



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:54 PM UTC

PDB ID : 7VOR / pdb_00007vor
EMDB ID : EMD-32058
Title : The structure of dimeric photosynthetic RC-LH1 supercomplex in Class-1
Authors : Cao, P.; Li, M.; Liu, L.N.
Deposited on : 2021-10-14
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

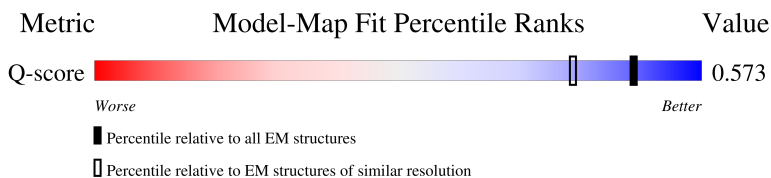
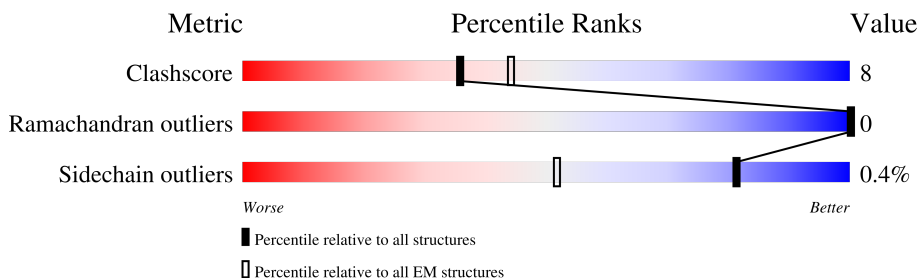
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 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	10492 (2.24 - 3.24)

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	L	282	
1	l	282	
2	M	308	
2	m	308	

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Mol	Chain	Length	Quality of chain
3	H	260	
3	h	260	
4	1	58	
4	3	58	
4	5	58	
4	6	58	
4	7	58	
4	9	58	
4	A	58	
4	D	58	
4	F	58	
4	I	58	
4	K	58	
4	O	58	
4	Q	58	
4	S	58	
4	U	58	
4	W	58	
4	a	58	
4	b1	58	
4	b9	58	
4	d	58	
4	f	58	
4	i	58	
4	k	58	

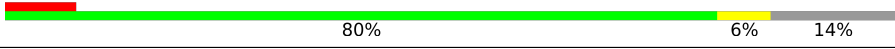
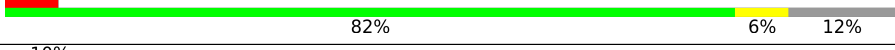
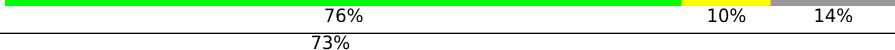
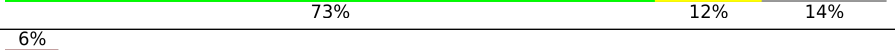
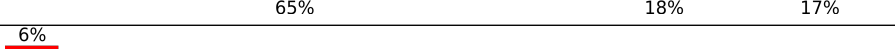
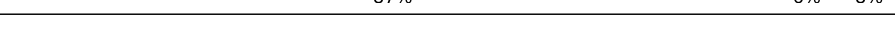
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Mol	Chain	Length	Quality of chain
4	o	58	
4	q	58	
4	s	58	
4	u	58	
4	w	58	
5	0	49	
5	2	49	
5	4	49	
5	8	49	
5	B	49	
5	C	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	V	49	
5	Z	49	
5	b	49	
5	b0	49	
5	b8	49	
5	c	49	
5	e	49	

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Mol	Chain	Length	Quality of chain
5	g	49	
5	j	49	
5	n	49	
5	p	49	
5	r	49	
5	t	49	
5	v	49	
5	z	49	
6	X	82	
6	x	82	
7	Y	53	
7	y	53	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 44980 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		
1	l	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	307	Total	C	N	O	S	0	0
			2445	1630	400	404	11		
2	m	307	Total	C	N	O	S	0	0
			2445	1630	400	404	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	260	Total	C	N	O	S	0	0
			1973	1264	335	363	11		
3	h	260	Total	C	N	O	S	0	0
			1973	1264	335	363	11		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	D	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	F	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	I	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	O	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	Q	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	S	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	U	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	W	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	3	52	Total	C	N	O	S	0	0
			437	299	70	66	2		
4	1	47	Total	C	N	O	S	0	0
			392	266	64	60	2		
4	7	48	Total	C	N	O	S	0	0
			403	277	62	61	3		
4	9	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	a	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	d	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	f	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	i	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	k	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	o	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	q	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	s	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	u	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	w	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	5	52	Total	C	N	O	S	0	0
			437	299	70	66	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	b1	47	Total	C	N	O	S	0	0
			392	266	64	60	2		
4	6	48	Total	C	N	O	S	0	0
			403	277	62	61	3		
4	b9	55	Total	C	N	O	S	0	0
			460	313	74	70	3		

- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	E	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	G	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	J	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	N	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	P	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	R	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	T	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	V	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	C	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	Z	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	2	38	Total	C	N	O	S	0	0
			309	206	50	52	1		
5	8	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	0	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	b	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	e	43	Total	C	N	O	S	0	0
			352	236	55	60	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	j	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	n	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	p	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	r	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	t	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	v	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	c	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	z	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	4	38	Total	C	N	O	S	0	0
			309	206	50	52	1		
5	b8	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	b0	44	Total	C	N	O	S	0	0
			360	240	56	63	1		

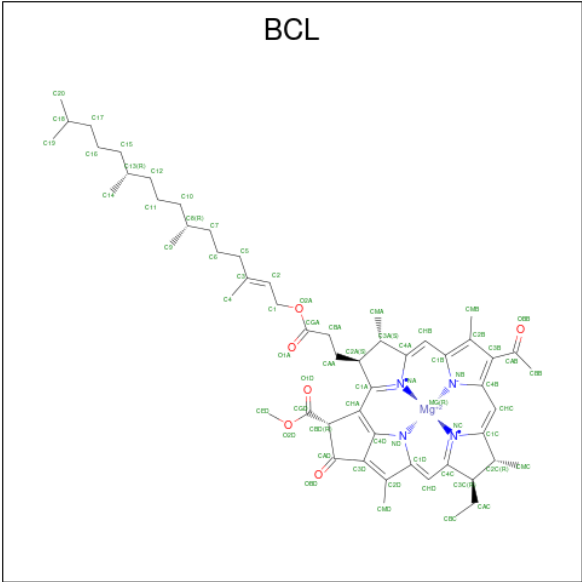
- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	68	Total	C	N	O	S	0	0
			529	345	93	88	3		
6	x	68	Total	C	N	O	S	0	0
			529	345	93	88	3		

- Molecule 7 is a protein called Rsp_7571 Protein-Y PufY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	49	Total	C	N	O	S	0	0
			361	248	55	55	3		
7	y	49	Total	C	N	O	S	0	0
			361	248	55	55	3		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 63	C 52	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	C	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
8	Z	1	Total 56	C 45	Mg 1	N 4	O 6	0
8	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
8	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
8	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	0	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	l	1	Total 63	C 52	Mg 1	N 4	O 6	0
8	m	1	Total 66	C 55	Mg 1	N 4	O 6	0

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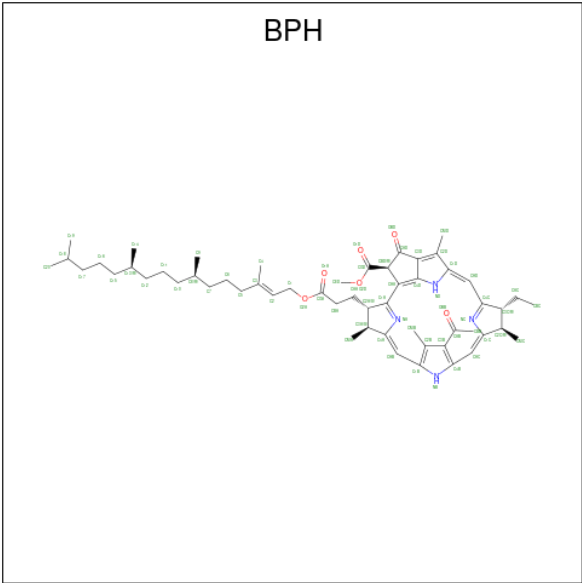
Mol	Chain	Residues	Atoms					AltConf
8	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	t	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	u	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	w	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	c	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
8	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
8	z	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	b1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	b9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	b0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



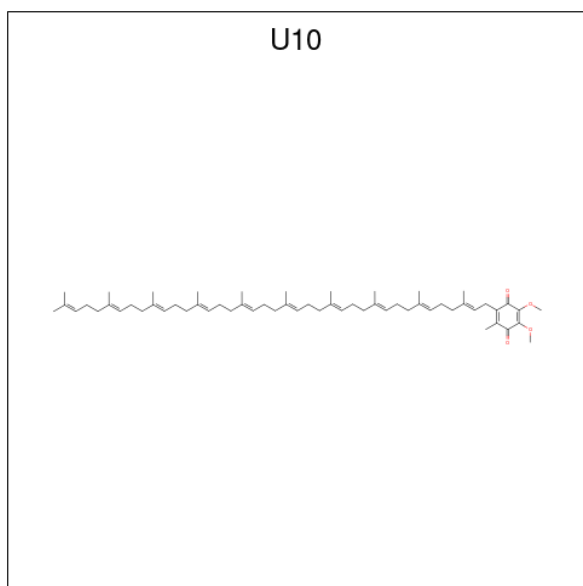
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			55	45	4	6	
9	l	1	Total	C	N	O	0
			65	55	4	6	

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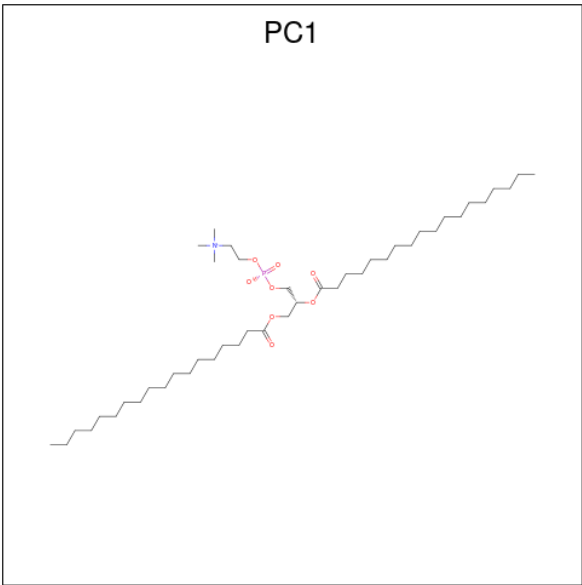
Mol	Chain	Residues	Atoms				AltConf
9	m	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 10 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	O		0
			38	34	4		
10	L	1	Total	C	O		0
			43	39	4		
10	M	1	Total	C	O		0
			48	44	4		
10	l	1	Total	C	O		0
			38	34	4		
10	l	1	Total	C	O		0
			43	39	4		
10	m	1	Total	C	O		0
			48	44	4		

- Molecule 11 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
11	H	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
11	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
11	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
11	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
11	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	l	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
11	h	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	h	1	Total	C	N	O	P	0
			34	24	1	8	1	
11	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
11	a	1	Total	C	N	O	P	0
			31	21	1	8	1	

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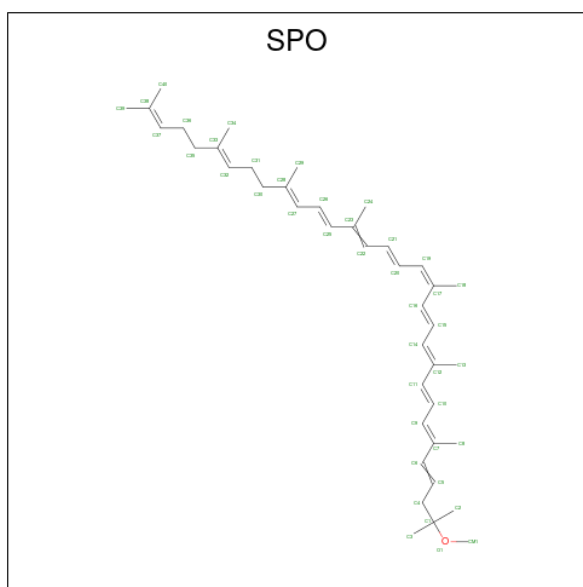
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Mol	Chain	Residues	Atoms					AltConf
11	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
11	d	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 12 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 13 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			42	41	1	
13	A	1	Total	C	O	0
			42	41	1	
13	B	1	Total	C	O	0
			42	41	1	
13	D	1	Total	C	O	0
			42	41	1	
13	E	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
13	E	1	Total	C	O	0
			42	41	1	
13	G	1	Total	C	O	0
			42	41	1	
13	G	1	Total	C	O	0
			42	41	1	
13	I	1	Total	C	O	0
			42	41	1	
13	J	1	Total	C	O	0
			42	41	1	
13	N	1	Total	C	O	0
			42	41	1	
13	O	1	Total	C	O	0
			42	41	1	
13	P	1	Total	C	O	0
			42	41	1	
13	Q	1	Total	C	O	0
			42	41	1	
13	Q	1	Total	C	O	0
			42	41	1	
13	Q	1	Total	C	O	0
			42	41	1	
13	S	1	Total	C	O	0
			42	41	1	
13	S	1	Total	C	O	0
			42	41	1	
13	U	1	Total	C	O	0
			42	41	1	
13	U	1	Total	C	O	0
			42	41	1	
13	C	1	Total	C	O	0
			42	41	1	
13	3	1	Total	C	O	0
			42	41	1	
13	3	1	Total	C	O	0
			42	41	1	
13	9	1	Total	C	O	0
			42	41	1	
13	0	1	Total	C	O	0
			42	41	1	
13	X	1	Total	C	O	0
			42	41	1	

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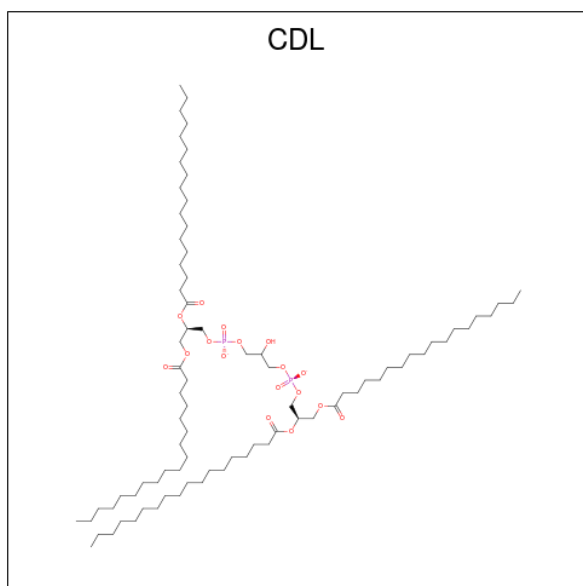
Mol	Chain	Residues	Atoms			AltConf
13	m	1	Total	C	O	0
			42	41	1	
13	a	1	Total	C	O	0
			42	41	1	
13	b	1	Total	C	O	0
			42	41	1	
13	d	1	Total	C	O	0
			42	41	1	
13	e	1	Total	C	O	0
			42	41	1	
13	e	1	Total	C	O	0
			42	41	1	
13	g	1	Total	C	O	0
			42	41	1	
13	g	1	Total	C	O	0
			42	41	1	
13	i	1	Total	C	O	0
			42	41	1	
13	j	1	Total	C	O	0
			42	41	1	
13	n	1	Total	C	O	0
			42	41	1	
13	o	1	Total	C	O	0
			42	41	1	
13	p	1	Total	C	O	0
			42	41	1	
13	q	1	Total	C	O	0
			42	41	1	
13	q	1	Total	C	O	0
			42	41	1	
13	q	1	Total	C	O	0
			42	41	1	
13	s	1	Total	C	O	0
			42	41	1	
13	s	1	Total	C	O	0
			42	41	1	
13	u	1	Total	C	O	0
			42	41	1	
13	u	1	Total	C	O	0
			42	41	1	
13	c	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
13	5	1	Total	C	O	0
			42	41	1	
13	5	1	Total	C	O	0
			42	41	1	
13	b9	1	Total	C	O	0
			42	41	1	
13	b0	1	Total	C	O	0
			42	41	1	
13	x	1	Total	C	O	0
			42	41	1	

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

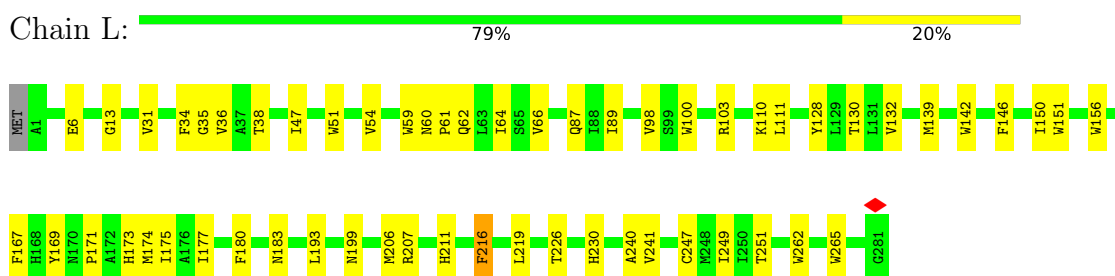


Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	O	P	0
			82	63	17	2	
14	F	1	Total	C	O	P	0
			63	44	17	2	
14	m	1	Total	C	O	P	0
			82	63	17	2	
14	f	1	Total	C	O	P	0
			63	44	17	2	

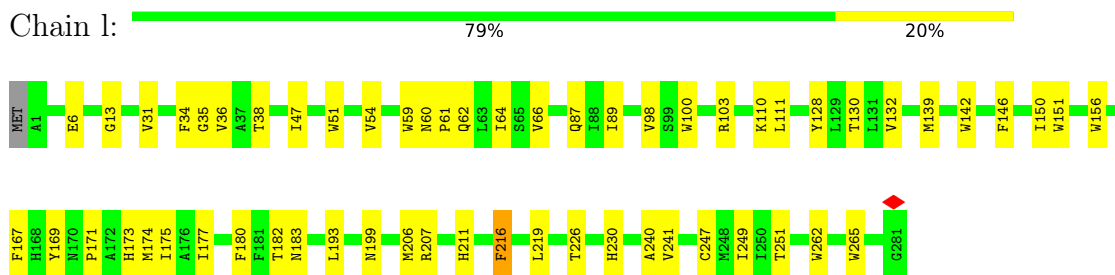
3 Residue-property plots

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

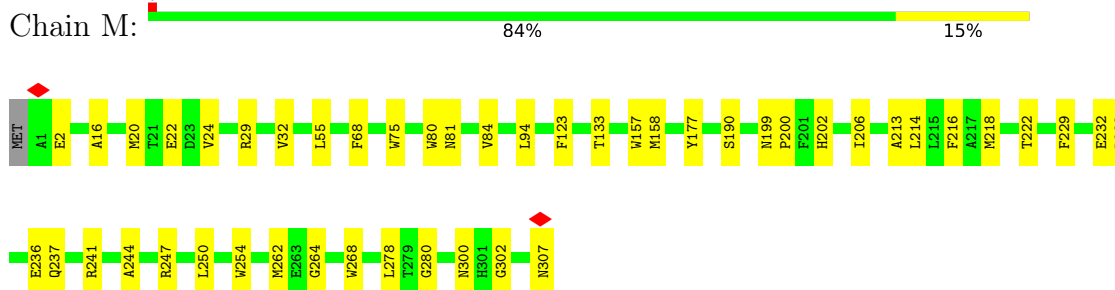
- Molecule 1: Reaction center protein L chain



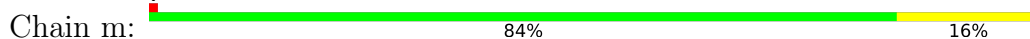
- Molecule 1: Reaction center protein L chain

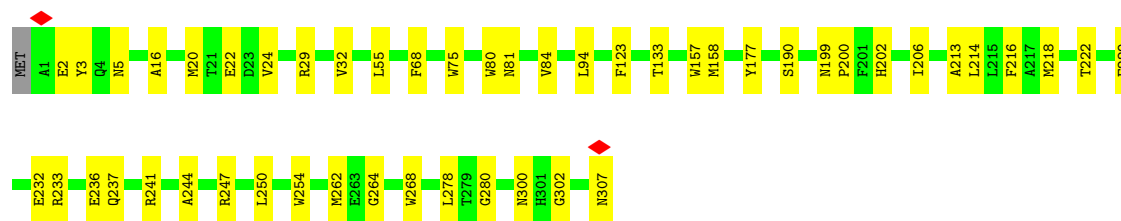


- Molecule 2: Reaction center protein M chain

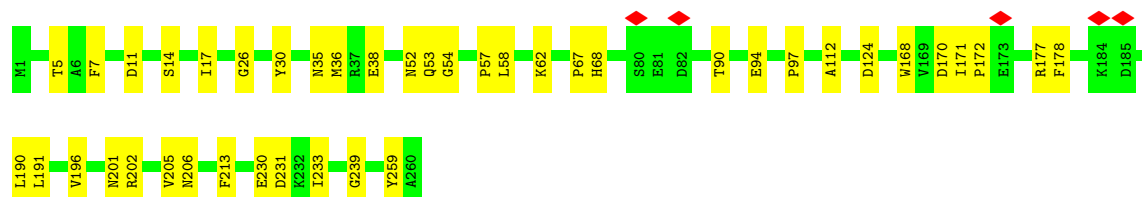
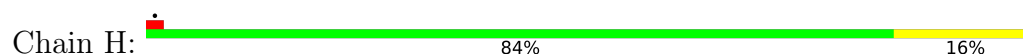


- Molecule 2: Reaction center protein M chain

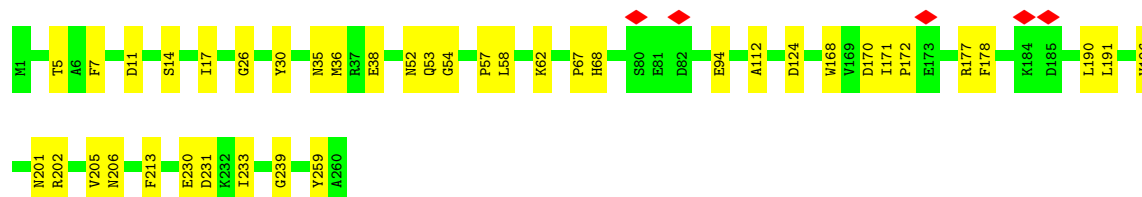
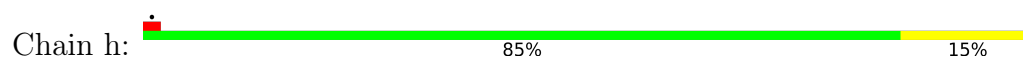




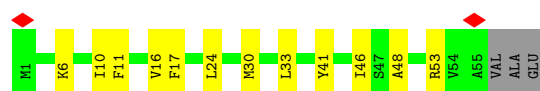
• Molecule 3: Reaction center protein H chain



• Molecule 3: Reaction center protein H chain



• Molecule 4: Light-harvesting protein B-875 alpha chain



• Molecule 4: Light-harvesting protein B-875 alpha chain

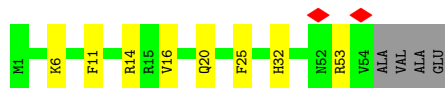
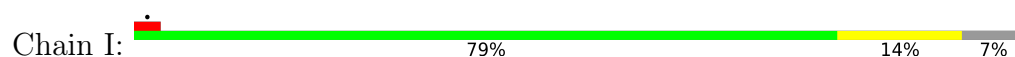


• Molecule 4: Light-harvesting protein B-875 alpha chain

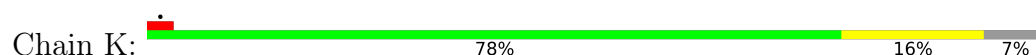




- Molecule 4: Light-harvesting protein B-875 alpha chain



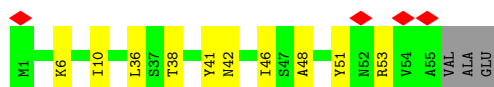
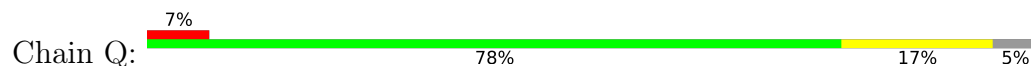
- Molecule 4: Light-harvesting protein B-875 alpha chain



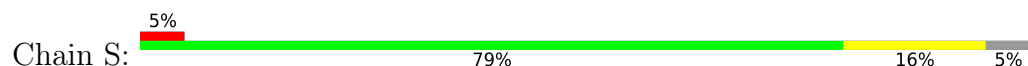
- Molecule 4: Light-harvesting protein B-875 alpha chain



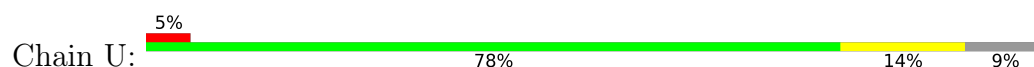
- Molecule 4: Light-harvesting protein B-875 alpha chain



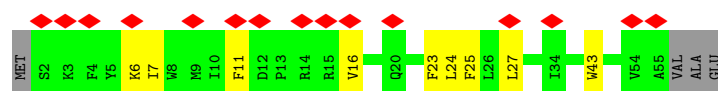
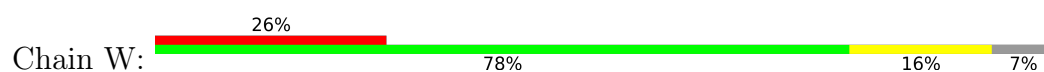
- Molecule 4: Light-harvesting protein B-875 alpha chain



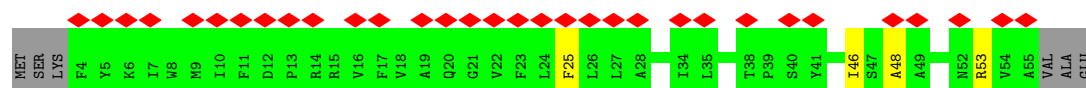
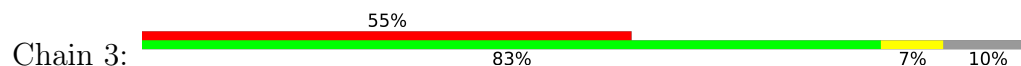
- Molecule 4: Light-harvesting protein B-875 alpha chain



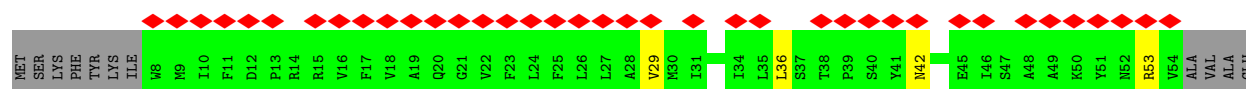
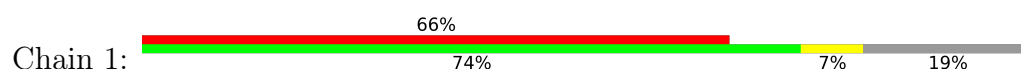
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



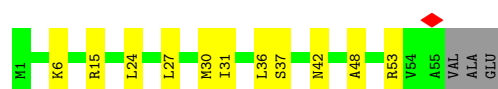
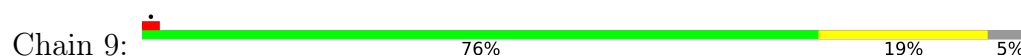
- Molecule 4: Light-harvesting protein B-875 alpha chain



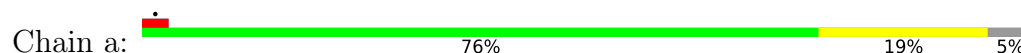
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



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- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain f:  71% 24% 5%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain i:  81% 12% 7%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain k:  78% 16% 7%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain o:  74% 17% 7%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain q:  78% 17% 5%



- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain s:  79% 16% 5%

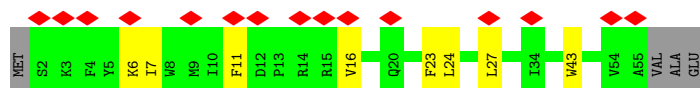
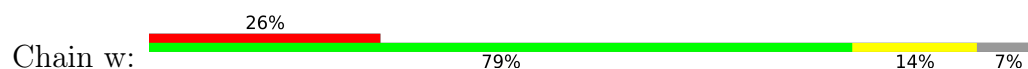


- Molecule 4: Light-harvesting protein B-875 alpha chain

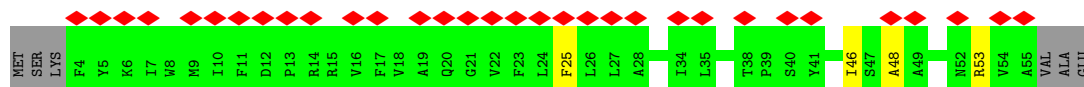
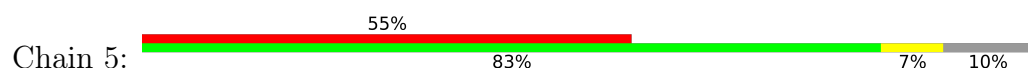
Chain u:  79% 12% 9%



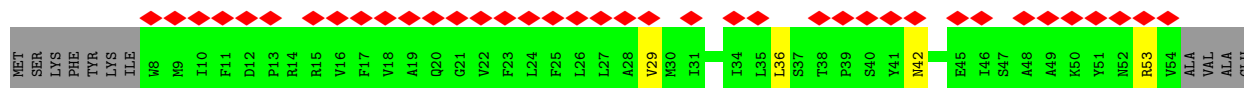
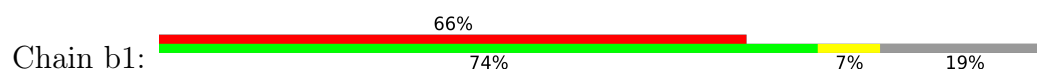
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



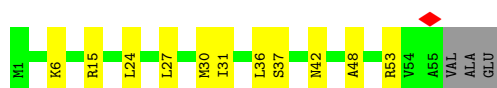
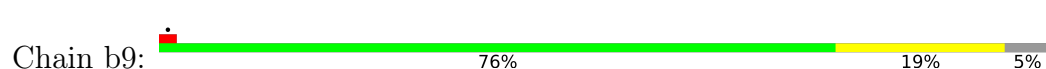
- Molecule 4: Light-harvesting protein B-875 alpha chain



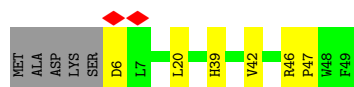
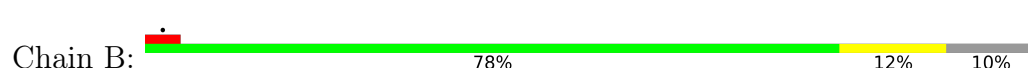
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 5: Light-harvesting protein B-875 beta chain



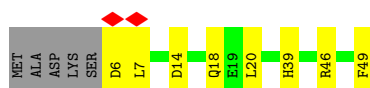
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain E:  82% 6% 12%



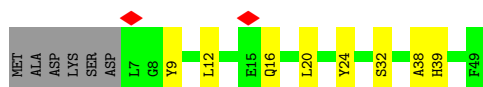
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain G:  73% 16% 10%



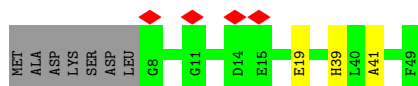
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain J:  71% 16% 12%



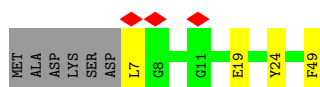
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain N:  80% 6% 14%



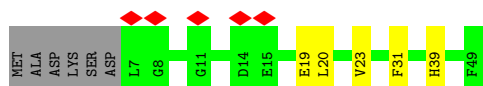
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain P:  80% 8% 12%



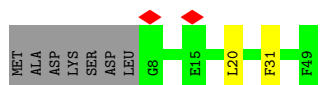
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain R:  78% 10% 12%

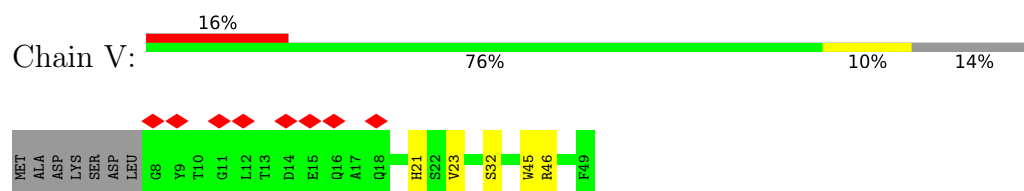


- Molecule 5: Light-harvesting protein B-875 beta chain

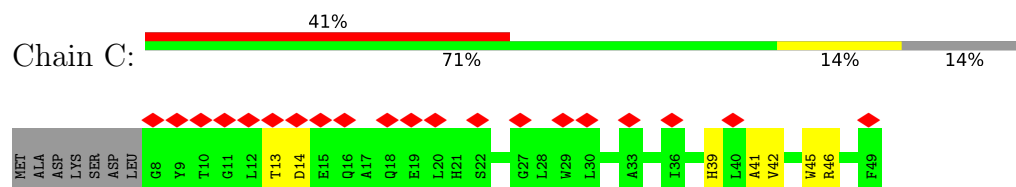
Chain T:  82% 14%



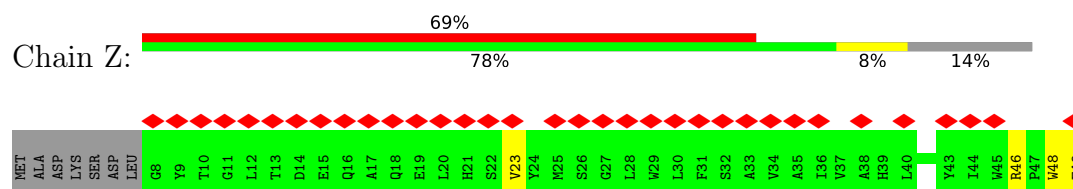
- Molecule 5: Light-harvesting protein B-875 beta chain



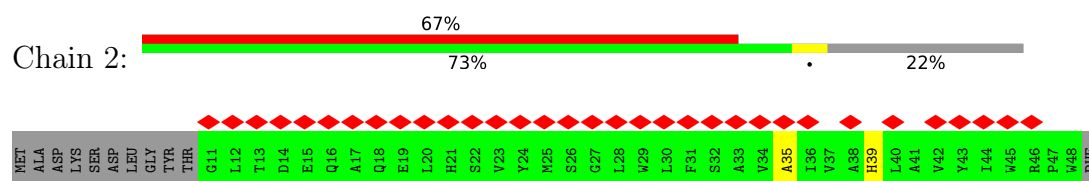
- Molecule 5: Light-harvesting protein B-875 beta chain



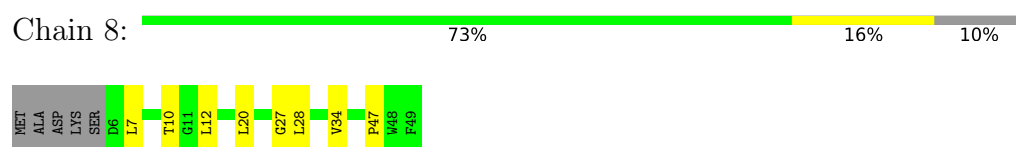
- Molecule 5: Light-harvesting protein B-875 beta chain



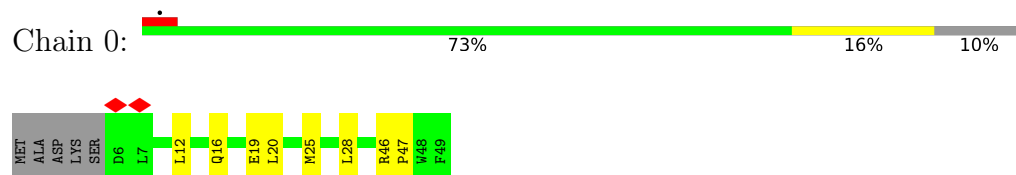
- Molecule 5: Light-harvesting protein B-875 beta chain



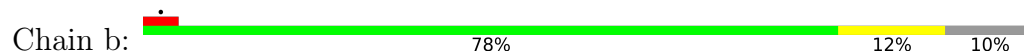
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain

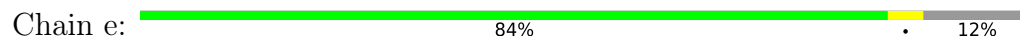


- Molecule 5: Light-harvesting protein B-875 beta chain

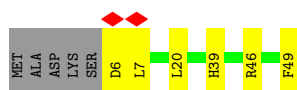
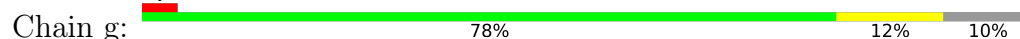




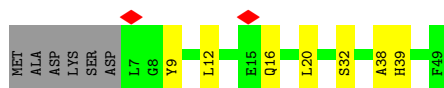
- Molecule 5: Light-harvesting protein B-875 beta chain



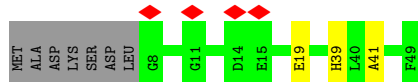
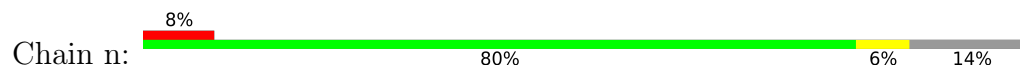
- Molecule 5: Light-harvesting protein B-875 beta chain



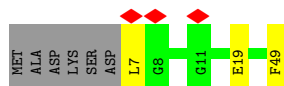
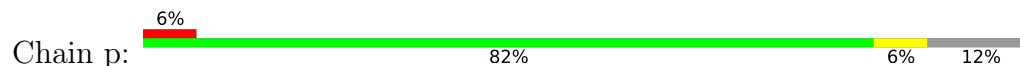
- Molecule 5: Light-harvesting protein B-875 beta chain



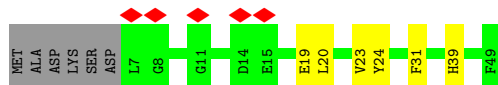
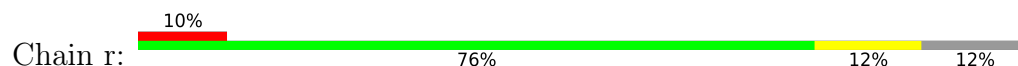
- Molecule 5: Light-harvesting protein B-875 beta chain



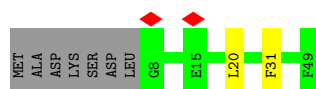
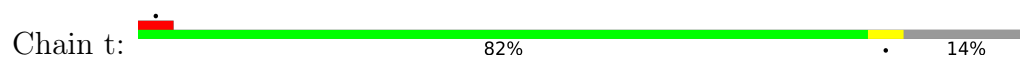
- Molecule 5: Light-harvesting protein B-875 beta chain



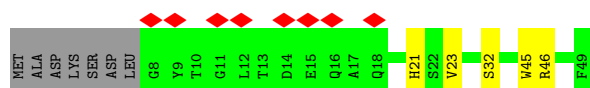
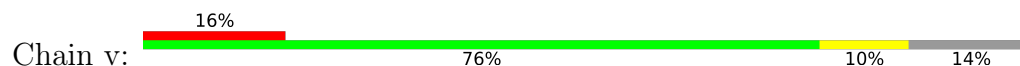
- Molecule 5: Light-harvesting protein B-875 beta chain



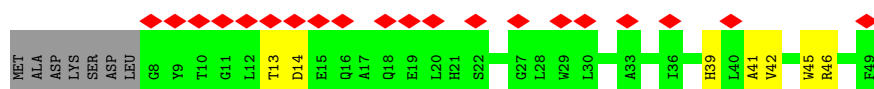
- Molecule 5: Light-harvesting protein B-875 beta chain



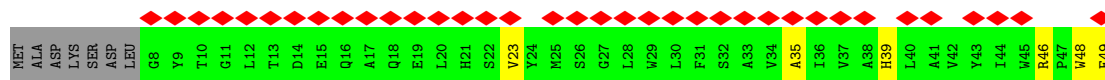
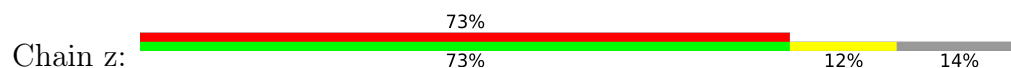
- Molecule 5: Light-harvesting protein B-875 beta chain



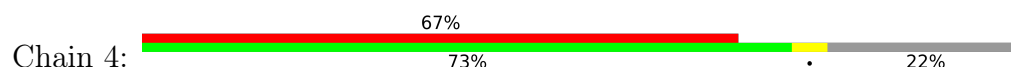
- Molecule 5: Light-harvesting protein B-875 beta chain



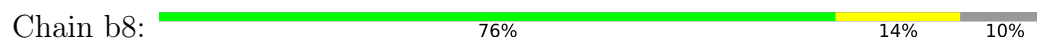
- Molecule 5: Light-harvesting protein B-875 beta chain



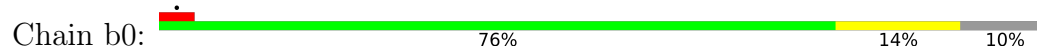
- Molecule 5: Light-harvesting protein B-875 beta chain



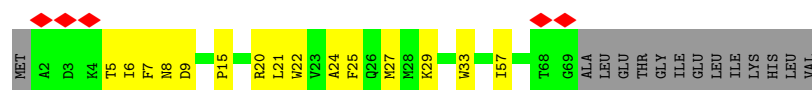
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain



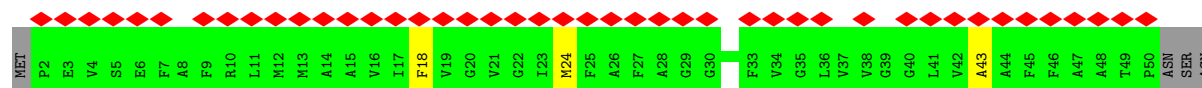
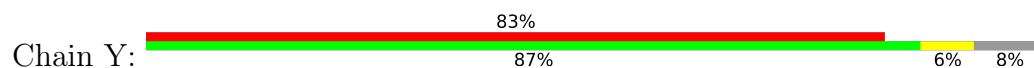
• Molecule 6: Intrinsic membrane protein PufX



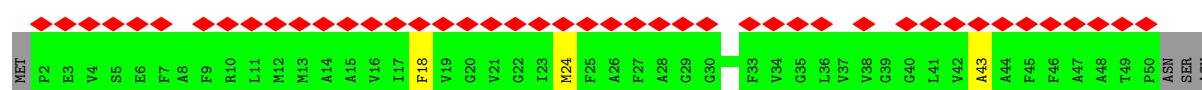
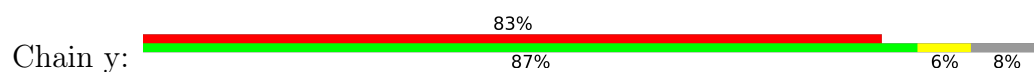
• Molecule 6: Intrinsic membrane protein PufX



• Molecule 7: Rsp_7571 Protein-Y PufY



• Molecule 7: Rsp_7571 Protein-Y PufY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	145392	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	432.63998, 432.63998, 432.63998	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, SPO, BPH, CDL, U10, FE2, PC1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.28	0/2320	0.31	0/3175
1	l	0.28	0/2320	0.31	0/3175
2	M	0.30	0/2538	0.31	0/3464
2	m	0.30	0/2538	0.31	0/3464
3	H	0.16	0/2024	0.25	0/2752
3	h	0.16	0/2024	0.25	0/2752
4	1	0.08	0/404	0.20	0/550
4	3	0.10	0/451	0.21	0/613
4	5	0.10	0/451	0.21	0/613
4	6	0.25	0/416	0.28	0/564
4	7	0.25	0/416	0.28	0/564
4	9	0.25	0/474	0.28	0/642
4	A	0.25	0/474	0.27	0/642
4	D	0.25	0/474	0.28	0/642
4	F	0.23	0/474	0.27	0/642
4	I	0.21	0/469	0.27	0/635
4	K	0.20	0/466	0.25	0/632
4	O	0.20	0/469	0.25	0/635
4	Q	0.20	0/474	0.24	0/642
4	S	0.21	0/474	0.26	0/642
4	U	0.14	0/461	0.24	0/625
4	W	0.13	0/466	0.24	0/632
4	a	0.25	0/474	0.27	0/642
4	b1	0.08	0/404	0.20	0/550
4	b9	0.25	0/474	0.28	0/642
4	d	0.25	0/474	0.28	0/642
4	f	0.23	0/474	0.27	0/642
4	i	0.21	0/469	0.27	0/635
4	k	0.20	0/466	0.25	0/632
4	o	0.20	0/469	0.25	0/635
4	q	0.20	0/474	0.24	0/642
4	s	0.21	0/474	0.26	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	u	0.14	0/461	0.23	0/625
4	w	0.13	0/466	0.24	0/632
5	0	0.24	0/373	0.24	0/510
5	2	0.09	0/320	0.16	0/439
5	4	0.09	0/320	0.16	0/439
5	8	0.23	0/373	0.23	0/510
5	B	0.23	0/373	0.23	0/510
5	C	0.12	0/357	0.19	0/488
5	E	0.23	0/365	0.27	0/499
5	G	0.21	0/373	0.23	0/510
5	J	0.17	0/365	0.23	0/499
5	N	0.19	0/357	0.22	0/488
5	P	0.26	0/365	0.22	0/499
5	R	0.18	0/365	0.21	0/499
5	T	0.17	0/357	0.23	0/488
5	V	0.16	0/357	0.21	0/488
5	Z	0.13	0/357	0.18	0/488
5	b	0.23	0/373	0.23	0/510
5	b0	0.24	0/373	0.24	0/510
5	b8	0.23	0/373	0.23	0/510
5	c	0.12	0/357	0.19	0/488
5	e	0.23	0/365	0.27	0/499
5	g	0.21	0/373	0.23	0/510
5	j	0.17	0/365	0.23	0/499
5	n	0.19	0/357	0.22	0/488
5	p	0.26	0/365	0.22	0/499
5	r	0.18	0/365	0.21	0/499
5	t	0.17	0/357	0.23	0/488
5	v	0.16	0/357	0.21	0/488
5	z	0.13	0/357	0.18	0/488
6	X	0.18	0/543	0.25	0/736
6	x	0.18	0/543	0.25	0/736
7	Y	0.10	0/373	0.18	0/505
7	y	0.10	0/373	0.18	0/505
All	All	0.22	0/38602	0.26	0/52570

