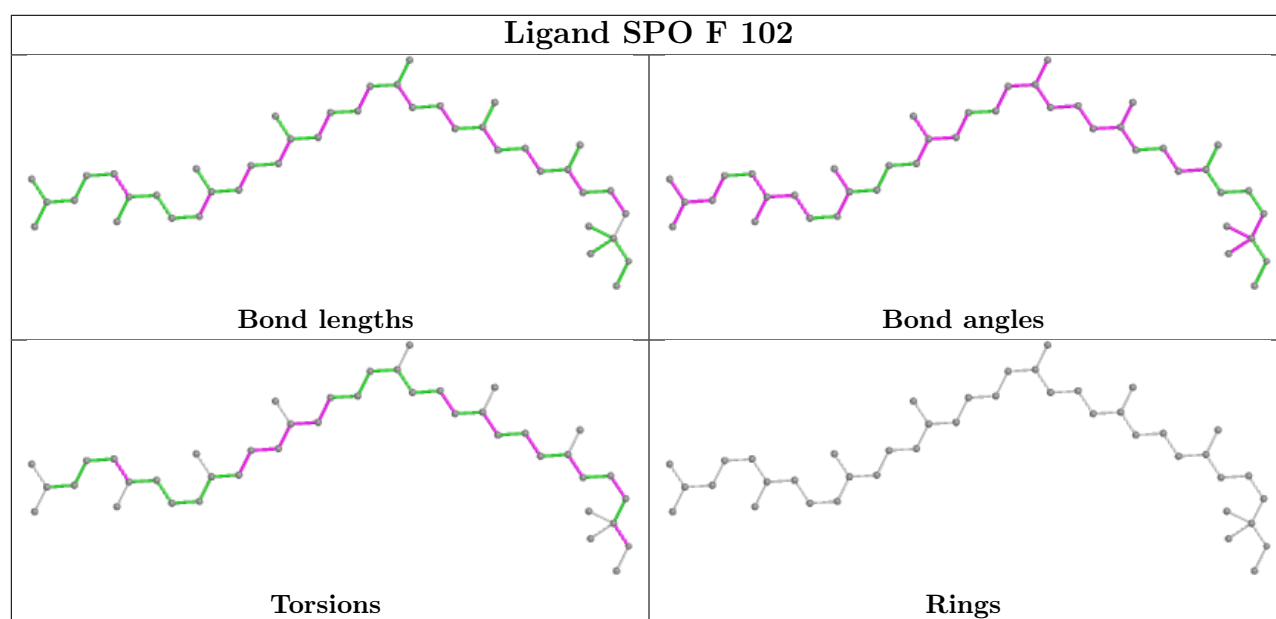
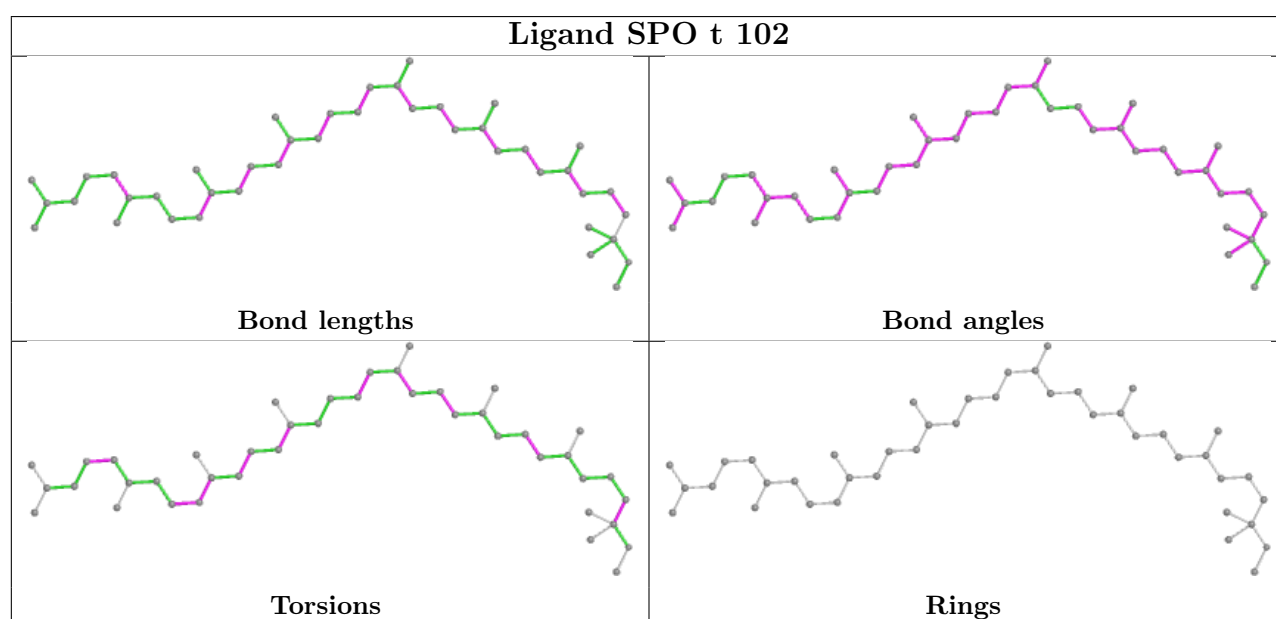
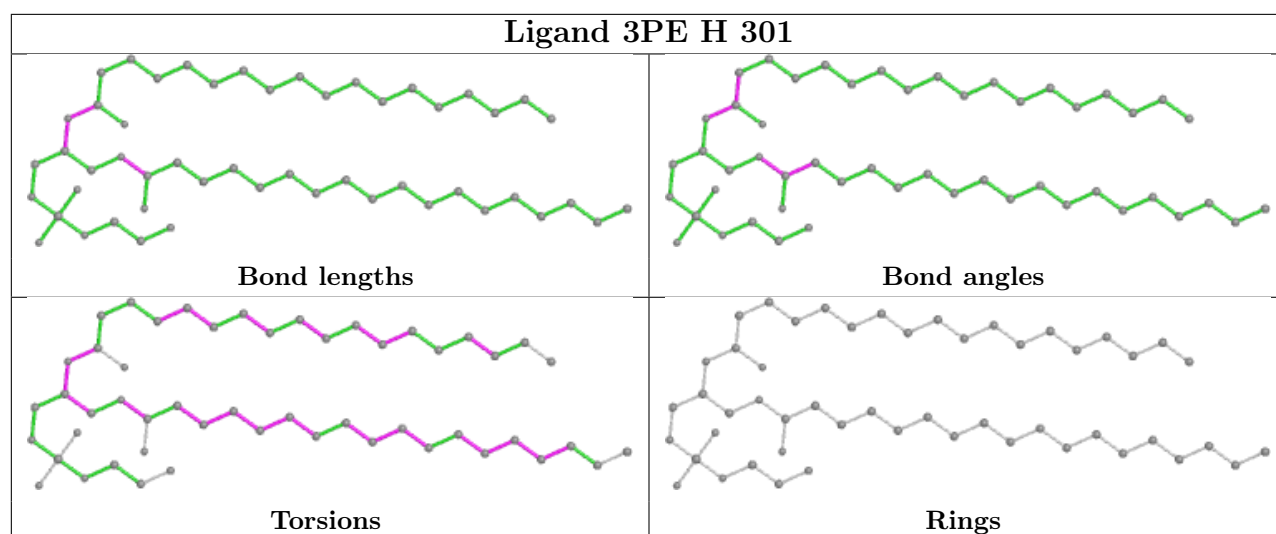


