



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:43 AM JST

PDB ID : 7VOT / pdb_00007vot
EMDB ID : EMD-32059
Title : The structure of dimeric photosynthetic RC-LH1 supercomplex in Class-2
Authors : Cao, P.; Li, M.; Liu, L.N.
Deposited on : 2021-10-14
Resolution : 2.90 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

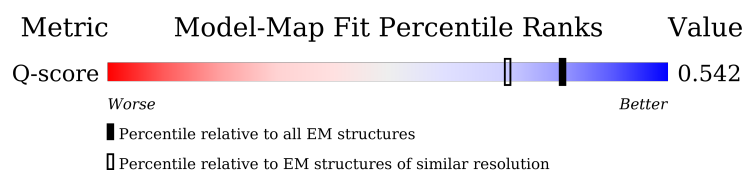
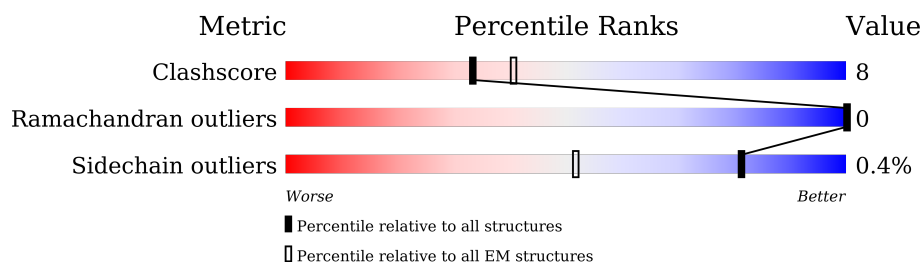
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	L	282	
1	l	282	
2	M	308	
2	m	308	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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 44984 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	258	Total	C	N	O	S	0	0
			1955	1252	333	359	11		
3	h	258	Total	C	N	O	S	0	0
			1955	1252	333	359	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		

Continued on next page...

Continued from previous page...

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	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	3	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	1	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	7	48	Total	C	N	O	S	0	0
			403	277	62	61	3		
4	9	54	Total	C	N	O	S	0	0
			455	310	73	69	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	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	5	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b1	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	6	48	Total	C	N	O	S	0	0
			403	277	62	61	3		
4	b9	54	Total	C	N	O	S	0	0
			455	310	73	69	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	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	J	42	Total	C	N	O	S	0	0
			344	230	54	59	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	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	Z	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	2	40	Total	C	N	O	S	0	0
			328	219	52	56	1		
5	8	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	0	43	Total	C	N	O	S	0	0
			352	236	55	60	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	j	42	Total	C	N	O	S	0	0
			344	230	54	59	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	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	z	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	4	40	Total	C	N	O	S	0	0
			328	219	52	56	1		
5	b8	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	b0	43	Total	C	N	O	S	0	0
			352	236	55	60	1		

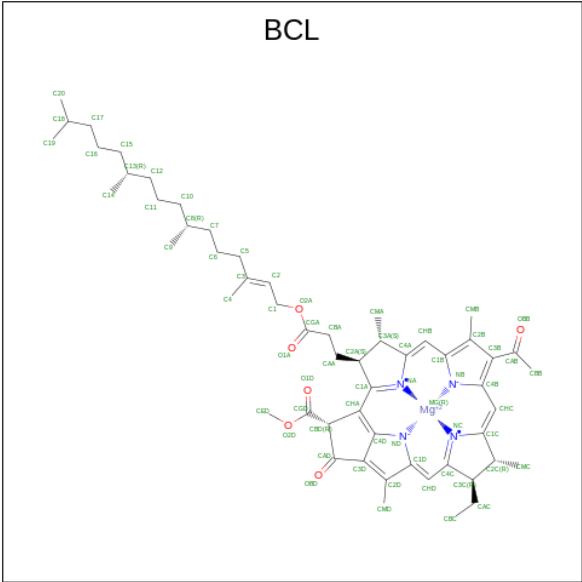
- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	52	Total	C	N	O	S	0	0
			404	268	70	63	3		
6	x	52	Total	C	N	O	S	0	0
			404	268	70	63	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	51	Total	C	N	O	S	0	0
			375	255	58	59	3		
7	y	51	Total	C	N	O	S	0	0
			375	255	58	59	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	L	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 61	C 50	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 61	C 50	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 61	C 50	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 66	C 55	Mg 1	N 4	O 6	0
8	Z	1	Total 57	C 46	Mg 1	N 4	O 6	0
8	1	1	Total 51	C 40	Mg 1	N 4	O 6	0
8	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
8	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	8	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	9	1	Total 56	C 45	Mg 1	N 4	O 6	0
8	0	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 63	C 52	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

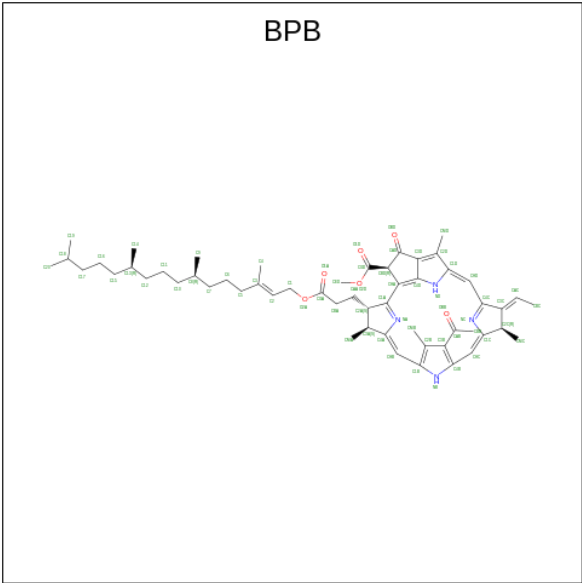
Mol	Chain	Residues	Atoms					AltConf
8	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 61	C 50	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 61	C 50	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 61	C 50	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	z	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
8	b1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
8	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	b8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	b9	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	b0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: C₅₅H₇₄N₄O₆).



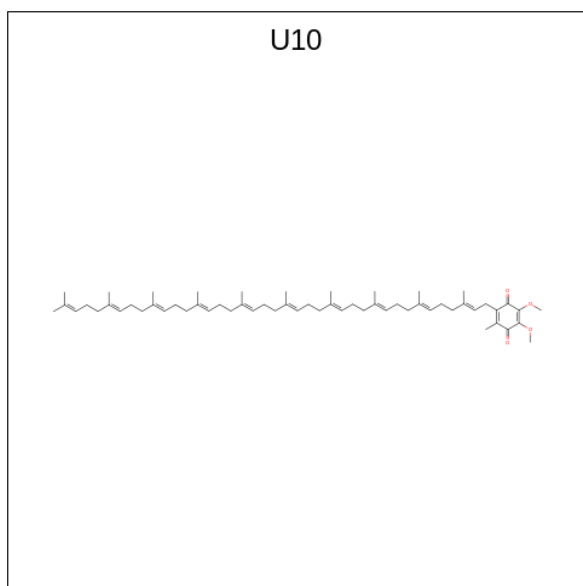
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			55	45	4	6	
9	l	1	Total	C	N	O	0
			65	55	4	6	

Continued on next page...

Continued from previous page...

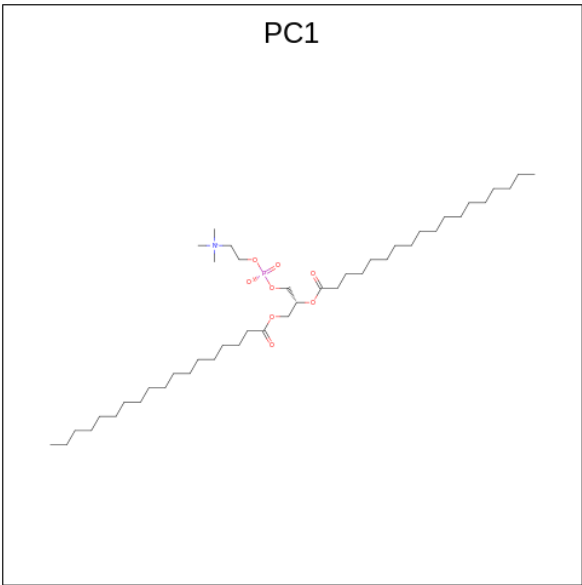
Mol	Chain	Residues	Atoms				AltConf
9	m	1	Total	C	N	O	0
			55	45	4	6	

- 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	M	1	Total	C	O		0
			38	34	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		
10	m	1	Total	C	O		0
			38	34	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
			32	22	1	8	1	
11	H	1	Total	C	N	O	P	0
			42	32	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
			36	26	1	8	1	
11	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
11	D	1	Total	C	N	O	P	0
			37	27	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
			32	22	1	8	1	
11	h	1	Total	C	N	O	P	0
			42	32	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	

Continued on next page...