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	41	0
1	l	2232	0	2187	43	0
2	M	2445	0	2359	38	0
2	m	2445	0	2359	38	0
3	H	1973	0	1981	35	0
3	h	1973	0	1981	34	0
4	1	392	0	405	5	0
4	3	437	0	452	3	0
4	5	437	0	452	3	0
4	6	403	0	422	10	0
4	7	403	0	422	10	0
4	9	460	0	482	9	0
4	A	460	0	482	11	0
4	D	460	0	482	16	0
4	F	460	0	482	12	0
4	I	455	0	477	8	0
4	K	452	0	470	7	0
4	O	455	0	477	11	0
4	Q	460	0	482	7	0
4	S	460	0	482	9	0
4	U	447	0	465	6	0
4	W	452	0	470	11	0
4	a	460	0	482	9	0
4	b1	392	0	405	5	0
4	b9	460	0	482	9	0
4	d	460	0	482	16	0
4	f	460	0	482	12	0
4	i	455	0	477	7	0
4	k	452	0	470	7	0
4	o	455	0	477	11	0
4	q	460	0	482	7	0
4	s	460	0	482	9	0
4	u	447	0	465	5	0
4	w	452	0	470	10	0
5	0	360	0	340	10	0
5	2	309	0	297	1	0
5	4	309	0	297	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	8	360	0	340	11	0
5	B	360	0	340	6	0
5	C	344	0	325	7	0
5	E	352	0	336	4	0
5	G	360	0	340	10	0
5	J	352	0	336	9	0
5	N	344	0	325	3	0
5	P	352	0	336	5	0
5	R	352	0	336	5	0
5	T	344	0	325	3	0
5	V	344	0	325	5	0
5	Z	344	0	325	4	0
5	b	360	0	340	6	0
5	b0	360	0	340	9	0
5	b8	360	0	340	10	0
5	c	344	0	325	7	0
5	e	352	0	336	2	0
5	g	360	0	340	9	0
5	j	352	0	336	8	0
5	n	344	0	325	3	0
5	p	352	0	336	4	0
5	r	352	0	336	6	0
5	t	344	0	325	3	0
5	v	344	0	325	5	0
5	z	344	0	325	5	0
6	X	529	0	533	17	0
6	x	529	0	533	17	0
7	Y	361	0	360	2	0
7	y	361	0	360	2	0
8	0	61	0	61	4	0
8	1	46	0	35	1	0
8	2	46	0	35	0	0
8	3	51	0	41	3	0
8	4	46	0	35	0	0
8	5	51	0	41	3	0
8	6	122	0	122	7	0
8	7	122	0	122	7	0
8	9	66	0	74	3	0
8	A	66	0	74	4	0
8	B	66	0	74	2	0
8	C	61	0	61	3	0
8	D	66	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	66	0	74	3	0
8	F	66	0	74	4	0
8	G	66	0	74	4	0
8	I	66	0	74	2	0
8	J	66	0	74	4	0
8	K	66	0	74	2	0
8	L	129	0	139	1	0
8	M	132	0	148	3	0
8	N	66	0	74	4	0
8	O	66	0	74	4	0
8	P	66	0	74	2	0
8	Q	66	0	74	2	0
8	R	66	0	74	3	0
8	S	66	0	74	3	0
8	T	66	0	74	1	0
8	U	66	0	74	1	0
8	V	66	0	74	6	0
8	W	66	0	74	10	0
8	Z	56	0	51	2	0
8	a	66	0	74	4	0
8	b	66	0	74	2	0
8	b0	61	0	61	3	0
8	b1	46	0	35	1	0
8	b9	66	0	74	3	0
8	c	61	0	61	3	0
8	d	66	0	74	3	0
8	e	66	0	74	3	0
8	f	66	0	74	4	0
8	g	66	0	74	3	0
8	i	66	0	74	2	0
8	j	66	0	74	4	0
8	k	66	0	74	1	0
8	l	129	0	139	1	0
8	m	132	0	148	5	0
8	n	66	0	74	6	0
8	o	66	0	74	4	0
8	p	66	0	74	1	0
8	q	66	0	74	3	0
8	r	66	0	74	3	0
8	s	66	0	74	2	0
8	t	66	0	74	1	0
8	u	66	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	v	66	0	74	7	0
8	w	66	0	74	10	0
8	z	56	0	51	2	0
9	L	65	0	76	2	0
9	M	55	0	53	2	0
9	l	65	0	76	3	0
9	m	55	0	53	3	0
10	L	81	0	102	3	0
10	M	48	0	63	1	0
10	l	81	0	102	4	0
10	m	48	0	63	2	0
11	A	114	0	150	14	0
11	D	39	0	52	4	0
11	H	77	0	102	6	0
11	L	79	0	106	7	0
11	a	114	0	150	12	0
11	d	39	0	52	3	0
11	h	77	0	102	8	0
11	l	79	0	106	7	0
12	M	1	0	0	0	0
12	m	1	0	0	0	0
13	0	42	0	60	2	0
13	3	84	0	120	8	0
13	5	84	0	120	9	0
13	9	42	0	60	6	0
13	A	42	0	60	5	0
13	B	42	0	60	3	0
13	C	42	0	60	6	0
13	D	42	0	60	2	0
13	E	84	0	120	5	0
13	G	84	0	120	9	0
13	I	42	0	60	2	0
13	J	42	0	60	1	0
13	M	42	0	60	3	0
13	N	42	0	60	1	0
13	O	42	0	60	1	0
13	P	42	0	60	2	0
13	Q	126	0	180	12	0
13	S	84	0	120	7	0
13	U	84	0	120	3	0
13	X	42	0	60	9	0
13	a	42	0	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	b	42	0	60	2	0
13	b0	42	0	60	1	0
13	b9	42	0	60	6	0
13	c	42	0	60	5	0
13	d	42	0	60	2	0
13	e	84	0	120	5	0
13	g	84	0	120	8	0
13	i	42	0	60	1	0
13	j	42	0	60	2	0
13	m	42	0	60	4	0
13	n	42	0	60	1	0
13	o	42	0	60	1	0
13	p	42	0	60	2	0
13	q	126	0	180	11	0
13	s	84	0	120	6	0
13	u	84	0	120	3	0
13	x	42	0	60	8	0
14	F	63	0	70	5	0
14	M	82	0	111	4	0
14	f	63	0	70	5	0
14	m	82	0	111	4	0
All	All	44980	0	46388	714	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.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:46:ILE:HG13	5:Z:46:ARG:HH12	1.46	0.80
6:x:20:ARG:HG2	13:x:101:SPO:H311	1.63	0.80
4:5:46:ILE:HG13	5:z:46:ARG:HH12	1.46	0.80
6:X:20:ARG:HG2	13:X:101:SPO:H311	1.63	0.78
4:F:3:LYS:HD2	4:F:6:LYS:HE2	1.70	0.74
3:H:54:GLY:O	4:D:15:ARG:NH1	2.21	0.73
3:h:52:ASN:HD22	11:a:104:PC1:H152	1.54	0.73
4:f:3:LYS:HD2	4:f:6:LYS:HE2	1.70	0.73
3:H:52:ASN:HD22	11:A:104:PC1:H152	1.54	0.72
3:h:54:GLY:O	4:d:15:ARG:NH1	2.21	0.72
3:h:57:PRO:HG3	11:d:101:PC1:H132	1.71	0.72
8:b9:101:BCL:H201	13:b9:102:SPO:H291	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:101:BCL:H201	13:9:102:SPO:H291	1.73	0.71
3:H:57:PRO:HG3	11:D:101:PC1:H132	1.71	0.70
4:7:6:LYS:NZ	5:0:19:GLU:OE2	2.24	0.70
4:6:6:LYS:NZ	5:b0:19:GLU:OE2	2.24	0.70
4:s:6:LYS:HD3	13:s:103:SPO:H393	1.76	0.67
4:S:6:LYS:HD3	13:S:103:SPO:H393	1.76	0.67
13:q:104:SPO:H362	5:t:20:LEU:HG	1.77	0.66
4:w:11:PHE:HB3	4:w:16:VAL:HG21	1.77	0.66
13:3:102:SPO:HM11	4:1:29:VAL:HG13	1.78	0.66
4:W:11:PHE:HB3	4:W:16:VAL:HG21	1.77	0.65
13:G:103:SPO:H351	8:I:101:BCL:H43	1.79	0.65
8:v:101:BCL:HAA1	8:v:101:BCL:H91	1.79	0.65
13:5:102:SPO:HM11	4:b1:29:VAL:HG13	1.78	0.65
13:Q:104:SPO:H362	5:T:20:LEU:HG	1.77	0.65
1:l:207:ARG:NH1	2:m:22:GLU:OE2	2.30	0.65
8:3:101:BCL:H43	13:3:103:SPO:H351	1.80	0.64
5:8:27:GLY:HA2	13:X:101:SPO:H343	1.79	0.64
2:m:75:TRP:HE1	13:m:406:SPO:HM13	1.62	0.64
4:O:20:GLN:HE21	13:O:102:SPO:H393	1.63	0.64
4:o:20:GLN:HE21	13:o:102:SPO:H393	1.63	0.64
1:L:207:ARG:NH1	2:M:22:GLU:OE2	2.30	0.64
13:g:103:SPO:H351	8:i:101:BCL:H43	1.79	0.64
5:b8:27:GLY:HA2	13:x:101:SPO:H343	1.79	0.63
8:V:101:BCL:HAA1	8:V:101:BCL:H91	1.79	0.63
2:M:75:TRP:HE1	13:M:406:SPO:HM13	1.62	0.63
13:9:102:SPO:H361	5:0:20:LEU:HD12	1.81	0.63
8:5:101:BCL:H43	13:5:103:SPO:H351	1.80	0.63
8:A:101:BCL:H201	13:A:102:SPO:H291	1.81	0.63
8:a:101:BCL:H201	13:a:102:SPO:H291	1.81	0.62
13:m:406:SPO:H391	4:o:30:MET:HG3	1.81	0.62
2:m:229:PHE:HB2	2:m:244:ALA:HB2	1.82	0.62
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.82	0.62
13:b9:102:SPO:H361	5:b0:20:LEU:HD12	1.81	0.62
4:F:24:LEU:HB2	8:F:101:BCL:H42	1.82	0.62
13:M:406:SPO:H391	4:O:30:MET:HG3	1.81	0.61
4:f:24:LEU:HB2	8:f:101:BCL:H42	1.82	0.61
4:Q:10:ILE:HD11	13:Q:104:SPO:H402	1.82	0.61
13:a:102:SPO:H393	4:b9:6:LYS:HD3	1.83	0.61
4:k:20:GLN:HG2	8:o:101:BCL:H101	1.81	0.61
4:k:11:PHE:HB3	4:k:16:VAL:HG21	1.81	0.61
13:A:102:SPO:H393	4:9:6:LYS:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:11:PHE:HB3	4:K:16:VAL:HG21	1.81	0.61
9:m:404:BPH:HBC3	9:m:404:BPH:HHD	1.83	0.61
14:F:102:CDL:H311	14:F:102:CDL:H111	1.83	0.60
3:h:54:GLY:HA2	11:a:104:PC1:H141	1.83	0.60
3:H:259:TYR:O	6:X:29:LYS:NZ	2.34	0.60
4:K:20:GLN:HG2	8:O:101:BCL:H101	1.81	0.60
9:M:404:BPH:HBC3	9:M:404:BPH:HHD	1.83	0.60
3:H:54:GLY:HA2	11:A:104:PC1:H141	1.83	0.60
5:C:45:TRP:HB2	13:C:102:SPO:H10	1.83	0.60
8:w:101:BCL:H43	13:c:102:SPO:H32	1.84	0.60
5:C:13:THR:HG22	5:C:14:ASP:N	2.16	0.60
4:q:10:ILE:HD11	13:q:104:SPO:H402	1.82	0.60
8:W:101:BCL:H43	13:C:102:SPO:H32	1.84	0.60
5:c:45:TRP:HB2	13:c:102:SPO:H10	1.83	0.60
14:f:102:CDL:H311	14:f:102:CDL:H111	1.83	0.60
5:c:13:THR:HG22	5:c:14:ASP:N	2.16	0.59
2:M:2:GLU:OE2	3:H:206:ASN:ND2	2.36	0.59
2:m:268:TRP:NE1	3:h:35:ASN:OD1	2.27	0.59
3:h:259:TYR:O	6:x:29:LYS:NZ	2.34	0.59
4:1:29:VAL:HG11	7:Y:24:MET:HE3	1.85	0.58
4:k:6:LYS:NZ	5:p:19:GLU:OE2	2.37	0.58
4:K:6:LYS:NZ	5:P:19:GLU:OE2	2.37	0.58
2:m:2:GLU:OE2	3:h:206:ASN:ND2	2.36	0.58
4:U:11:PHE:HB3	4:U:16:VAL:HG21	1.85	0.58
5:2:35:ALA:O	5:2:39:HIS:ND1	2.30	0.58
1:l:130:THR:HG23	1:l:249:ILE:HD13	1.86	0.58
4:u:11:PHE:HB3	4:u:16:VAL:HG21	1.85	0.57
1:L:130:THR:HG23	1:L:249:ILE:HD13	1.86	0.57
11:l:307:PC1:H261	4:a:30:MET:HG3	1.86	0.57
4:b1:29:VAL:HG11	7:y:24:MET:HE3	1.85	0.57
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.86	0.57
13:Q:104:SPO:H403	5:T:20:LEU:HD12	1.86	0.57
13:q:104:SPO:H403	5:t:20:LEU:HD12	1.86	0.57
11:L:307:PC1:H261	4:A:30:MET:HG3	1.86	0.57
6:X:7:PHE:HE1	5:b8:12:LEU:HD21	1.70	0.57
2:m:237:GLN:HB2	2:m:262:MET:HG2	1.86	0.57
13:c:102:SPO:H182	13:c:102:SPO:H14	1.87	0.57
13:b9:102:SPO:H361	5:b0:20:LEU:CD1	2.35	0.56
2:m:241:ARG:NH1	3:h:38:GLU:OE1	2.39	0.56
1:l:150:ILE:HD11	11:h:301:PC1:H2B2	1.88	0.56
5:z:46:ARG:HH21	4:b1:53:ARG:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.41	0.56
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.39	0.56
13:9:102:SPO:H361	5:0:20:LEU:CD1	2.35	0.56
1:l:169:TYR:HA	1:l:174:MET:HE3	1.88	0.56
1:L:150:ILE:HD11	11:H:301:PC1:H2B2	1.88	0.56
5:P:49:PHE:O	4:Q:51:TYR:OH	2.22	0.56
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.87	0.56
4:d:6:LYS:HB3	13:g:101:SPO:H402	1.88	0.56
1:L:169:TYR:HA	1:L:174:MET:HE3	1.88	0.55
5:8:12:LEU:HD21	6:x:7:PHE:HE1	1.70	0.55
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.72	0.55
1:l:173:HIS:CE1	1:l:177:ILE:HD11	2.41	0.55
5:Z:46:ARG:HH21	4:1:53:ARG:HG3	1.70	0.55
3:h:196:VAL:HG12	3:h:205:VAL:HG22	1.87	0.55
4:D:6:LYS:HB3	13:G:101:SPO:H402	1.88	0.55
2:M:268:TRP:NE1	3:H:35:ASN:OD1	2.27	0.55
4:w:7:ILE:HB	13:5:102:SPO:H32	1.88	0.55
1:L:34:PHE:O	1:L:38:THR:OG1	2.22	0.55
13:C:102:SPO:H182	13:C:102:SPO:H14	1.87	0.55
3:H:54:GLY:HA3	11:H:302:PC1:H153	1.88	0.54
4:W:7:ILE:HB	13:3:102:SPO:H32	1.88	0.54
2:m:232:GLU:OE2	3:h:177:ARG:NH1	2.40	0.54
5:p:7:LEU:HD21	13:q:102:SPO:H391	1.88	0.54
3:h:54:GLY:HA3	11:h:302:PC1:H153	1.88	0.54
3:h:191:LEU:HD11	3:h:213:PHE:HE2	1.72	0.54
13:G:103:SPO:H351	8:I:101:BCL:C4	2.38	0.54
1:l:226:THR:O	1:l:230:HIS:ND1	2.36	0.54
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.73	0.54
5:P:7:LEU:HD21	13:Q:102:SPO:H391	1.88	0.54
4:d:11:PHE:HB3	4:d:16:VAL:HG21	1.89	0.54
4:i:32:HIS:CE1	8:j:101:BCL:HMD3	2.43	0.54
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.43	0.53
2:M:232:GLU:OE2	3:H:177:ARG:NH1	2.40	0.53
4:D:11:PHE:HB3	4:D:16:VAL:HG21	1.89	0.53
2:m:94:LEU:HB3	2:m:177:TYR:HB2	1.90	0.53
4:I:32:HIS:CE1	8:J:101:BCL:HMD3	2.43	0.53
1:l:36:VAL:HA	10:m:405:U10:H403	1.90	0.53
4:S:11:PHE:HB3	4:S:16:VAL:HG21	1.91	0.53
1:l:38:THR:HG21	1:l:100:TRP:HE3	1.73	0.53
1:L:36:VAL:HA	10:M:405:U10:H403	1.90	0.53
1:l:34:PHE:O	1:l:38:THR:OG1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:202:HIS:CE1	2:m:206:ILE:HD11	2.43	0.53
5:b:47:PRO:O	4:d:53:ARG:NH2	2.42	0.53
3:h:5:THR:HG22	3:h:11:ASP:HB3	1.91	0.53
3:h:68:HIS:NE2	3:h:124:ASP:O	2.42	0.53
3:h:201:ASN:HD21	3:h:202:ARG:HH11	1.57	0.53
13:g:103:SPO:H351	8:i:101:BCL:C4	2.38	0.53
4:w:6:LYS:HD3	13:5:102:SPO:H403	1.91	0.53
2:M:233:ARG:NE	2:M:236:GLU:OE1	2.36	0.53
4:W:6:LYS:HD3	13:3:102:SPO:H403	1.91	0.53
3:H:201:ASN:HD21	3:H:202:ARG:HH11	1.57	0.53
2:M:94:LEU:HB3	2:M:177:TYR:HB2	1.90	0.52
2:m:233:ARG:NE	2:m:236:GLU:OE1	2.36	0.52
3:H:5:THR:HG22	3:H:11:ASP:HB3	1.91	0.52
5:B:47:PRO:O	4:D:53:ARG:NH2	2.42	0.52
4:9:48:ALA:HA	4:9:53:ARG:HD2	1.92	0.52
4:b9:48:ALA:HA	4:b9:53:ARG:HD2	1.92	0.52
1:l:171:PRO:HG2	10:l:305:U10:H212	1.92	0.52
4:D:48:ALA:HB1	4:D:54:VAL:HG23	1.92	0.52
4:d:15:ARG:HD2	11:d:101:PC1:H11	1.92	0.52
5:R:39:HIS:CG	8:R:101:BCL:H91	2.45	0.52
4:q:36:LEU:O	4:q:42:ASN:ND2	2.42	0.52
4:Q:36:LEU:O	4:Q:42:ASN:ND2	2.42	0.52
4:s:11:PHE:HB3	4:s:16:VAL:HG21	1.91	0.52
5:R:31:PHE:HE2	8:R:101:BCL:HBA1	1.75	0.51
1:L:6:GLU:HA	2:M:250:LEU:HD11	1.92	0.51
4:a:11:PHE:HB3	4:a:16:VAL:HG21	1.91	0.51
5:4:35:ALA:O	5:4:39:HIS:ND1	2.30	0.51
2:M:68:PHE:HZ	4:S:30:MET:HB2	1.76	0.51
4:O:11:PHE:HB3	4:O:16:VAL:HG21	1.93	0.51
1:l:6:GLU:HA	2:m:250:LEU:HD11	1.92	0.51
5:n:39:HIS:CG	8:n:102:BCL:H91	2.46	0.51
5:r:31:PHE:HE2	8:r:101:BCL:HBA1	1.75	0.51
5:r:39:HIS:CG	8:r:101:BCL:H91	2.45	0.51
1:L:171:PRO:HG2	10:L:305:U10:H212	1.92	0.51
3:H:68:HIS:NE2	3:H:124:ASP:O	2.42	0.51
4:A:11:PHE:HB3	4:A:16:VAL:HG21	1.91	0.51
2:M:81:ASN:HB3	2:M:84:VAL:HB	1.93	0.51
2:m:233:ARG:NH2	3:h:230:GLU:OE1	2.44	0.51
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.93	0.51
2:M:233:ARG:NH2	3:H:230:GLU:OE1	2.44	0.51
2:m:68:PHE:HZ	4:s:30:MET:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:z:101:BCL:HBB3	8:b1:101:BCL:CHC	2.41	0.51
4:d:48:ALA:HB1	4:d:54:VAL:HG23	1.92	0.51
4:o:24:LEU:HB2	8:o:101:BCL:H42	1.93	0.51
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.29	0.50
1:L:226:THR:O	1:L:230:HIS:ND1	2.36	0.50
2:M:233:ARG:HH11	3:H:177:ARG:NH1	2.09	0.50
4:O:24:LEU:HB2	8:O:101:BCL:H42	1.93	0.50
4:D:15:ARG:HD2	11:D:101:PC1:H11	1.92	0.50
4:1:36:LEU:O	4:1:42:ASN:ND2	2.44	0.50
8:e:102:BCL:C2B	8:e:102:BCL:H112	2.41	0.50
5:b8:7:LEU:HD21	5:b0:16:GLN:HB3	1.93	0.50
6:X:7:PHE:CE2	6:X:9:ASP:HB3	2.47	0.50
4:o:11:PHE:HB3	4:o:16:VAL:HG21	1.93	0.50
5:N:39:HIS:CG	8:N:102:BCL:H91	2.46	0.50
8:E:102:BCL:H112	8:E:102:BCL:C2B	2.41	0.50
4:i:11:PHE:HB3	4:i:16:VAL:HG21	1.93	0.50
8:w:101:BCL:HHD	5:c:42:VAL:HG21	1.94	0.50
1:L:31:VAL:O	1:L:35:GLY:HA3	2.12	0.50
3:H:190:LEU:HB2	3:H:233:ILE:HD13	1.94	0.50
11:H:301:PC1:H261	14:F:102:CDL:H341	1.94	0.50
8:Z:101:BCL:HBB3	8:1:101:BCL:CHC	2.41	0.50
2:m:81:ASN:HB3	2:m:84:VAL:HB	1.93	0.50
2:m:16:ALA:HB1	2:m:32:VAL:HG21	1.93	0.50
5:p:49:PHE:O	4:q:51:TYR:OH	2.22	0.50
5:v:32:SER:CB	8:v:101:BCL:H2	2.42	0.50
4:b1:36:LEU:O	4:b1:42:ASN:ND2	2.44	0.50
5:B:6:ASP:OD1	5:B:6:ASP:N	2.44	0.50
3:h:190:LEU:HB2	3:h:233:ILE:HD13	1.94	0.50
1:L:62:GLN:HB3	1:L:151:TRP:CD1	2.47	0.50
1:l:175:ILE:HD11	10:l:305:U10:H13	1.94	0.50
6:x:7:PHE:CE2	6:x:9:ASP:HB3	2.47	0.50
8:W:101:BCL:HHD	5:C:42:VAL:HG21	1.94	0.49
1:l:87:GLN:HE21	1:l:142:TRP:CD1	2.29	0.49
5:G:6:ASP:OD1	5:J:16:GLN:NE2	2.42	0.49
11:A:104:PC1:H133	11:A:104:PC1:H12	1.94	0.49
5:V:32:SER:CB	8:V:101:BCL:H2	2.42	0.49
3:h:7:PHE:CZ	4:f:34:ILE:HG12	2.47	0.49
8:v:101:BCL:HMA1	8:w:101:BCL:HMA1	1.93	0.49
1:l:62:GLN:HB3	1:l:151:TRP:CD1	2.47	0.49
4:W:24:LEU:HB2	8:W:101:BCL:H42	1.95	0.49
14:m:407:CDL:H602	3:h:26:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:w:24:LEU:HB2	8:w:101:BCL:H42	1.95	0.49
5:8:7:LEU:HD21	5:0:16:GLN:HB3	1.93	0.49
2:m:233:ARG:HH11	3:h:177:ARG:NH1	2.09	0.49
11:h:301:PC1:H261	14:f:102:CDL:H341	1.94	0.49
4:o:17:PHE:CZ	13:p:101:SPO:H342	2.47	0.49
1:L:175:ILE:HD11	10:L:305:U10:H13	1.94	0.49
14:M:407:CDL:H602	3:H:26:GLY:HA3	1.95	0.49
5:G:49:PHE:HD2	8:G:102:BCL:H171	1.77	0.49
1:l:31:VAL:O	1:l:35:GLY:HA3	2.12	0.49
1:l:219:LEU:HD11	2:m:133:THR:HG22	1.95	0.49
8:l:302:BCL:H152	9:l:303:BPH:H172	1.95	0.49
2:M:218:MET:O	2:M:222:THR:OG1	2.30	0.49
8:3:101:BCL:C4	13:3:103:SPO:H351	2.42	0.49
5:c:39:HIS:ND1	8:c:101:BCL:H91	2.28	0.49
5:g:6:ASP:OD1	5:j:16:GLN:NE2	2.42	0.48
8:V:101:BCL:HMA1	8:W:101:BCL:HMA1	1.93	0.48
1:l:47:ILE:HG21	4:b9:30:MET:HE2	1.95	0.48
5:g:49:PHE:HD2	8:g:102:BCL:H171	1.77	0.48
5:j:39:HIS:CG	8:j:101:BCL:H91	2.47	0.48
4:o:32:HIS:CE1	8:o:101:BCL:NA	2.81	0.48
4:6:14:ARG:HB3	6:x:22:TRP:CZ2	2.48	0.48
8:L:302:BCL:H152	9:L:303:BPH:H172	1.95	0.48
4:O:17:PHE:CZ	13:P:101:SPO:H342	2.47	0.48
11:a:104:PC1:H133	11:a:104:PC1:H12	1.94	0.48
4:I:11:PHE:HB3	4:I:16:VAL:HG21	1.93	0.48
5:J:39:HIS:CG	8:J:101:BCL:H91	2.47	0.48
5:b:46:ARG:NH1	4:d:53:ARG:HG2	2.29	0.48
6:x:20:ARG:HG2	13:x:101:SPO:C31	2.41	0.48
3:H:7:PHE:CZ	4:F:34:ILE:HG12	2.47	0.48
4:D:10:ILE:HG23	4:F:14:ARG:HG2	1.96	0.48
4:7:14:ARG:HB3	6:X:22:TRP:CZ2	2.48	0.48
4:9:24:LEU:HB2	8:9:101:BCL:H42	1.95	0.48
2:m:218:MET:O	2:m:222:THR:OG1	2.30	0.48
13:q:104:SPO:H362	13:q:104:SPO:H341	1.49	0.48
5:B:46:ARG:NH1	4:D:53:ARG:HG2	2.29	0.48
4:b9:27:LEU:O	4:b9:31:ILE:HG13	2.14	0.48
11:A:103:PC1:O22	4:9:15:ARG:NH2	2.47	0.48
8:W:101:BCL:H2A	13:C:102:SPO:H25	1.96	0.48
5:b:6:ASP:N	5:b:6:ASP:OD1	2.44	0.48
5:C:39:HIS:ND1	8:C:101:BCL:H91	2.28	0.48
1:L:13:GLY:O	1:L:110:LYS:NZ	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:ILE:HG21	4:9:30:MET:HE2	1.95	0.48
1:L:139:MET:HA	6:X:57:ILE:HG21	1.96	0.48
4:O:32:HIS:CE1	8:O:101:BCL:NA	2.81	0.48
5:8:27:GLY:HA3	13:X:101:SPO:C27	2.44	0.48
4:o:6:LYS:HB3	13:q:102:SPO:H402	1.96	0.48
4:O:6:LYS:HB3	13:Q:102:SPO:H402	1.96	0.47
5:8:7:LEU:HD22	5:0:12:LEU:HD22	1.96	0.47
8:5:101:BCL:C4	13:5:103:SPO:H351	2.42	0.47
4:9:27:LEU:O	4:9:31:ILE:HG13	2.14	0.47
3:h:168:TRP:HB2	3:h:178:PHE:HB2	1.96	0.47
11:h:301:PC1:H122	14:f:102:CDL:OB9	2.14	0.47
5:b8:7:LEU:HD22	5:b0:12:LEU:HD22	1.96	0.47
1:L:6:GLU:OE2	2:M:254:TRP:NE1	2.36	0.47
2:M:24:VAL:HG11	2:M:29:ARG:HH21	1.80	0.47
11:H:301:PC1:H122	14:F:102:CDL:OB9	2.14	0.47
5:g:49:PHE:CG	13:g:103:SPO:H11	2.49	0.47
5:j:9:TYR:OH	4:k:12:ASP:OD1	2.30	0.47
5:b0:25:MET:SD	5:b0:28:LEU:HD23	2.55	0.47
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.96	0.47
10:l:305:U10:H271	10:l:305:U10:H251	1.40	0.47
4:b9:24:LEU:HB2	8:b9:101:BCL:H42	1.95	0.47
1:L:241:VAL:HG21	9:L:303:BPH:HBC3	1.97	0.47
5:G:49:PHE:CG	13:G:103:SPO:H11	2.49	0.47
13:3:102:SPO:H82	4:1:29:VAL:HG22	1.97	0.47
13:A:102:SPO:H362	5:B:20:LEU:HG	1.97	0.47
1:l:241:VAL:HG21	9:l:303:BPH:HBC3	1.97	0.47
13:a:102:SPO:H362	5:b:20:LEU:HG	1.97	0.47
11:a:103:PC1:O22	4:b9:15:ARG:NH2	2.47	0.47
4:d:10:ILE:HG23	4:f:14:ARG:HG2	1.96	0.47
1:L:199:ASN:OD1	3:H:62:LYS:NZ	2.47	0.47
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.95	0.47
4:O:38:THR:OG1	4:O:40:SER:O	2.23	0.47
13:P:101:SPO:H341	13:P:101:SPO:H361	1.46	0.47
4:d:43:TRP:HA	4:d:46:ILE:HD12	1.97	0.47
13:d:103:SPO:H341	13:d:103:SPO:H361	1.48	0.47
5:b8:27:GLY:HA3	13:x:101:SPO:C27	2.44	0.47
2:M:199:ASN:HB3	2:M:202:HIS:HB3	1.97	0.47
4:7:9:MET:HE3	13:9:102:SPO:H402	1.97	0.47
5:8:47:PRO:O	4:9:53:ARG:NH2	2.42	0.47
4:6:9:MET:HE3	13:b9:102:SPO:H402	1.97	0.47
8:w:101:BCL:H2A	13:c:102:SPO:H25	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:66:VAL:HG11	1:l:89:ILE:HD12	1.97	0.46
1:L:66:VAL:HG11	1:L:89:ILE:HD12	1.97	0.46
1:l:6:GLU:OE2	2:m:254:TRP:NE1	2.36	0.46
13:b:102:SPO:H361	13:b:102:SPO:H341	1.50	0.46
1:L:146:PHE:HB3	1:L:156:TRP:CD2	2.50	0.46
5:B:39:HIS:CE1	8:B:101:BCL:H91	2.50	0.46
8:B:101:BCL:H61	8:B:101:BCL:H2	1.73	0.46
1:l:139:MET:HA	6:x:57:ILE:HG21	1.96	0.46
2:m:190:SER:HB2	8:m:403:BCL:H3C	1.97	0.46
2:m:199:ASN:HB3	2:m:202:HIS:HB3	1.97	0.46
13:x:101:SPO:H362	13:x:101:SPO:H341	1.61	0.46
2:M:190:SER:HB2	8:M:403:BCL:H3C	1.97	0.46
2:m:24:VAL:HG11	2:m:29:ARG:HH21	1.80	0.46
2:M:300:ASN:OD1	2:M:307:ASN:ND2	2.49	0.46
4:D:43:TRP:HA	4:D:46:ILE:HD12	1.97	0.46
5:0:25:MET:SD	5:0:28:LEU:HD23	2.55	0.46
1:l:146:PHE:HB3	1:l:156:TRP:CD2	2.50	0.46
5:V:32:SER:HB3	8:V:101:BCL:H2	1.96	0.46
8:0:101:BCL:H62	8:0:101:BCL:H92	1.80	0.46
14:m:407:CDL:H162	14:m:407:CDL:H762	1.98	0.46
8:f:101:BCL:H201	13:g:101:SPO:H291	1.97	0.46
13:s:103:SPO:H351	5:v:23:VAL:HG11	1.98	0.46
5:v:32:SER:HB3	8:v:101:BCL:H2	1.96	0.46
13:5:102:SPO:H82	4:b1:29:VAL:HG22	1.97	0.46
6:x:24:ALA:HB2	13:x:101:SPO:H291	1.98	0.46
5:G:39:HIS:CE1	8:G:102:BCL:H91	2.51	0.46
1:l:180:PHE:CD2	1:l:240:ALA:HB1	2.51	0.46
13:j:102:SPO:H362	13:j:102:SPO:H341	1.87	0.46
13:p:101:SPO:H361	13:p:101:SPO:H341	1.46	0.46
5:g:39:HIS:CE1	8:g:102:BCL:H91	2.51	0.46
14:M:407:CDL:H162	14:M:407:CDL:H762	1.98	0.46
13:0:102:SPO:H361	13:0:102:SPO:H341	1.77	0.46
7:Y:18:PHE:HB2	7:Y:43:ALA:HB2	1.98	0.46
14:m:407:CDL:H512	3:h:30:TYR:CZ	2.51	0.46
13:e:103:SPO:H392	4:f:20:GLN:NE2	2.31	0.46
11:L:306:PC1:H111	11:L:306:PC1:H142	1.68	0.46
14:M:407:CDL:H512	3:H:30:TYR:CZ	2.51	0.46
3:H:36:MET:HE2	3:H:58:LEU:HD23	1.98	0.46
5:C:13:THR:CG2	5:C:14:ASP:N	2.78	0.46
3:h:14:SER:HA	3:h:17:ILE:HG22	1.98	0.46
4:d:51:TYR:HB2	4:d:53:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:102:SPO:H341	13:3:102:SPO:H362	1.47	0.45
4:7:13:PRO:HB3	5:8:20:LEU:HD21	1.99	0.45
7:y:18:PHE:HB2	7:y:43:ALA:HB2	1.98	0.45
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.51	0.45
8:V:101:BCL:H111	8:V:101:BCL:H72	1.86	0.45
11:l:306:PC1:H142	11:l:306:PC1:H111	1.68	0.45
5:b:39:HIS:CE1	8:b:101:BCL:H91	2.50	0.45
4:q:38:THR:HG21	4:s:44:LEU:HD13	1.98	0.45
8:b0:101:BCL:H62	8:b0:101:BCL:H2	1.75	0.45
8:0:101:BCL:H62	8:0:101:BCL:H2	1.75	0.45
3:h:36:MET:HE2	3:h:58:LEU:HD23	1.98	0.45
8:7:101:BCL:H61	8:7:101:BCL:H41	1.75	0.45
6:X:24:ALA:HB2	13:X:101:SPO:H291	1.98	0.45
3:H:14:SER:HA	3:H:17:ILE:HG22	1.98	0.45
4:U:24:LEU:HB2	8:U:101:BCL:H42	1.99	0.45
2:m:300:ASN:OD1	2:m:307:ASN:ND2	2.49	0.45
4:f:48:ALA:HA	4:f:53:ARG:HD3	1.99	0.45
8:n:102:BCL:H61	8:n:102:BCL:H2	1.82	0.45
4:A:10:ILE:HD11	13:E:101:SPO:H403	1.99	0.45
13:E:103:SPO:H392	4:F:20:GLN:NE2	2.31	0.45
5:T:31:PHE:HE2	8:T:101:BCL:HBA1	1.82	0.45
1:l:167:PHE:HE1	1:l:251:THR:HG21	1.82	0.45
13:m:406:SPO:H361	13:m:406:SPO:H341	1.72	0.45
4:u:24:LEU:HB2	8:u:101:BCL:H42	1.99	0.45
5:c:13:THR:CG2	5:c:14:ASP:N	2.78	0.45
13:b9:102:SPO:H341	5:b0:20:LEU:HD12	1.98	0.45
8:F:101:BCL:H201	13:G:101:SPO:H291	1.97	0.45
8:A:101:BCL:HHD	5:B:42:VAL:HG21	1.98	0.45
4:F:11:PHE:HE1	4:I:14:ARG:HG3	1.82	0.45
4:Q:38:THR:HG21	4:S:44:LEU:HD13	1.98	0.45
13:9:102:SPO:H341	5:0:20:LEU:HD12	1.98	0.45
1:l:199:ASN:OD1	3:h:62:LYS:NZ	2.47	0.45
11:l:306:PC1:H242	6:x:33:TRP:HB3	1.99	0.45
2:m:123:PHE:HA	2:m:157:TRP:HH2	1.82	0.45
8:a:101:BCL:HHD	5:b:42:VAL:HG21	1.98	0.45
2:M:123:PHE:HA	2:M:157:TRP:HH2	1.82	0.45
4:D:24:LEU:HB2	8:D:102:BCL:H42	1.98	0.45
8:S:101:BCL:HHC	8:S:101:BCL:OBB	2.17	0.45
13:S:103:SPO:H351	5:V:23:VAL:HG11	1.98	0.45
4:a:10:ILE:HD11	13:e:101:SPO:H403	1.99	0.45
4:d:24:LEU:HB2	8:d:102:BCL:H42	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:102:SPO:H361	13:s:102:SPO:H341	1.54	0.45
5:t:31:PHE:HE2	8:t:101:BCL:HBA1	1.82	0.45
11:L:306:PC1:H242	6:X:33:TRP:HB3	1.99	0.45
4:K:24:LEU:HB2	8:K:101:BCL:H42	1.99	0.45
6:X:20:ARG:HG2	13:X:101:SPO:C31	2.41	0.45
4:6:13:PRO:HB3	5:b8:20:LEU:HD21	1.99	0.45
1:L:262:TRP:O	1:L:265:TRP:HD1	2.00	0.44
13:B:102:SPO:H341	13:B:102:SPO:H361	1.50	0.44
8:N:102:BCL:H92	8:N:102:BCL:H62	1.76	0.44
4:U:20:GLN:HE21	13:U:102:SPO:H392	1.82	0.44
4:W:43:TRP:CZ2	8:W:101:BCL:HHC	2.52	0.44
8:a:101:BCL:HHC	8:a:101:BCL:OBB	2.17	0.44
8:e:102:BCL:H61	8:e:102:BCL:H2	1.79	0.44
4:6:35:LEU:HD11	8:6:102:BCL:HHD	1.99	0.44
4:w:43:TRP:CZ2	8:w:101:BCL:HHC	2.52	0.44
6:x:27:MET:HE1	13:x:101:SPO:H243	2.00	0.44
13:D:103:SPO:H341	13:D:103:SPO:H361	1.48	0.44
4:a:48:ALA:HA	4:a:53:ARG:HD3	1.99	0.44
1:L:167:PHE:HE1	1:L:251:THR:HG21	1.82	0.44
2:M:80:TRP:CH2	4:S:34:ILE:HG12	2.52	0.44
2:M:278:LEU:HD11	14:M:407:CDL:H822	2.00	0.44
11:A:105:PC1:H131	4:D:14:ARG:C	2.43	0.44
4:D:51:TYR:HB2	4:D:53:ARG:HD2	1.98	0.44
8:7:101:BCL:H52	8:7:101:BCL:H8	1.83	0.44
6:X:15:PRO:HB2	6:x:5:THR:HG23	2.00	0.44
5:b8:28:LEU:HD13	13:x:101:SPO:C20	2.48	0.44
8:b9:101:BCL:OBB	8:b9:101:BCL:HHC	2.18	0.44
4:7:35:LEU:HD11	8:7:102:BCL:HHD	1.99	0.44
6:X:27:MET:HE1	13:X:101:SPO:H243	2.00	0.44
4:f:11:PHE:HE1	4:i:14:ARG:HG3	1.82	0.44
4:b9:36:LEU:O	4:b9:42:ASN:ND2	2.51	0.44
3:H:259:TYR:OH	6:x:20:ARG:NH1	2.51	0.44
4:A:24:LEU:HB2	8:A:101:BCL:H42	2.00	0.44
4:A:41:TYR:H	4:A:46:ILE:HD11	1.83	0.44
13:3:102:SPO:H351	5:Z:23:VAL:HG11	2.00	0.44
4:9:36:LEU:O	4:9:42:ASN:ND2	2.51	0.44
2:m:55:LEU:HD23	2:m:55:LEU:HA	1.87	0.44
13:j:102:SPO:H32A	5:n:41:ALA:HB2	2.00	0.44
8:n:102:BCL:H92	8:n:102:BCL:H62	1.76	0.44
4:s:7:ILE:HB	13:s:103:SPO:H32	2.00	0.44
4:u:48:ALA:HA	4:u:53:ARG:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:17:PHE:CZ	13:A:102:SPO:H342	2.53	0.44
4:A:48:ALA:HA	4:A:53:ARG:HD3	1.99	0.44
5:G:7:LEU:HD13	5:J:12:LEU:HD11	1.99	0.44
8:P:102:BCL:H62	8:P:102:BCL:H2	1.80	0.44
6:X:5:THR:HG23	6:x:15:PRO:HB2	2.00	0.44
1:l:207:ARG:HD2	1:l:211:HIS:CD2	2.53	0.44
4:a:17:PHE:CZ	13:a:102:SPO:H342	2.53	0.44
8:v:101:BCL:H111	8:v:101:BCL:H72	1.86	0.44
10:L:305:U10:H121	10:L:305:U10:H101	1.79	0.44
8:A:101:BCL:HHC	8:A:101:BCL:OBB	2.17	0.44
11:A:103:PC1:H133	11:A:103:PC1:H112	1.80	0.44
13:J:102:SPO:H32A	5:N:41:ALA:HB2	2.00	0.44
4:S:7:ILE:HB	13:S:103:SPO:H32	2.00	0.44
1:l:262:TRP:O	1:l:265:TRP:HD1	2.00	0.44
2:m:80:TRP:CH2	4:s:34:ILE:HG12	2.52	0.44
4:F:48:ALA:HA	4:F:53:ARG:HD3	1.99	0.44
4:Q:48:ALA:HA	4:Q:53:ARG:HB2	2.00	0.44
4:U:48:ALA:HA	4:U:53:ARG:HB2	2.00	0.44
11:a:105:PC1:H131	4:d:14:ARG:C	2.43	0.44
8:b:101:BCL:H61	8:b:101:BCL:H2	1.73	0.44
5:g:7:LEU:HD13	5:j:12:LEU:HD11	1.99	0.44
13:5:102:SPO:H362	13:5:102:SPO:H341	1.47	0.44
1:L:59:TRP:CH2	11:L:307:PC1:H272	2.53	0.43
1:L:60:ASN:HD21	11:H:301:PC1:H143	1.82	0.43
1:l:13:GLY:O	1:l:110:LYS:NZ	2.36	0.43
1:l:60:ASN:HD21	11:h:301:PC1:H143	1.82	0.43
1:l:111:LEU:O	2:m:247:ARG:NH1	2.51	0.43
4:a:41:TYR:H	4:a:46:ILE:HD11	1.83	0.43
8:d:102:BCL:OBB	8:d:102:BCL:HHC	2.18	0.43
5:g:20:LEU:HA	13:g:101:SPO:H37	1.99	0.43
4:u:20:GLN:HE21	13:u:102:SPO:H392	1.83	0.43
13:u:102:SPO:H362	13:u:102:SPO:H341	1.79	0.43
2:m:278:LEU:HD11	14:m:407:CDL:H822	2.00	0.43
5:G:46:ARG:HG2	4:I:53:ARG:NH2	2.33	0.43
4:3:48:ALA:HA	4:3:53:ARG:HD3	2.00	0.43
4:a:24:LEU:HB2	8:a:101:BCL:H42	2.00	0.43
4:o:38:THR:OG1	4:o:40:SER:O	2.23	0.43
8:c:101:BCL:H92	8:c:101:BCL:H62	1.80	0.43
6:X:20:ARG:NH1	3:h:259:TYR:OH	2.51	0.43
11:h:302:PC1:H111	11:h:302:PC1:H133	1.78	0.43
5:g:46:ARG:HG2	4:i:53:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:w:101:BCL:H8	8:w:101:BCL:H121	1.80	0.43
13:5:102:SPO:H351	5:z:23:VAL:HG11	2.00	0.43
1:L:111:LEU:O	2:M:247:ARG:NH1	2.51	0.43
1:L:207:ARG:HD2	1:L:211:HIS:CD2	2.53	0.43
13:U:103:SPO:H42	8:3:101:BCL:HBB2	2.00	0.43
8:D:102:BCL:OBB	8:D:102:BCL:HHC	2.18	0.43
13:D:103:SPO:H42	5:E:44:ILE:HD12	2.01	0.43
4:I:6:LYS:HB3	13:N:101:SPO:H402	2.01	0.43
8:j:101:BCL:H112	8:j:101:BCL:C2B	2.49	0.43
4:q:48:ALA:HA	4:q:53:ARG:HB2	2.00	0.43
13:E:103:SPO:H362	8:F:101:BCL:H41	2.00	0.43
4:F:23:PHE:HE1	4:I:25:PHE:CE1	2.37	0.43
5:G:20:LEU:HA	13:G:101:SPO:H37	2.00	0.43
8:Q:101:BCL:OBB	8:Q:101:BCL:HHC	2.19	0.43
13:Q:104:SPO:H342	4:S:17:PHE:CZ	2.53	0.43
1:l:54:VAL:HG21	4:a:33:LEU:HD22	2.01	0.43
13:e:103:SPO:H362	8:f:101:BCL:H41	2.00	0.43
4:i:6:LYS:HB3	13:n:101:SPO:H402	2.01	0.43
5:z:35:ALA:O	5:z:39:HIS:ND1	2.48	0.43
8:N:102:BCL:H112	8:N:102:BCL:C2B	2.49	0.43
4:W:43:TRP:CE3	8:W:101:BCL:HBC2	2.54	0.43
4:f:23:PHE:HE1	4:i:25:PHE:CE1	2.37	0.43
13:g:103:SPO:H181	5:j:38:ALA:HB1	2.00	0.43
4:k:24:LEU:HB2	8:k:101:BCL:H42	1.99	0.43
11:D:101:PC1:H151	4:F:15:ARG:HA	2.00	0.43
4:F:17:PHE:CZ	13:G:101:SPO:H342	2.54	0.43
4:W:23:PHE:HE1	4:3:25:PHE:CE1	2.37	0.43
4:W:43:TRP:CE3	8:W:101:BCL:H2C	2.54	0.43
13:C:102:SPO:H26	13:C:102:SPO:H241	1.89	0.43
13:b0:102:SPO:H31	13:b0:102:SPO:H5	1.70	0.43
4:F:33:LEU:HD13	14:F:102:CDL:H532	2.01	0.43
5:J:32:SER:HB2	8:J:101:BCL:H42	2.01	0.43
8:W:101:BCL:H8	8:W:101:BCL:H121	1.80	0.43
5:8:28:LEU:HD13	13:X:101:SPO:C20	2.48	0.43
1:l:59:TRP:CH2	11:l:307:PC1:H272	2.53	0.43
11:l:307:PC1:H132	11:l:307:PC1:H112	1.79	0.43
11:d:101:PC1:H151	4:f:15:ARG:HA	2.00	0.43
4:w:43:TRP:CE3	8:w:101:BCL:H2C	2.54	0.43
8:6:101:BCL:H52	8:6:101:BCL:H8	1.83	0.43
4:W:27:LEU:HD23	8:C:101:BCL:HED3	2.00	0.42
8:f:101:BCL:HHC	8:f:101:BCL:OBB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:w:43:TRP:CE3	8:w:101:BCL:HBC2	2.54	0.42
13:B:102:SPO:H31	13:B:102:SPO:H5	1.76	0.42
4:D:30:MET:HG3	14:F:102:CDL:H121	2.02	0.42
10:m:405:U10:H33	10:m:405:U10:H372	1.88	0.42
13:m:406:SPO:H26	13:m:406:SPO:H241	1.88	0.42
11:a:103:PC1:H372	11:a:104:PC1:H231	2.02	0.42
4:f:17:PHE:CZ	13:g:101:SPO:H342	2.54	0.42
8:6:101:BCL:H141	5:b8:34:VAL:HG21	2.01	0.42
8:b0:101:BCL:OBB	8:b0:101:BCL:HHC	2.20	0.42
1:L:206:MET:O	3:H:67:PRO:HG3	2.19	0.42
8:D:102:BCL:H121	8:D:102:BCL:H8	1.97	0.42
8:G:102:BCL:H92	8:G:102:BCL:H62	1.78	0.42
13:d:103:SPO:H42	5:e:44:ILE:HD12	2.01	0.42
4:q:41:TYR:H	4:q:46:ILE:HD11	1.83	0.42
13:s:103:SPO:H26	13:s:103:SPO:H241	1.90	0.42
4:w:27:LEU:HD23	8:c:101:BCL:HED3	2.00	0.42
4:6:46:ILE:H	4:6:46:ILE:HG13	1.63	0.42
8:6:101:BCL:OBB	8:6:101:BCL:HHC	2.19	0.42
3:H:90:THR:OG1	3:H:97:PRO:O	2.27	0.42
11:A:104:PC1:H112	11:A:104:PC1:H132	1.71	0.42
13:G:103:SPO:H181	5:J:38:ALA:HB1	2.00	0.42
13:i:102:SPO:H341	5:j:20:LEU:HG	2.01	0.42
13:u:103:SPO:H42	8:5:101:BCL:HBB2	2.00	0.42
4:6:42:ASN:ND2	4:6:45:GLU:HB2	2.34	0.42
2:M:200:PRO:HB2	3:H:17:ILE:HD13	2.02	0.42
3:H:112:ALA:HB2	3:H:239:GLY:HA3	2.01	0.42
13:A:102:SPO:H362	13:A:102:SPO:H341	1.64	0.42
5:E:39:HIS:ND1	8:E:102:BCL:H91	2.34	0.42
13:Q:104:SPO:H362	13:Q:104:SPO:H341	1.49	0.42
5:R:19:GLU:O	5:R:23:VAL:HG23	2.20	0.42
8:9:101:BCL:OBB	8:9:101:BCL:HHC	2.18	0.42
11:l:307:PC1:H352	11:l:307:PC1:H321	1.79	0.42
4:f:33:LEU:HD13	14:f:102:CDL:H532	2.01	0.42
8:n:102:BCL:H112	8:n:102:BCL:C2B	2.49	0.42
13:q:104:SPO:H342	4:s:17:PHE:CZ	2.53	0.42
8:s:101:BCL:OBB	8:s:101:BCL:HHC	2.17	0.42
8:J:101:BCL:C2B	8:J:101:BCL:H112	2.49	0.42
13:Q:102:SPO:H341	5:R:20:LEU:HD12	2.02	0.42
4:S:3:LYS:HD2	4:S:6:LYS:HE2	2.02	0.42
4:7:42:ASN:ND2	4:7:45:GLU:HB2	2.34	0.42
13:X:101:SPO:H362	13:X:101:SPO:H341	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:264:GLY:HA3	3:h:35:ASN:ND2	2.35	0.42
11:a:103:PC1:H112	11:a:103:PC1:H133	1.80	0.42
8:q:101:BCL:OBB	8:q:101:BCL:HHC	2.19	0.42
13:q:102:SPO:H341	5:r:20:LEU:HD12	2.02	0.42
4:5:48:ALA:HA	4:5:53:ARG:HD3	2.00	0.42
13:b9:102:SPO:C36	5:b0:20:LEU:HD12	2.49	0.42
8:7:101:BCL:H141	5:8:34:VAL:HG21	2.01	0.42
6:X:27:MET:HE2	6:X:27:MET:HB3	1.89	0.42
5:e:39:HIS:ND1	8:e:102:BCL:H91	2.34	0.42
5:z:48:TRP:CD2	8:z:101:BCL:H2C	2.55	0.42
4:U:8:TRP:CD1	5:V:21:HIS:HB2	2.55	0.42
8:7:101:BCL:OBB	8:7:101:BCL:HHC	2.19	0.42
1:l:206:MET:O	3:h:67:PRO:HG3	2.19	0.42
4:d:30:MET:HG3	14:f:102:CDL:H121	2.02	0.42
5:p:7:LEU:HG	13:q:102:SPO:H401	2.02	0.42
1:L:128:TYR:O	1:L:132:VAL:HG22	2.20	0.42
11:L:307:PC1:H112	11:L:307:PC1:H132	1.79	0.42
3:H:53:GLN:H	11:A:105:PC1:H143	1.85	0.42
8:F:101:BCL:HHC	8:F:101:BCL:OBB	2.19	0.42
4:O:43:TRP:CE3	8:O:101:BCL:H2C	2.55	0.42
5:P:7:LEU:HG	13:Q:102:SPO:H401	2.02	0.42
4:Q:41:TYR:H	4:Q:46:ILE:HD11	1.83	0.42
4:W:7:ILE:HD12	4:W:7:ILE:HA	1.86	0.42
13:0:102:SPO:H31	13:0:102:SPO:H5	1.70	0.42
3:h:112:ALA:HB2	3:h:239:GLY:HA3	2.01	0.42
4:w:23:PHE:HE1	4:5:25:PHE:CE1	2.37	0.42
4:6:10:ILE:HD11	5:b8:7:LEU:HD12	2.02	0.42
5:b8:47:PRO:O	4:b9:53:ARG:NH2	2.42	0.42
3:H:170:ASP:OD1	3:H:172:PRO:HD2	2.19	0.42
4:Q:6:LYS:HD3	13:Q:104:SPO:H393	2.00	0.42
13:S:102:SPO:H361	13:S:102:SPO:H341	1.54	0.42
5:V:45:TRP:CE3	5:V:46:ARG:HB2	2.55	0.42
5:C:41:ALA:HB1	13:C:102:SPO:H81	2.02	0.42
4:s:3:LYS:HD2	4:s:6:LYS:HE2	2.02	0.42
4:u:8:TRP:CD1	5:v:21:HIS:HB2	2.55	0.42
1:L:51:TRP:HE1	4:9:37:SER:CB	2.33	0.41
1:L:54:VAL:HG21	4:A:33:LEU:HD22	2.01	0.41
1:L:98:VAL:HG11	11:L:306:PC1:H3B2	2.02	0.41
3:H:94:GLU:CD	11:A:103:PC1:H143	2.45	0.41
4:A:53:ARG:NH2	5:0:46:ARG:HG3	2.35	0.41
5:C:45:TRP:CE3	5:C:46:ARG:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:193:LEU:HD22	1:l:216:PHE:CD2	2.55	0.41
9:l:303:BPH:H162	9:l:303:BPH:H192	1.84	0.41
3:h:53:GLN:H	11:a:105:PC1:H143	1.85	0.41
5:j:32:SER:HB2	8:j:101:BCL:H42	2.01	0.41
4:q:6:LYS:HD3	13:q:104:SPO:H393	2.00	0.41
1:L:193:LEU:HD22	1:L:216:PHE:CD2	2.55	0.41
2:M:264:GLY:HA3	3:H:35:ASN:ND2	2.35	0.41
13:M:406:SPO:H26	13:M:406:SPO:H241	1.88	0.41
4:k:32:HIS:CE1	8:n:102:BCL:HMD1	2.56	0.41
5:c:45:TRP:CE3	5:c:46:ARG:HB2	2.55	0.41
4:D:16:VAL:HG22	11:D:101:PC1:H31	2.02	0.41
10:l:305:U10:H121	10:l:305:U10:H101	1.79	0.41
3:h:170:ASP:OD1	3:h:172:PRO:HD2	2.19	0.41
3:h:171:ILE:HB	3:h:172:PRO:HD3	2.02	0.41
13:q:103:SPO:H311	13:q:103:SPO:H291	1.87	0.41
5:c:41:ALA:HB1	13:c:102:SPO:H81	2.02	0.41
1:L:183:ASN:ND2	2:M:213:ALA:HA	2.36	0.41
1:L:211:HIS:CE1	2:M:20:MET:HE2	2.56	0.41
13:S:102:SPO:H26	13:S:102:SPO:H241	1.94	0.41
13:9:102:SPO:C36	5:0:20:LEU:HD12	2.49	0.41
1:l:51:TRP:HE1	4:b9:37:SER:CB	2.33	0.41
1:l:128:TYR:O	1:l:132:VAL:HG22	2.20	0.41
3:h:94:GLU:CD	11:a:103:PC1:H143	2.45	0.41
13:B:102:SPO:H16	8:0:101:BCL:H141	2.02	0.41
8:0:101:BCL:HHC	8:0:101:BCL:OBB	2.19	0.41
11:A:103:PC1:H372	11:A:104:PC1:H231	2.02	0.41
8:S:101:BCL:HED3	13:S:102:SPO:H25	2.03	0.41
5:Z:48:TRP:CD2	8:Z:101:BCL:H2C	2.55	0.41
8:7:102:BCL:HHC	8:7:102:BCL:OBB	2.21	0.41
13:X:101:SPO:H26	13:X:101:SPO:H241	1.85	0.41
1:l:103:ARG:NH2	2:m:254:TRP:O	2.54	0.41
1:l:211:HIS:CE1	2:m:20:MET:HE2	2.56	0.41
4:a:53:ARG:NH2	5:b0:46:ARG:HG3	2.35	0.41
5:r:19:GLU:O	5:r:23:VAL:HG23	2.20	0.41
8:6:101:BCL:H61	8:6:101:BCL:H41	1.75	0.41
1:L:103:ARG:NH2	2:M:254:TRP:O	2.54	0.41
2:M:302:GLY:HA3	11:H:301:PC1:H141	2.03	0.41
4:A:53:ARG:NH2	5:0:47:PRO:O	2.46	0.41
4:S:11:PHE:HB3	4:S:16:VAL:CG2	2.51	0.41
8:C:101:BCL:H62	8:C:101:BCL:H2	1.90	0.41
13:e:101:SPO:H82	4:f:29:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:r:39:HIS:CD2	8:r:101:BCL:H91	2.56	0.41
8:M:402:BCL:H2	9:M:404:BPH:HMB2	2.03	0.41
4:I:6:LYS:HE3	5:N:19:GLU:OE2	2.20	0.41
4:O:20:GLN:HE22	5:P:24:TYR:HE1	1.69	0.41
13:U:102:SPO:H362	13:U:102:SPO:H341	1.79	0.41
11:a:105:PC1:C13	4:d:14:ARG:HB2	2.51	0.41
5:g:49:PHE:CD2	8:g:102:BCL:H171	2.56	0.41
4:i:6:LYS:HE3	5:n:19:GLU:OE2	2.20	0.41
11:L:307:PC1:H321	11:L:307:PC1:H352	1.79	0.41
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.02	0.41
5:E:39:HIS:CG	8:E:102:BCL:H91	2.56	0.41
13:G:103:SPO:H362	13:G:103:SPO:H341	1.74	0.41
4:I:20:GLN:HE22	5:J:24:TYR:HE1	1.68	0.41
5:J:9:TYR:OH	4:K:12:ASP:OD1	2.30	0.41
4:K:32:HIS:CE1	8:N:102:BCL:HMD1	2.56	0.41
8:P:102:BCL:HBB3	8:Q:101:BCL:CHC	2.51	0.41
5:R:39:HIS:CD2	8:R:101:BCL:H91	2.56	0.41
4:7:32:HIS:CE1	8:7:102:BCL:HMD3	2.56	0.41
6:X:25:PHE:CD1	6:x:21:LEU:HD21	2.56	0.41
1:l:61:PRO:HA	1:l:64:ILE:HD12	2.02	0.41
2:m:3:TYR:CZ	2:m:5:ASN:HA	2.56	0.41
2:m:200:PRO:HB2	3:h:17:ILE:HD13	2.02	0.41
2:m:302:GLY:HA3	11:h:301:PC1:H141	2.03	0.41
8:m:403:BCL:HHC	8:m:403:BCL:OBB	2.21	0.41
8:n:102:BCL:H162	8:n:102:BCL:H192	1.86	0.41
4:o:43:TRP:CE3	8:o:101:BCL:H2C	2.55	0.41
8:p:102:BCL:HBB3	8:q:101:BCL:CHC	2.51	0.41
5:v:45:TRP:CE3	5:v:46:ARG:HB2	2.55	0.41
8:v:101:BCL:HBB3	8:w:101:BCL:C1C	2.51	0.41
4:6:32:HIS:CE1	8:6:102:BCL:HMD3	2.56	0.41
4:A:6:LYS:HE3	5:E:19:GLU:OE2	2.21	0.41
8:D:102:BCL:H201	13:E:101:SPO:H291	2.03	0.41
4:U:23:PHE:HE1	4:W:25:PHE:CE1	2.39	0.41
1:l:98:VAL:HG11	11:l:306:PC1:H3B2	2.02	0.41
5:r:24:TYR:CE2	8:s:101:BCL:H171	2.56	0.41
4:6:38:THR:O	4:6:42:ASN:HB2	2.21	0.41
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.57	0.40
11:A:105:PC1:H111	11:A:105:PC1:H133	1.69	0.40
13:E:101:SPO:H82	4:F:29:VAL:HG23	2.03	0.40
5:G:7:LEU:CD2	5:J:12:LEU:HG	2.51	0.40
5:G:14:ASP:OD2	5:G:18:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:49:PHE:CD2	8:G:102:BCL:H171	2.56	0.40
13:I:102:SPO:H341	5:J:20:LEU:HG	2.01	0.40
1:l:35:GLY:HA2	1:l:103:ARG:HD2	2.03	0.40
2:m:157:TRP:CE3	2:m:158:MET:HG2	2.56	0.40
13:b:102:SPO:H16	8:b0:101:BCL:H141	2.02	0.40
4:o:24:LEU:HD23	4:o:24:LEU:HA	1.94	0.40
4:s:11:PHE:HB3	4:s:16:VAL:CG2	2.51	0.40
13:s:102:SPO:HM12	13:s:102:SPO:H42	1.91	0.40
2:M:250:LEU:HA	2:M:250:LEU:HD23	1.78	0.40
11:A:105:PC1:H131	4:D:14:ARG:HB2	2.03	0.40
8:V:101:BCL:HBB3	8:W:101:BCL:C1C	2.51	0.40
4:7:10:ILE:HD11	5:8:7:LEU:HD12	2.02	0.40
1:l:183:ASN:ND2	2:m:213:ALA:HA	2.36	0.40
9:m:404:BPH:H6C1	9:m:404:BPH:H4C1	1.82	0.40
4:d:1:MET:HE2	4:d:1:MET:HB3	1.98	0.40
13:5:103:SPO:H26	13:5:103:SPO:H241	1.88	0.40
11:A:103:PC1:H222	11:A:103:PC1:H252	1.93	0.40
11:A:105:PC1:C13	4:D:14:ARG:HB2	2.51	0.40
13:I:102:SPO:H31	8:K:101:BCL:HBB2	2.03	0.40
6:X:6:ILE:O	6:X:8:ASN:ND2	2.54	0.40
11:a:105:PC1:H151	4:d:15:ARG:HA	2.04	0.40
4:k:51:TYR:HB2	4:k:53:ARG:HD2	2.03	0.40
8:q:101:BCL:H193	8:q:101:BCL:H161	1.89	0.40
8:6:102:BCL:OBB	8:6:102:BCL:HHC	2.21	0.40
2:M:280:GLY:HA2	8:M:403:BCL:HED2	2.03	0.40
4:K:51:TYR:HB2	4:K:53:ARG:HD2	2.03	0.40
4:O:7:ILE:HB	13:Q:102:SPO:H32	2.04	0.40
8:S:101:BCL:H41	13:S:102:SPO:H351	2.03	0.40
1:l:182:THR:HG23	8:m:402:BCL:H42	2.04	0.40
11:h:301:PC1:H231	11:h:301:PC1:H321	2.04	0.40
8:d:102:BCL:H201	13:e:101:SPO:H291	2.03	0.40
5:g:7:LEU:CD2	5:j:12:LEU:HG	2.51	0.40
1:L:61:PRO:HA	1:L:64:ILE:HD12	2.02	0.40
2:M:55:LEU:HA	2:M:55:LEU:HD23	1.87	0.40
13:Q:103:SPO:H361	13:Q:103:SPO:H341	1.78	0.40
4:7:11:PHE:C	5:8:10:THR:HG21	2.46	0.40
4:7:38:THR:O	4:7:42:ASN:HB2	2.21	0.40
6:X:21:LEU:HD21	6:x:25:PHE:CD1	2.56	0.40
2:m:280:GLY:HA2	8:m:403:BCL:HED2	2.03	0.40
8:m:402:BCL:H2	9:m:404:BPH:HMB2	2.03	0.40
11:a:104:PC1:H112	11:a:104:PC1:H132	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:o:11:PHE:HD1	4:o:11:PHE:HA	1.76	0.40
8:v:101:BCL:HBA2	8:v:101:BCL:H3A	1.80	0.40
4:w:7:ILE:HD12	4:w:7:ILE:HA	1.86	0.40
6:x:6:ILE:O	6:x:8:ASN:ND2	2.54	0.40
6:x:22:TRP:O	6:x:26:GLN:HG2	2.21	0.40

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	L	279/282 (99%)	272 (98%)	7 (2%)	0	100	100
1	l	279/282 (99%)	272 (98%)	7 (2%)	0	100	100
2	M	305/308 (99%)	299 (98%)	6 (2%)	0	100	100
2	m	305/308 (99%)	299 (98%)	6 (2%)	0	100	100
3	H	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
3	h	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
4	1	45/58 (78%)	45 (100%)	0	0	100	100
4	3	50/58 (86%)	49 (98%)	1 (2%)	0	100	100
4	5	50/58 (86%)	49 (98%)	1 (2%)	0	100	100
4	6	46/58 (79%)	44 (96%)	2 (4%)	0	100	100
4	7	46/58 (79%)	44 (96%)	2 (4%)	0	100	100
4	9	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	A	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	D	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	F	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	I	52/58 (90%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	52/58 (90%)	52 (100%)	0	0	100	100
4	O	52/58 (90%)	52 (100%)	0	0	100	100
4	Q	53/58 (91%)	50 (94%)	3 (6%)	0	100	100
4	S	53/58 (91%)	53 (100%)	0	0	100	100
4	U	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	W	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	a	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	b1	45/58 (78%)	45 (100%)	0	0	100	100
4	b9	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	d	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	f	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	i	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	k	52/58 (90%)	52 (100%)	0	0	100	100
4	o	52/58 (90%)	52 (100%)	0	0	100	100
4	q	53/58 (91%)	50 (94%)	3 (6%)	0	100	100
4	s	53/58 (91%)	53 (100%)	0	0	100	100
4	u	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	w	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
5	0	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	2	36/49 (74%)	36 (100%)	0	0	100	100
5	4	36/49 (74%)	36 (100%)	0	0	100	100
5	8	42/49 (86%)	42 (100%)	0	0	100	100
5	B	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	C	40/49 (82%)	40 (100%)	0	0	100	100
5	E	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	G	42/49 (86%)	42 (100%)	0	0	100	100
5	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	N	40/49 (82%)	40 (100%)	0	0	100	100
5	P	41/49 (84%)	41 (100%)	0	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	40/49 (82%)	40 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	V	40/49 (82%)	40 (100%)	0	0	100	100
5	Z	40/49 (82%)	40 (100%)	0	0	100	100
5	b	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	b0	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	b8	42/49 (86%)	42 (100%)	0	0	100	100
5	c	40/49 (82%)	40 (100%)	0	0	100	100
5	e	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	g	42/49 (86%)	42 (100%)	0	0	100	100
5	j	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	n	40/49 (82%)	40 (100%)	0	0	100	100
5	p	41/49 (84%)	41 (100%)	0	0	100	100
5	r	41/49 (84%)	41 (100%)	0	0	100	100
5	t	40/49 (82%)	40 (100%)	0	0	100	100
5	v	40/49 (82%)	40 (100%)	0	0	100	100
5	z	40/49 (82%)	40 (100%)	0	0	100	100
6	X	66/82 (80%)	64 (97%)	2 (3%)	0	100	100
6	x	66/82 (80%)	64 (97%)	2 (3%)	0	100	100
7	Y	47/53 (89%)	47 (100%)	0	0	100	100
7	y	47/53 (89%)	47 (100%)	0	0	100	100
All	All	4482/4966 (90%)	4402 (98%)	80 (2%)	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	L	220/221 (100%)	218 (99%)	2 (1%)	70	82
1	l	220/221 (100%)	218 (99%)	2 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	240/241 (100%)	238 (99%)	2 (1%)	73	83
2	m	240/241 (100%)	238 (99%)	2 (1%)	73	83
3	H	208/208 (100%)	207 (100%)	1 (0%)	81	88
3	h	208/208 (100%)	207 (100%)	1 (0%)	81	88
4	1	42/51 (82%)	42 (100%)	0	100	100
4	3	46/51 (90%)	46 (100%)	0	100	100
4	5	46/51 (90%)	46 (100%)	0	100	100
4	6	44/51 (86%)	44 (100%)	0	100	100
4	7	44/51 (86%)	44 (100%)	0	100	100
4	9	49/51 (96%)	49 (100%)	0	100	100
4	A	49/51 (96%)	49 (100%)	0	100	100
4	D	49/51 (96%)	49 (100%)	0	100	100
4	F	49/51 (96%)	49 (100%)	0	100	100
4	I	49/51 (96%)	49 (100%)	0	100	100
4	K	48/51 (94%)	48 (100%)	0	100	100
4	O	49/51 (96%)	48 (98%)	1 (2%)	48	67
4	Q	49/51 (96%)	49 (100%)	0	100	100
4	S	49/51 (96%)	49 (100%)	0	100	100
4	U	48/51 (94%)	48 (100%)	0	100	100
4	W	48/51 (94%)	48 (100%)	0	100	100
4	a	49/51 (96%)	49 (100%)	0	100	100
4	b1	42/51 (82%)	42 (100%)	0	100	100
4	b9	49/51 (96%)	49 (100%)	0	100	100
4	d	49/51 (96%)	49 (100%)	0	100	100
4	f	49/51 (96%)	49 (100%)	0	100	100
4	i	49/51 (96%)	49 (100%)	0	100	100
4	k	48/51 (94%)	48 (100%)	0	100	100
4	o	49/51 (96%)	48 (98%)	1 (2%)	48	67
4	q	49/51 (96%)	49 (100%)	0	100	100
4	s	49/51 (96%)	49 (100%)	0	100	100
4	u	48/51 (94%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	w	48/51 (94%)	48 (100%)	0	100	100
5	0	36/40 (90%)	36 (100%)	0	100	100
5	2	31/40 (78%)	31 (100%)	0	100	100
5	4	31/40 (78%)	31 (100%)	0	100	100
5	8	36/40 (90%)	36 (100%)	0	100	100
5	B	36/40 (90%)	36 (100%)	0	100	100
5	C	34/40 (85%)	34 (100%)	0	100	100
5	E	35/40 (88%)	35 (100%)	0	100	100
5	G	36/40 (90%)	36 (100%)	0	100	100
5	J	35/40 (88%)	35 (100%)	0	100	100
5	N	34/40 (85%)	34 (100%)	0	100	100
5	P	35/40 (88%)	35 (100%)	0	100	100
5	R	35/40 (88%)	35 (100%)	0	100	100
5	T	34/40 (85%)	34 (100%)	0	100	100
5	V	34/40 (85%)	34 (100%)	0	100	100
5	Z	34/40 (85%)	33 (97%)	1 (3%)	37	59
5	b	36/40 (90%)	36 (100%)	0	100	100
5	b0	36/40 (90%)	36 (100%)	0	100	100
5	b8	36/40 (90%)	36 (100%)	0	100	100
5	c	34/40 (85%)	34 (100%)	0	100	100
5	e	35/40 (88%)	35 (100%)	0	100	100
5	g	36/40 (90%)	36 (100%)	0	100	100
5	j	35/40 (88%)	35 (100%)	0	100	100
5	n	34/40 (85%)	34 (100%)	0	100	100
5	p	35/40 (88%)	35 (100%)	0	100	100
5	r	35/40 (88%)	35 (100%)	0	100	100
5	t	34/40 (85%)	34 (100%)	0	100	100
5	v	34/40 (85%)	34 (100%)	0	100	100
5	z	34/40 (85%)	33 (97%)	1 (3%)	37	59
6	X	54/66 (82%)	54 (100%)	0	100	100
6	x	54/66 (82%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Y	33/37 (89%)	33 (100%)	0	100	100
7	y	33/37 (89%)	33 (100%)	0	100	100
All	All	3816/4094 (93%)	3802 (100%)	14 (0%)	81	90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	216	PHE
1	L	247	CYS
2	M	214	LEU
2	M	216	PHE
3	H	231	ASP
4	O	11	PHE
5	Z	49	PHE
1	l	216	PHE
1	l	247	CYS
2	m	214	LEU
2	m	216	PHE
3	h	231	ASP
4	o	11	PHE
5	z	49	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	264	GLN
2	M	28	ASN
2	M	259	ASN
2	M	299	GLN
3	H	204	HIS
4	D	42	ASN
4	D	52	ASN
5	E	16	GLN
5	N	16	GLN
4	U	42	ASN
4	7	20	GLN
4	7	42	ASN
5	0	16	GLN
6	X	8	ASN
6	X	66	ASN

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Mol	Chain	Res	Type
1	l	264	GLN
2	m	28	ASN
2	m	259	ASN
2	m	307	ASN
4	d	42	ASN
5	e	16	GLN
4	f	42	ASN
5	n	16	GLN
4	u	42	ASN
4	6	42	ASN
5	b0	16	GLN
6	x	66	ASN

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 148 ligands modelled in this entry, 2 are monoatomic - leaving 146 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	BCL	b9	101	-	69,74,74	1.11	6 (8%)	79,115,115	1.43	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	l	302	-	66,71,74	1.12	7 (10%)	75,111,115	1.36	8 (10%)
10	U10	M	405	-	48,48,63	2.71	14 (29%)	60,61,79	1.72	15 (25%)
8	BCL	S	101	-	69,74,74	1.13	7 (10%)	79,115,115	1.43	11 (13%)
11	PC1	A	105	-	37,37,53	0.58	0	43,45,61	0.61	1 (2%)
13	SPO	q	104	-	41,41,41	0.20	0	47,50,50	0.23	0
8	BCL	Q	101	-	69,74,74	1.12	6 (8%)	79,115,115	1.45	12 (15%)
8	BCL	A	101	-	69,74,74	1.12	7 (10%)	79,115,115	1.42	10 (12%)
13	SPO	U	102	-	41,41,41	0.20	0	47,50,50	0.40	0
8	BCL	W	101	-	69,74,74	1.08	5 (7%)	79,115,115	1.40	8 (10%)
10	U10	m	405	-	48,48,63	2.71	14 (29%)	60,61,79	1.72	15 (25%)
8	BCL	7	102	-	64,69,74	1.10	5 (7%)	73,109,115	1.46	11 (15%)
8	BCL	L	302	-	66,71,74	1.12	7 (10%)	75,111,115	1.36	8 (10%)
8	BCL	i	101	-	69,74,74	1.10	7 (10%)	79,115,115	1.42	9 (11%)
8	BCL	w	101	-	69,74,74	1.08	5 (7%)	79,115,115	1.40	8 (10%)
11	PC1	L	306	-	38,38,53	1.17	4 (10%)	44,46,61	1.21	3 (6%)
8	BCL	J	101	-	69,74,74	1.08	5 (7%)	79,115,115	1.33	7 (8%)
13	SPO	a	102	-	41,41,41	0.26	0	47,50,50	0.26	0
8	BCL	C	101	-	64,69,74	1.11	6 (9%)	73,109,115	1.33	8 (10%)
13	SPO	S	102	-	41,41,41	0.22	0	47,50,50	0.26	0
13	SPO	c	102	-	41,41,41	0.21	0	47,50,50	0.43	0
8	BCL	r	101	-	69,74,74	1.08	4 (5%)	79,115,115	1.28	8 (10%)
8	BCL	f	101	-	69,74,74	1.13	5 (7%)	79,115,115	1.43	10 (12%)
13	SPO	m	406	-	41,41,41	0.26	0	47,50,50	0.32	0
8	BCL	K	101	-	69,74,74	1.12	6 (8%)	79,115,115	1.40	10 (12%)
8	BCL	k	101	-	69,74,74	1.12	6 (8%)	79,115,115	1.40	10 (12%)
8	BCL	b1	101	-	49,54,74	1.26	5 (10%)	55,91,115	1.52	7 (12%)
8	BCL	6	102	-	64,69,74	1.10	5 (7%)	73,109,115	1.46	11 (15%)
13	SPO	G	101	-	41,41,41	0.21	0	47,50,50	0.20	0
13	SPO	g	103	-	41,41,41	0.20	0	47,50,50	0.36	0
11	PC1	L	307	-	39,39,53	1.16	4 (10%)	45,47,61	1.14	3 (6%)
13	SPO	C	102	-	41,41,41	0.21	0	47,50,50	0.43	0
8	BCL	5	101	-	54,59,74	1.26	4 (7%)	61,97,115	1.54	8 (13%)
8	BCL	R	101	-	69,74,74	1.08	4 (5%)	79,115,115	1.28	8 (10%)
13	SPO	p	101	-	41,41,41	0.20	0	47,50,50	0.22	0
8	BCL	U	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.39	9 (11%)
8	BCL	0	101	-	64,69,74	1.13	5 (7%)	73,109,115	1.53	12 (16%)
8	BCL	g	102	-	69,74,74	1.10	5 (7%)	79,115,115	1.37	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	SPO	i	102	-	41,41,41	0.20	0	47,50,50	0.23	0
14	CDL	M	407	-	81,81,99	1.03	9 (11%)	87,93,111	1.21	6 (6%)
11	PC1	a	103	-	44,44,53	1.11	4 (9%)	50,52,61	1.21	3 (6%)
8	BCL	c	101	-	64,69,74	1.11	5 (7%)	73,109,115	1.33	8 (10%)
8	BCL	s	101	-	69,74,74	1.13	7 (10%)	79,115,115	1.43	11 (13%)
13	SPO	b9	102	-	41,41,41	0.27	0	47,50,50	0.27	0
8	BCL	M	403	-	69,74,74	1.16	7 (10%)	79,115,115	1.42	9 (11%)
8	BCL	T	101	-	69,74,74	1.08	4 (5%)	79,115,115	1.31	9 (11%)
10	U10	L	305	-	43,43,63	2.74	13 (30%)	54,55,79	1.76	14 (25%)
9	BPH	l	303	-	59,70,70	1.17	3 (5%)	59,101,101	2.04	11 (18%)
8	BCL	3	101	-	54,59,74	1.26	4 (7%)	61,97,115	1.54	8 (13%)
13	SPO	Q	104	-	41,41,41	0.20	0	47,50,50	0.23	0
8	BCL	9	101	-	69,74,74	1.11	6 (8%)	79,115,115	1.43	10 (12%)
8	BCL	e	102	-	69,74,74	1.09	4 (5%)	79,115,115	1.35	9 (11%)
8	BCL	M	402	-	69,74,74	1.11	7 (10%)	79,115,115	1.38	7 (8%)
11	PC1	l	307	-	39,39,53	1.16	4 (10%)	45,47,61	1.14	3 (6%)
8	BCL	u	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.39	9 (11%)
13	SPO	N	101	-	41,41,41	0.20	0	47,50,50	0.19	0
13	SPO	9	102	-	41,41,41	0.27	0	47,50,50	0.27	0
11	PC1	l	306	-	38,38,53	1.17	4 (10%)	44,46,61	1.21	3 (6%)
8	BCL	l	301	-	69,74,74	1.13	7 (10%)	79,115,115	1.34	11 (13%)
8	BCL	n	102	-	69,74,74	1.09	5 (7%)	79,115,115	1.34	8 (10%)
8	BCL	1	101	-	49,54,74	1.26	5 (10%)	55,91,115	1.52	7 (12%)
11	PC1	H	302	-	33,33,53	1.28	6 (18%)	39,41,61	1.11	3 (7%)
11	PC1	A	103	-	44,44,53	1.11	4 (9%)	50,52,61	1.22	3 (6%)
13	SPO	5	102	-	41,41,41	0.19	0	47,50,50	0.31	0
8	BCL	I	101	-	69,74,74	1.10	7 (10%)	79,115,115	1.42	9 (11%)
13	SPO	d	103	-	41,41,41	0.21	0	47,50,50	0.27	0
13	SPO	q	102	-	41,41,41	0.21	0	47,50,50	0.24	0
13	SPO	M	406	-	41,41,41	0.26	0	47,50,50	0.32	0
13	SPO	5	103	-	41,41,41	0.17	0	47,50,50	0.31	0
8	BCL	P	102	-	69,74,74	1.08	4 (5%)	79,115,115	1.34	9 (11%)
10	U10	l	304	-	38,38,63	2.68	12 (31%)	48,49,79	1.76	13 (27%)
11	PC1	a	105	-	37,37,53	0.58	0	43,45,61	0.61	1 (2%)
13	SPO	j	102	-	41,41,41	0.19	0	47,50,50	0.28	0
9	BPH	m	404	-	49,60,70	1.28	4 (8%)	47,89,101	2.09	9 (19%)
8	BCL	j	101	-	69,74,74	1.08	5 (7%)	79,115,115	1.32	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	SPO	S	103	-	41,41,41	0.23	0	47,50,50	0.31	0
13	SPO	E	103	-	41,41,41	0.21	0	47,50,50	0.37	0
11	PC1	H	301	-	42,42,53	1.14	5 (11%)	48,50,61	1.18	3 (6%)
13	SPO	A	102	-	41,41,41	0.25	0	47,50,50	0.26	0
8	BCL	b	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.46	10 (12%)
8	BCL	6	101	-	64,69,74	1.12	4 (6%)	73,109,115	1.46	12 (16%)
8	BCL	o	101	-	69,74,74	1.09	6 (8%)	79,115,115	1.40	7 (8%)
13	SPO	O	102	-	41,41,41	0.23	0	47,50,50	0.40	0
13	SPO	P	101	-	41,41,41	0.20	0	47,50,50	0.22	0
13	SPO	e	103	-	41,41,41	0.21	0	47,50,50	0.37	0
13	SPO	G	103	-	41,41,41	0.20	0	47,50,50	0.36	0
13	SPO	X	101	-	41,41,41	0.25	0	47,50,50	0.35	0
8	BCL	p	102	-	69,74,74	1.08	4 (5%)	79,115,115	1.34	9 (11%)
11	PC1	a	104	-	30,30,53	1.34	4 (13%)	36,38,61	1.21	3 (8%)
13	SPO	e	101	-	41,41,41	0.24	0	47,50,50	0.22	0
8	BCL	D	102	-	69,74,74	1.13	6 (8%)	79,115,115	1.42	11 (13%)
8	BCL	7	101	-	64,69,74	1.12	4 (6%)	73,109,115	1.46	12 (16%)
8	BCL	4	101	-	49,54,74	1.25	4 (8%)	55,91,115	1.46	6 (10%)
11	PC1	A	104	-	30,30,53	1.34	4 (13%)	36,38,61	1.21	3 (8%)
8	BCL	O	101	-	69,74,74	1.09	6 (8%)	79,115,115	1.40	7 (8%)
11	PC1	h	301	-	42,42,53	1.14	5 (11%)	48,50,61	1.18	3 (6%)
10	U10	L	304	-	38,38,63	2.68	12 (31%)	48,49,79	1.76	13 (27%)
8	BCL	G	102	-	69,74,74	1.11	5 (7%)	79,115,115	1.37	9 (11%)
8	BCL	m	403	-	69,74,74	1.16	7 (10%)	79,115,115	1.43	9 (11%)
13	SPO	B	102	-	41,41,41	0.25	0	47,50,50	0.24	0
13	SPO	Q	102	-	41,41,41	0.21	0	47,50,50	0.24	0
13	SPO	u	102	-	41,41,41	0.20	0	47,50,50	0.40	0
13	SPO	J	102	-	41,41,41	0.19	0	47,50,50	0.27	0
13	SPO	Q	103	-	41,41,41	0.21	0	47,50,50	0.48	1 (2%)
14	CDL	f	102	-	62,62,99	1.16	8 (12%)	68,74,111	1.28	6 (8%)
13	SPO	q	103	-	41,41,41	0.21	0	47,50,50	0.48	1 (2%)
8	BCL	B	101	-	69,74,74	1.10	5 (7%)	79,115,115	1.46	10 (12%)
13	SPO	s	103	-	41,41,41	0.23	0	47,50,50	0.31	0
8	BCL	F	101	-	69,74,74	1.12	5 (7%)	79,115,115	1.43	10 (12%)
8	BCL	Z	101	-	59,64,74	1.16	3 (5%)	67,103,115	1.34	6 (8%)
8	BCL	z	101	-	59,64,74	1.17	3 (5%)	67,103,115	1.35	6 (8%)
8	BCL	2	101	-	49,54,74	1.25	4 (8%)	55,91,115	1.46	6 (10%)
13	SPO	g	101	-	41,41,41	0.21	0	47,50,50	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	b0	101	-	64,69,74	1.13	5 (7%)	73,109,115	1.53	12 (16%)
13	SPO	E	101	-	41,41,41	0.24	0	47,50,50	0.22	0
13	SPO	o	102	-	41,41,41	0.23	0	47,50,50	0.40	0
13	SPO	I	102	-	41,41,41	0.20	0	47,50,50	0.23	0
8	BCL	d	102	-	69,74,74	1.13	6 (8%)	79,115,115	1.42	11 (13%)
13	SPO	u	103	-	41,41,41	0.19	0	47,50,50	0.31	0
14	CDL	m	407	-	81,81,99	1.03	9 (11%)	87,93,111	1.21	6 (6%)
9	BPH	M	404	-	49,60,70	1.28	4 (8%)	47,89,101	2.09	9 (19%)
8	BCL	t	101	-	69,74,74	1.08	4 (5%)	79,115,115	1.31	9 (11%)
13	SPO	U	103	-	41,41,41	0.18	0	47,50,50	0.31	0
8	BCL	q	101	-	69,74,74	1.12	6 (8%)	79,115,115	1.44	12 (15%)
8	BCL	N	102	-	69,74,74	1.09	5 (7%)	79,115,115	1.34	9 (11%)
13	SPO	n	101	-	41,41,41	0.20	0	47,50,50	0.19	0
8	BCL	m	402	-	69,74,74	1.11	7 (10%)	79,115,115	1.38	7 (8%)
11	PC1	h	302	-	33,33,53	1.28	6 (18%)	39,41,61	1.11	3 (7%)
8	BCL	v	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.35	10 (12%)
13	SPO	x	101	-	41,41,41	0.25	0	47,50,50	0.35	0
13	SPO	0	102	-	41,41,41	0.25	0	47,50,50	0.27	0
13	SPO	3	102	-	41,41,41	0.19	0	47,50,50	0.31	0
13	SPO	b	102	-	41,41,41	0.25	0	47,50,50	0.24	0
10	U10	l	305	-	43,43,63	2.73	13 (30%)	54,55,79	1.76	14 (25%)
13	SPO	3	103	-	41,41,41	0.17	0	47,50,50	0.31	0
8	BCL	V	101	-	69,74,74	1.09	5 (7%)	79,115,115	1.35	10 (12%)
14	CDL	F	102	-	62,62,99	1.16	8 (12%)	68,74,111	1.28	6 (8%)
9	BPH	L	303	-	59,70,70	1.17	3 (5%)	59,101,101	2.04	11 (18%)
8	BCL	E	102	-	69,74,74	1.09	4 (5%)	79,115,115	1.35	9 (11%)
11	PC1	D	101	-	38,38,53	1.20	5 (13%)	44,46,61	1.21	3 (6%)
13	SPO	s	102	-	41,41,41	0.22	0	47,50,50	0.26	0
13	SPO	D	103	-	41,41,41	0.21	0	47,50,50	0.27	0
11	PC1	d	101	-	38,38,53	1.20	5 (13%)	44,46,61	1.21	3 (6%)
8	BCL	L	301	-	69,74,74	1.13	7 (10%)	79,115,115	1.34	11 (13%)
13	SPO	b0	102	-	41,41,41	0.25	0	47,50,50	0.27	0
8	BCL	a	101	-	69,74,74	1.12	7 (10%)	79,115,115	1.42	10 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	b9	101	-	-	1/41/137/137	-
8	BCL	l	302	-	-	0/38/134/137	-
10	U10	M	405	-	-	10/45/69/87	0/1/1/1
8	BCL	S	101	-	-	0/41/137/137	-
11	PC1	A	105	-	-	18/41/41/57	-
13	SPO	q	104	-	-	12/47/47/47	-
8	BCL	Q	101	-	-	2/41/137/137	-
8	BCL	A	101	-	-	3/41/137/137	-
13	SPO	U	102	-	-	8/47/47/47	-
8	BCL	W	101	-	-	0/41/137/137	-
10	U10	m	405	-	-	10/45/69/87	0/1/1/1
8	BCL	7	102	-	-	7/35/131/137	-
8	BCL	L	302	-	-	0/38/134/137	-
8	BCL	i	101	-	-	2/41/137/137	-
8	BCL	w	101	-	-	0/41/137/137	-
11	PC1	L	306	-	-	12/42/42/57	-
8	BCL	J	101	-	-	4/41/137/137	-
13	SPO	a	102	-	-	12/47/47/47	-
8	BCL	C	101	-	-	3/35/131/137	-
13	SPO	S	102	-	-	14/47/47/47	-
13	SPO	c	102	-	-	16/47/47/47	-
8	BCL	r	101	-	-	3/41/137/137	-
8	BCL	f	101	-	-	2/41/137/137	-
13	SPO	m	406	-	-	9/47/47/47	-
8	BCL	K	101	-	-	1/41/137/137	-
8	BCL	k	101	-	-	1/41/137/137	-
8	BCL	b1	101	-	-	0/17/113/137	-
8	BCL	6	102	-	-	7/35/131/137	-
13	SPO	G	101	-	-	11/47/47/47	-
13	SPO	g	103	-	-	11/47/47/47	-
11	PC1	L	307	-	-	19/43/43/57	-
13	SPO	C	102	-	-	16/47/47/47	-
8	BCL	5	101	-	-	0/23/119/137	-
8	BCL	R	101	-	-	3/41/137/137	-
13	SPO	p	101	-	-	10/47/47/47	-
8	BCL	U	101	-	-	0/41/137/137	-
8	BCL	0	101	-	-	3/35/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	g	102	-	-	1/41/137/137	-
13	SPO	i	102	-	-	12/47/47/47	-
14	CDL	M	407	-	-	26/92/92/110	-
11	PC1	a	103	-	-	17/48/48/57	-
8	BCL	c	101	-	-	3/35/131/137	-
8	BCL	s	101	-	-	0/41/137/137	-
13	SPO	b9	102	-	-	15/47/47/47	-
8	BCL	M	403	-	-	0/41/137/137	-
8	BCL	T	101	-	-	3/41/137/137	-
10	U10	L	305	-	-	10/39/63/87	0/1/1/1
9	BPH	l	303	-	-	2/37/105/105	0/5/6/6
8	BCL	3	101	-	-	0/23/119/137	-
13	SPO	Q	104	-	-	12/47/47/47	-
8	BCL	9	101	-	-	1/41/137/137	-
8	BCL	e	102	-	-	6/41/137/137	-
8	BCL	M	402	-	-	4/41/137/137	-
11	PC1	l	307	-	-	19/43/43/57	-
8	BCL	u	101	-	-	0/41/137/137	-
13	SPO	N	101	-	-	10/47/47/47	-
13	SPO	9	102	-	-	15/47/47/47	-
11	PC1	l	306	-	-	12/42/42/57	-
8	BCL	l	301	-	-	0/41/137/137	-
8	BCL	n	102	-	-	4/41/137/137	-
8	BCL	1	101	-	-	0/17/113/137	-
11	PC1	H	302	-	-	13/37/37/57	-
11	PC1	A	103	-	-	17/48/48/57	-
13	SPO	5	102	-	-	13/47/47/47	-
8	BCL	I	101	-	-	2/41/137/137	-
13	SPO	d	103	-	-	16/47/47/47	-
13	SPO	q	102	-	-	9/47/47/47	-
13	SPO	M	406	-	-	9/47/47/47	-
13	SPO	5	103	-	-	12/47/47/47	-
8	BCL	P	102	-	-	3/41/137/137	-
10	U10	l	304	-	-	14/33/57/87	0/1/1/1
11	PC1	a	105	-	-	18/41/41/57	-
13	SPO	j	102	-	-	13/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BPH	m	404	-	-	3/25/93/105	0/5/6/6
8	BCL	j	101	-	-	4/41/137/137	-
13	SPO	S	103	-	-	9/47/47/47	-
13	SPO	E	103	-	-	16/47/47/47	-
11	PC1	H	301	-	-	11/46/46/57	-
13	SPO	A	102	-	-	12/47/47/47	-
8	BCL	b	101	-	-	4/41/137/137	-
8	BCL	6	101	-	-	4/35/131/137	-
8	BCL	o	101	-	-	0/41/137/137	-
13	SPO	O	102	-	-	15/47/47/47	-
13	SPO	P	101	-	-	10/47/47/47	-
13	SPO	e	103	-	-	16/47/47/47	-
13	SPO	G	103	-	-	11/47/47/47	-
13	SPO	X	101	-	-	9/47/47/47	-
8	BCL	p	102	-	-	3/41/137/137	-
11	PC1	a	104	-	-	16/34/34/57	-
13	SPO	e	101	-	-	11/47/47/47	-
8	BCL	D	102	-	-	1/41/137/137	-
8	BCL	7	101	-	-	4/35/131/137	-
8	BCL	4	101	-	-	2/17/113/137	-
11	PC1	A	104	-	-	16/34/34/57	-
8	BCL	O	101	-	-	0/41/137/137	-
11	PC1	h	301	-	-	11/46/46/57	-
10	U10	L	304	-	-	14/33/57/87	0/1/1/1
8	BCL	G	102	-	-	1/41/137/137	-
8	BCL	m	403	-	-	0/41/137/137	-
13	SPO	B	102	-	-	14/47/47/47	-
13	SPO	Q	102	-	-	9/47/47/47	-
13	SPO	u	102	-	-	8/47/47/47	-
13	SPO	J	102	-	-	13/47/47/47	-
13	SPO	Q	103	-	-	11/47/47/47	-
14	CDL	f	102	-	-	29/73/73/110	-
13	SPO	q	103	-	-	11/47/47/47	-
8	BCL	B	101	-	-	4/41/137/137	-
13	SPO	s	103	-	-	9/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	F	101	-	-	2/41/137/137	-
8	BCL	Z	101	-	-	4/29/125/137	-
8	BCL	z	101	-	-	4/29/125/137	-
8	BCL	2	101	-	-	2/17/113/137	-
13	SPO	g	101	-	-	11/47/47/47	-
8	BCL	b0	101	-	-	3/35/131/137	-
13	SPO	E	101	-	-	11/47/47/47	-
13	SPO	o	102	-	-	15/47/47/47	-
13	SPO	I	102	-	-	12/47/47/47	-
8	BCL	d	102	-	-	1/41/137/137	-
13	SPO	u	103	-	-	9/47/47/47	-
14	CDL	m	407	-	-	26/92/92/110	-
9	BPH	M	404	-	-	3/25/93/105	0/5/6/6
8	BCL	t	101	-	-	3/41/137/137	-
13	SPO	U	103	-	-	9/47/47/47	-
8	BCL	q	101	-	-	2/41/137/137	-
8	BCL	N	102	-	-	4/41/137/137	-
13	SPO	n	101	-	-	10/47/47/47	-
8	BCL	m	402	-	-	4/41/137/137	-
11	PC1	h	302	-	-	13/37/37/57	-
8	BCL	v	101	-	-	3/41/137/137	-
13	SPO	x	101	-	-	9/47/47/47	-
13	SPO	0	102	-	-	14/47/47/47	-
13	SPO	3	102	-	-	13/47/47/47	-
13	SPO	b	102	-	-	14/47/47/47	-
10	U10	l	305	-	-	10/39/63/87	0/1/1/1
13	SPO	3	103	-	-	12/47/47/47	-
8	BCL	V	101	-	-	3/41/137/137	-
14	CDL	F	102	-	-	29/73/73/110	-
9	BPH	L	303	-	-	2/37/105/105	0/5/6/6
8	BCL	E	102	-	-	6/41/137/137	-
11	PC1	D	101	-	-	12/42/42/57	-
13	SPO	s	102	-	-	14/47/47/47	-
13	SPO	D	103	-	-	16/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PC1	d	101	-	-	12/42/42/57	-
8	BCL	L	301	-	-	0/41/137/137	-
13	SPO	b0	102	-	-	14/47/47/47	-
8	BCL	a	101	-	-	3/41/137/137	-