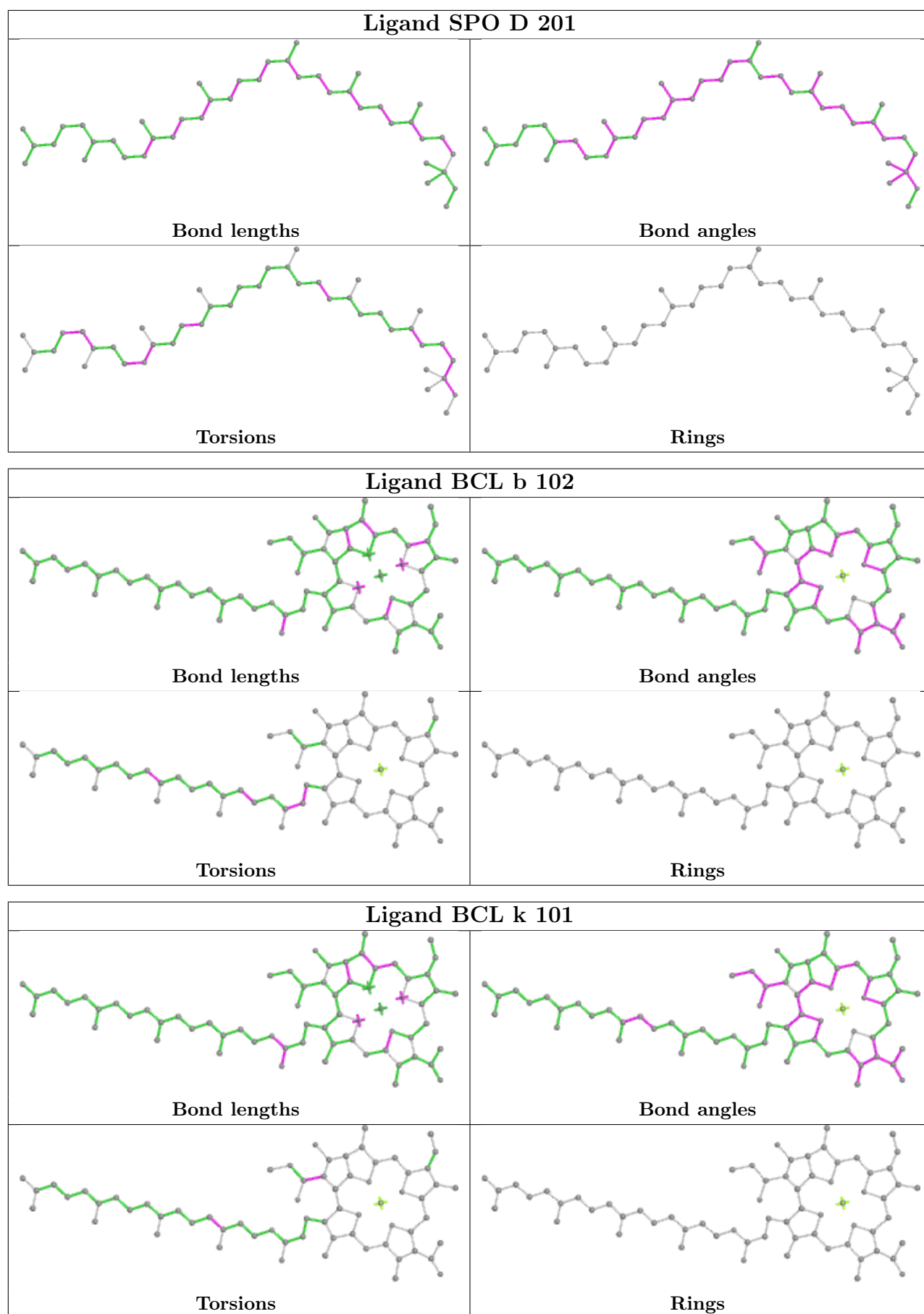


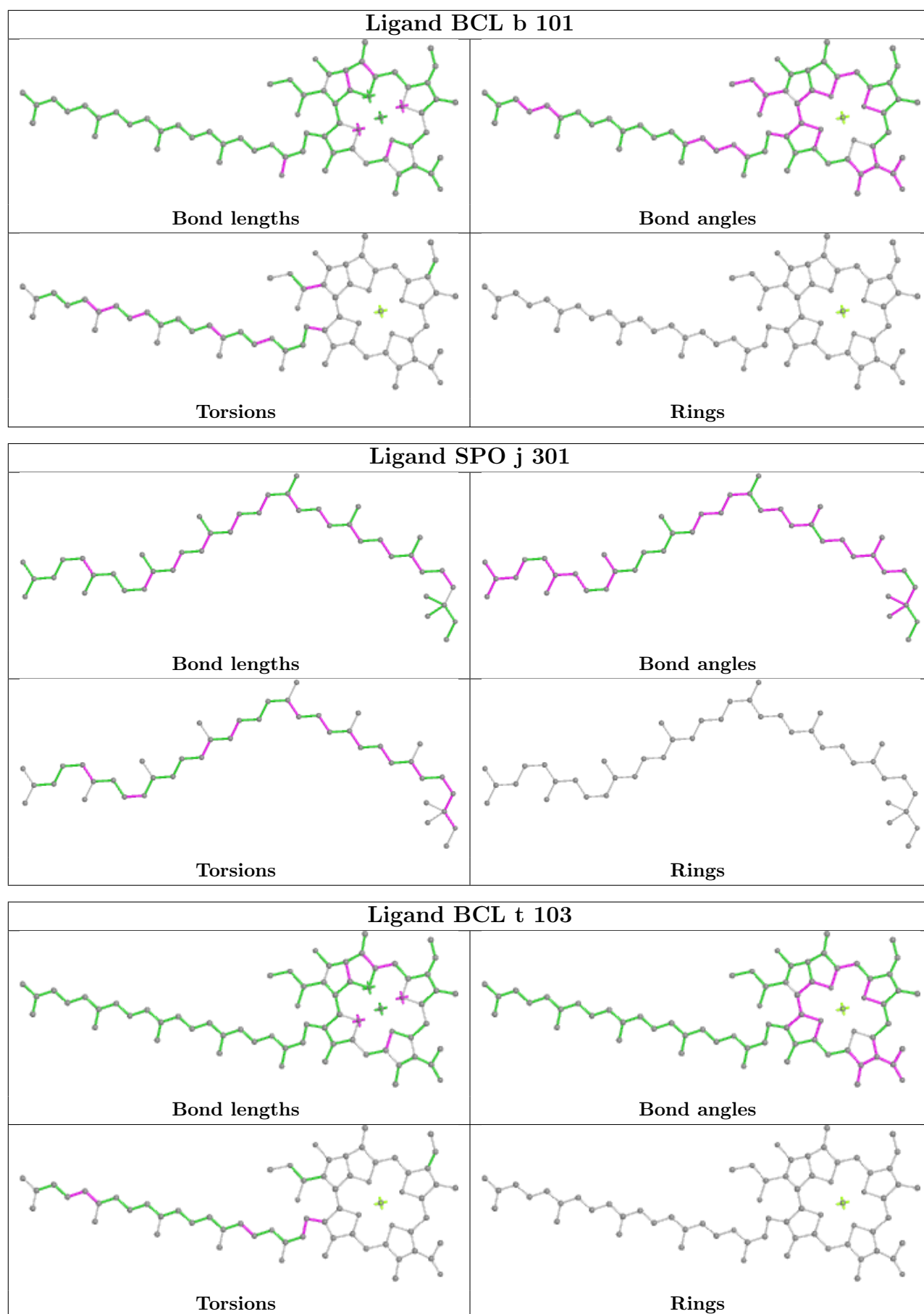


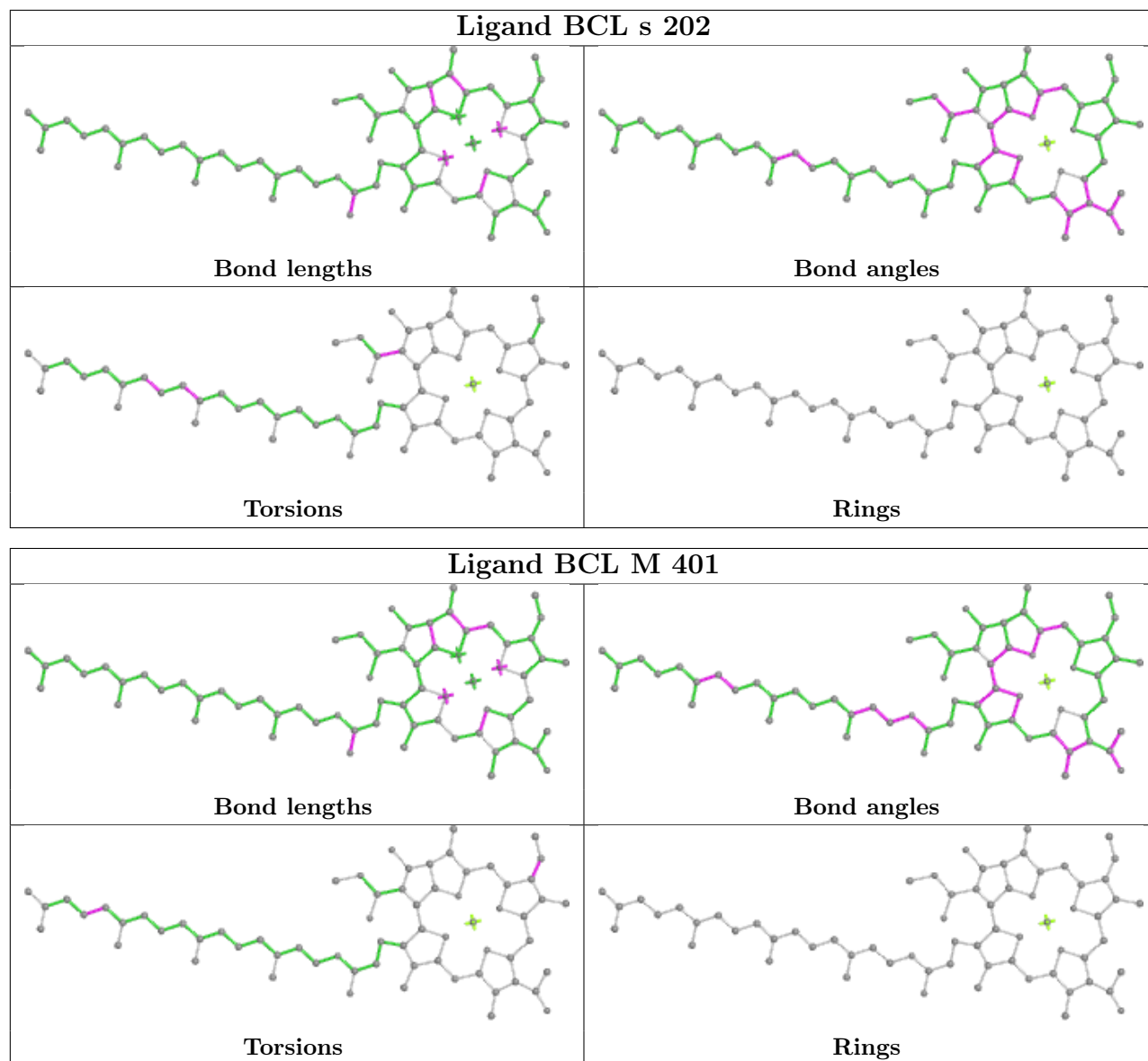




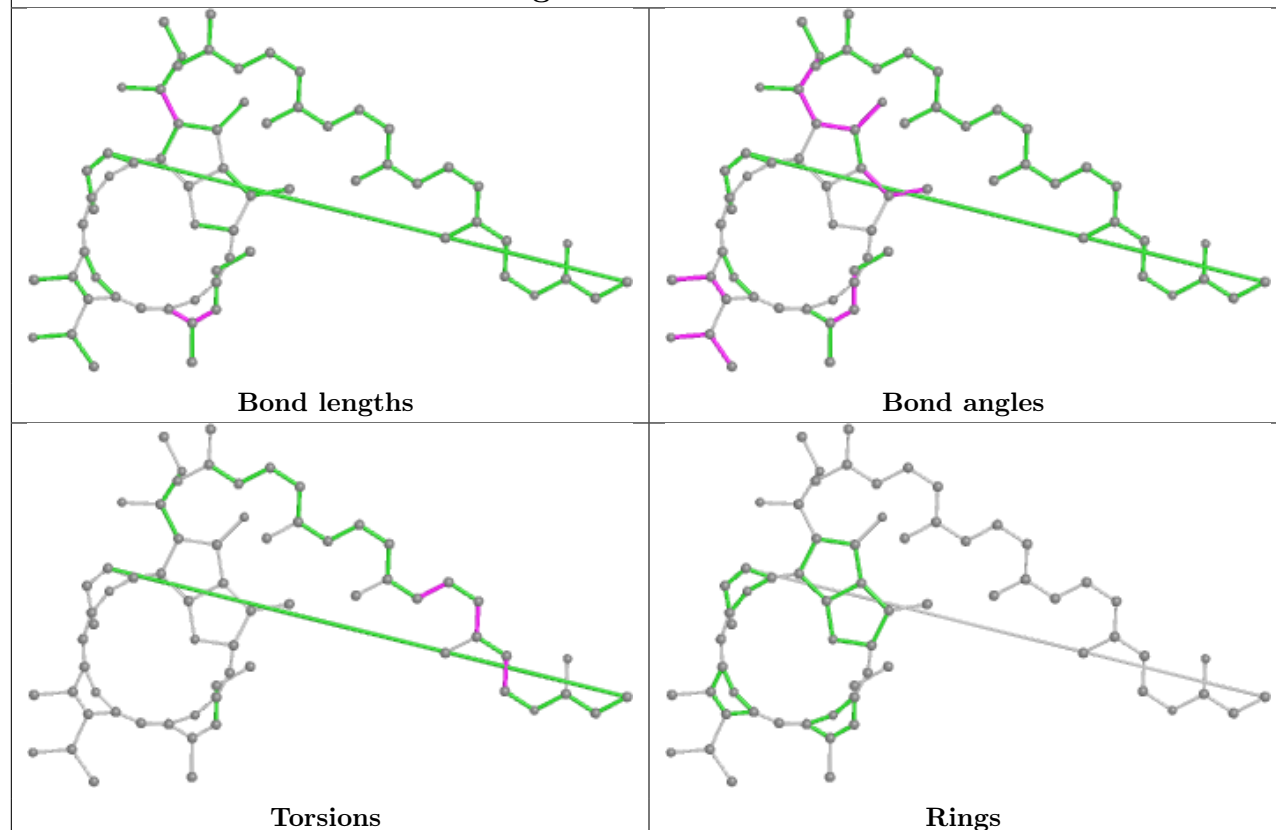




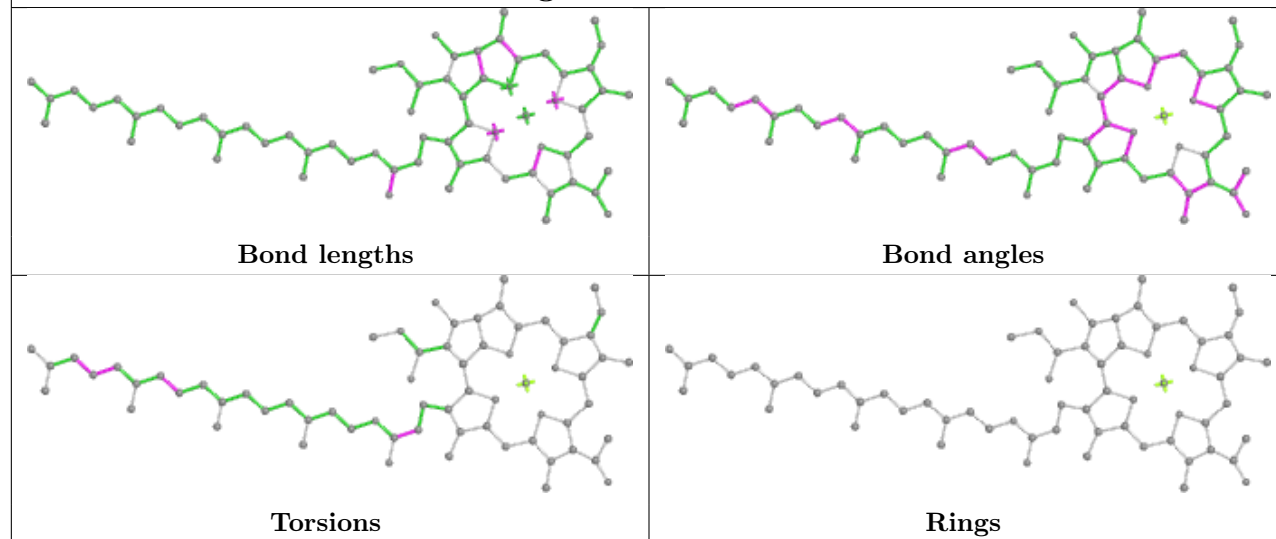


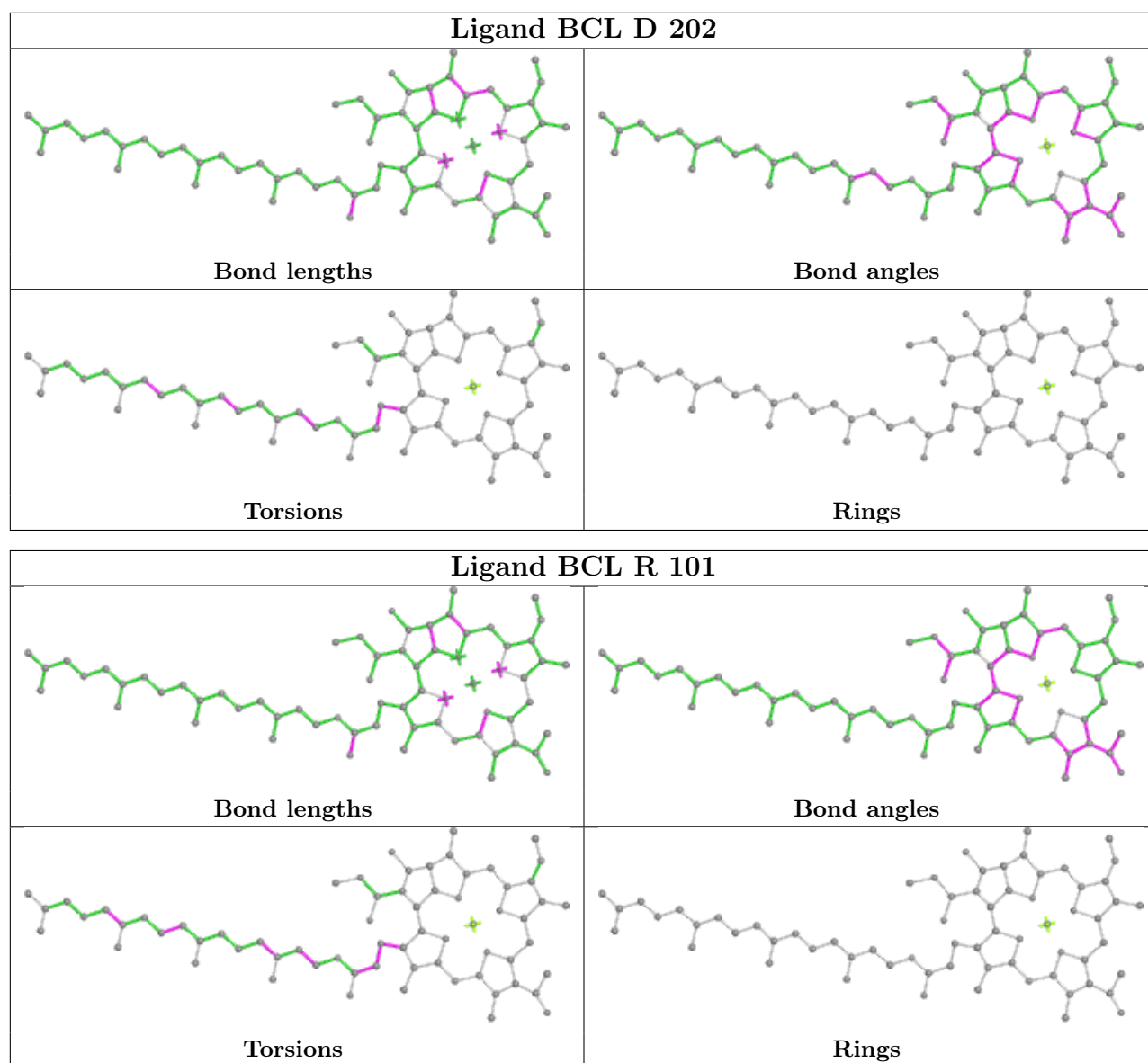


Ligand BPH L 302

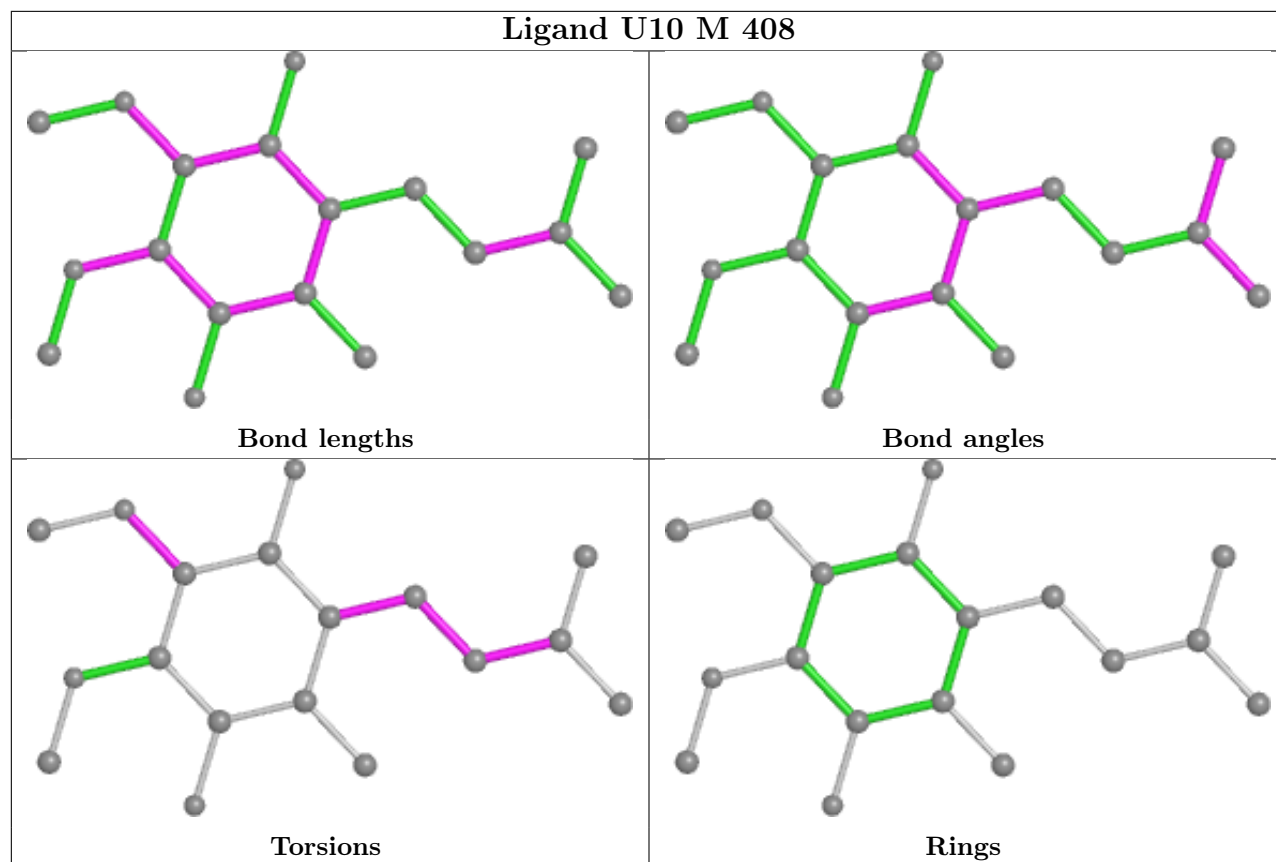


Ligand BCL a 101