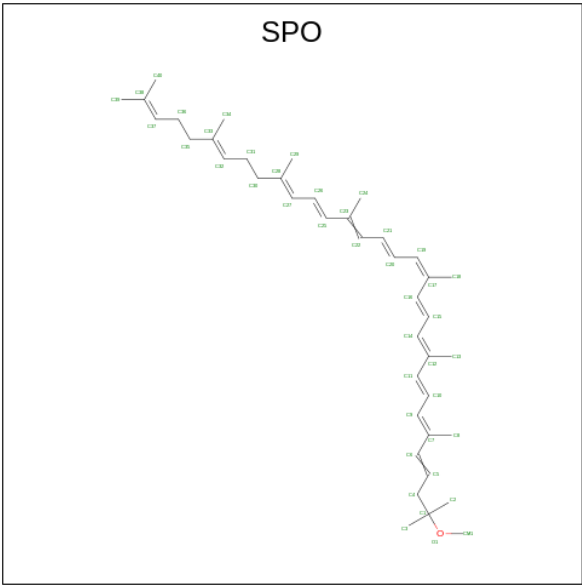
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
11	a	1	Total	C	N	O	P	0
			31	21	1	8	1	
11	a	1	Total	C	N	O	P	0
			36	26	1	8	1	
11	d	1	Total	C	N	O	P	0
			40	30	1	8	1	
11	d	1	Total	C	N	O	P	0
			37	27	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	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
13	D	1	Total 42	C 41	O 1	0
13	E	1	Total 42	C 41	O 1	0
13	F	1	Total 42	C 41	O 1	0
13	F	1	Total 42	C 41	O 1	0
13	I	1	Total 42	C 41	O 1	0
13	I	1	Total 42	C 41	O 1	0
13	J	1	Total 42	C 41	O 1	0
13	N	1	Total 42	C 41	O 1	0
13	N	1	Total 42	C 41	O 1	0
13	O	1	Total 42	C 41	O 1	0
13	R	1	Total 42	C 41	O 1	0
13	R	1	Total 42	C 41	O 1	0
13	R	1	Total 42	C 41	O 1	0
13	S	1	Total 42	C 41	O 1	0
13	U	1	Total 42	C 41	O 1	0
13	V	1	Total 42	C 41	O 1	0
13	V	1	Total 42	C 41	O 1	0
13	C	1	Total 42	C 41	O 1	0
13	3	1	Total 42	C 41	O 1	0
13	3	1	Total 42	C 41	O 1	0
13	7	1	Total 42	C 41	O 1	0

Continued on next page...

Continued from previous page...

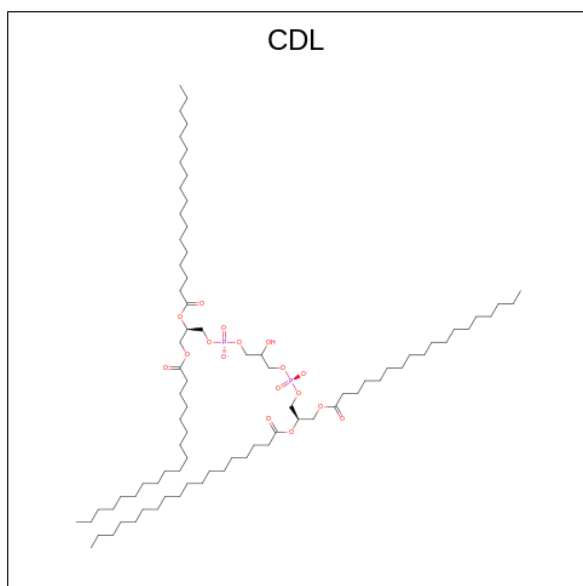
Mol	Chain	Residues	Atoms			AltConf
13	9	1	Total 42	C 41	O 1	0
13	0	1	Total 42	C 41	O 1	0
13	m	1	Total 42	C 41	O 1	0
13	a	1	Total 42	C 41	O 1	0
13	b	1	Total 42	C 41	O 1	0
13	d	1	Total 42	C 41	O 1	0
13	e	1	Total 42	C 41	O 1	0
13	f	1	Total 42	C 41	O 1	0
13	f	1	Total 42	C 41	O 1	0
13	i	1	Total 42	C 41	O 1	0
13	i	1	Total 42	C 41	O 1	0
13	j	1	Total 42	C 41	O 1	0
13	n	1	Total 42	C 41	O 1	0
13	n	1	Total 42	C 41	O 1	0
13	o	1	Total 42	C 41	O 1	0
13	r	1	Total 42	C 41	O 1	0
13	r	1	Total 42	C 41	O 1	0
13	r	1	Total 42	C 41	O 1	0
13	s	1	Total 42	C 41	O 1	0
13	u	1	Total 42	C 41	O 1	0
13	v	1	Total 42	C 41	O 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
13	v	1	Total	C	O	0
			42	41	1	
13	c	1	Total	C	O	0
			42	41	1	
13	5	1	Total	C	O	0
			42	41	1	
13	5	1	Total	C	O	0
			42	41	1	
13	6	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	

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

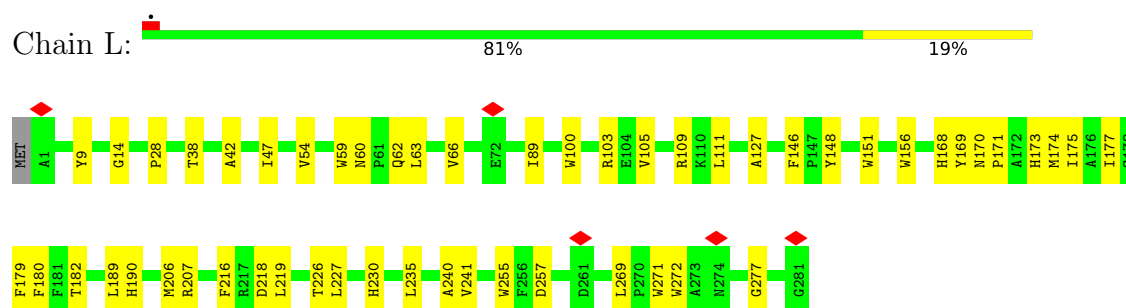


Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	O	P	0
			76	57	17	2	
14	H	1	Total	C	O	P	0
			63	44	17	2	
14	m	1	Total	C	O	P	0
			76	57	17	2	
14	h	1	Total	C	O	P	0
			63	44	17	2	

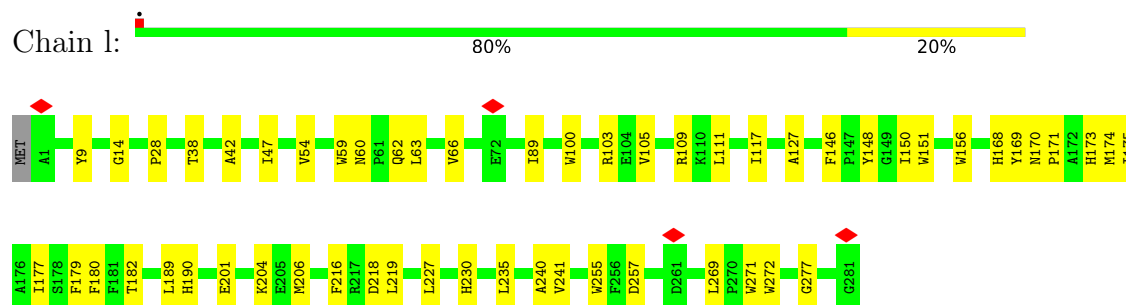
3 Residue-property plots

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.

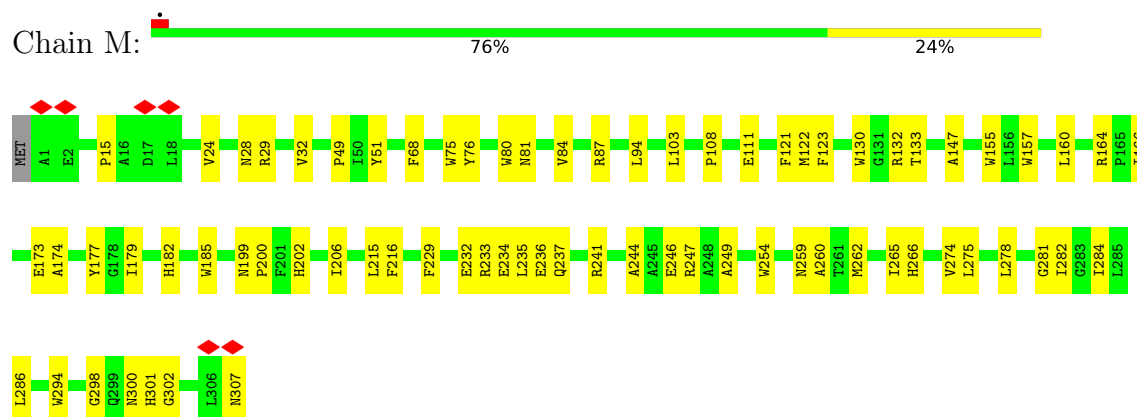
- Molecule 1: Reaction center protein L chain