All (531) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	305	U10	C13-C14	6.27	1.47	1.33
10	l	305	U10	C13-C14	6.27	1.47	1.33
10	L	305	U10	C8-C9	6.22	1.47	1.33
10	l	305	U10	C8-C9	6.19	1.47	1.33
10	L	305	U10	C28-C29	6.18	1.47	1.33
10	l	305	U10	C28-C29	6.18	1.47	1.33
10	L	305	U10	C18-C19	6.13	1.47	1.33
10	l	305	U10	C18-C19	6.13	1.47	1.33
10	L	305	U10	C23-C24	6.12	1.47	1.33
10	l	305	U10	C23-C24	6.12	1.47	1.33
10	L	304	U10	C18-C19	6.10	1.47	1.33
10	l	304	U10	C18-C19	6.10	1.47	1.33
10	L	304	U10	C23-C24	6.05	1.47	1.33
10	l	304	U10	C23-C24	6.05	1.47	1.33
10	M	405	U10	C33-C34	6.03	1.46	1.33
10	m	405	U10	C33-C34	6.03	1.46	1.33
10	L	304	U10	C8-C9	6.02	1.46	1.33
10	l	304	U10	C8-C9	6.02	1.46	1.33
10	m	405	U10	C28-C29	6.01	1.46	1.33
10	L	304	U10	C13-C14	6.01	1.46	1.33
10	l	304	U10	C13-C14	6.01	1.46	1.33
10	M	405	U10	C28-C29	6.01	1.46	1.33
10	M	405	U10	C13-C14	5.98	1.46	1.33
10	m	405	U10	C13-C14	5.98	1.46	1.33
10	M	405	U10	C23-C24	5.96	1.46	1.33
10	m	405	U10	C23-C24	5.96	1.46	1.33
10	M	405	U10	C18-C19	5.95	1.46	1.33
10	m	405	U10	C18-C19	5.95	1.46	1.33
10	M	405	U10	C8-C9	5.91	1.46	1.33
10	m	405	U10	C8-C9	5.91	1.46	1.33
10	M	405	U10	O3-C3	-5.66	1.23	1.36
10	m	405	U10	O3-C3	-5.66	1.23	1.36
10	M	405	U10	O4-C4	-5.61	1.23	1.36
10	m	405	U10	O4-C4	-5.61	1.23	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	305	U10	O3-C3	-5.50	1.23	1.36
10	l	305	U10	O3-C3	-5.50	1.23	1.36
10	L	305	U10	O4-C4	-5.46	1.23	1.36
10	l	305	U10	O4-C4	-5.46	1.23	1.36
10	L	304	U10	O4-C4	-5.44	1.23	1.36
10	l	304	U10	O4-C4	-5.44	1.23	1.36
10	L	304	U10	O3-C3	-5.38	1.23	1.36
10	l	304	U10	O3-C3	-5.38	1.23	1.36
10	l	304	U10	C28-C29	5.01	1.47	1.32
10	L	304	U10	C28-C29	4.99	1.47	1.32
10	L	305	U10	C33-C34	4.97	1.47	1.32
10	l	305	U10	C33-C34	4.97	1.47	1.32
8	3	101	BCL	MG-NA	4.95	2.18	2.06
8	5	101	BCL	MG-NA	4.95	2.18	2.06
10	M	405	U10	C38-C39	4.93	1.47	1.32
10	m	405	U10	C38-C39	4.93	1.47	1.32
8	z	101	BCL	MG-NA	4.86	2.17	2.06
8	Z	101	BCL	MG-NA	4.85	2.17	2.06
8	2	101	BCL	MG-NA	4.76	2.17	2.06
8	4	101	BCL	MG-NA	4.76	2.17	2.06
8	1	101	BCL	MG-NA	4.76	2.17	2.06
8	b1	101	BCL	MG-NA	4.76	2.17	2.06
8	c	101	BCL	MG-NA	4.72	2.17	2.06
8	C	101	BCL	MG-NA	4.71	2.17	2.06
8	J	101	BCL	MG-NA	4.67	2.17	2.06
8	j	101	BCL	MG-NA	4.67	2.17	2.06
8	Q	101	BCL	MG-NA	4.66	2.17	2.06
8	q	101	BCL	MG-NA	4.66	2.17	2.06
8	g	102	BCL	MG-NA	4.66	2.17	2.06
8	G	102	BCL	MG-NA	4.65	2.17	2.06
8	P	102	BCL	MG-NA	4.64	2.17	2.06
8	p	102	BCL	MG-NA	4.64	2.17	2.06
8	S	101	BCL	MG-NA	4.64	2.17	2.06
8	s	101	BCL	MG-NA	4.64	2.17	2.06
8	W	101	BCL	MG-NA	4.63	2.17	2.06
8	w	101	BCL	MG-NA	4.63	2.17	2.06
8	n	102	BCL	MG-NA	4.63	2.17	2.06
8	R	101	BCL	MG-NA	4.63	2.17	2.06
8	r	101	BCL	MG-NA	4.63	2.17	2.06
8	N	102	BCL	MG-NA	4.62	2.17	2.06
8	T	101	BCL	MG-NA	4.61	2.17	2.06
8	t	101	BCL	MG-NA	4.61	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	101	BCL	MG-NA	4.61	2.17	2.06
8	u	101	BCL	MG-NA	4.61	2.17	2.06
8	E	102	BCL	MG-NA	4.59	2.17	2.06
8	e	102	BCL	MG-NA	4.59	2.17	2.06
8	B	101	BCL	MG-NA	4.58	2.17	2.06
8	b	101	BCL	MG-NA	4.58	2.17	2.06
9	M	404	BPH	CBD-CGD	-4.57	1.46	1.52
9	m	404	BPH	CBD-CGD	-4.57	1.46	1.52
8	V	101	BCL	MG-NA	4.54	2.17	2.06
8	v	101	BCL	MG-NA	4.54	2.17	2.06
8	0	101	BCL	MG-NA	4.53	2.17	2.06
8	F	101	BCL	MG-NA	4.52	2.17	2.06
8	f	101	BCL	MG-NA	4.52	2.17	2.06
8	K	101	BCL	MG-NA	4.51	2.17	2.06
8	k	101	BCL	MG-NA	4.51	2.17	2.06
8	M	403	BCL	MG-NA	4.51	2.17	2.06
8	m	403	BCL	MG-NA	4.51	2.17	2.06
8	b0	101	BCL	MG-NA	4.49	2.16	2.06
9	L	303	BPH	CBD-CGD	-4.49	1.46	1.52
9	l	303	BPH	CBD-CGD	-4.46	1.46	1.52
8	D	102	BCL	MG-NA	4.42	2.16	2.06
8	d	102	BCL	MG-NA	4.42	2.16	2.06
8	7	102	BCL	MG-NA	4.37	2.16	2.06
8	6	102	BCL	MG-NA	4.37	2.16	2.06
8	M	402	BCL	MG-NA	4.34	2.16	2.06
8	m	402	BCL	MG-NA	4.34	2.16	2.06
8	9	101	BCL	MG-NA	4.30	2.16	2.06
8	b9	101	BCL	MG-NA	4.30	2.16	2.06
8	L	301	BCL	MG-NA	4.29	2.16	2.06
8	l	301	BCL	MG-NA	4.28	2.16	2.06
8	a	101	BCL	MG-NA	4.27	2.16	2.06
8	A	101	BCL	MG-NA	4.27	2.16	2.06
8	7	101	BCL	MG-NA	4.26	2.16	2.06
8	6	101	BCL	MG-NA	4.26	2.16	2.06
8	l	302	BCL	MG-NA	4.25	2.16	2.06
8	L	302	BCL	MG-NA	4.23	2.16	2.06
8	I	101	BCL	MG-NA	4.21	2.16	2.06
8	i	101	BCL	MG-NA	4.21	2.16	2.06
8	O	101	BCL	MG-NA	4.20	2.16	2.06
8	o	101	BCL	MG-NA	4.20	2.16	2.06
9	L	303	BPH	C3D-CAD	-3.60	1.40	1.47
9	l	303	BPH	C3D-CAD	-3.60	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	5	101	BCL	MG-NC	3.59	2.14	2.06
8	3	101	BCL	MG-NC	3.58	2.14	2.06
8	1	101	BCL	MG-NC	3.53	2.14	2.06
8	b1	101	BCL	MG-NC	3.53	2.14	2.06
8	2	101	BCL	MG-NC	3.52	2.14	2.06
8	4	101	BCL	MG-NC	3.52	2.14	2.06
8	z	101	BCL	MG-NC	3.46	2.14	2.06
8	Z	101	BCL	MG-NC	3.45	2.14	2.06
9	M	404	BPH	C3D-CAD	-3.41	1.41	1.47
9	m	404	BPH	C3D-CAD	-3.41	1.41	1.47
10	M	405	U10	C3-C2	-3.38	1.39	1.48
10	m	405	U10	C3-C2	-3.38	1.39	1.48
10	M	405	U10	C4-C5	-3.37	1.39	1.48
10	m	405	U10	C4-C5	-3.37	1.39	1.48
10	L	305	U10	C4-C5	-3.31	1.39	1.48
10	l	305	U10	C4-C5	-3.31	1.39	1.48
8	T	101	BCL	MG-NC	3.30	2.14	2.06
8	t	101	BCL	MG-NC	3.30	2.14	2.06
8	u	101	BCL	MG-NC	3.30	2.14	2.06
8	v	101	BCL	MG-NC	3.30	2.14	2.06
8	U	101	BCL	MG-NC	3.29	2.14	2.06
8	V	101	BCL	MG-NC	3.29	2.14	2.06
10	L	304	U10	C4-C5	-3.25	1.39	1.48
10	l	304	U10	C4-C5	-3.25	1.39	1.48
8	j	101	BCL	MG-NC	3.23	2.14	2.06
8	f	101	BCL	MG-NC	3.23	2.13	2.06
8	F	101	BCL	MG-NC	3.22	2.13	2.06
8	q	101	BCL	MG-NC	3.22	2.13	2.06
8	Q	101	BCL	MG-NC	3.22	2.13	2.06
8	J	101	BCL	MG-NC	3.22	2.13	2.06
8	G	102	BCL	MG-NC	3.21	2.13	2.06
8	R	101	BCL	MG-NC	3.19	2.13	2.06
8	r	101	BCL	MG-NC	3.19	2.13	2.06
8	C	101	BCL	MG-NC	3.17	2.13	2.06
8	g	102	BCL	MG-NC	3.17	2.13	2.06
8	c	101	BCL	MG-NC	3.17	2.13	2.06
8	w	101	BCL	MG-NC	3.14	2.13	2.06
8	N	102	BCL	MG-NC	3.14	2.13	2.06
8	W	101	BCL	MG-NC	3.14	2.13	2.06
8	P	102	BCL	MG-NC	3.14	2.13	2.06
8	p	102	BCL	MG-NC	3.14	2.13	2.06
10	L	305	U10	C3-C2	-3.12	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	l	305	U10	C3-C2	-3.12	1.39	1.48
8	s	101	BCL	MG-NC	3.11	2.13	2.06
8	S	101	BCL	MG-NC	3.11	2.13	2.06
8	n	102	BCL	MG-NC	3.10	2.13	2.06
8	E	102	BCL	MG-NC	3.09	2.13	2.06
8	e	102	BCL	MG-NC	3.09	2.13	2.06
8	K	101	BCL	MG-NC	3.03	2.13	2.06
8	k	101	BCL	MG-NC	3.03	2.13	2.06
8	A	101	BCL	MG-NC	3.01	2.13	2.06
8	a	101	BCL	MG-NC	3.01	2.13	2.06
8	D	102	BCL	MG-NC	2.95	2.13	2.06
8	d	102	BCL	MG-NC	2.95	2.13	2.06
8	b0	101	BCL	MG-NC	2.95	2.13	2.06
8	B	101	BCL	MG-NC	2.94	2.13	2.06
8	b	101	BCL	MG-NC	2.94	2.13	2.06
8	0	101	BCL	MG-NC	2.94	2.13	2.06
8	7	102	BCL	MG-NC	2.94	2.13	2.06
8	6	102	BCL	MG-NC	2.94	2.13	2.06
8	9	101	BCL	MG-NC	2.92	2.13	2.06
8	b9	101	BCL	MG-NC	2.92	2.13	2.06
8	7	101	BCL	MG-NC	2.92	2.13	2.06
8	6	101	BCL	MG-NC	2.92	2.13	2.06
8	m	402	BCL	MG-NC	2.88	2.13	2.06
11	d	101	PC1	O21-C2	-2.88	1.39	1.46
8	i	101	BCL	MG-NC	2.88	2.13	2.06
10	L	304	U10	C3-C2	-2.88	1.40	1.48
10	l	304	U10	C3-C2	-2.88	1.40	1.48
8	I	101	BCL	MG-NC	2.88	2.13	2.06
8	M	402	BCL	MG-NC	2.87	2.13	2.06
11	D	101	PC1	O21-C2	-2.84	1.39	1.46
14	M	407	CDL	OA6-CA4	-2.83	1.39	1.46
14	m	407	CDL	OA6-CA4	-2.83	1.39	1.46
11	A	104	PC1	O21-C2	-2.78	1.40	1.46
11	a	104	PC1	O21-C2	-2.78	1.40	1.46
14	M	407	CDL	OB6-CB4	-2.77	1.40	1.46
14	m	407	CDL	OB6-CB4	-2.77	1.40	1.46
8	L	301	BCL	MG-NC	2.77	2.12	2.06
8	l	301	BCL	MG-NC	2.77	2.12	2.06
10	M	405	U10	C6-C5	-2.77	1.38	1.46
10	m	405	U10	C6-C5	-2.77	1.38	1.46
8	O	101	BCL	MG-NC	2.77	2.12	2.06
8	o	101	BCL	MG-NC	2.77	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	301	BCL	O1A-CGA	-2.74	1.14	1.22
14	F	102	CDL	OB6-CB4	-2.73	1.40	1.46
14	f	102	CDL	OB6-CB4	-2.73	1.40	1.46
8	L	301	BCL	O1A-CGA	-2.73	1.14	1.22
11	H	301	PC1	O21-C2	-2.73	1.40	1.46
11	h	301	PC1	O21-C2	-2.73	1.40	1.46
14	f	102	CDL	OA6-CA4	-2.73	1.40	1.46
11	L	307	PC1	O21-C2	-2.72	1.40	1.46
11	l	307	PC1	O21-C2	-2.72	1.40	1.46
14	F	102	CDL	OA6-CA4	-2.71	1.40	1.46
11	A	103	PC1	O21-C2	-2.71	1.40	1.46
11	a	103	PC1	O21-C2	-2.71	1.40	1.46
10	L	305	U10	C6-C5	-2.70	1.38	1.46
10	l	305	U10	C6-C5	-2.70	1.38	1.46
8	L	302	BCL	MG-NC	2.65	2.12	2.06
8	l	302	BCL	MG-NC	2.65	2.12	2.06
10	L	304	U10	C6-C5	-2.65	1.39	1.46
10	l	304	U10	C6-C5	-2.65	1.39	1.46
11	L	306	PC1	O21-C2	-2.64	1.40	1.46
11	l	306	PC1	O21-C2	-2.64	1.40	1.46
8	Q	101	BCL	C3B-C4B	2.58	1.46	1.41
8	q	101	BCL	C3B-C4B	2.58	1.46	1.41
8	M	403	BCL	MG-NC	2.58	2.12	2.06
8	m	403	BCL	MG-NC	2.58	2.12	2.06
10	M	405	U10	C1-C2	-2.56	1.38	1.47
10	m	405	U10	C1-C2	-2.56	1.38	1.47
8	L	302	BCL	C1D-C2D	-2.55	1.40	1.45
8	l	302	BCL	C1D-C2D	-2.55	1.40	1.45
8	M	403	BCL	C3B-C4B	2.55	1.46	1.41
8	m	403	BCL	C3B-C4B	2.55	1.46	1.41
8	S	101	BCL	C3B-C4B	2.53	1.46	1.41
8	s	101	BCL	C3B-C4B	2.53	1.46	1.41
8	D	102	BCL	C3B-C4B	2.53	1.46	1.41
8	d	102	BCL	C3B-C4B	2.53	1.46	1.41
11	H	302	PC1	O21-C2	-2.52	1.40	1.46
11	h	302	PC1	O21-C2	-2.52	1.40	1.46
8	e	102	BCL	C1D-C2D	-2.51	1.40	1.45
8	M	403	BCL	C3D-C4D	-2.49	1.38	1.44
8	m	403	BCL	C3D-C4D	-2.49	1.38	1.44
8	E	102	BCL	C1D-C2D	-2.48	1.40	1.45
8	7	101	BCL	C3B-C4B	2.48	1.46	1.41
8	6	101	BCL	C3B-C4B	2.48	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	303	BPH	C3B-C4B	2.48	1.45	1.41
9	l	303	BPH	C3B-C4B	2.48	1.45	1.41
11	H	302	PC1	O21-C21	2.45	1.41	1.34
11	h	302	PC1	O21-C21	2.45	1.41	1.34
8	M	403	BCL	CBD-CGD	-2.45	1.45	1.52
8	m	403	BCL	CBD-CGD	-2.45	1.45	1.52
14	F	102	CDL	OA8-CA7	2.45	1.40	1.33
14	f	102	CDL	OA8-CA7	2.45	1.40	1.33
11	H	301	PC1	O31-C3	-2.44	1.39	1.45
11	h	301	PC1	O31-C3	-2.44	1.39	1.45
14	M	407	CDL	OA8-CA7	2.44	1.40	1.33
14	m	407	CDL	OA8-CA7	2.44	1.40	1.33
11	A	103	PC1	O31-C31	2.43	1.40	1.33
11	a	103	PC1	O31-C31	2.43	1.40	1.33
8	A	101	BCL	C3B-C4B	2.43	1.45	1.41
8	a	101	BCL	C3B-C4B	2.43	1.45	1.41
8	L	302	BCL	C3D-C4D	-2.42	1.38	1.44
8	l	302	BCL	C3D-C4D	-2.42	1.38	1.44
8	M	402	BCL	C3D-C4D	-2.42	1.38	1.44
8	m	402	BCL	C3D-C4D	-2.42	1.38	1.44
8	T	101	BCL	C1D-C2D	-2.42	1.40	1.45
8	t	101	BCL	C1D-C2D	-2.42	1.40	1.45
8	9	101	BCL	C1D-C2D	-2.40	1.40	1.45
8	b9	101	BCL	C1D-C2D	-2.40	1.40	1.45
8	3	101	BCL	C3B-C4B	2.39	1.45	1.41
8	W	101	BCL	CHD-C1D	2.39	1.43	1.38
8	w	101	BCL	CHD-C1D	2.39	1.43	1.38
8	l	301	BCL	C3B-C4B	2.39	1.45	1.41
11	l	307	PC1	O31-C31	2.38	1.40	1.33
8	7	102	BCL	C3D-C4D	-2.38	1.38	1.44
8	6	102	BCL	C3D-C4D	-2.38	1.38	1.44
14	F	102	CDL	OB8-CB7	2.38	1.40	1.33
14	f	102	CDL	OB8-CB7	2.38	1.40	1.33
8	B	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	b	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	7	102	BCL	C1D-C2D	-2.38	1.40	1.45
8	6	102	BCL	C1D-C2D	-2.38	1.40	1.45
8	U	101	BCL	C3B-C4B	2.38	1.45	1.41
8	u	101	BCL	C3B-C4B	2.38	1.45	1.41
8	V	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	v	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	0	101	BCL	C1D-C2D	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b0	101	BCL	C1D-C2D	-2.37	1.40	1.45
8	0	101	BCL	C3D-C4D	-2.37	1.38	1.44
8	b0	101	BCL	C3D-C4D	-2.37	1.38	1.44
14	m	407	CDL	OB8-CB7	2.37	1.40	1.33
8	5	101	BCL	C3B-C4B	2.37	1.45	1.41
11	L	306	PC1	O31-C31	2.36	1.40	1.33
11	l	306	PC1	O31-C31	2.36	1.40	1.33
14	M	407	CDL	OB8-CB7	2.36	1.40	1.33
11	L	307	PC1	O31-C31	2.36	1.40	1.33
8	D	102	BCL	C3D-C4D	-2.35	1.38	1.44
8	d	102	BCL	C3D-C4D	-2.35	1.38	1.44
8	L	301	BCL	C3B-C4B	2.34	1.45	1.41
8	N	102	BCL	C1D-C2D	-2.34	1.40	1.45
8	n	102	BCL	C1D-C2D	-2.34	1.40	1.45
8	E	102	BCL	C3D-C4D	-2.34	1.38	1.44
8	e	102	BCL	C3D-C4D	-2.34	1.38	1.44
8	G	102	BCL	C1D-C2D	-2.34	1.40	1.45
8	g	102	BCL	C1D-C2D	-2.34	1.40	1.45
8	B	101	BCL	C3D-C4D	-2.34	1.38	1.44
8	b	101	BCL	C3D-C4D	-2.34	1.38	1.44
11	D	101	PC1	O31-C31	2.33	1.40	1.33
11	d	101	PC1	O31-C31	2.33	1.40	1.33
11	A	104	PC1	O31-C3	-2.32	1.40	1.45
11	a	104	PC1	O31-C3	-2.32	1.40	1.45
8	2	101	BCL	CHD-C1D	2.32	1.42	1.38
8	4	101	BCL	CHD-C1D	2.32	1.42	1.38
8	A	101	BCL	C1D-C2D	-2.32	1.40	1.45
8	a	101	BCL	C1D-C2D	-2.32	1.40	1.45
8	M	402	BCL	C1D-C2D	-2.30	1.40	1.45
8	m	402	BCL	C1D-C2D	-2.30	1.40	1.45
11	H	302	PC1	O31-C31	2.29	1.40	1.33
11	h	302	PC1	O31-C31	2.29	1.40	1.33
8	7	101	BCL	C3D-C4D	-2.29	1.39	1.44
8	6	101	BCL	C3D-C4D	-2.29	1.39	1.44
8	A	101	BCL	C3D-C4D	-2.29	1.39	1.44
8	a	101	BCL	C3D-C4D	-2.29	1.39	1.44
8	N	102	BCL	C3D-C4D	-2.29	1.39	1.44
8	n	102	BCL	C3D-C4D	-2.29	1.39	1.44
10	L	304	U10	C1-C2	-2.29	1.39	1.47
10	l	304	U10	C1-C2	-2.29	1.39	1.47
8	D	102	BCL	O1A-CGA	-2.29	1.15	1.22
8	d	102	BCL	O1A-CGA	-2.29	1.15	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	302	PC1	O31-C3	-2.28	1.40	1.45
11	h	302	PC1	O31-C3	-2.28	1.40	1.45
8	l	101	BCL	C3B-C4B	2.28	1.45	1.41
8	b1	101	BCL	C3B-C4B	2.28	1.45	1.41
8	K	101	BCL	C3B-C4B	2.28	1.45	1.41
8	k	101	BCL	C3B-C4B	2.28	1.45	1.41
8	K	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	k	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	9	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	b9	101	BCL	C3D-C4D	-2.28	1.39	1.44
10	l	305	U10	C1-C2	-2.28	1.39	1.47
8	M	403	BCL	O1A-CGA	-2.27	1.15	1.22
8	m	403	BCL	O1A-CGA	-2.27	1.15	1.22
8	L	301	BCL	C3D-C4D	-2.27	1.39	1.44
8	l	301	BCL	C3D-C4D	-2.27	1.39	1.44
10	L	305	U10	C1-C2	-2.27	1.39	1.47
8	l	101	BCL	CHD-C1D	2.27	1.42	1.38
8	b1	101	BCL	CHD-C1D	2.27	1.42	1.38
11	A	104	PC1	O31-C31	2.26	1.39	1.33
11	a	104	PC1	O31-C31	2.26	1.39	1.33
8	R	101	BCL	C3D-C4D	-2.26	1.39	1.44
8	r	101	BCL	C3D-C4D	-2.26	1.39	1.44
8	L	301	BCL	C1D-C2D	-2.26	1.40	1.45
8	l	301	BCL	C1D-C2D	-2.26	1.40	1.45
8	G	102	BCL	C3D-C4D	-2.26	1.39	1.44
8	g	102	BCL	C3D-C4D	-2.26	1.39	1.44
8	p	102	BCL	C1D-C2D	-2.25	1.40	1.45
8	Q	101	BCL	C3D-C4D	-2.25	1.39	1.44
8	T	101	BCL	C3D-C4D	-2.25	1.39	1.44
8	t	101	BCL	C3D-C4D	-2.25	1.39	1.44
8	P	102	BCL	C3D-C4D	-2.24	1.39	1.44
8	p	102	BCL	C3D-C4D	-2.24	1.39	1.44
8	F	101	BCL	C3B-C4B	2.24	1.45	1.41
8	f	101	BCL	C3B-C4B	2.24	1.45	1.41
8	P	102	BCL	C1D-C2D	-2.23	1.40	1.45
10	L	304	U10	C6-C1	2.23	1.39	1.35
10	l	304	U10	C6-C1	2.23	1.39	1.35
8	S	101	BCL	C3D-C4D	-2.23	1.39	1.44
8	s	101	BCL	C3D-C4D	-2.22	1.39	1.44
8	J	101	BCL	C3D-C4D	-2.22	1.39	1.44
8	j	101	BCL	C3D-C4D	-2.22	1.39	1.44
11	D	101	PC1	O31-C3	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	305	U10	C6-C1	2.22	1.39	1.35
10	l	305	U10	C6-C1	2.22	1.39	1.35
11	l	307	PC1	O31-C3	-2.22	1.40	1.45
8	D	102	BCL	C1D-C2D	-2.22	1.40	1.45
8	d	102	BCL	C1D-C2D	-2.22	1.40	1.45
8	L	302	BCL	O1A-CGA	-2.22	1.15	1.22
8	l	302	BCL	O1A-CGA	-2.22	1.15	1.22
8	V	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	v	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	I	101	BCL	C1D-C2D	-2.21	1.41	1.45
8	i	101	BCL	C1D-C2D	-2.21	1.41	1.45
8	S	101	BCL	C1D-C2D	-2.21	1.41	1.45
8	s	101	BCL	C1D-C2D	-2.21	1.41	1.45
11	A	103	PC1	O31-C3	-2.21	1.40	1.45
11	a	103	PC1	O31-C3	-2.21	1.40	1.45
8	q	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	O	101	BCL	C1D-C2D	-2.20	1.41	1.45
8	o	101	BCL	C1D-C2D	-2.20	1.41	1.45
8	O	101	BCL	C3D-C4D	-2.20	1.39	1.44
8	o	101	BCL	C3D-C4D	-2.20	1.39	1.44
11	d	101	PC1	O31-C3	-2.20	1.40	1.45
8	M	403	BCL	C1D-C2D	-2.20	1.41	1.45
8	f	101	BCL	C3D-C4D	-2.20	1.39	1.44
11	L	307	PC1	O31-C3	-2.19	1.40	1.45
8	m	403	BCL	C1D-C2D	-2.19	1.41	1.45
8	I	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	i	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	R	101	BCL	C1D-C2D	-2.19	1.41	1.45
8	r	101	BCL	C1D-C2D	-2.19	1.41	1.45
14	M	407	CDL	OB8-CB6	-2.18	1.40	1.45
14	m	407	CDL	OB8-CB6	-2.18	1.40	1.45
8	F	101	BCL	C3D-C4D	-2.18	1.39	1.44
14	M	407	CDL	OA8-CA6	-2.18	1.40	1.45
14	m	407	CDL	OA8-CA6	-2.18	1.40	1.45
8	9	101	BCL	O1A-CGA	-2.18	1.16	1.22
8	b9	101	BCL	O1A-CGA	-2.18	1.16	1.22
11	L	306	PC1	O31-C3	-2.17	1.40	1.45
11	l	306	PC1	O31-C3	-2.17	1.40	1.45
11	H	301	PC1	O31-C31	2.17	1.39	1.33
11	h	301	PC1	O31-C31	2.17	1.39	1.33
8	J	101	BCL	C1D-C2D	-2.17	1.41	1.45
8	j	101	BCL	C1D-C2D	-2.17	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	101	BCL	C3B-C4B	2.17	1.45	1.41
8	b9	101	BCL	C3B-C4B	2.17	1.45	1.41
8	f	101	BCL	C1D-C2D	-2.15	1.41	1.45
8	0	101	BCL	C3B-C4B	2.15	1.45	1.41
8	b0	101	BCL	C3B-C4B	2.15	1.45	1.41
8	Q	101	BCL	C1D-C2D	-2.15	1.41	1.45
8	q	101	BCL	C1D-C2D	-2.15	1.41	1.45
8	M	402	BCL	C3B-C4B	2.14	1.45	1.41
8	m	402	BCL	C3B-C4B	2.14	1.45	1.41
8	K	101	BCL	C1D-C2D	-2.14	1.41	1.45
8	k	101	BCL	C1D-C2D	-2.14	1.41	1.45
8	F	101	BCL	C1D-C2D	-2.14	1.41	1.45
8	C	101	BCL	CHD-C1D	2.13	1.42	1.38
8	c	101	BCL	CHD-C1D	2.13	1.42	1.38
8	I	101	BCL	CHD-C1D	2.13	1.42	1.38
8	i	101	BCL	CHD-C1D	2.13	1.42	1.38
8	O	101	BCL	C3B-C4B	2.13	1.45	1.41
8	o	101	BCL	C3B-C4B	2.13	1.45	1.41
8	W	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	w	101	BCL	C3D-C4D	-2.13	1.39	1.44
14	F	102	CDL	OB8-CB6	-2.13	1.40	1.45
14	f	102	CDL	OB8-CB6	-2.13	1.40	1.45
8	K	101	BCL	O1A-CGA	-2.12	1.16	1.22
8	k	101	BCL	O1A-CGA	-2.12	1.16	1.22
11	A	103	PC1	O21-C21	2.12	1.40	1.34
11	a	103	PC1	O21-C21	2.12	1.40	1.34
11	H	301	PC1	O21-C21	2.12	1.40	1.34
11	h	301	PC1	O21-C21	2.12	1.40	1.34
11	L	306	PC1	O21-C21	2.12	1.40	1.34
11	l	306	PC1	O21-C21	2.12	1.40	1.34
8	M	402	BCL	CHD-C1D	2.11	1.42	1.38
8	m	402	BCL	CHD-C1D	2.11	1.42	1.38
14	F	102	CDL	OA6-CA5	2.11	1.40	1.34
14	f	102	CDL	OA6-CA5	2.11	1.40	1.34
8	U	101	BCL	C3D-C4D	-2.10	1.39	1.44
8	u	101	BCL	C3D-C4D	-2.10	1.39	1.44
8	3	101	BCL	CHD-C1D	2.10	1.42	1.38
8	5	101	BCL	CHD-C1D	2.10	1.42	1.38
8	G	102	BCL	C3B-C4B	2.09	1.45	1.41
8	g	102	BCL	C3B-C4B	2.09	1.45	1.41
11	L	307	PC1	O21-C21	2.09	1.40	1.34
11	d	101	PC1	O21-C21	2.09	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	407	CDL	OB6-CB5	2.09	1.40	1.34
14	m	407	CDL	OB6-CB5	2.09	1.40	1.34
14	M	407	CDL	OA6-CA5	2.09	1.40	1.34
14	m	407	CDL	OA6-CA5	2.09	1.40	1.34
8	L	302	BCL	C3B-C4B	2.08	1.45	1.41
8	I	101	BCL	O1A-CGA	-2.08	1.16	1.22
8	i	101	BCL	O1A-CGA	-2.08	1.16	1.22
8	O	101	BCL	CHD-C1D	2.07	1.42	1.38
14	f	102	CDL	OB6-CB5	2.07	1.40	1.34
9	M	404	BPH	C1C-C2C	-2.07	1.47	1.51
9	m	404	BPH	C1C-C2C	-2.07	1.47	1.51
10	M	405	U10	C6-C1	2.07	1.38	1.35
10	m	405	U10	C6-C1	2.07	1.38	1.35
11	A	104	PC1	O21-C21	2.07	1.40	1.34
11	a	104	PC1	O21-C21	2.07	1.40	1.34
8	J	101	BCL	C3B-C4B	2.07	1.45	1.41
8	j	101	BCL	C3B-C4B	2.07	1.45	1.41
8	w	101	BCL	C3B-C4B	2.07	1.45	1.41
8	I	101	BCL	C3B-C4B	2.07	1.45	1.41
8	i	101	BCL	C3B-C4B	2.07	1.45	1.41
8	V	101	BCL	C3B-C4B	2.07	1.45	1.41
8	v	101	BCL	C3B-C4B	2.07	1.45	1.41
8	L	302	BCL	CHD-C1D	2.06	1.42	1.38
8	l	302	BCL	CHD-C1D	2.06	1.42	1.38
11	l	307	PC1	O21-C21	2.06	1.40	1.34
8	Q	101	BCL	CHD-C1D	2.06	1.42	1.38
8	q	101	BCL	CHD-C1D	2.06	1.42	1.38
8	2	101	BCL	C3B-C4B	2.06	1.45	1.41
8	4	101	BCL	C3B-C4B	2.06	1.45	1.41
14	F	102	CDL	OB6-CB5	2.06	1.40	1.34
8	S	101	BCL	O1A-CGA	-2.06	1.16	1.22
8	s	101	BCL	O1A-CGA	-2.06	1.16	1.22
8	C	101	BCL	C3B-C4B	2.06	1.45	1.41
8	c	101	BCL	C3B-C4B	2.06	1.45	1.41
11	D	101	PC1	O21-C21	2.06	1.40	1.34
8	l	301	BCL	CHD-C1D	2.06	1.42	1.38
14	M	407	CDL	PB2-OB4	-2.06	1.45	1.55
14	m	407	CDL	PB2-OB4	-2.06	1.45	1.55
8	l	302	BCL	C3B-C4B	2.06	1.45	1.41
14	F	102	CDL	OA8-CA6	-2.05	1.40	1.45
14	f	102	CDL	OA8-CA6	-2.05	1.40	1.45
11	H	301	PC1	P-O12	-2.05	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	h	301	PC1	P-O12	-2.05	1.45	1.55
8	S	101	BCL	CHD-C1D	2.05	1.42	1.38
8	s	101	BCL	CHD-C1D	2.05	1.42	1.38
8	U	101	BCL	C1D-C2D	-2.05	1.41	1.45
8	z	101	BCL	CHD-C1D	2.05	1.42	1.38
8	W	101	BCL	C3B-C4B	2.03	1.45	1.41
8	B	101	BCL	C3B-C4B	2.03	1.45	1.41
8	b	101	BCL	C3B-C4B	2.03	1.45	1.41
8	Z	101	BCL	CHD-C1D	2.03	1.42	1.38
8	o	101	BCL	CHD-C1D	2.03	1.42	1.38
11	H	302	PC1	C12-N	-2.03	1.45	1.51
11	h	302	PC1	C12-N	-2.03	1.45	1.51
8	M	402	BCL	CBD-CGD	-2.03	1.46	1.52
8	m	402	BCL	CBD-CGD	-2.03	1.46	1.52
8	A	101	BCL	O1A-CGA	-2.03	1.16	1.22
8	a	101	BCL	O1A-CGA	-2.03	1.16	1.22
8	N	102	BCL	C3B-C4B	2.02	1.45	1.41
8	n	102	BCL	C3B-C4B	2.02	1.45	1.41
8	C	101	BCL	C3D-C4D	-2.02	1.39	1.44
8	c	101	BCL	C3D-C4D	-2.02	1.39	1.44
8	u	101	BCL	C1D-C2D	-2.02	1.41	1.45
8	l	101	BCL	C3D-C4D	-2.01	1.39	1.44
8	b1	101	BCL	C3D-C4D	-2.01	1.39	1.44
11	D	101	PC1	P-O12	-2.01	1.46	1.55
11	d	101	PC1	P-O12	-2.01	1.46	1.55
8	L	301	BCL	CHD-C1D	2.01	1.42	1.38
8	C	101	BCL	C1D-C2D	-2.01	1.41	1.45
8	7	102	BCL	C3B-C4B	2.01	1.45	1.41
11	H	302	PC1	P-O12	-2.01	1.46	1.55
11	h	302	PC1	P-O12	-2.01	1.46	1.55
8	6	102	BCL	C3B-C4B	2.01	1.45	1.41
8	A	101	BCL	CBD-CGD	-2.00	1.46	1.52
8	a	101	BCL	CBD-CGD	-2.00	1.46	1.52
9	M	404	BPH	C3B-C4B	2.00	1.44	1.41
9	m	404	BPH	C3B-C4B	2.00	1.44	1.41

All (777) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	303	BPH	C4D-CHA-CBD	-10.65	103.35	108.45
9	l	303	BPH	C4D-CHA-CBD	-10.65	103.35	108.45
9	M	404	BPH	C4D-CHA-CBD	-10.19	103.56	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	m	404	BPH	C4D-CHA-CBD	-10.19	103.56	108.45
8	m	403	BCL	C4D-CHA-C1A	5.57	127.89	121.24
8	M	403	BCL	C4D-CHA-C1A	5.55	127.87	121.24
8	I	101	BCL	C4D-CHA-C1A	5.50	127.81	121.24
8	i	101	BCL	C4D-CHA-C1A	5.50	127.80	121.24
8	Q	101	BCL	C4D-CHA-C1A	5.40	127.68	121.24
8	q	101	BCL	C4D-CHA-C1A	5.40	127.68	121.24
8	k	101	BCL	C4D-CHA-C1A	5.37	127.65	121.24
8	O	101	BCL	C4D-CHA-C1A	5.36	127.64	121.24
8	o	101	BCL	C4D-CHA-C1A	5.36	127.64	121.24
8	D	102	BCL	C4D-CHA-C1A	5.36	127.63	121.24
8	d	102	BCL	C4D-CHA-C1A	5.36	127.63	121.24
8	K	101	BCL	C4D-CHA-C1A	5.35	127.62	121.24
8	U	101	BCL	C4D-CHA-C1A	5.35	127.62	121.24
8	u	101	BCL	C4D-CHA-C1A	5.35	127.62	121.24
8	F	101	BCL	C4D-CHA-C1A	5.34	127.61	121.24
8	f	101	BCL	C4D-CHA-C1A	5.34	127.61	121.24
8	S	101	BCL	C4D-CHA-C1A	5.33	127.60	121.24
8	s	101	BCL	C4D-CHA-C1A	5.33	127.60	121.24
8	B	101	BCL	C4D-CHA-C1A	5.33	127.60	121.24
8	b	101	BCL	C4D-CHA-C1A	5.33	127.60	121.24
8	9	101	BCL	C4D-CHA-C1A	5.32	127.59	121.24
8	b9	101	BCL	C4D-CHA-C1A	5.32	127.59	121.24
8	M	402	BCL	C4D-CHA-C1A	5.31	127.58	121.24
8	m	402	BCL	C4D-CHA-C1A	5.31	127.58	121.24
8	A	101	BCL	C4D-CHA-C1A	5.30	127.56	121.24
8	a	101	BCL	C4D-CHA-C1A	5.30	127.56	121.24
8	J	101	BCL	C4D-CHA-C1A	5.29	127.55	121.24
8	j	101	BCL	C4D-CHA-C1A	5.29	127.55	121.24
8	3	101	BCL	C4D-CHA-C1A	5.28	127.54	121.24
8	5	101	BCL	C4D-CHA-C1A	5.28	127.54	121.24
8	z	101	BCL	C4D-CHA-C1A	5.27	127.53	121.24
8	0	101	BCL	C4D-CHA-C1A	5.26	127.51	121.24
8	b0	101	BCL	C4D-CHA-C1A	5.26	127.51	121.24
8	7	101	BCL	C4D-CHA-C1A	5.25	127.51	121.24
8	6	101	BCL	C4D-CHA-C1A	5.25	127.51	121.24
8	w	101	BCL	C4D-CHA-C1A	5.25	127.50	121.24
8	1	101	BCL	C4D-CHA-C1A	5.24	127.50	121.24
8	b1	101	BCL	C4D-CHA-C1A	5.24	127.50	121.24
8	Z	101	BCL	C4D-CHA-C1A	5.24	127.50	121.24
8	W	101	BCL	C4D-CHA-C1A	5.23	127.48	121.24
8	R	101	BCL	C4D-CHA-C1A	5.23	127.48	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	101	BCL	C4D-CHA-C1A	5.23	127.48	121.24
8	r	101	BCL	C4D-CHA-C1A	5.23	127.48	121.24
8	c	101	BCL	C4D-CHA-C1A	5.23	127.48	121.24
8	l	302	BCL	C4D-CHA-C1A	5.22	127.47	121.24
8	L	302	BCL	C4D-CHA-C1A	5.20	127.44	121.24
8	n	102	BCL	C4D-CHA-C1A	5.19	127.43	121.24
8	e	102	BCL	C4D-CHA-C1A	5.18	127.42	121.24
8	N	102	BCL	C4D-CHA-C1A	5.17	127.41	121.24
8	E	102	BCL	C4D-CHA-C1A	5.17	127.41	121.24
8	7	102	BCL	C4D-CHA-C1A	5.14	127.37	121.24
8	6	102	BCL	C4D-CHA-C1A	5.14	127.37	121.24
8	V	101	BCL	C4D-CHA-C1A	5.12	127.35	121.24
8	v	101	BCL	C4D-CHA-C1A	5.12	127.35	121.24
8	P	102	BCL	C4D-CHA-C1A	5.11	127.33	121.24
8	p	102	BCL	C4D-CHA-C1A	5.11	127.33	121.24
8	T	101	BCL	C4D-CHA-C1A	5.08	127.30	121.24
8	t	101	BCL	C4D-CHA-C1A	5.08	127.30	121.24
8	g	102	BCL	C4D-CHA-C1A	5.05	127.27	121.24
8	G	102	BCL	C4D-CHA-C1A	5.02	127.23	121.24
8	2	101	BCL	C4D-CHA-C1A	5.00	127.20	121.24
8	4	101	BCL	C4D-CHA-C1A	5.00	127.20	121.24
8	L	301	BCL	C4D-CHA-C1A	4.91	127.10	121.24
8	l	301	BCL	C4D-CHA-C1A	4.88	127.06	121.24
8	0	101	BCL	C1-C2-C3	4.67	133.84	126.20
8	b0	101	BCL	C1-C2-C3	4.67	133.84	126.20
8	B	101	BCL	C1-C2-C3	4.54	133.63	126.20
8	b	101	BCL	C1-C2-C3	4.54	133.63	126.20
11	A	103	PC1	O21-C21-C22	4.31	120.80	111.48
11	a	103	PC1	O21-C21-C22	4.31	120.80	111.48
11	L	306	PC1	O21-C21-C22	4.28	120.75	111.48
11	l	306	PC1	O21-C21-C22	4.28	120.75	111.48
10	L	305	U10	C7-C8-C9	-4.22	119.56	126.83
10	l	305	U10	C7-C8-C9	-4.21	119.59	126.83
9	m	404	BPH	C4D-ND-C1D	-4.14	103.91	108.87
10	L	305	U10	C17-C18-C19	-4.14	118.15	127.62
10	l	305	U10	C17-C18-C19	-4.14	118.15	127.62
9	L	303	BPH	C4D-ND-C1D	-4.14	103.92	108.87
9	l	303	BPH	C4D-ND-C1D	-4.14	103.92	108.87
9	M	404	BPH	C4D-ND-C1D	-4.12	103.94	108.87
8	m	403	BCL	C4A-NA-C1A	4.08	108.54	106.68
8	M	403	BCL	C4A-NA-C1A	4.08	108.54	106.68
10	L	304	U10	C7-C8-C9	-4.07	119.81	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	l	304	U10	C7-C8-C9	-4.07	119.81	126.83
11	A	104	PC1	O21-C21-C22	4.04	120.22	111.48
11	a	104	PC1	O21-C21-C22	4.04	120.22	111.48
14	F	102	CDL	OA6-CA5-C11	4.04	120.21	111.48
14	f	102	CDL	OA6-CA5-C11	4.04	120.21	111.48
8	L	302	BCL	C1D-ND-C4D	-4.03	103.48	106.31
8	l	302	BCL	C1D-ND-C4D	-4.03	103.48	106.31
8	W	101	BCL	C1D-ND-C4D	-3.99	103.51	106.31
8	w	101	BCL	C1D-ND-C4D	-3.99	103.51	106.31
11	H	301	PC1	O21-C21-C22	3.97	120.08	111.48
11	h	301	PC1	O21-C21-C22	3.97	120.08	111.48
11	D	101	PC1	O21-C21-C22	3.97	120.07	111.48
11	d	101	PC1	O21-C21-C22	3.96	120.05	111.48
8	M	402	BCL	CHD-C1D-ND	-3.91	119.30	124.80
8	m	402	BCL	CHD-C1D-ND	-3.91	119.30	124.80
8	o	101	BCL	C4A-NA-C1A	3.90	108.46	106.68
14	F	102	CDL	OB6-CB5-C51	3.89	119.90	111.48
14	f	102	CDL	OB6-CB5-C51	3.89	119.89	111.48
8	Q	101	BCL	C4A-NA-C1A	3.87	108.44	106.68
8	q	101	BCL	C4A-NA-C1A	3.87	108.44	106.68
8	I	101	BCL	CHD-C1D-ND	-3.87	119.36	124.80
8	i	101	BCL	CHD-C1D-ND	-3.87	119.36	124.80
8	S	101	BCL	C4A-NA-C1A	3.86	108.44	106.68
8	s	101	BCL	C4A-NA-C1A	3.86	108.44	106.68
8	o	101	BCL	C1D-ND-C4D	-3.83	103.63	106.31
8	O	101	BCL	C4A-NA-C1A	3.82	108.42	106.68
8	O	101	BCL	C1D-ND-C4D	-3.82	103.63	106.31
14	M	407	CDL	OB6-CB5-C51	3.82	119.75	111.48
14	m	407	CDL	OB6-CB5-C51	3.82	119.75	111.48
14	M	407	CDL	OA6-CA5-C11	3.82	119.75	111.48
14	m	407	CDL	OA6-CA5-C11	3.82	119.75	111.48
8	I	101	BCL	C1D-ND-C4D	-3.81	103.64	106.31
8	i	101	BCL	C1D-ND-C4D	-3.81	103.64	106.31
8	9	101	BCL	C4A-NA-C1A	3.79	108.41	106.68
8	b9	101	BCL	C4A-NA-C1A	3.79	108.41	106.68
8	D	102	BCL	C4A-NA-C1A	3.76	108.40	106.68
8	7	102	BCL	C11-C10-C8	3.76	128.46	115.97
8	6	102	BCL	C11-C10-C8	3.76	128.46	115.97
8	O	101	BCL	CHD-C1D-ND	-3.74	119.54	124.80
8	o	101	BCL	CHD-C1D-ND	-3.73	119.55	124.80
8	2	101	BCL	CHD-C1D-ND	-3.73	119.55	124.80
8	4	101	BCL	CHD-C1D-ND	-3.73	119.56	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	302	BCL	CHD-C1D-ND	-3.71	119.58	124.80
8	W	101	BCL	CHD-C1D-ND	-3.71	119.58	124.80
8	l	302	BCL	CHD-C1D-ND	-3.71	119.58	124.80
8	w	101	BCL	CHD-C1D-ND	-3.71	119.58	124.80
8	F	101	BCL	C4A-NA-C1A	3.71	108.37	106.68
8	f	101	BCL	C4A-NA-C1A	3.71	108.37	106.68
8	z	101	BCL	CHD-C1D-ND	-3.70	119.60	124.80
11	l	307	PC1	O21-C21-C22	3.70	119.48	111.48
8	d	102	BCL	C4A-NA-C1A	3.69	108.36	106.68
11	L	307	PC1	O21-C21-C22	3.69	119.47	111.48
8	Z	101	BCL	CHD-C1D-ND	-3.68	119.63	124.80
8	U	101	BCL	C1D-ND-C4D	-3.68	103.73	106.31
8	u	101	BCL	C1D-ND-C4D	-3.68	103.73	106.31
8	K	101	BCL	C4A-NA-C1A	3.67	108.36	106.68
8	k	101	BCL	C4A-NA-C1A	3.67	108.36	106.68
11	H	302	PC1	O21-C21-C22	3.67	119.42	111.48
11	h	302	PC1	O21-C21-C22	3.67	119.42	111.48
8	M	402	BCL	C1D-ND-C4D	-3.67	103.74	106.31
8	m	402	BCL	C1D-ND-C4D	-3.67	103.74	106.31
10	L	305	U10	C22-C23-C24	-3.66	119.24	127.62
10	l	305	U10	C22-C23-C24	-3.65	119.26	127.62
8	A	101	BCL	C1D-ND-C4D	-3.64	103.76	106.31
8	a	101	BCL	C1D-ND-C4D	-3.64	103.76	106.31
8	D	102	BCL	C1D-ND-C4D	-3.62	103.77	106.31
8	d	102	BCL	C1D-ND-C4D	-3.62	103.77	106.31
8	f	101	BCL	CHD-C1D-ND	-3.61	119.72	124.80
8	5	101	BCL	C1-C2-C3	-3.61	120.93	126.76
8	3	101	BCL	C1-C2-C3	-3.60	120.94	126.76
8	Q	101	BCL	C1D-ND-C4D	-3.60	103.79	106.31
8	1	101	BCL	CHD-C1D-ND	-3.59	119.75	124.80
8	b1	101	BCL	CHD-C1D-ND	-3.59	119.75	124.80
8	K	101	BCL	C1D-ND-C4D	-3.59	103.79	106.31
8	k	101	BCL	C1D-ND-C4D	-3.59	103.79	106.31
8	U	101	BCL	CHD-C1D-ND	-3.59	119.75	124.80
8	u	101	BCL	CHD-C1D-ND	-3.59	119.75	124.80
8	I	101	BCL	C4A-NA-C1A	3.58	108.31	106.68
8	i	101	BCL	C4A-NA-C1A	3.58	108.31	106.68
8	l	301	BCL	CHD-C1D-ND	-3.58	119.76	124.80
8	2	101	BCL	C1D-ND-C4D	-3.58	103.80	106.31
8	F	101	BCL	CHD-C1D-ND	-3.58	119.76	124.80
8	L	301	BCL	CHD-C1D-ND	-3.58	119.77	124.80
8	4	101	BCL	C1D-ND-C4D	-3.57	103.81	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	101	BCL	CHD-C1D-ND	-3.57	119.78	124.80
8	D	102	BCL	CHD-C1D-ND	-3.57	119.78	124.80
8	d	102	BCL	CHD-C1D-ND	-3.57	119.78	124.80
8	1	101	BCL	C1D-ND-C4D	-3.57	103.81	106.31
8	b1	101	BCL	C1D-ND-C4D	-3.57	103.81	106.31
8	w	101	BCL	C4A-NA-C1A	3.57	108.31	106.68
8	A	101	BCL	CHD-C1D-ND	-3.56	119.79	124.80
8	9	101	BCL	CHD-C1D-ND	-3.56	119.79	124.80
8	b9	101	BCL	CHD-C1D-ND	-3.56	119.79	124.80
8	m	403	BCL	C1D-ND-C4D	-3.56	103.81	106.31
8	9	101	BCL	C1D-ND-C4D	-3.55	103.82	106.31
8	b9	101	BCL	C1D-ND-C4D	-3.55	103.82	106.31
8	Q	101	BCL	CHD-C1D-ND	-3.55	119.81	124.80
10	L	304	U10	C17-C18-C19	-3.55	119.51	127.62
10	l	304	U10	C17-C18-C19	-3.55	119.51	127.62
9	m	404	BPH	C3D-C4D-ND	3.54	112.25	107.71
8	7	101	BCL	CHD-C1D-ND	-3.54	119.82	124.80
8	6	101	BCL	CHD-C1D-ND	-3.54	119.82	124.80
8	C	101	BCL	CHD-C1D-ND	-3.54	119.82	124.80
8	c	101	BCL	CHD-C1D-ND	-3.54	119.82	124.80
8	q	101	BCL	CHD-C1D-ND	-3.54	119.83	124.80
8	J	101	BCL	CHD-C1D-ND	-3.53	119.83	124.80
8	L	301	BCL	C1D-ND-C4D	-3.53	103.84	106.31
8	K	101	BCL	CHD-C1D-ND	-3.53	119.84	124.80
8	k	101	BCL	CHD-C1D-ND	-3.53	119.84	124.80
8	S	101	BCL	C1D-ND-C4D	-3.53	103.84	106.31
8	q	101	BCL	C1D-ND-C4D	-3.52	103.84	106.31
10	M	405	U10	C27-C28-C29	-3.52	119.56	127.62
8	F	101	BCL	C1-C2-C3	-3.52	120.43	126.20
8	f	101	BCL	C1-C2-C3	-3.52	120.43	126.20
9	M	404	BPH	C3D-C4D-ND	3.52	112.22	107.71
10	m	405	U10	C27-C28-C29	-3.52	119.57	127.62
8	s	101	BCL	C1D-ND-C4D	-3.52	103.84	106.31
8	A	101	BCL	C4A-NA-C1A	3.52	108.28	106.68
8	a	101	BCL	C4A-NA-C1A	3.52	108.28	106.68
8	m	403	BCL	CHD-C1D-ND	-3.51	119.86	124.80
8	R	101	BCL	CHD-C1D-ND	-3.51	119.87	124.80
8	r	101	BCL	CHD-C1D-ND	-3.51	119.87	124.80
8	j	101	BCL	CHD-C1D-ND	-3.51	119.87	124.80
8	U	101	BCL	C4A-NA-C1A	3.50	108.28	106.68
8	u	101	BCL	C4A-NA-C1A	3.50	108.28	106.68
8	M	403	BCL	C1D-ND-C4D	-3.50	103.85	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	403	BCL	CHD-C1D-ND	-3.49	119.89	124.80
8	c	101	BCL	C1D-ND-C4D	-3.48	103.87	106.31
8	W	101	BCL	C4A-NA-C1A	3.48	108.27	106.68
8	l	301	BCL	C1D-ND-C4D	-3.48	103.87	106.31
8	3	101	BCL	CHD-C1D-ND	-3.46	119.93	124.80
8	5	101	BCL	CHD-C1D-ND	-3.46	119.93	124.80
8	G	102	BCL	CHD-C1D-ND	-3.46	119.94	124.80
8	g	102	BCL	CHD-C1D-ND	-3.46	119.94	124.80
8	C	101	BCL	C1D-ND-C4D	-3.45	103.89	106.31
8	S	101	BCL	CHD-C1D-ND	-3.45	119.94	124.80
8	s	101	BCL	CHD-C1D-ND	-3.45	119.95	124.80
8	3	101	BCL	C4A-NA-C1A	3.44	108.25	106.68
8	5	101	BCL	C4A-NA-C1A	3.44	108.25	106.68
8	V	101	BCL	CHD-C1D-ND	-3.44	119.96	124.80
8	v	101	BCL	CHD-C1D-ND	-3.44	119.96	124.80
8	F	101	BCL	C1D-ND-C4D	-3.43	103.91	106.31
8	f	101	BCL	C1D-ND-C4D	-3.43	103.91	106.31
8	G	102	BCL	C1-C2-C3	3.43	131.81	126.20
8	g	102	BCL	C1-C2-C3	3.43	131.81	126.20
8	1	101	BCL	C4A-NA-C1A	3.42	108.24	106.68
8	b1	101	BCL	C4A-NA-C1A	3.42	108.24	106.68
8	7	101	BCL	C1D-ND-C4D	-3.42	103.91	106.31
8	6	101	BCL	C1D-ND-C4D	-3.42	103.91	106.31
9	L	303	BPH	C3D-C4D-ND	3.42	112.09	107.71
9	l	303	BPH	C3D-C4D-ND	3.42	112.09	107.71
8	z	101	BCL	C1D-ND-C4D	-3.41	103.92	106.31
10	M	405	U10	C32-C33-C34	-3.41	119.83	127.62
10	m	405	U10	C32-C33-C34	-3.41	119.83	127.62
8	7	102	BCL	CHD-C1D-ND	-3.39	120.03	124.80
8	6	102	BCL	CHD-C1D-ND	-3.39	120.03	124.80
8	3	101	BCL	C1D-ND-C4D	-3.39	103.93	106.31
8	B	101	BCL	CHD-C1D-ND	-3.39	120.03	124.80
8	P	102	BCL	CHD-C1D-ND	-3.39	120.04	124.80
8	p	102	BCL	CHD-C1D-ND	-3.39	120.04	124.80
10	L	304	U10	C22-C23-C24	-3.38	119.88	127.62
10	l	304	U10	C22-C23-C24	-3.38	119.88	127.62
8	b	101	BCL	CHD-C1D-ND	-3.37	120.05	124.80
8	Z	101	BCL	C1D-ND-C4D	-3.37	103.95	106.31
10	M	405	U10	C12-C13-C14	-3.36	119.93	127.62
10	m	405	U10	C12-C13-C14	-3.36	119.93	127.62
8	5	101	BCL	C1D-ND-C4D	-3.34	103.97	106.31
8	0	101	BCL	CHD-C1D-ND	-3.33	120.12	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b0	101	BCL	CHD-C1D-ND	-3.33	120.12	124.80
8	G	102	BCL	C1D-ND-C4D	-3.32	103.98	106.31
8	g	102	BCL	C1D-ND-C4D	-3.32	103.98	106.31
8	T	101	BCL	CHD-C1D-ND	-3.32	120.13	124.80
8	t	101	BCL	CHD-C1D-ND	-3.32	120.13	124.80
10	L	305	U10	C27-C28-C29	-3.31	120.04	127.62
10	l	305	U10	C27-C28-C29	-3.31	120.04	127.62
8	N	102	BCL	CHD-C1D-ND	-3.31	120.14	124.80
10	M	405	U10	C17-C18-C19	-3.30	120.06	127.62
10	m	405	U10	C17-C18-C19	-3.30	120.06	127.62
8	7	101	BCL	C4A-NA-C1A	3.30	108.18	106.68
8	6	101	BCL	C4A-NA-C1A	3.30	108.18	106.68
8	J	101	BCL	C1D-ND-C4D	-3.29	104.00	106.31
8	j	101	BCL	C1D-ND-C4D	-3.29	104.00	106.31
8	7	102	BCL	C1D-ND-C4D	-3.29	104.01	106.31
8	6	102	BCL	C1D-ND-C4D	-3.29	104.01	106.31
8	n	102	BCL	CHD-C1D-ND	-3.28	120.18	124.80
10	L	305	U10	C15-C14-C16	3.28	120.92	115.23
10	l	305	U10	C15-C14-C16	3.28	120.92	115.23
8	N	102	BCL	C1D-ND-C4D	-3.28	104.01	106.31
8	n	102	BCL	C1D-ND-C4D	-3.28	104.01	106.31
10	M	405	U10	C22-C23-C24	-3.27	120.14	127.62
10	m	405	U10	C22-C23-C24	-3.27	120.14	127.62
8	E	102	BCL	C1D-ND-C4D	-3.27	104.02	106.31
8	R	101	BCL	C1D-ND-C4D	-3.27	104.02	106.31
8	r	101	BCL	C1D-ND-C4D	-3.27	104.02	106.31
8	E	102	BCL	CHD-C1D-ND	-3.26	120.21	124.80
8	e	102	BCL	CHD-C1D-ND	-3.26	120.21	124.80
8	e	102	BCL	C1D-ND-C4D	-3.24	104.04	106.31
10	M	405	U10	C25-C24-C26	3.24	120.85	115.23
10	m	405	U10	C25-C24-C26	3.24	120.85	115.23
10	L	304	U10	C15-C14-C16	3.24	120.84	115.23
10	l	304	U10	C15-C14-C16	3.24	120.84	115.23
10	l	304	U10	C12-C13-C14	-3.23	120.23	127.62
8	V	101	BCL	C1D-ND-C4D	-3.23	104.05	106.31
8	v	101	BCL	C1D-ND-C4D	-3.23	104.05	106.31
10	L	304	U10	C12-C13-C14	-3.22	120.24	127.62
8	b0	101	BCL	CHA-C1A-NA	-3.22	119.11	126.39
8	B	101	BCL	C1D-ND-C4D	-3.21	104.06	106.31
8	b	101	BCL	C1D-ND-C4D	-3.21	104.06	106.31
9	M	404	BPH	OBD-CAD-CBD	-3.21	121.11	125.82
8	0	101	BCL	CHA-C1A-NA	-3.20	119.14	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	304	U10	C25-C24-C26	3.20	120.78	115.23
8	B	101	BCL	CHA-C1A-NA	-3.20	119.14	126.39
8	b	101	BCL	CHA-C1A-NA	-3.20	119.14	126.39
8	T	101	BCL	C1D-ND-C4D	-3.19	104.07	106.31
8	t	101	BCL	C1D-ND-C4D	-3.19	104.07	106.31
10	l	304	U10	C25-C24-C26	3.19	120.76	115.23
9	m	404	BPH	OBD-CAD-CBD	-3.19	121.15	125.82
8	P	102	BCL	C1D-ND-C4D	-3.19	104.08	106.31
8	m	403	BCL	CHA-C1A-NA	-3.18	119.19	126.39
10	m	405	U10	C35-C34-C36	3.18	120.75	115.23
8	M	403	BCL	CHA-C1A-NA	-3.17	119.21	126.39
10	M	405	U10	C35-C34-C36	3.17	120.73	115.23
8	0	101	BCL	C1D-ND-C4D	-3.17	104.09	106.31
8	b0	101	BCL	C1D-ND-C4D	-3.17	104.09	106.31
8	e	102	BCL	CHA-C1A-NA	-3.16	119.24	126.39
8	E	102	BCL	CHA-C1A-NA	-3.16	119.25	126.39
8	g	102	BCL	CHA-C1A-NA	-3.15	119.26	126.39
8	W	101	BCL	CHA-C1A-NA	-3.15	119.26	126.39
8	w	101	BCL	CHA-C1A-NA	-3.15	119.26	126.39
8	p	102	BCL	CHA-C1A-NA	-3.15	119.27	126.39
8	p	102	BCL	C1D-ND-C4D	-3.14	104.11	106.31
8	G	102	BCL	CHA-C1A-NA	-3.14	119.28	126.39
8	P	102	BCL	CHA-C1A-NA	-3.13	119.29	126.39
8	V	101	BCL	CHA-C1A-NA	-3.13	119.30	126.39
8	v	101	BCL	CHA-C1A-NA	-3.13	119.30	126.39
8	K	101	BCL	C1-C2-C3	-3.12	121.08	126.20
8	T	101	BCL	CHA-C1A-NA	-3.12	119.33	126.39
8	k	101	BCL	C1-C2-C3	-3.10	121.11	126.20
8	t	101	BCL	CHA-C1A-NA	-3.10	119.36	126.39
8	7	102	BCL	CHA-C1A-NA	-3.10	119.37	126.39
8	6	102	BCL	CHA-C1A-NA	-3.10	119.37	126.39
10	L	304	U10	C7-C6-C1	-3.10	119.58	124.89
10	l	304	U10	C7-C6-C1	-3.10	119.58	124.89
8	U	101	BCL	CHA-C1A-NA	-3.09	119.38	126.39
8	u	101	BCL	CHA-C1A-NA	-3.09	119.38	126.39
9	L	303	BPH	OBD-CAD-CBD	-3.09	121.28	125.82
8	M	402	BCL	C2A-C1A-CHA	3.09	129.24	123.87
8	m	402	BCL	C2A-C1A-CHA	3.09	129.24	123.87
8	I	101	BCL	CHA-C1A-NA	-3.08	119.41	126.39
8	i	101	BCL	CHA-C1A-NA	-3.08	119.41	126.39
8	A	101	BCL	CHA-C1A-NA	-3.08	119.41	126.39
8	a	101	BCL	CHA-C1A-NA	-3.08	119.41	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	101	BCL	CHA-C1A-NA	-3.08	119.41	126.39
8	r	101	BCL	CHA-C1A-NA	-3.08	119.41	126.39
9	l	303	BPH	OBD-CAD-CBD	-3.08	121.31	125.82
8	k	101	BCL	CHA-C1A-NA	-3.08	119.42	126.39
8	3	101	BCL	CHA-C1A-NA	-3.07	119.43	126.39
8	5	101	BCL	CHA-C1A-NA	-3.07	119.43	126.39
8	K	101	BCL	CHA-C1A-NA	-3.06	119.45	126.39
8	O	101	BCL	CHA-C1A-NA	-3.06	119.46	126.39
8	1	101	BCL	CHA-C1A-NA	-3.06	119.47	126.39
8	b1	101	BCL	CHA-C1A-NA	-3.06	119.47	126.39
8	F	101	BCL	CHA-C1A-NA	-3.06	119.47	126.39
8	N	102	BCL	CHA-C1A-NA	-3.06	119.47	126.39
8	f	101	BCL	CHA-C1A-NA	-3.06	119.47	126.39
8	n	102	BCL	CHA-C1A-NA	-3.06	119.47	126.39
8	Q	101	BCL	CHA-C1A-NA	-3.05	119.48	126.39
8	q	101	BCL	CHA-C1A-NA	-3.05	119.48	126.39
8	z	101	BCL	CHA-C1A-NA	-3.05	119.48	126.39
8	Z	101	BCL	C4A-NA-C1A	3.05	108.07	106.68
8	o	101	BCL	CHA-C1A-NA	-3.05	119.49	126.39
8	9	101	BCL	CHA-C1A-NA	-3.05	119.49	126.39
8	b9	101	BCL	CHA-C1A-NA	-3.05	119.49	126.39
8	z	101	BCL	C4A-NA-C1A	3.04	108.07	106.68
8	S	101	BCL	CHA-C1A-NA	-3.04	119.51	126.39
8	s	101	BCL	CHA-C1A-NA	-3.04	119.51	126.39
8	Z	101	BCL	CHA-C1A-NA	-3.03	119.52	126.39
8	J	101	BCL	CHA-C1A-NA	-3.03	119.53	126.39
8	j	101	BCL	CHA-C1A-NA	-3.03	119.53	126.39
8	7	101	BCL	CHA-C1A-NA	-3.03	119.54	126.39
8	6	101	BCL	CHA-C1A-NA	-3.03	119.54	126.39
8	N	102	BCL	C4A-NA-C1A	3.02	108.06	106.68
8	n	102	BCL	C4A-NA-C1A	3.02	108.06	106.68
8	M	402	BCL	C4A-NA-C1A	3.02	108.06	106.68
8	m	402	BCL	C4A-NA-C1A	3.02	108.06	106.68
8	E	102	BCL	C4A-NA-C1A	3.02	108.06	106.68
8	e	102	BCL	C4A-NA-C1A	3.02	108.06	106.68
8	M	402	BCL	CHA-C1A-NA	-3.00	119.59	126.39
8	m	402	BCL	CHA-C1A-NA	-3.00	119.59	126.39
8	W	101	BCL	C2A-C1A-CHA	3.00	129.08	123.87
8	w	101	BCL	C2A-C1A-CHA	3.00	129.08	123.87
8	s	101	BCL	C1-C2-C3	-3.00	121.28	126.20
8	S	101	BCL	C1-C2-C3	-3.00	121.28	126.20
11	A	103	PC1	O31-C31-C32	2.99	120.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	103	PC1	O31-C31-C32	2.99	120.95	111.83
8	D	102	BCL	CHA-C1A-NA	-2.99	119.62	126.39
8	d	102	BCL	CHA-C1A-NA	-2.99	119.62	126.39
8	J	101	BCL	C4A-NA-C1A	2.99	108.04	106.68
8	j	101	BCL	C4A-NA-C1A	2.99	108.04	106.68
8	C	101	BCL	CHA-C1A-NA	-2.98	119.65	126.39
8	c	101	BCL	CHA-C1A-NA	-2.98	119.65	126.39
8	i	101	BCL	C1-C2-C3	-2.95	121.36	126.20
8	l	302	BCL	CHA-C1A-NA	-2.95	119.71	126.39
8	7	102	BCL	C2A-C1A-CHA	2.95	128.99	123.87
8	6	102	BCL	C2A-C1A-CHA	2.94	128.98	123.87
8	O	101	BCL	C2A-C1A-CHA	2.94	128.97	123.87
8	o	101	BCL	C2A-C1A-CHA	2.94	128.97	123.87
8	L	302	BCL	CHA-C1A-NA	-2.94	119.74	126.39
8	2	101	BCL	C2A-C1A-CHA	2.94	128.96	123.87
14	F	102	CDL	OB8-CB7-C71	2.94	120.79	111.83
14	f	102	CDL	OB8-CB7-C71	2.94	120.79	111.83
8	Q	101	BCL	C16-C15-C13	2.93	125.71	115.97
8	q	101	BCL	C16-C15-C13	2.93	125.71	115.97
8	I	101	BCL	C1-C2-C3	-2.93	121.40	126.20
8	4	101	BCL	C2A-C1A-CHA	2.92	128.93	123.87
8	2	101	BCL	CHA-C1A-NA	-2.91	119.80	126.39
8	4	101	BCL	CHA-C1A-NA	-2.91	119.80	126.39
8	B	101	BCL	C2A-C1A-CHA	2.91	128.92	123.87
8	b	101	BCL	C2A-C1A-CHA	2.91	128.92	123.87
8	g	102	BCL	C2A-C1A-CHA	2.90	128.90	123.87
8	L	301	BCL	CHA-C1A-NA	-2.89	119.84	126.39
8	b0	101	BCL	C2A-C1A-CHA	2.89	128.89	123.87
8	C	101	BCL	C2A-C1A-CHA	2.89	128.89	123.87
8	c	101	BCL	C2A-C1A-CHA	2.89	128.89	123.87
8	V	101	BCL	C2A-C1A-CHA	2.89	128.89	123.87
8	v	101	BCL	C2A-C1A-CHA	2.89	128.89	123.87
8	7	102	BCL	C4A-NA-C1A	2.89	108.00	106.68
8	G	102	BCL	C2A-C1A-CHA	2.89	128.88	123.87
8	P	102	BCL	C6-C7-C8	-2.89	106.36	115.97
8	p	102	BCL	C6-C7-C8	-2.89	106.36	115.97
8	0	101	BCL	C2A-C1A-CHA	2.88	128.87	123.87
8	z	101	BCL	C2A-C1A-CHA	2.88	128.87	123.87
8	l	302	BCL	C2A-C1A-CHA	2.88	128.86	123.87
8	P	102	BCL	C4A-NA-C1A	2.88	107.99	106.68
8	l	301	BCL	CHA-C1A-NA	-2.88	119.87	126.39
9	L	303	BPH	C2D-C1D-ND	2.88	111.51	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	303	BPH	C2D-C1D-ND	2.88	111.51	109.43
8	6	102	BCL	C4A-NA-C1A	2.87	107.99	106.68
8	Z	101	BCL	C2A-C1A-CHA	2.87	128.85	123.87
8	L	302	BCL	C2A-C1A-CHA	2.86	128.83	123.87
8	e	102	BCL	C2A-C1A-CHA	2.86	128.83	123.87
8	A	101	BCL	C2A-C1A-CHA	2.86	128.83	123.87
8	P	102	BCL	C2A-C1A-CHA	2.86	128.83	123.87
8	a	101	BCL	C2A-C1A-CHA	2.86	128.83	123.87
8	p	102	BCL	C2A-C1A-CHA	2.86	128.83	123.87
8	E	102	BCL	C2A-C1A-CHA	2.86	128.82	123.87
14	m	407	CDL	OB8-CB7-C71	2.86	120.54	111.83
11	D	101	PC1	O31-C31-C32	2.85	120.52	111.83
11	d	101	PC1	O31-C31-C32	2.85	120.52	111.83
14	M	407	CDL	OB8-CB7-C71	2.84	120.51	111.83
11	H	301	PC1	O31-C31-C32	2.84	120.49	111.83
11	h	301	PC1	O31-C31-C32	2.84	120.49	111.83
8	L	301	BCL	C2A-C1A-CHA	2.83	128.78	123.87
8	p	102	BCL	C4A-NA-C1A	2.83	107.97	106.68
10	L	305	U10	C25-C24-C26	2.82	120.13	115.23
10	l	305	U10	C25-C24-C26	2.82	120.13	115.23
10	L	305	U10	C30-C29-C31	2.82	120.12	115.23
10	l	305	U10	C30-C29-C31	2.82	120.12	115.23
8	N	102	BCL	C2A-C1A-CHA	2.82	128.76	123.87
8	n	102	BCL	C2A-C1A-CHA	2.82	128.76	123.87
8	N	102	BCL	C1-C2-C3	2.81	130.80	126.20
8	n	102	BCL	C1-C2-C3	2.81	130.80	126.20
8	l	301	BCL	C2A-C1A-CHA	2.81	128.74	123.87
10	M	405	U10	C15-C14-C16	2.80	120.09	115.23
10	m	405	U10	C15-C14-C16	2.80	120.09	115.23
8	0	101	BCL	C6-C7-C8	-2.80	106.66	115.97
8	b0	101	BCL	C6-C7-C8	-2.80	106.66	115.97
8	9	101	BCL	C2A-C1A-CHA	2.80	128.72	123.87
8	b9	101	BCL	C2A-C1A-CHA	2.80	128.72	123.87
10	L	305	U10	C10-C9-C11	2.80	120.08	115.23
10	l	305	U10	C10-C9-C11	2.80	120.08	115.23
8	T	101	BCL	C2A-C1A-CHA	2.80	128.72	123.87
8	m	403	BCL	C2A-C1A-CHA	2.79	128.71	123.87
8	t	101	BCL	C2A-C1A-CHA	2.79	128.70	123.87
8	M	403	BCL	C2A-C1A-CHA	2.78	128.70	123.87
9	L	303	BPH	CMB-C2B-C3B	2.78	130.25	124.68
9	l	303	BPH	CMB-C2B-C3B	2.78	130.25	124.68
8	w	101	BCL	C1-C2-C3	-2.78	121.64	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	302	BCL	C4A-NA-C1A	2.78	107.95	106.68
8	l	302	BCL	C4A-NA-C1A	2.78	107.95	106.68
8	F	101	BCL	C2A-C1A-CHA	2.78	128.69	123.87
8	f	101	BCL	C2A-C1A-CHA	2.78	128.69	123.87
8	k	101	BCL	C2A-C1A-CHA	2.77	128.68	123.87
8	C	101	BCL	C4A-NA-C1A	2.77	107.94	106.68
8	c	101	BCL	C4A-NA-C1A	2.77	107.94	106.68
8	W	101	BCL	C1-C2-C3	-2.76	121.67	126.20
14	M	407	CDL	OA8-CA7-C31	2.76	120.25	111.83
14	m	407	CDL	OA8-CA7-C31	2.76	120.25	111.83
8	J	101	BCL	C2A-C1A-CHA	2.76	128.66	123.87
8	j	101	BCL	C2A-C1A-CHA	2.76	128.66	123.87
8	K	101	BCL	C2A-C1A-CHA	2.76	128.65	123.87
8	3	101	BCL	C2A-C1A-CHA	2.75	128.64	123.87
8	5	101	BCL	C2A-C1A-CHA	2.75	128.64	123.87
8	7	101	BCL	C2A-C1A-CHA	2.74	128.63	123.87
8	6	101	BCL	C2A-C1A-CHA	2.74	128.63	123.87
9	M	404	BPH	O2D-CGD-CBD	2.74	113.96	110.95
9	m	404	BPH	O2D-CGD-CBD	2.74	113.96	110.95
10	M	405	U10	C10-C9-C11	2.74	119.98	115.23
10	m	405	U10	C10-C9-C11	2.74	119.98	115.23
8	I	101	BCL	C2A-C1A-CHA	2.72	128.59	123.87
8	i	101	BCL	C2A-C1A-CHA	2.72	128.58	123.87
8	B	101	BCL	C4A-NA-C1A	2.71	107.92	106.68
8	b	101	BCL	C4A-NA-C1A	2.71	107.92	106.68
8	R	101	BCL	C2A-C1A-CHA	2.71	128.57	123.87
8	r	101	BCL	C2A-C1A-CHA	2.71	128.57	123.87
8	D	102	BCL	C2A-C1A-CHA	2.71	128.56	123.87
8	d	102	BCL	C2A-C1A-CHA	2.71	128.56	123.87
9	m	404	BPH	C2D-C1D-ND	2.70	111.38	109.43
10	M	405	U10	C30-C29-C31	2.69	119.89	115.23
10	m	405	U10	C30-C29-C31	2.69	119.89	115.23
8	p	102	BCL	C1-C2-C3	2.68	130.59	126.20
11	A	105	PC1	O12-P-O14	2.68	124.90	112.44
8	U	101	BCL	C2A-C1A-CHA	2.67	128.51	123.87
8	u	101	BCL	C2A-C1A-CHA	2.67	128.51	123.87
11	a	105	PC1	O12-P-O14	2.67	124.88	112.44
8	P	102	BCL	C1-C2-C3	2.67	130.57	126.20
11	L	306	PC1	O31-C31-C32	2.67	119.98	111.83
11	l	306	PC1	O31-C31-C32	2.67	119.98	111.83
8	2	101	BCL	C4A-NA-C1A	2.67	107.89	106.68
8	4	101	BCL	C4A-NA-C1A	2.67	107.89	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	405	U10	C20-C19-C21	2.66	119.85	115.23
10	m	405	U10	C20-C19-C21	2.66	119.85	115.23
10	L	304	U10	C1M-C1-C6	-2.66	120.08	124.45
10	l	304	U10	C1M-C1-C6	-2.66	120.08	124.45
9	M	404	BPH	C2D-C1D-ND	2.66	111.35	109.43
11	L	307	PC1	O31-C31-C32	2.65	119.93	111.83
11	l	307	PC1	O31-C31-C32	2.65	119.92	111.83
10	L	305	U10	C1M-C1-C6	-2.64	120.11	124.45
10	l	305	U10	C1M-C1-C6	-2.64	120.11	124.45
8	S	101	BCL	C2A-C1A-CHA	2.63	128.44	123.87
8	s	101	BCL	C2A-C1A-CHA	2.63	128.44	123.87
8	Q	101	BCL	C2A-C1A-CHA	2.61	128.40	123.87
8	q	101	BCL	C2A-C1A-CHA	2.61	128.40	123.87
14	F	102	CDL	OA8-CA7-C31	2.59	119.74	111.83
14	f	102	CDL	OA8-CA7-C31	2.59	119.74	111.83
11	A	104	PC1	O12-P-O14	-2.59	100.39	112.44
8	M	403	BCL	CMB-C2B-C1B	-2.59	121.48	125.42
8	m	403	BCL	CMB-C2B-C1B	-2.59	121.48	125.42
11	a	104	PC1	O12-P-O14	-2.59	100.41	112.44
8	A	101	BCL	CMB-C2B-C1B	-2.58	121.49	125.42
8	a	101	BCL	CMB-C2B-C1B	-2.58	121.49	125.42
8	R	101	BCL	C4A-NA-C1A	2.57	107.85	106.68
8	r	101	BCL	C4A-NA-C1A	2.57	107.85	106.68
8	S	101	BCL	CMB-C2B-C1B	-2.57	121.50	125.42
8	s	101	BCL	CMB-C2B-C1B	-2.57	121.50	125.42
8	t	101	BCL	C4A-NA-C1A	2.57	107.85	106.68
8	M	403	BCL	OBB-CAB-CBB	-2.57	114.02	119.77
8	m	403	BCL	OBB-CAB-CBB	-2.57	114.02	119.77
8	O	101	BCL	C1-C2-C3	-2.57	121.99	126.20
8	B	101	BCL	C6-C7-C8	-2.55	107.48	115.97
8	b	101	BCL	C6-C7-C8	-2.55	107.48	115.97
8	o	101	BCL	C1-C2-C3	-2.55	122.02	126.20
11	A	104	PC1	O31-C31-C32	2.55	119.61	111.83
11	a	104	PC1	O31-C31-C32	2.55	119.61	111.83
9	l	303	BPH	C1-C2-C3	-2.55	122.02	126.20
9	L	303	BPH	C1-C2-C3	-2.54	122.03	126.20
11	H	302	PC1	O31-C31-C32	2.54	119.58	111.83
11	h	302	PC1	O31-C31-C32	2.54	119.58	111.83
8	6	101	BCL	CMB-C2B-C1B	-2.54	121.56	125.42
8	7	101	BCL	CMB-C2B-C1B	-2.53	121.56	125.42
8	0	101	BCL	C4A-NA-C1A	2.53	107.83	106.68
8	6	102	BCL	CAB-C3B-C2B	2.53	133.00	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	102	CDL	OA4-PA1-OA3	-2.53	100.68	112.44
14	f	102	CDL	OA4-PA1-OA3	-2.53	100.68	112.44
8	7	102	BCL	CAB-C3B-C2B	2.53	133.00	127.74
8	U	101	BCL	C1-C2-C3	-2.52	122.07	126.20
8	u	101	BCL	C1-C2-C3	-2.52	122.07	126.20
10	l	304	U10	C10-C9-C11	2.52	119.60	115.23
8	Q	101	BCL	CMB-C2B-C1B	-2.52	121.59	125.42
8	q	101	BCL	CMB-C2B-C1B	-2.52	121.59	125.42
10	L	304	U10	C10-C9-C11	2.51	119.59	115.23
8	l	101	BCL	C2A-C1A-CHA	2.51	128.22	123.87
8	b1	101	BCL	C2A-C1A-CHA	2.51	128.22	123.87
8	T	101	BCL	C4A-NA-C1A	2.50	107.82	106.68
11	H	301	PC1	O12-P-O14	-2.49	100.85	112.44
11	h	301	PC1	O12-P-O14	-2.49	100.85	112.44
14	F	102	CDL	OB4-PB2-OB3	-2.48	100.89	112.44
14	f	102	CDL	OB4-PB2-OB3	-2.48	100.89	112.44
9	M	404	BPH	CMB-C2B-C3B	2.48	129.64	124.68
9	m	404	BPH	CMB-C2B-C3B	2.48	129.64	124.68
10	L	305	U10	C20-C19-C21	2.48	119.53	115.23
10	l	305	U10	C20-C19-C21	2.48	119.53	115.23
8	b0	101	BCL	C4A-NA-C1A	2.47	107.81	106.68
11	D	101	PC1	O12-P-O14	-2.47	100.96	112.44
11	d	101	PC1	O12-P-O14	-2.47	100.96	112.44
10	L	305	U10	C12-C13-C14	-2.46	121.99	127.62
10	l	305	U10	C12-C13-C14	-2.46	121.99	127.62
14	M	407	CDL	OA4-PA1-OA3	-2.45	101.03	112.44
14	m	407	CDL	OA4-PA1-OA3	-2.45	101.03	112.44
8	G	102	BCL	C6-C7-C8	-2.44	107.84	115.97
8	g	102	BCL	C6-C7-C8	-2.44	107.84	115.97
8	0	101	BCL	CAB-C3B-C2B	2.44	132.81	127.74
8	b0	101	BCL	CAB-C3B-C2B	2.44	132.81	127.74
14	m	407	CDL	OB4-PB2-OB3	-2.43	101.13	112.44
14	M	407	CDL	OB4-PB2-OB3	-2.43	101.15	112.44
8	V	101	BCL	C4A-NA-C1A	2.42	107.78	106.68
8	v	101	BCL	C4A-NA-C1A	2.42	107.78	106.68
8	K	101	BCL	C1C-NC-C4C	2.40	107.77	106.68
8	k	101	BCL	C1C-NC-C4C	2.40	107.77	106.68
11	A	103	PC1	O12-P-O14	-2.39	101.31	112.44
11	a	103	PC1	O12-P-O14	-2.39	101.31	112.44
8	D	102	BCL	CMB-C2B-C1B	-2.39	121.78	125.42
8	d	102	BCL	CMB-C2B-C1B	-2.39	121.78	125.42
8	b9	101	BCL	CMB-C2B-C1B	-2.39	121.78	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	403	BCL	CAB-C3B-C2B	2.39	132.71	127.74
8	m	403	BCL	CAB-C3B-C2B	2.39	132.71	127.74
8	G	102	BCL	C4A-NA-C1A	2.39	107.77	106.68
10	M	405	U10	C7-C8-C9	-2.39	122.71	126.83
10	m	405	U10	C7-C8-C9	-2.39	122.71	126.83
8	9	101	BCL	CMB-C2B-C1B	-2.39	121.78	125.42
8	V	101	BCL	CBA-CAA-C2A	-2.38	106.70	113.79
8	v	101	BCL	CBA-CAA-C2A	-2.38	106.70	113.79
10	l	304	U10	C31-C29-C30	2.38	120.07	114.59
10	L	305	U10	C7-C6-C1	-2.38	120.81	124.89
10	l	305	U10	C7-C6-C1	-2.38	120.81	124.89
8	9	101	BCL	C1C-NC-C4C	2.38	107.77	106.68
10	L	304	U10	C31-C29-C30	2.37	120.04	114.59
9	L	303	BPH	C11-C10-C8	-2.37	108.09	115.97
9	l	303	BPH	C11-C10-C8	-2.37	108.09	115.97
8	b9	101	BCL	C1C-NC-C4C	2.36	107.76	106.68
8	L	301	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
8	l	301	BCL	CMB-C2B-C1B	-2.35	121.84	125.42
8	D	102	BCL	OBB-CAB-CBB	-2.35	114.51	119.77
8	d	102	BCL	OBB-CAB-CBB	-2.35	114.51	119.77
9	L	303	BPH	OBB-CAB-CBB	-2.35	115.19	120.19
9	l	303	BPH	OBB-CAB-CBB	-2.35	115.19	120.19
8	d	102	BCL	C1C-NC-C4C	2.35	107.75	106.68
9	L	303	BPH	CMD-C2D-C3D	2.34	129.36	124.68
9	l	303	BPH	CMD-C2D-C3D	2.34	129.36	124.68
8	g	102	BCL	C4A-NA-C1A	2.34	107.75	106.68
8	S	101	BCL	CAB-C3B-C2B	2.34	132.60	127.74
8	s	101	BCL	CAB-C3B-C2B	2.34	132.60	127.74
8	A	101	BCL	C1C-NC-C4C	2.34	107.75	106.68
8	a	101	BCL	C1C-NC-C4C	2.34	107.75	106.68
13	q	103	SPO	C1-C4-C5	-2.32	106.96	112.98
13	Q	103	SPO	C1-C4-C5	-2.32	106.97	112.98
10	L	304	U10	C20-C19-C21	2.31	119.24	115.23
10	l	304	U10	C20-C19-C21	2.31	119.24	115.23
11	L	306	PC1	O12-P-O14	-2.31	101.70	112.44
11	l	306	PC1	O12-P-O14	-2.31	101.70	112.44
10	L	305	U10	C36-C34-C35	2.31	119.90	114.59
10	l	305	U10	C36-C34-C35	2.31	119.90	114.59
8	Q	101	BCL	OBB-CAB-CBB	-2.30	114.62	119.77
8	q	101	BCL	OBB-CAB-CBB	-2.30	114.62	119.77
11	l	307	PC1	O12-P-O14	-2.30	101.75	112.44
8	A	101	BCL	OBB-CAB-CBB	-2.29	114.63	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	101	BCL	OBB-CAB-CBB	-2.29	114.63	119.77
8	9	101	BCL	CAB-C3B-C2B	2.29	132.50	127.74
8	b9	101	BCL	CAB-C3B-C2B	2.29	132.50	127.74
11	L	307	PC1	O12-P-O14	-2.29	101.79	112.44
8	L	301	BCL	C4A-NA-C1A	2.29	107.72	106.68
8	l	301	BCL	C4A-NA-C1A	2.29	107.72	106.68
8	7	101	BCL	OBB-CAB-CBB	-2.29	114.65	119.77
8	6	101	BCL	OBB-CAB-CBB	-2.29	114.65	119.77
10	M	405	U10	C41-C39-C40	2.28	119.83	114.59
10	m	405	U10	C41-C39-C40	2.28	119.83	114.59
8	S	101	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
8	s	101	BCL	OBB-CAB-CBB	-2.28	114.67	119.77
8	Q	101	BCL	CAB-C3B-C2B	2.27	132.47	127.74
8	q	101	BCL	CAB-C3B-C2B	2.27	132.47	127.74
8	D	102	BCL	C1C-NC-C4C	2.27	107.72	106.68
8	A	101	BCL	CAB-C3B-C2B	2.27	132.46	127.74
8	a	101	BCL	CAB-C3B-C2B	2.27	132.46	127.74
8	F	101	BCL	CAB-C3B-C2B	2.27	132.46	127.74
8	f	101	BCL	CMB-C2B-C1B	-2.27	121.96	125.42
8	V	101	BCL	CAA-CBA-CGA	2.27	119.65	113.21
8	v	101	BCL	CAA-CBA-CGA	2.27	119.65	113.21
8	7	101	BCL	C1C-NC-C4C	2.26	107.71	106.68
8	t	101	BCL	C1-C2-C3	2.26	129.89	126.20
8	F	101	BCL	CMB-C2B-C1B	-2.25	121.99	125.42
8	K	101	BCL	CAB-C3B-C2B	2.25	132.42	127.74
8	k	101	BCL	CAB-C3B-C2B	2.25	132.42	127.74
8	f	101	BCL	CAB-C3B-C2B	2.25	132.41	127.74
8	C	101	BCL	C6-C7-C8	-2.25	108.50	115.97
8	c	101	BCL	C6-C7-C8	-2.25	108.50	115.97
8	T	101	BCL	C1-C2-C3	2.24	129.88	126.20
8	0	101	BCL	CMB-C2B-C1B	-2.24	122.00	125.42
8	b0	101	BCL	CMB-C2B-C1B	-2.24	122.00	125.42
8	W	101	BCL	C11-C10-C8	-2.24	108.51	115.97
8	w	101	BCL	C11-C10-C8	-2.24	108.51	115.97
8	E	102	BCL	CAB-C3B-C2B	2.24	132.40	127.74
8	e	102	BCL	CAB-C3B-C2B	2.24	132.40	127.74
8	Q	101	BCL	C1C-NC-C4C	2.24	107.70	106.68
8	U	101	BCL	CAB-C3B-C2B	2.24	132.39	127.74
8	u	101	BCL	CAB-C3B-C2B	2.24	132.39	127.74
8	7	102	BCL	CMB-C2B-C1B	-2.23	122.02	125.42
8	6	102	BCL	CMB-C2B-C1B	-2.23	122.02	125.42
8	6	101	BCL	C1-C2-C3	-2.23	122.54	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	101	BCL	C1-C2-C3	-2.23	122.55	126.20
9	M	404	BPH	CMD-C2D-C3D	2.22	129.12	124.68
9	m	404	BPH	CMD-C2D-C3D	2.22	129.12	124.68
8	6	101	BCL	C1C-NC-C4C	2.22	107.69	106.68
11	H	302	PC1	O12-P-O14	-2.22	102.11	112.44
11	h	302	PC1	O12-P-O14	-2.22	102.11	112.44
8	D	102	BCL	CAB-C3B-C2B	2.22	132.35	127.74
8	3	101	BCL	CAB-C3B-C2B	2.22	132.35	127.74
8	L	302	BCL	CMB-C2B-C1B	-2.22	122.05	125.42
8	l	302	BCL	CMB-C2B-C1B	-2.22	122.05	125.42
8	R	101	BCL	CAB-C3B-C2B	2.21	132.34	127.74
8	7	102	BCL	C1-C2-C3	2.21	129.82	126.20
8	9	101	BCL	OBB-CAB-CBB	-2.21	114.82	119.77
8	b9	101	BCL	OBB-CAB-CBB	-2.21	114.82	119.77
8	d	102	BCL	CAB-C3B-C2B	2.21	132.34	127.74
8	q	101	BCL	C1C-NC-C4C	2.21	107.69	106.68
8	5	101	BCL	CAB-C3B-C2B	2.20	132.32	127.74
8	L	301	BCL	CAB-C3B-C2B	2.20	132.32	127.74
8	l	301	BCL	CAB-C3B-C2B	2.20	132.32	127.74
8	r	101	BCL	CAB-C3B-C2B	2.20	132.31	127.74
9	l	303	BPH	O2D-CGD-CBD	2.20	113.36	110.95
8	S	101	BCL	C1C-NC-C4C	2.20	107.68	106.68
8	s	101	BCL	C1C-NC-C4C	2.20	107.68	106.68
8	r	101	BCL	C1C-NC-C4C	2.19	107.68	106.68
8	T	101	BCL	C11-C10-C8	2.19	123.25	115.97
8	t	101	BCL	C11-C10-C8	2.19	123.25	115.97
8	6	102	BCL	C1-C2-C3	2.19	129.78	126.20
10	L	304	U10	C6-C1-C2	2.19	120.90	119.17
10	l	304	U10	C6-C1-C2	2.19	120.90	119.17
8	7	101	BCL	CAB-C3B-C2B	2.18	132.28	127.74
8	6	101	BCL	CAB-C3B-C2B	2.18	132.28	127.74
8	L	301	BCL	OBB-CAB-CBB	-2.18	114.89	119.77
9	L	303	BPH	O2D-CGD-CBD	2.17	113.33	110.95
8	7	101	BCL	C6-C7-C8	-2.17	108.75	115.97
8	6	101	BCL	C6-C7-C8	-2.17	108.75	115.97
8	P	102	BCL	CAB-C3B-C2B	2.16	132.24	127.74
8	p	102	BCL	CAB-C3B-C2B	2.16	132.24	127.74
8	Q	101	BCL	C17-C16-C15	2.16	122.95	113.28
8	l	301	BCL	OBB-CAB-CBB	-2.16	114.94	119.77
8	q	101	BCL	C17-C16-C15	2.15	122.93	113.28
8	V	101	BCL	C6-C7-C8	2.15	123.13	115.97
8	v	101	BCL	C6-C7-C8	2.15	123.13	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	101	BCL	C6-C5-C3	2.15	118.71	113.47
8	v	101	BCL	C6-C5-C3	2.15	118.71	113.47
8	E	102	BCL	C1-C2-C3	2.14	129.71	126.20
8	K	101	BCL	CMB-C2B-C1B	-2.14	122.16	125.42
8	k	101	BCL	CMB-C2B-C1B	-2.14	122.16	125.42
8	0	101	BCL	OBb-CAB-CBB	-2.14	114.97	119.77
8	b0	101	BCL	OBb-CAB-CBB	-2.14	114.97	119.77
8	e	102	BCL	C1-C2-C3	2.14	129.70	126.20
8	R	101	BCL	C1C-NC-C4C	2.13	107.65	106.68
8	7	102	BCL	OBb-CAB-CBB	-2.13	115.00	119.77
8	T	101	BCL	C6-C7-C8	-2.13	108.89	115.97
8	t	101	BCL	C6-C7-C8	-2.13	108.89	115.97
8	I	101	BCL	CAB-C3B-C2B	2.13	132.16	127.74
8	L	301	BCL	C4D-C3D-CAD	-2.12	105.80	108.11
8	l	301	BCL	C4D-C3D-CAD	-2.12	105.80	108.11
10	M	405	U10	C37-C38-C39	-2.12	120.56	127.64
10	m	405	U10	C37-C38-C39	-2.12	120.56	127.64
8	6	102	BCL	OBb-CAB-CBB	-2.12	115.01	119.77
8	D	102	BCL	C1-C2-C3	-2.11	122.74	126.20
8	d	102	BCL	C1-C2-C3	-2.11	122.74	126.20
8	i	101	BCL	CAB-C3B-C2B	2.11	132.13	127.74
8	M	402	BCL	CMB-C2B-C1B	-2.10	122.22	125.42
8	m	402	BCL	CMB-C2B-C1B	-2.10	122.22	125.42
8	l	101	BCL	CAB-C3B-C2B	2.10	132.10	127.74
8	b1	101	BCL	CAB-C3B-C2B	2.10	132.10	127.74
8	F	101	BCL	OBb-CAB-CBB	-2.10	115.08	119.77
8	f	101	BCL	OBb-CAB-CBB	-2.10	115.08	119.77
8	L	301	BCL	C1C-NC-C4C	2.09	107.63	106.68
8	l	301	BCL	C1C-NC-C4C	2.09	107.63	106.68
8	C	101	BCL	C1-C2-C3	2.09	129.62	126.20
10	L	305	U10	C32-C33-C34	-2.09	120.69	127.64
10	l	305	U10	C32-C33-C34	-2.09	120.69	127.64
8	B	101	BCL	CAB-C3B-C2B	2.08	132.06	127.74
8	b	101	BCL	CAB-C3B-C2B	2.08	132.06	127.74
8	E	102	BCL	C6-C7-C8	-2.07	109.07	115.97
8	e	102	BCL	C6-C7-C8	-2.07	109.07	115.97
8	c	101	BCL	C1-C2-C3	2.06	129.58	126.20
8	0	101	BCL	C1C-NC-C4C	2.06	107.62	106.68
8	b0	101	BCL	C1C-NC-C4C	2.06	107.62	106.68
8	l	302	BCL	CAB-C3B-C2B	2.05	131.99	127.74
10	l	304	U10	C27-C28-C29	-2.04	120.83	127.64
8	U	101	BCL	CMB-C2B-C1B	-2.04	122.31	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	u	101	BCL	CMB-C2B-C1B	-2.04	122.31	125.42
8	G	102	BCL	C1C-NC-C4C	2.04	107.61	106.68
10	L	304	U10	C27-C28-C29	-2.03	120.86	127.64
8	L	302	BCL	CAB-C3B-C2B	2.03	131.96	127.74
9	M	404	BPH	OBB-CAB-CBB	-2.02	115.88	120.19
9	m	404	BPH	OBB-CAB-CBB	-2.02	115.88	120.19
8	J	101	BCL	C6-C7-C8	-2.02	109.24	115.97
8	j	101	BCL	C6-C7-C8	-2.02	109.24	115.97
8	B	101	BCL	CMB-C2B-C1B	-2.02	122.35	125.42
8	b	101	BCL	CMB-C2B-C1B	-2.02	122.35	125.42
8	I	101	BCL	CMB-C2B-C1B	-2.01	122.35	125.42
8	i	101	BCL	CMB-C2B-C1B	-2.01	122.35	125.42
8	N	102	BCL	C1C-NC-C4C	2.01	107.60	106.68
10	M	405	U10	C7-C6-C1	-2.01	121.45	124.89
10	m	405	U10	C7-C6-C1	-2.01	121.45	124.89
8	N	102	BCL	C6-C7-C8	-2.00	109.31	115.97
8	n	102	BCL	C6-C7-C8	-2.00	109.31	115.97
8	j	101	BCL	CAB-C3B-C2B	2.00	131.90	127.74

There are no chirality outliers.