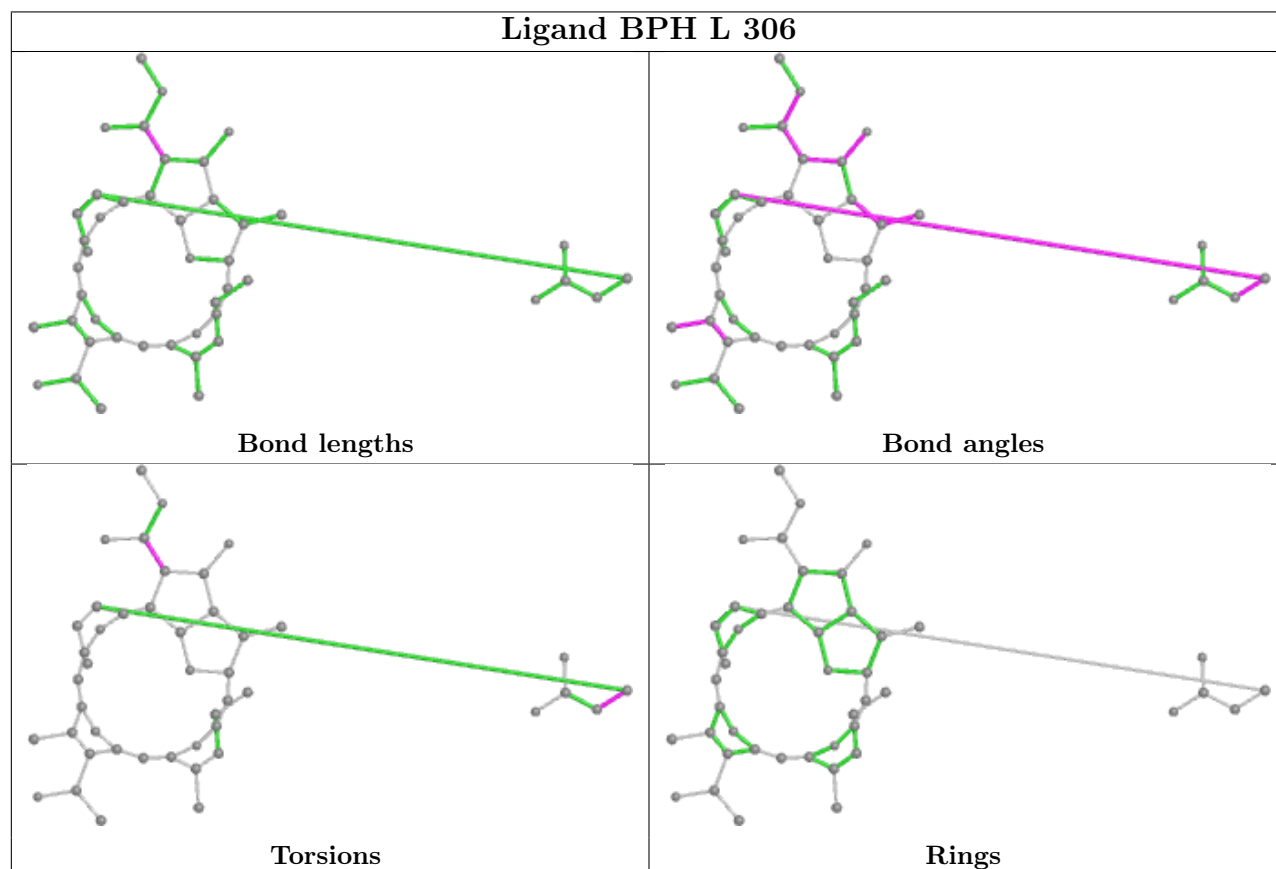


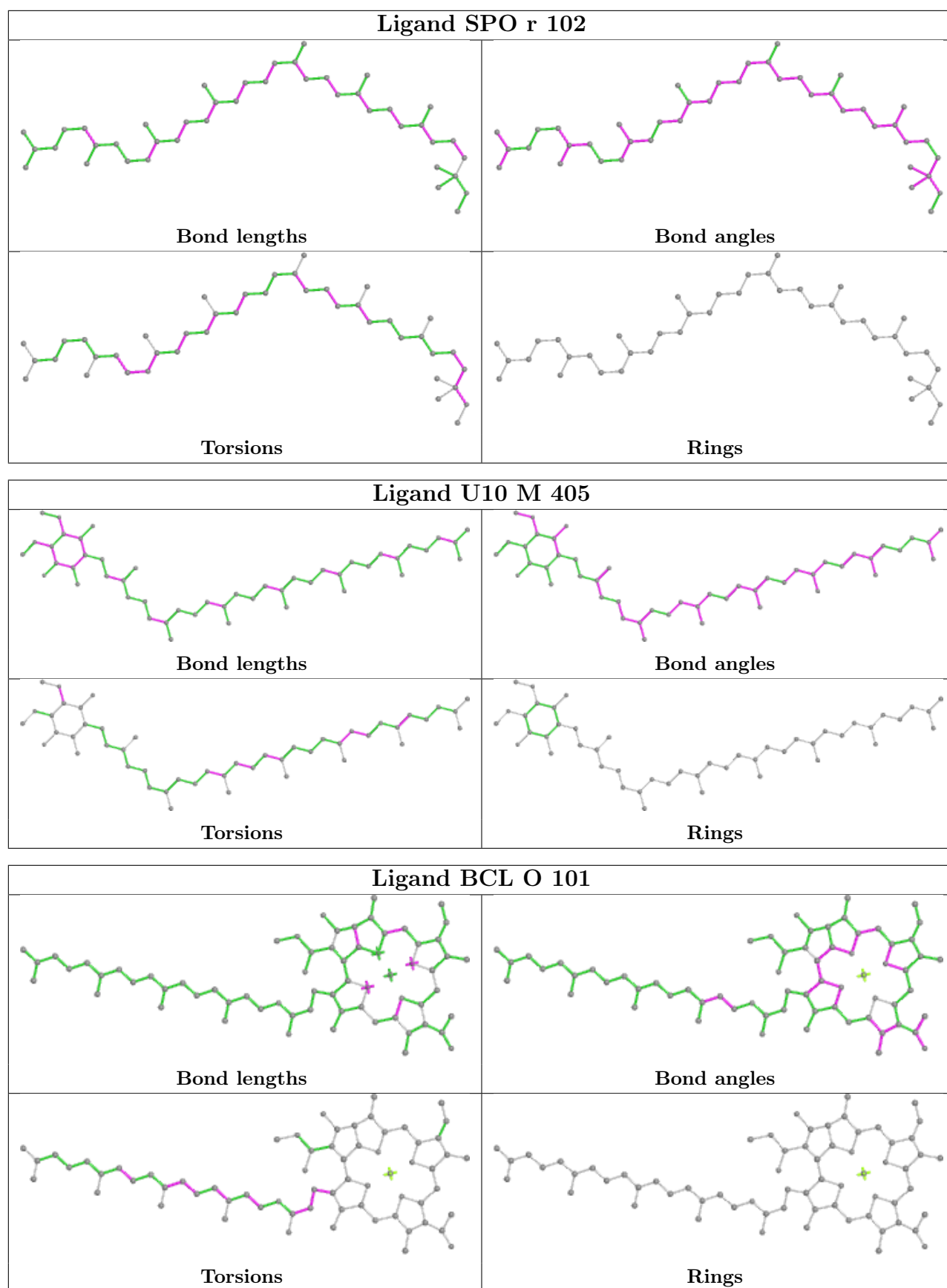


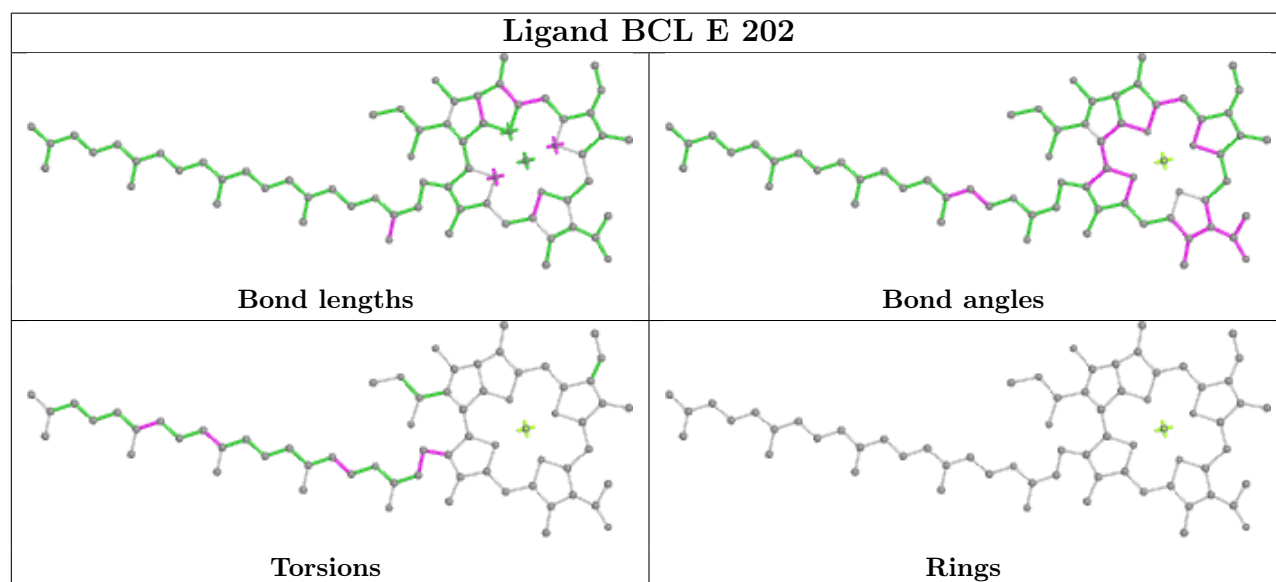
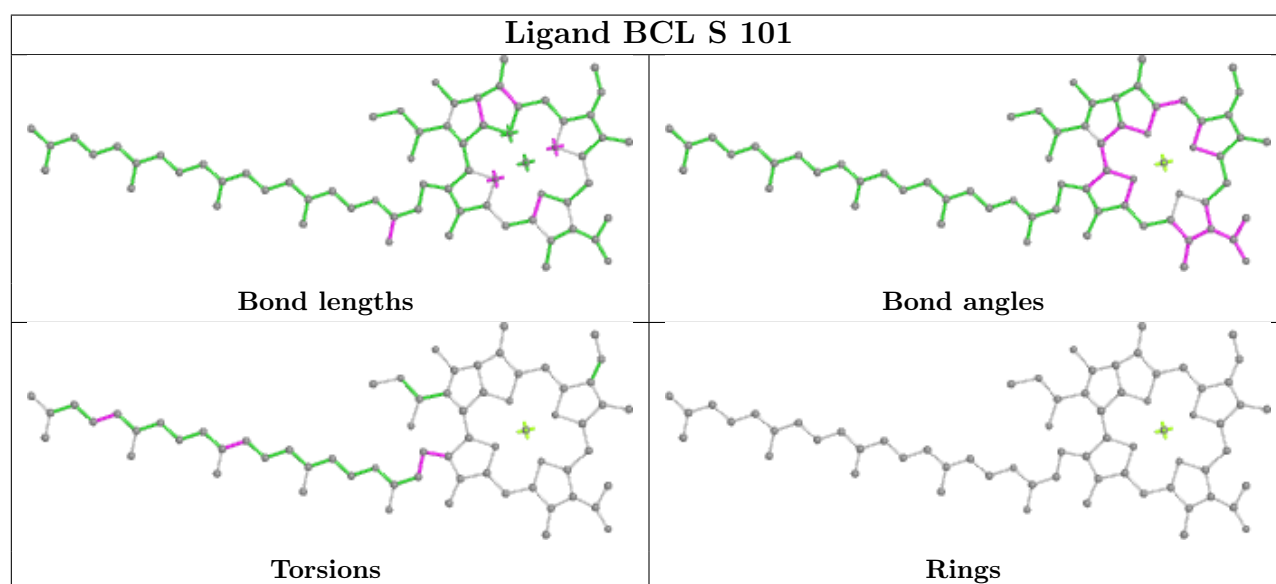
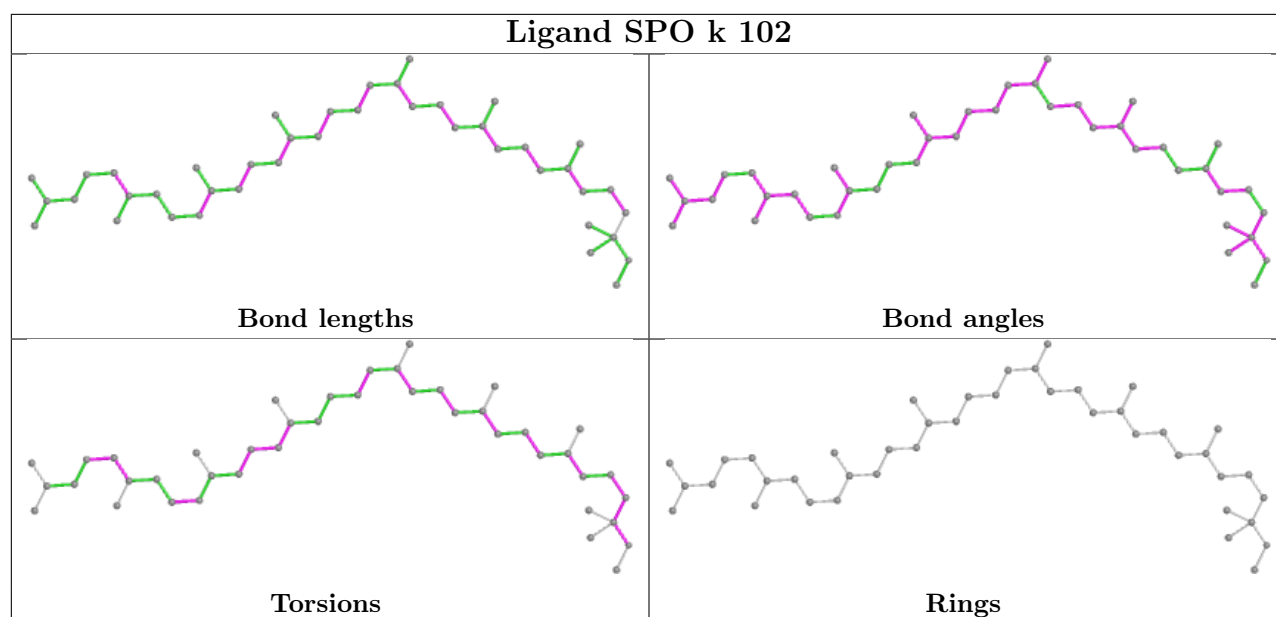
Ligand U10 M 408



Ligand BPH L 306







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.

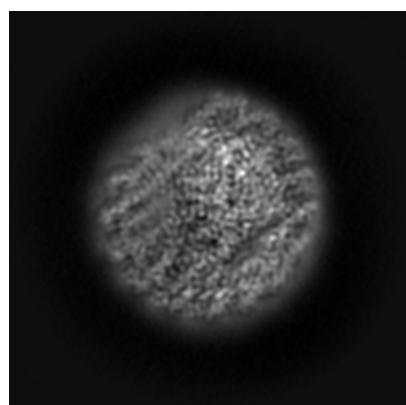