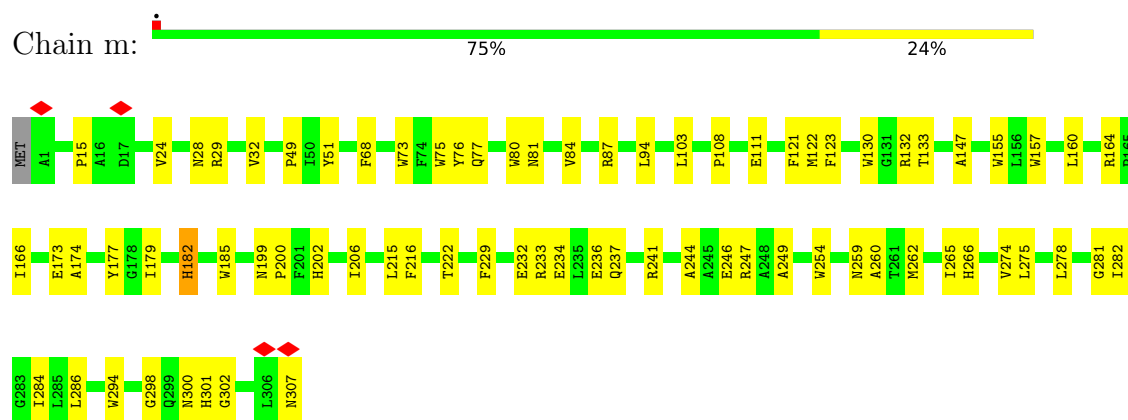
- Molecule 1: Reaction center protein L chain



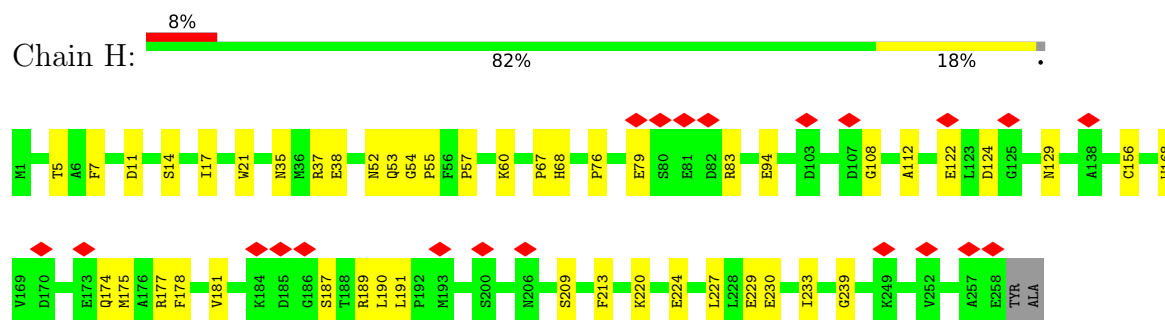
- Molecule 2: Reaction center protein M chain



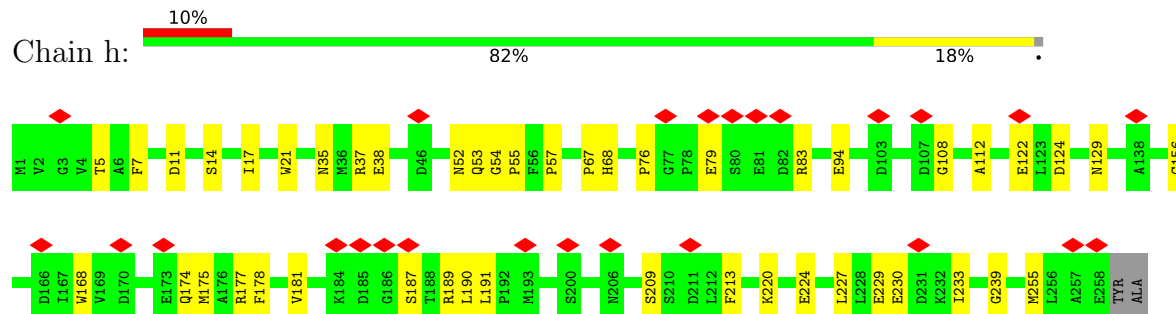
- Molecule 2: Reaction center protein M chain



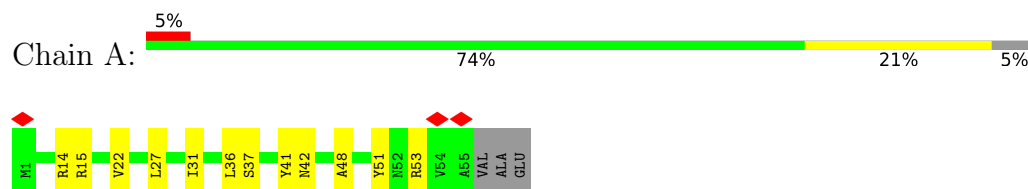
- Molecule 3: Reaction center protein H chain



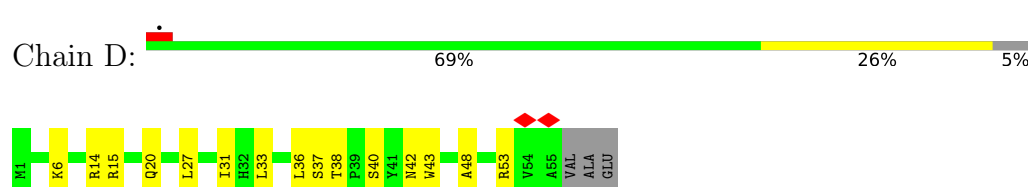
- Molecule 3: Reaction center protein H chain



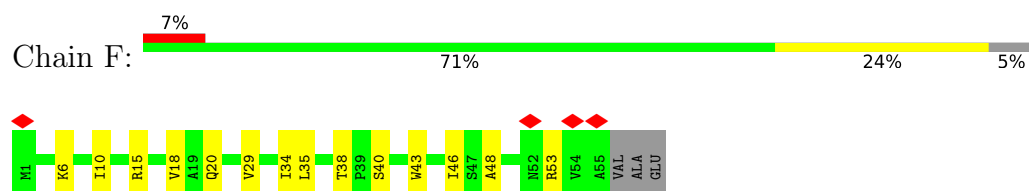
- Molecule 4: Light-harvesting protein B-875 alpha chain



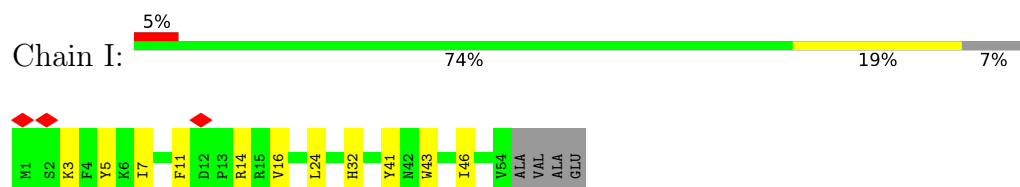
- Molecule 4: Light-harvesting protein B-875 alpha chain



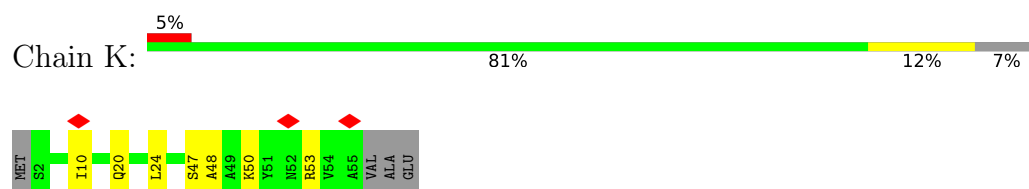
- Molecule 4: Light-harvesting protein B-875 alpha chain



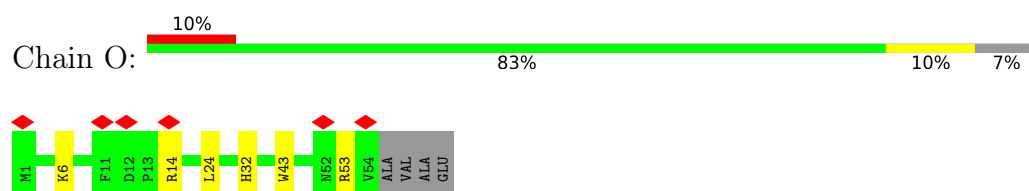
- Molecule 4: Light-harvesting protein B-875 alpha chain



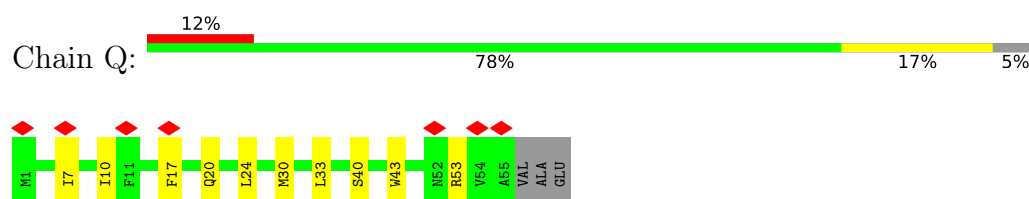
- Molecule 4: Light-harvesting protein B-875 alpha chain