All (1186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	7	101	BCL	C2-C3-C5-C6
8	7	101	BCL	C4-C3-C5-C6
8	6	101	BCL	C4-C3-C5-C6
10	L	305	U10	C24-C26-C27-C28
10	l	305	U10	C24-C26-C27-C28
11	L	306	PC1	C11-O13-P-O12
11	L	306	PC1	C11-O13-P-O14
11	L	306	PC1	C11-O13-P-O11
11	L	306	PC1	C1-O11-P-O12
11	L	306	PC1	C1-O11-P-O14
11	L	306	PC1	C1-O11-P-O13
11	L	306	PC1	O21-C2-C3-O31
11	L	307	PC1	C11-O13-P-O12
11	L	307	PC1	C11-O13-P-O14
11	L	307	PC1	C11-O13-P-O11
11	L	307	PC1	C1-O11-P-O12
11	L	307	PC1	C1-O11-P-O13
11	L	307	PC1	O11-C1-C2-O21
11	H	301	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
11	H	302	PC1	C1-O11-P-O14
11	H	302	PC1	O13-C11-C12-N
11	H	302	PC1	O21-C2-C3-O31
11	A	103	PC1	C11-O13-P-O14
11	A	103	PC1	C1-O11-P-O12
11	A	103	PC1	C1-O11-P-O14
11	A	103	PC1	C1-O11-P-O13
11	A	104	PC1	C1-O11-P-O14
11	A	104	PC1	C1-O11-P-O13
11	A	104	PC1	C12-C11-O13-P
11	A	104	PC1	O11-C1-C2-O21
11	A	105	PC1	C11-O13-P-O14
11	A	105	PC1	C11-O13-P-O11
11	A	105	PC1	C1-O11-P-O12
11	A	105	PC1	C1-O11-P-O13
11	D	101	PC1	C11-O13-P-O12
11	D	101	PC1	C1-O11-P-O12
11	D	101	PC1	C1-O11-P-O14
11	D	101	PC1	C1-O11-P-O13
11	D	101	PC1	O13-C11-C12-N
11	l	306	PC1	C11-O13-P-O12
11	l	306	PC1	C11-O13-P-O14
11	l	306	PC1	C11-O13-P-O11
11	l	306	PC1	C1-O11-P-O12
11	l	306	PC1	C1-O11-P-O14
11	l	306	PC1	C1-O11-P-O13
11	l	306	PC1	O21-C2-C3-O31
11	l	307	PC1	C11-O13-P-O12
11	l	307	PC1	C11-O13-P-O14
11	l	307	PC1	C11-O13-P-O11
11	l	307	PC1	C1-O11-P-O12
11	l	307	PC1	C1-O11-P-O13
11	l	307	PC1	O11-C1-C2-O21
11	h	301	PC1	O13-C11-C12-N
11	h	302	PC1	C1-O11-P-O14
11	h	302	PC1	O13-C11-C12-N
11	h	302	PC1	O21-C2-C3-O31
11	a	103	PC1	C11-O13-P-O14
11	a	103	PC1	C1-O11-P-O12
11	a	103	PC1	C1-O11-P-O14
11	a	103	PC1	C1-O11-P-O13
11	a	104	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
11	a	104	PC1	C1-O11-P-O13
11	a	104	PC1	C12-C11-O13-P
11	a	104	PC1	O11-C1-C2-O21
11	a	105	PC1	C11-O13-P-O14
11	a	105	PC1	C11-O13-P-O11
11	a	105	PC1	C1-O11-P-O12
11	a	105	PC1	C1-O11-P-O13
11	d	101	PC1	C11-O13-P-O12
11	d	101	PC1	C1-O11-P-O12
11	d	101	PC1	C1-O11-P-O14
11	d	101	PC1	C1-O11-P-O13
11	d	101	PC1	O13-C11-C12-N
13	M	406	SPO	C4-C1-O1-CM1
13	A	102	SPO	C10-C11-C12-C13
13	B	102	SPO	O1-C1-C4-C5
13	B	102	SPO	C2-C1-C4-C5
13	B	102	SPO	C3-C1-C4-C5
13	B	102	SPO	C5-C6-C7-C8
13	B	102	SPO	C5-C6-C7-C9
13	B	102	SPO	C10-C11-C12-C13
13	B	102	SPO	C10-C11-C12-C14
13	D	103	SPO	O1-C1-C4-C5
13	D	103	SPO	C2-C1-C4-C5
13	D	103	SPO	C3-C1-C4-C5
13	D	103	SPO	C5-C6-C7-C8
13	D	103	SPO	C5-C6-C7-C9
13	D	103	SPO	C10-C11-C12-C13
13	D	103	SPO	C10-C11-C12-C14
13	E	101	SPO	C10-C11-C12-C13
13	E	101	SPO	C10-C11-C12-C14
13	E	101	SPO	C33-C35-C36-C37
13	E	103	SPO	C5-C6-C7-C8
13	E	103	SPO	C5-C6-C7-C9
13	E	103	SPO	C10-C11-C12-C13
13	E	103	SPO	C10-C11-C12-C14
13	G	101	SPO	C10-C11-C12-C14
13	G	103	SPO	C10-C11-C12-C13
13	G	103	SPO	C10-C11-C12-C14
13	G	103	SPO	C27-C28-C30-C31
13	G	103	SPO	C29-C28-C30-C31
13	I	102	SPO	C10-C11-C12-C13
13	I	102	SPO	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
13	J	102	SPO	O1-C1-C4-C5
13	J	102	SPO	C2-C1-C4-C5
13	J	102	SPO	C3-C1-C4-C5
13	J	102	SPO	C10-C11-C12-C13
13	J	102	SPO	C10-C11-C12-C14
13	J	102	SPO	C32-C33-C35-C36
13	J	102	SPO	C34-C33-C35-C36
13	N	101	SPO	C10-C11-C12-C13
13	N	101	SPO	C10-C11-C12-C14
13	N	101	SPO	C15-C16-C17-C19
13	N	101	SPO	C33-C35-C36-C37
13	O	102	SPO	O1-C1-C4-C5
13	O	102	SPO	C2-C1-C4-C5
13	O	102	SPO	C3-C1-C4-C5
13	O	102	SPO	C15-C16-C17-C19
13	O	102	SPO	C22-C23-C25-C26
13	P	101	SPO	C10-C11-C12-C13
13	P	101	SPO	C10-C11-C12-C14
13	Q	102	SPO	C10-C11-C12-C13
13	Q	102	SPO	C10-C11-C12-C14
13	Q	103	SPO	C5-C6-C7-C8
13	Q	103	SPO	C5-C6-C7-C9
13	Q	103	SPO	C10-C11-C12-C13
13	Q	103	SPO	C10-C11-C12-C14
13	Q	104	SPO	C10-C11-C12-C13
13	Q	104	SPO	C10-C11-C12-C14
13	S	102	SPO	O1-C1-C4-C5
13	S	102	SPO	C3-C1-C4-C5
13	S	102	SPO	C5-C6-C7-C8
13	S	102	SPO	C5-C6-C7-C9
13	S	102	SPO	C10-C11-C12-C13
13	S	102	SPO	C10-C11-C12-C14
13	S	102	SPO	C27-C28-C30-C31
13	S	102	SPO	C29-C28-C30-C31
13	S	103	SPO	C5-C6-C7-C8
13	S	103	SPO	C5-C6-C7-C9
13	S	103	SPO	C10-C11-C12-C14
13	U	102	SPO	C10-C11-C12-C13
13	U	102	SPO	C10-C11-C12-C14
13	U	102	SPO	C34-C33-C35-C36
13	C	102	SPO	C11-C10-C9-C7
13	C	102	SPO	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	C	102	SPO	C10-C11-C12-C14
13	C	102	SPO	C15-C16-C17-C19
13	3	102	SPO	C10-C11-C12-C13
13	3	102	SPO	C10-C11-C12-C14
13	3	102	SPO	C15-C16-C17-C19
13	3	103	SPO	C5-C6-C7-C8
13	3	103	SPO	C11-C10-C9-C7
13	3	103	SPO	C10-C11-C12-C14
13	9	102	SPO	C15-C16-C17-C18
13	9	102	SPO	C15-C16-C17-C19
13	0	102	SPO	O1-C1-C4-C5
13	0	102	SPO	C2-C1-C4-C5
13	0	102	SPO	C3-C1-C4-C5
13	0	102	SPO	C1-C4-C5-C6
13	0	102	SPO	C10-C11-C12-C13
13	0	102	SPO	C10-C11-C12-C14
13	X	101	SPO	C10-C11-C12-C13
13	X	101	SPO	C10-C11-C12-C14
13	X	101	SPO	C15-C16-C17-C19
13	X	101	SPO	C32-C33-C35-C36
13	X	101	SPO	C34-C33-C35-C36
13	m	406	SPO	C4-C1-O1-CM1
13	a	102	SPO	C10-C11-C12-C13
13	b	102	SPO	O1-C1-C4-C5
13	b	102	SPO	C2-C1-C4-C5
13	b	102	SPO	C3-C1-C4-C5
13	b	102	SPO	C5-C6-C7-C8
13	b	102	SPO	C5-C6-C7-C9
13	b	102	SPO	C10-C11-C12-C13
13	b	102	SPO	C10-C11-C12-C14
13	d	103	SPO	O1-C1-C4-C5
13	d	103	SPO	C2-C1-C4-C5
13	d	103	SPO	C3-C1-C4-C5
13	d	103	SPO	C5-C6-C7-C8
13	d	103	SPO	C5-C6-C7-C9
13	d	103	SPO	C10-C11-C12-C13
13	d	103	SPO	C10-C11-C12-C14
13	e	101	SPO	C10-C11-C12-C13
13	e	101	SPO	C10-C11-C12-C14
13	e	101	SPO	C33-C35-C36-C37
13	e	103	SPO	C5-C6-C7-C8
13	e	103	SPO	C5-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
13	e	103	SPO	C10-C11-C12-C13
13	e	103	SPO	C10-C11-C12-C14
13	g	101	SPO	C10-C11-C12-C14
13	g	103	SPO	C10-C11-C12-C13
13	g	103	SPO	C10-C11-C12-C14
13	g	103	SPO	C27-C28-C30-C31
13	g	103	SPO	C29-C28-C30-C31
13	i	102	SPO	C10-C11-C12-C13
13	i	102	SPO	C15-C16-C17-C19
13	j	102	SPO	O1-C1-C4-C5
13	j	102	SPO	C2-C1-C4-C5
13	j	102	SPO	C3-C1-C4-C5
13	j	102	SPO	C10-C11-C12-C13
13	j	102	SPO	C10-C11-C12-C14
13	j	102	SPO	C32-C33-C35-C36
13	j	102	SPO	C34-C33-C35-C36
13	n	101	SPO	C10-C11-C12-C13
13	n	101	SPO	C10-C11-C12-C14
13	n	101	SPO	C15-C16-C17-C19
13	n	101	SPO	C33-C35-C36-C37
13	o	102	SPO	O1-C1-C4-C5
13	o	102	SPO	C2-C1-C4-C5
13	o	102	SPO	C3-C1-C4-C5
13	o	102	SPO	C15-C16-C17-C19
13	o	102	SPO	C22-C23-C25-C26
13	p	101	SPO	C10-C11-C12-C13
13	p	101	SPO	C10-C11-C12-C14
13	q	102	SPO	C10-C11-C12-C13
13	q	102	SPO	C10-C11-C12-C14
13	q	103	SPO	C5-C6-C7-C8
13	q	103	SPO	C5-C6-C7-C9
13	q	103	SPO	C10-C11-C12-C13
13	q	103	SPO	C10-C11-C12-C14
13	q	104	SPO	C10-C11-C12-C13
13	q	104	SPO	C10-C11-C12-C14
13	s	102	SPO	O1-C1-C4-C5
13	s	102	SPO	C3-C1-C4-C5
13	s	102	SPO	C5-C6-C7-C8
13	s	102	SPO	C5-C6-C7-C9
13	s	102	SPO	C10-C11-C12-C13
13	s	102	SPO	C10-C11-C12-C14
13	s	102	SPO	C27-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
13	s	102	SPO	C29-C28-C30-C31
13	s	103	SPO	C5-C6-C7-C8
13	s	103	SPO	C5-C6-C7-C9
13	s	103	SPO	C10-C11-C12-C14
13	u	102	SPO	C10-C11-C12-C13
13	u	102	SPO	C10-C11-C12-C14
13	u	102	SPO	C34-C33-C35-C36
13	c	102	SPO	C11-C10-C9-C7
13	c	102	SPO	C10-C11-C12-C13
13	c	102	SPO	C10-C11-C12-C14
13	c	102	SPO	C15-C16-C17-C19
13	5	102	SPO	C10-C11-C12-C13
13	5	102	SPO	C10-C11-C12-C14
13	5	102	SPO	C15-C16-C17-C19
13	5	103	SPO	C5-C6-C7-C8
13	5	103	SPO	C11-C10-C9-C7
13	5	103	SPO	C10-C11-C12-C14
13	b9	102	SPO	C15-C16-C17-C18
13	b9	102	SPO	C15-C16-C17-C19
13	b0	102	SPO	O1-C1-C4-C5
13	b0	102	SPO	C2-C1-C4-C5
13	b0	102	SPO	C3-C1-C4-C5
13	b0	102	SPO	C1-C4-C5-C6
13	b0	102	SPO	C10-C11-C12-C13
13	b0	102	SPO	C10-C11-C12-C14
13	x	101	SPO	C10-C11-C12-C13
13	x	101	SPO	C10-C11-C12-C14
13	x	101	SPO	C15-C16-C17-C19
13	x	101	SPO	C32-C33-C35-C36
13	x	101	SPO	C34-C33-C35-C36
14	M	407	CDL	CA3-OA5-PA1-OA2
14	M	407	CDL	CA3-OA5-PA1-OA3
14	M	407	CDL	C51-CB5-OB6-CB4
14	F	102	CDL	CA2-OA2-PA1-OA3
14	F	102	CDL	CA2-OA2-PA1-OA4
14	F	102	CDL	CA2-OA2-PA1-OA5
14	F	102	CDL	CA3-OA5-PA1-OA2
14	F	102	CDL	CA3-OA5-PA1-OA4
14	F	102	CDL	C11-CA5-OA6-CA4
14	F	102	CDL	CB2-OB2-PB2-OB3
14	F	102	CDL	CB2-OB2-PB2-OB4
14	F	102	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
14	m	407	CDL	CA3-OA5-PA1-OA2
14	m	407	CDL	CA3-OA5-PA1-OA3
14	m	407	CDL	C51-CB5-OB6-CB4
14	f	102	CDL	CA2-OA2-PA1-OA3
14	f	102	CDL	CA2-OA2-PA1-OA4
14	f	102	CDL	CA2-OA2-PA1-OA5
14	f	102	CDL	CA3-OA5-PA1-OA2
14	f	102	CDL	CA3-OA5-PA1-OA4
14	f	102	CDL	C11-CA5-OA6-CA4
14	f	102	CDL	CB2-OB2-PB2-OB3
14	f	102	CDL	CB2-OB2-PB2-OB4
14	f	102	CDL	CB2-OB2-PB2-OB5
11	A	105	PC1	O32-C31-O31-C3
11	a	105	PC1	O32-C31-O31-C3
14	F	102	CDL	OA9-CA7-OA8-CA6
14	f	102	CDL	OA9-CA7-OA8-CA6
11	L	307	PC1	O22-C21-O21-C2
11	l	307	PC1	O22-C21-O21-C2
14	M	407	CDL	OB7-CB5-OB6-CB4
14	F	102	CDL	OA7-CA5-OA6-CA4
14	m	407	CDL	OB7-CB5-OB6-CB4
14	f	102	CDL	OA7-CA5-OA6-CA4
11	A	105	PC1	C32-C31-O31-C3
11	a	105	PC1	C32-C31-O31-C3
14	F	102	CDL	C31-CA7-OA8-CA6
14	f	102	CDL	C31-CA7-OA8-CA6
11	L	307	PC1	C22-C21-O21-C2
11	l	307	PC1	C22-C21-O21-C2
8	7	102	BCL	C4-C3-C5-C6
8	6	102	BCL	C4-C3-C5-C6
9	M	404	BPH	C4-C3-C5-C6
9	m	404	BPH	C4-C3-C5-C6
13	A	102	SPO	C34-C33-C35-C36
13	G	103	SPO	C34-C33-C35-C36
13	P	101	SPO	C34-C33-C35-C36
13	Q	103	SPO	C29-C28-C30-C31
13	Q	104	SPO	C34-C33-C35-C36
13	C	102	SPO	C29-C28-C30-C31
13	3	102	SPO	C34-C33-C35-C36
13	3	103	SPO	C29-C28-C30-C31
13	3	103	SPO	C34-C33-C35-C36
13	9	102	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
13	a	102	SPO	C34-C33-C35-C36
13	g	103	SPO	C34-C33-C35-C36
13	p	101	SPO	C34-C33-C35-C36
13	q	103	SPO	C29-C28-C30-C31
13	q	104	SPO	C34-C33-C35-C36
13	c	102	SPO	C29-C28-C30-C31
13	5	102	SPO	C34-C33-C35-C36
13	5	103	SPO	C29-C28-C30-C31
13	5	103	SPO	C34-C33-C35-C36
13	b9	102	SPO	C34-C33-C35-C36
8	6	101	BCL	C2-C3-C5-C6
9	M	404	BPH	C2-C3-C5-C6
9	m	404	BPH	C2-C3-C5-C6
13	G	103	SPO	C32-C33-C35-C36
13	P	101	SPO	C32-C33-C35-C36
13	Q	103	SPO	C27-C28-C30-C31
13	Q	104	SPO	C32-C33-C35-C36
13	U	102	SPO	C32-C33-C35-C36
13	C	102	SPO	C27-C28-C30-C31
13	3	102	SPO	C32-C33-C35-C36
13	3	103	SPO	C27-C28-C30-C31
13	3	103	SPO	C32-C33-C35-C36
13	9	102	SPO	C32-C33-C35-C36
13	g	103	SPO	C32-C33-C35-C36
13	p	101	SPO	C32-C33-C35-C36
13	q	103	SPO	C27-C28-C30-C31
13	q	104	SPO	C32-C33-C35-C36
13	u	102	SPO	C32-C33-C35-C36
13	c	102	SPO	C27-C28-C30-C31
13	5	102	SPO	C32-C33-C35-C36
13	5	103	SPO	C27-C28-C30-C31
13	5	103	SPO	C32-C33-C35-C36
13	b9	102	SPO	C32-C33-C35-C36
8	0	101	BCL	C2A-CAA-CBA-CGA
8	b0	101	BCL	C2A-CAA-CBA-CGA
11	A	105	PC1	C11-C12-N-C13
11	a	105	PC1	C11-C12-N-C13
10	M	405	U10	C37-C38-C39-C40
10	m	405	U10	C37-C38-C39-C40
10	L	305	U10	C25-C24-C26-C27
10	l	305	U10	C25-C24-C26-C27
13	B	102	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
13	D	103	SPO	C34-C33-C35-C36
13	Q	103	SPO	C34-C33-C35-C36
13	S	102	SPO	C34-C33-C35-C36
13	0	102	SPO	C29-C28-C30-C31
13	0	102	SPO	C34-C33-C35-C36
13	b	102	SPO	C34-C33-C35-C36
13	d	103	SPO	C34-C33-C35-C36
13	q	103	SPO	C34-C33-C35-C36
13	s	102	SPO	C34-C33-C35-C36
13	b0	102	SPO	C29-C28-C30-C31
13	b0	102	SPO	C34-C33-C35-C36
10	L	305	U10	C23-C24-C26-C27
10	l	305	U10	C23-C24-C26-C27
13	M	406	SPO	C32-C33-C35-C36
13	A	102	SPO	C32-C33-C35-C36
13	B	102	SPO	C32-C33-C35-C36
13	D	103	SPO	C32-C33-C35-C36
13	Q	103	SPO	C32-C33-C35-C36
13	S	102	SPO	C32-C33-C35-C36
13	0	102	SPO	C32-C33-C35-C36
13	m	406	SPO	C32-C33-C35-C36
13	a	102	SPO	C32-C33-C35-C36
13	b	102	SPO	C32-C33-C35-C36
13	d	103	SPO	C32-C33-C35-C36
13	q	103	SPO	C32-C33-C35-C36
13	s	102	SPO	C32-C33-C35-C36
13	b0	102	SPO	C32-C33-C35-C36
10	L	304	U10	C14-C16-C17-C18
10	L	304	U10	C19-C21-C22-C23
10	l	304	U10	C14-C16-C17-C18
10	l	304	U10	C19-C21-C22-C23
13	A	102	SPO	C33-C35-C36-C37
13	B	102	SPO	C33-C35-C36-C37
13	D	103	SPO	C33-C35-C36-C37
13	E	103	SPO	C28-C30-C31-C32
13	E	103	SPO	C33-C35-C36-C37
13	G	101	SPO	C33-C35-C36-C37
13	I	102	SPO	C33-C35-C36-C37
13	P	101	SPO	C33-C35-C36-C37
13	Q	102	SPO	C33-C35-C36-C37
13	S	103	SPO	C33-C35-C36-C37
13	U	103	SPO	C33-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
13	3	102	SPO	C33-C35-C36-C37
13	a	102	SPO	C33-C35-C36-C37
13	b	102	SPO	C33-C35-C36-C37
13	d	103	SPO	C33-C35-C36-C37
13	e	103	SPO	C28-C30-C31-C32
13	e	103	SPO	C33-C35-C36-C37
13	g	101	SPO	C33-C35-C36-C37
13	i	102	SPO	C33-C35-C36-C37
13	p	101	SPO	C33-C35-C36-C37
13	q	102	SPO	C33-C35-C36-C37
13	s	103	SPO	C33-C35-C36-C37
13	u	103	SPO	C33-C35-C36-C37
13	5	102	SPO	C33-C35-C36-C37
8	N	102	BCL	C2A-CAA-CBA-CGA
8	n	102	BCL	C2A-CAA-CBA-CGA
13	E	103	SPO	C11-C10-C9-C7
13	G	103	SPO	C12-C14-C15-C16
13	O	102	SPO	C11-C10-C9-C7
13	e	103	SPO	C11-C10-C9-C7
13	g	103	SPO	C12-C14-C15-C16
13	o	102	SPO	C11-C10-C9-C7
13	M	406	SPO	C34-C33-C35-C36
13	m	406	SPO	C34-C33-C35-C36
8	7	102	BCL	C2-C3-C5-C6
8	6	102	BCL	C2-C3-C5-C6
13	0	102	SPO	C27-C28-C30-C31
13	b0	102	SPO	C27-C28-C30-C31
13	A	102	SPO	C15-C16-C17-C18
13	E	101	SPO	C15-C16-C17-C18
13	G	101	SPO	C10-C11-C12-C13
13	I	102	SPO	C15-C16-C17-C18
13	J	102	SPO	C5-C6-C7-C8
13	N	101	SPO	C15-C16-C17-C18
13	O	102	SPO	C5-C6-C7-C8
13	O	102	SPO	C15-C16-C17-C18
13	O	102	SPO	C24-C23-C25-C26
13	S	103	SPO	C10-C11-C12-C13
13	C	102	SPO	C15-C16-C17-C18
13	3	102	SPO	C15-C16-C17-C18
13	3	103	SPO	C10-C11-C12-C13
13	9	102	SPO	C10-C11-C12-C13
13	X	101	SPO	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	a	102	SPO	C15-C16-C17-C18
13	e	101	SPO	C15-C16-C17-C18
13	g	101	SPO	C10-C11-C12-C13
13	i	102	SPO	C15-C16-C17-C18
13	j	102	SPO	C5-C6-C7-C8
13	n	101	SPO	C15-C16-C17-C18
13	o	102	SPO	C5-C6-C7-C8
13	o	102	SPO	C15-C16-C17-C18
13	o	102	SPO	C24-C23-C25-C26
13	s	103	SPO	C10-C11-C12-C13
13	c	102	SPO	C15-C16-C17-C18
13	5	102	SPO	C15-C16-C17-C18
13	5	103	SPO	C10-C11-C12-C13
13	b9	102	SPO	C10-C11-C12-C13
13	x	101	SPO	C15-C16-C17-C18
13	A	102	SPO	C10-C11-C12-C14
13	I	102	SPO	C10-C11-C12-C14
13	J	102	SPO	C5-C6-C7-C9
13	3	103	SPO	C5-C6-C7-C9
13	9	102	SPO	C10-C11-C12-C14
13	a	102	SPO	C10-C11-C12-C14
13	i	102	SPO	C10-C11-C12-C14
13	j	102	SPO	C5-C6-C7-C9
13	5	103	SPO	C5-C6-C7-C9
13	b9	102	SPO	C10-C11-C12-C14
8	J	101	BCL	C2A-CAA-CBA-CGA
8	j	101	BCL	C2A-CAA-CBA-CGA
10	M	405	U10	C37-C38-C39-C41
10	m	405	U10	C37-C38-C39-C41
11	A	104	PC1	C22-C21-O21-C2
11	a	104	PC1	C22-C21-O21-C2
14	M	407	CDL	OB6-CB4-CB6-OB8
14	m	407	CDL	OB6-CB4-CB6-OB8
10	L	305	U10	C12-C11-C9-C10
10	l	305	U10	C12-C11-C9-C10
13	0	102	SPO	C11-C10-C9-C7
13	b0	102	SPO	C11-C10-C9-C7
10	L	304	U10	C9-C11-C12-C13
10	L	304	U10	C24-C26-C27-C28
10	L	305	U10	C29-C31-C32-C33
10	l	304	U10	C9-C11-C12-C13
10	l	304	U10	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
10	l	305	U10	C29-C31-C32-C33
13	Q	104	SPO	C33-C35-C36-C37
13	q	104	SPO	C33-C35-C36-C37
11	A	103	PC1	C31-C32-C33-C34
11	a	103	PC1	C31-C32-C33-C34
8	B	101	BCL	C2A-CAA-CBA-CGA
8	G	102	BCL	C2A-CAA-CBA-CGA
8	P	102	BCL	C2A-CAA-CBA-CGA
8	R	101	BCL	C2A-CAA-CBA-CGA
8	T	101	BCL	C2A-CAA-CBA-CGA
8	b	101	BCL	C2A-CAA-CBA-CGA
8	g	102	BCL	C2A-CAA-CBA-CGA
8	p	102	BCL	C2A-CAA-CBA-CGA
8	r	101	BCL	C2A-CAA-CBA-CGA
8	t	101	BCL	C2A-CAA-CBA-CGA
13	I	102	SPO	C11-C10-C9-C7
13	O	102	SPO	C12-C14-C15-C16
13	X	101	SPO	C11-C10-C9-C7
13	i	102	SPO	C11-C10-C9-C7
13	o	102	SPO	C12-C14-C15-C16
13	x	101	SPO	C11-C10-C9-C7
11	A	104	PC1	O22-C21-O21-C2
11	A	105	PC1	O22-C21-O21-C2
11	a	104	PC1	O22-C21-O21-C2
11	a	105	PC1	O22-C21-O21-C2
11	A	105	PC1	C11-C12-N-C15
11	a	105	PC1	C11-C12-N-C15
13	E	103	SPO	C29-C28-C30-C31
13	e	103	SPO	C29-C28-C30-C31
11	A	105	PC1	C22-C21-O21-C2
11	a	105	PC1	C22-C21-O21-C2
14	F	102	CDL	O1-C1-CA2-OA2
14	f	102	CDL	O1-C1-CA2-OA2
14	M	407	CDL	C71-CB7-OB8-CB6
14	m	407	CDL	C71-CB7-OB8-CB6
13	G	101	SPO	C15-C16-C17-C18
13	G	103	SPO	C15-C16-C17-C18
13	Q	102	SPO	C15-C16-C17-C18
13	S	103	SPO	C15-C16-C17-C18
13	U	103	SPO	C10-C11-C12-C13
13	C	102	SPO	C5-C6-C7-C8
13	g	101	SPO	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	g	103	SPO	C15-C16-C17-C18
13	q	102	SPO	C15-C16-C17-C18
13	s	103	SPO	C15-C16-C17-C18
13	u	103	SPO	C10-C11-C12-C13
13	c	102	SPO	C5-C6-C7-C8
13	G	103	SPO	C15-C16-C17-C19
13	O	102	SPO	C5-C6-C7-C9
13	C	102	SPO	C5-C6-C7-C9
13	g	103	SPO	C15-C16-C17-C19
13	o	102	SPO	C5-C6-C7-C9
13	c	102	SPO	C5-C6-C7-C9
8	E	102	BCL	C2A-CAA-CBA-CGA
8	7	102	BCL	C2A-CAA-CBA-CGA
8	e	102	BCL	C2A-CAA-CBA-CGA
8	6	102	BCL	C2A-CAA-CBA-CGA
11	A	105	PC1	C11-C12-N-C14
11	a	105	PC1	C11-C12-N-C14
14	F	102	CDL	C71-C72-C73-C74
14	f	102	CDL	C71-C72-C73-C74
11	L	307	PC1	C22-C23-C24-C25
11	l	307	PC1	C22-C23-C24-C25
11	L	307	PC1	C23-C24-C25-C26
11	l	307	PC1	C23-C24-C25-C26
11	L	307	PC1	C1-C2-C3-O31
11	l	307	PC1	C1-C2-C3-O31
14	M	407	CDL	OB9-CB7-OB8-CB6
14	m	407	CDL	OB9-CB7-OB8-CB6
11	H	301	PC1	C37-C38-C39-C3A
11	h	301	PC1	C37-C38-C39-C3A
13	G	101	SPO	C34-C33-C35-C36
13	g	101	SPO	C34-C33-C35-C36
10	L	305	U10	C12-C11-C9-C8
10	l	305	U10	C12-C11-C9-C8
13	E	103	SPO	C27-C28-C30-C31
13	e	103	SPO	C27-C28-C30-C31
11	A	103	PC1	C32-C33-C34-C35
11	a	103	PC1	C32-C33-C34-C35
13	E	101	SPO	C5-C6-C7-C8
13	E	103	SPO	C15-C16-C17-C18
13	Q	102	SPO	C5-C6-C7-C8
13	9	102	SPO	C5-C6-C7-C8
13	e	103	SPO	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	q	102	SPO	C5-C6-C7-C8
13	b9	102	SPO	C5-C6-C7-C8
13	E	103	SPO	C1-C4-C5-C6
13	G	103	SPO	C1-C4-C5-C6
13	e	103	SPO	C1-C4-C5-C6
13	g	103	SPO	C1-C4-C5-C6
13	E	101	SPO	C5-C6-C7-C9
13	E	101	SPO	C15-C16-C17-C19
13	Q	102	SPO	C5-C6-C7-C9
13	9	102	SPO	C5-C6-C7-C9
13	e	101	SPO	C5-C6-C7-C9
13	e	101	SPO	C15-C16-C17-C19
13	q	102	SPO	C5-C6-C7-C9
13	b9	102	SPO	C5-C6-C7-C9
8	R	101	BCL	C4-C3-C5-C6
8	r	101	BCL	C4-C3-C5-C6
13	G	101	SPO	C32-C33-C35-C36
13	g	101	SPO	C32-C33-C35-C36
11	A	103	PC1	C23-C24-C25-C26
11	a	103	PC1	C23-C24-C25-C26
13	S	102	SPO	C33-C35-C36-C37
13	s	102	SPO	C33-C35-C36-C37
11	L	306	PC1	C21-C22-C23-C24
11	l	306	PC1	C21-C22-C23-C24
11	D	101	PC1	O21-C2-C3-O31
11	d	101	PC1	O21-C2-C3-O31
11	H	301	PC1	C36-C37-C38-C39
11	h	301	PC1	C36-C37-C38-C39
10	L	304	U10	C27-C28-C29-C30
10	l	304	U10	C27-C28-C29-C30
14	M	407	CDL	C11-CA5-OA6-CA4
14	F	102	CDL	C51-CB5-OB6-CB4
14	m	407	CDL	C11-CA5-OA6-CA4
14	f	102	CDL	C51-CB5-OB6-CB4
11	L	306	PC1	O11-C1-C2-C3
11	A	104	PC1	O11-C1-C2-C3
11	A	105	PC1	O11-C1-C2-C3
11	l	306	PC1	O11-C1-C2-C3
11	a	104	PC1	O11-C1-C2-C3
11	a	105	PC1	O11-C1-C2-C3
9	L	303	BPH	C11-C10-C8-C7
9	l	303	BPH	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	S	102	SPO	C2-C1-C4-C5
13	9	102	SPO	C3-C1-C4-C5
13	s	102	SPO	C2-C1-C4-C5
13	b9	102	SPO	C3-C1-C4-C5
11	A	104	PC1	C21-C22-C23-C24
11	a	104	PC1	C21-C22-C23-C24
8	J	101	BCL	C4-C3-C5-C6
8	j	101	BCL	C4-C3-C5-C6
8	E	102	BCL	C2-C3-C5-C6
8	R	101	BCL	C2-C3-C5-C6
8	Z	101	BCL	C2-C3-C5-C6
8	e	102	BCL	C2-C3-C5-C6
8	r	101	BCL	C2-C3-C5-C6
8	z	101	BCL	C2-C3-C5-C6
9	L	303	BPH	C11-C10-C8-C9
9	l	303	BPH	C11-C10-C8-C9
13	A	102	SPO	C11-C10-C9-C7
13	a	102	SPO	C11-C10-C9-C7
11	A	104	PC1	C1-C2-C3-O31
11	D	101	PC1	C1-C2-C3-O31
11	a	104	PC1	C1-C2-C3-O31
11	d	101	PC1	C1-C2-C3-O31
14	f	102	CDL	C73-C74-C75-C76
14	F	102	CDL	C73-C74-C75-C76
8	E	102	BCL	C4-C3-C5-C6
8	e	102	BCL	C4-C3-C5-C6
10	L	304	U10	C20-C19-C21-C22
10	l	304	U10	C20-C19-C21-C22
10	L	304	U10	C18-C19-C21-C22
10	l	304	U10	C18-C19-C21-C22
13	G	101	SPO	C5-C6-C7-C8
13	I	102	SPO	C5-C6-C7-C8
13	N	101	SPO	C5-C6-C7-C8
13	P	101	SPO	C5-C6-C7-C8
13	Q	104	SPO	C5-C6-C7-C8
13	U	103	SPO	C5-C6-C7-C8
13	3	102	SPO	C5-C6-C7-C8
13	X	101	SPO	C5-C6-C7-C8
13	e	101	SPO	C5-C6-C7-C8
13	g	101	SPO	C5-C6-C7-C8
13	i	102	SPO	C5-C6-C7-C8
13	n	101	SPO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	p	101	SPO	C5-C6-C7-C8
13	q	104	SPO	C5-C6-C7-C8
13	u	103	SPO	C5-C6-C7-C8
13	5	102	SPO	C5-C6-C7-C8
13	x	101	SPO	C5-C6-C7-C8
13	G	101	SPO	C5-C6-C7-C9
13	G	101	SPO	C15-C16-C17-C19
13	I	102	SPO	C5-C6-C7-C9
13	N	101	SPO	C5-C6-C7-C9
13	Q	102	SPO	C15-C16-C17-C19
13	Q	104	SPO	C5-C6-C7-C9
13	S	103	SPO	C15-C16-C17-C19
13	X	101	SPO	C5-C6-C7-C9
13	g	101	SPO	C5-C6-C7-C9
13	g	101	SPO	C15-C16-C17-C19
13	i	102	SPO	C5-C6-C7-C9
13	n	101	SPO	C5-C6-C7-C9
13	q	102	SPO	C15-C16-C17-C19
13	q	104	SPO	C5-C6-C7-C9
13	s	103	SPO	C15-C16-C17-C19
13	x	101	SPO	C5-C6-C7-C9
11	H	301	PC1	C32-C31-O31-C3
11	h	301	PC1	C32-C31-O31-C3
8	7	102	BCL	O2A-C1-C2-C3
8	6	102	BCL	O2A-C1-C2-C3
13	3	102	SPO	C11-C10-C9-C7
13	5	102	SPO	C11-C10-C9-C7
11	D	101	PC1	O11-C1-C2-O21
11	d	101	PC1	O11-C1-C2-O21
14	M	407	CDL	OA5-CA3-CA4-OA6
14	m	407	CDL	OA5-CA3-CA4-OA6
8	J	101	BCL	C2-C3-C5-C6
8	N	102	BCL	C2-C3-C5-C6
8	j	101	BCL	C2-C3-C5-C6
8	n	102	BCL	C2-C3-C5-C6
11	L	307	PC1	O21-C2-C3-O31
11	l	307	PC1	O21-C2-C3-O31
14	F	102	CDL	OA6-CA4-CA6-OA8
14	F	102	CDL	OB6-CB4-CB6-OB8
14	f	102	CDL	OA6-CA4-CA6-OA8
14	f	102	CDL	OB6-CB4-CB6-OB8
11	d	101	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
11	D	101	PC1	C22-C23-C24-C25
10	M	405	U10	C34-C36-C37-C38
10	m	405	U10	C34-C36-C37-C38
14	M	407	CDL	C55-C56-C57-C58
14	m	407	CDL	C55-C56-C57-C58
13	M	406	SPO	C2-C1-O1-CM1
13	m	406	SPO	C2-C1-O1-CM1
14	M	407	CDL	OA5-CA3-CA4-CA6
14	m	407	CDL	OA5-CA3-CA4-CA6
8	N	102	BCL	C4-C3-C5-C6
8	Z	101	BCL	C4-C3-C5-C6
8	n	102	BCL	C4-C3-C5-C6
8	z	101	BCL	C4-C3-C5-C6
10	M	405	U10	C30-C29-C31-C32
10	M	405	U10	C35-C34-C36-C37
10	m	405	U10	C30-C29-C31-C32
10	m	405	U10	C35-C34-C36-C37
13	D	103	SPO	C11-C10-C9-C7
13	Q	103	SPO	C25-C26-C27-C28
13	C	102	SPO	C25-C26-C27-C28
13	9	102	SPO	C11-C10-C9-C7
13	d	103	SPO	C11-C10-C9-C7
13	q	103	SPO	C25-C26-C27-C28
13	c	102	SPO	C25-C26-C27-C28
13	b9	102	SPO	C11-C10-C9-C7
13	M	406	SPO	C15-C16-C17-C18
13	m	406	SPO	C15-C16-C17-C18
11	H	301	PC1	O32-C31-O31-C3
11	h	301	PC1	O32-C31-O31-C3
11	H	301	PC1	C29-C2A-C2B-C2C
11	h	301	PC1	C29-C2A-C2B-C2C
14	m	407	CDL	C61-C62-C63-C64
13	A	102	SPO	C15-C16-C17-C19
13	U	103	SPO	C5-C6-C7-C9
13	a	102	SPO	C15-C16-C17-C19
13	u	103	SPO	C5-C6-C7-C9
14	M	407	CDL	C61-C62-C63-C64
8	C	101	BCL	C2A-CAA-CBA-CGA
8	c	101	BCL	C2A-CAA-CBA-CGA
11	L	306	PC1	C1-C2-C3-O31
11	H	302	PC1	C1-C2-C3-O31
11	A	103	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
11	A	105	PC1	C1-C2-C3-O31
11	l	306	PC1	C1-C2-C3-O31
11	h	302	PC1	C1-C2-C3-O31
11	a	103	PC1	C1-C2-C3-O31
11	a	105	PC1	C1-C2-C3-O31
14	M	407	CDL	CB3-CB4-CB6-OB8
14	m	407	CDL	CB3-CB4-CB6-OB8
8	P	102	BCL	C4-C3-C5-C6
8	C	101	BCL	C4-C3-C5-C6
8	p	102	BCL	C4-C3-C5-C6
8	c	101	BCL	C4-C3-C5-C6
8	P	102	BCL	C2-C3-C5-C6
8	p	102	BCL	C2-C3-C5-C6
10	M	405	U10	C28-C29-C31-C32
10	m	405	U10	C28-C29-C31-C32
11	L	306	PC1	O11-C1-C2-O21
11	A	103	PC1	O11-C1-C2-O21
11	A	105	PC1	O11-C1-C2-O21
11	l	306	PC1	O11-C1-C2-O21
11	a	103	PC1	O11-C1-C2-O21
11	a	105	PC1	O11-C1-C2-O21
14	M	407	CDL	C56-C57-C58-C59
14	m	407	CDL	C56-C57-C58-C59
10	L	304	U10	C27-C28-C29-C31
10	l	304	U10	C27-C28-C29-C31
11	A	103	PC1	O21-C2-C3-O31
11	A	105	PC1	O21-C2-C3-O31
11	a	103	PC1	O21-C2-C3-O31
11	a	105	PC1	O21-C2-C3-O31
14	M	407	CDL	OA6-CA4-CA6-OA8
14	m	407	CDL	OA6-CA4-CA6-OA8
11	h	301	PC1	C34-C35-C36-C37
8	C	101	BCL	C2-C3-C5-C6
8	c	101	BCL	C2-C3-C5-C6
10	M	405	U10	C33-C34-C36-C37
10	m	405	U10	C33-C34-C36-C37
11	H	301	PC1	C34-C35-C36-C37
10	L	305	U10	C19-C21-C22-C23
10	l	305	U10	C19-C21-C22-C23
13	C	102	SPO	C33-C35-C36-C37
13	3	103	SPO	C33-C35-C36-C37
13	c	102	SPO	C33-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
13	5	103	SPO	C33-C35-C36-C37
13	B	102	SPO	C11-C10-C9-C7
13	b	102	SPO	C11-C10-C9-C7
11	A	103	PC1	C27-C28-C29-C2A
11	a	103	PC1	C27-C28-C29-C2A
11	H	302	PC1	O11-C1-C2-C3
11	h	302	PC1	O11-C1-C2-C3
13	A	102	SPO	C5-C6-C7-C8
13	O	102	SPO	C10-C11-C12-C13
13	U	102	SPO	C5-C6-C7-C8
13	0	102	SPO	C5-C6-C7-C8
13	a	102	SPO	C5-C6-C7-C8
13	o	102	SPO	C10-C11-C12-C13
13	u	102	SPO	C5-C6-C7-C8
13	b0	102	SPO	C5-C6-C7-C8
13	B	102	SPO	C1-C4-C5-C6
13	b	102	SPO	C1-C4-C5-C6
10	L	305	U10	C27-C28-C29-C30
10	l	305	U10	C27-C28-C29-C30
13	A	102	SPO	C5-C6-C7-C9
13	O	102	SPO	C10-C11-C12-C14
13	P	101	SPO	C5-C6-C7-C9
13	U	102	SPO	C5-C6-C7-C9
13	U	103	SPO	C10-C11-C12-C14
13	3	102	SPO	C5-C6-C7-C9
13	0	102	SPO	C5-C6-C7-C9
13	a	102	SPO	C5-C6-C7-C9
13	o	102	SPO	C10-C11-C12-C14
13	p	101	SPO	C5-C6-C7-C9
13	u	102	SPO	C5-C6-C7-C9
13	u	103	SPO	C10-C11-C12-C14
13	5	102	SPO	C5-C6-C7-C9
13	b0	102	SPO	C5-C6-C7-C9
14	M	407	CDL	OA7-CA5-OA6-CA4
14	F	102	CDL	OB7-CB5-OB6-CB4
14	m	407	CDL	OA7-CA5-OA6-CA4
14	f	102	CDL	OB7-CB5-OB6-CB4
13	N	101	SPO	C11-C10-C9-C7
13	n	101	SPO	C11-C10-C9-C7
10	L	304	U10	C5-C4-O4-C4M
10	L	305	U10	C5-C4-O4-C4M
10	l	304	U10	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
10	l	305	U10	C5-C4-O4-C4M
11	H	302	PC1	O11-C1-C2-O21
11	h	302	PC1	O11-C1-C2-O21
14	M	407	CDL	CA3-CA4-CA6-OA8
14	m	407	CDL	CA3-CA4-CA6-OA8
10	L	304	U10	C25-C24-C26-C27
10	l	304	U10	C25-C24-C26-C27
11	H	302	PC1	C12-C11-O13-P
11	h	302	PC1	C12-C11-O13-P
11	A	104	PC1	O21-C2-C3-O31
11	a	104	PC1	O21-C2-C3-O31
14	M	407	CDL	C62-C63-C64-C65
14	m	407	CDL	C62-C63-C64-C65
13	3	102	SPO	C12-C14-C15-C16
13	5	102	SPO	C12-C14-C15-C16
11	L	307	PC1	O13-C11-C12-N
11	l	307	PC1	O13-C11-C12-N
13	U	103	SPO	C29-C28-C30-C31
13	u	103	SPO	C29-C28-C30-C31
13	Q	104	SPO	C15-C16-C17-C18
13	q	104	SPO	C15-C16-C17-C18
13	E	103	SPO	C15-C16-C17-C19
13	e	103	SPO	C15-C16-C17-C19
14	F	102	CDL	C72-C73-C74-C75
14	f	102	CDL	C72-C73-C74-C75
11	L	307	PC1	O11-C1-C2-C3
11	D	101	PC1	O11-C1-C2-C3
11	l	307	PC1	O11-C1-C2-C3
11	d	101	PC1	O11-C1-C2-C3
14	F	102	CDL	OB5-CB3-CB4-CB6
14	f	102	CDL	OB5-CB3-CB4-CB6
11	h	302	PC1	C33-C34-C35-C36
13	9	102	SPO	C2-C1-C4-C5
13	b9	102	SPO	C2-C1-C4-C5
11	H	302	PC1	C33-C34-C35-C36
11	H	301	PC1	C2-C1-O11-P
11	A	104	PC1	C2-C1-O11-P
11	h	301	PC1	C2-C1-O11-P
11	a	104	PC1	C2-C1-O11-P
14	F	102	CDL	OB5-CB3-CB4-OB6
14	f	102	CDL	OB5-CB3-CB4-OB6
11	A	104	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
11	a	104	PC1	C11-C12-N-C13
13	D	103	SPO	C12-C14-C15-C16
13	Q	103	SPO	C12-C14-C15-C16
13	Q	104	SPO	C11-C10-C9-C7
13	d	103	SPO	C12-C14-C15-C16
13	q	103	SPO	C12-C14-C15-C16
13	q	104	SPO	C11-C10-C9-C7
14	M	407	CDL	C12-C13-C14-C15
14	m	407	CDL	C12-C13-C14-C15
11	L	307	PC1	C1-O11-P-O14
11	H	301	PC1	C11-O13-P-O14
11	H	302	PC1	C1-O11-P-O13
11	A	103	PC1	C11-O13-P-O12
11	A	103	PC1	C11-O13-P-O11
11	A	104	PC1	C11-O13-P-O14
11	A	105	PC1	C11-O13-P-O12
11	l	307	PC1	C1-O11-P-O14
11	h	301	PC1	C11-O13-P-O14
11	h	302	PC1	C1-O11-P-O13
11	a	103	PC1	C11-O13-P-O12
11	a	103	PC1	C11-O13-P-O11
11	a	104	PC1	C11-O13-P-O14
11	a	105	PC1	C11-O13-P-O12
13	J	102	SPO	C12-C14-C15-C16
13	S	102	SPO	C11-C10-C9-C7
13	3	102	SPO	C17-C19-C20-C21
13	j	102	SPO	C12-C14-C15-C16
13	s	102	SPO	C11-C10-C9-C7
13	5	102	SPO	C17-C19-C20-C21
14	M	407	CDL	CA2-OA2-PA1-OA3
14	M	407	CDL	CA3-OA5-PA1-OA4
14	F	102	CDL	CB3-OB5-PB2-OB2
14	F	102	CDL	CB3-OB5-PB2-OB3
14	m	407	CDL	CA2-OA2-PA1-OA3
14	m	407	CDL	CA3-OA5-PA1-OA4
14	f	102	CDL	CB3-OB5-PB2-OB2
14	f	102	CDL	CB3-OB5-PB2-OB3
10	L	304	U10	C23-C24-C26-C27
10	l	304	U10	C23-C24-C26-C27
13	U	103	SPO	C27-C28-C30-C31
13	u	103	SPO	C27-C28-C30-C31
11	H	302	PC1	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
11	h	302	PC1	C34-C35-C36-C37
13	B	102	SPO	C9-C10-C11-C12
13	D	103	SPO	C9-C10-C11-C12
13	E	103	SPO	C9-C10-C11-C12
13	G	103	SPO	C9-C10-C11-C12
13	J	102	SPO	C9-C10-C11-C12
13	S	102	SPO	C9-C10-C11-C12
13	C	102	SPO	C14-C15-C16-C17
13	0	102	SPO	C9-C10-C11-C12
13	b	102	SPO	C9-C10-C11-C12
13	d	103	SPO	C9-C10-C11-C12
13	e	103	SPO	C9-C10-C11-C12
13	g	103	SPO	C9-C10-C11-C12
13	j	102	SPO	C9-C10-C11-C12
13	s	102	SPO	C9-C10-C11-C12
13	c	102	SPO	C14-C15-C16-C17
13	b0	102	SPO	C9-C10-C11-C12
13	C	102	SPO	C28-C30-C31-C32
13	3	103	SPO	C28-C30-C31-C32
13	c	102	SPO	C28-C30-C31-C32
13	5	103	SPO	C28-C30-C31-C32
14	M	407	CDL	C33-C34-C35-C36
14	m	407	CDL	C33-C34-C35-C36
8	7	102	BCL	C6-C7-C8-C9
8	6	102	BCL	C6-C7-C8-C9
11	d	101	PC1	C21-C22-C23-C24
11	D	101	PC1	C21-C22-C23-C24
13	J	102	SPO	C29-C28-C30-C31
13	j	102	SPO	C29-C28-C30-C31
14	M	407	CDL	C59-C60-C61-C62
14	m	407	CDL	C59-C60-C61-C62
10	M	405	U10	C24-C26-C27-C28
10	m	405	U10	C24-C26-C27-C28
14	F	102	CDL	CA3-CA4-CA6-OA8
14	F	102	CDL	CB3-CB4-CB6-OB8
14	f	102	CDL	CA3-CA4-CA6-OA8
14	f	102	CDL	CB3-CB4-CB6-OB8
13	M	406	SPO	C3-C1-O1-CM1
13	m	406	SPO	C3-C1-O1-CM1
13	Q	104	SPO	C15-C16-C17-C19
13	q	104	SPO	C15-C16-C17-C19
13	P	101	SPO	C11-C10-C9-C7

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Mol	Chain	Res	Type	Atoms
13	p	101	SPO	C11-C10-C9-C7
8	B	101	BCL	C4-C3-C5-C6
8	b	101	BCL	C4-C3-C5-C6
11	H	302	PC1	C36-C37-C38-C39
11	h	302	PC1	C36-C37-C38-C39
8	A	101	BCL	C11-C10-C8-C9
8	a	101	BCL	C11-C10-C8-C9
11	H	302	PC1	C32-C31-O31-C3
11	h	302	PC1	C32-C31-O31-C3
11	A	103	PC1	C32-C31-O31-C3
11	a	103	PC1	C32-C31-O31-C3
10	L	304	U10	C12-C11-C9-C10
10	l	304	U10	C12-C11-C9-C10
13	N	101	SPO	C29-C28-C30-C31
13	P	101	SPO	C29-C28-C30-C31
13	Q	104	SPO	C29-C28-C30-C31
13	n	101	SPO	C29-C28-C30-C31
13	p	101	SPO	C29-C28-C30-C31
13	q	104	SPO	C29-C28-C30-C31
13	9	102	SPO	C33-C35-C36-C37
13	b9	102	SPO	C33-C35-C36-C37
8	A	101	BCL	C11-C10-C8-C7
8	a	101	BCL	C11-C10-C8-C7
11	A	104	PC1	C11-C12-N-C14
11	a	104	PC1	C11-C12-N-C14
11	L	307	PC1	O21-C21-C22-C23
11	l	307	PC1	O21-C21-C22-C23
13	E	103	SPO	C8-C7-C9-C10
13	C	102	SPO	C13-C12-C14-C15
13	e	103	SPO	C8-C7-C9-C10
13	c	102	SPO	C13-C12-C14-C15
13	M	406	SPO	C15-C16-C17-C19
13	m	406	SPO	C15-C16-C17-C19
8	M	402	BCL	C4-C3-C5-C6
8	m	402	BCL	C4-C3-C5-C6
13	9	102	SPO	C29-C28-C30-C31
13	b9	102	SPO	C29-C28-C30-C31
10	M	405	U10	C5-C4-O4-C4M
10	m	405	U10	C5-C4-O4-C4M
11	H	302	PC1	O32-C31-O31-C3
11	h	302	PC1	O32-C31-O31-C3
8	Q	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	q	101	BCL	C8-C10-C11-C12
13	D	103	SPO	C25-C26-C27-C28
13	d	103	SPO	C25-C26-C27-C28
13	I	102	SPO	C29-C28-C30-C31
13	I	102	SPO	C34-C33-C35-C36
13	i	102	SPO	C29-C28-C30-C31
13	i	102	SPO	C34-C33-C35-C36
13	Q	104	SPO	C27-C28-C30-C31
13	q	104	SPO	C27-C28-C30-C31
11	A	103	PC1	O32-C31-O31-C3
11	a	103	PC1	O32-C31-O31-C3
10	L	304	U10	C3-C4-O4-C4M
10	l	304	U10	C3-C4-O4-C4M
11	A	104	PC1	C11-C12-N-C15
11	a	104	PC1	C11-C12-N-C15
13	E	103	SPO	C6-C7-C9-C10
13	C	102	SPO	C11-C12-C14-C15
13	e	103	SPO	C6-C7-C9-C10
13	c	102	SPO	C11-C12-C14-C15
13	D	103	SPO	C29-C28-C30-C31
13	G	101	SPO	C29-C28-C30-C31
13	O	102	SPO	C29-C28-C30-C31
13	d	103	SPO	C29-C28-C30-C31
13	g	101	SPO	C29-C28-C30-C31
13	o	102	SPO	C29-C28-C30-C31
8	M	402	BCL	C2-C3-C5-C6
8	m	402	BCL	C2-C3-C5-C6
10	L	304	U10	C12-C11-C9-C8
10	l	304	U10	C12-C11-C9-C8
8	M	402	BCL	C11-C10-C8-C7
8	m	402	BCL	C11-C10-C8-C7
11	A	105	PC1	C24-C25-C26-C27
11	a	105	PC1	C24-C25-C26-C27
13	3	103	SPO	C15-C16-C17-C18
13	5	103	SPO	C15-C16-C17-C18
8	b9	101	BCL	C4-C3-C5-C6
13	A	102	SPO	C29-C28-C30-C31
13	U	102	SPO	C29-C28-C30-C31
13	a	102	SPO	C29-C28-C30-C31
13	u	102	SPO	C29-C28-C30-C31
8	B	101	BCL	C2-C3-C5-C6
8	b	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	I	102	SPO	C27-C28-C30-C31
13	N	101	SPO	C27-C28-C30-C31
13	P	101	SPO	C27-C28-C30-C31
13	9	102	SPO	C27-C28-C30-C31
13	i	102	SPO	C27-C28-C30-C31
13	n	101	SPO	C27-C28-C30-C31
13	p	101	SPO	C27-C28-C30-C31
13	b9	102	SPO	C27-C28-C30-C31
8	D	102	BCL	C8-C10-C11-C12
8	d	102	BCL	C8-C10-C11-C12
8	F	101	BCL	C11-C10-C8-C9
8	f	101	BCL	C11-C10-C8-C9
8	B	101	BCL	C10-C11-C12-C13
8	b	101	BCL	C10-C11-C12-C13
13	U	103	SPO	C11-C10-C9-C7
13	u	103	SPO	C11-C10-C9-C7
8	K	101	BCL	C4-C3-C5-C6
8	9	101	BCL	C4-C3-C5-C6
8	k	101	BCL	C4-C3-C5-C6
13	E	101	SPO	C29-C28-C30-C31
13	e	101	SPO	C29-C28-C30-C31
13	S	103	SPO	C29-C28-C30-C31
13	S	103	SPO	C34-C33-C35-C36
13	s	103	SPO	C29-C28-C30-C31
13	s	103	SPO	C34-C33-C35-C36
8	V	101	BCL	C4-C3-C5-C6
8	v	101	BCL	C4-C3-C5-C6
13	B	102	SPO	C29-C28-C30-C31
13	E	101	SPO	C34-C33-C35-C36
13	b	102	SPO	C29-C28-C30-C31
13	e	101	SPO	C34-C33-C35-C36
13	A	102	SPO	C27-C28-C30-C31
13	E	101	SPO	C27-C28-C30-C31
13	a	102	SPO	C27-C28-C30-C31
13	e	101	SPO	C27-C28-C30-C31
8	E	102	BCL	C10-C11-C12-C13
8	e	102	BCL	C10-C11-C12-C13
11	A	103	PC1	C28-C29-C2A-C2B
11	a	103	PC1	C28-C29-C2A-C2B
13	M	406	SPO	C1-C4-C5-C6
13	Q	103	SPO	C1-C4-C5-C6
13	m	406	SPO	C1-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
13	q	103	SPO	C1-C4-C5-C6
8	M	402	BCL	C11-C10-C8-C9
8	I	101	BCL	C11-C10-C8-C9
8	m	402	BCL	C11-C10-C8-C9
8	i	101	BCL	C11-C10-C8-C9
11	L	307	PC1	C36-C37-C38-C39
11	l	307	PC1	C36-C37-C38-C39
13	J	102	SPO	C27-C28-C30-C31
13	j	102	SPO	C27-C28-C30-C31
8	7	102	BCL	C8-C10-C11-C12
8	6	102	BCL	C8-C10-C11-C12
14	M	407	CDL	C31-C32-C33-C34
14	m	407	CDL	C31-C32-C33-C34
8	2	101	BCL	CAA-CBA-CGA-O2A
8	4	101	BCL	CAA-CBA-CGA-O2A
10	L	305	U10	C15-C14-C16-C17
10	l	305	U10	C15-C14-C16-C17
13	3	102	SPO	C29-C28-C30-C31
13	5	102	SPO	C29-C28-C30-C31
8	Z	101	BCL	CAA-CBA-CGA-O2A
8	z	101	BCL	CAA-CBA-CGA-O2A
11	L	306	PC1	O21-C21-C22-C23
11	l	306	PC1	O21-C21-C22-C23
8	2	101	BCL	CAA-CBA-CGA-O1A
8	4	101	BCL	CAA-CBA-CGA-O1A
11	D	101	PC1	C24-C25-C26-C27
11	d	101	PC1	C24-C25-C26-C27
8	A	101	BCL	C8-C10-C11-C12
8	a	101	BCL	C8-C10-C11-C12
11	A	103	PC1	O11-C1-C2-C3
11	a	103	PC1	O11-C1-C2-C3
13	Q	102	SPO	C34-C33-C35-C36
13	9	102	SPO	O1-C1-C4-C5
13	b9	102	SPO	O1-C1-C4-C5
8	F	101	BCL	C11-C10-C8-C7
8	I	101	BCL	C11-C10-C8-C7
8	V	101	BCL	C6-C7-C8-C10
8	f	101	BCL	C11-C10-C8-C7
8	i	101	BCL	C11-C10-C8-C7
8	v	101	BCL	C6-C7-C8-C10
8	n	102	BCL	C10-C11-C12-C13
8	N	102	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	M	406	SPO	C33-C35-C36-C37
13	m	406	SPO	C33-C35-C36-C37
8	E	102	BCL	CAA-CBA-CGA-O2A
8	e	102	BCL	CAA-CBA-CGA-O2A
11	H	301	PC1	O21-C21-C22-C23
11	h	301	PC1	O21-C21-C22-C23
13	q	102	SPO	C34-C33-C35-C36
8	T	101	BCL	C2-C3-C5-C6
8	t	101	BCL	C2-C3-C5-C6
13	G	101	SPO	C27-C28-C30-C31
13	g	101	SPO	C27-C28-C30-C31
11	A	105	PC1	C36-C37-C38-C39
11	a	105	PC1	C36-C37-C38-C39
8	T	101	BCL	C4-C3-C5-C6
8	t	101	BCL	C4-C3-C5-C6
13	I	102	SPO	C32-C33-C35-C36
13	O	102	SPO	C27-C28-C30-C31
13	i	102	SPO	C32-C33-C35-C36
13	o	102	SPO	C27-C28-C30-C31
8	V	101	BCL	C6-C7-C8-C9
8	v	101	BCL	C6-C7-C8-C9
10	M	405	U10	C25-C24-C26-C27
10	m	405	U10	C25-C24-C26-C27
11	l	307	PC1	C32-C33-C34-C35
13	D	103	SPO	C27-C28-C30-C31
13	d	103	SPO	C27-C28-C30-C31
13	E	101	SPO	C11-C10-C9-C7
13	E	103	SPO	C17-C19-C20-C21
13	C	102	SPO	C17-C19-C20-C21
13	e	101	SPO	C11-C10-C9-C7
13	e	103	SPO	C17-C19-C20-C21
13	c	102	SPO	C17-C19-C20-C21
11	L	307	PC1	C32-C33-C34-C35
8	0	101	BCL	C4-C3-C5-C6
8	b0	101	BCL	C4-C3-C5-C6
9	M	404	BPH	C2-C1-O2A-CGA
9	m	404	BPH	C2-C1-O2A-CGA
8	7	101	BCL	C11-C10-C8-C7
8	6	101	BCL	C11-C10-C8-C7
11	L	307	PC1	O31-C31-C32-C33
11	l	307	PC1	O31-C31-C32-C33
14	F	102	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
13	U	103	SPO	C2-C1-C4-C5
13	u	103	SPO	C2-C1-C4-C5
14	f	102	CDL	C52-C53-C54-C55
14	F	102	CDL	OB9-CB7-OB8-CB6
14	f	102	CDL	OB9-CB7-OB8-CB6
8	0	101	BCL	C2-C3-C5-C6
8	b0	101	BCL	C2-C3-C5-C6
8	7	102	BCL	CAA-CBA-CGA-O2A
8	6	102	BCL	CAA-CBA-CGA-O2A
14	F	102	CDL	C71-CB7-OB8-CB6
14	f	102	CDL	C71-CB7-OB8-CB6
13	Q	102	SPO	C11-C10-C9-C7
13	q	102	SPO	C11-C10-C9-C7
8	E	102	BCL	CAA-CBA-CGA-O1A
11	A	104	PC1	O21-C21-C22-C23
11	a	104	PC1	O21-C21-C22-C23
13	U	102	SPO	C27-C28-C30-C31
13	u	102	SPO	C27-C28-C30-C31
8	J	101	BCL	C10-C11-C12-C13
8	j	101	BCL	C10-C11-C12-C13
8	Z	101	BCL	CAA-CBA-CGA-O1A
8	e	102	BCL	CAA-CBA-CGA-O1A
8	z	101	BCL	CAA-CBA-CGA-O1A
11	H	301	PC1	O22-C21-C22-C23
11	h	301	PC1	O22-C21-C22-C23
14	M	407	CDL	C72-C71-CB7-OB8
14	m	407	CDL	C72-C71-CB7-OB8
8	Q	101	BCL	CAD-CBD-CGD-O2D
8	q	101	BCL	CAD-CBD-CGD-O2D
8	7	101	BCL	C8-C10-C11-C12
8	6	101	BCL	C8-C10-C11-C12
14	M	407	CDL	C12-C11-CA5-OA6
14	m	407	CDL	C12-C11-CA5-OA6

There are no ring outliers.