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30656. These allow visual inspection of the internal detail of the map and identification of artifacts.

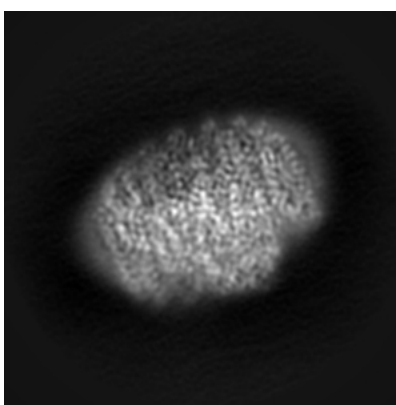
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

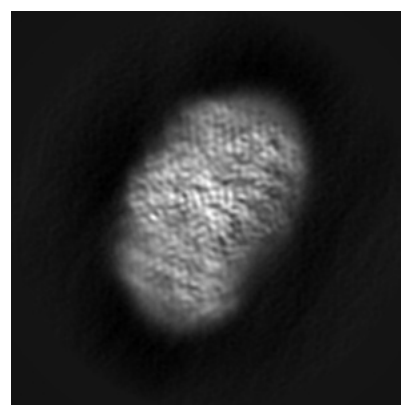
6.1.1 Primary map



X



Y

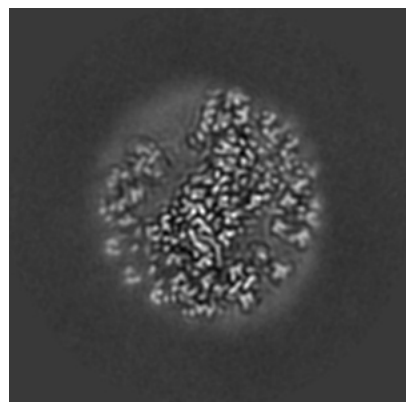