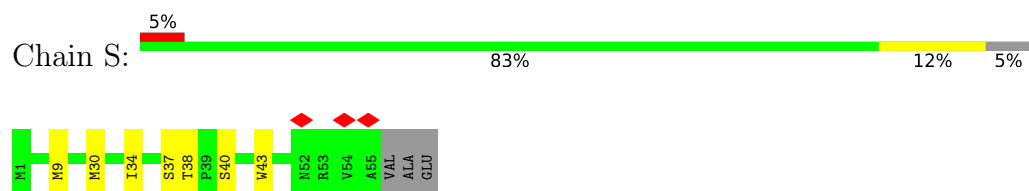
- Molecule 4: Light-harvesting protein B-875 alpha chain



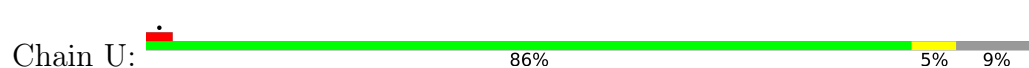
- Molecule 4: Light-harvesting protein B-875 alpha chain

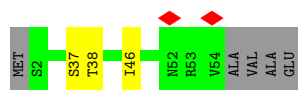


- Molecule 4: Light-harvesting protein B-875 alpha chain

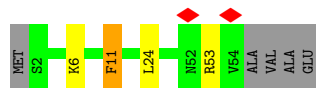
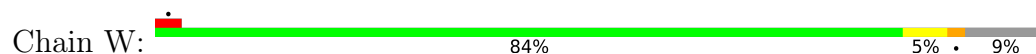


- Molecule 4: Light-harvesting protein B-875 alpha chain

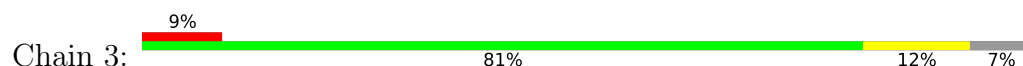




- Molecule 4: Light-harvesting protein B-875 alpha chain



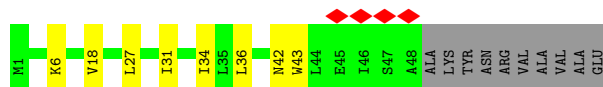
- Molecule 4: Light-harvesting protein B-875 alpha chain



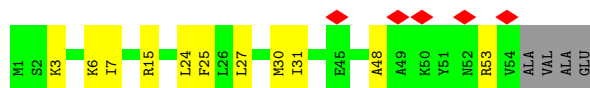
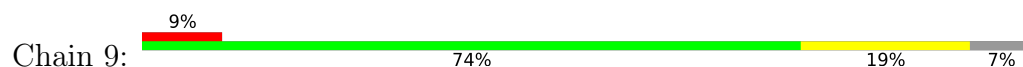
- Molecule 4: Light-harvesting protein B-875 alpha chain



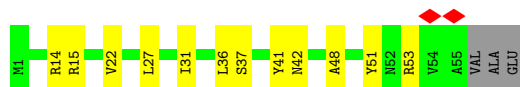
- Molecule 4: Light-harvesting protein B-875 alpha chain



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



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



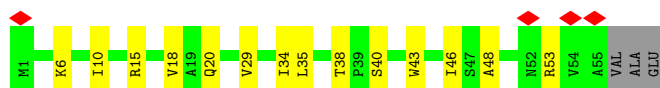
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain d:  74% 21% 5%



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

Chain f:  71% 24% 5%



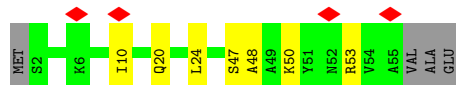
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain i:  74% 19% 7%



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

Chain k:  81% 12% 7%



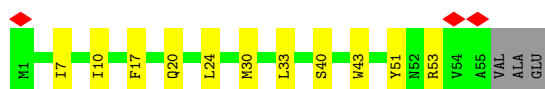
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain o:  79% 14% 7%



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

Chain q:  76% 19% 5%



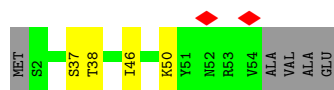
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain s:  83% 12% 5%



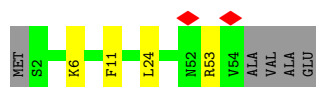
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain u:  84% 7% 9%



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

Chain w:  84% 7% 9%



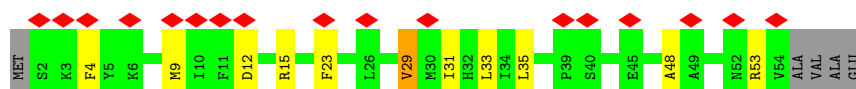
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 5:  9% 81% 12% 7%



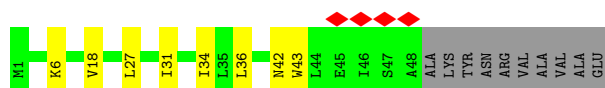
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain b1:  29% 72% 17% 9%



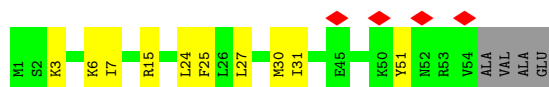
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 6:  7% 69% 14% 17%



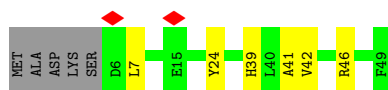
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain b9:  7% 76% 17% 7%

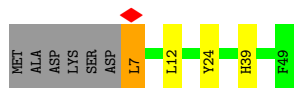
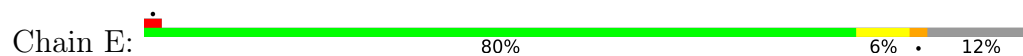


- Molecule 5: Light-harvesting protein B-875 beta chain

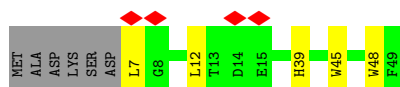
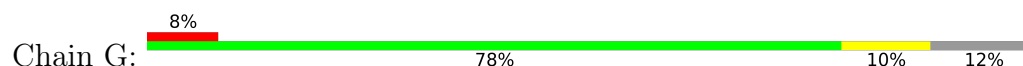
Chain B:  78% 12% 10%



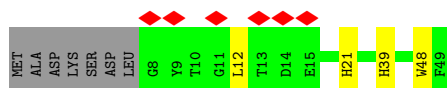
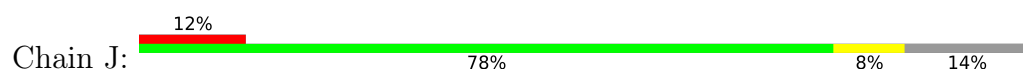
- Molecule 5: Light-harvesting protein B-875 beta chain



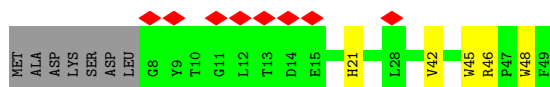
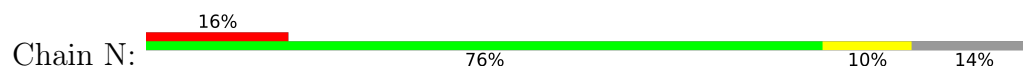
- Molecule 5: Light-harvesting protein B-875 beta chain



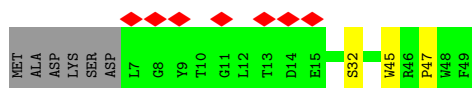
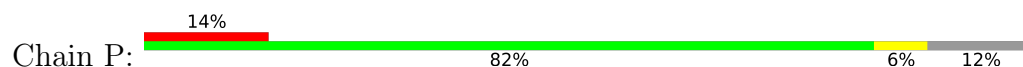
- Molecule 5: Light-harvesting protein B-875 beta chain



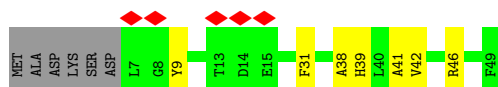
- Molecule 5: Light-harvesting protein B-875 beta chain



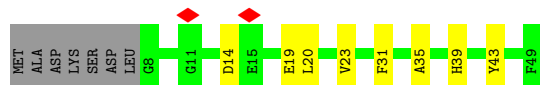
- Molecule 5: Light-harvesting protein B-875 beta chain