140 monomers are involved in 406 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	b9	101	BCL	3	0
8	l	302	BCL	1	0
10	M	405	U10	1	0
8	S	101	BCL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	105	PC1	5	0
13	q	104	SPO	6	0
8	Q	101	BCL	2	0
8	A	101	BCL	4	0
13	U	102	SPO	2	0
8	W	101	BCL	10	0
10	m	405	U10	2	0
8	7	102	BCL	3	0
8	L	302	BCL	1	0
8	i	101	BCL	2	0
8	w	101	BCL	10	0
11	L	306	PC1	3	0
8	J	101	BCL	4	0
13	a	102	SPO	4	0
8	C	101	BCL	3	0
13	S	102	SPO	4	0
13	c	102	SPO	5	0
8	r	101	BCL	3	0
8	f	101	BCL	4	0
13	m	406	SPO	4	0
8	K	101	BCL	2	0
8	k	101	BCL	1	0
8	b1	101	BCL	1	0
8	6	102	BCL	3	0
13	G	101	SPO	4	0
13	g	103	SPO	4	0
11	L	307	PC1	4	0
13	C	102	SPO	6	0
8	5	101	BCL	3	0
8	R	101	BCL	3	0
13	p	101	SPO	2	0
8	U	101	BCL	1	0
8	0	101	BCL	4	0
8	g	102	BCL	3	0
13	i	102	SPO	1	0
14	M	407	CDL	4	0
11	a	103	PC1	4	0
8	c	101	BCL	3	0
8	s	101	BCL	2	0
13	b9	102	SPO	6	0
8	M	403	BCL	2	0
8	T	101	BCL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	305	U10	3	0
9	l	303	BPH	3	0
8	3	101	BCL	3	0
13	Q	104	SPO	6	0
8	9	101	BCL	3	0
8	e	102	BCL	3	0
8	M	402	BCL	1	0
11	l	307	PC1	4	0
8	u	101	BCL	1	0
13	N	101	SPO	1	0
13	9	102	SPO	6	0
11	l	306	PC1	3	0
8	n	102	BCL	6	0
8	1	101	BCL	1	0
11	H	302	PC1	1	0
11	A	103	PC1	5	0
13	5	102	SPO	6	0
8	I	101	BCL	2	0
13	d	103	SPO	2	0
13	q	102	SPO	4	0
13	M	406	SPO	3	0
13	5	103	SPO	3	0
8	P	102	BCL	2	0
11	a	105	PC1	4	0
13	j	102	SPO	2	0
9	m	404	BPH	3	0
8	j	101	BCL	4	0
13	S	103	SPO	3	0
13	E	103	SPO	2	0
11	H	301	PC1	5	0
13	A	102	SPO	5	0
8	b	101	BCL	2	0
8	6	101	BCL	4	0
8	o	101	BCL	4	0
13	O	102	SPO	1	0
13	P	101	SPO	2	0
13	e	103	SPO	2	0
13	G	103	SPO	5	0
13	X	101	SPO	9	0
8	p	102	BCL	1	0
11	a	104	PC1	5	0
13	e	101	SPO	3	0

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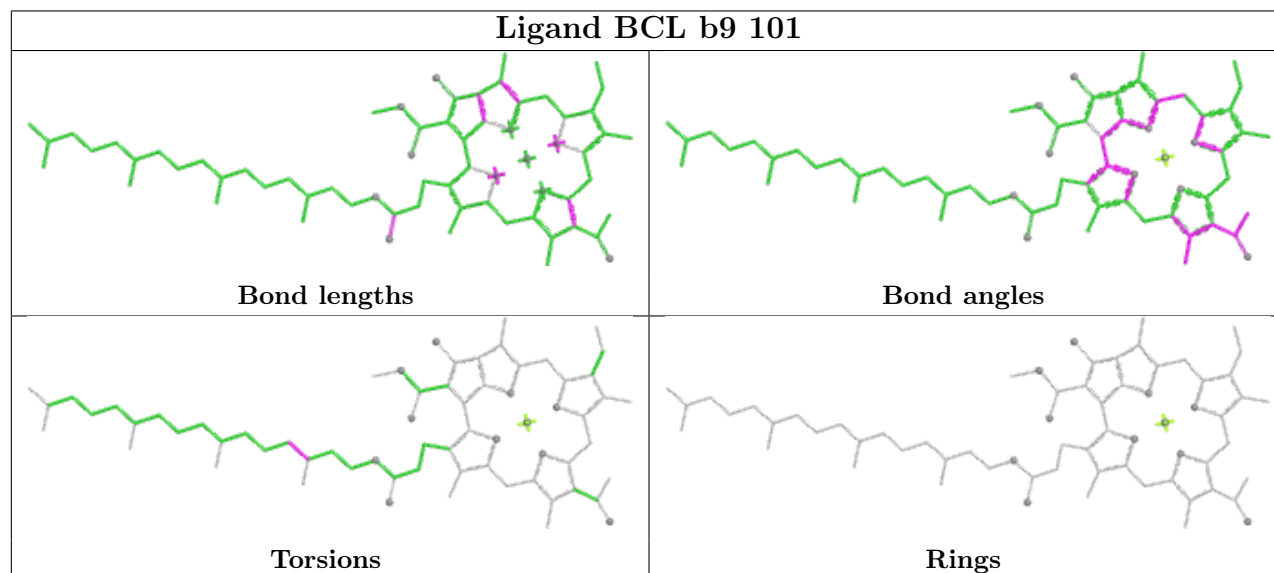
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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8	7	101	BCL	4	0
11	A	104	PC1	5	0
8	O	101	BCL	4	0
11	h	301	PC1	6	0
8	G	102	BCL	4	0
8	m	403	BCL	3	0
13	B	102	SPO	3	0
13	Q	102	SPO	5	0
13	u	102	SPO	2	0
13	J	102	SPO	1	0
13	Q	103	SPO	1	0
14	f	102	CDL	5	0
13	q	103	SPO	1	0
8	B	101	BCL	2	0
13	s	103	SPO	4	0
8	F	101	BCL	4	0
8	Z	101	BCL	2	0
8	z	101	BCL	2	0
13	g	101	SPO	4	0
8	b0	101	BCL	3	0
13	E	101	SPO	3	0
13	o	102	SPO	1	0
13	I	102	SPO	2	0
8	d	102	BCL	3	0
13	u	103	SPO	1	0
14	m	407	CDL	4	0
9	M	404	BPH	2	0
8	t	101	BCL	1	0
13	U	103	SPO	1	0
8	q	101	BCL	3	0
8	N	102	BCL	4	0
13	n	101	SPO	1	0
8	m	402	BCL	2	0
11	h	302	PC1	2	0
8	v	101	BCL	7	0
13	x	101	SPO	8	0
13	0	102	SPO	2	0
13	3	102	SPO	6	0
13	b	102	SPO	2	0
10	l	305	U10	4	0
13	3	103	SPO	2	0

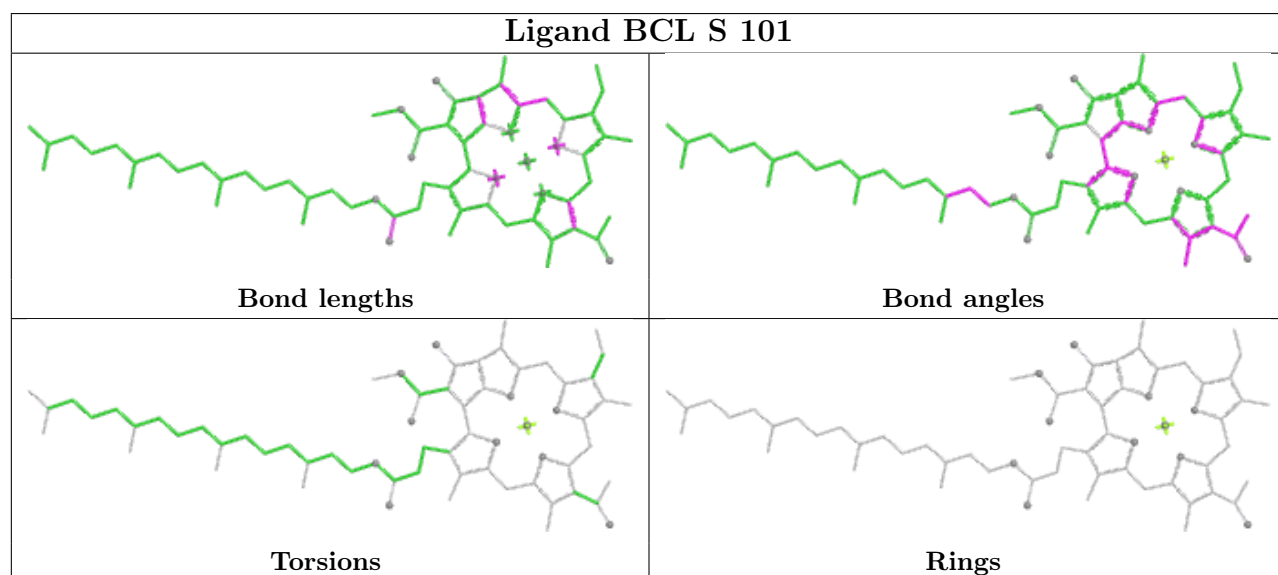
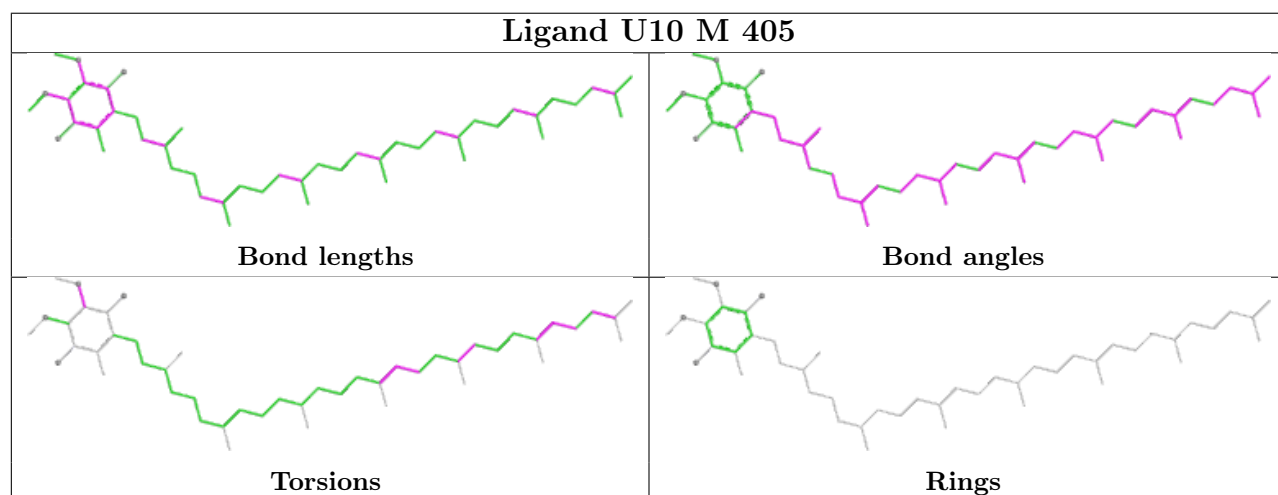
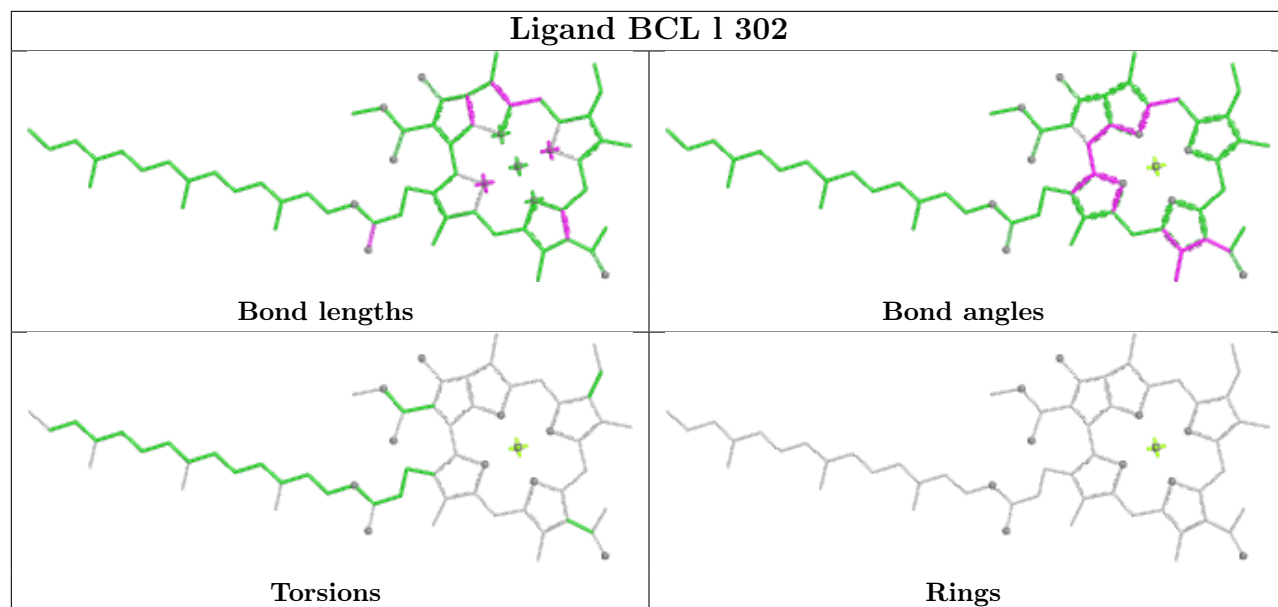
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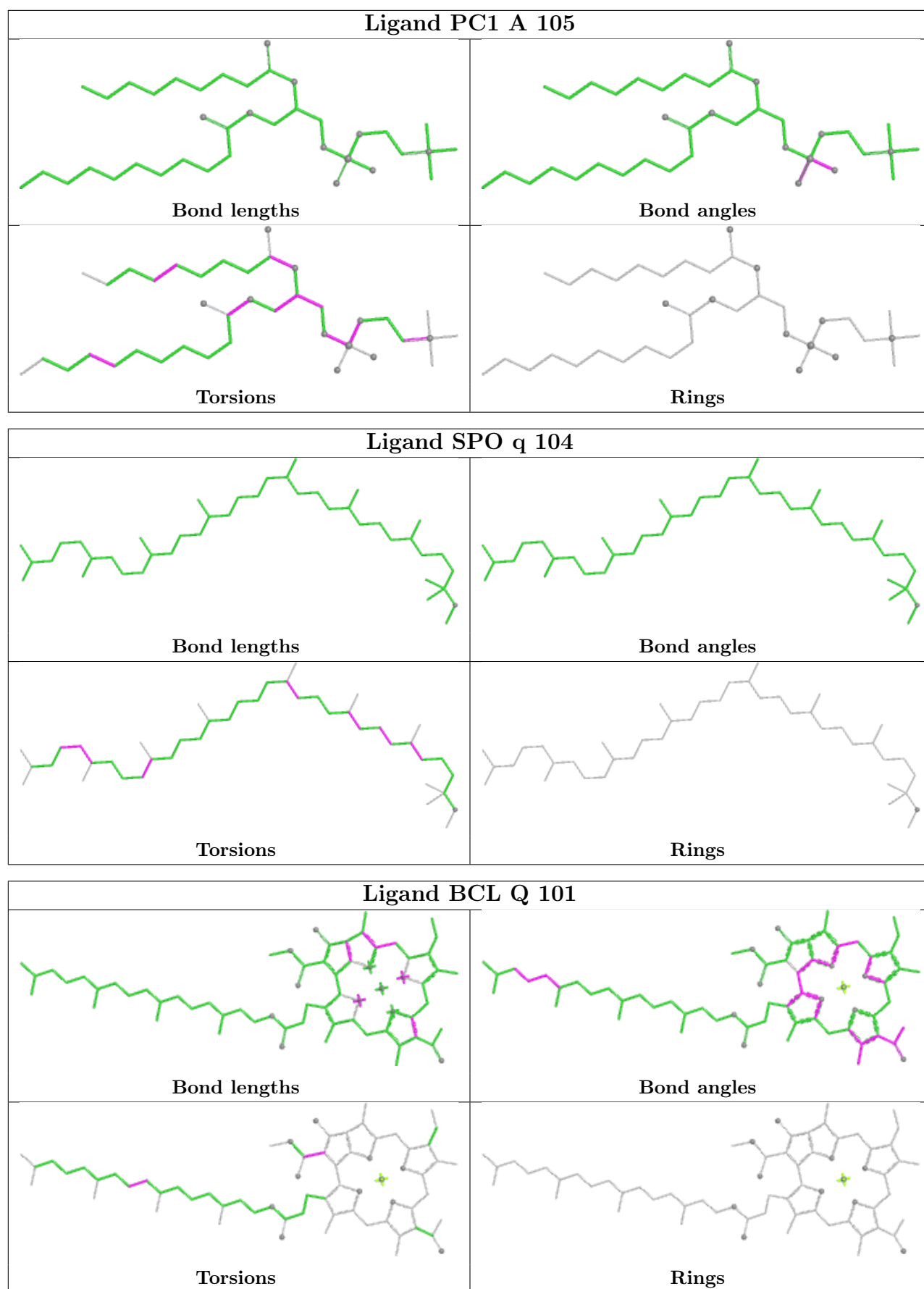
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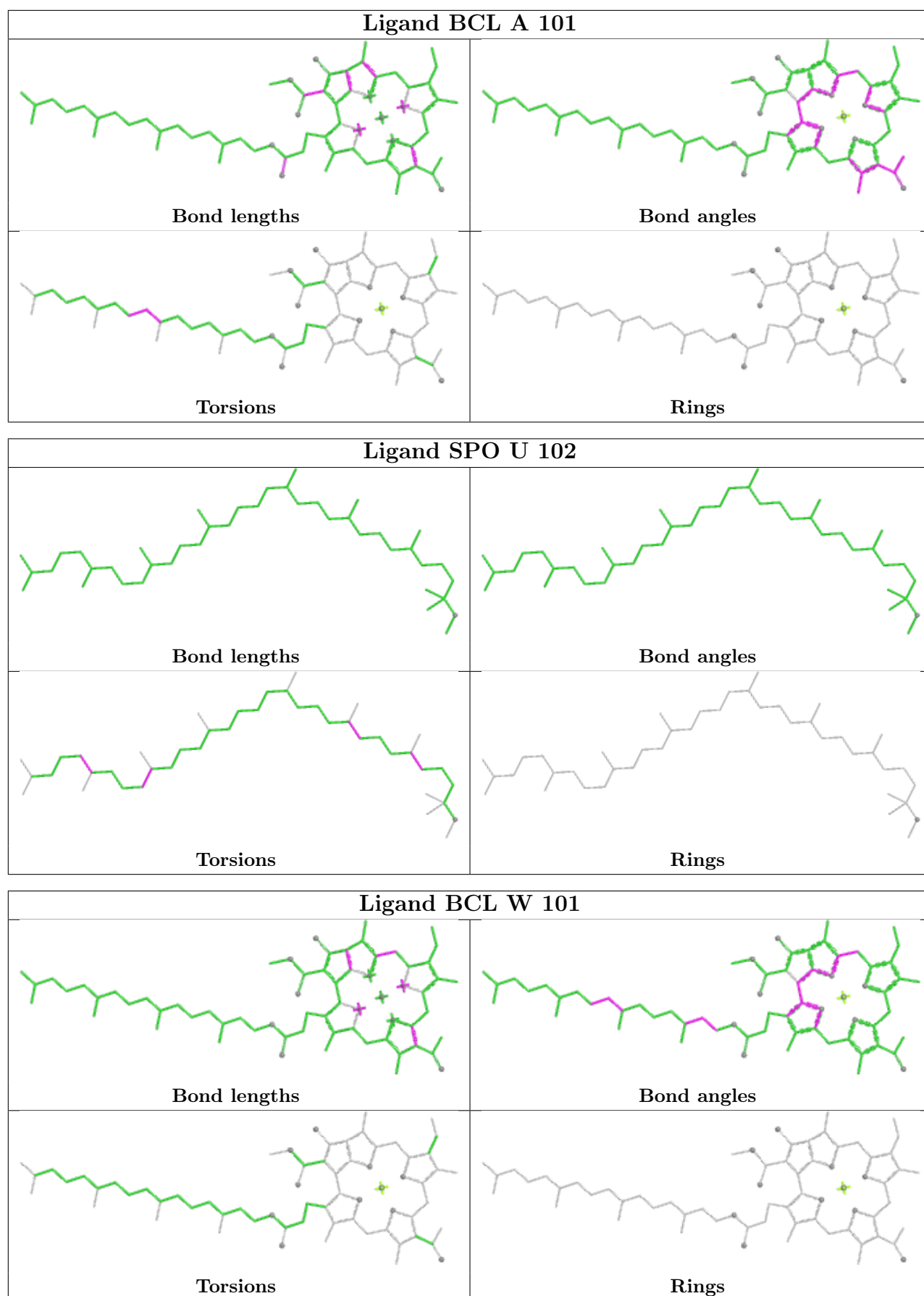
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	V	101	BCL	6	0
14	F	102	CDL	5	0
9	L	303	BPH	2	0
8	E	102	BCL	3	0
11	D	101	PC1	4	0
13	s	102	SPO	2	0
13	D	103	SPO	2	0
11	d	101	PC1	3	0
13	b0	102	SPO	1	0
8	a	101	BCL	4	0

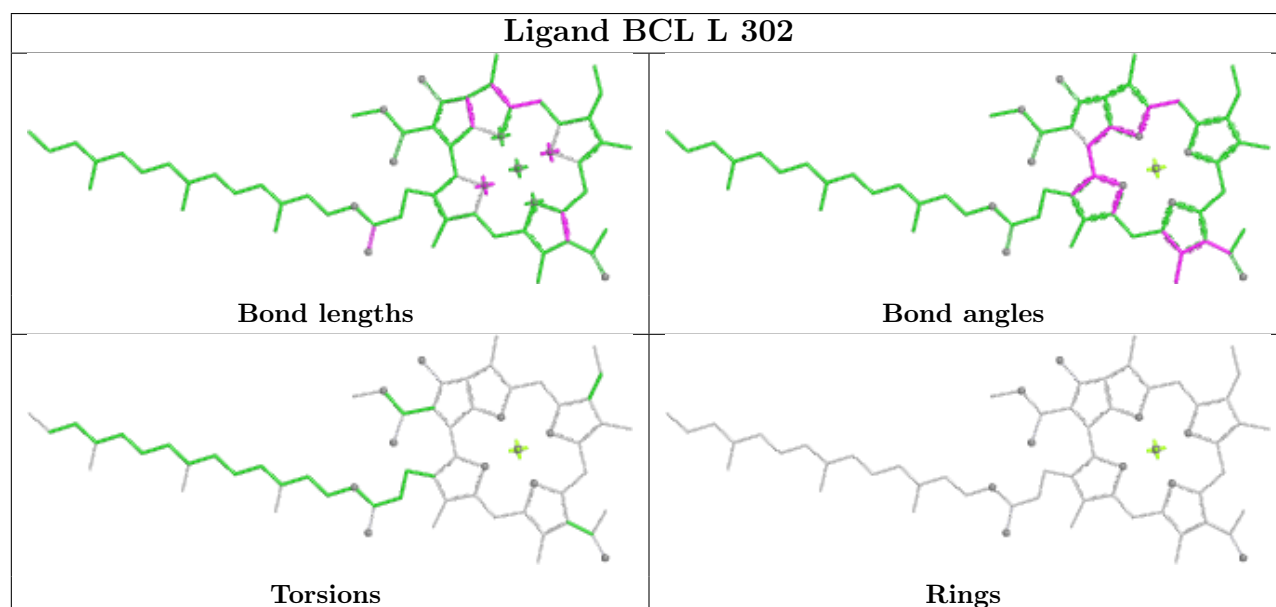
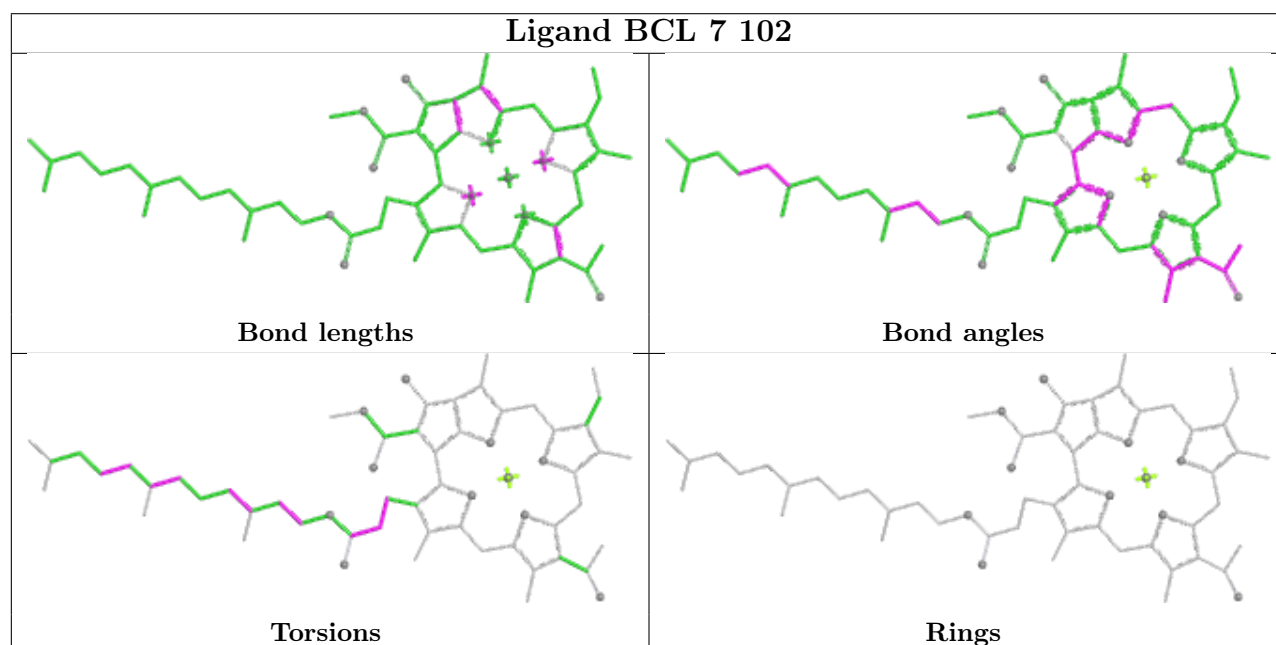
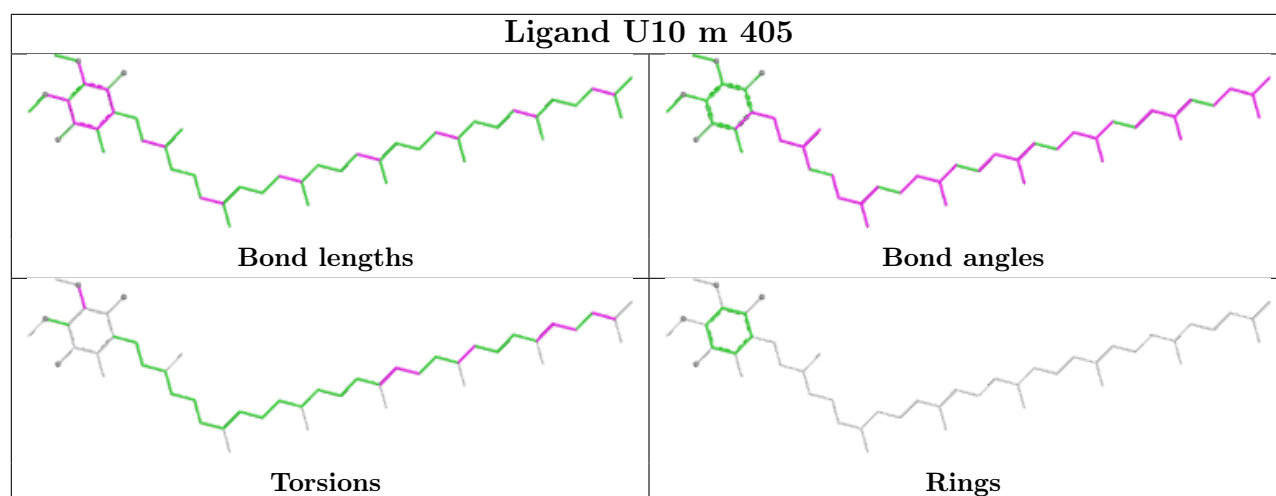
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

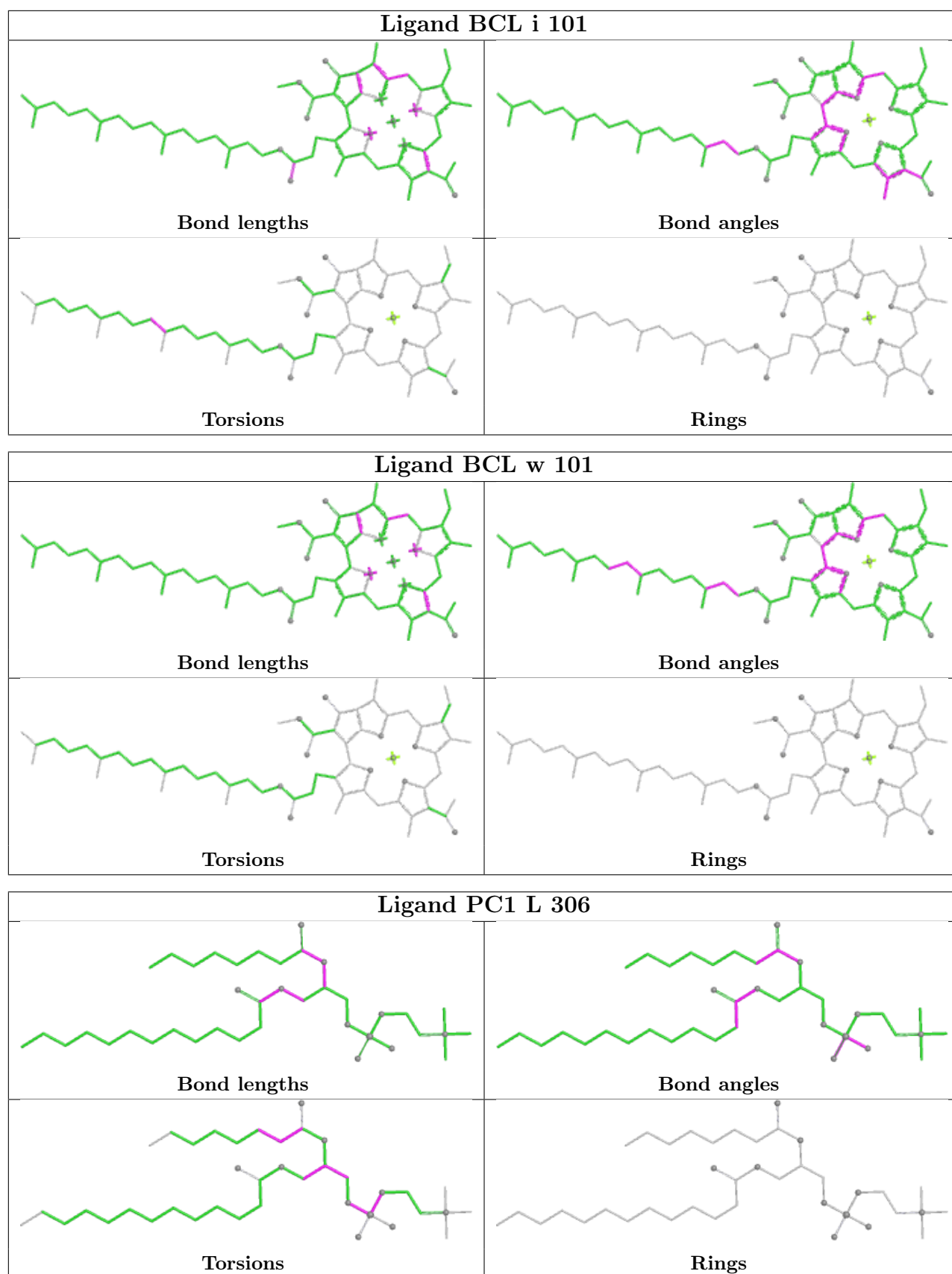


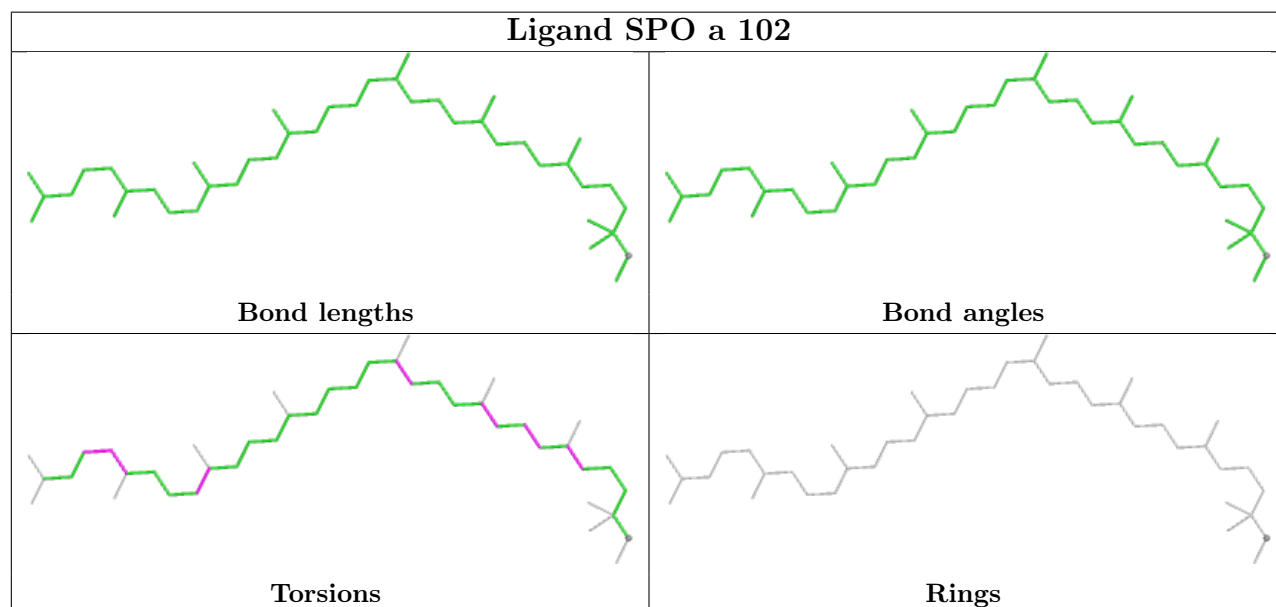
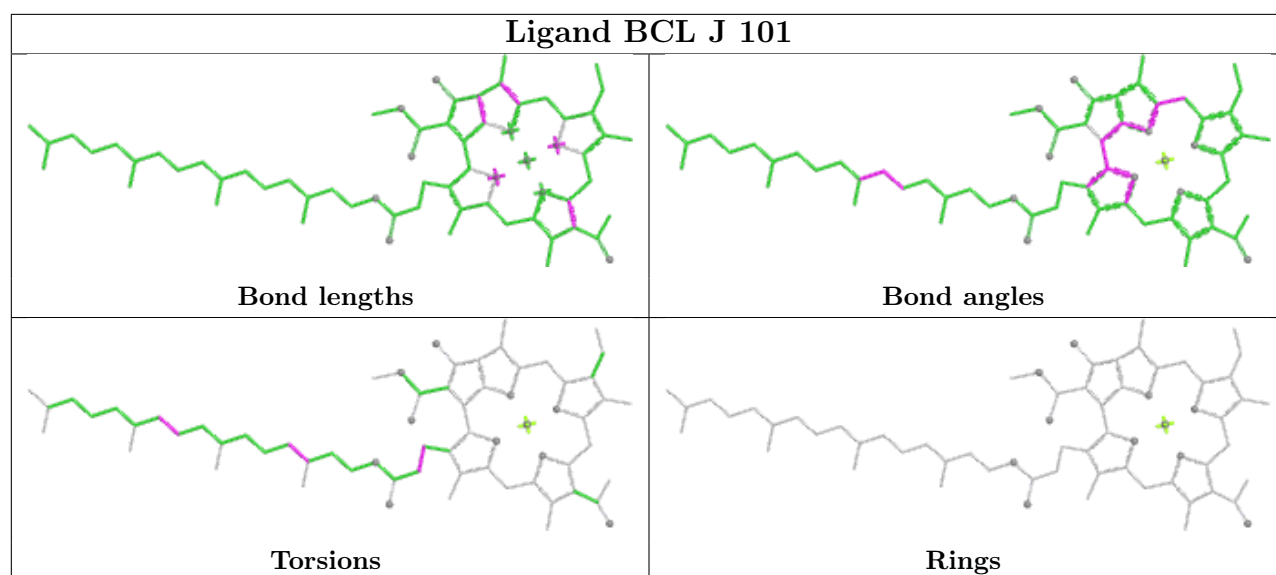


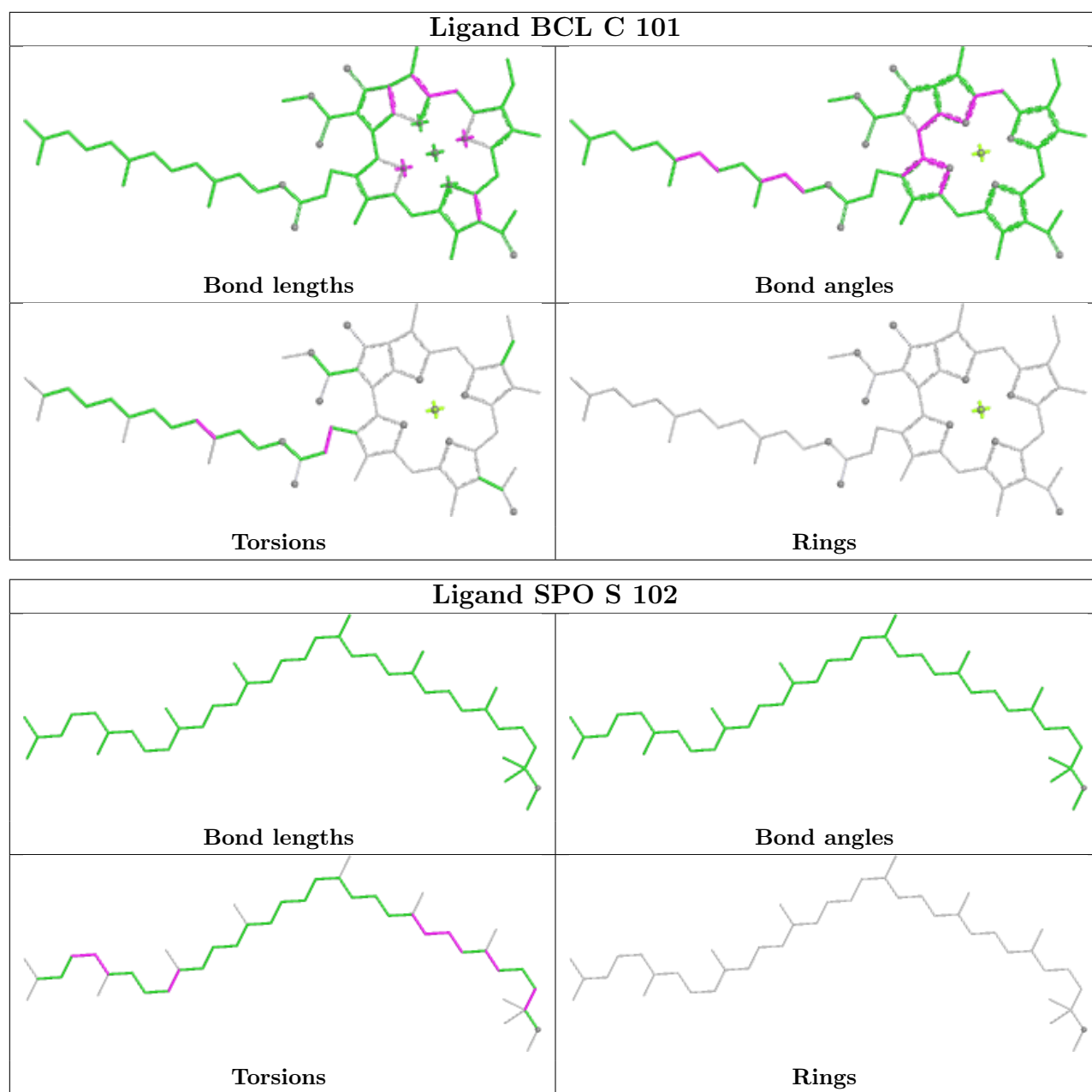


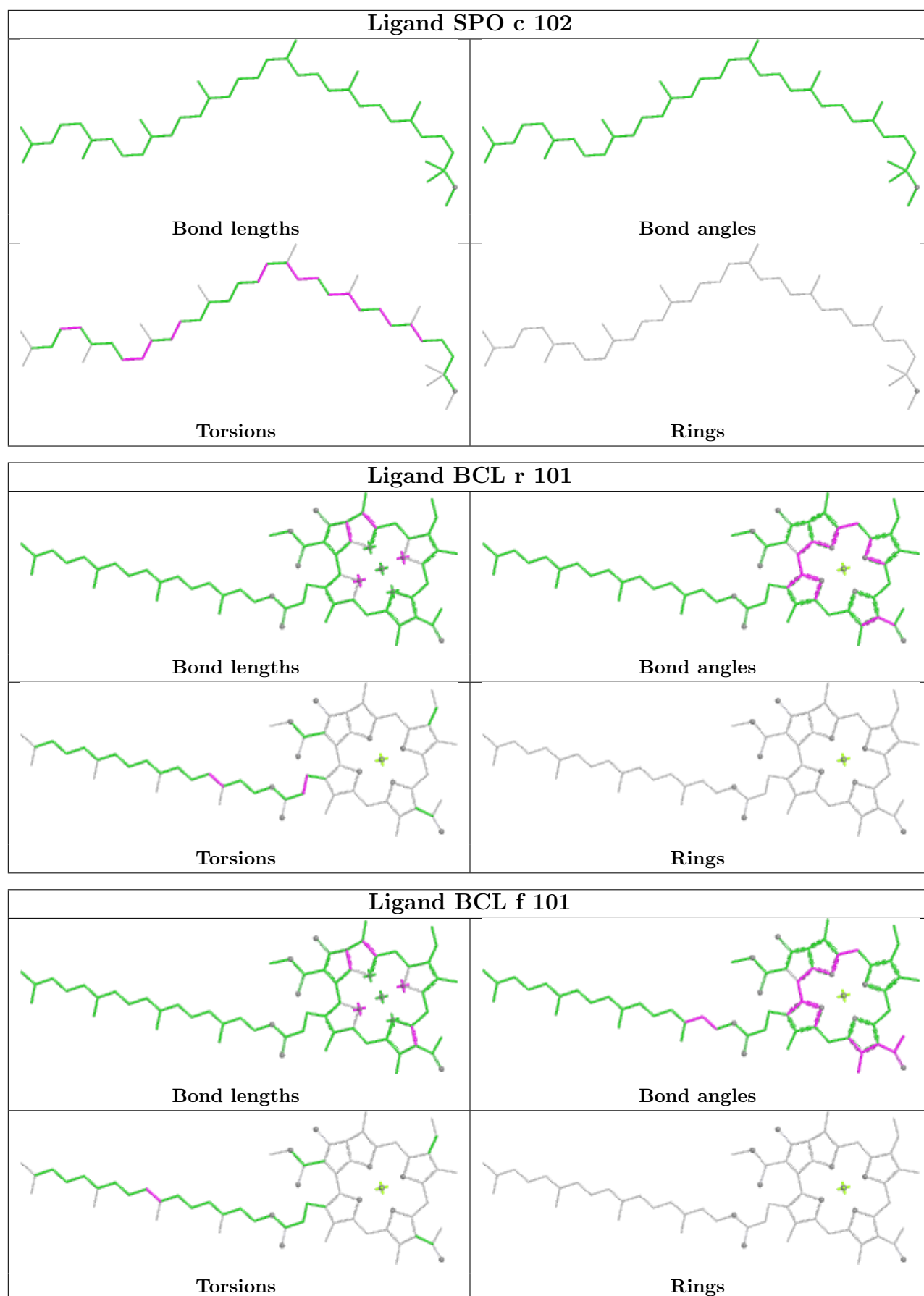


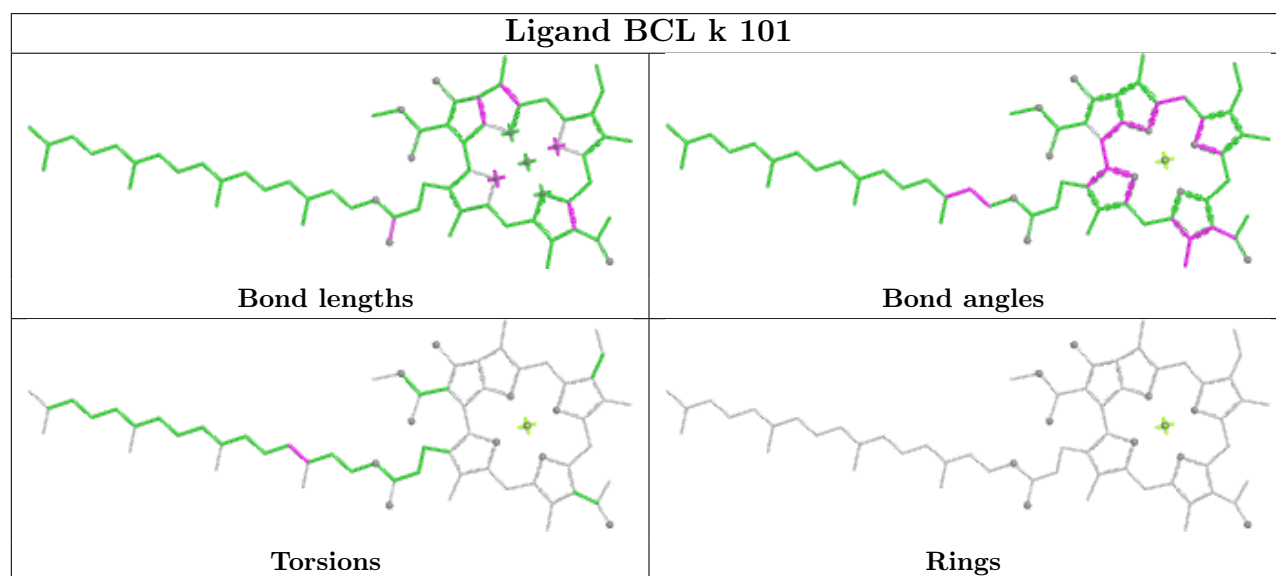
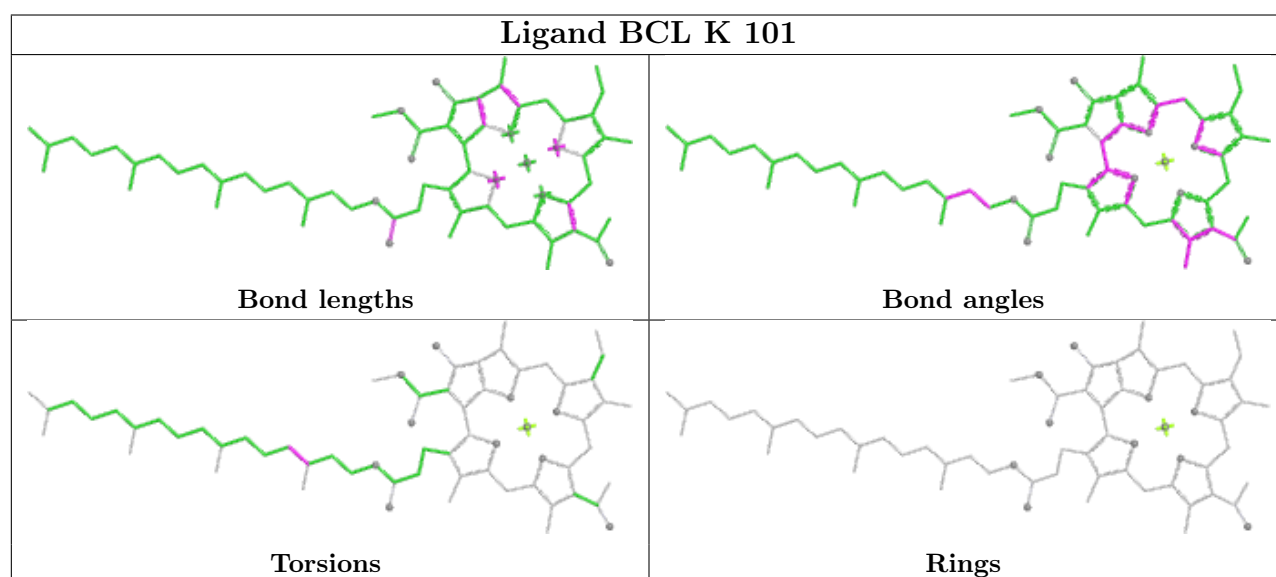
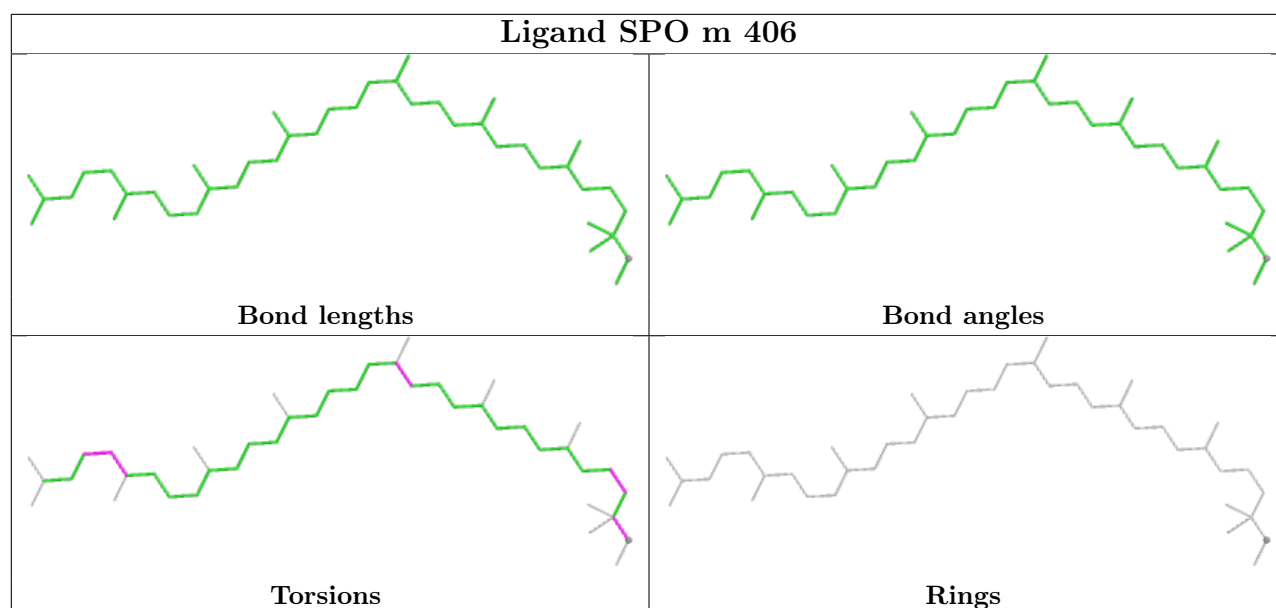


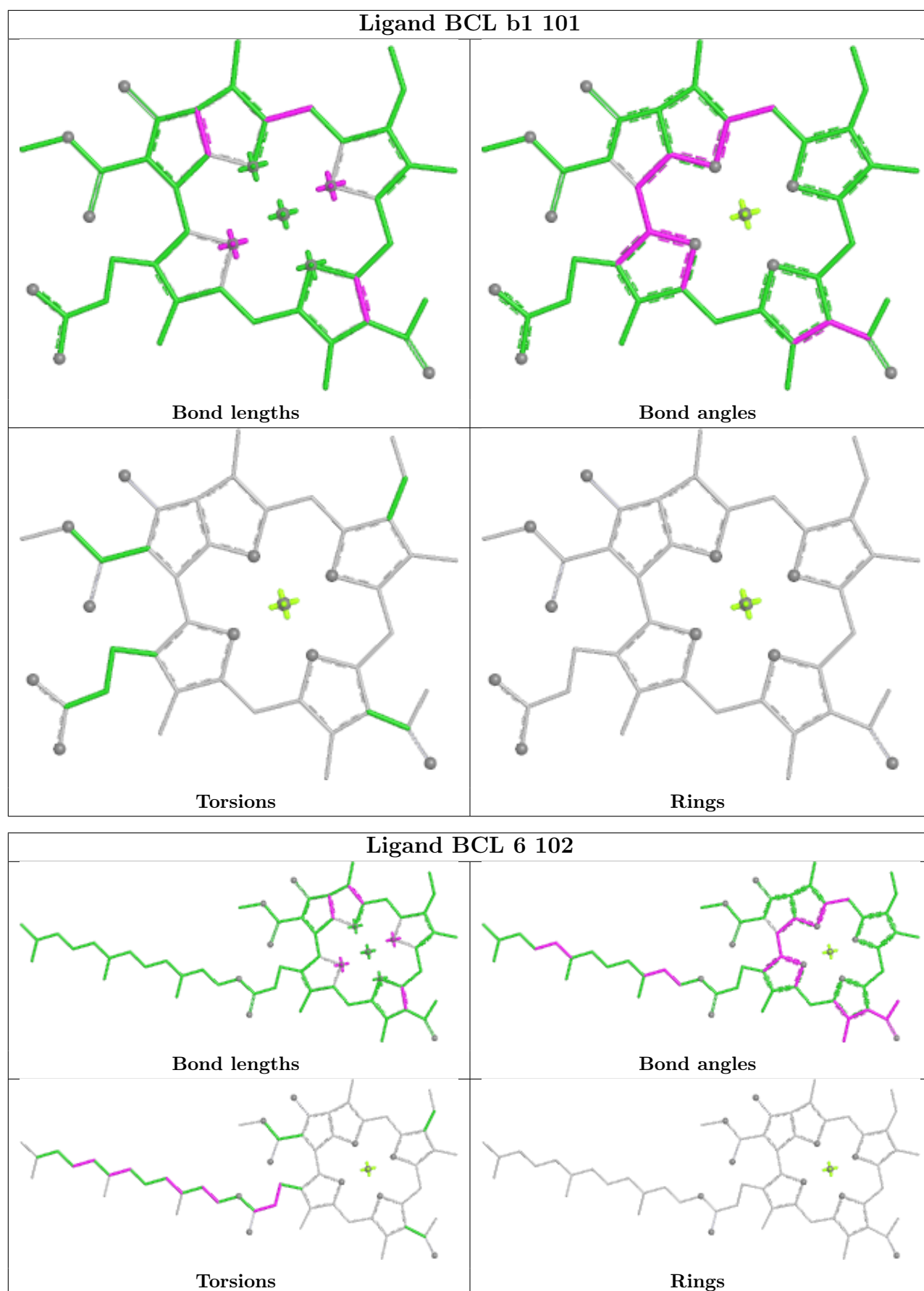


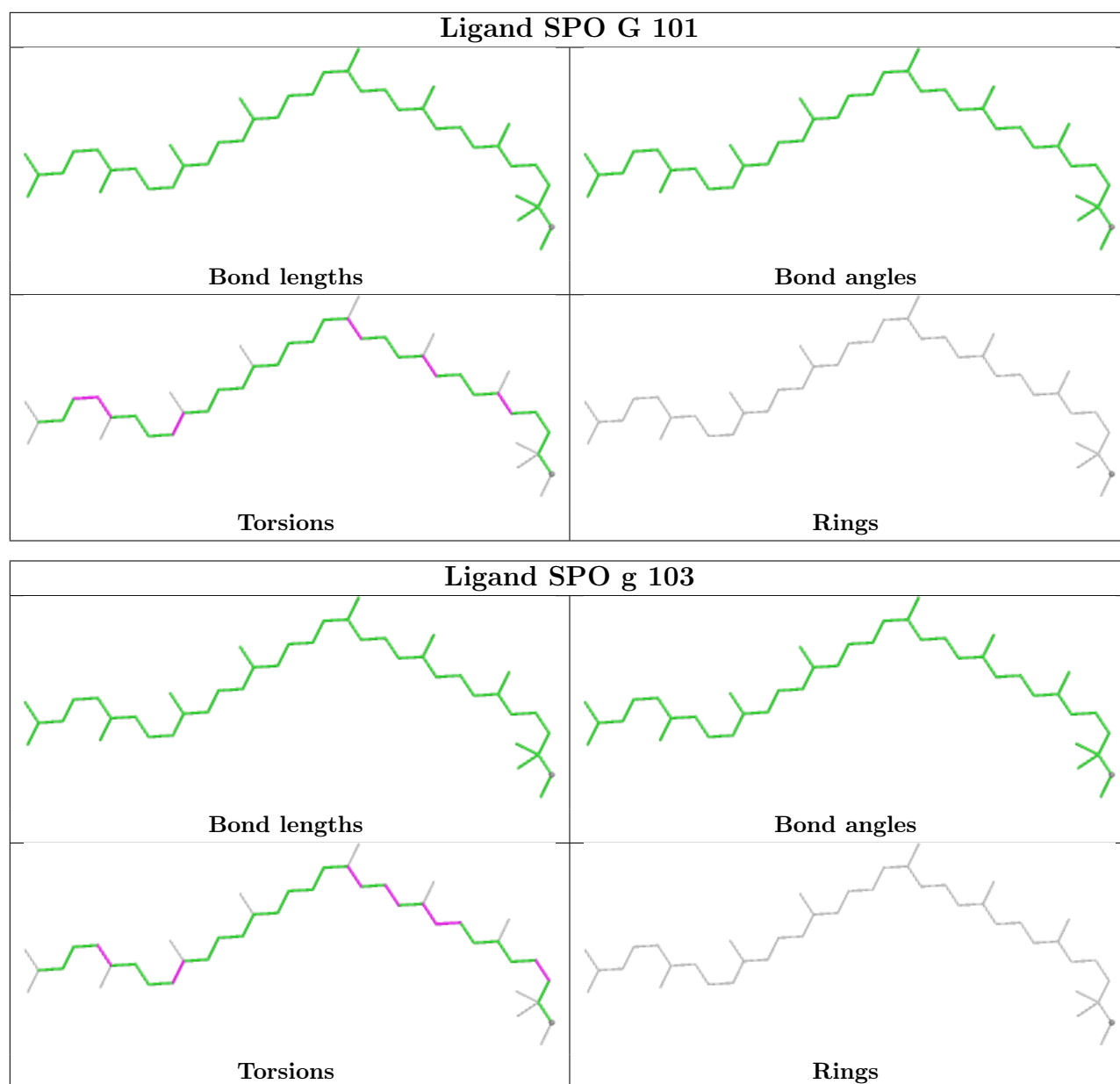


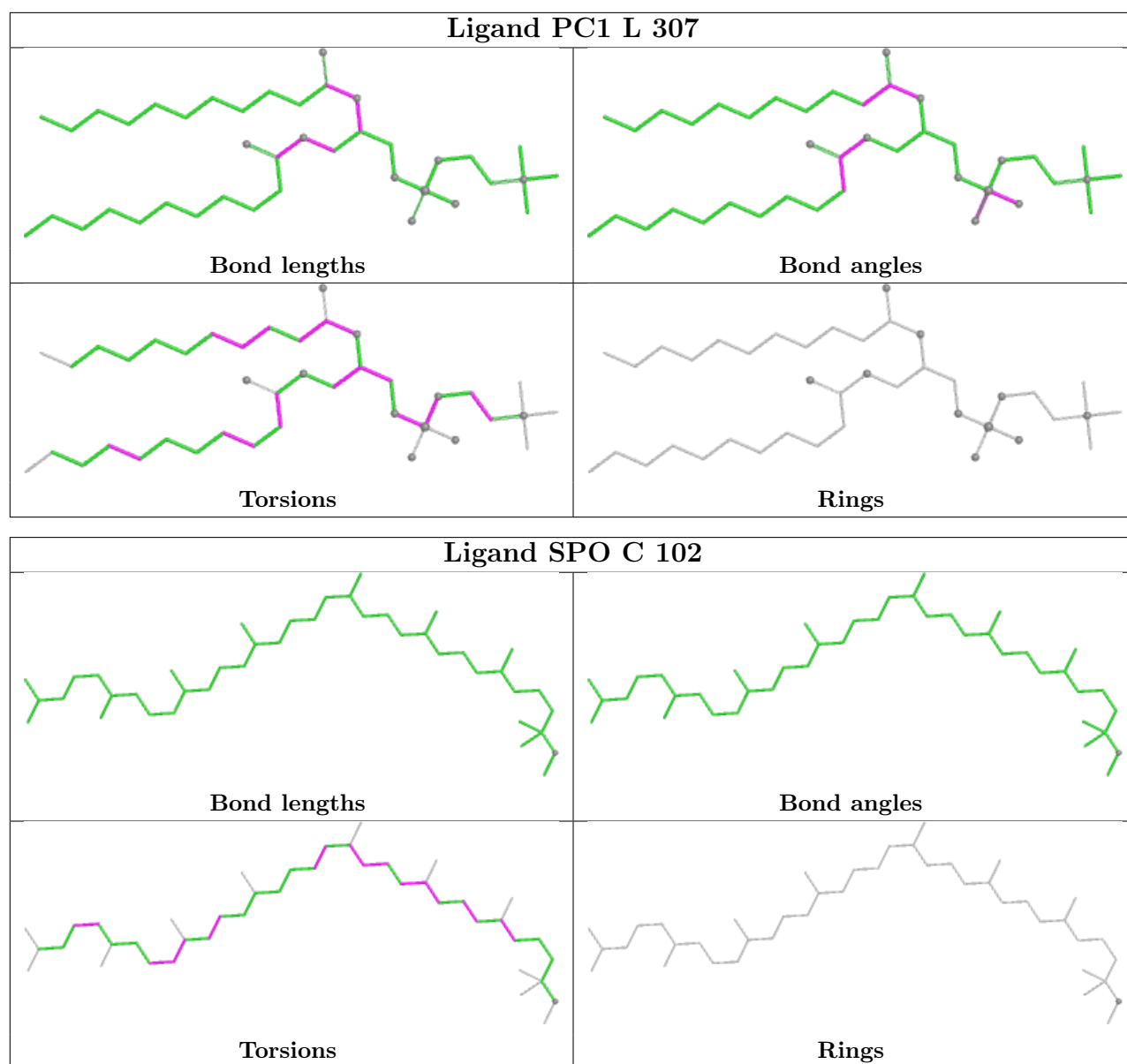


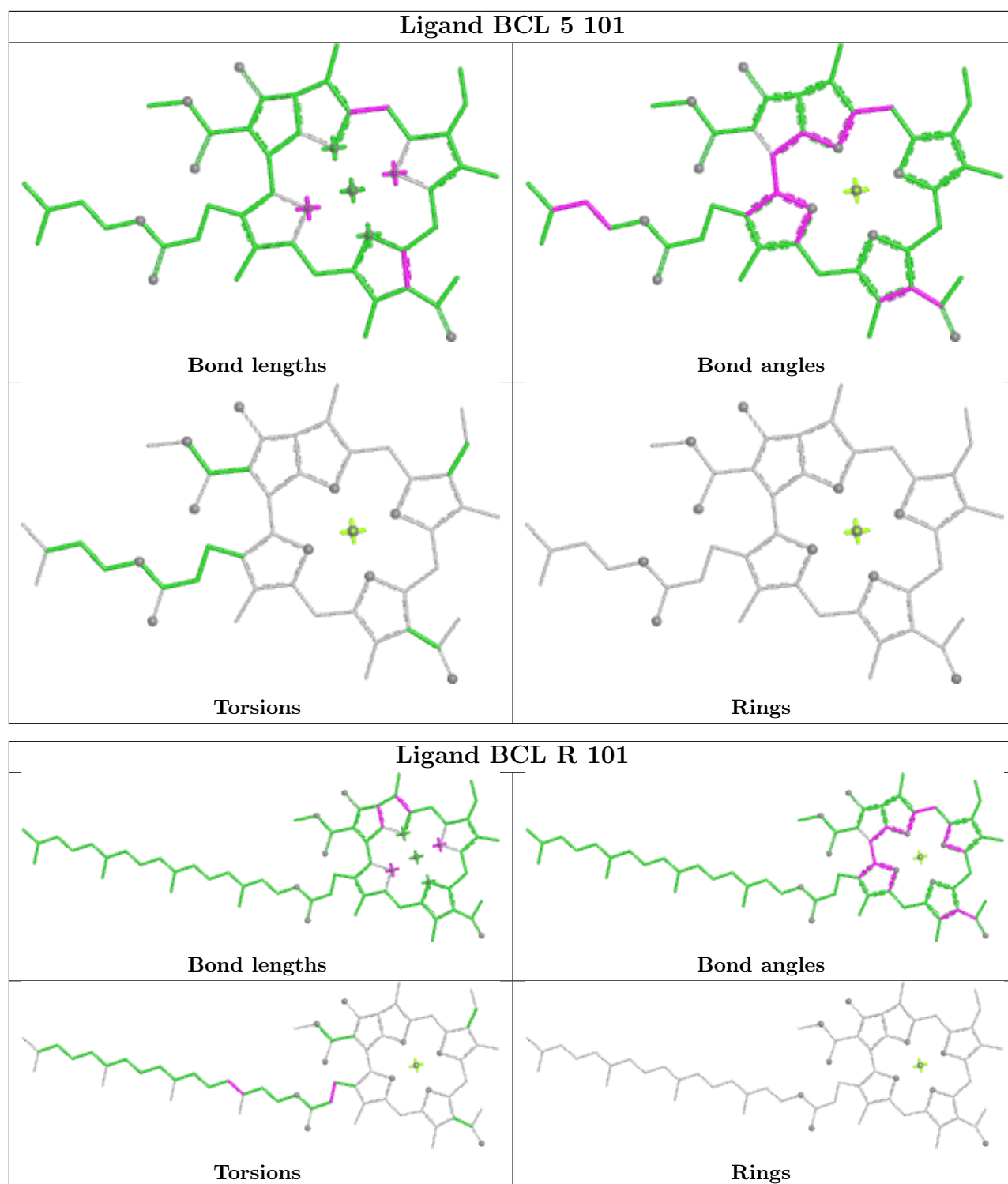


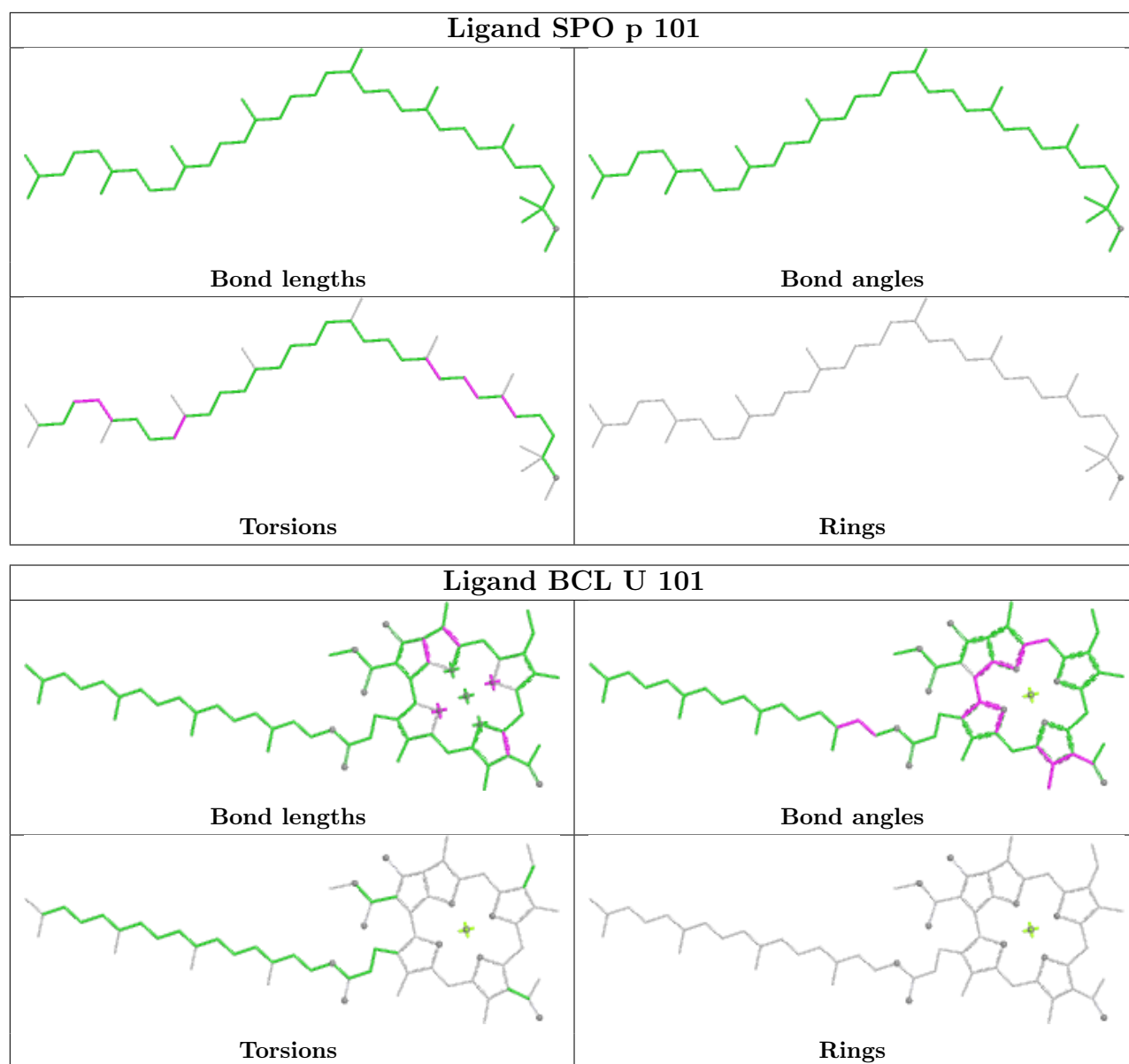


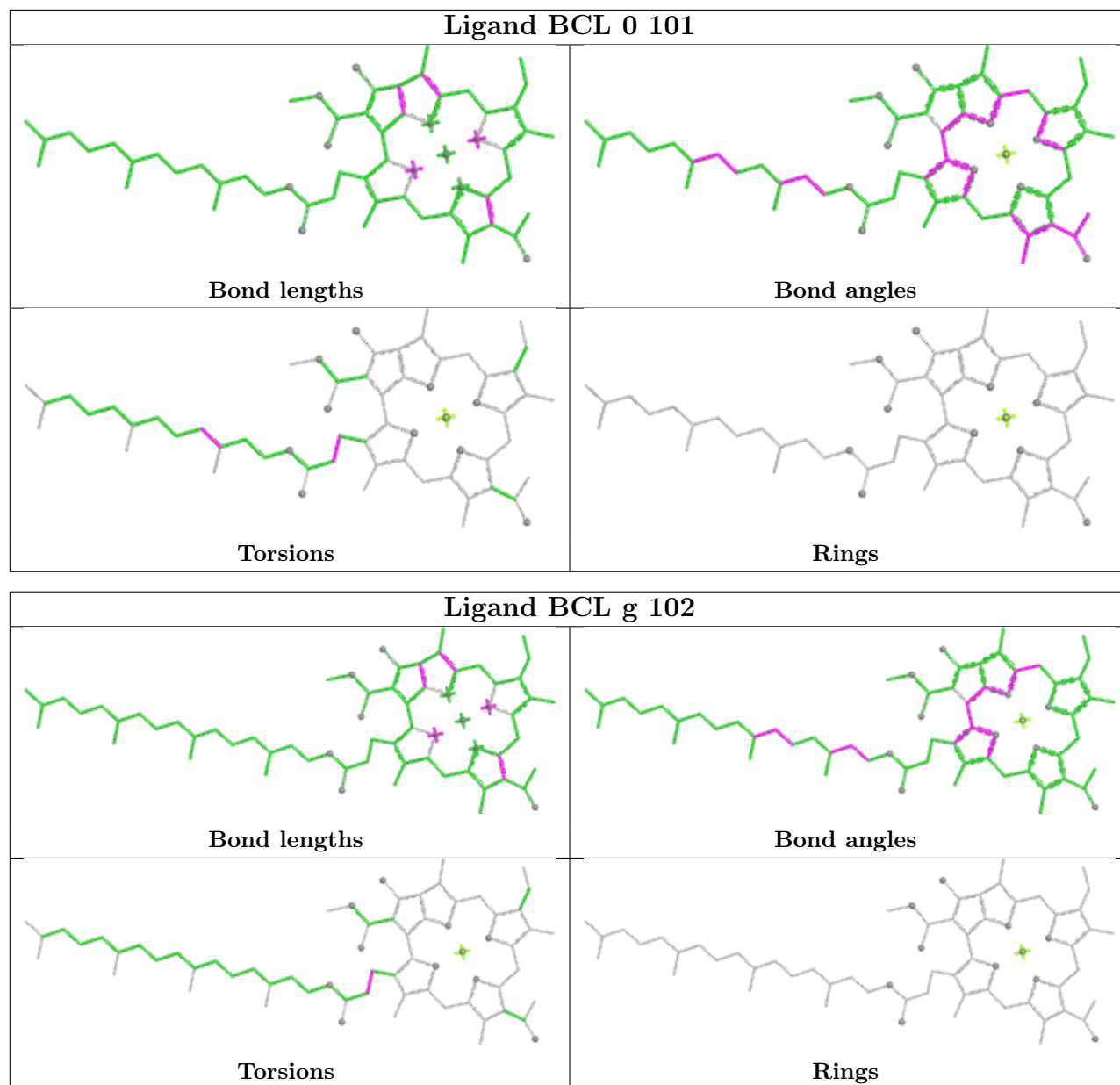


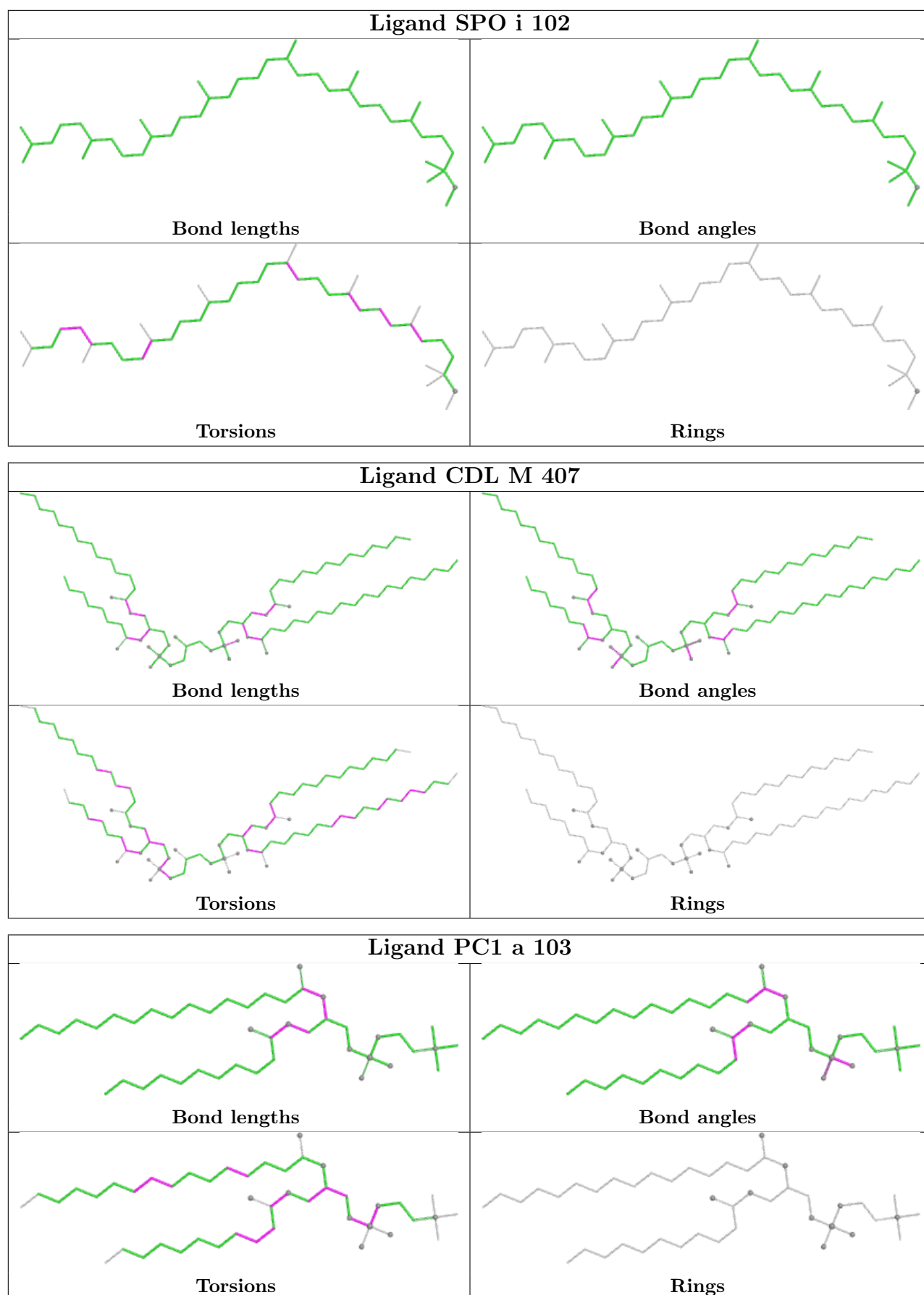


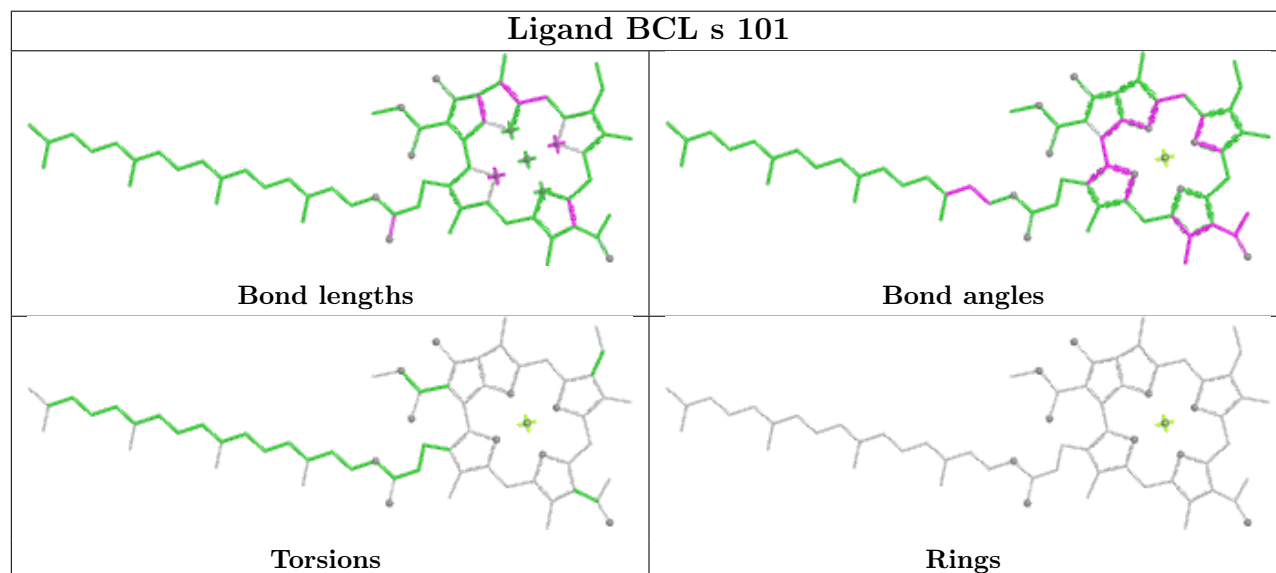
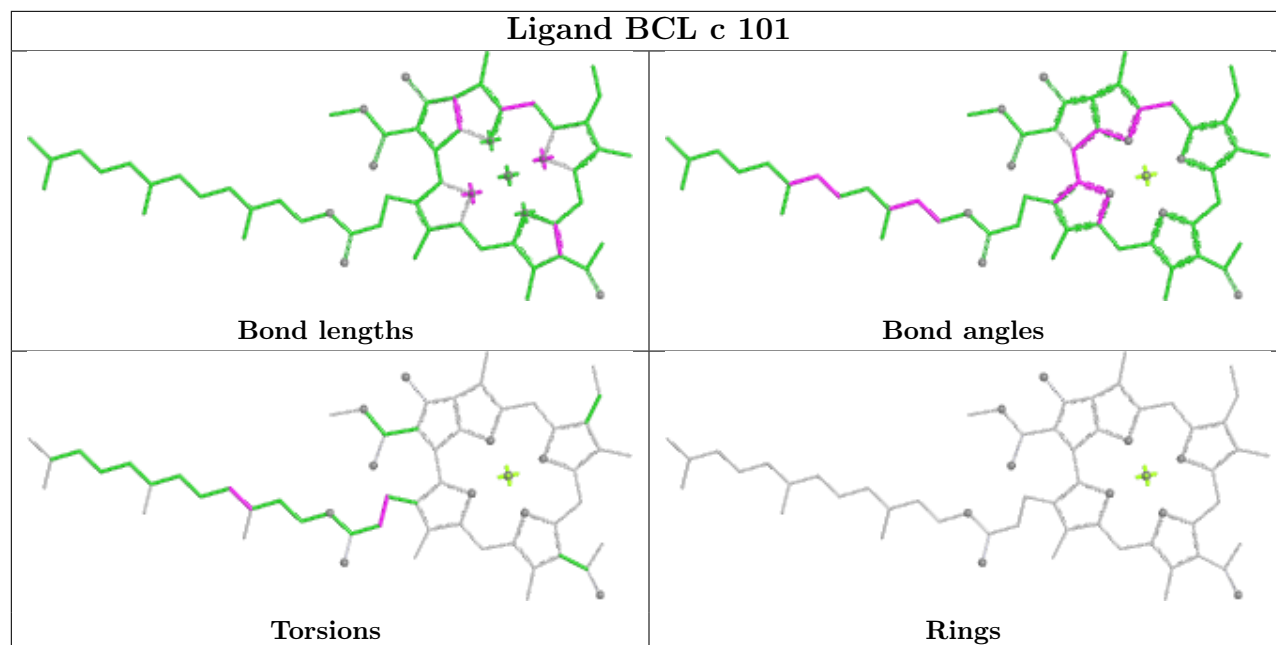