Z

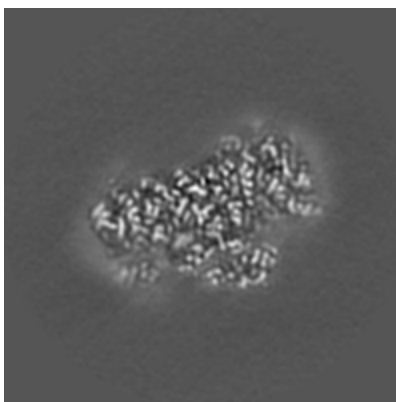
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

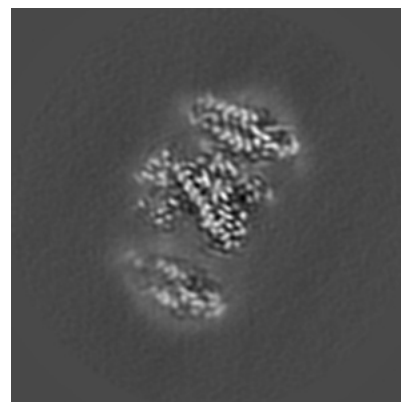
6.2.1 Primary map



X Index: 130



Y Index: 130

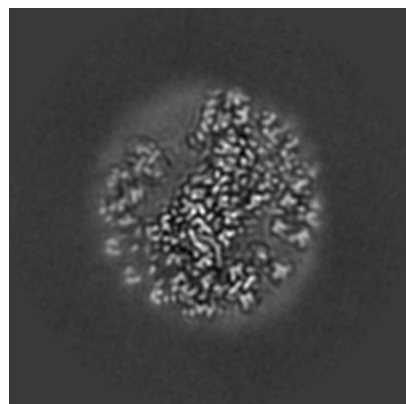


Z Index: 130

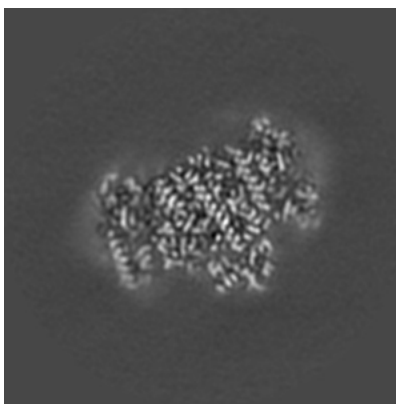
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