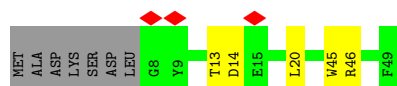
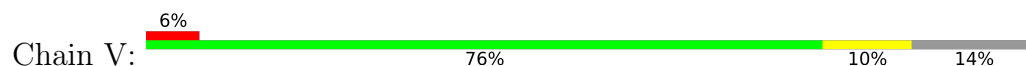
- Molecule 5: Light-harvesting protein B-875 beta chain



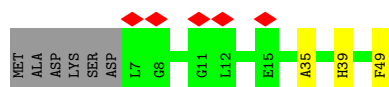
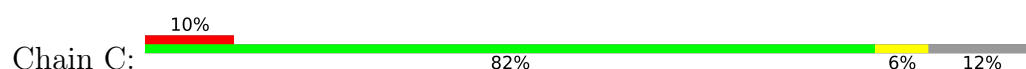
- Molecule 5: Light-harvesting protein B-875 beta chain



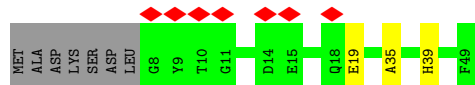
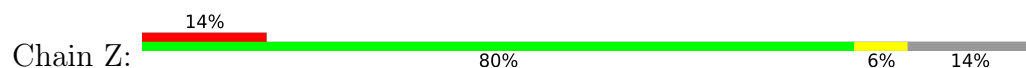
- Molecule 5: Light-harvesting protein B-875 beta chain



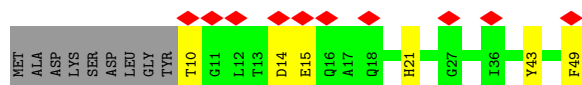
- Molecule 5: Light-harvesting protein B-875 beta chain



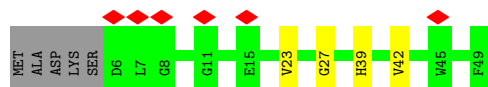
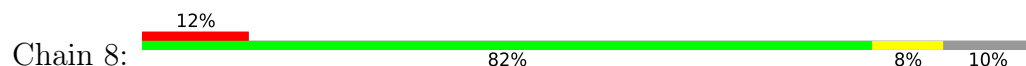
- Molecule 5: Light-harvesting protein B-875 beta chain



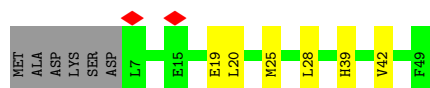
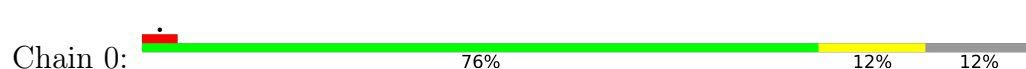
- Molecule 5: Light-harvesting protein B-875 beta chain



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



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



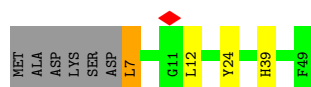
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain b: 



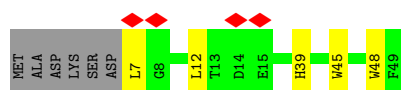
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain e: 



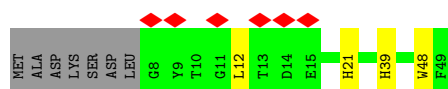
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain g: 



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

Chain j: 



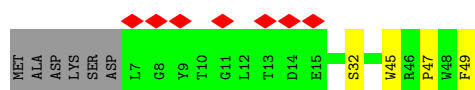
- Molecule 5: Light-harvesting protein B-875 beta chain

Chain n: 



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

Chain p: 

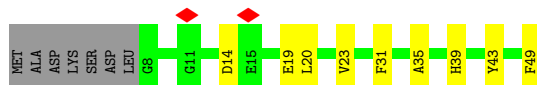


- Molecule 5: Light-harvesting protein B-875 beta chain

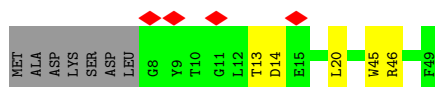
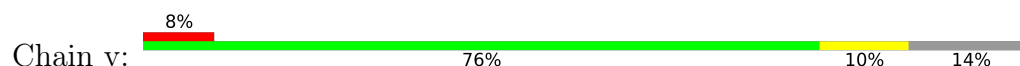
Chain r: 



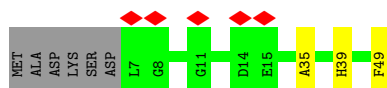
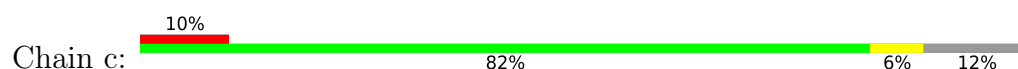
- Molecule 5: Light-harvesting protein B-875 beta chain



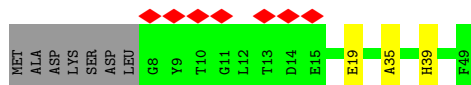
- Molecule 5: Light-harvesting protein B-875 beta chain



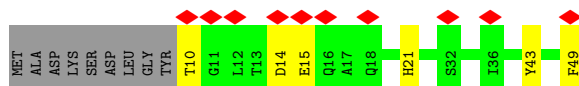
- Molecule 5: Light-harvesting protein B-875 beta chain



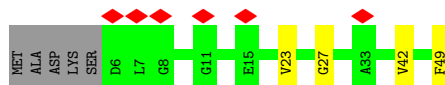
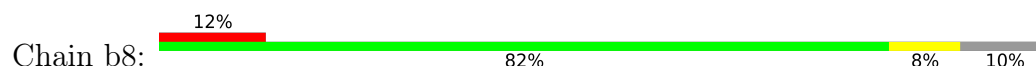
- Molecule 5: Light-harvesting protein B-875 beta chain



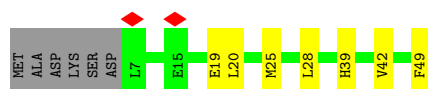
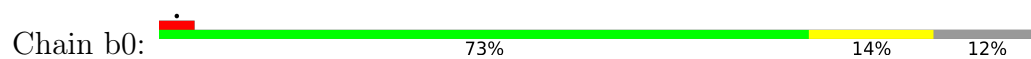
- Molecule 5: Light-harvesting protein B-875 beta chain



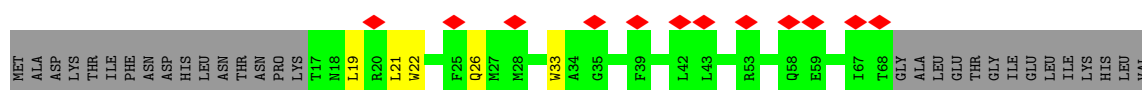
- Molecule 5: Light-harvesting protein B-875 beta chain



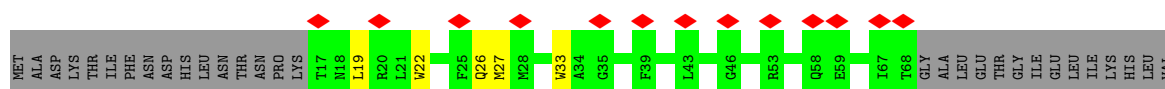
- Molecule 5: Light-harvesting protein B-875 beta chain



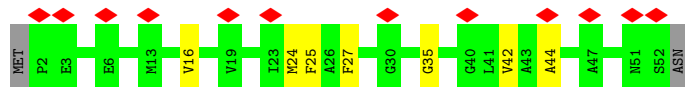
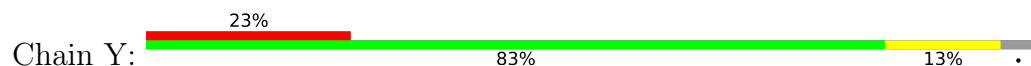
- Molecule 6: Intrinsic membrane protein PufX



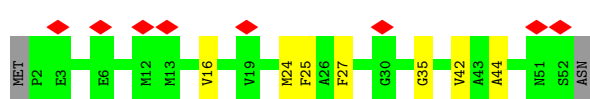
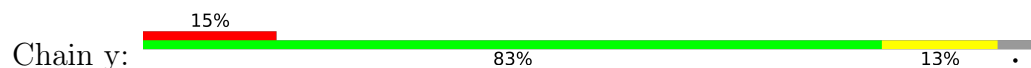
- Molecule 6: Intrinsic membrane protein PufX