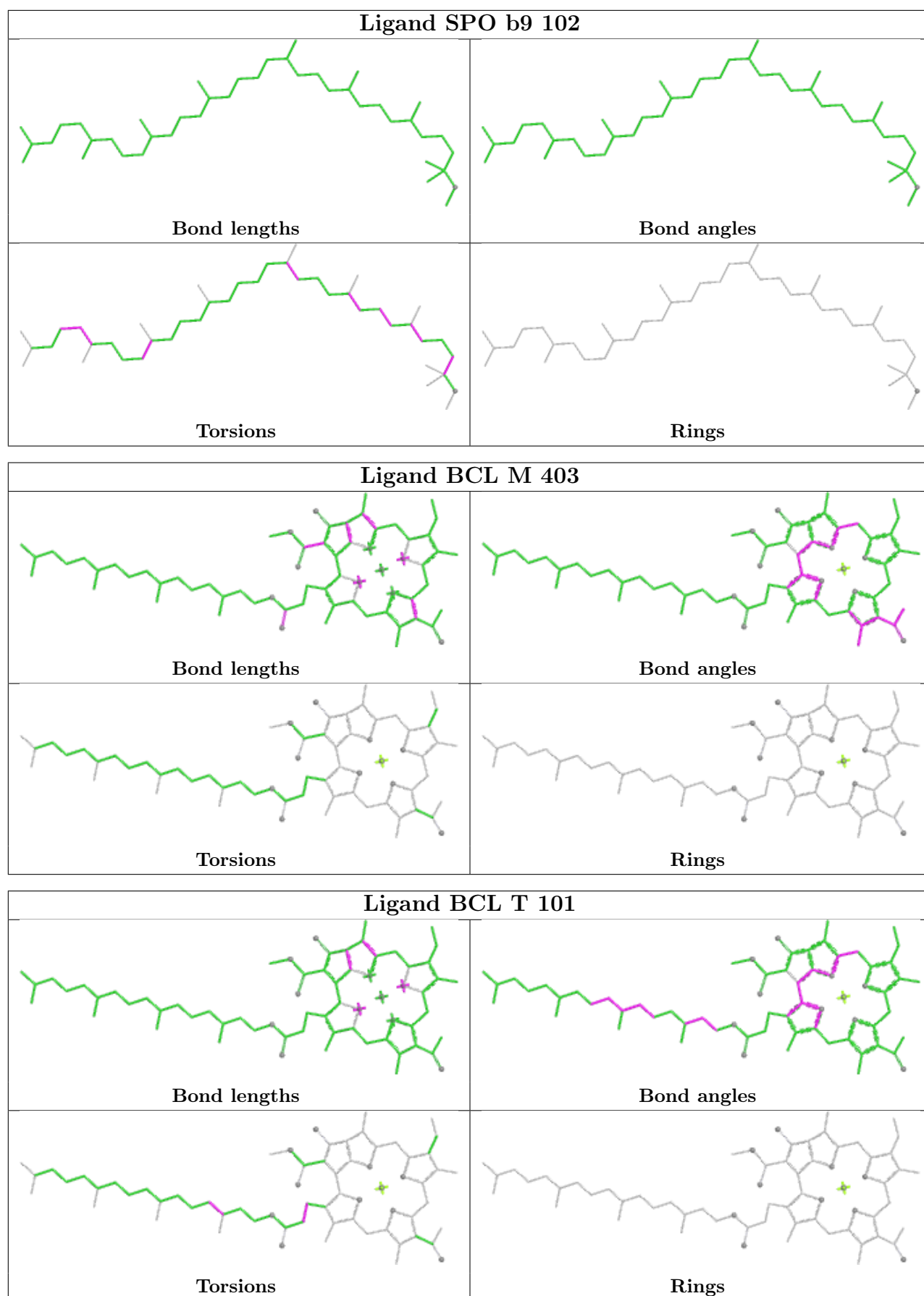


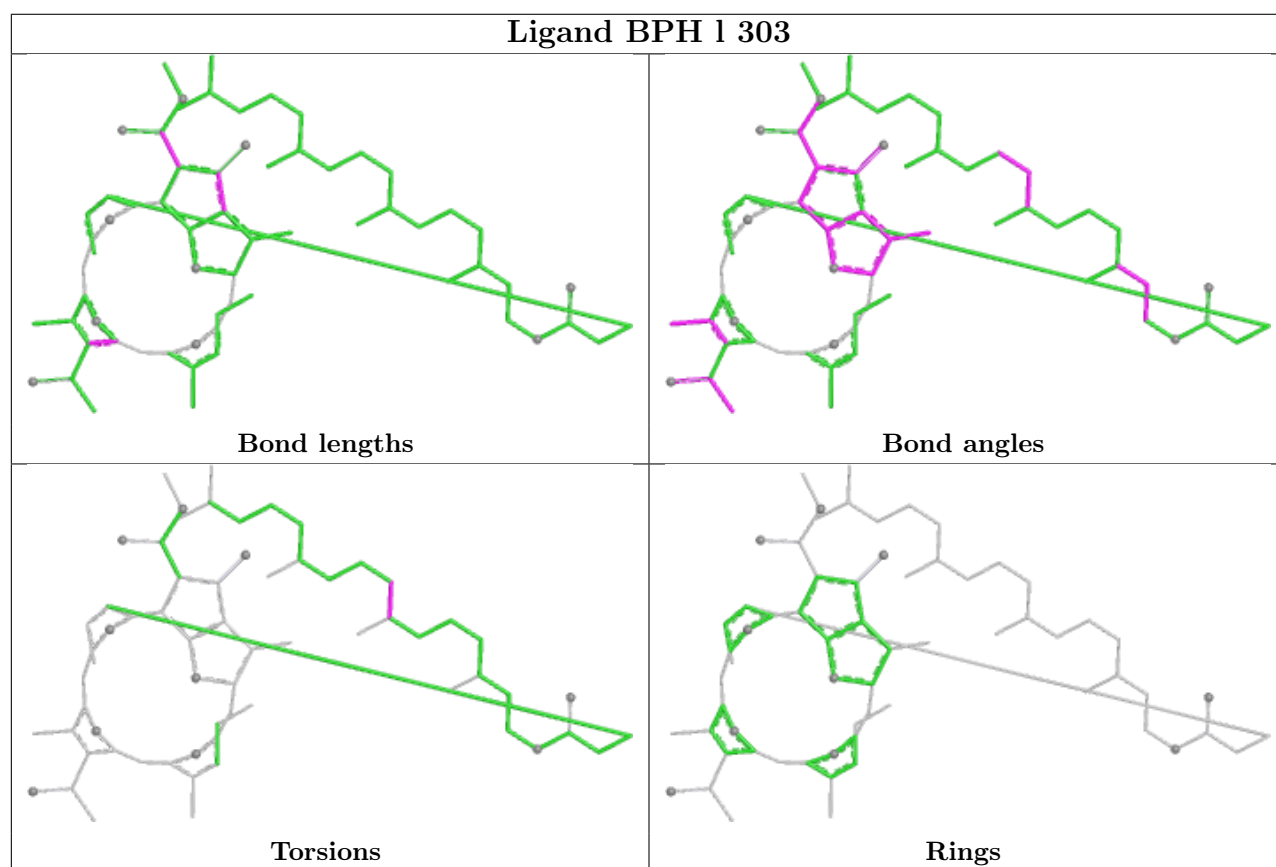
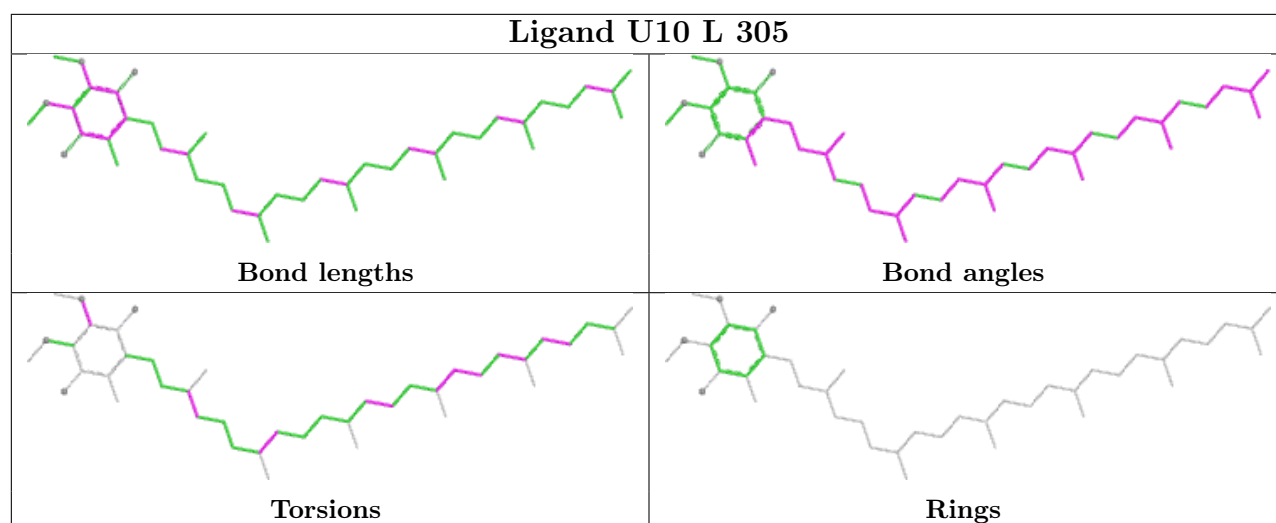


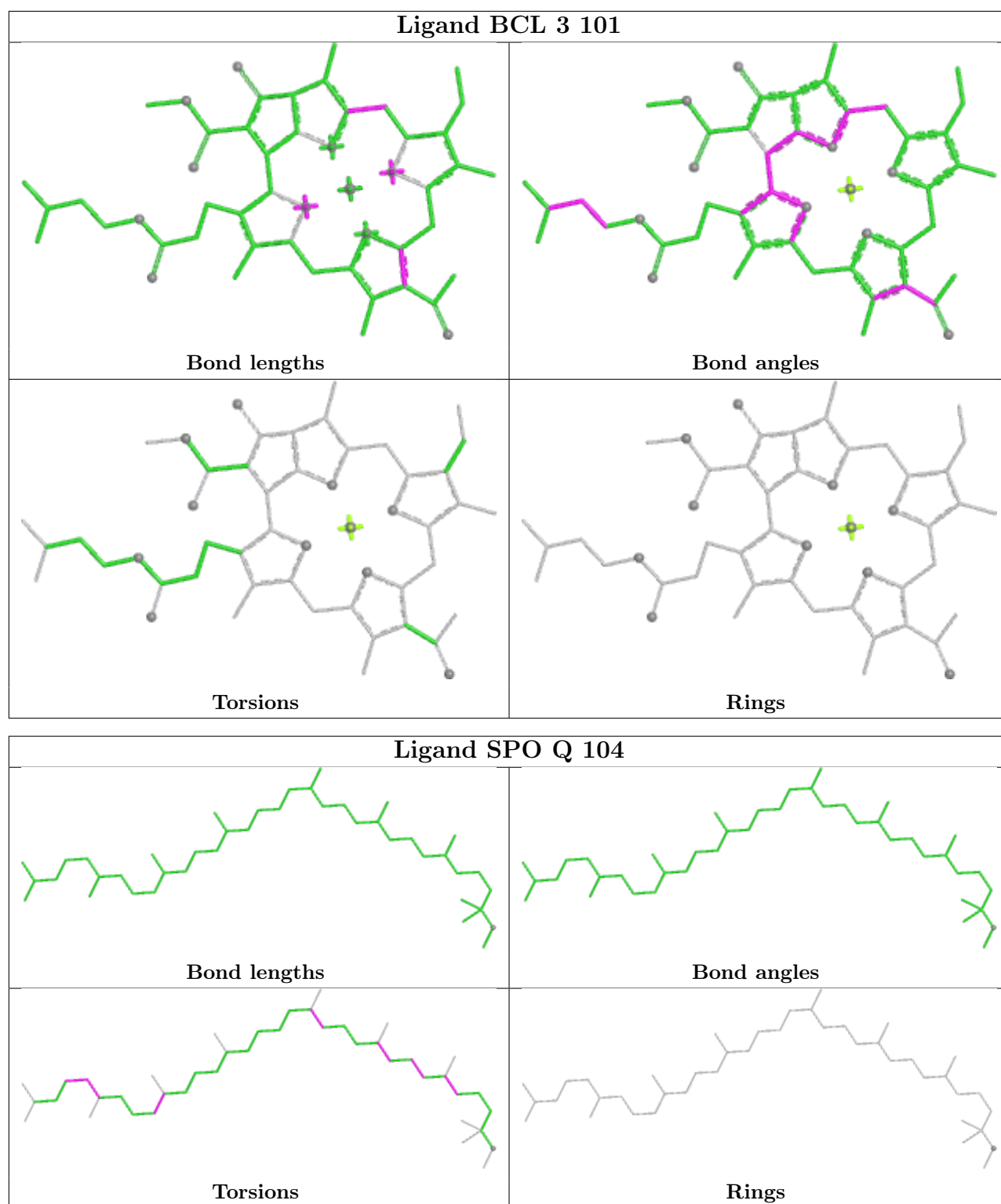


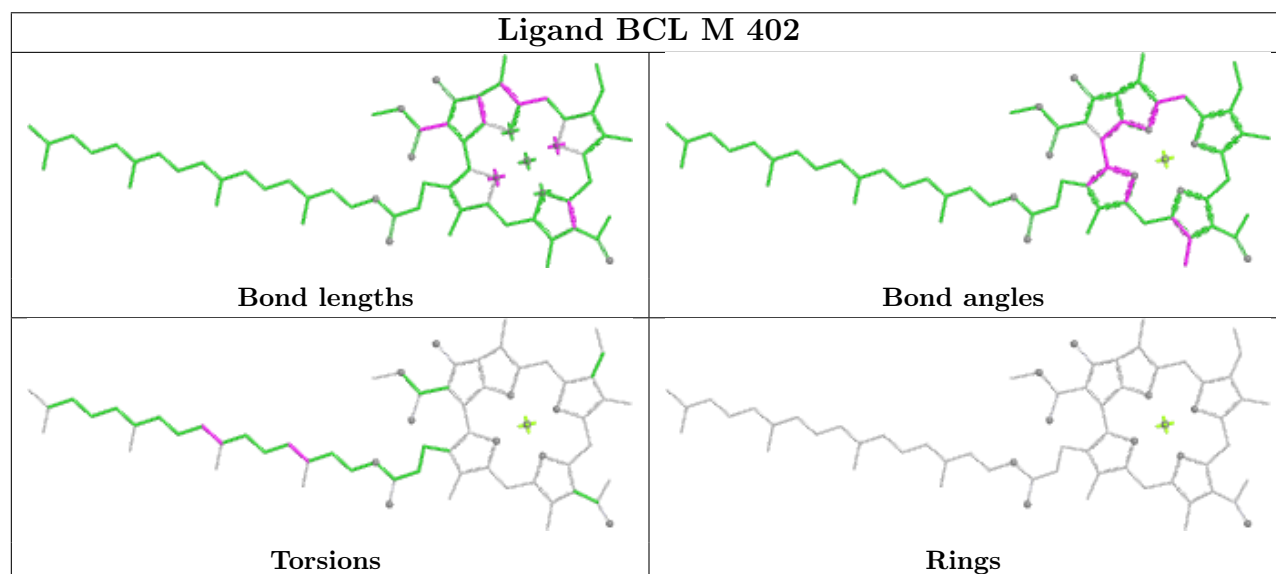
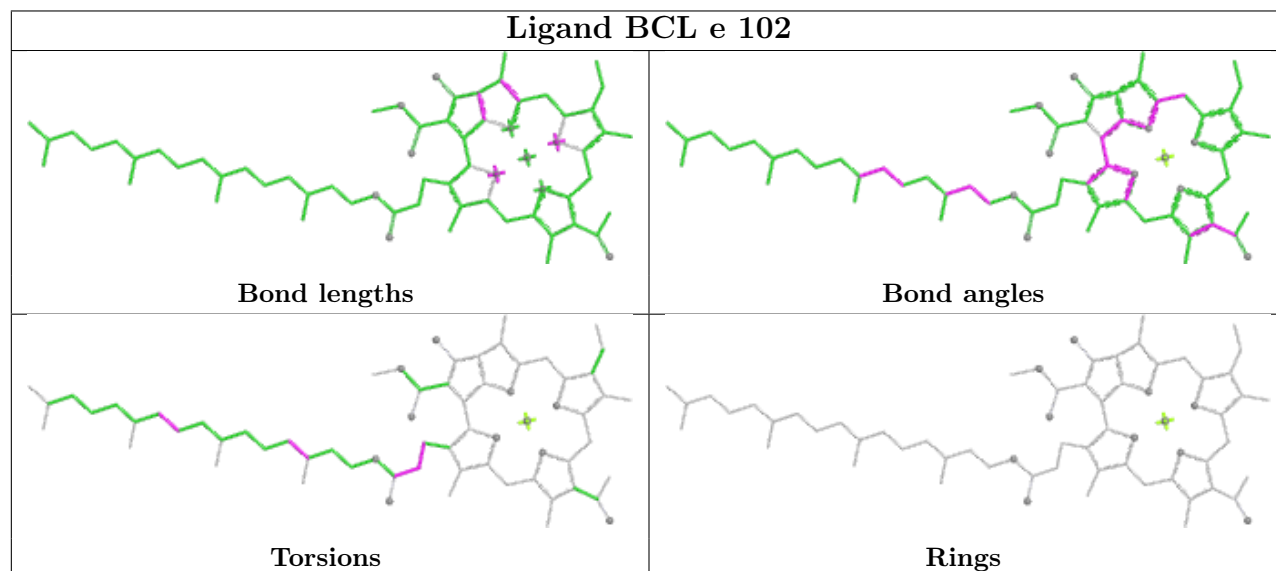
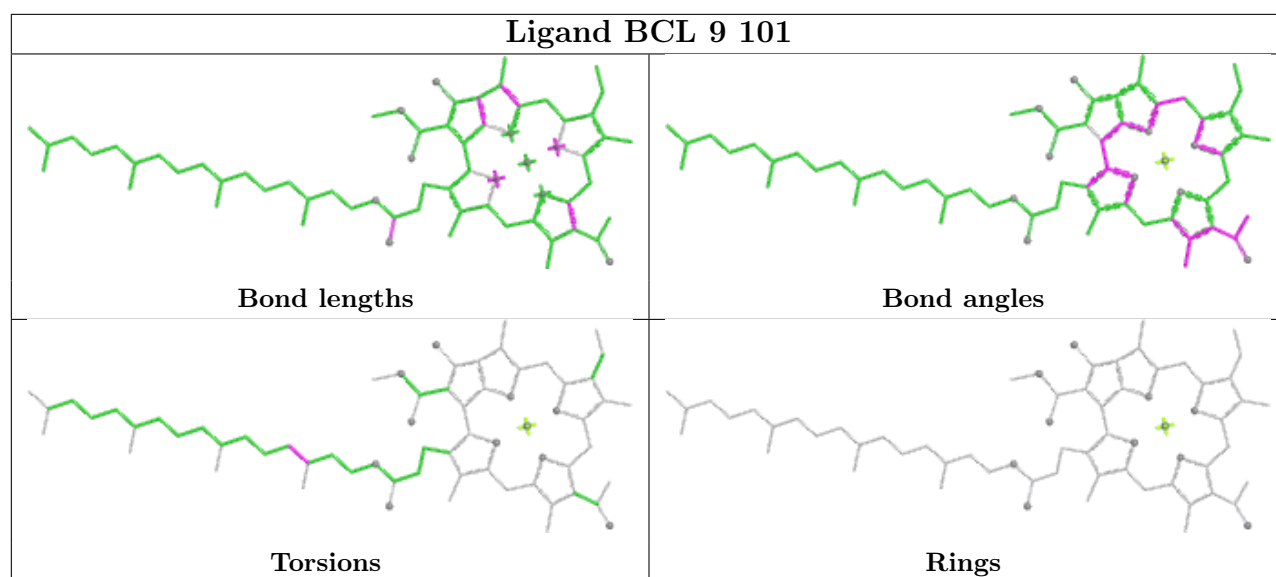


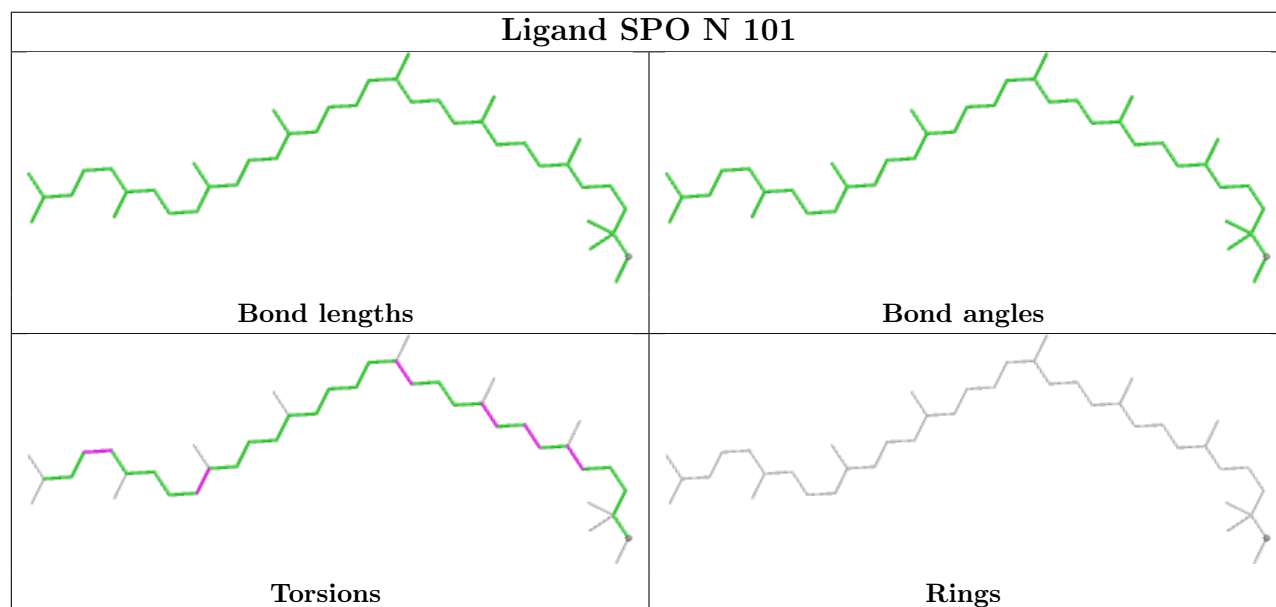
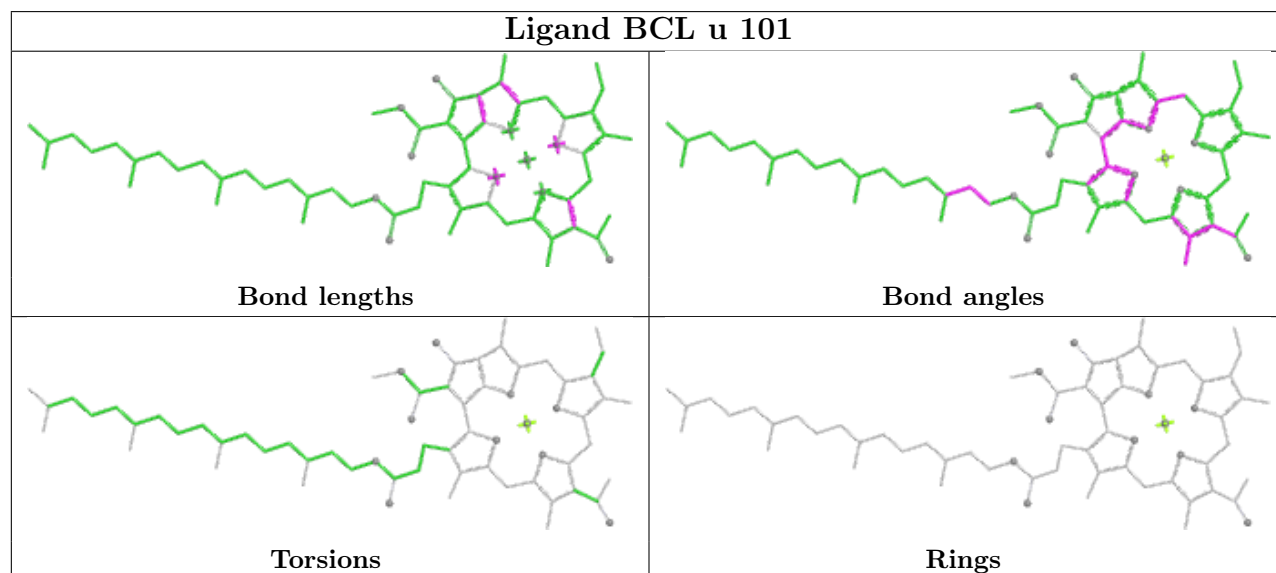
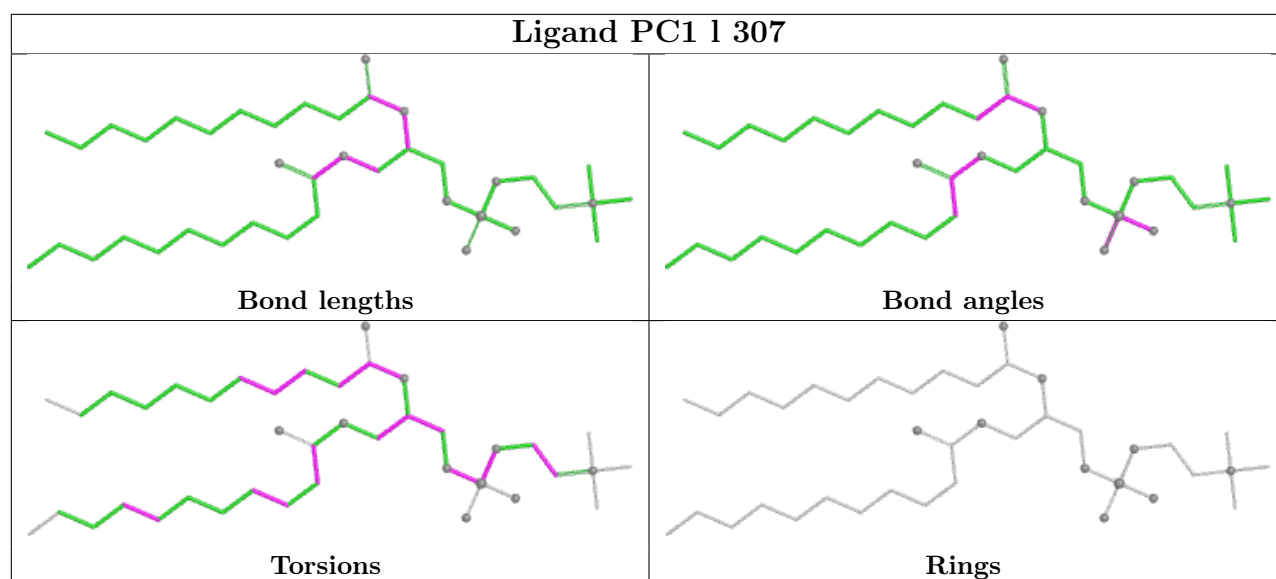


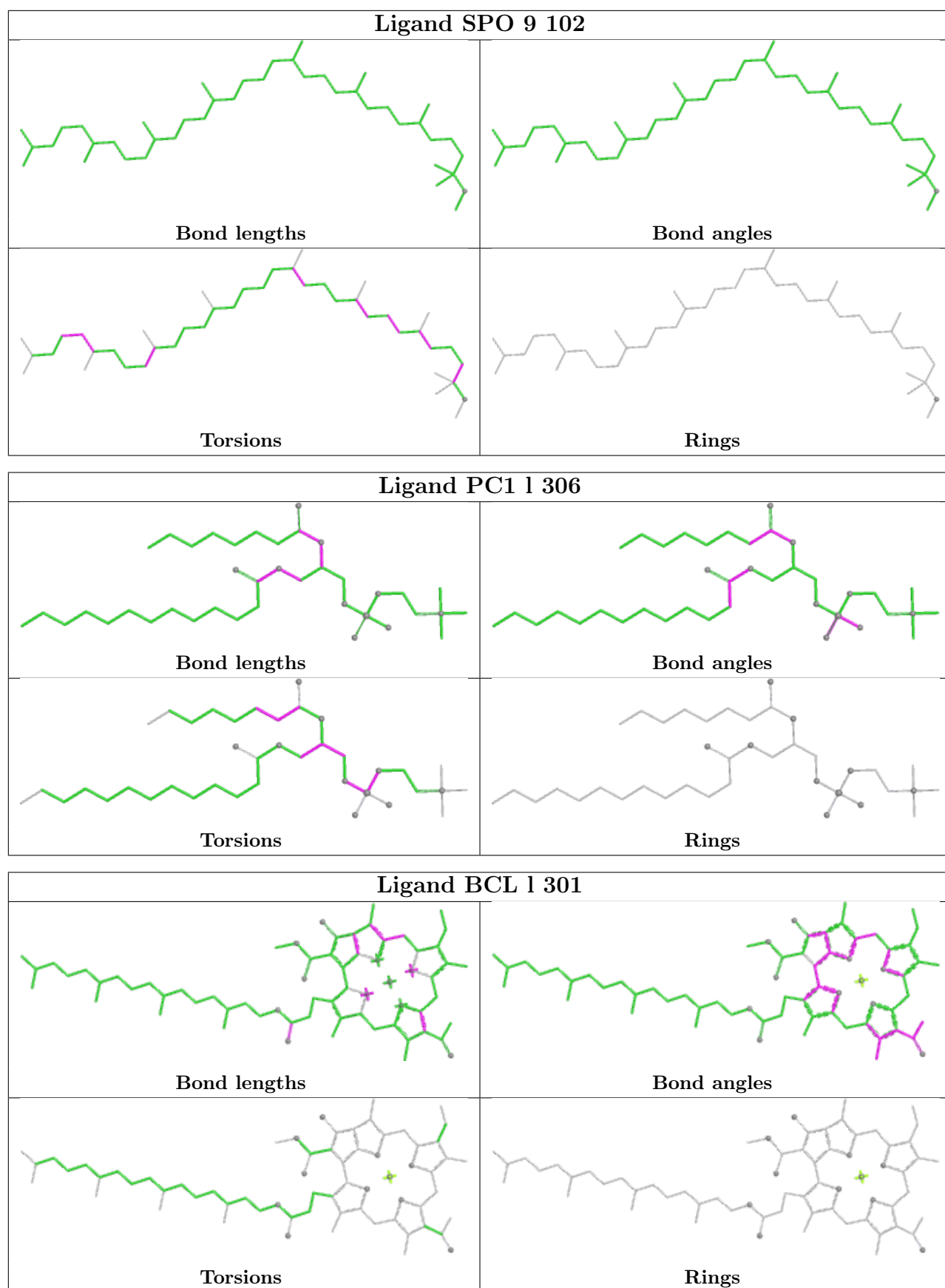


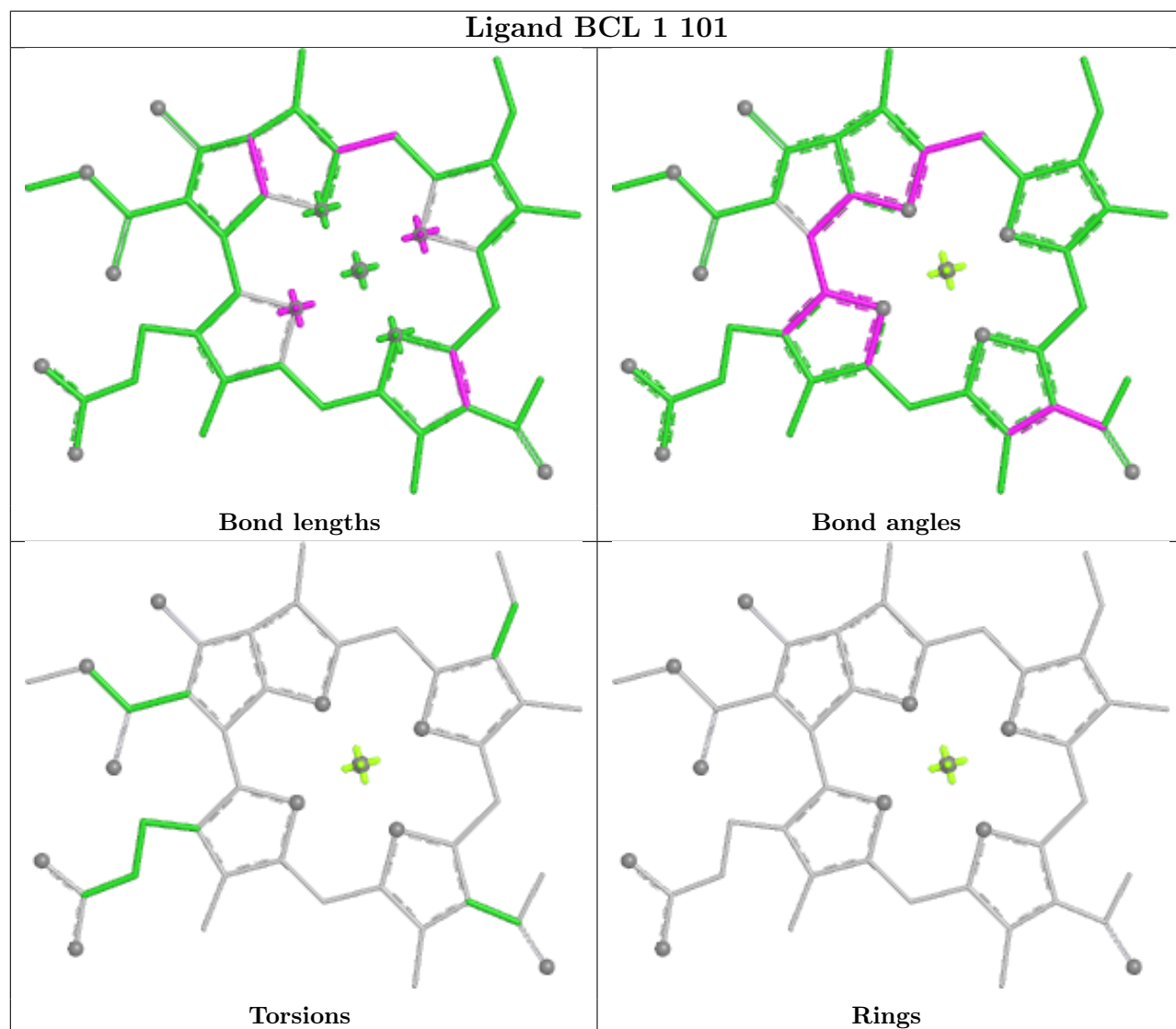
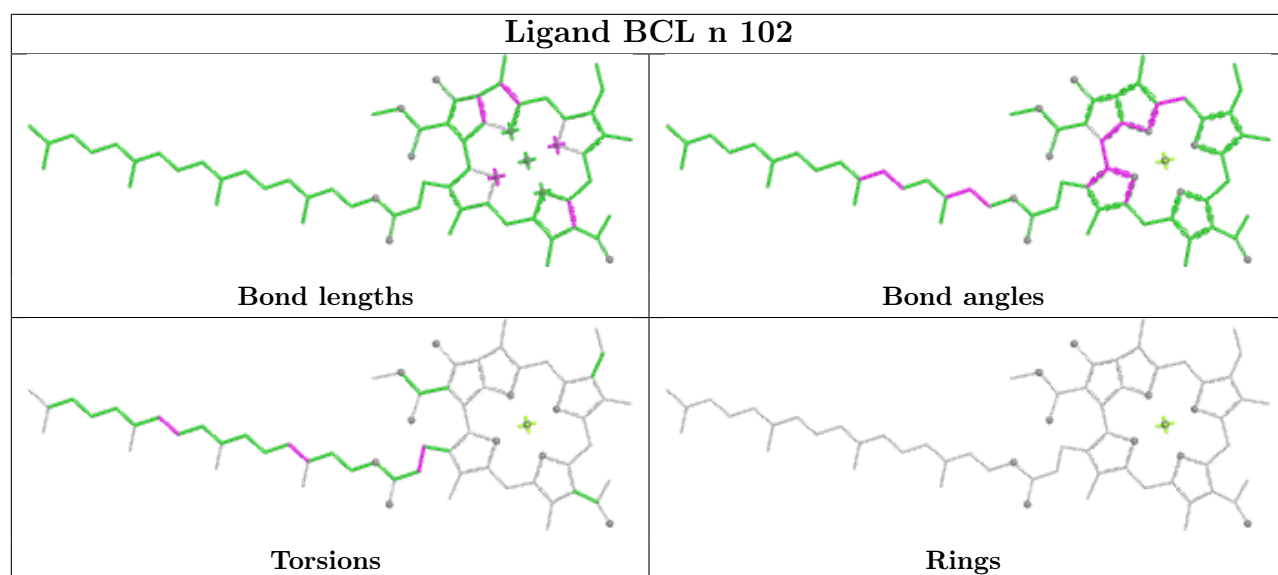


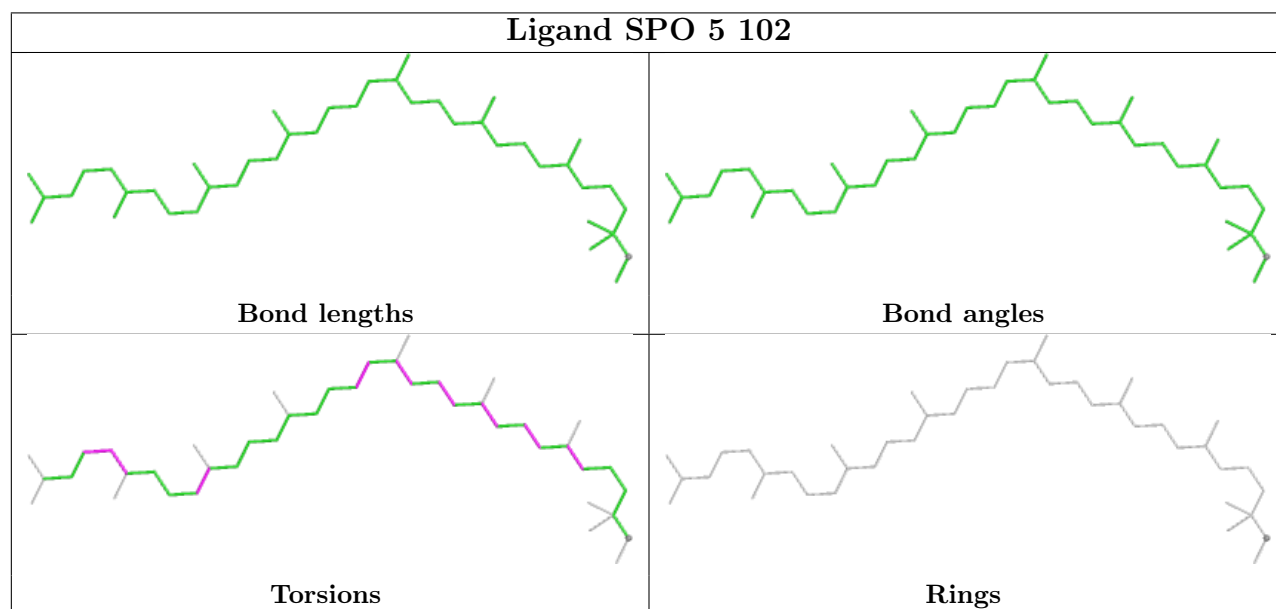
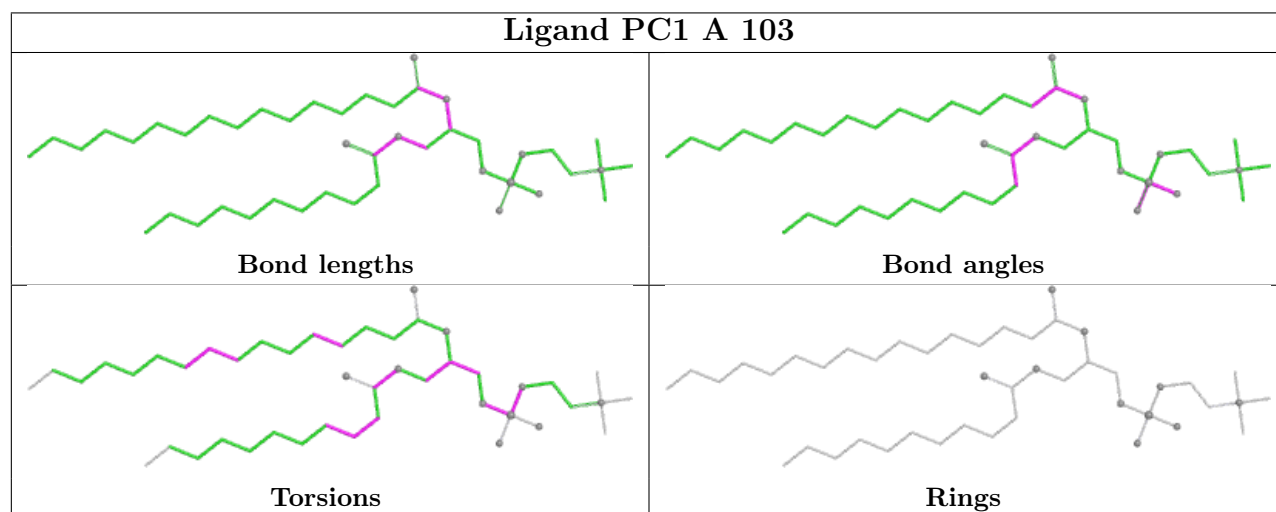
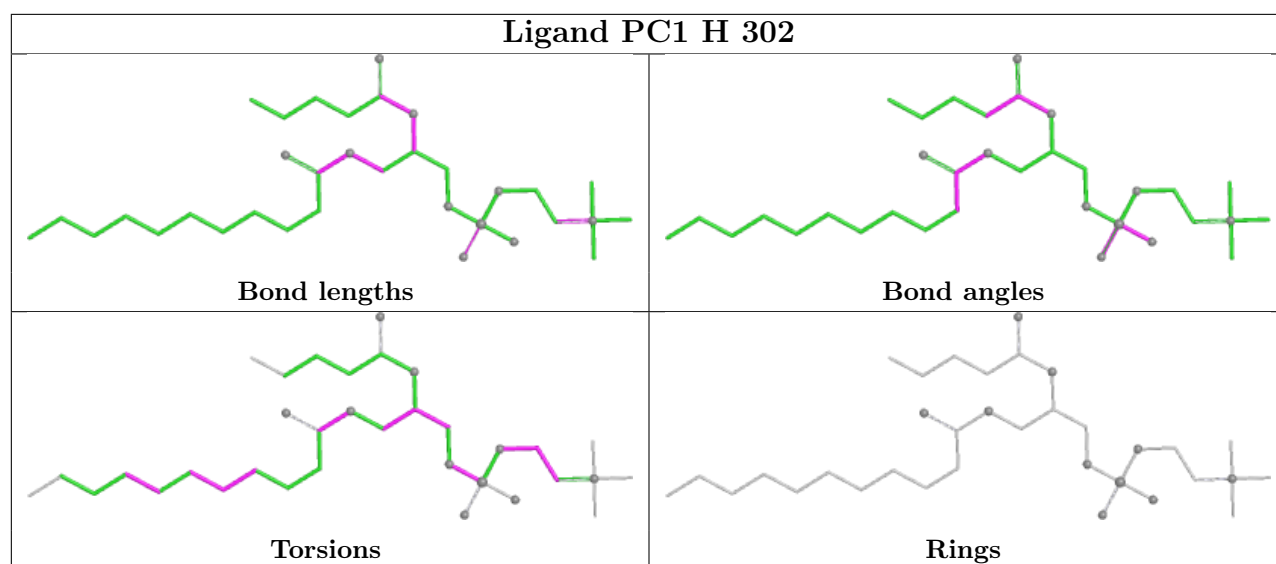


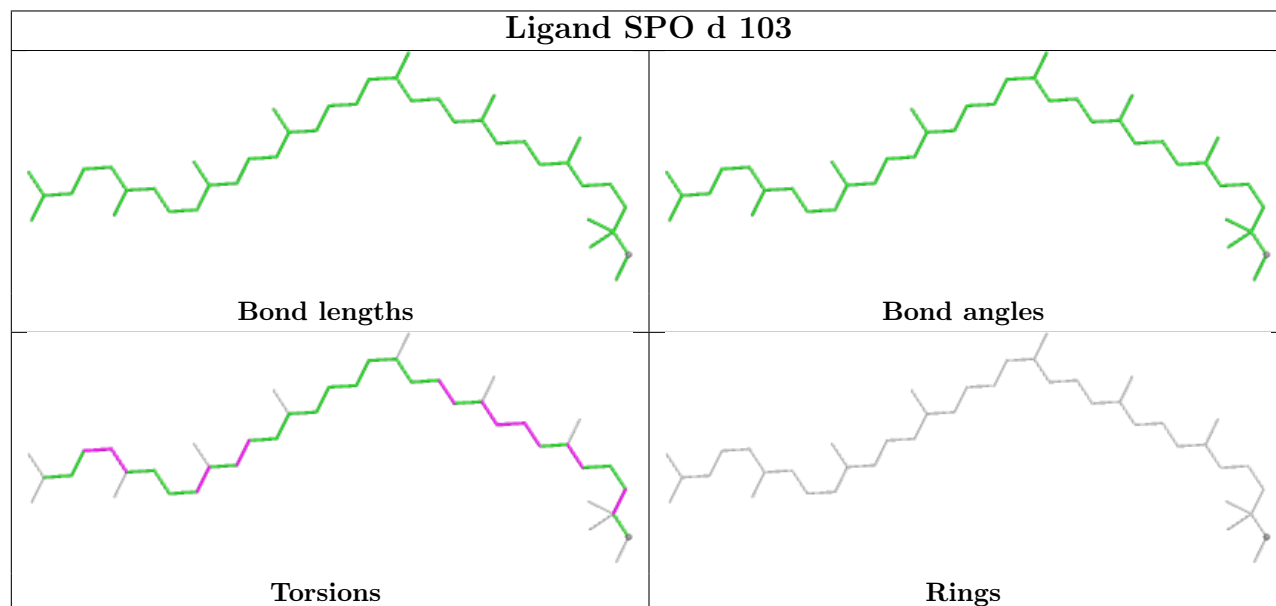
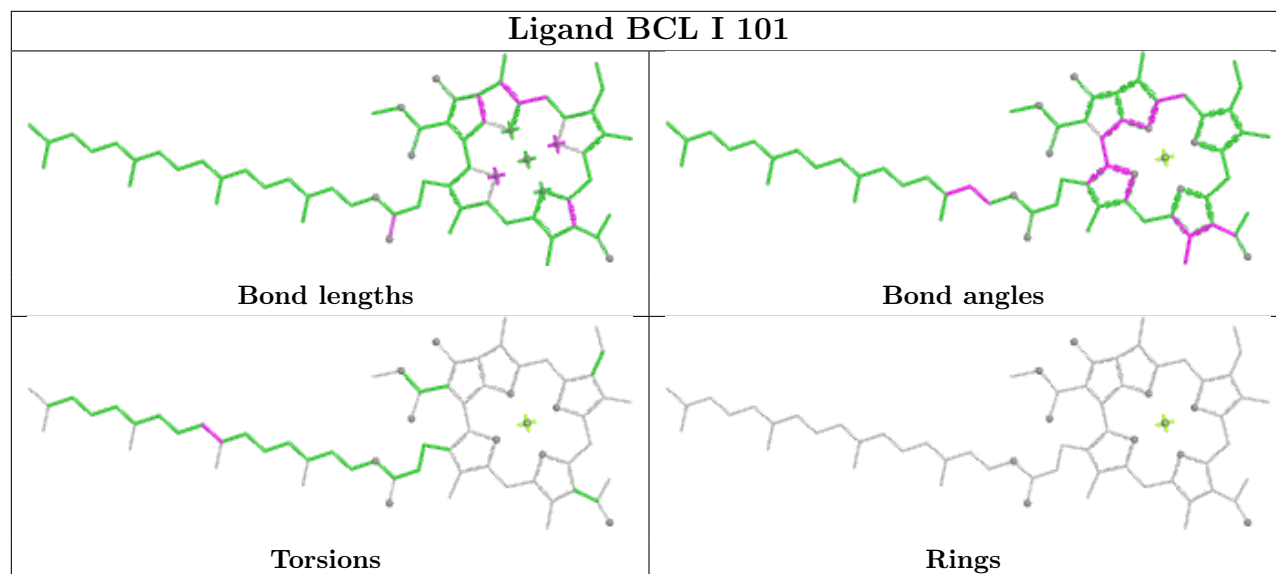


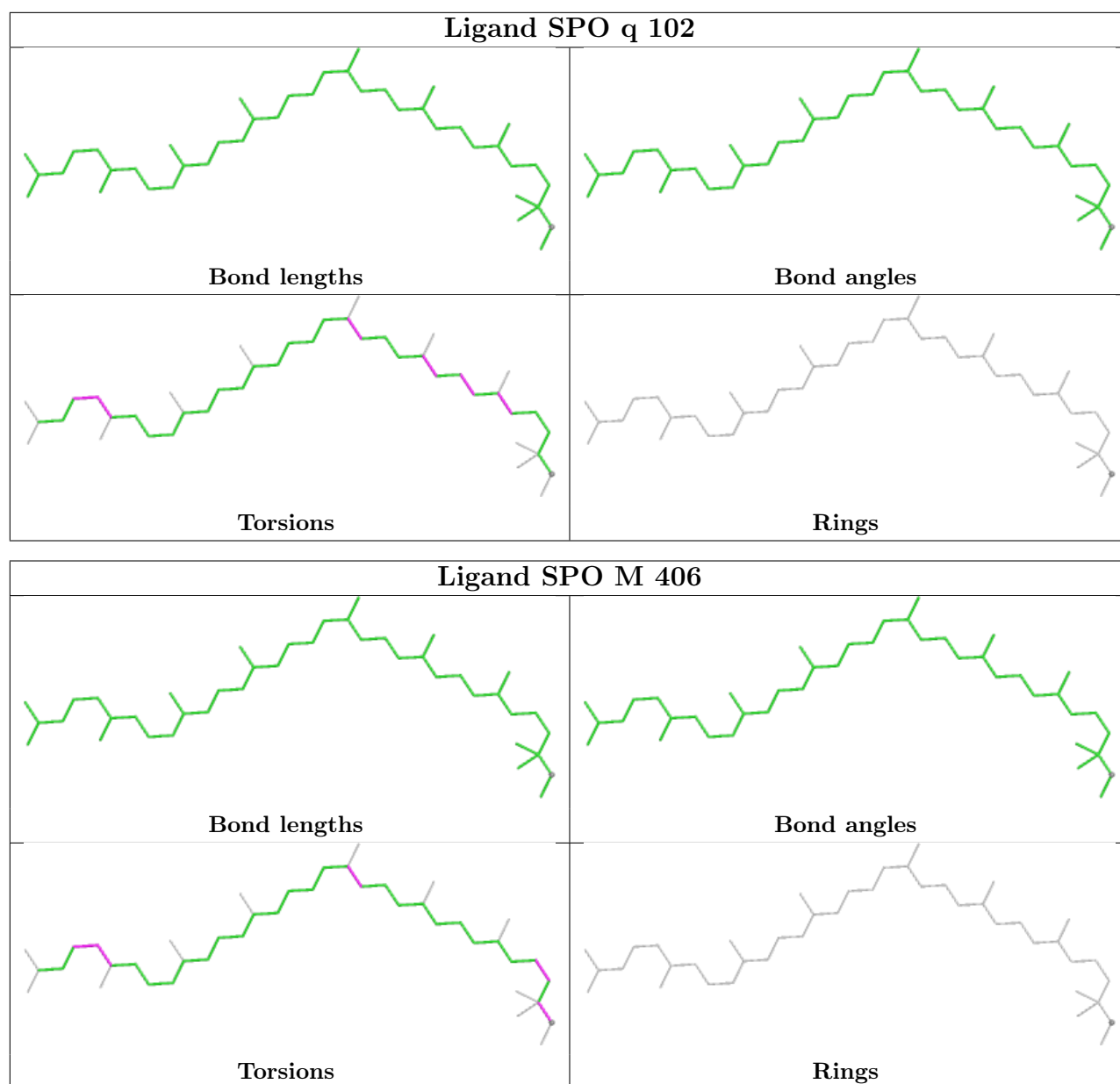


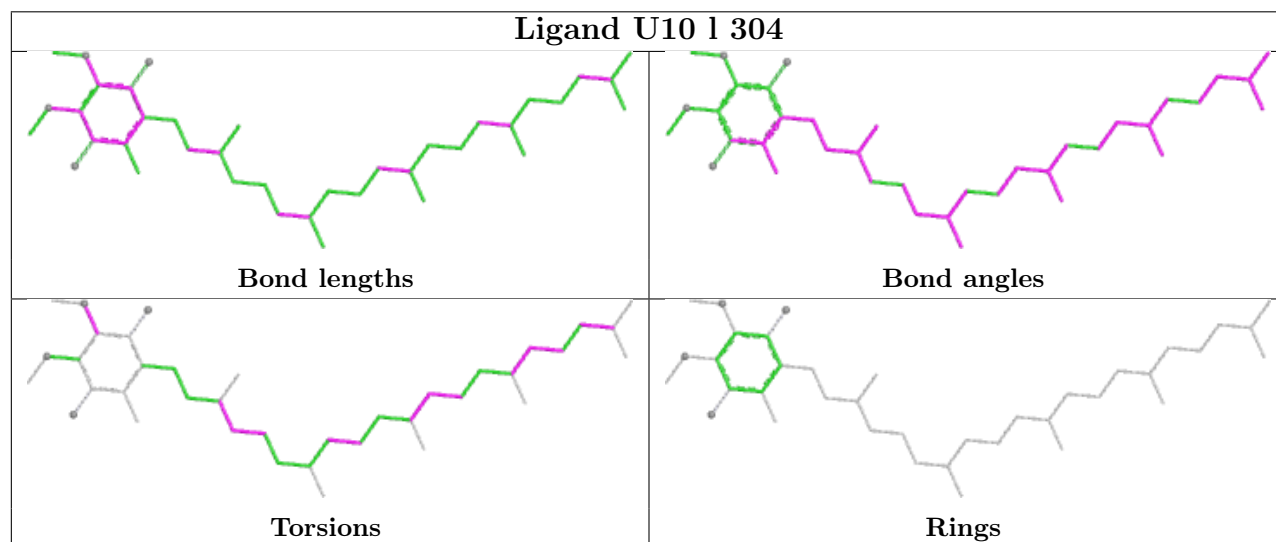
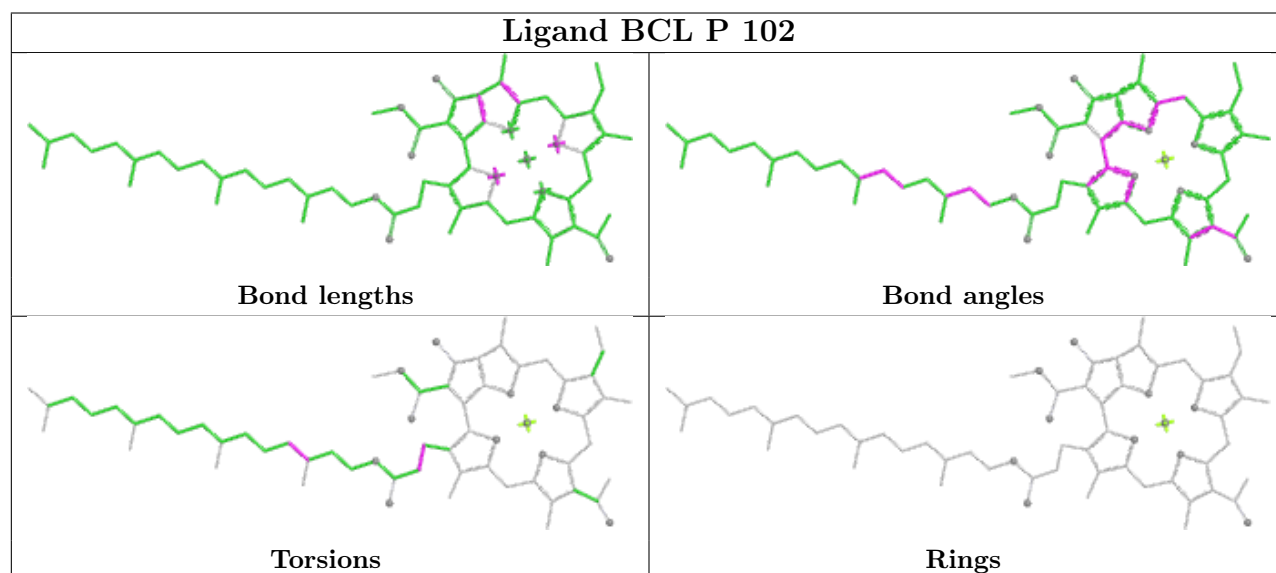
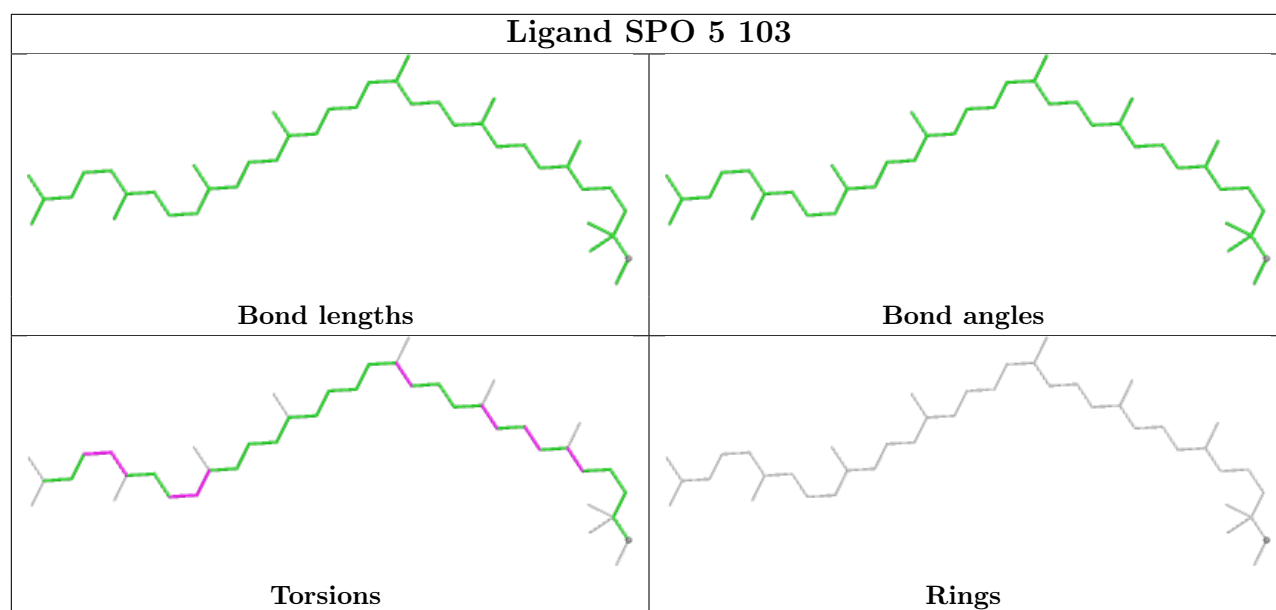


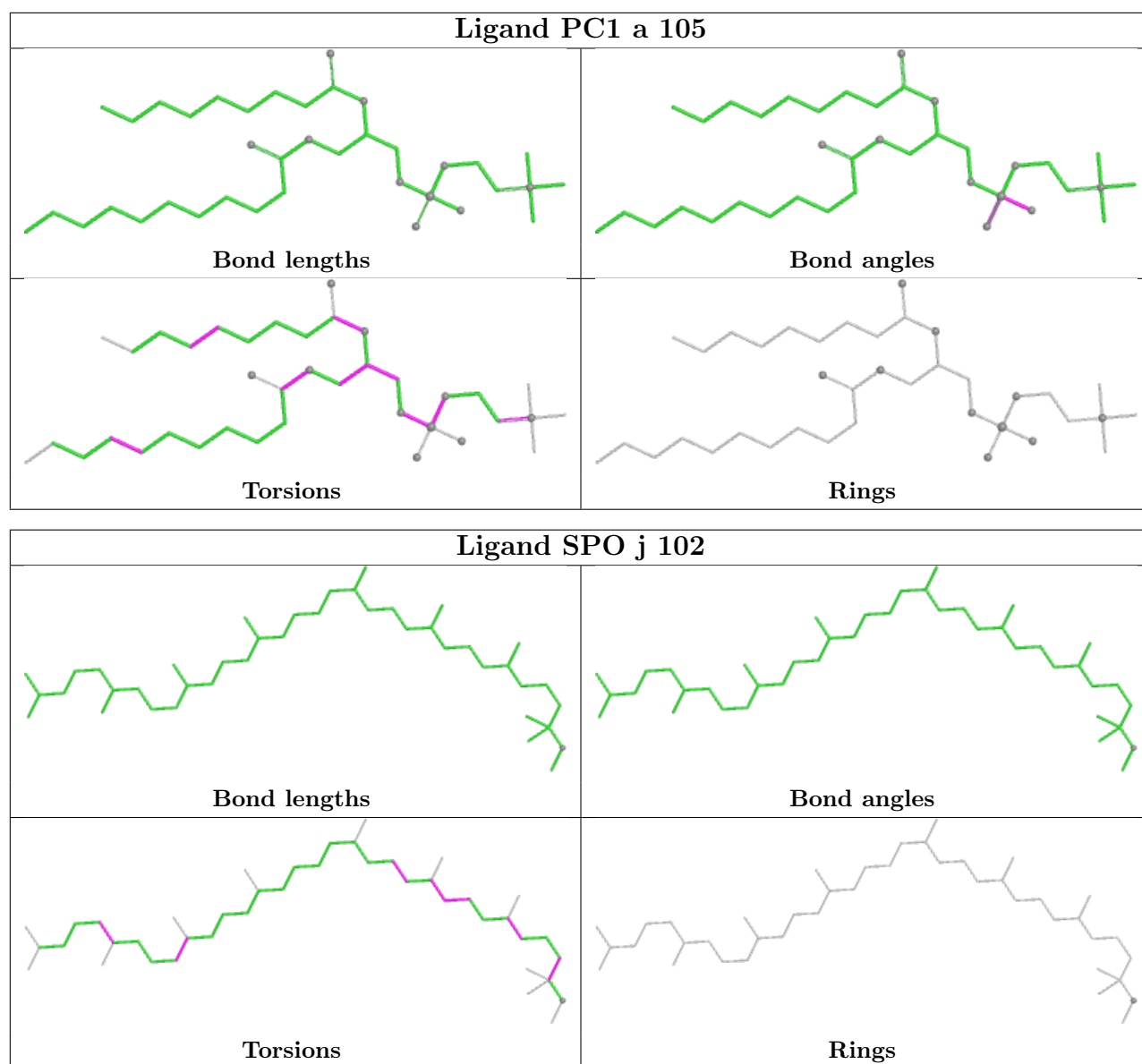


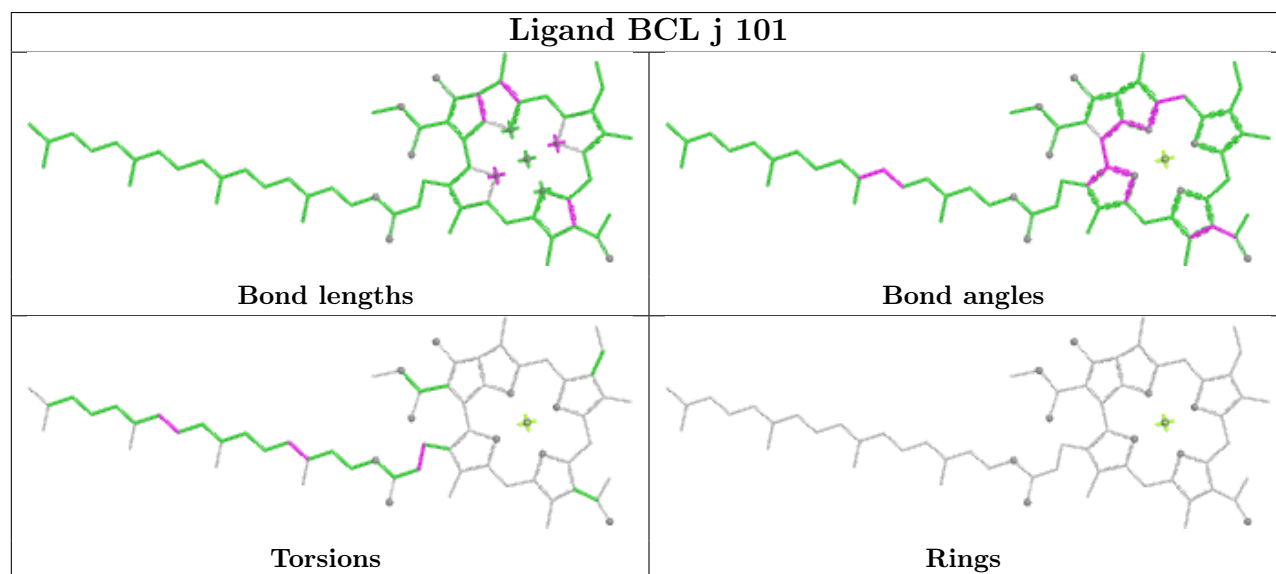
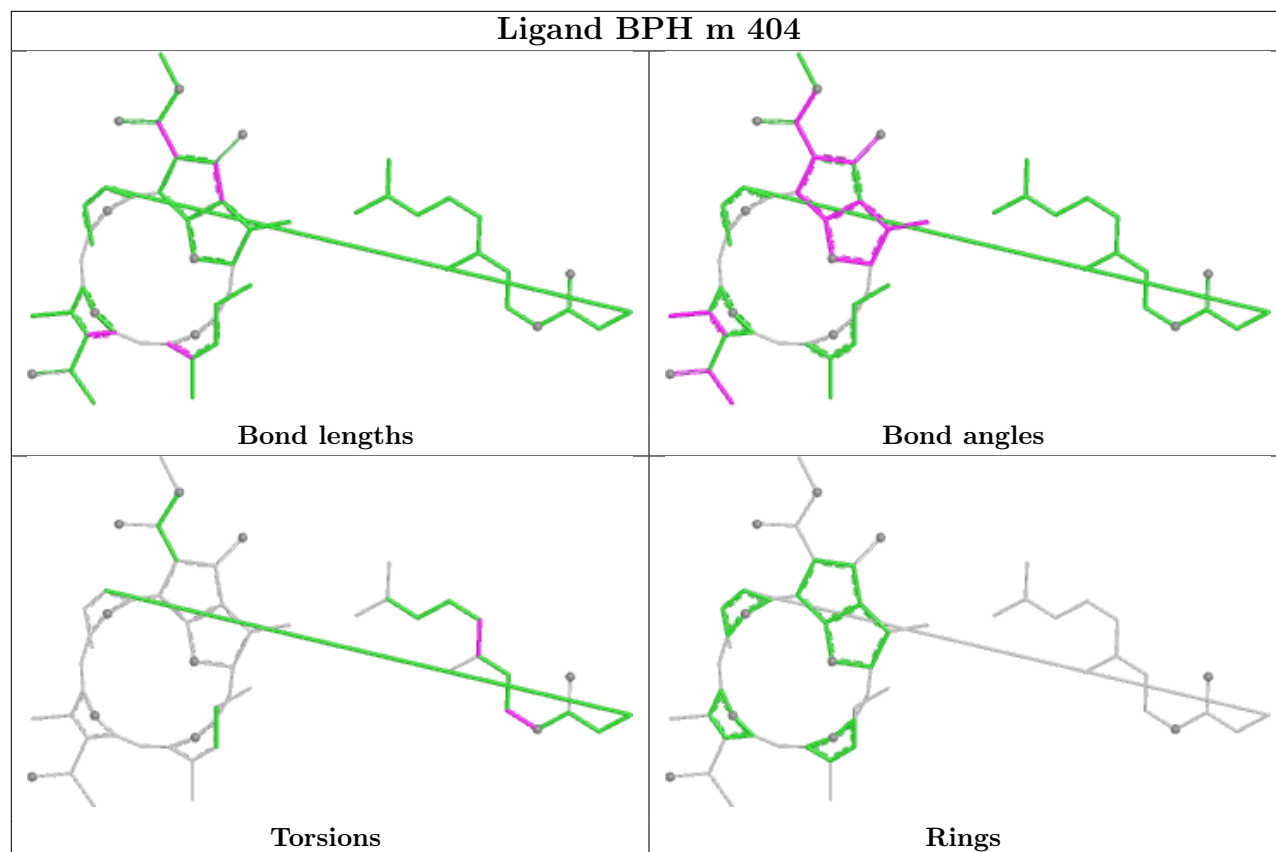


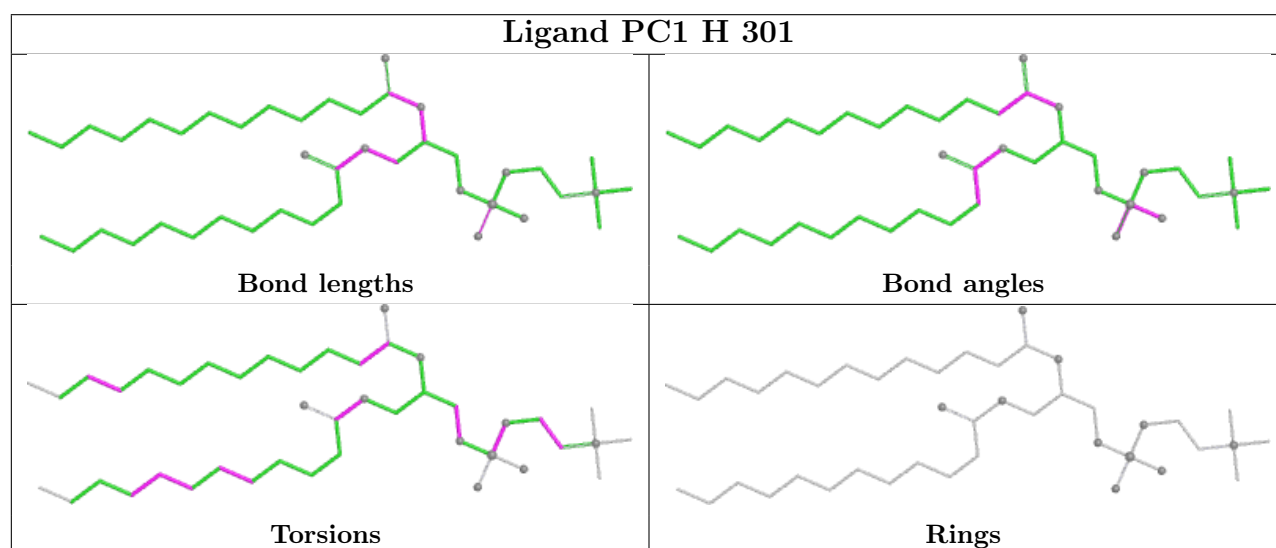
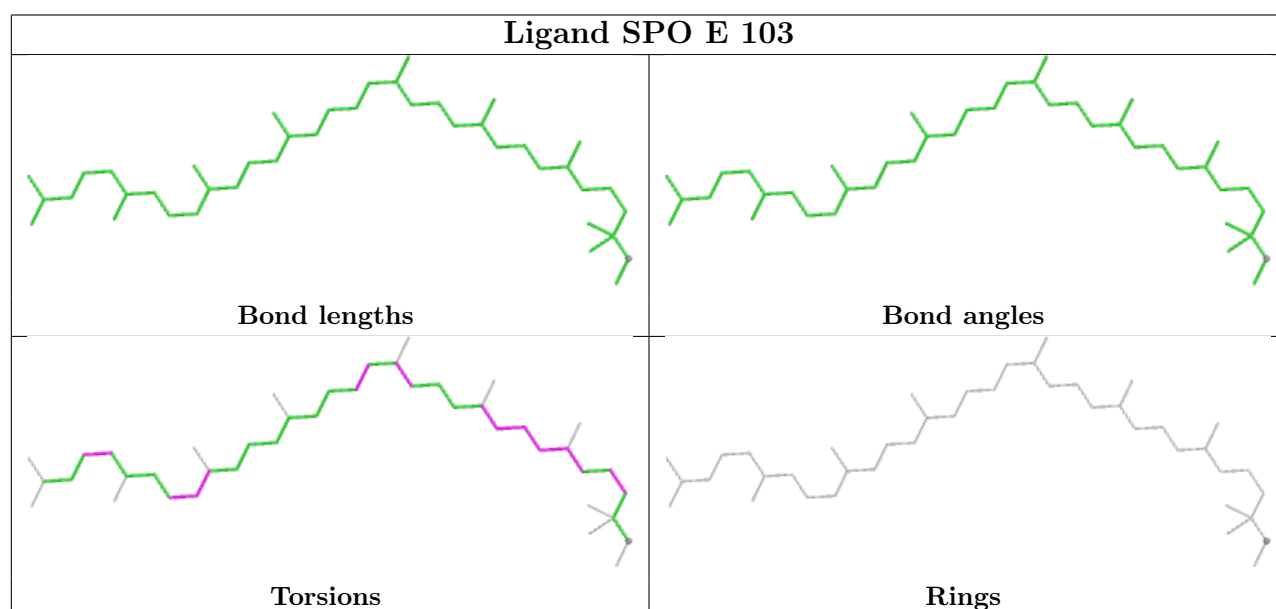
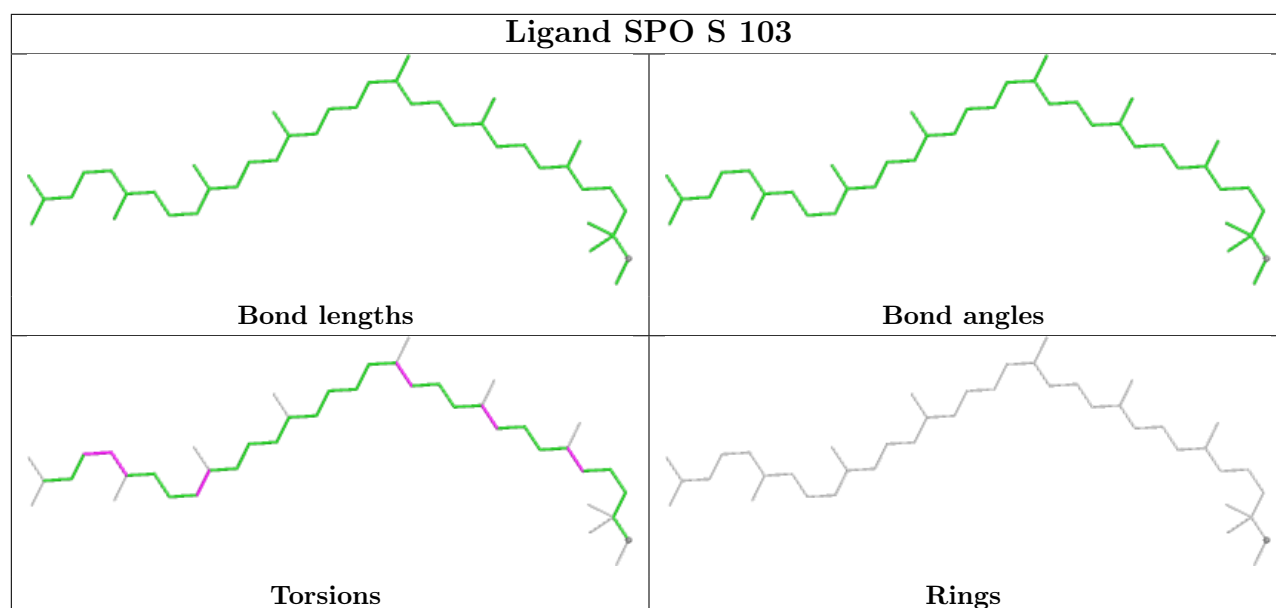