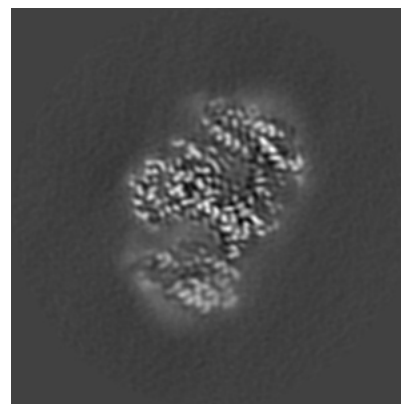
6.3.1 Primary map



X Index: 130



Y Index: 140

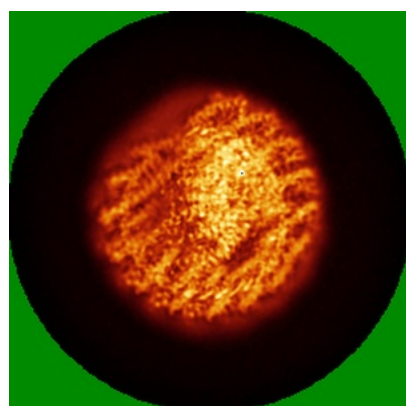


Z Index: 150

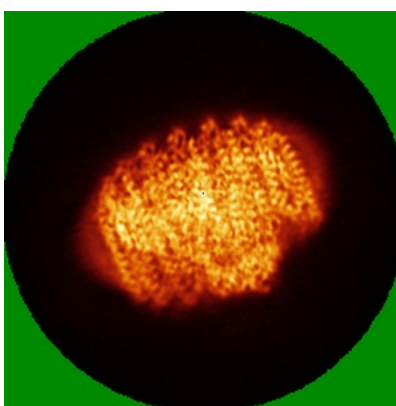
The images above show the largest variance slices of the map in three orthogonal directions.

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

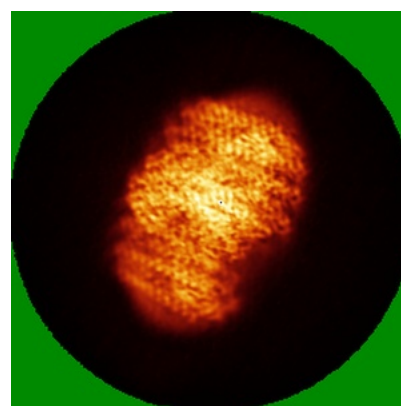
6.4.1 Primary map



X



Y

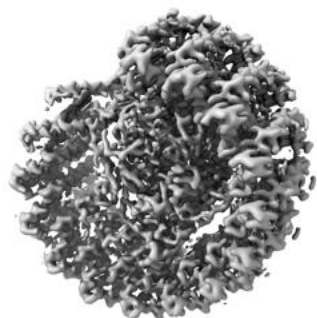


Z

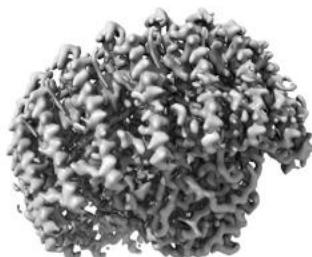
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

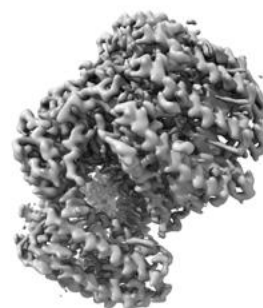
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

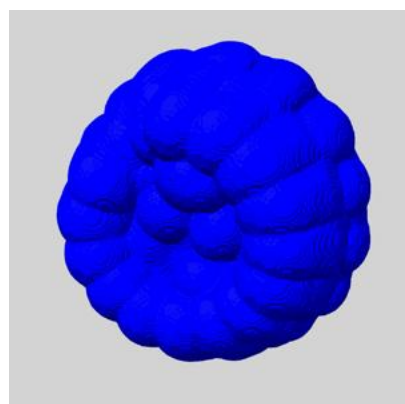
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

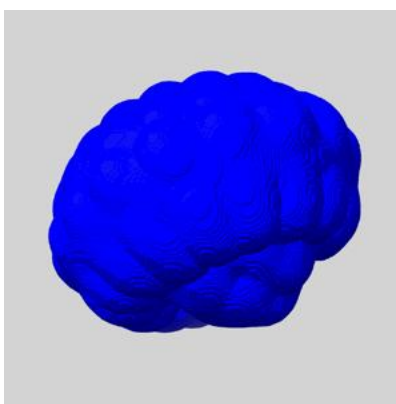
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

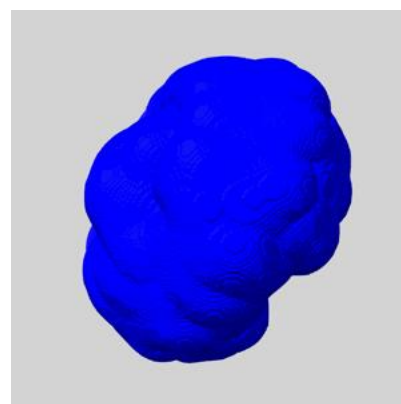
6.6.1 emd_30656_msk_1.map [i](#)