- 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, Not provided	
Number of particles used	147085	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)	1800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	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: FE2, BCL, BPB, PC1, CDL, U10, SPO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.20	0/2320	0.26	0/3175
1	l	0.21	0/2320	0.26	0/3175
2	M	0.23	0/2538	0.28	0/3464
2	m	0.23	0/2538	0.28	0/3464
3	H	0.15	0/2005	0.25	0/2727
3	h	0.15	0/2005	0.25	0/2727
4	1	0.10	0/461	0.21	0/625
4	3	0.13	0/469	0.21	0/635
4	5	0.13	0/469	0.21	0/635
4	6	0.14	0/416	0.24	0/564
4	7	0.14	0/416	0.24	0/564
4	9	0.17	0/469	0.26	0/635
4	A	0.18	0/474	0.25	0/642
4	D	0.19	0/474	0.25	0/642
4	F	0.17	0/474	0.24	0/642
4	I	0.14	0/469	0.23	0/635
4	K	0.14	0/466	0.23	0/632
4	O	0.14	0/469	0.24	0/635
4	Q	0.16	0/474	0.31	0/642
4	S	0.18	0/474	0.24	0/642
4	U	0.17	0/461	0.29	0/625
4	W	0.16	0/461	0.25	0/625
4	a	0.19	0/474	0.25	0/642
4	b1	0.11	0/461	0.21	0/625
4	b9	0.17	0/469	0.26	0/635
4	d	0.19	0/474	0.25	0/642
4	f	0.17	0/474	0.24	0/642
4	i	0.14	0/469	0.23	0/635
4	k	0.14	0/466	0.23	0/632
4	o	0.15	0/469	0.25	0/635
4	q	0.17	0/474	0.31	0/642
4	s	0.18	0/474	0.24	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	u	0.17	0/461	0.29	0/625
4	w	0.16	0/461	0.25	0/625
5	0	0.14	0/365	0.20	0/499
5	2	0.10	0/340	0.21	0/465
5	4	0.10	0/340	0.21	0/465
5	8	0.11	0/373	0.16	0/510
5	B	0.15	0/373	0.20	0/510
5	C	0.12	0/365	0.19	0/499
5	E	0.16	0/365	0.23	0/499
5	G	0.14	0/365	0.20	0/499
5	J	0.12	0/357	0.19	0/488
5	N	0.11	0/357	0.18	0/488
5	P	0.11	0/365	0.19	0/499
5	R	0.13	0/365	0.22	0/499
5	T	0.14	0/357	0.20	0/488
5	V	0.15	0/357	0.19	0/488
5	Z	0.10	0/357	0.19	0/488
5	b	0.16	0/373	0.20	0/510
5	b0	0.14	0/365	0.20	0/499
5	b8	0.12	0/373	0.17	0/510
5	c	0.12	0/365	0.19	0/499
5	e	0.16	0/365	0.23	0/499
5	g	0.14	0/365	0.20	0/499
5	j	0.12	0/357	0.19	0/488
5	n	0.11	0/357	0.18	0/488
5	p	0.11	0/365	0.19	0/499
5	r	0.13	0/365	0.22	0/499
5	t	0.14	0/357	0.20	0/488
5	v	0.15	0/357	0.19	0/488
5	z	0.11	0/357	0.19	0/488
6	X	0.13	0/415	0.21	0/562
6	x	0.13	0/415	0.21	0/562
7	Y	0.12	0/387	0.21	0/524
7	y	0.13	0/387	0.21	0/524
All	All	0.17	0/38474	0.24	0/52384