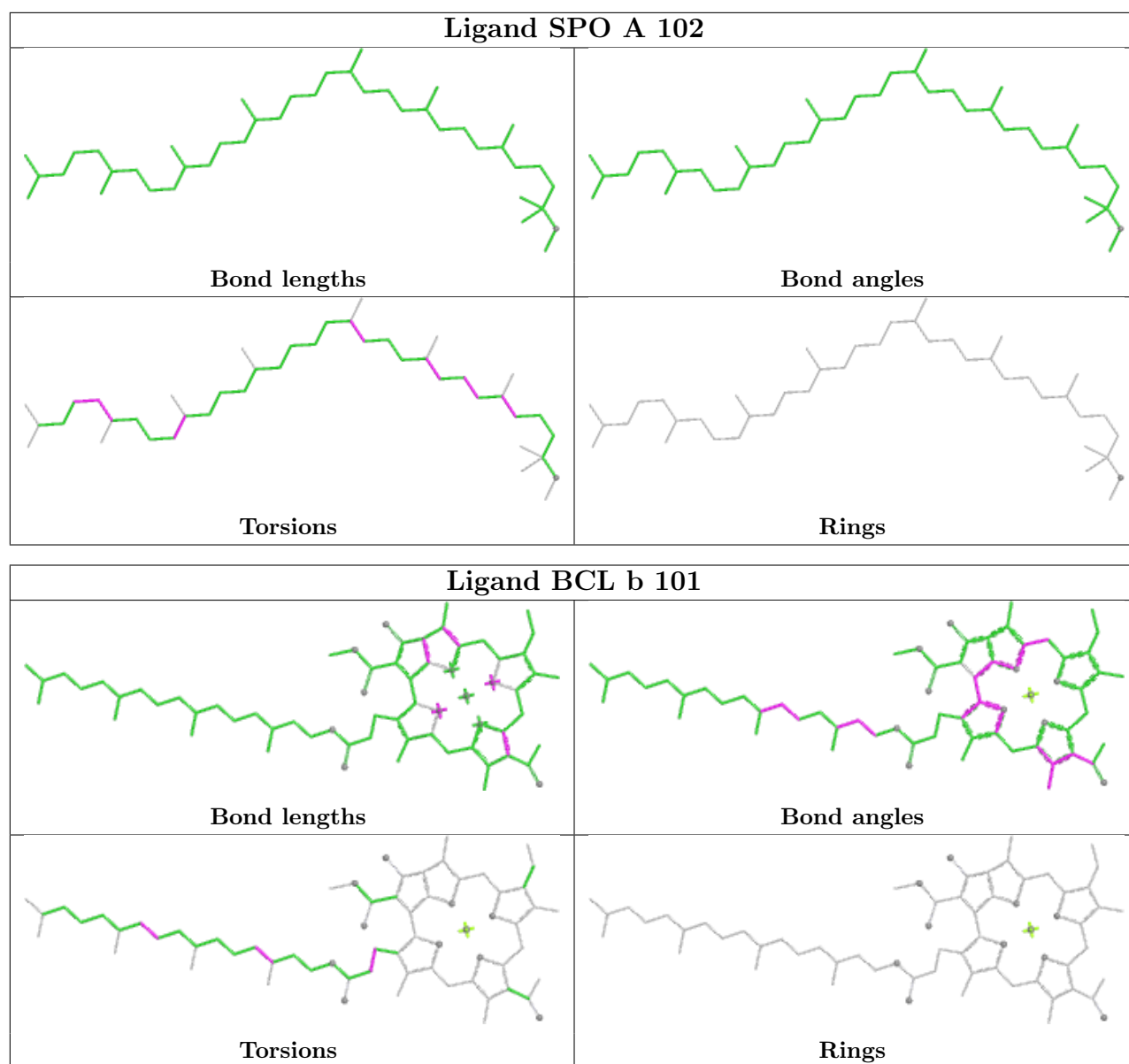


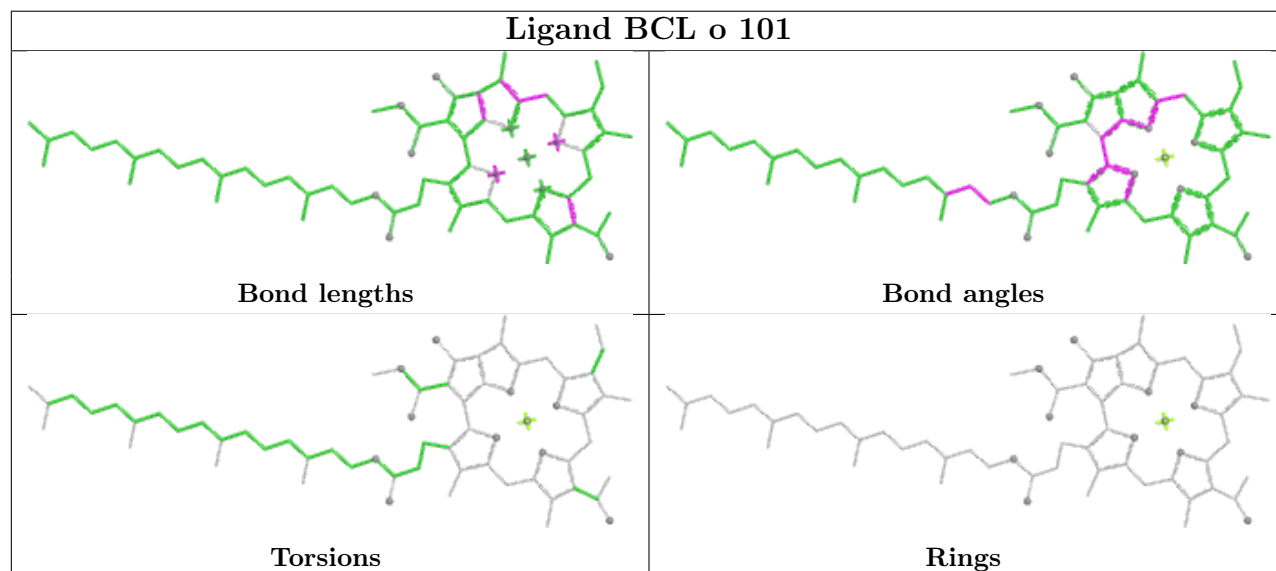
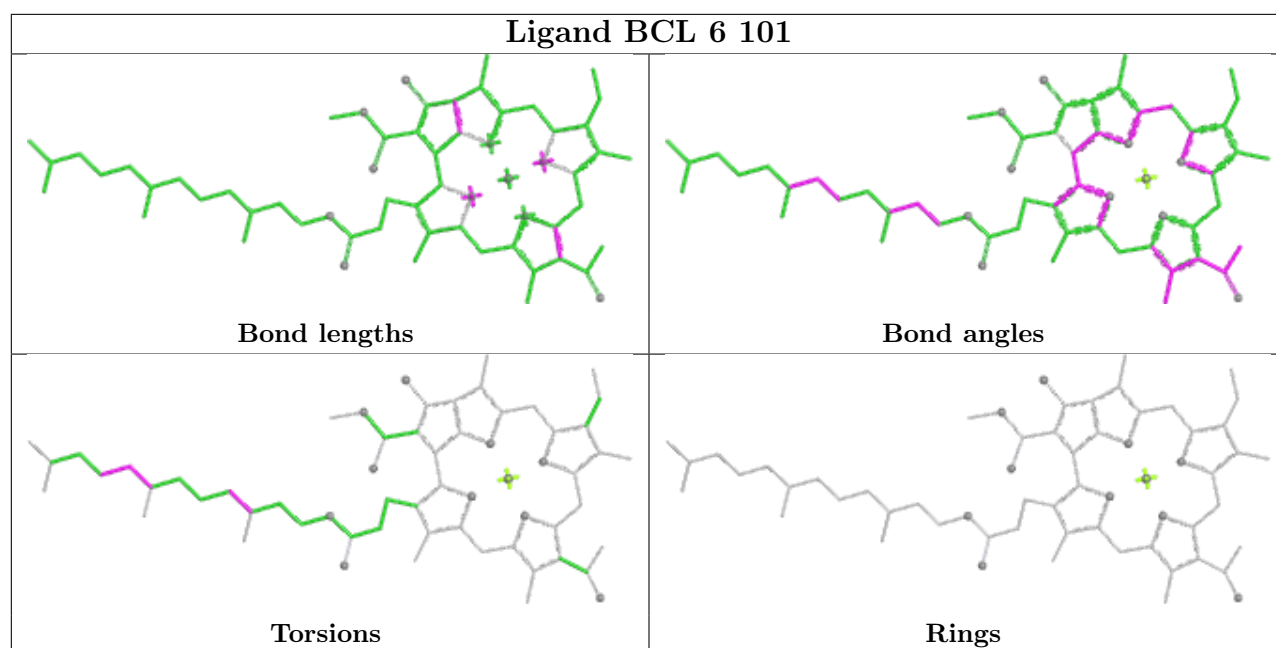


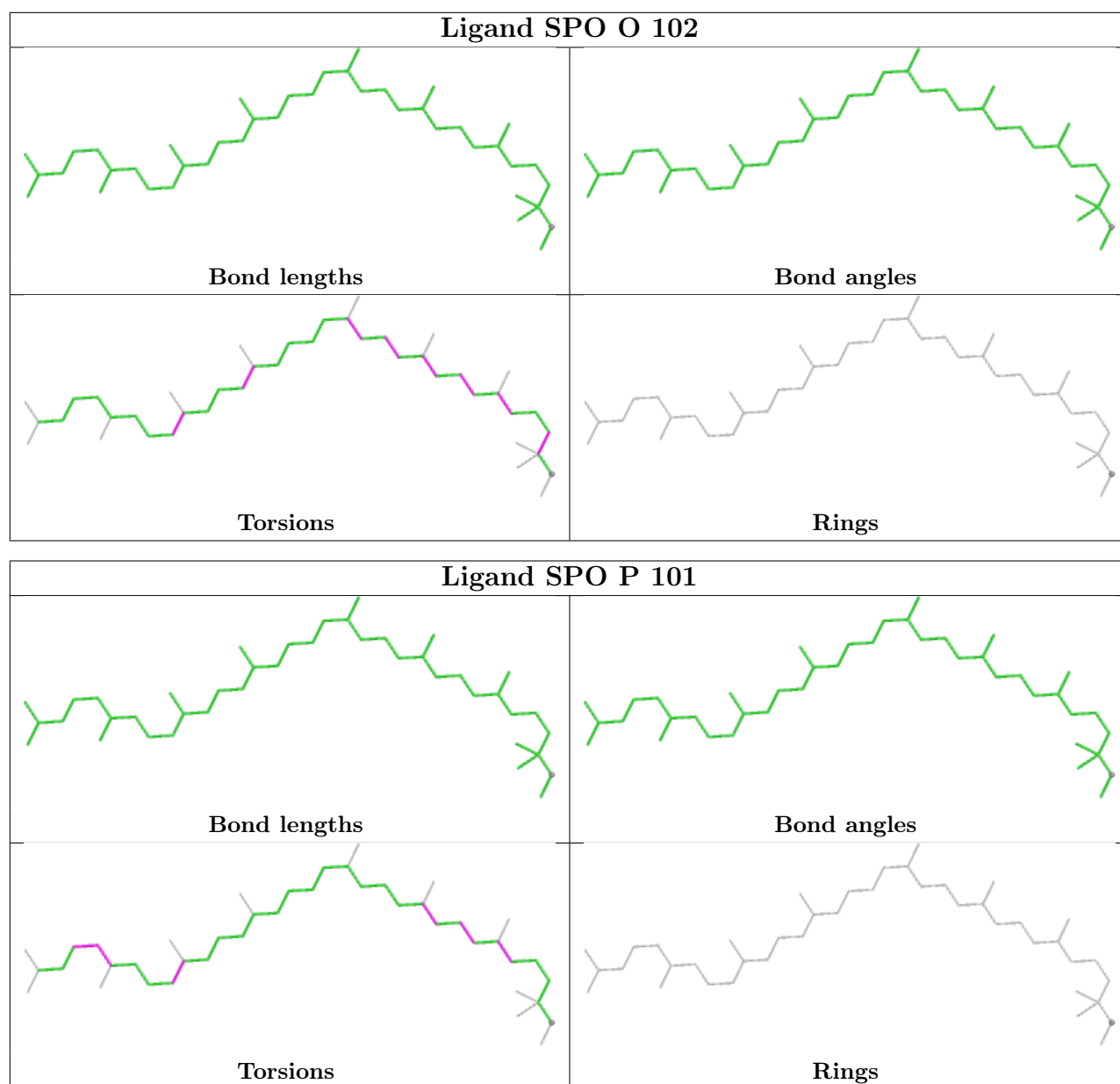


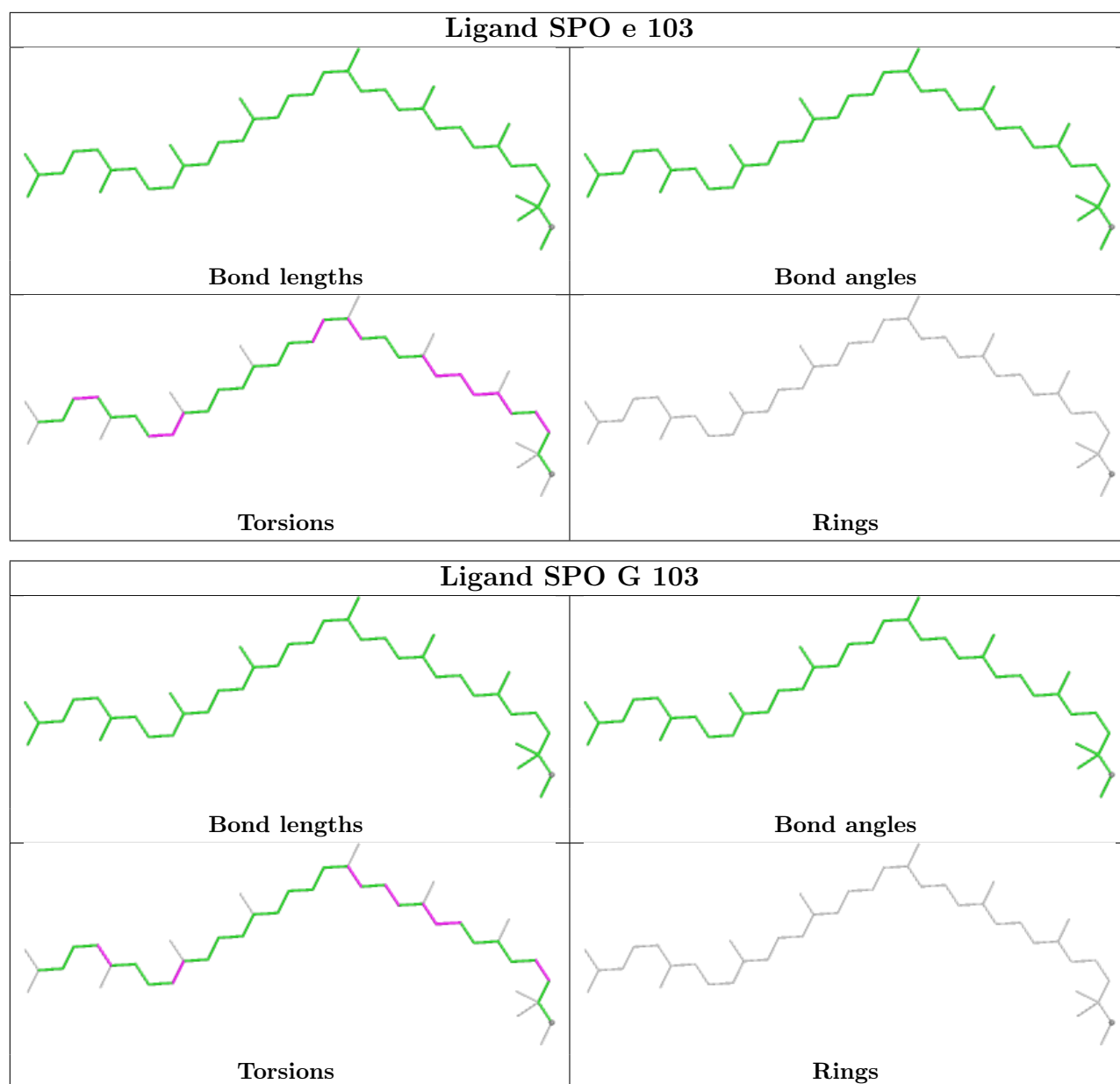


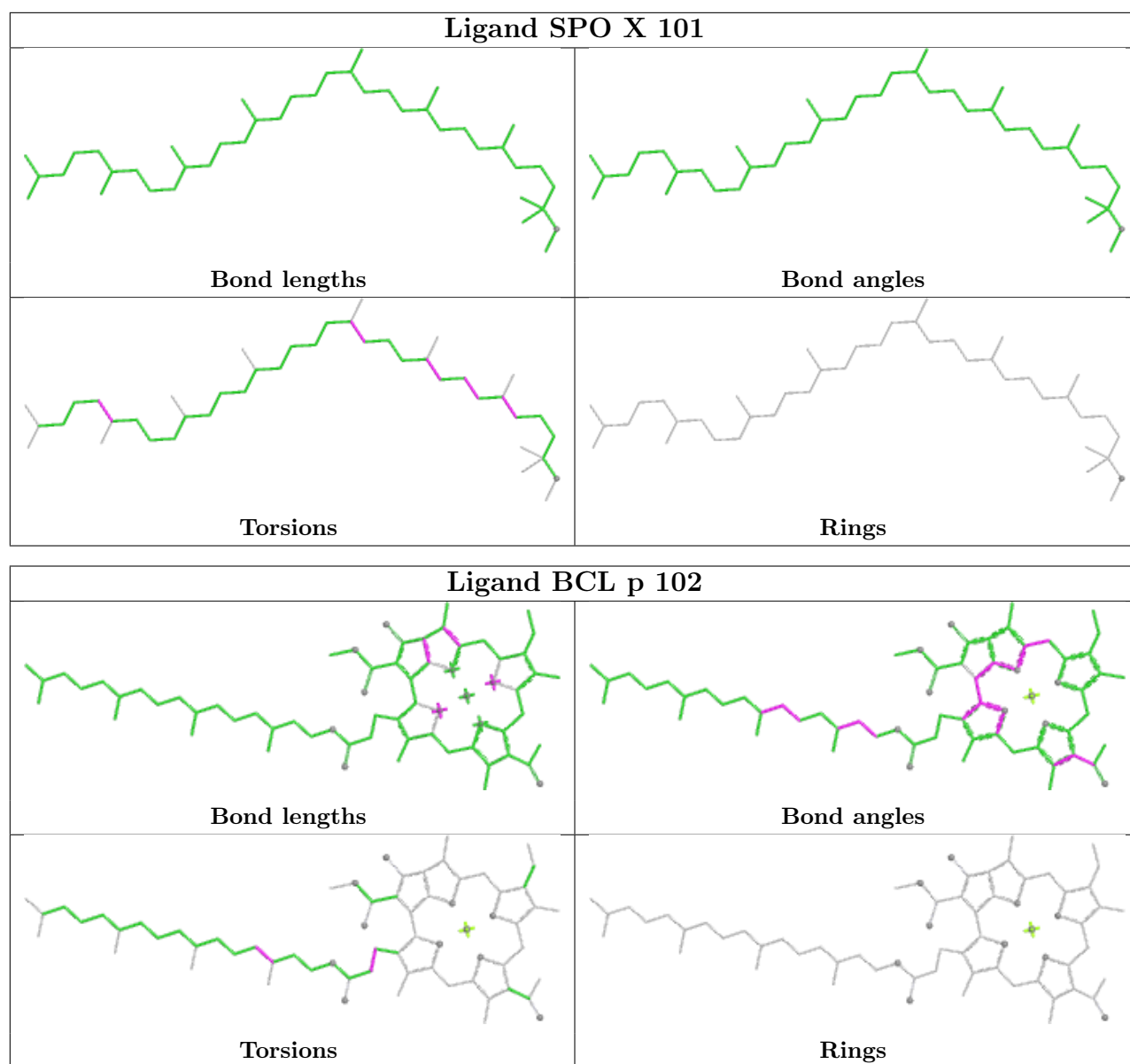


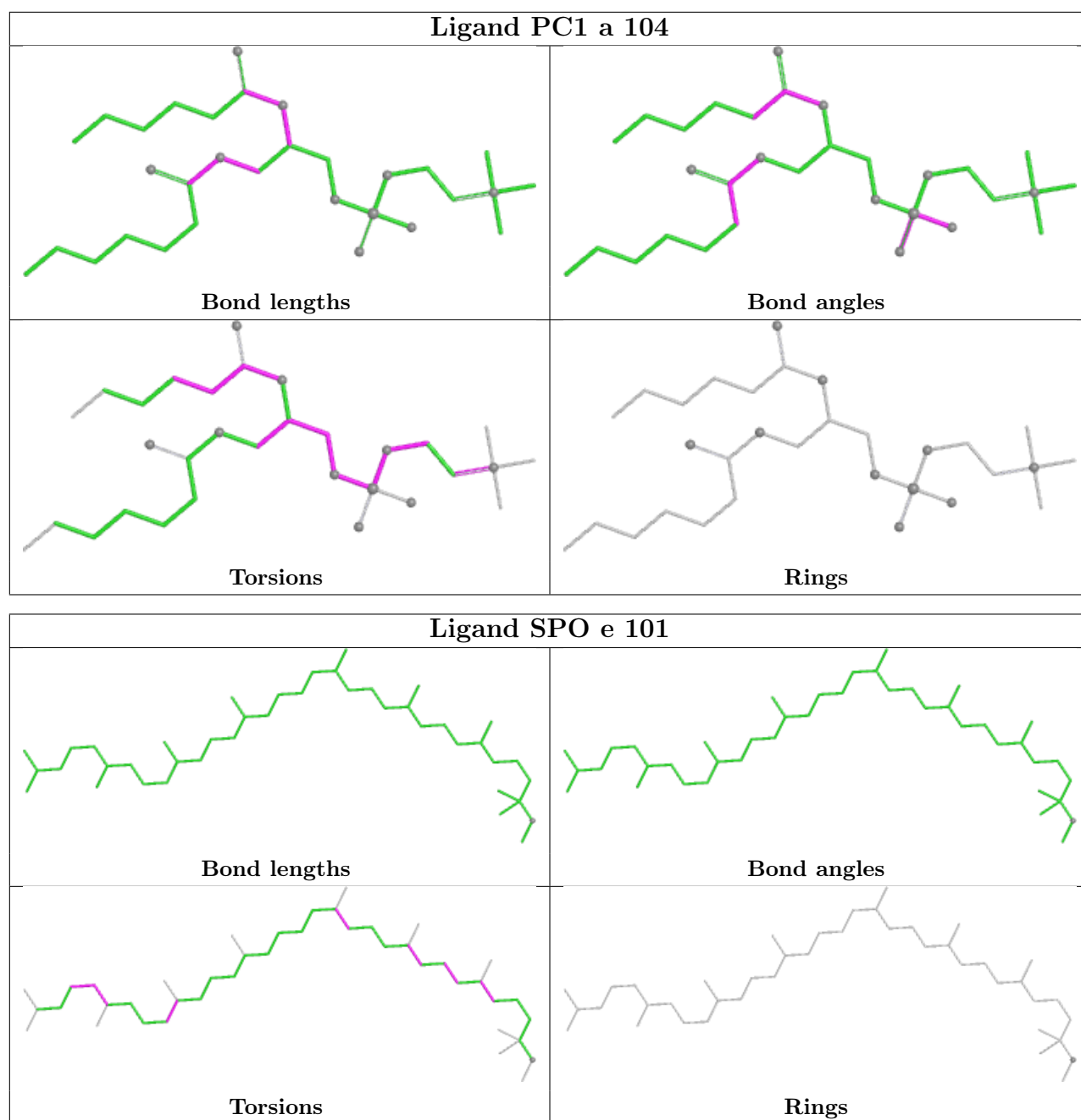


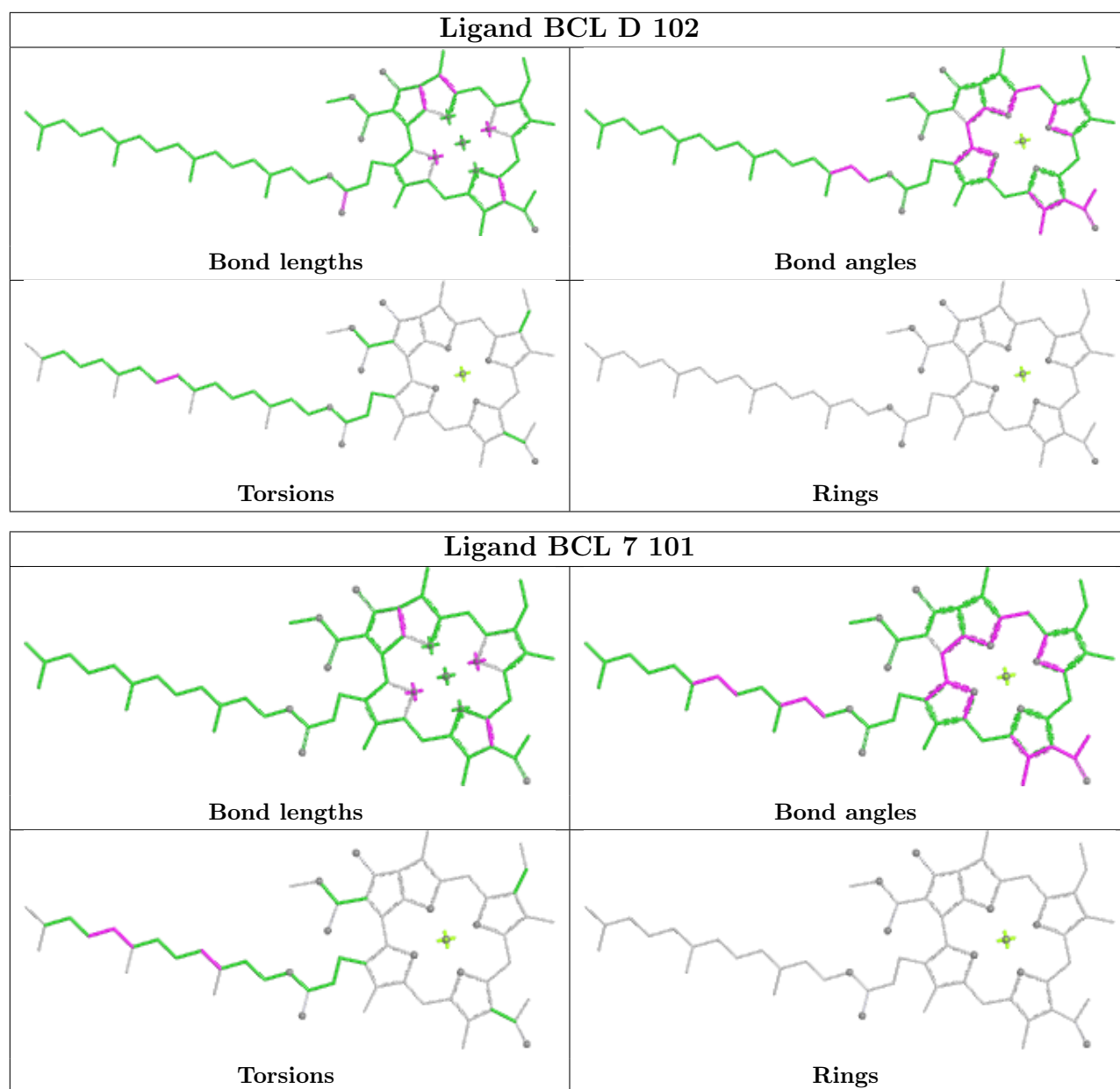




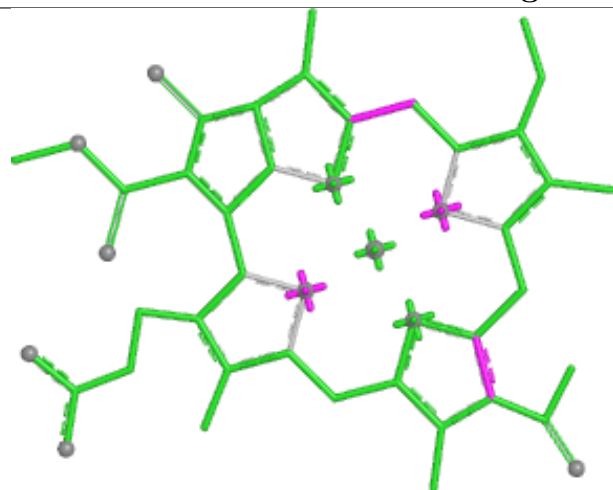




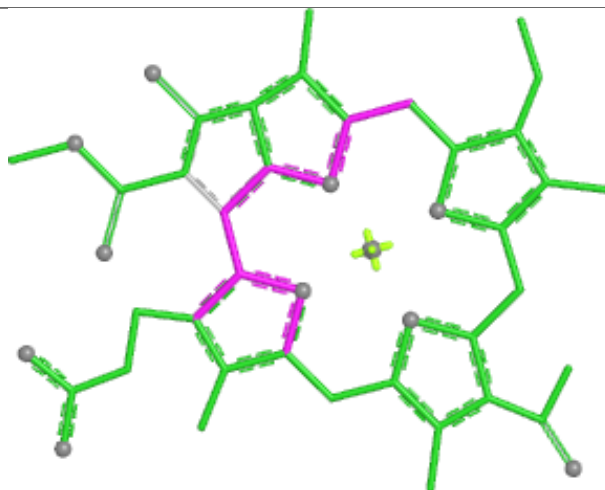




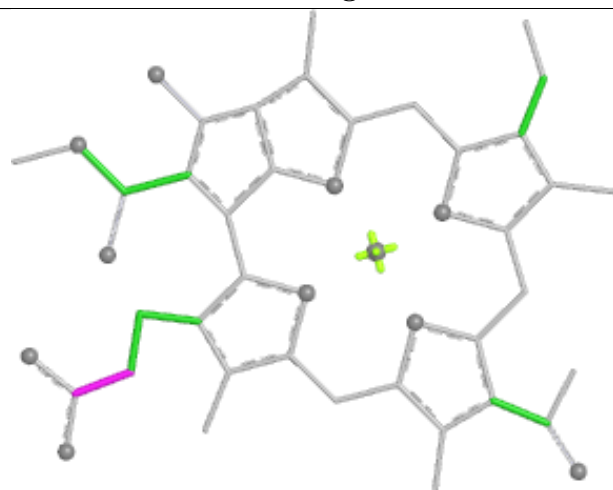
Ligand BCL 4 101



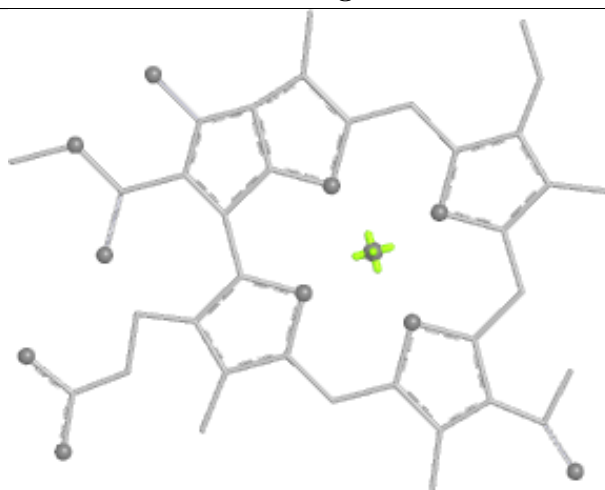
Bond lengths



Bond angles

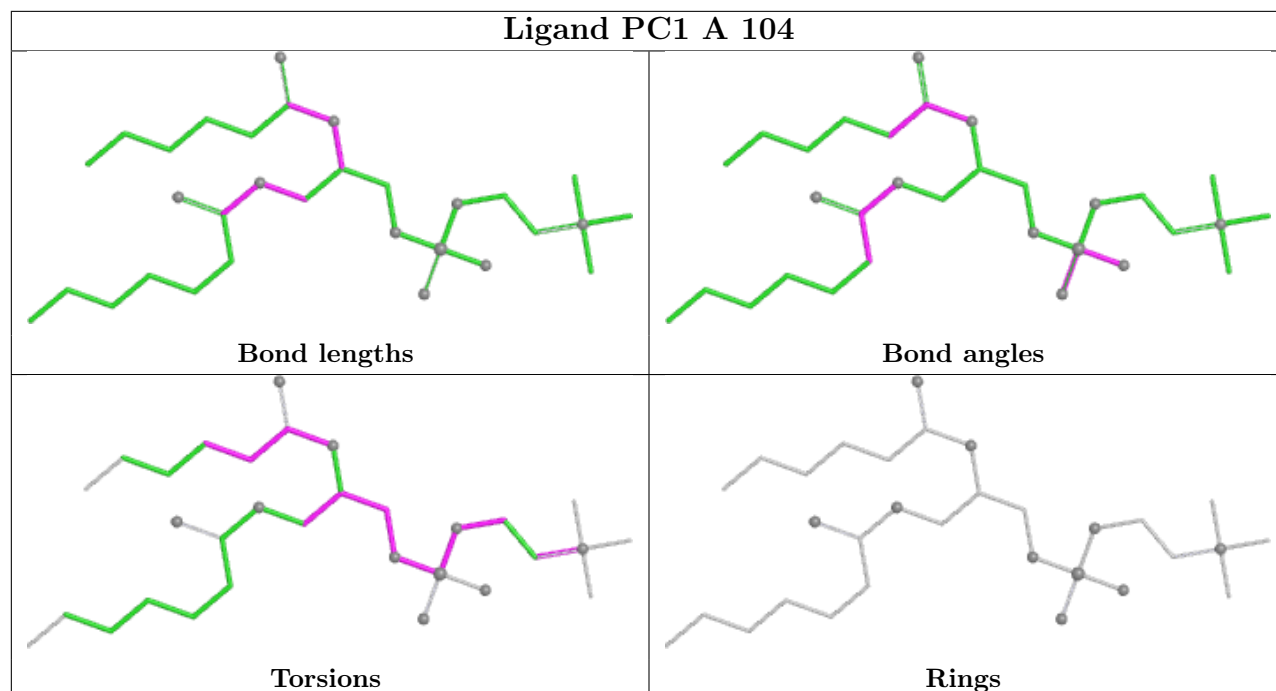


Torsions

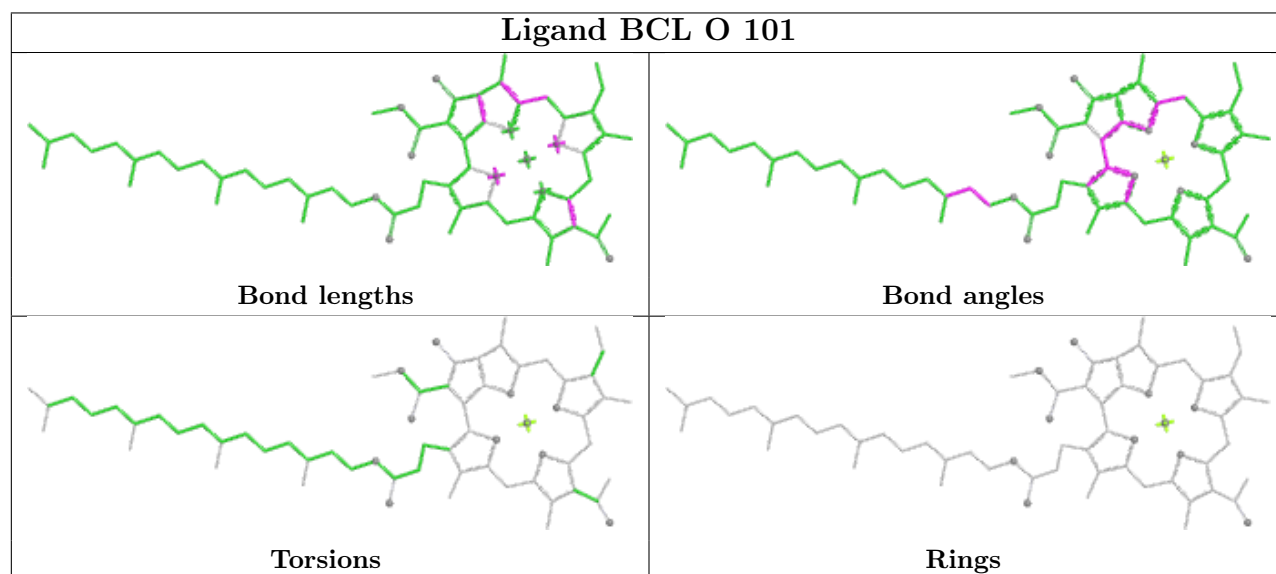


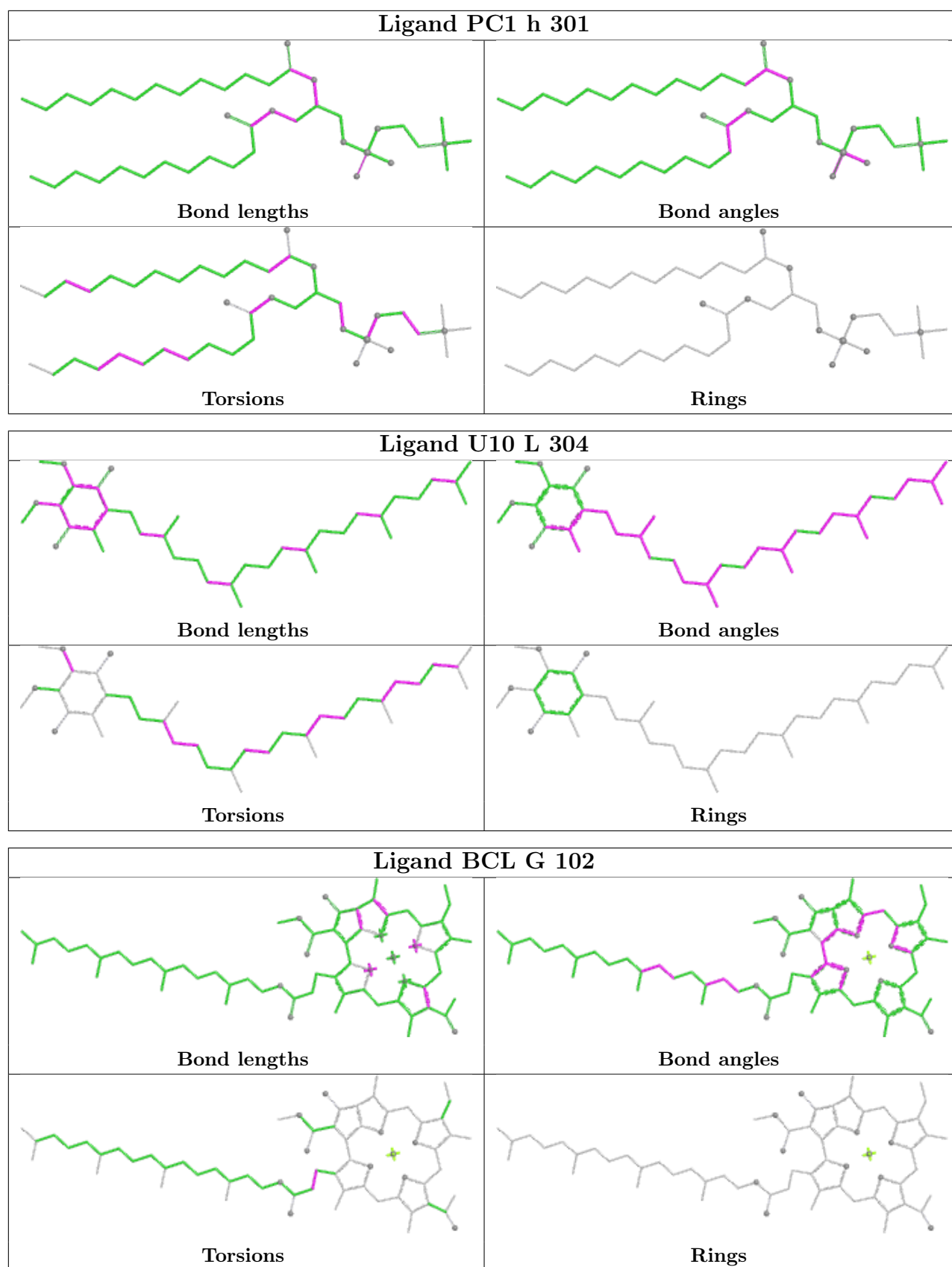
Rings

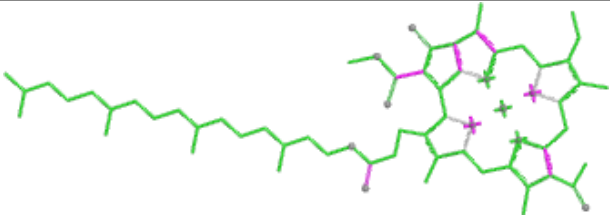
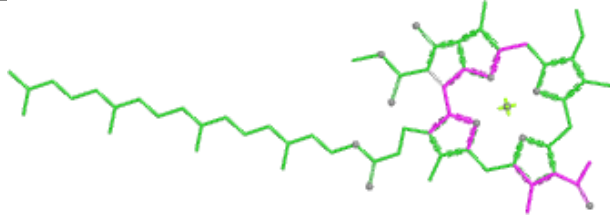
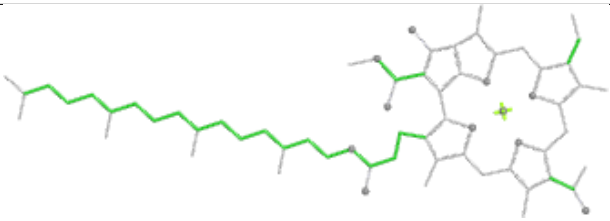
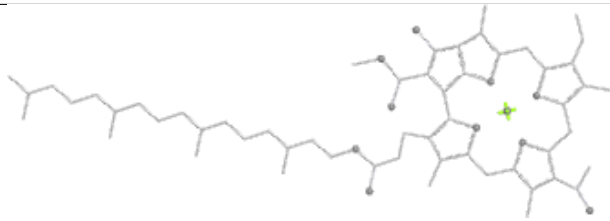
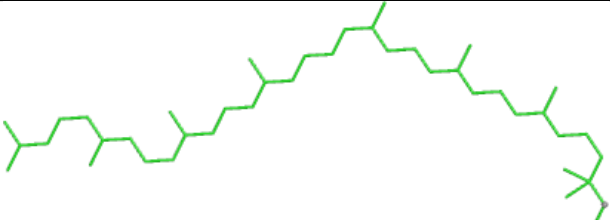
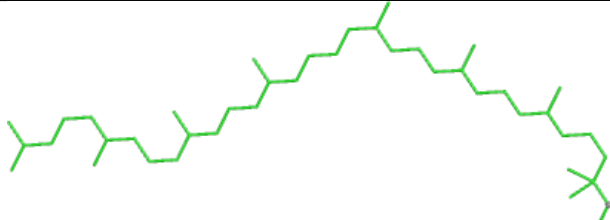
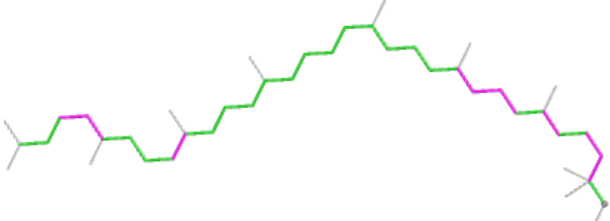
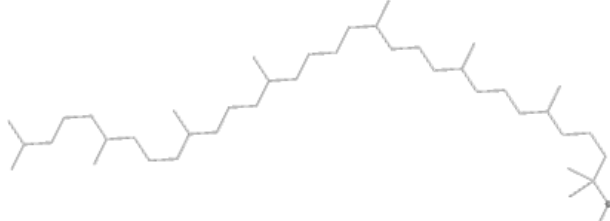
Ligand PC1 A 104

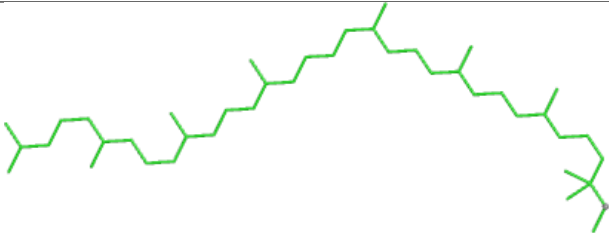
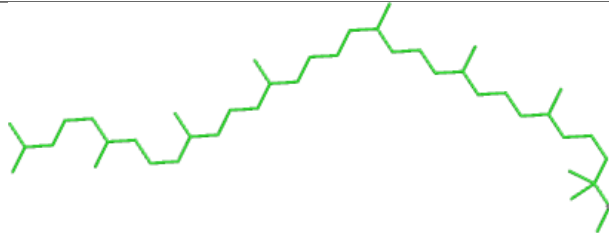
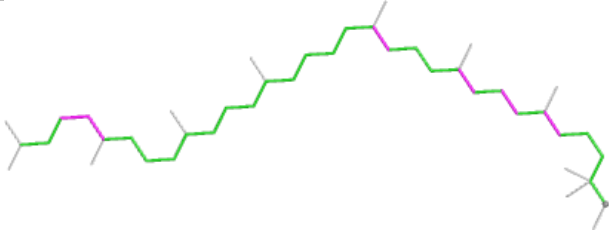
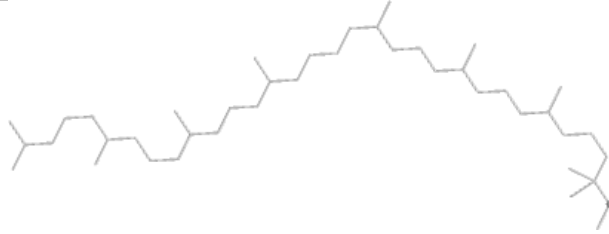
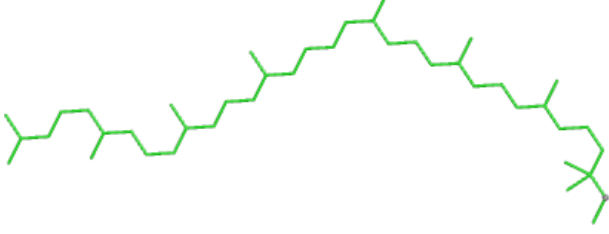
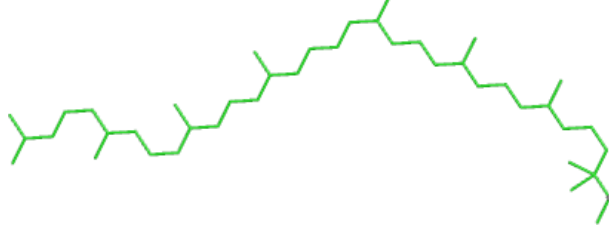
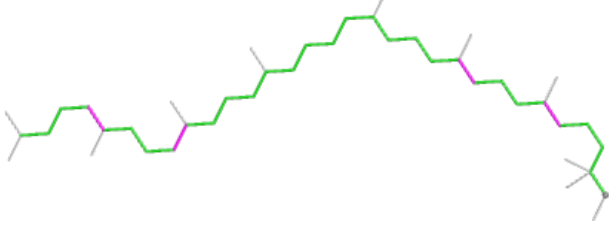
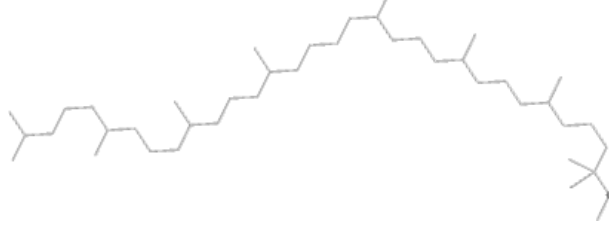


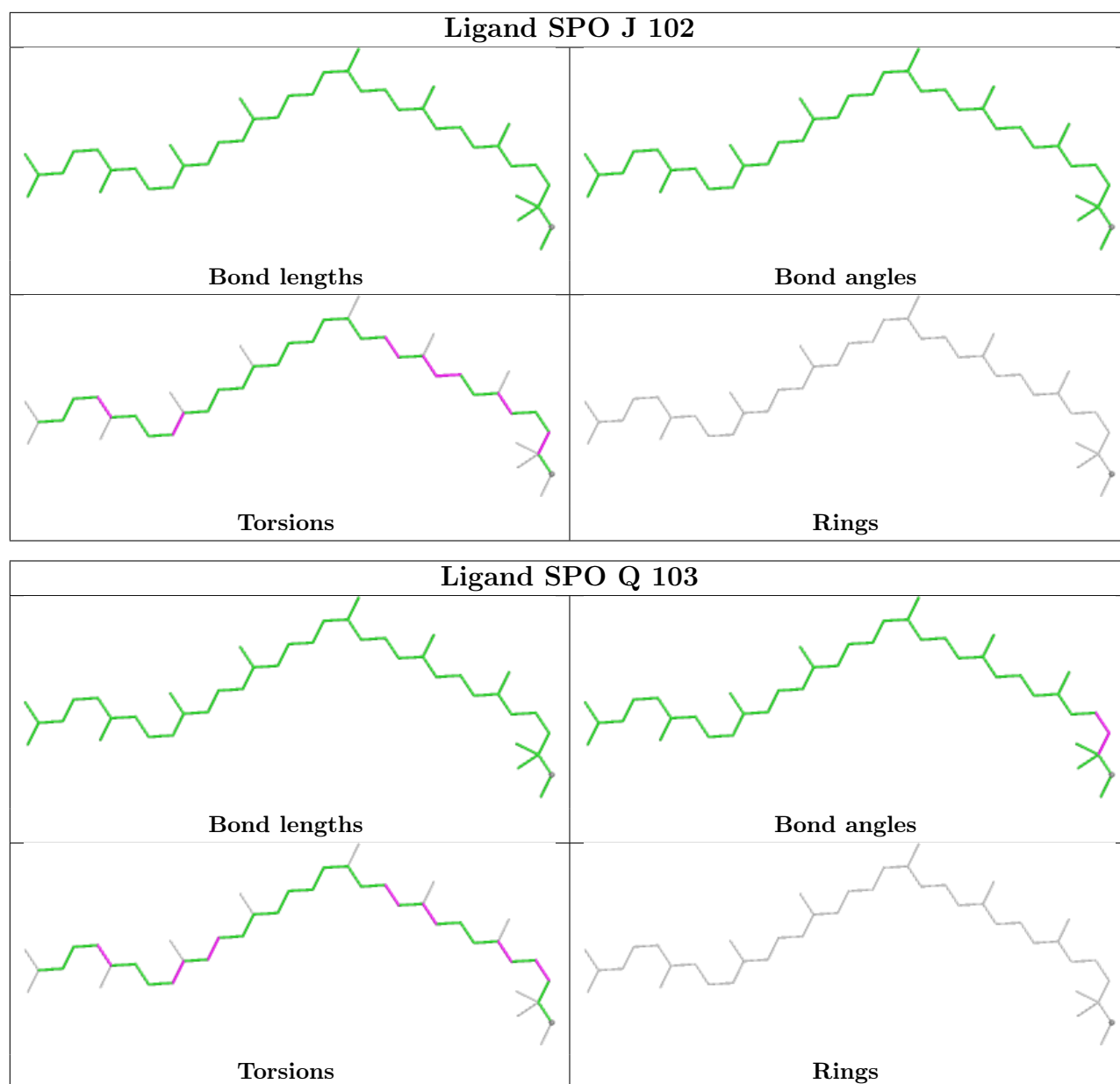
Ligand BCL O 101

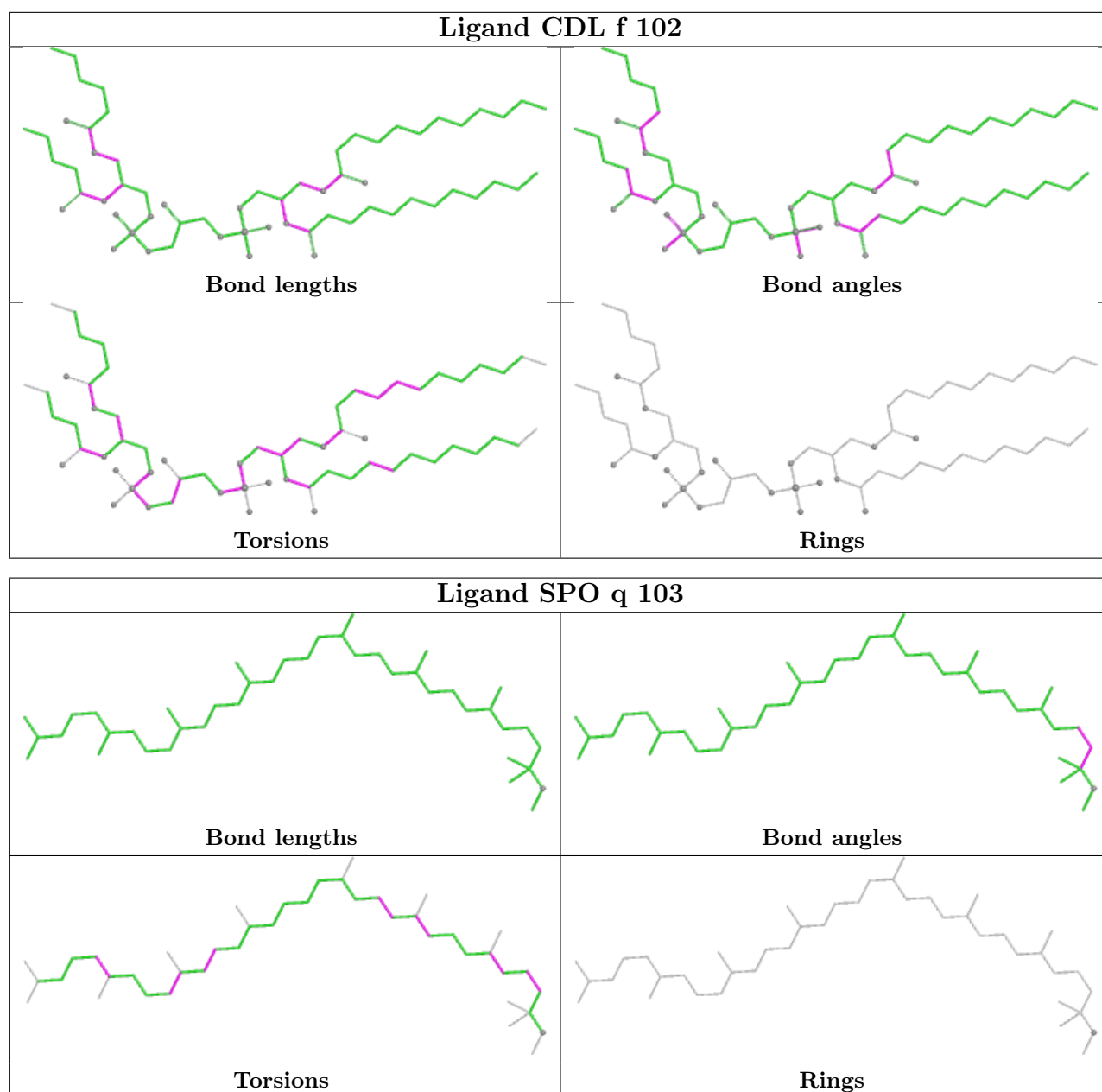


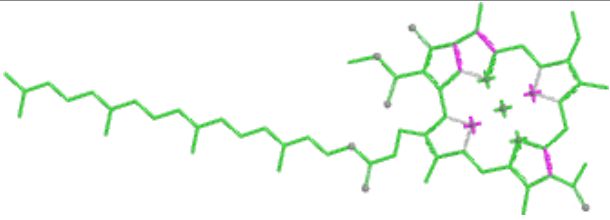
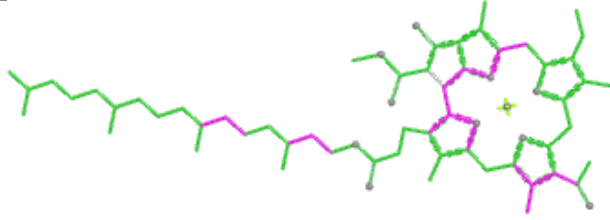
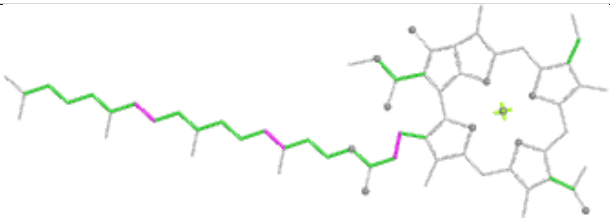
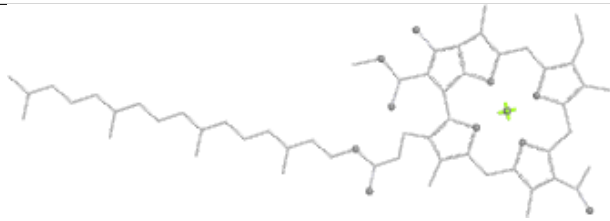
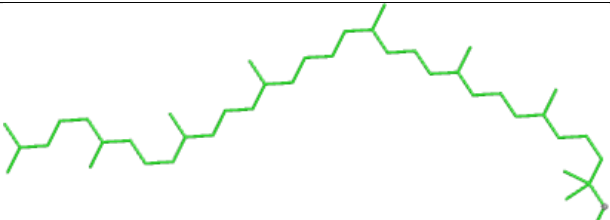
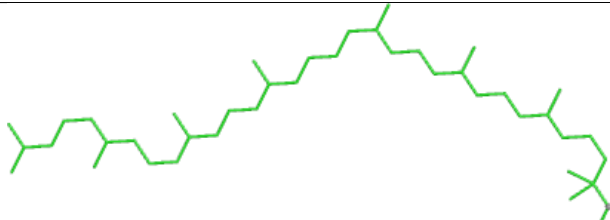
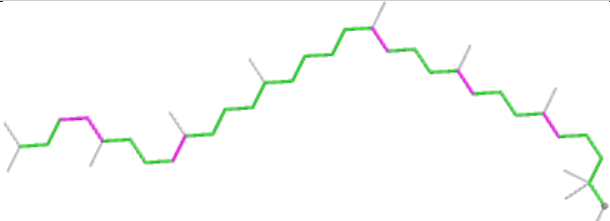
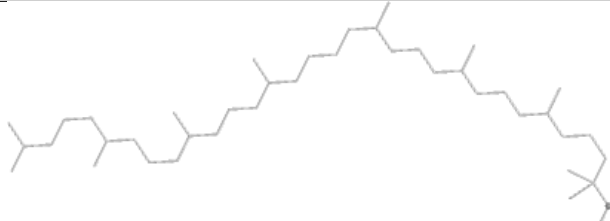
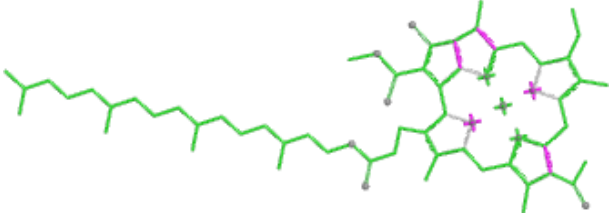
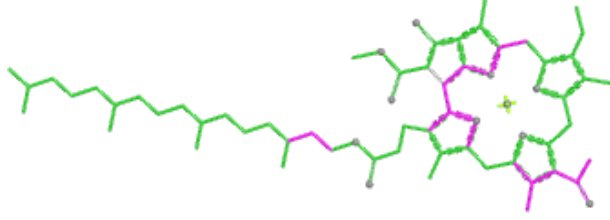
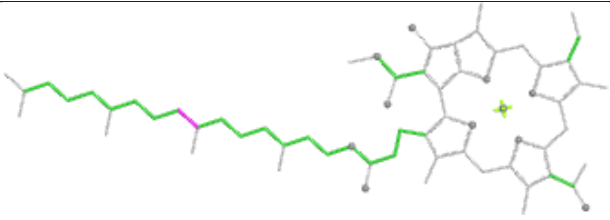
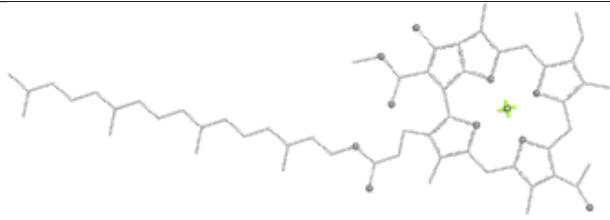


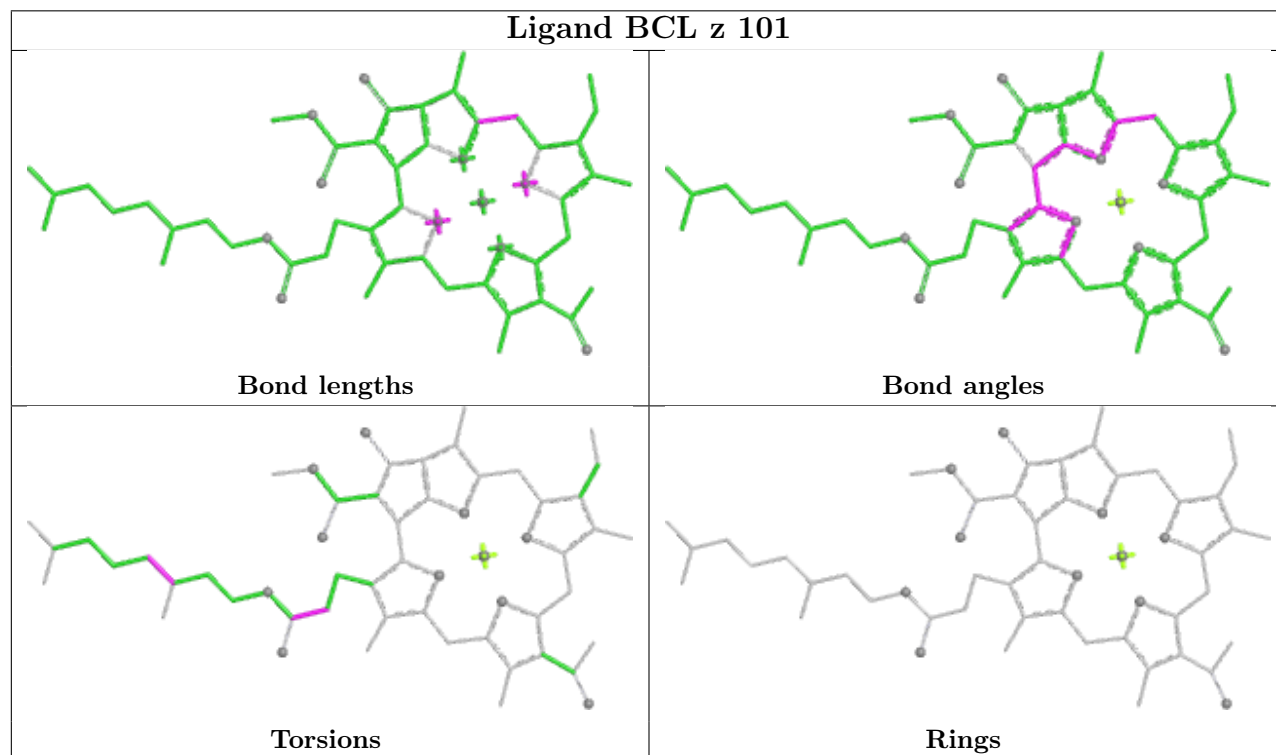
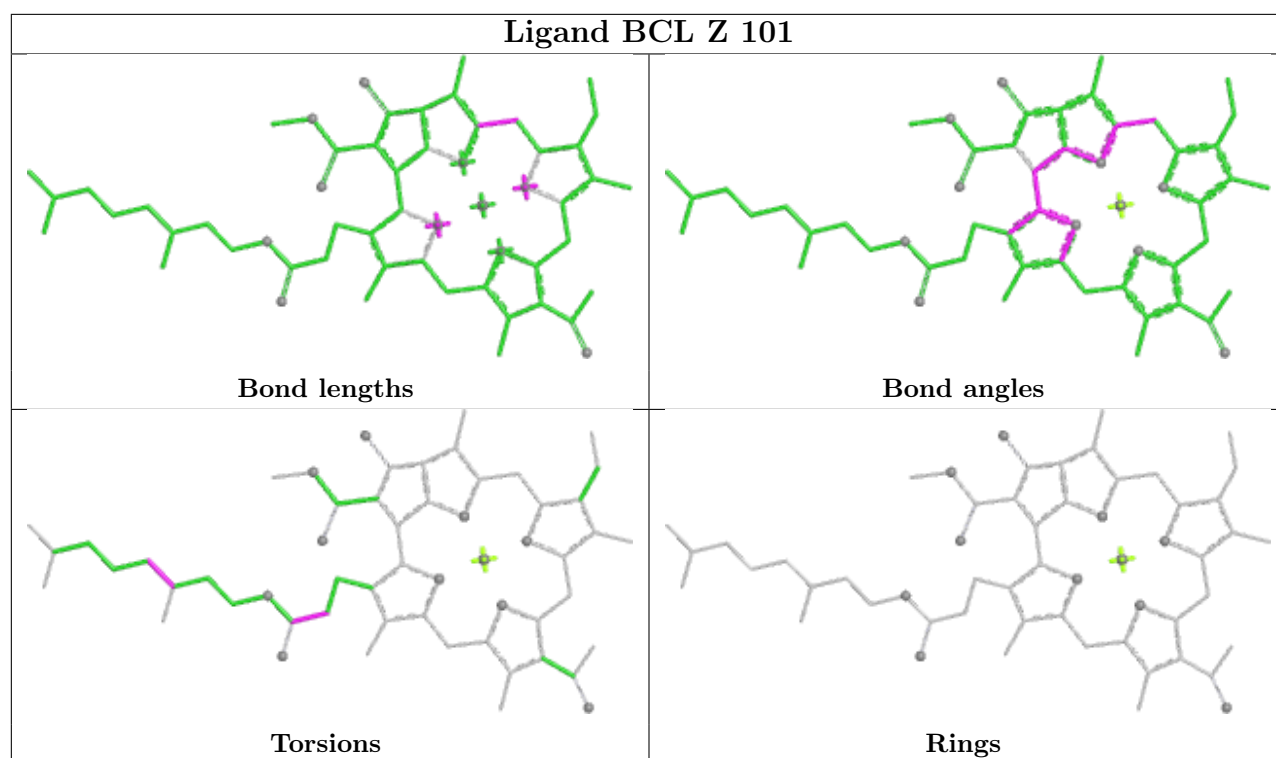
Ligand BCL m 403	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO B 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

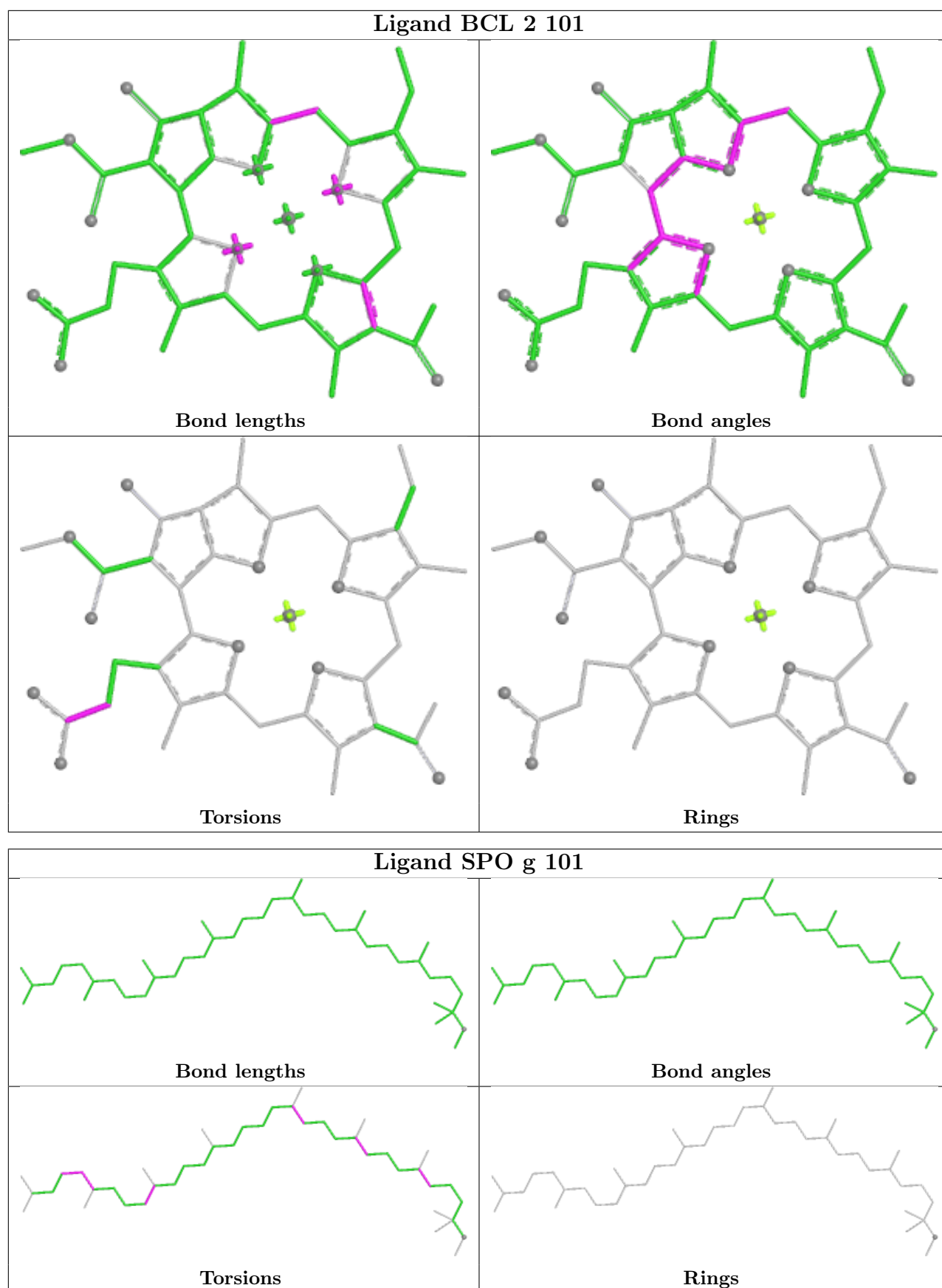
Ligand SPO Q 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO u 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

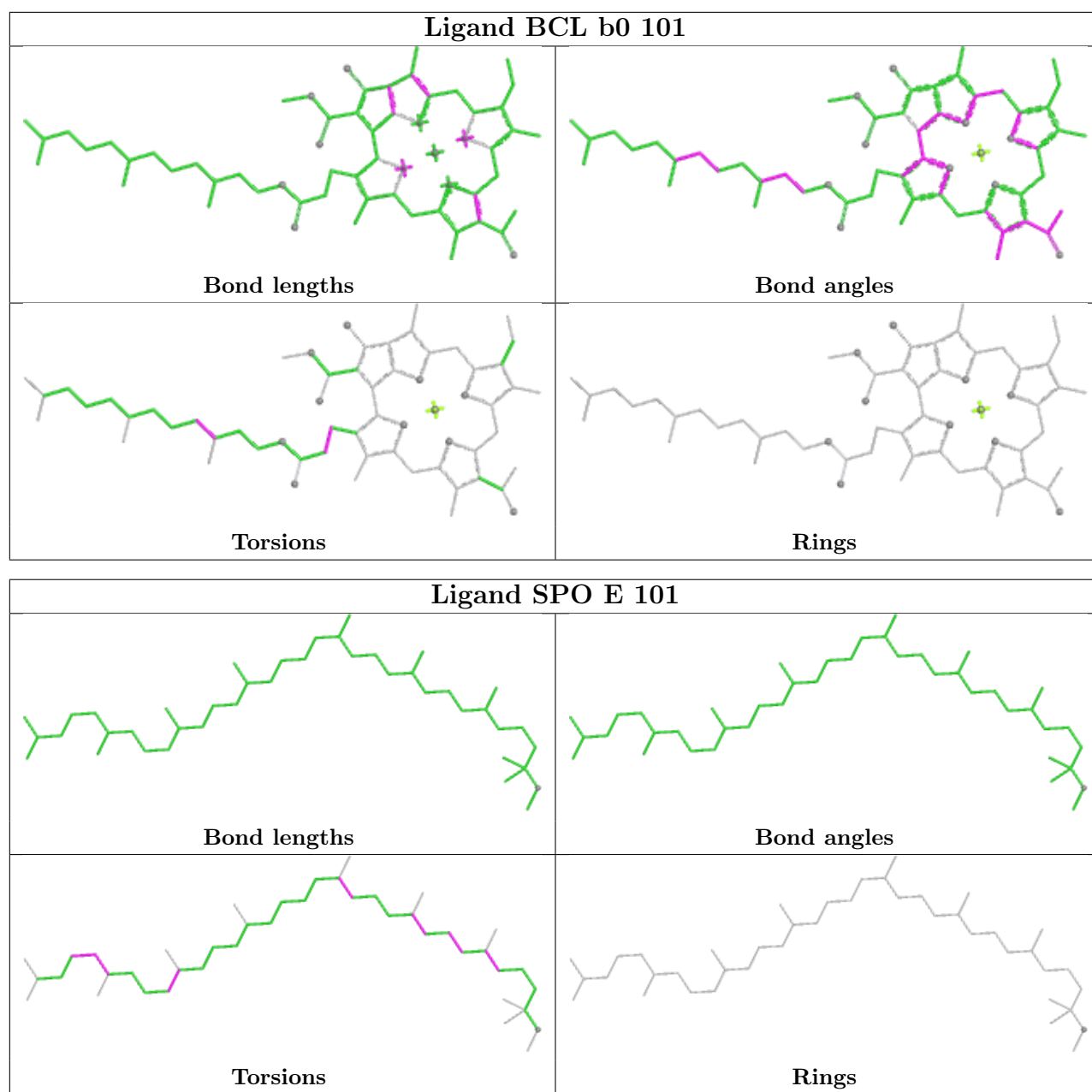


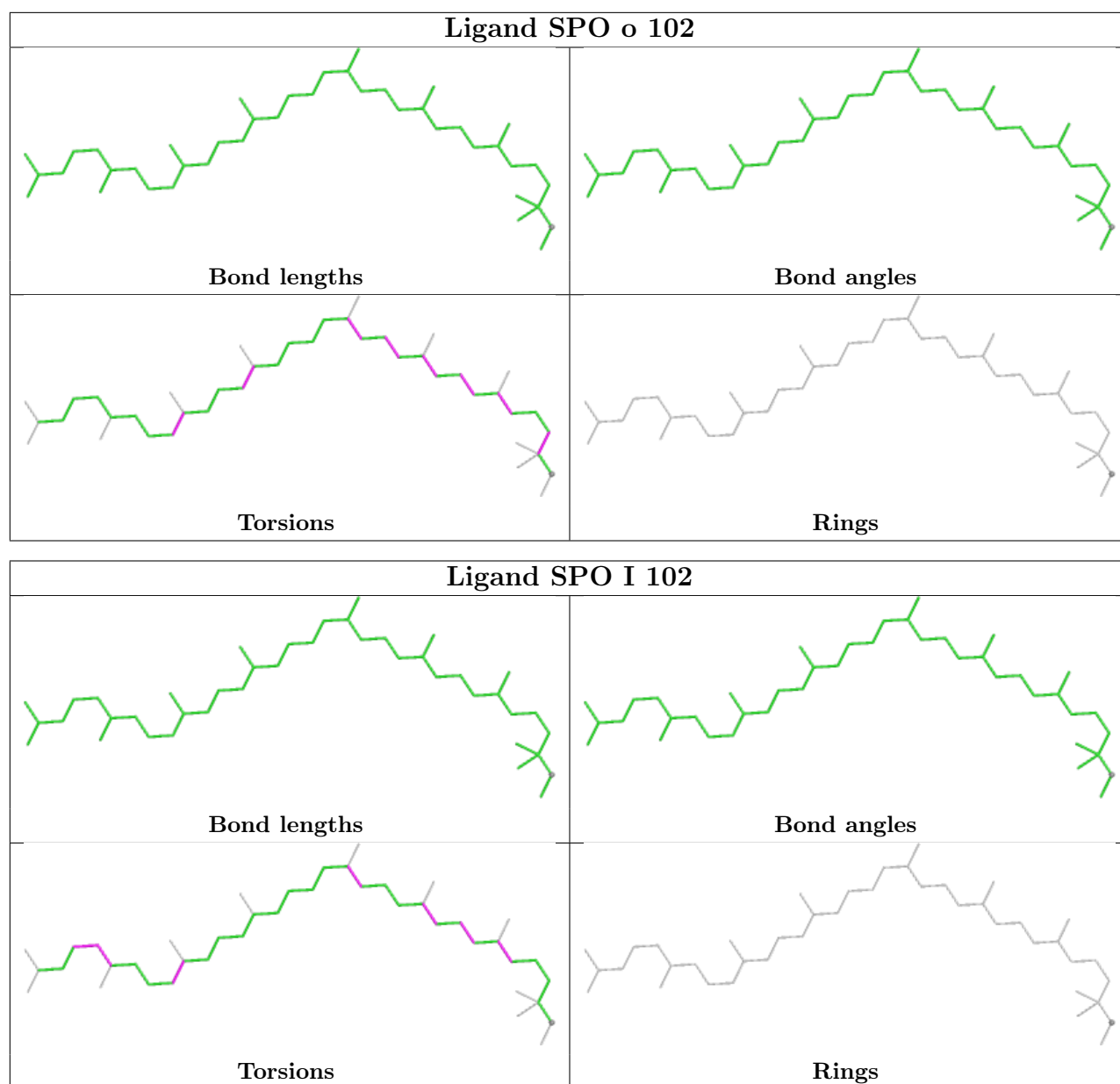


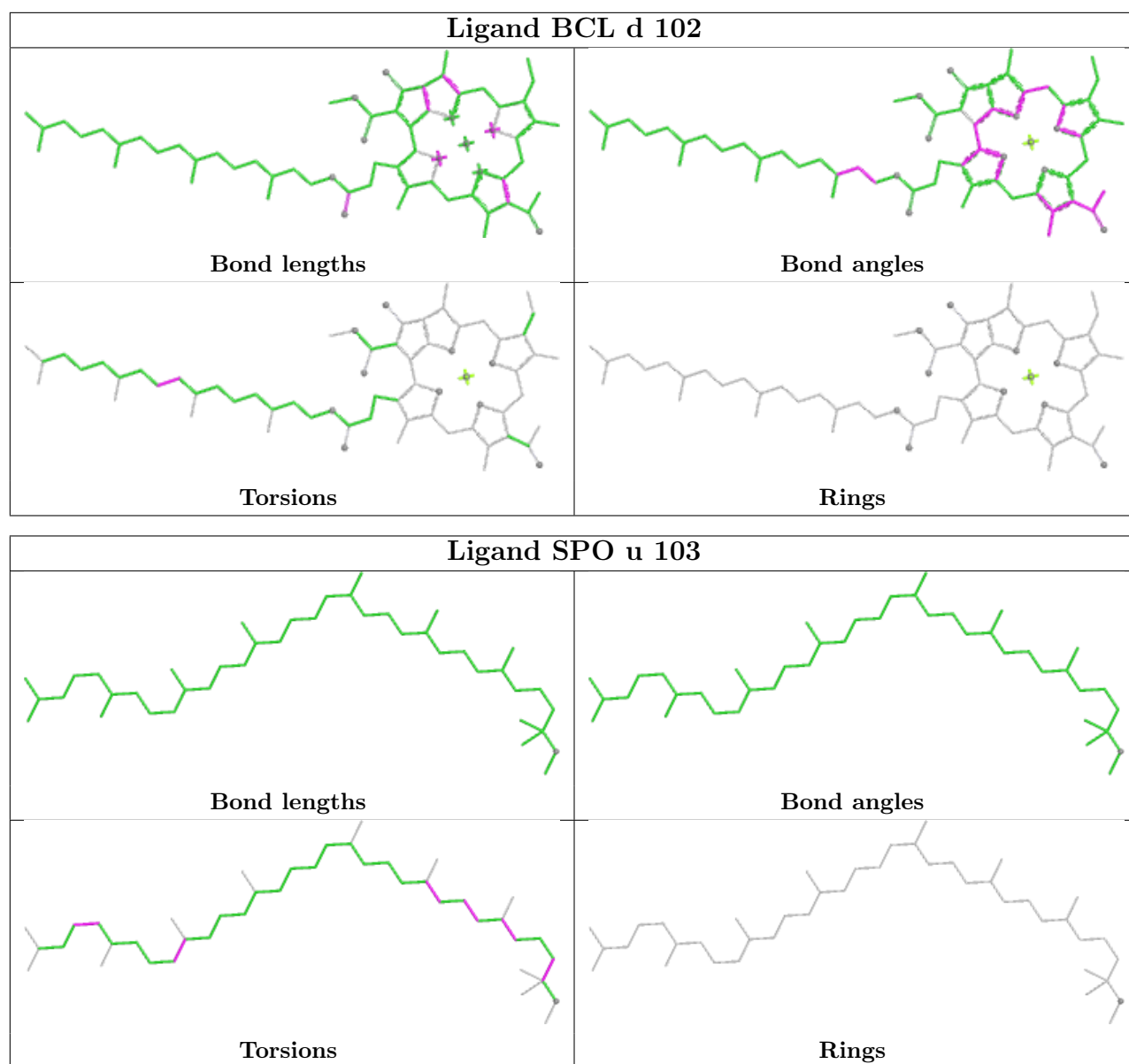
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO s 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL F 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