X



Y

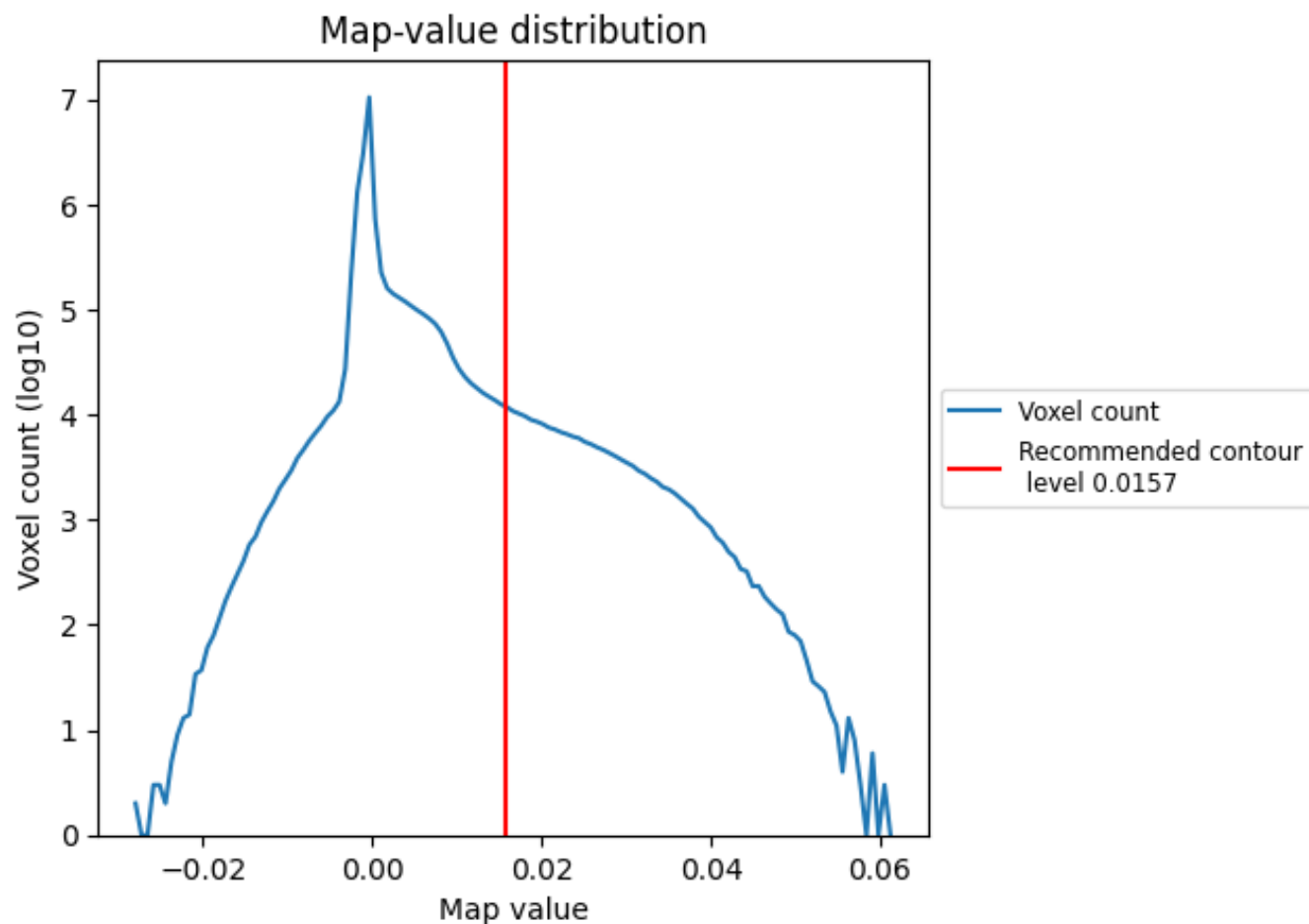


Z

7 Map analysis [i](#)

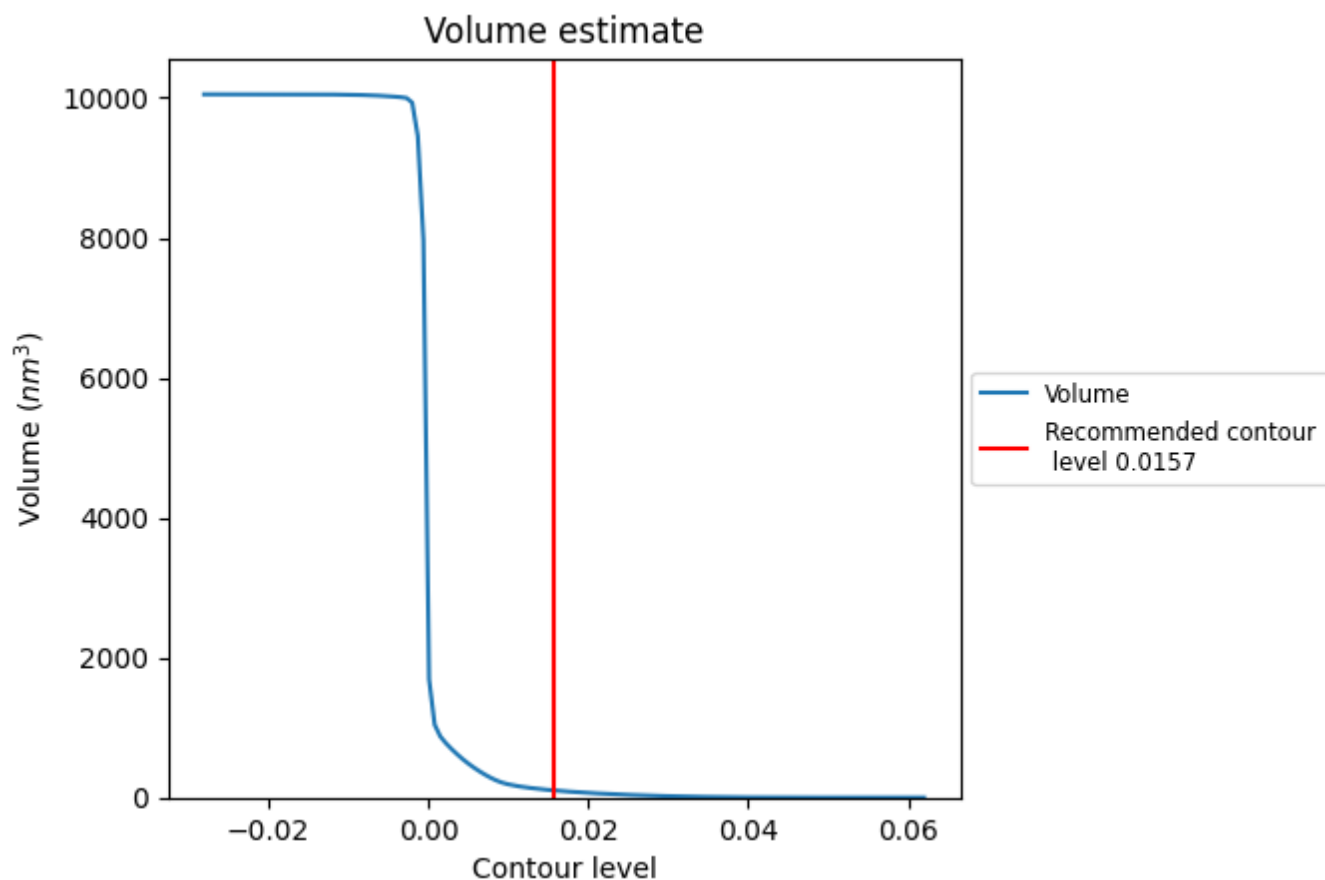
This section contains the results of statistical analysis of the map.

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.

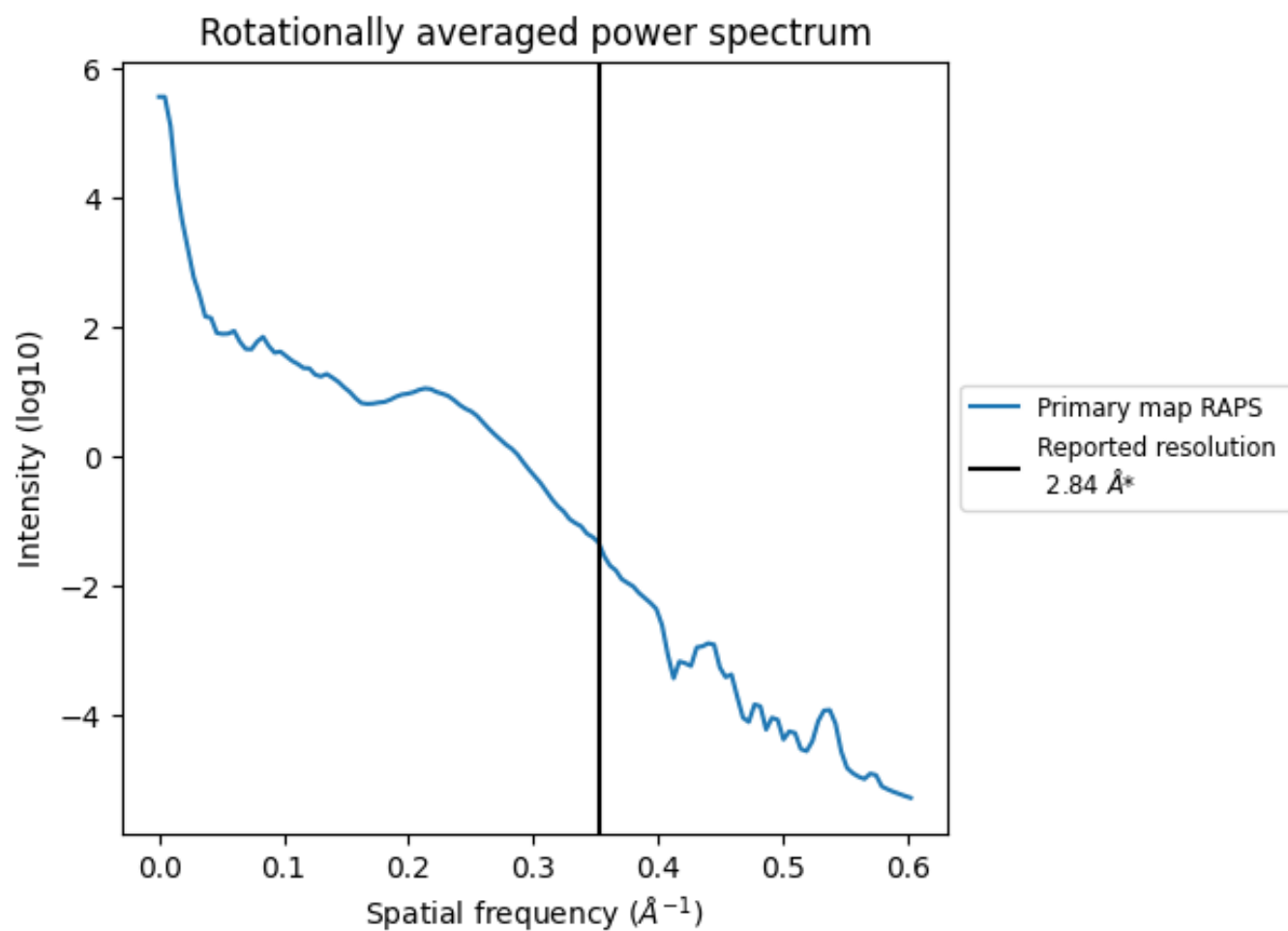
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 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 ⓘ

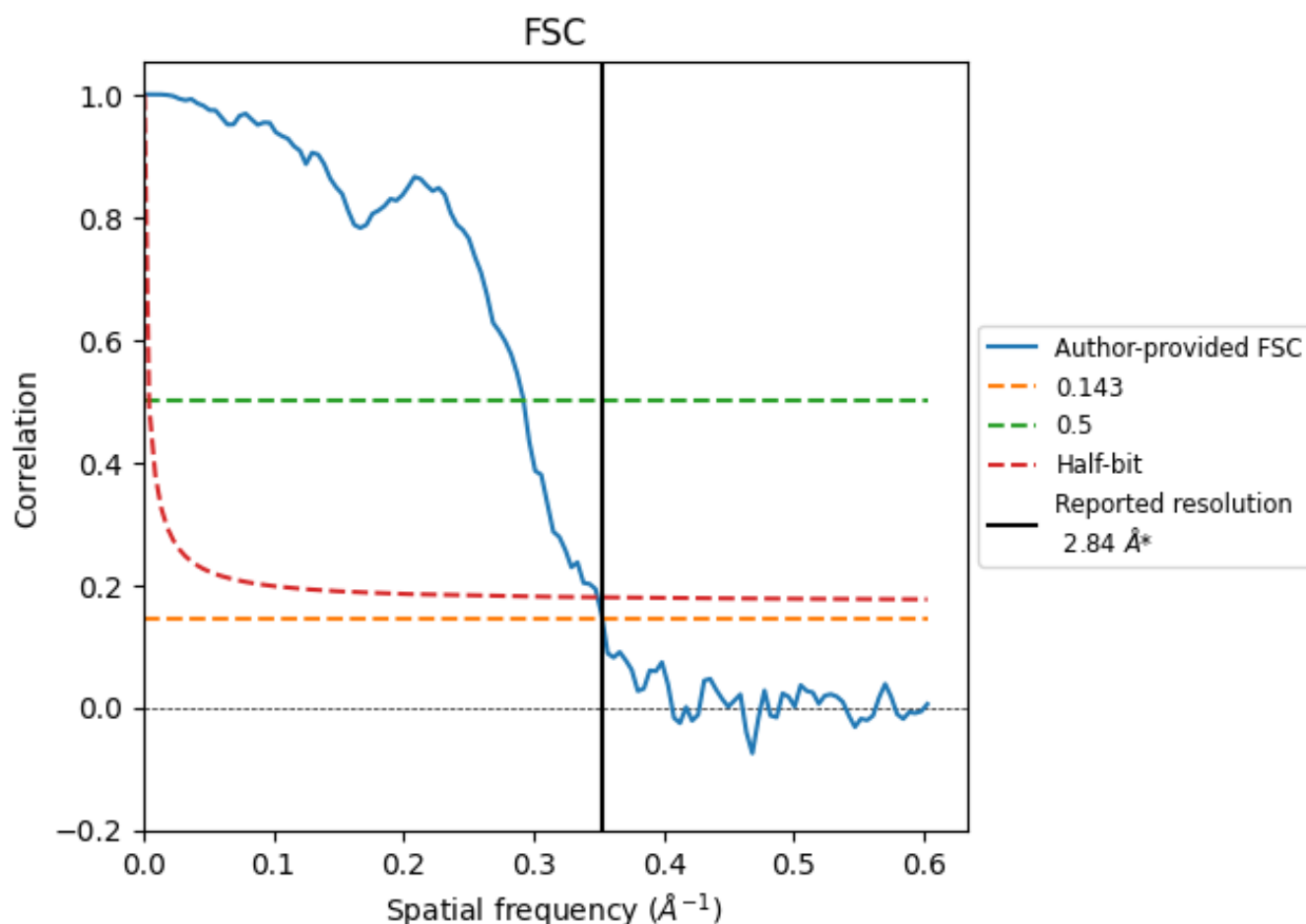


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 0.352 Å⁻¹

8.2 Resolution estimates [i](#)

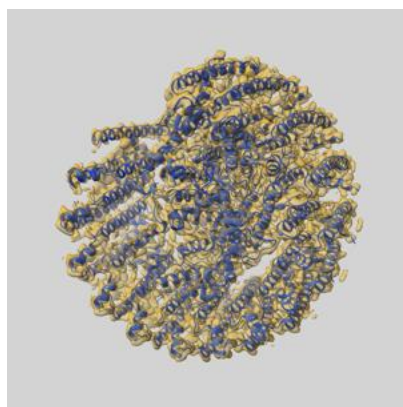
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.83	3.42	2.86
Unmasked-calculated*	-	-	-

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

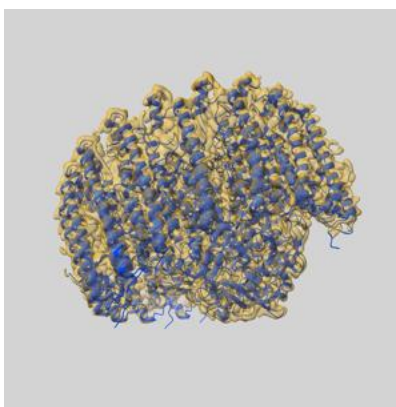
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30656 and PDB model 7DDQ. Per-residue inclusion information can be found in section [3](#) on page [13](#).