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	49	0
1	l	2232	0	2187	52	0
2	M	2445	0	2359	59	0
2	m	2445	0	2359	59	0
3	H	1955	0	1967	40	0
3	h	1955	0	1967	41	0
4	1	447	0	465	10	0
4	3	455	0	477	6	0
4	5	455	0	477	6	0
4	6	403	0	422	6	0
4	7	403	0	422	6	0
4	9	455	0	477	8	0
4	A	460	0	482	9	0
4	D	460	0	482	16	0
4	F	460	0	482	13	0
4	I	455	0	477	11	0
4	K	452	0	470	6	0
4	O	455	0	477	8	0
4	Q	460	0	482	12	0
4	S	460	0	482	6	0
4	U	447	0	465	3	0
4	W	447	0	465	4	0
4	a	460	0	482	11	0
4	b1	447	0	465	11	0
4	b9	455	0	477	8	0
4	d	460	0	482	14	0
4	f	460	0	482	13	0
4	i	455	0	477	11	0
4	k	452	0	470	6	0
4	o	455	0	477	9	0
4	q	460	0	482	13	0
4	s	460	0	482	6	0
4	u	447	0	465	4	0
4	w	447	0	465	3	0
5	0	352	0	336	6	0
5	2	328	0	313	4	0
5	4	328	0	313	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	8	360	0	340	4	0
5	B	360	0	340	7	0
5	C	352	0	336	2	0
5	E	352	0	336	4	0
5	G	352	0	336	6	0
5	J	344	0	325	5	0
5	N	344	0	325	5	0
5	P	352	0	336	3	0
5	R	352	0	336	7	0
5	T	344	0	325	7	0
5	V	344	0	325	4	0
5	Z	344	0	325	2	0
5	b	360	0	340	8	0
5	b0	352	0	336	7	0
5	b8	360	0	340	4	0
5	c	352	0	336	2	0
5	e	352	0	336	4	0
5	g	352	0	336	6	0
5	j	344	0	325	5	0
5	n	344	0	325	5	0
5	p	352	0	336	4	0
5	r	352	0	336	7	0
5	t	344	0	325	8	0
5	v	344	0	325	4	0
5	z	344	0	325	2	0
6	X	404	0	414	4	0
6	x	404	0	414	4	0
7	Y	375	0	371	6	0
7	y	375	0	371	7	0
8	0	61	0	61	2	0
8	1	51	0	41	0	0
8	2	56	0	51	1	0
8	3	66	0	74	4	0
8	4	56	0	51	2	0
8	5	66	0	74	4	0
8	6	61	0	61	2	0
8	7	61	0	61	2	0
8	8	61	0	61	2	0
8	9	56	0	51	4	0
8	A	66	0	74	4	0
8	B	66	0	74	3	0
8	C	61	0	61	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	66	0	74	5	0
8	E	66	0	74	2	0
8	F	66	0	74	4	0
8	G	66	0	74	5	0
8	I	66	0	74	5	0
8	J	61	0	61	5	0
8	K	66	0	74	4	0
8	L	195	0	213	10	0
8	M	66	0	74	1	0
8	N	61	0	61	5	0
8	O	66	0	74	10	0
8	P	61	0	61	4	0
8	Q	66	0	74	6	0
8	R	66	0	74	3	0
8	S	66	0	74	5	0
8	T	66	0	74	3	0
8	U	66	0	74	1	0
8	V	66	0	74	2	0
8	W	66	0	74	2	0
8	Z	57	0	53	0	0
8	a	66	0	74	3	0
8	b	66	0	74	5	0
8	b0	61	0	61	2	0
8	b1	51	0	41	0	0
8	b8	61	0	61	0	0
8	b9	56	0	51	4	0
8	c	61	0	61	2	0
8	d	66	0	74	6	0
8	e	66	0	74	2	0
8	f	66	0	74	5	0
8	g	66	0	74	5	0
8	i	66	0	74	6	0
8	j	61	0	61	5	0
8	k	66	0	74	4	0
8	l	195	0	213	11	0
8	m	66	0	74	1	0
8	n	61	0	61	5	0
8	o	66	0	74	10	0
8	p	61	0	61	4	0
8	q	66	0	74	6	0
8	r	66	0	74	3	0
8	s	66	0	74	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	t	66	0	74	4	0
8	u	66	0	74	2	0
8	v	66	0	74	1	0
8	w	66	0	74	1	0
8	z	57	0	53	0	0
9	L	65	0	74	5	0
9	M	55	0	51	2	0
9	l	65	0	74	4	0
9	m	55	0	51	2	0
10	L	81	0	102	8	0
10	M	86	0	110	3	0
10	l	81	0	102	9	0
10	m	86	0	110	3	0
11	A	112	0	146	13	0
11	D	77	0	102	7	0
11	H	76	0	100	8	0
11	L	71	0	90	5	0
11	a	112	0	146	12	0
11	d	77	0	102	7	0
11	h	76	0	100	10	0
11	l	71	0	90	5	0
12	M	1	0	0	0	0
12	m	1	0	0	0	0
13	0	42	0	60	0	0
13	3	84	0	120	7	0
13	5	84	0	120	6	0
13	6	42	0	60	5	0
13	7	42	0	60	5	0
13	9	42	0	60	3	0
13	A	42	0	60	4	0
13	B	42	0	60	2	0
13	C	42	0	60	2	0
13	D	42	0	60	2	0
13	E	42	0	60	0	0
13	F	84	0	120	6	0
13	I	84	0	120	4	0
13	J	42	0	60	4	0
13	M	42	0	60	5	0
13	N	84	0	120	7	0
13	O	42	0	60	3	0
13	R	126	0	180	13	0
13	S	42	0	60	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	U	42	0	60	3	0
13	V	84	0	120	1	0
13	a	42	0	60	4	0
13	b	42	0	60	2	0
13	b0	42	0	60	1	0
13	b9	42	0	60	2	0
13	c	42	0	60	2	0
13	d	42	0	60	2	0
13	e	42	0	60	0	0
13	f	84	0	120	7	0
13	i	84	0	120	3	0
13	j	42	0	60	4	0
13	m	42	0	60	5	0
13	n	84	0	120	6	0
13	o	42	0	60	2	0
13	r	126	0	180	12	0
13	s	42	0	60	4	0
13	u	42	0	60	2	0
13	v	84	0	120	1	0
14	H	63	0	70	2	0
14	M	76	0	96	4	0
14	h	63	0	70	2	0
14	m	76	0	96	1	0
All	All	44984	0	46412	754	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 (754) 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)
2:M:234:GLU:OE1	2:M:266:HIS:CE1	2.27	0.88
2:m:234:GLU:OE1	2:m:266:HIS:CE1	2.27	0.86
1:l:230:HIS:CE1	2:m:234:GLU:OE2	2.30	0.84
1:L:230:HIS:CE1	2:M:234:GLU:OE2	2.30	0.83
13:N:103:SPO:H10	5:P:45:TRP:HB2	1.69	0.75
13:n:103:SPO:H10	5:p:45:TRP:HB2	1.69	0.74
2:m:229:PHE:HB2	2:m:244:ALA:HB2	1.70	0.73
5:B:7:LEU:HD21	5:E:12:LEU:HB3	1.70	0.73
1:L:111:LEU:O	2:M:247:ARG:NH1	2.21	0.73
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:7:LEU:HD21	5:e:12:LEU:HB3	1.70	0.73
1:l:111:LEU:O	2:m:247:ARG:NH1	2.21	0.73
4:Q:24:LEU:HB2	8:Q:101:BCL:H42	1.71	0.72
3:h:54:GLY:O	4:d:15:ARG:NH1	2.23	0.72
4:q:24:LEU:HB2	8:q:101:BCL:H42	1.71	0.71
3:H:54:GLY:O	4:D:15:ARG:NH1	2.23	0.71
4:b1:29:VAL:HG11	7:y:24:MET:HG2	1.74	0.69
4:1:29:VAL:HG11	7:Y:24:MET:HG2	1.74	0.69
3:h:57:PRO:HG3	11:d:102:PC1:H132	1.75	0.67
4:b1:35:LEU:HD11	8:4:101:BCL:HHD	1.76	0.67
4:1:35:LEU:HD11	8:2:101:BCL:HHD	1.76	0.67
3:H:57:PRO:HG3	11:D:102:PC1:H132	1.76	0.67
3:h:94:GLU:O	4:b9:15:ARG:NH1	2.29	0.66
1:L:169:TYR:HA	1:L:174:MET:HE3	1.77	0.66
1:l:169:TYR:HA	1:l:174:MET:HE3	1.78	0.66
3:H:94:GLU:O	4:9:15:ARG:NH1	2.29	0.66
9:M:403:BPB:H55	9:M:403:BPB:HHD	1.79	0.65
9:m:403:BPB:HHD	9:m:403:BPB:H55	1.79	0.64
3:h:52:ASN:HD22	11:a:104:PC1:H153	1.62	0.64
3:H:52:ASN:HD22	11:A:104:PC1:H153	1.62	0.64
1:l:175:ILE:HG23	10:l:304:U10:H28	1.79	0.64
4:7:34:ILE:HD12	13:7:102:SPO:H32A	1.79	0.63
4:6:34:ILE:HD12	13:6:102:SPO:H32A	1.79	0.63
4:a:48:ALA:HA	4:a:53:ARG:HD3	1.80	0.63
4:A:48:ALA:HA	4:A:53:ARG:HD3	1.80	0.63
1:L:175:ILE:HG23	10:L:304:U10:H28	1.79	0.63
2:m:234:GLU:OE1	2:m:266:HIS:HE1	1.73	0.63
2:M:260:ALA:HA	3:H:35:ASN:HB3	1.81	0.62
8:l:302:BCL:H141	11:h:301:PC1:H2C1	1.81	0.62
3:h:129:ASN:ND2	3:h:224:GLU:OE1	2.32	0.62
1:l:66:VAL:HG11	1:l:89:ILE:HD12	1.79	0.62
4:6:6:LYS:NZ	5:b0:19:GLU:OE2	2.31	0.62
1:L:66:VAL:HG11	1:L:89:ILE:HD12	1.79	0.62
2:m:260:ALA:HA	3:h:35:ASN:HB3	1.81	0.62
5:t:35:ALA:O	5:t:39:HIS:ND1	2.25	0.62
4:W:6:LYS:NZ	5:Z:19:GLU:OE2	2.33	0.61
4:W:24:LEU:HB2	8:W:101:BCL:H42	1.81	0.61
1:l:255:TRP:HE3	10:l:305:U10:H28	1.65	0.61
4:w:24:LEU:HB2	8:w:101:BCL:H42	1.81	0.61
4:3:26:LEU:HD21	7:Y:42:VAL:HG21	1.82	0.61
11:l:306:PC1:H11	4:6:18:VAL:HG11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:w:6:LYS:NZ	5:z:19:GLU:OE2	2.33	0.61
4:1:9:MET:O	5:2:10:THR:N	2.33	0.61
8:v:101:BCL:H2	8:v:101:BCL:H72	1.83	0.61
4:b1:9:MET:O	5:4:10:THR:N	2.33	0.60
8:V:101:BCL:H2	8:V:101:BCL:H72	1.83	0.60
4:5:26:LEU:HD21	7:y:42:VAL:HG21	1.82	0.60
3:H:129:ASN:ND2	3:H:224:GLU:OE1	2.32	0.60
1:L:255:TRP:HE3	10:L:305:U10:H28	1.65	0.60
8:L:302:BCL:H141	11:H:301:PC1:H2C1	1.81	0.60
11:L:306:PC1:H11	4:7:18:VAL:HG11	1.83	0.60
3:h:11:ASP:H	3:h:14:SER:HB2	1.66	0.60