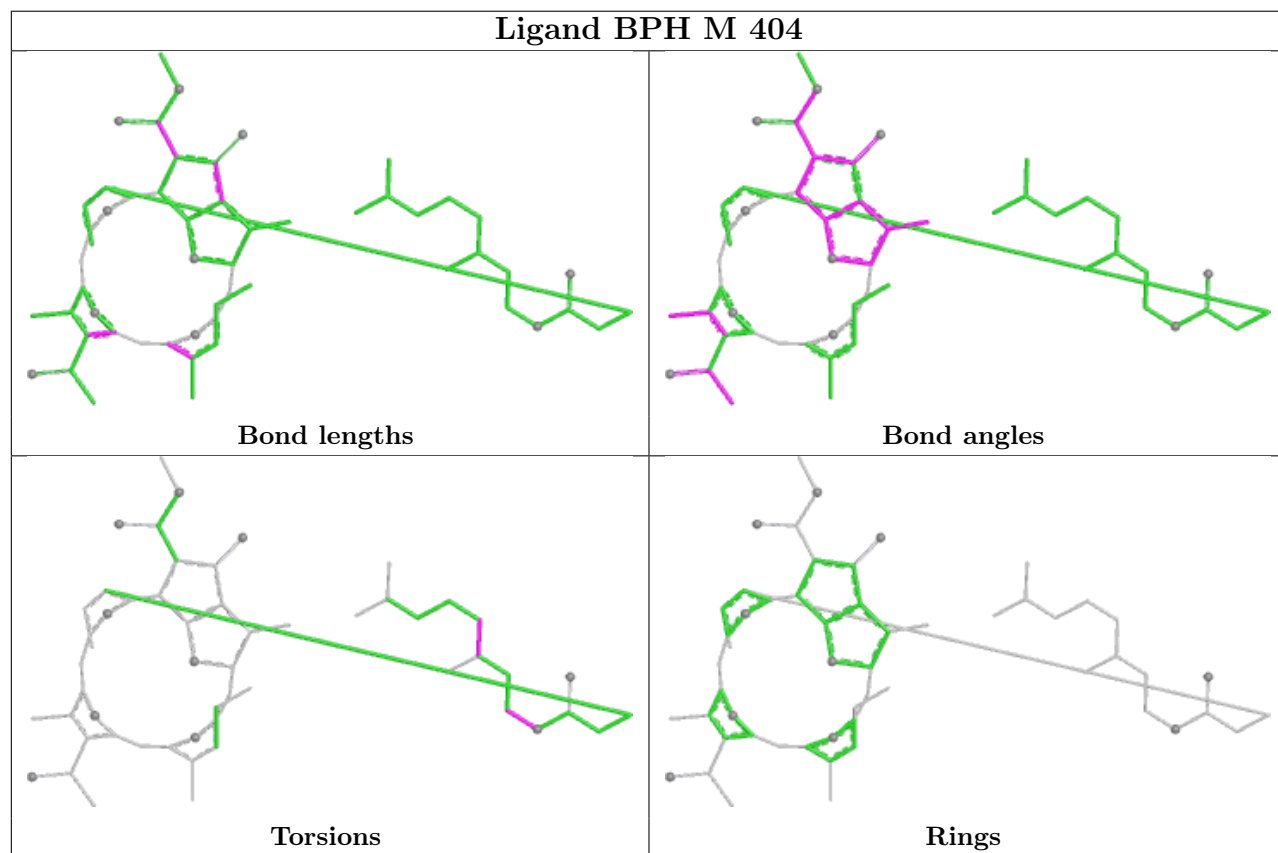
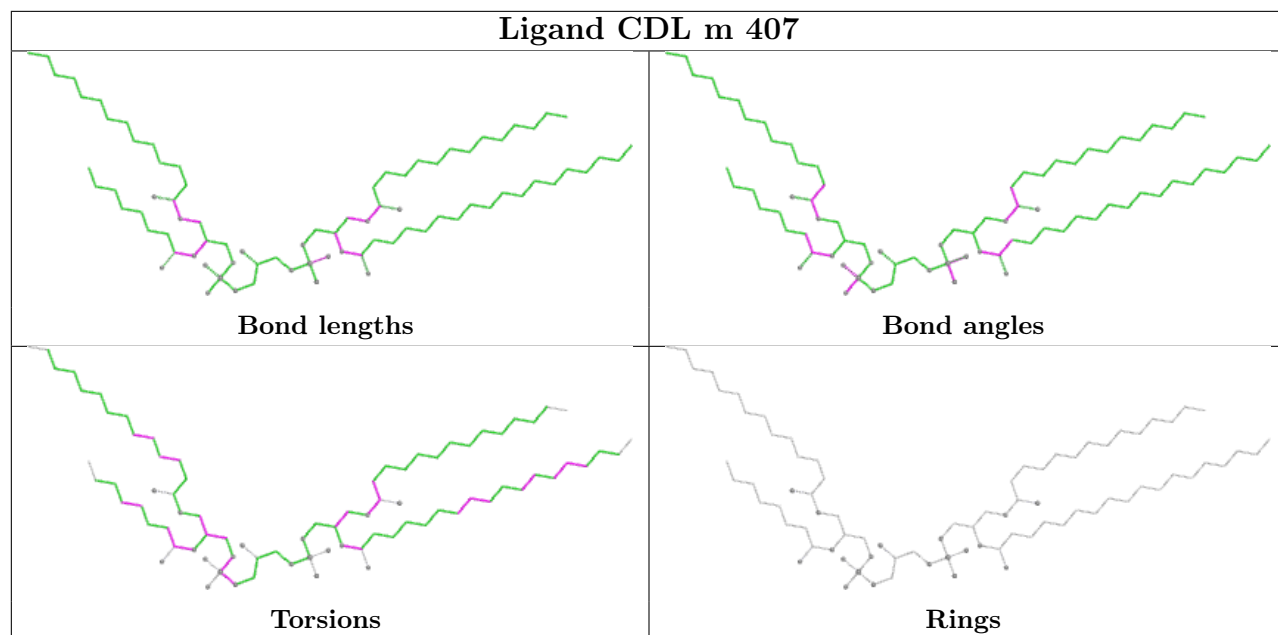


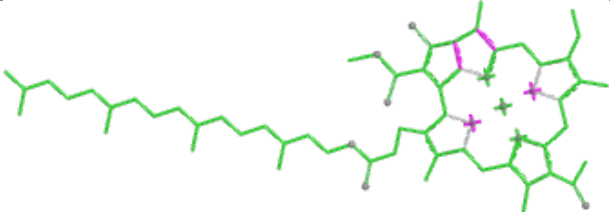
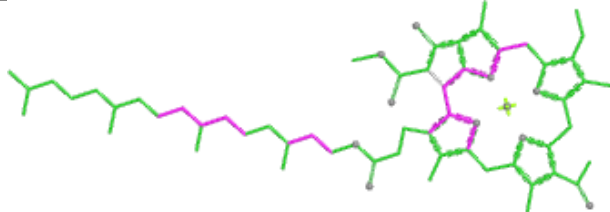
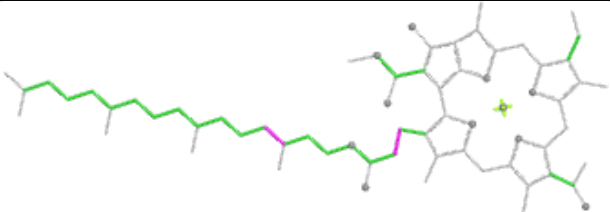
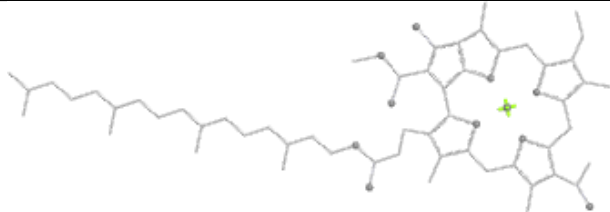
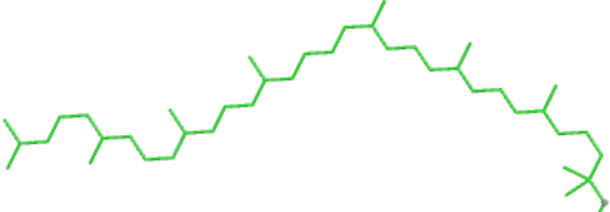
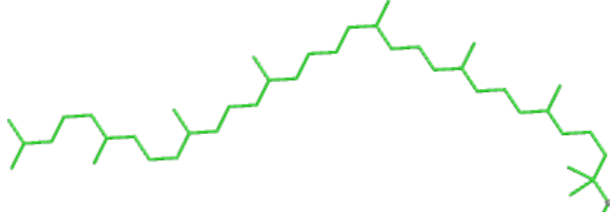
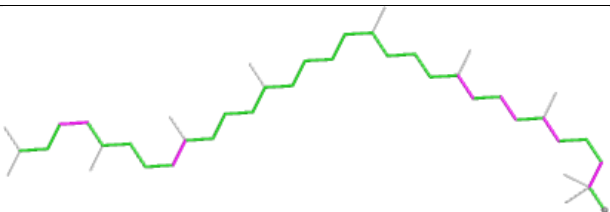
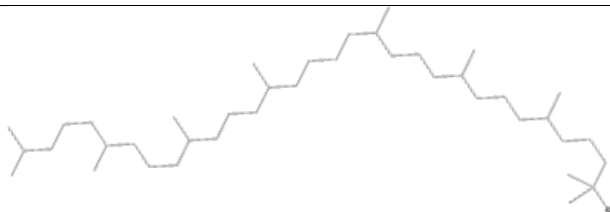
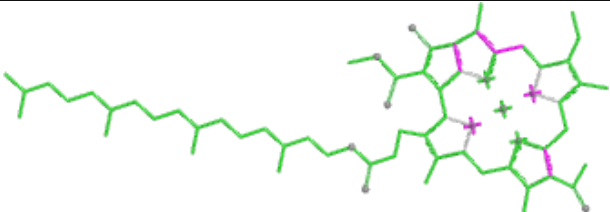
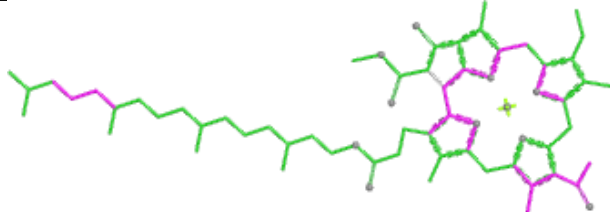
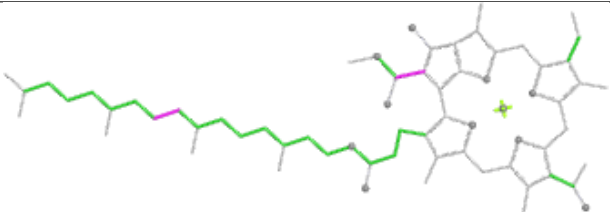
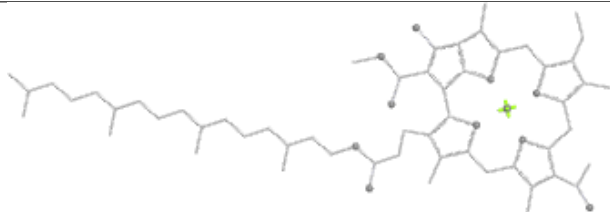


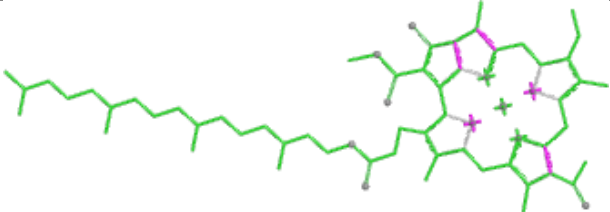
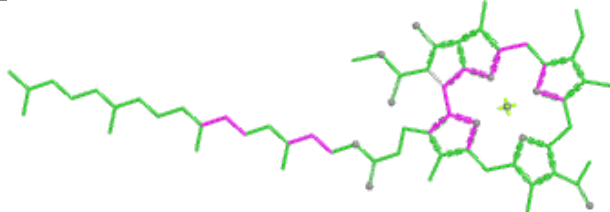
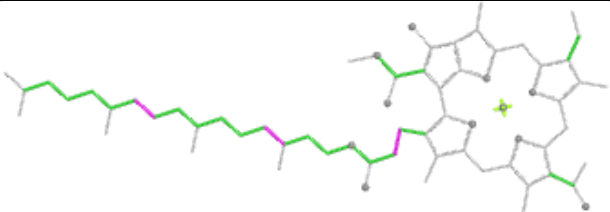
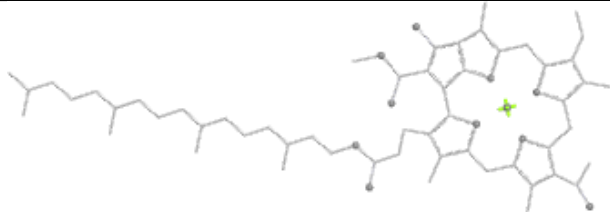
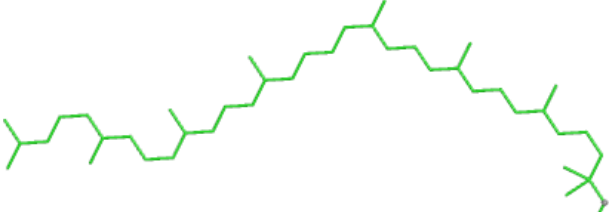
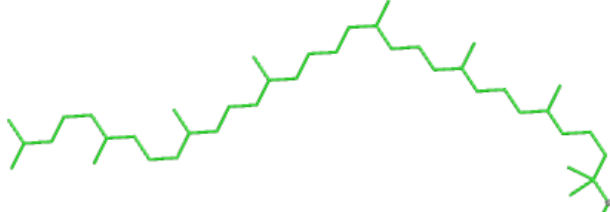
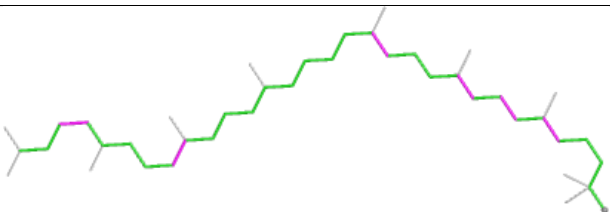
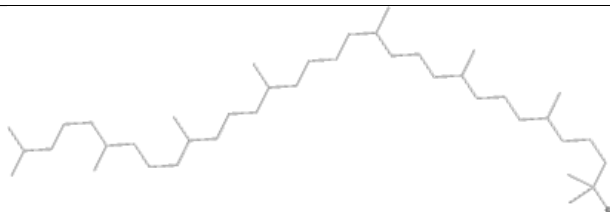
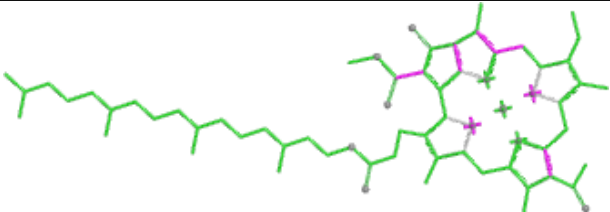
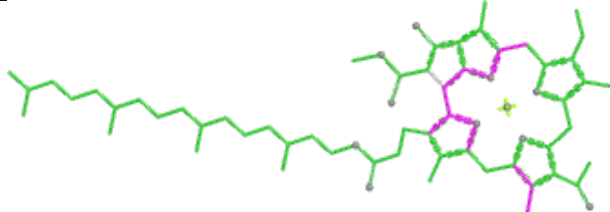
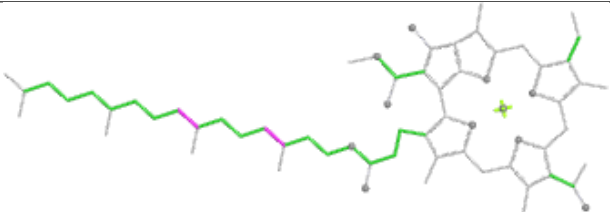
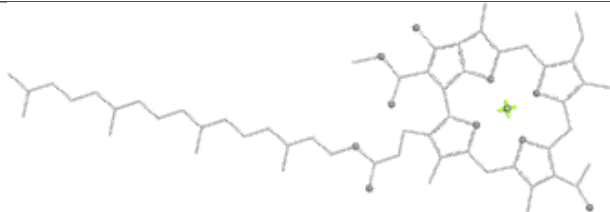


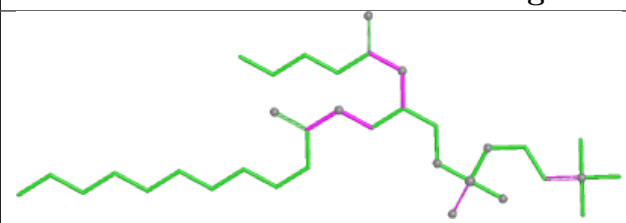
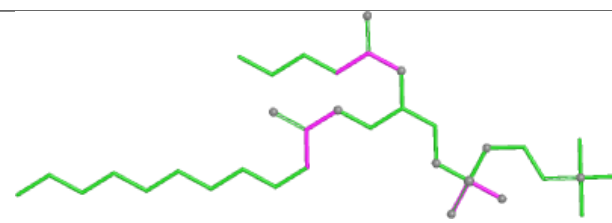
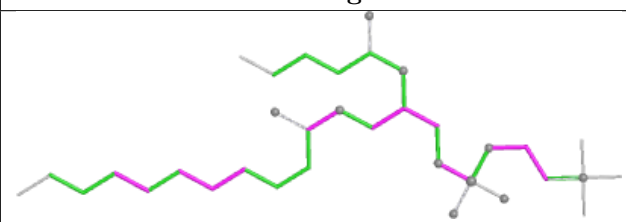
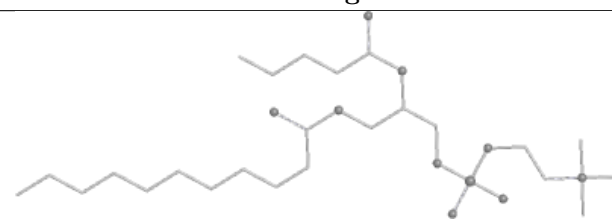


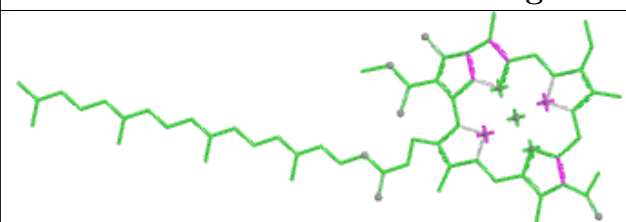
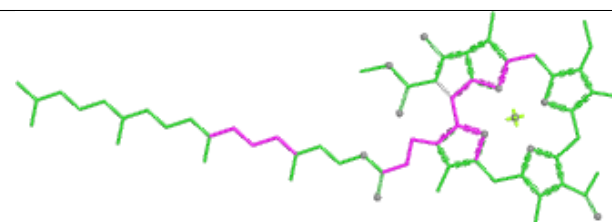
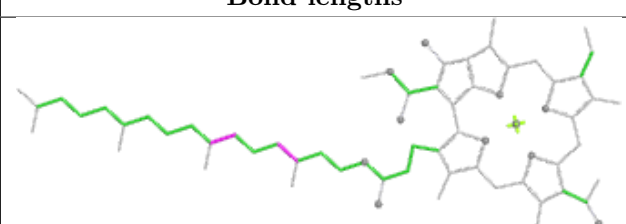
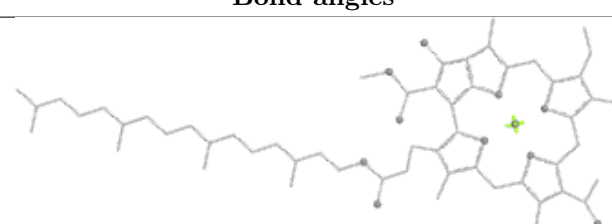


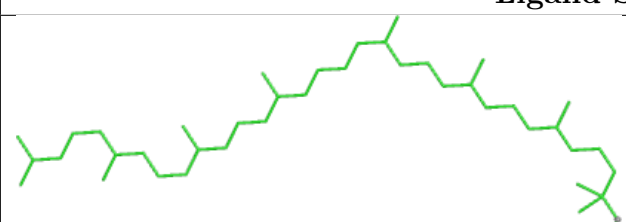
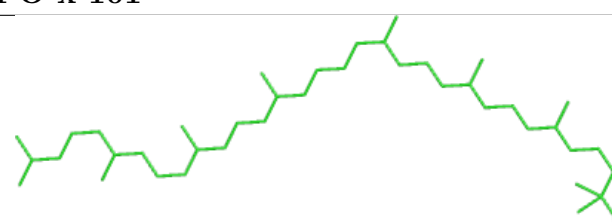
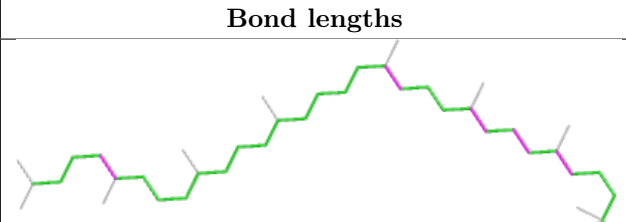
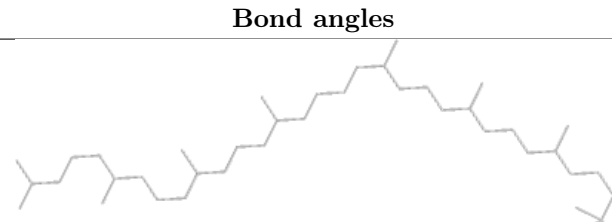


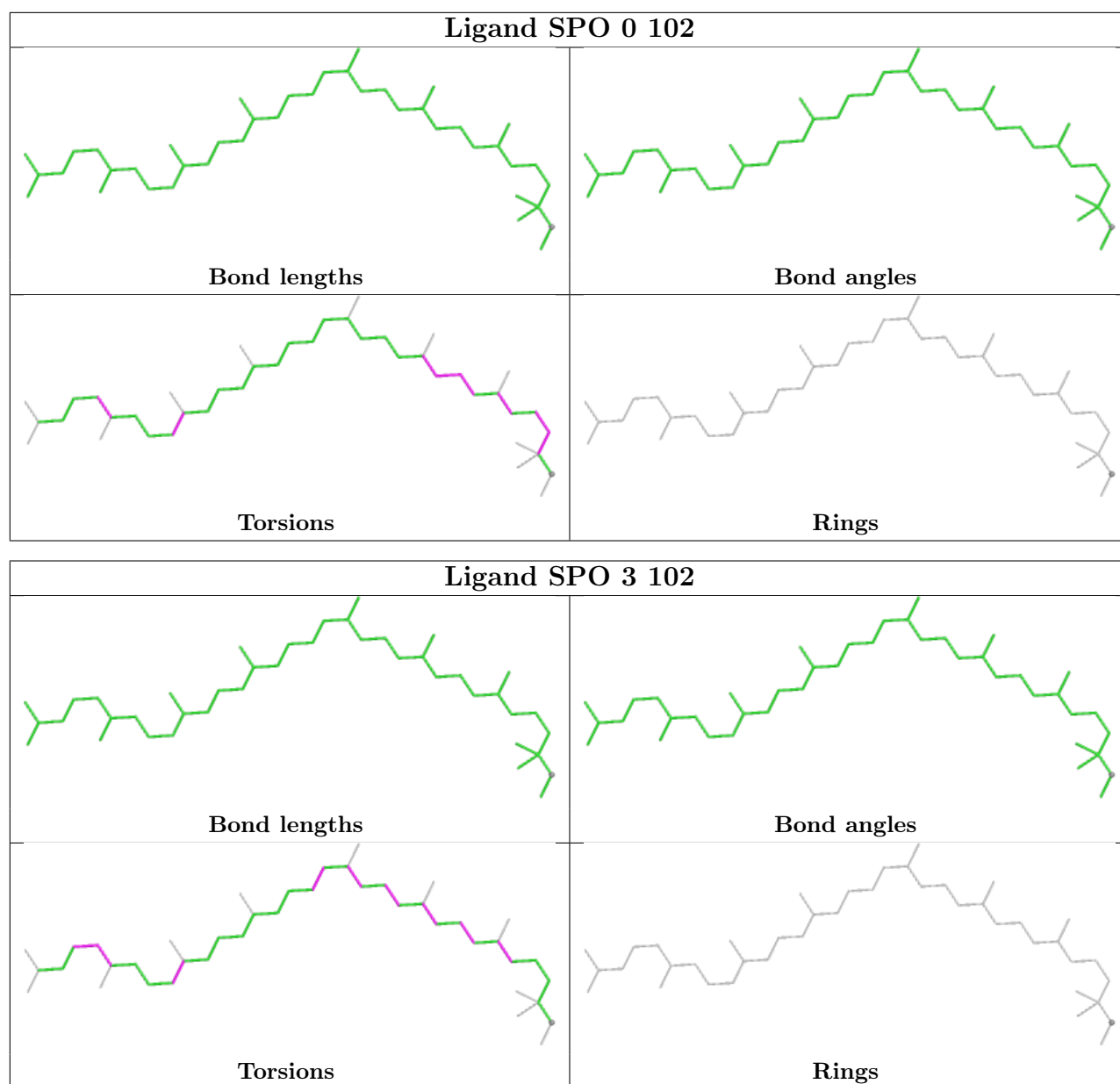
Ligand BCL t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO U 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL q 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

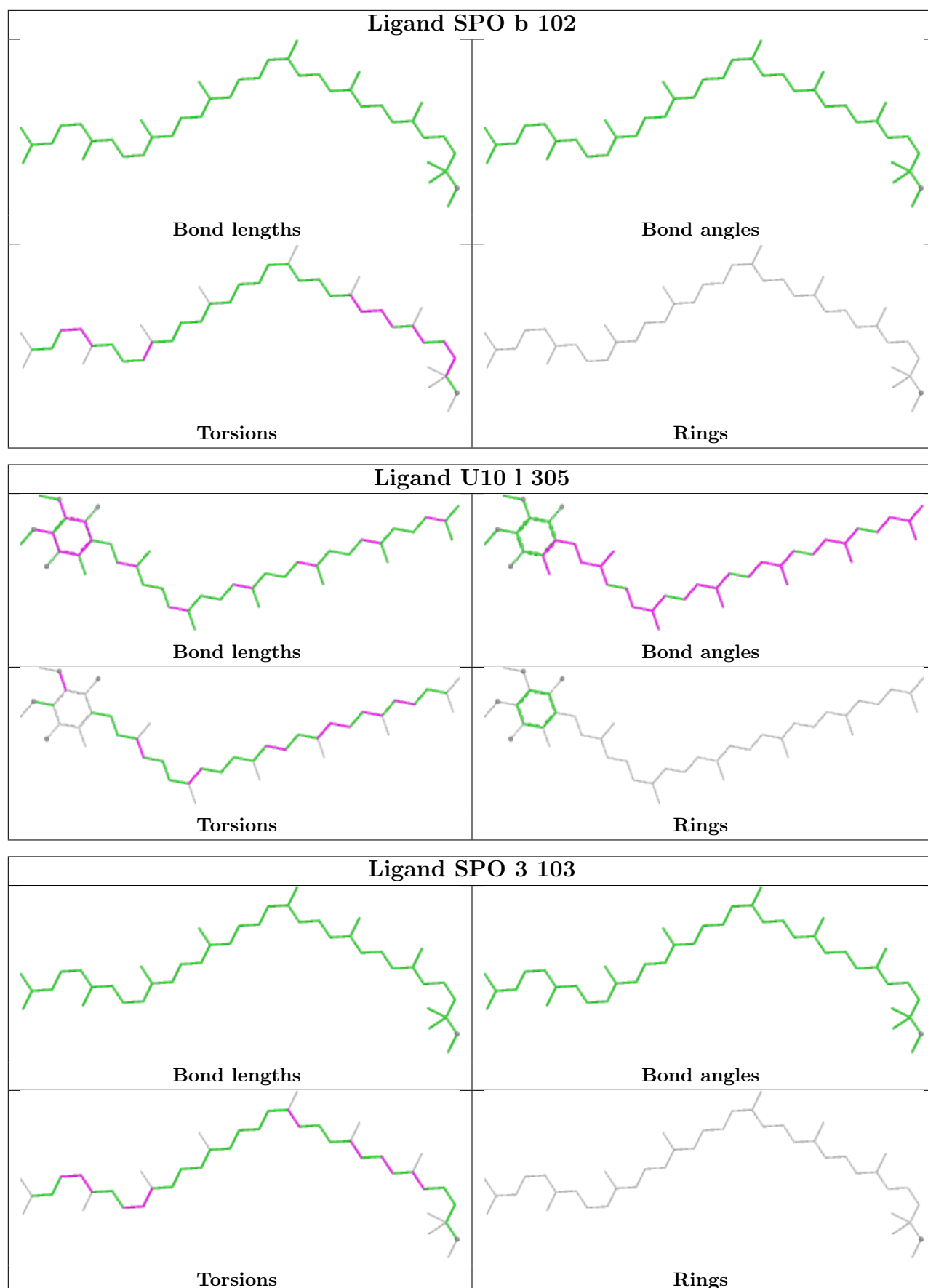
Ligand BCL N 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO n 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL m 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

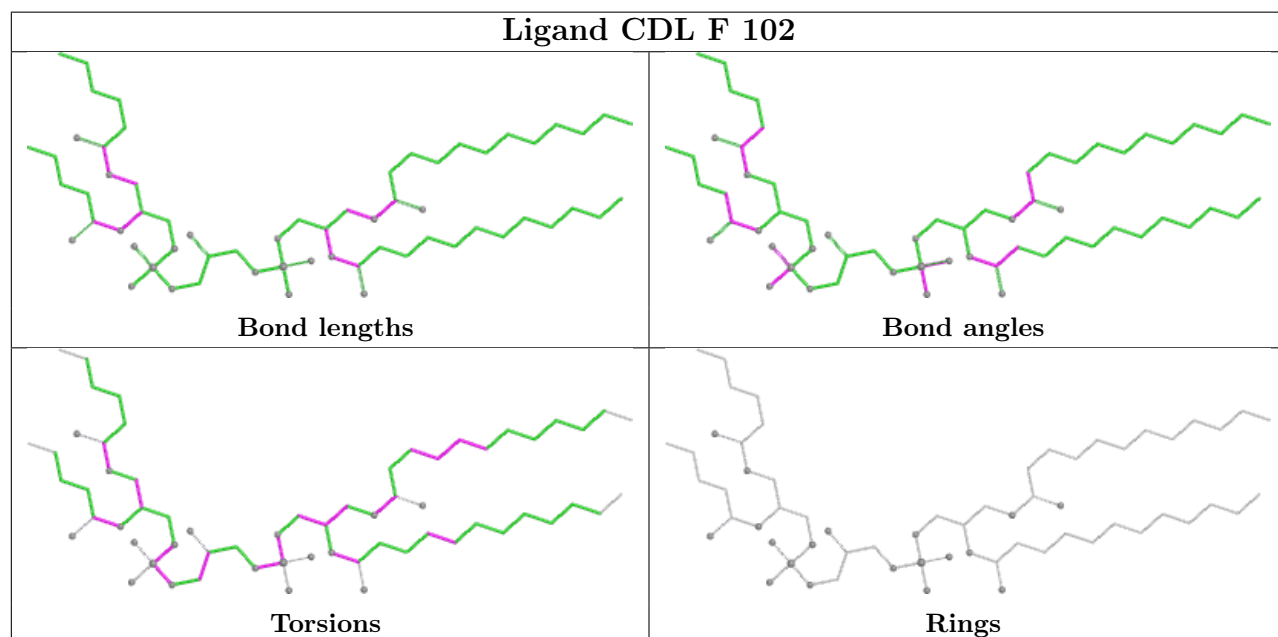
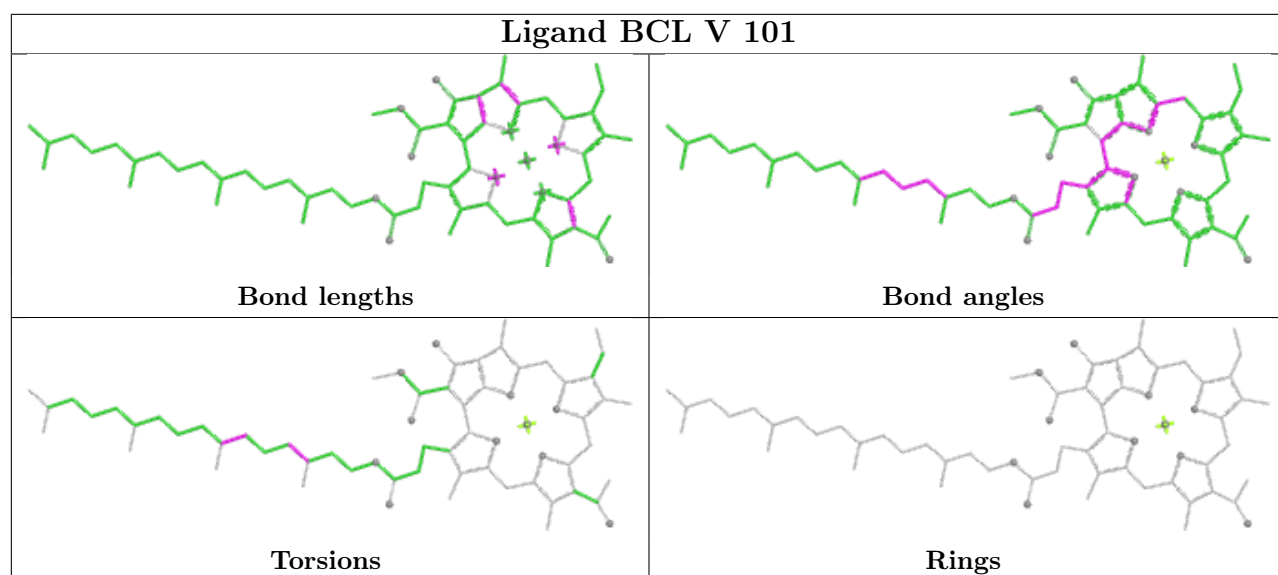
Ligand PC1 h 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL v 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

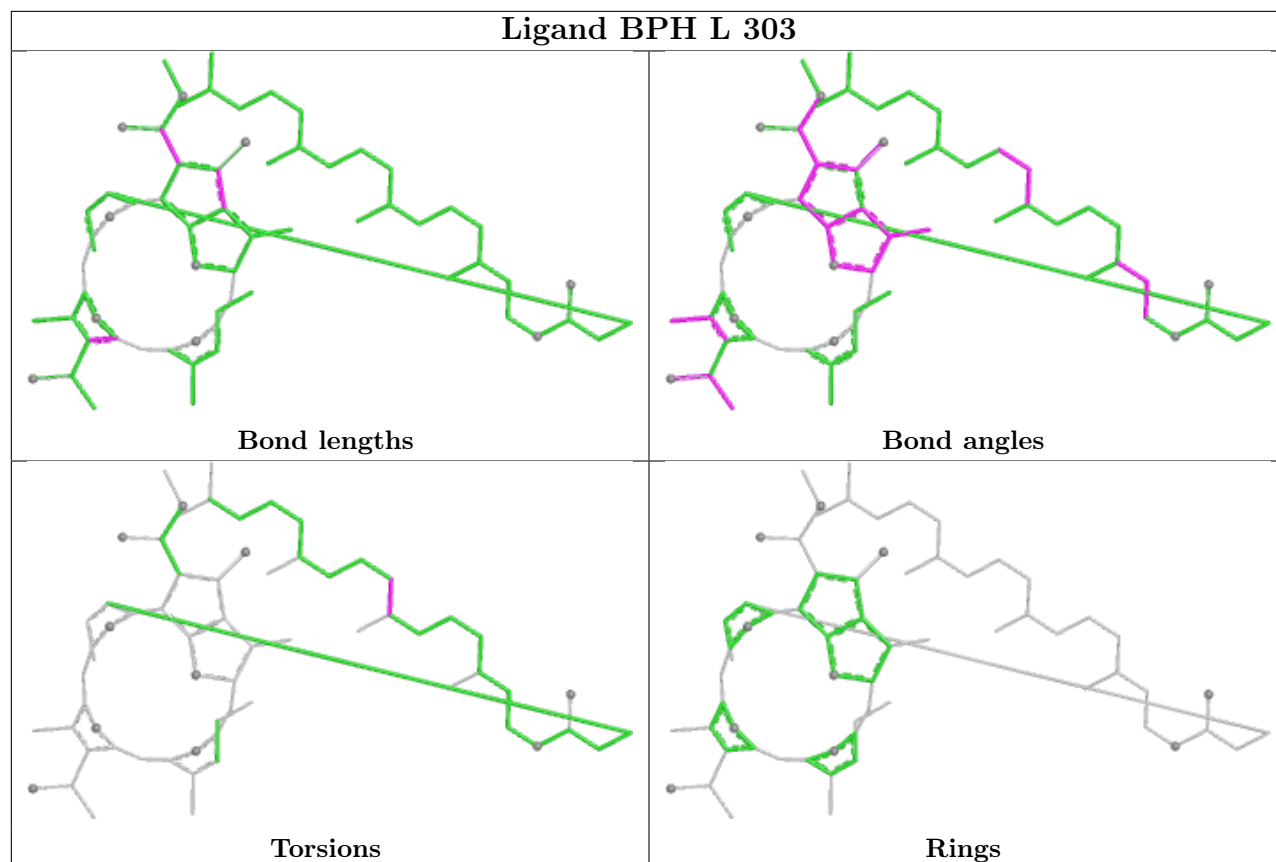
Ligand SPO x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



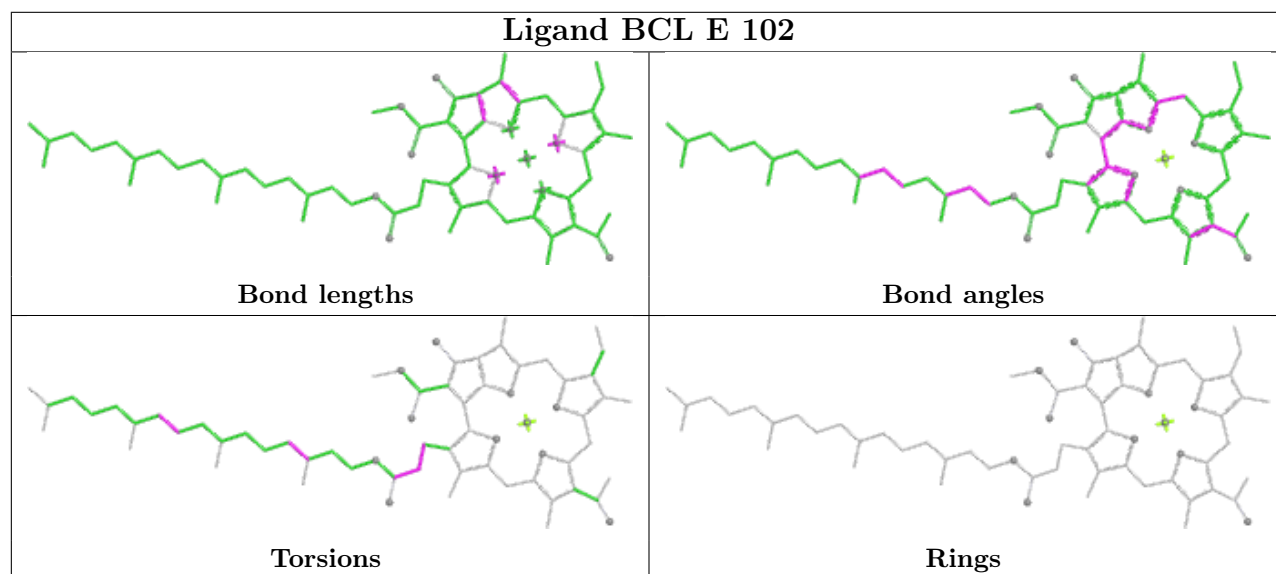


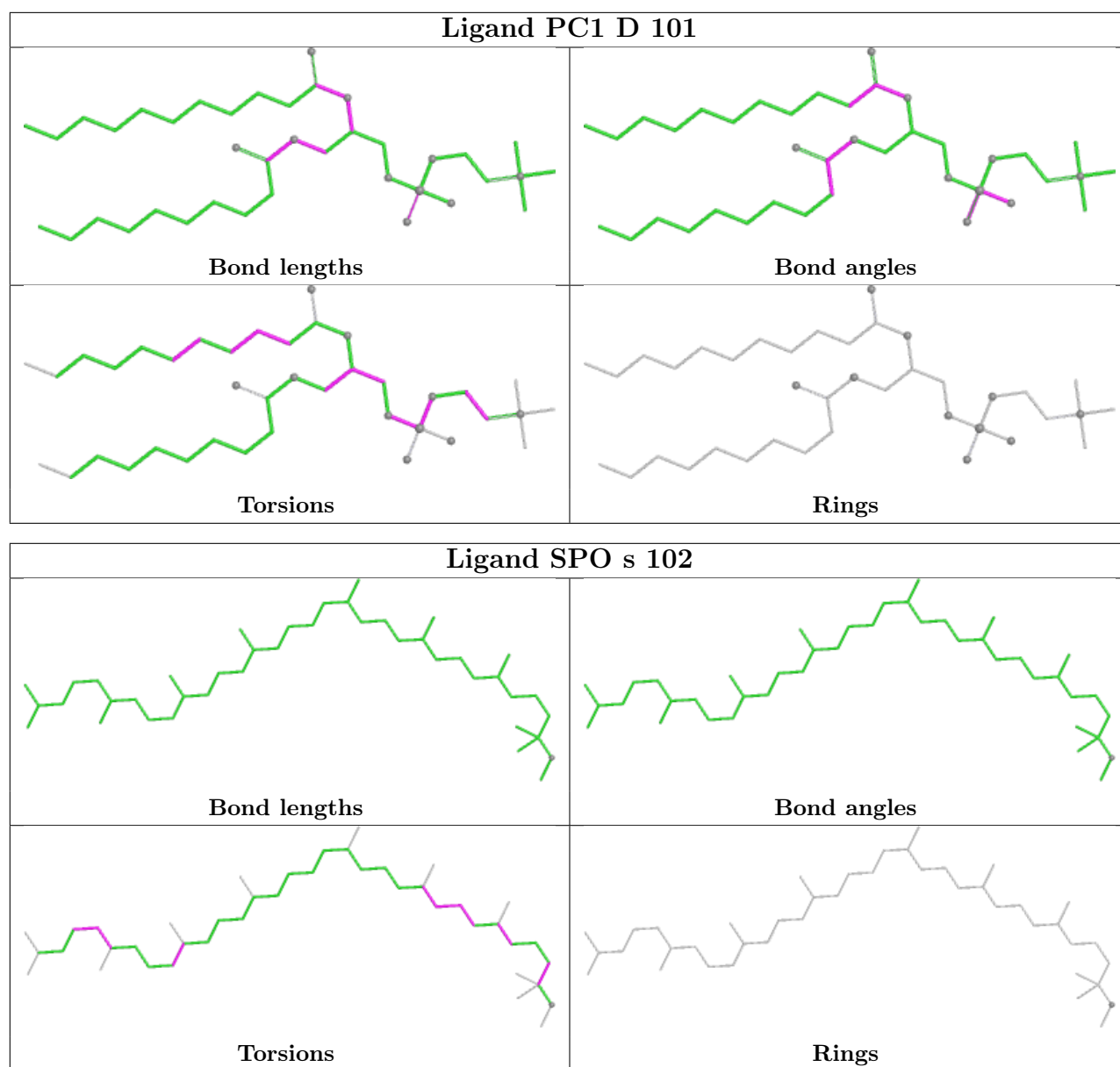


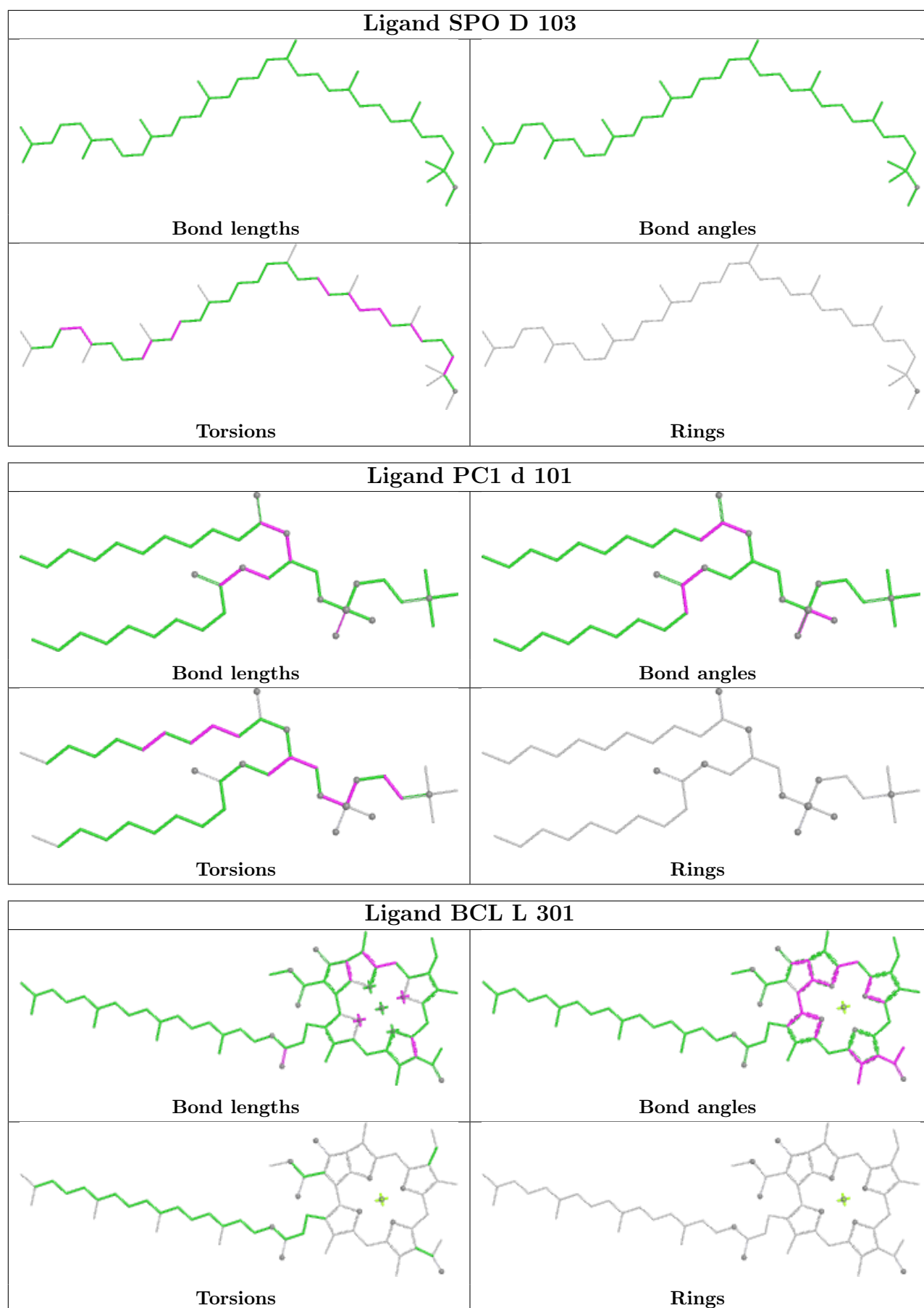
Ligand BPH L 303

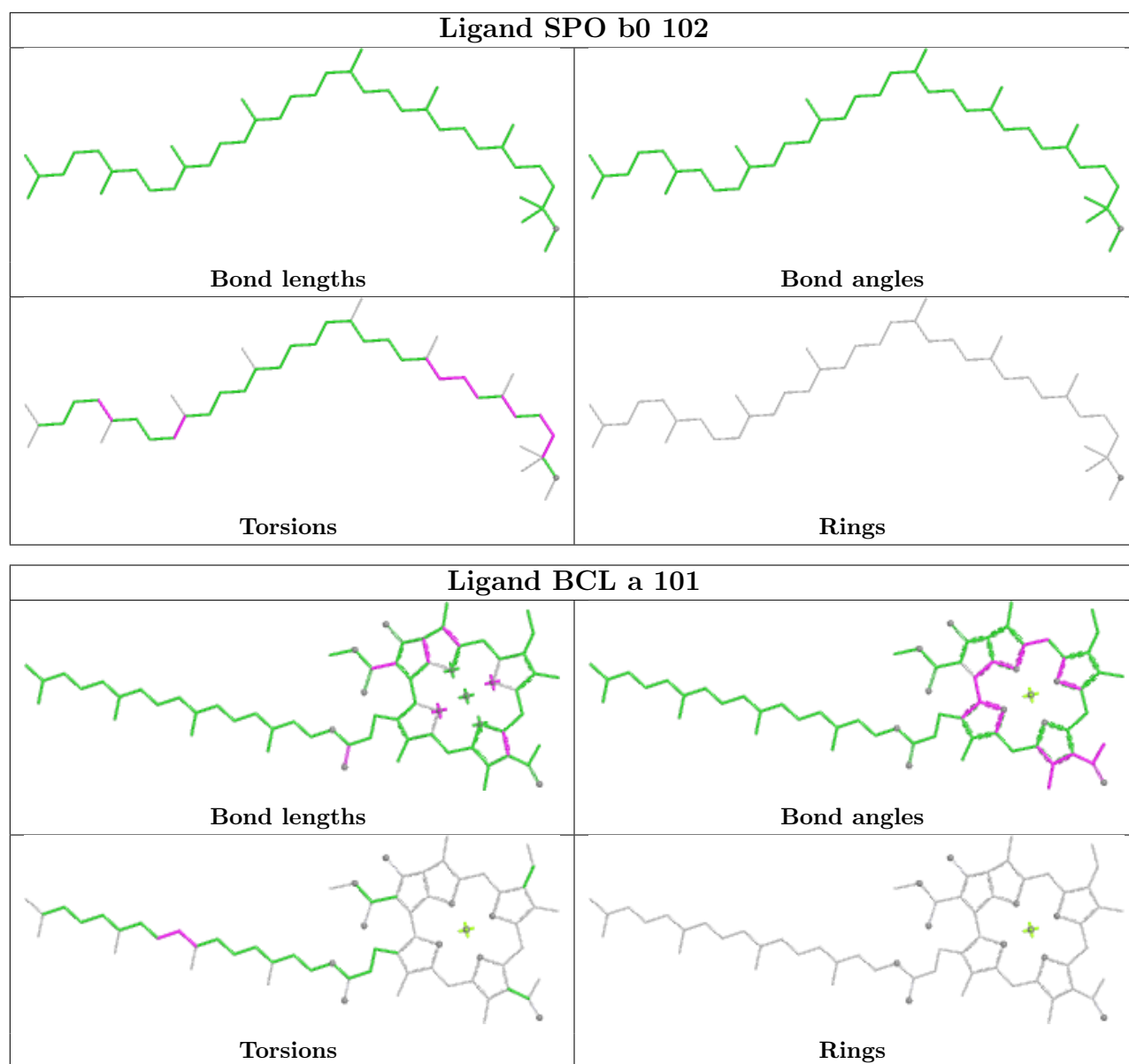


Ligand BCL E 102









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.

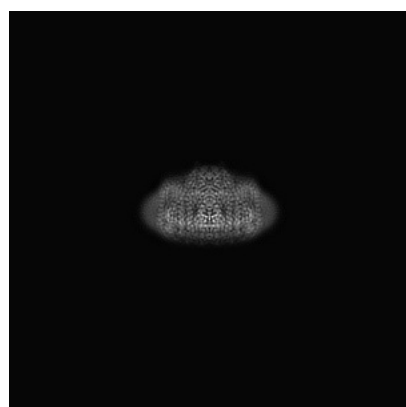
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32058. These allow visual inspection of the internal detail of the map and identification of artifacts.

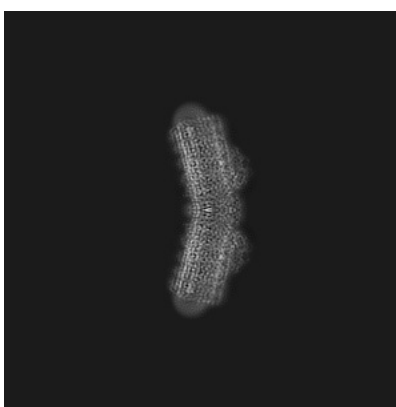
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

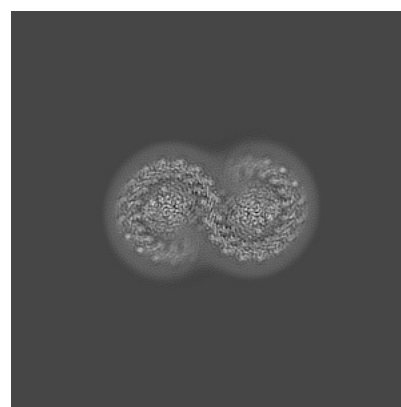
6.1.1 Primary map



X



Y

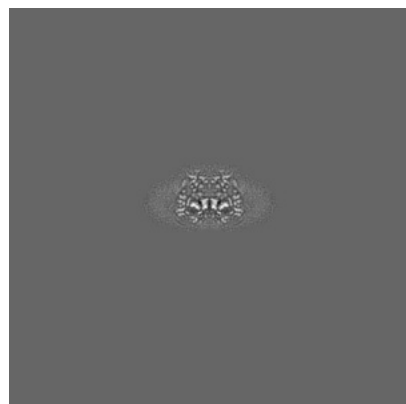


Z

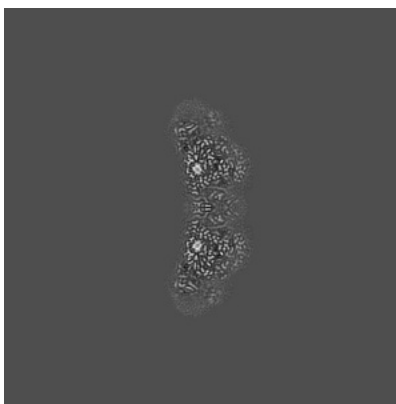
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

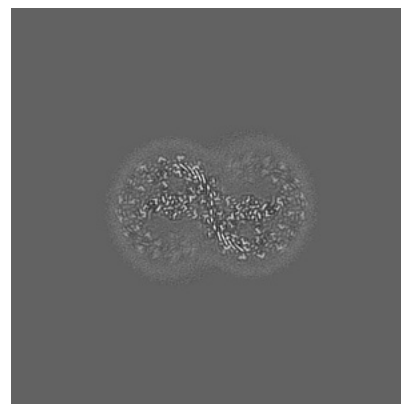
6.2.1 Primary map



X Index: 208



Y Index: 208

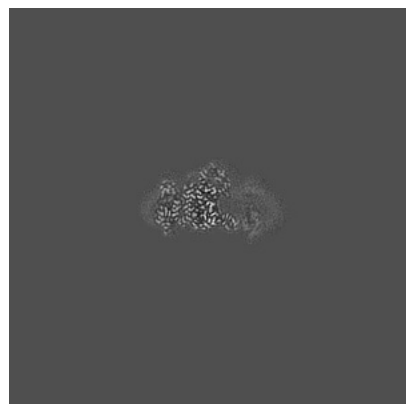


Z Index: 208

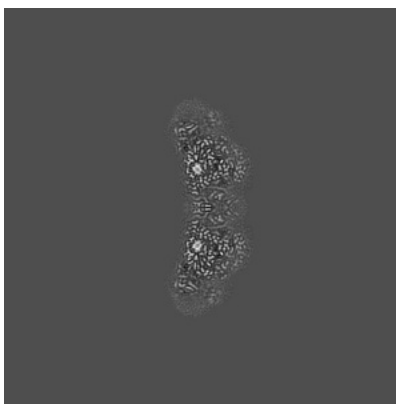
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

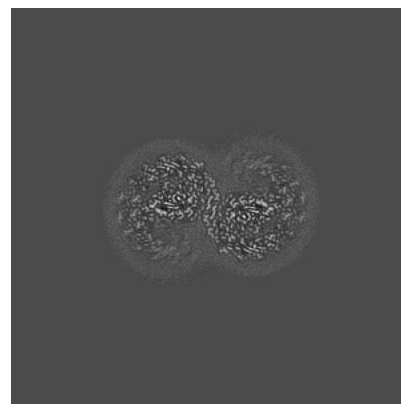
6.3.1 Primary map



X Index: 257



Y Index: 208

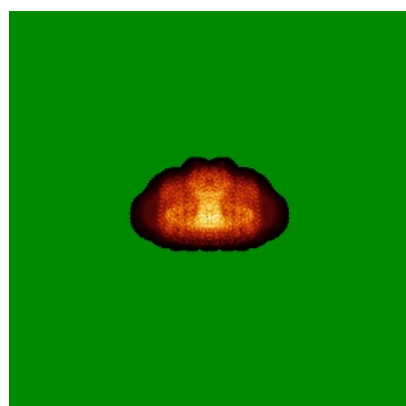


Z Index: 202

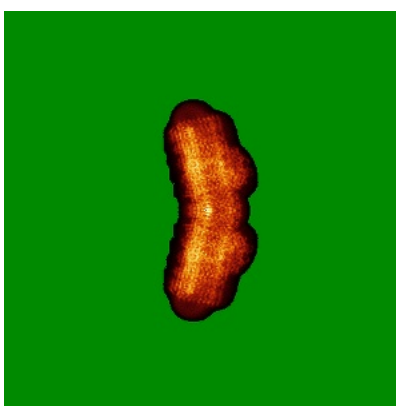
The images above show the largest variance slices of the map in three orthogonal directions.

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

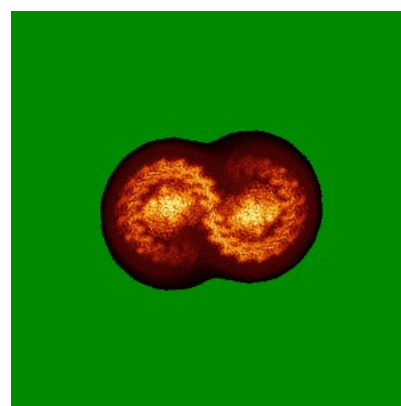
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

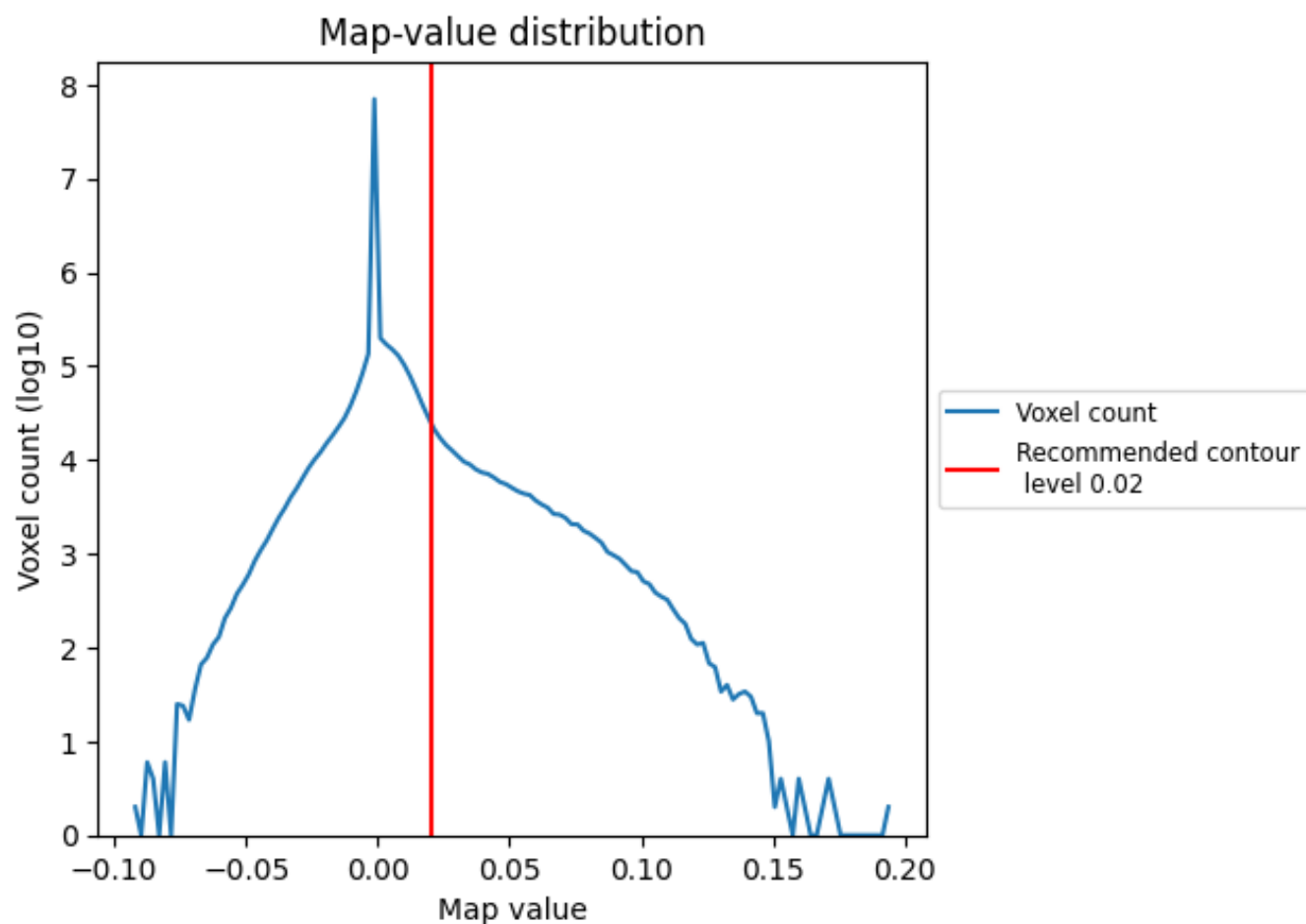
6.6 Mask visualisation

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

7 Map analysis [i](#)

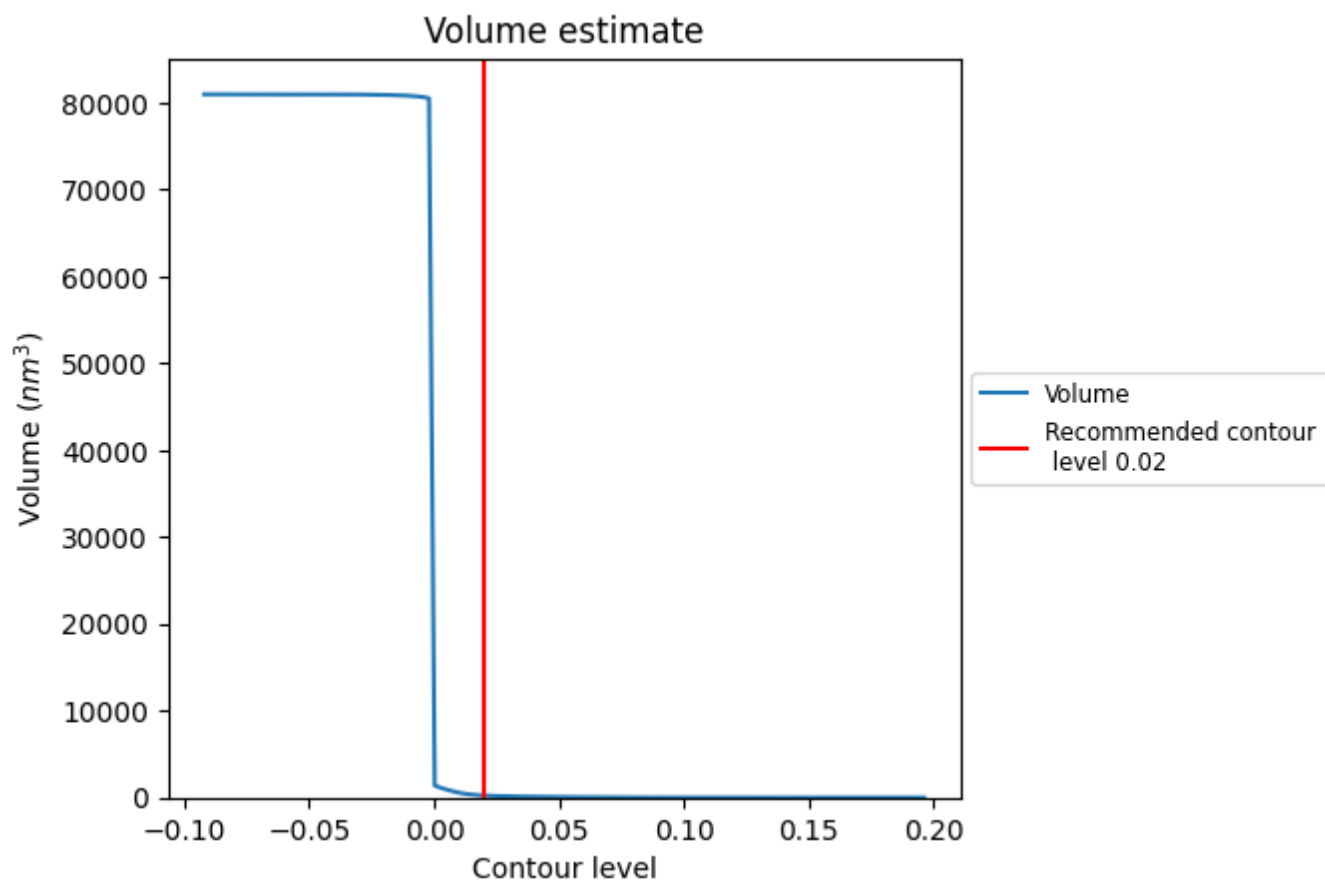
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

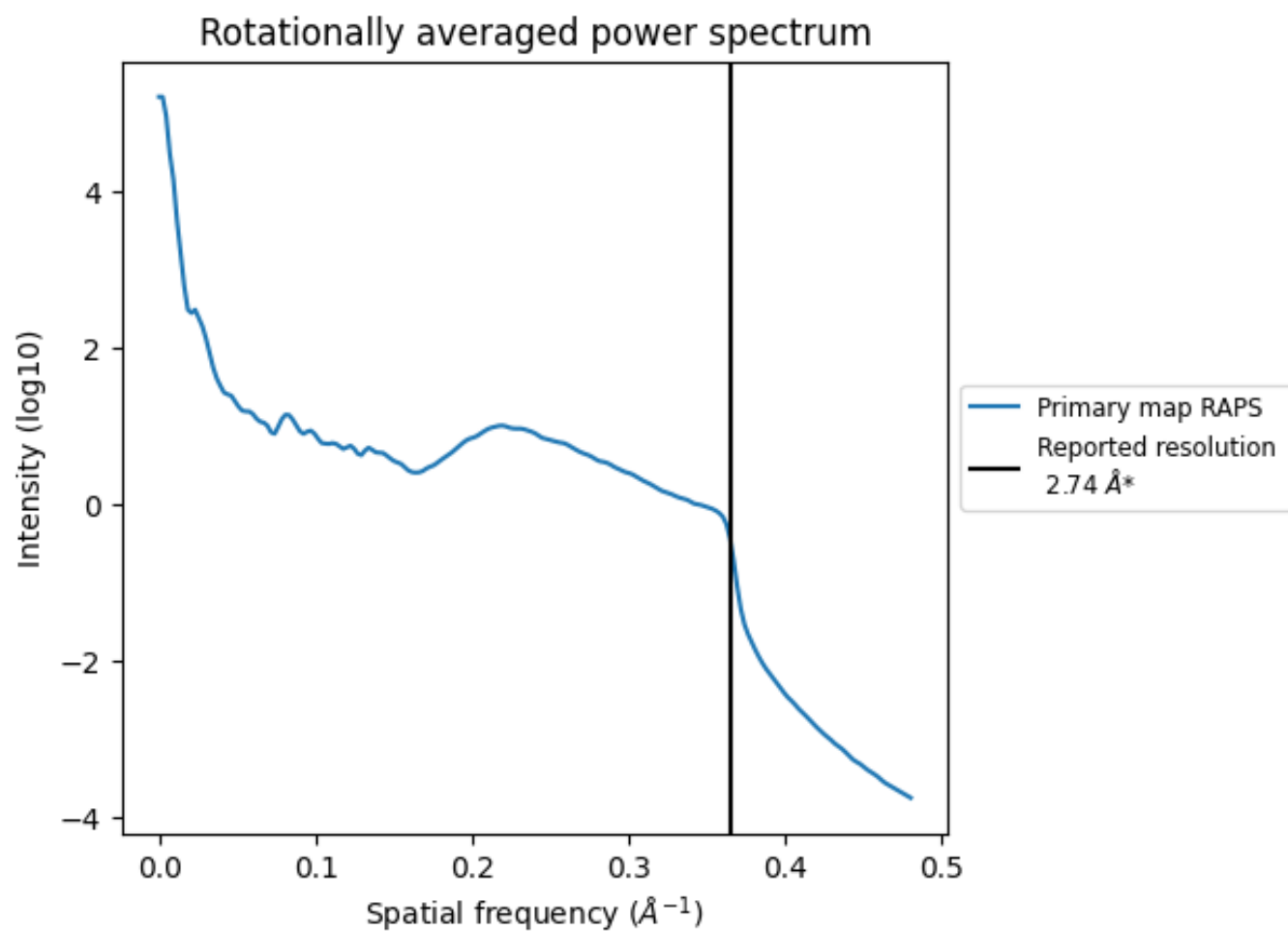
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm^3 ; this corresponds to an approximate mass of 211 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 0.365 Å⁻¹

8 Fourier-Shell correlation

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

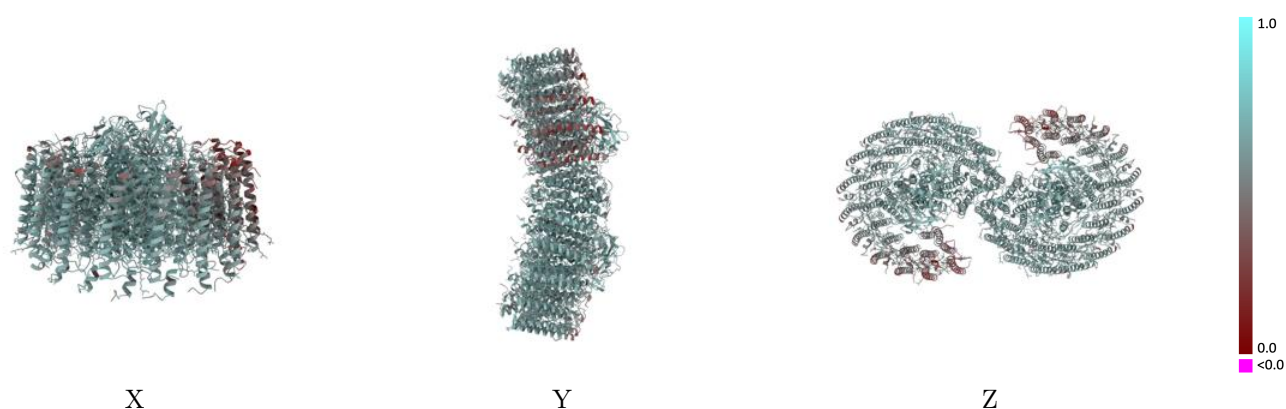
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32058 and PDB model 7VOR. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

This section was not generated.

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

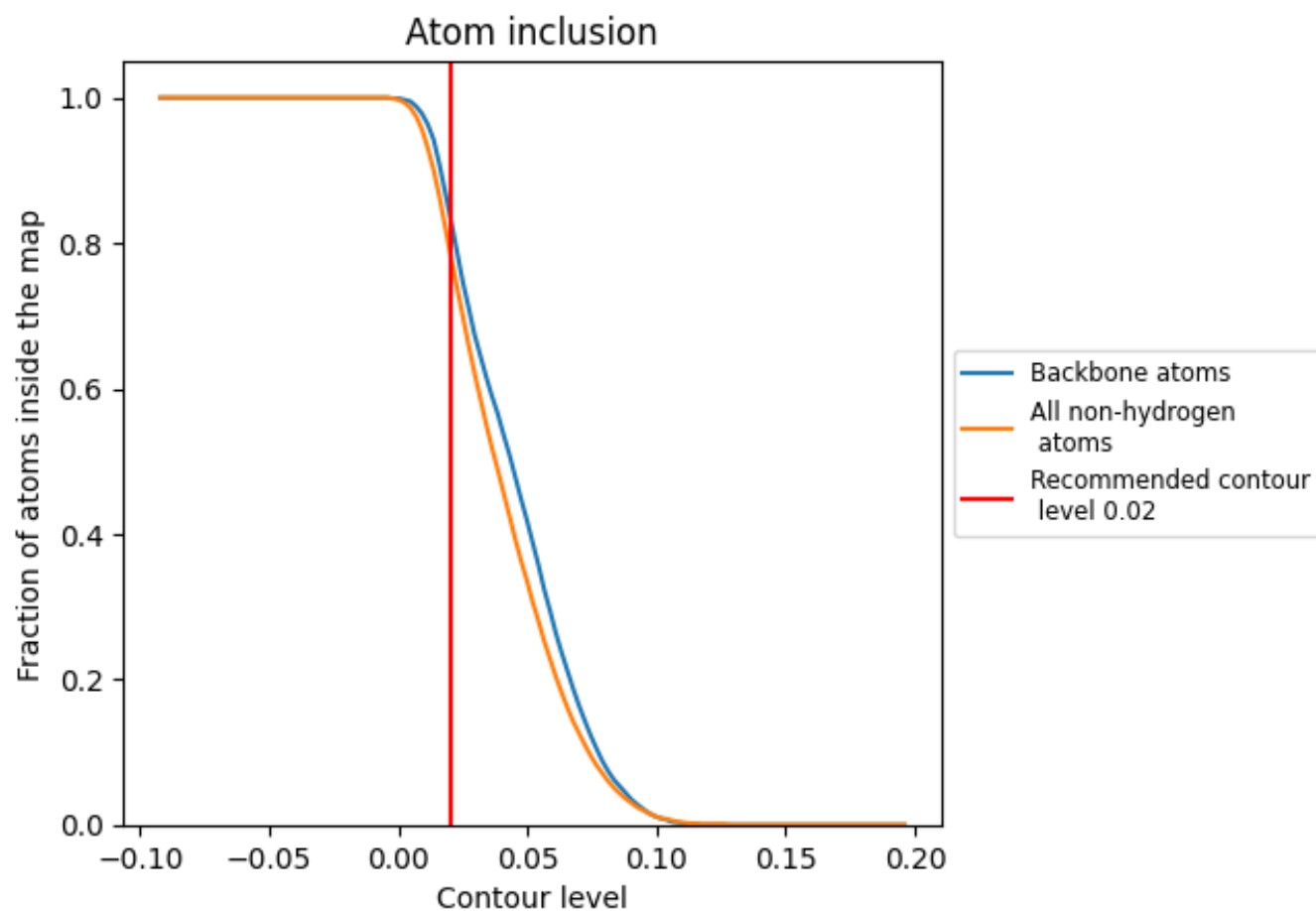


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7890	 0.5730
0	 0.8740	 0.6040
1	 0.2550	 0.3540
2	 0.1720	 0.3220
3	 0.3640	 0.4140
4	 0.1720	 0.3260
5	 0.3660	 0.4140
6	 0.9060	 0.6190
7	 0.9060	 0.6190
8	 0.8950	 0.6040
9	 0.9290	 0.6210
A	 0.8980	 0.6140
B	 0.8680	 0.6040
C	 0.4600	 0.4220
D	 0.8870	 0.6130
E	 0.8650	 0.5910
F	 0.8470	 0.5930
G	 0.8050	 0.5790
H	 0.8450	 0.5980
I	 0.8630	 0.5960
J	 0.8080	 0.5760
K	 0.8250	 0.5830
L	 0.9390	 0.6410
M	 0.9360	 0.6360
N	 0.7930	 0.5680
O	 0.8140	 0.5780
P	 0.7860	 0.5730
Q	 0.8130	 0.5830
R	 0.7860	 0.5580
S	 0.7800	 0.5730
T	 0.7690	 0.5450
U	 0.7100	 0.5370
V	 0.6580	 0.4820
W	 0.5610	 0.4640
X	 0.8080	 0.5830



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Chain	Atom inclusion	Q-score
Y	 0.2150	 0.4160
Z	 0.2860	 0.3440
a	 0.8980	 0.6160
b	 0.8660	 0.6110
b0	 0.8710	 0.6100
b1	 0.2570	 0.3580
b8	 0.8950	 0.6080
b9	 0.9260	 0.6240
c	 0.4580	 0.4240
d	 0.8830	 0.6170
e	 0.8610	 0.5960
f	 0.8480	 0.5950
g	 0.8070	 0.5860
h	 0.8420	 0.5980
i	 0.8650	 0.6010
j	 0.8080	 0.5790
k	 0.8250	 0.5850
l	 0.9380	 0.6400
m	 0.9350	 0.6370
n	 0.7950	 0.5730
o	 0.8140	 0.5800
p	 0.7860	 0.5750
q	 0.8160	 0.5850
r	 0.7830	 0.5610
s	 0.7810	 0.5760
t	 0.7710	 0.5460
u	 0.7080	 0.5420
v	 0.6610	 0.4840
w	 0.5590	 0.4640
x	 0.8080	 0.5800
y	 0.2150	 0.4180
z	 0.2830	 0.3490