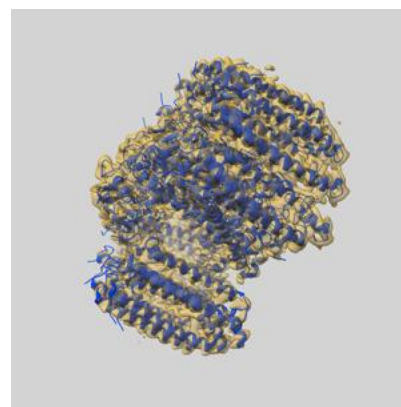
9.1 Map-model overlay [i](#)



X



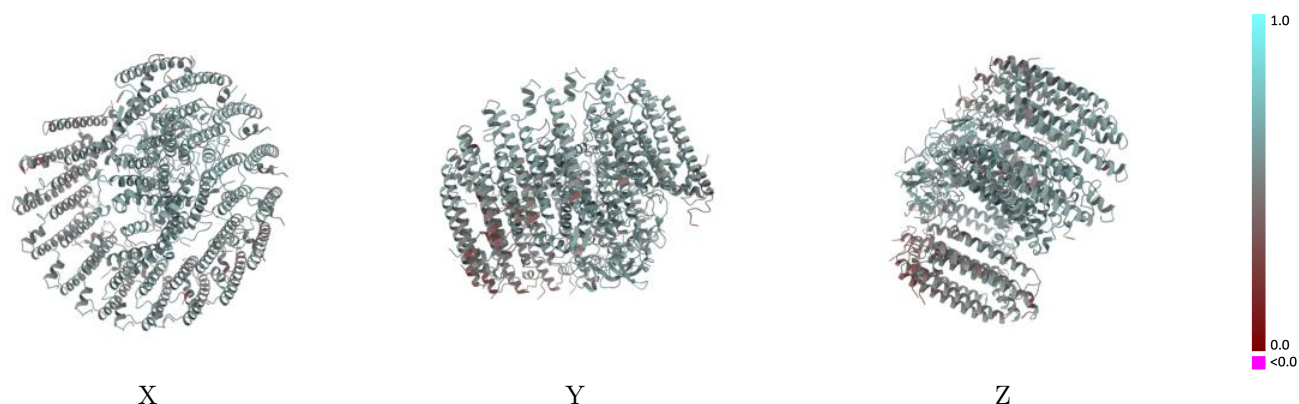
Y



Z

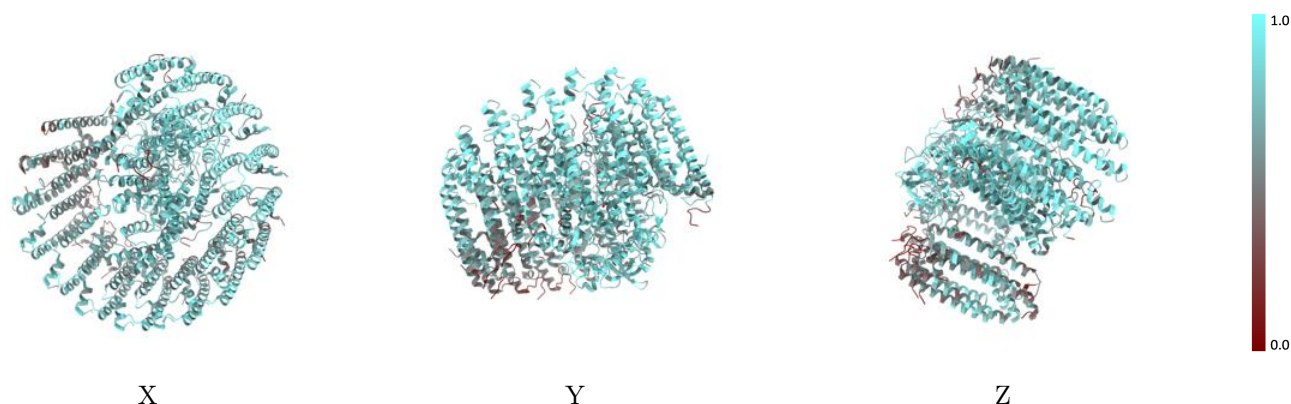
The images above show the 3D surface view of the map at the recommended contour level 0.0157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



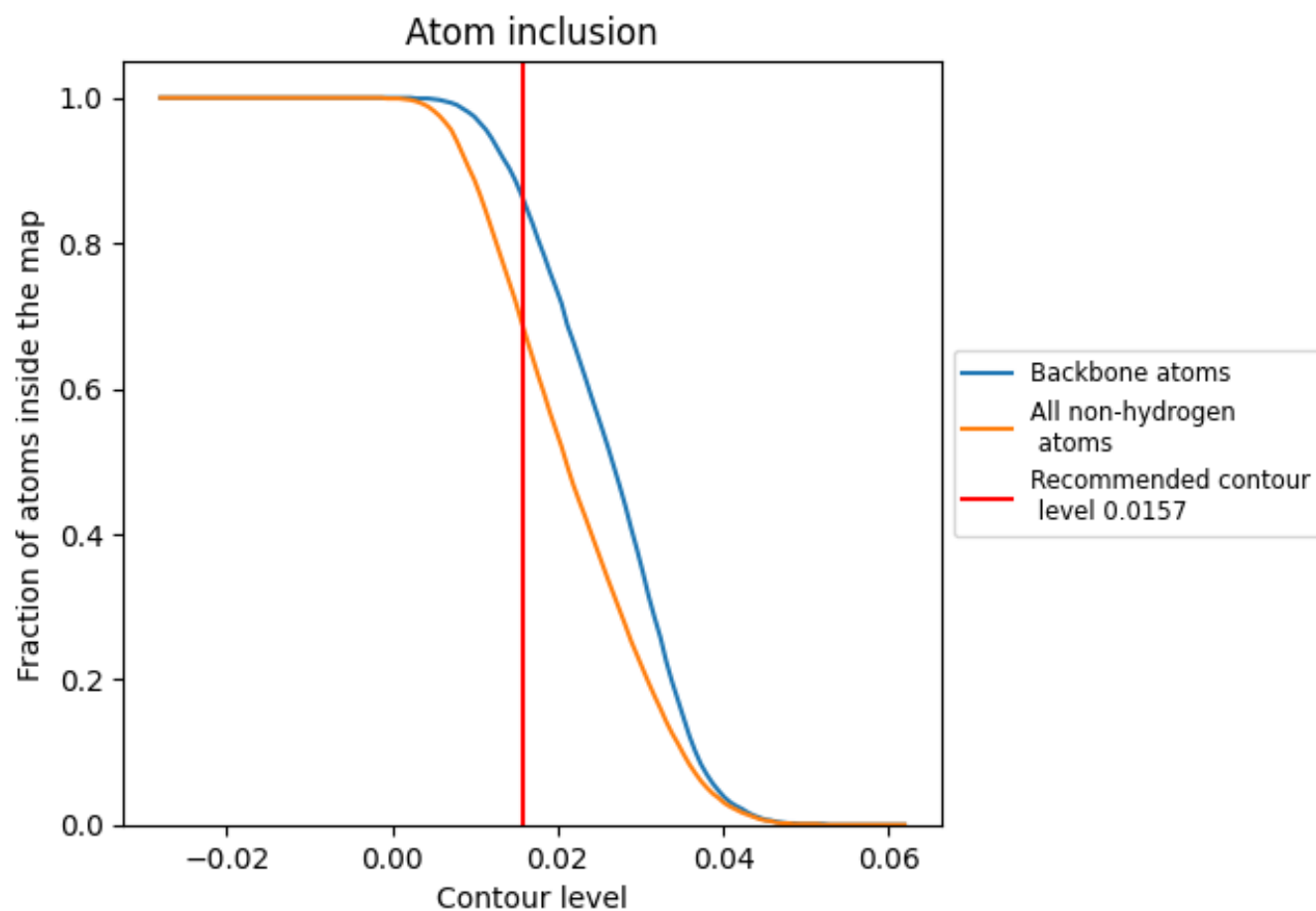
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0157).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% 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 (0.0157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6900	 0.5380
A	 0.7260	 0.5420
B	 0.7720	 0.5540
D	 0.7330	 0.5600
E	 0.6700	 0.5270
F	 0.6420	 0.5260
G	 0.6420	 0.5080
H	 0.7990	 0.5740
I	 0.5510	 0.4670
J	 0.6300	 0.4970
K	 0.6710	 0.5240
L	 0.8110	 0.5900
M	 0.8100	 0.5890
N	 0.5900	 0.4990
O	 0.5700	 0.4800
R	 0.5230	 0.4660
S	 0.5460	 0.4510
T	 0.5630	 0.4640
U	 0.5720	 0.4900
X	 0.5120	 0.5240
a	 0.7100	 0.5580
b	 0.7610	 0.5710
d	 0.7570	 0.5680
e	 0.7630	 0.5680
f	 0.7500	 0.5520
g	 0.6540	 0.5190
i	 0.6410	 0.5110
j	 0.6180	 0.5120
k	 0.6650	 0.5340
n	 0.6870	 0.5380
o	 0.6510	 0.5120
r	 0.5430	 0.4730
s	 0.5480	 0.4870
t	 0.5400	 0.4910
u	 0.5070	 0.4940