5:T:35:ALA:O	5:T:39:HIS:ND1	2.25	0.60
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.34	0.59
2:m:75:TRP:HE1	13:m:405:SPO:HM12	1.67	0.59
8:l:301:BCL:HBC2	8:m:402:BCL:HBC2	1.85	0.59
3:H:11:ASP:H	3:H:14:SER:HB2	1.66	0.59
2:m:241:ARG:NH1	3:h:38:GLU:OE1	2.34	0.59
2:M:75:TRP:HE1	13:M:405:SPO:HM12	1.67	0.59
4:Q:17:PHE:CD1	13:R:103:SPO:H392	2.38	0.59
8:L:301:BCL:HBC2	8:M:402:BCL:HBC2	1.85	0.59
4:q:17:PHE:CD1	13:r:103:SPO:H392	2.38	0.59
4:D:33:LEU:HD13	11:D:101:PC1:H332	1.85	0.59
13:N:103:SPO:H343	8:O:101:BCL:H61	1.85	0.58
11:d:102:PC1:H133	4:f:18:VAL:HG21	1.85	0.58
4:d:33:LEU:HD13	11:d:101:PC1:H332	1.85	0.58
13:n:103:SPO:H343	8:o:101:BCL:H61	1.86	0.58
4:3:48:ALA:HA	4:3:53:ARG:HD3	1.84	0.58
5:g:48:TRP:HZ2	8:g:101:BCL:H122	1.69	0.58
4:o:24:LEU:HB2	8:o:101:BCL:H42	1.85	0.58
13:f:103:SPO:H10	5:g:45:TRP:HB2	1.86	0.58
5:G:48:TRP:HZ2	8:G:101:BCL:H122	1.69	0.57
4:5:48:ALA:HA	4:5:53:ARG:HD3	1.84	0.57
2:M:232:GLU:OE2	3:H:177:ARG:NH1	2.37	0.57
5:G:7:LEU:HD13	5:J:12:LEU:HD11	1.86	0.57
4:D:36:LEU:O	4:D:42:ASN:ND2	2.37	0.57
5:T:31:PHE:HE2	8:T:101:BCL:HBA1	1.69	0.57
2:M:234:GLU:OE1	2:M:266:HIS:HE1	1.73	0.57
2:m:164:ARG:HH12	2:m:173:GLU:HB3	1.70	0.57
4:k:10:ILE:O	4:o:14:ARG:NH1	2.38	0.57
4:O:24:LEU:HB2	8:O:101:BCL:H42	1.85	0.57
13:7:102:SPO:H31	8:9:101:BCL:HBB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:232:GLU:OE2	3:h:177:ARG:NH1	2.37	0.57
11:D:102:PC1:H133	4:F:18:VAL:HG21	1.86	0.57
4:d:36:LEU:O	4:d:42:ASN:ND2	2.37	0.57
8:L:302:BCL:H152	9:L:303:BPB:H17A	1.86	0.57
5:t:31:PHE:HE2	8:t:101:BCL:HBA1	1.69	0.57
1:L:60:ASN:HD22	1:L:63:LEU:HG	1.70	0.56
13:F:103:SPO:H10	5:G:45:TRP:HB2	1.86	0.56
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.87	0.56
4:K:10:ILE:O	4:O:14:ARG:NH1	2.38	0.56
8:a:101:BCL:H201	13:a:102:SPO:H291	1.87	0.56
3:h:83:ARG:NH2	3:h:108:GLY:O	2.38	0.56
13:d:104:SPO:H21A	8:f:101:BCL:HBB2	1.87	0.56
2:M:164:ARG:HH12	2:M:173:GLU:HB3	1.70	0.56
4:Q:10:ILE:HG23	5:R:9:TYR:HD2	1.70	0.56
4:9:24:LEU:HB2	8:9:101:BCL:H42	1.88	0.56
5:g:7:LEU:HD13	5:j:12:LEU:HD11	1.86	0.56
13:6:102:SPO:H31	8:b9:101:BCL:HBB2	1.86	0.56
13:J:102:SPO:H33	4:K:50:LYS:HE2	1.87	0.56
4:K:24:LEU:HB2	8:K:101:BCL:H42	1.87	0.56
4:b9:24:LEU:HB2	8:b9:101:BCL:H42	1.88	0.56
4:7:6:LYS:NZ	5:0:19:GLU:OE2	2.31	0.56
13:D:104:SPO:H21A	8:F:101:BCL:HBB2	1.87	0.56
13:j:102:SPO:H33	4:k:50:LYS:HE2	1.87	0.55
4:k:24:LEU:HB2	8:k:101:BCL:H42	1.87	0.55
13:j:102:SPO:H25	8:k:101:BCL:H2A	1.89	0.55
8:A:101:BCL:H201	13:A:102:SPO:H291	1.87	0.55
8:l:302:BCL:H152	9:l:303:BPB:H17A	1.86	0.55
5:e:39:HIS:CG	8:e:101:BCL:H91	2.41	0.55
4:q:10:ILE:HG23	5:r:9:TYR:HD2	1.70	0.55
1:l:60:ASN:HD22	1:l:63:LEU:HG	1.70	0.55
2:M:81:ASN:HB3	2:M:84:VAL:HB	1.89	0.55
3:H:83:ARG:NH2	3:H:108:GLY:O	2.38	0.55
3:H:191:LEU:HD11	3:H:213:PHE:HE1	1.72	0.55
3:h:191:LEU:HD11	3:h:213:PHE:HE1	1.72	0.55
11:a:105:PC1:H131	4:d:14:ARG:HB3	1.89	0.55
3:h:54:GLY:HA2	11:a:104:PC1:H141	1.88	0.55
4:5:24:LEU:HB2	8:5:101:BCL:H42	1.88	0.55
3:h:122:GLU:HB2	3:h:227:LEU:HD21	1.87	0.55
3:H:54:GLY:HA2	11:A:104:PC1:H141	1.88	0.55
13:J:102:SPO:H25	8:K:101:BCL:H2A	1.89	0.54
5:E:39:HIS:CG	8:E:101:BCL:H91	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:81:ASN:HB3	2:m:84:VAL:HB	1.89	0.54
5:n:21:HIS:HE1	8:o:101:BCL:H193	1.73	0.54
11:A:105:PC1:H131	4:D:14:ARG:HB3	1.89	0.54
1:l:28:PRO:HD3	11:a:104:PC1:H111	1.90	0.54
3:h:156:CYS:SG	3:h:209:SER:OG	2.64	0.54
1:L:28:PRO:HD3	11:A:104:PC1:H111	1.90	0.54
2:m:94:LEU:HB3	2:m:177:TYR:HB2	1.90	0.54
4:K:48:ALA:HA	4:K:53:ARG:HB2	1.90	0.53
5:P:47:PRO:O	4:Q:53:ARG:NH2	2.41	0.53
4:3:24:LEU:HB2	8:3:101:BCL:H42	1.88	0.53
4:s:38:THR:OG1	4:s:40:SER:O	2.24	0.53
2:M:81:ASN:ND2	4:U:37:SER:OG	2.41	0.53
4:q:17:PHE:CG	13:r:103:SPO:H392	2.43	0.53
4:b9:3:LYS:HE2	4:b9:6:LYS:HE2	1.91	0.53
1:L:168:HIS:NE2	8:L:301:BCL:OBB	2.33	0.53
11:l:308:PC1:H151	4:u:38:THR:HG22	1.90	0.53
4:Q:17:PHE:CG	13:R:103:SPO:H392	2.43	0.53
1:l:241:VAL:HG21	9:l:303:BPB:H55	1.91	0.53
4:O:32:HIS:CE1	8:O:101:BCL:NA	2.77	0.53
2:m:81:ASN:ND2	4:u:37:SER:OG	2.41	0.53
1:l:219:LEU:HD11	2:m:133:THR:HG22	1.91	0.53
5:b0:39:HIS:CE1	8:b0:101:BCL:H91	2.44	0.53
11:L:308:PC1:H151	4:U:38:THR:HG22	1.90	0.52
2:M:94:LEU:HB3	2:M:177:TYR:HB2	1.90	0.52
4:F:48:ALA:HA	4:F:53:ARG:HD3	1.91	0.52
5:N:21:HIS:HE1	8:O:101:BCL:H193	1.73	0.52
4:f:48:ALA:HA	4:f:53:ARG:HD3	1.91	0.52
5:p:47:PRO:O	4:q:53:ARG:NH2	2.41	0.52
1:L:241:VAL:HG21	9:L:303:BPB:H55	1.91	0.52
1:L:255:TRP:CE3	10:L:305:U10:H28	2.43	0.52
5:T:19:GLU:O	5:T:23:VAL:HG23	2.09	0.52
4:9:3:LYS:HE2	4:9:6:LYS:HE2	1.91	0.52
5:0:39:HIS:CE1	8:0:101:BCL:H91	2.44	0.52
5:J:39:HIS:CG	8:J:101:BCL:H91	2.45	0.52
4:k:48:ALA:HA	4:k:53:ARG:HB2	1.90	0.52
5:r:39:HIS:CG	8:r:102:BCL:H91	2.45	0.52
5:t:19:GLU:O	5:t:23:VAL:HG23	2.09	0.52
4:o:32:HIS:CE1	8:o:101:BCL:NA	2.77	0.52
1:l:255:TRP:CE3	10:l:305:U10:H28	2.43	0.51
2:m:233:ARG:HE	2:m:236:GLU:CD	2.18	0.51
4:f:6:LYS:HD3	13:i:102:SPO:H393	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b1:48:ALA:HA	4:b1:53:ARG:HD3	1.92	0.51
1:L:170:ASN:HB3	1:L:173:HIS:HB2	1.92	0.51
4:1:48:ALA:HA	4:1:53:ARG:HD3	1.92	0.51
3:h:68:HIS:NE2	3:h:124:ASP:O	2.42	0.51
8:F:101:BCL:H2A	13:F:103:SPO:H25	1.93	0.51
4:O:43:TRP:NE1	8:O:101:BCL:OBB	2.43	0.51
2:m:241:ARG:HH22	3:h:79:GLU:CD	2.18	0.51
1:l:170:ASN:HB3	1:l:173:HIS:HB2	1.92	0.51
5:j:39:HIS:CG	8:j:101:BCL:H91	2.45	0.51
5:4:43:TYR:HE2	5:4:49:PHE:H	1.59	0.51
8:P:101:BCL:H52	13:R:103:SPO:H242	1.93	0.51
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.91	0.51
4:5:31:ILE:HG12	13:5:102:SPO:H31	1.92	0.51
1:L:190:HIS:HA	10:L:304:U10:O2	2.11	0.50
2:M:241:ARG:HH22	3:H:79:GLU:CD	2.19	0.50
5:R:41:ALA:HB1	13:R:103:SPO:H81	1.94	0.50
1:l:103:ARG:NH2	2:m:254:TRP:O	2.44	0.50
5:v:13:THR:HG22	5:v:14:ASP:N	2.26	0.50
1:L:103:ARG:NH2	2:M:254:TRP:O	2.44	0.50
5:R:39:HIS:CG	8:R:102:BCL:H91	2.45	0.50
2:m:160:LEU:HD23	2:m:284:ILE:HG21	1.92	0.50
2:M:160:LEU:HD23	2:M:284:ILE:HG21	1.92	0.50
2:m:199:ASN:HB3	2:m:202:HIS:HB3	1.94	0.50
8:f:101:BCL:H2A	13:f:103:SPO:H25	1.93	0.50
2:M:233:ARG:HE	2:M:236:GLU:CD	2.18	0.50
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.94	0.50
13:7:102:SPO:H10	4:9:25:PHE:HE1	1.76	0.50
8:n:102:BCL:HHD	8:n:102:BCL:HBC3	1.94	0.50
1:L:151:TRP:HZ2	11:H:301:PC1:H341	1.77	0.50
1:L:277:GLY:O	2:M:87:ARG:NH2	2.45	0.50
5:V:13:THR:HG22	5:V:14:ASP:N	2.26	0.50
4:o:43:TRP:NE1	8:o:101:BCL:OBB	2.43	0.50
13:6:102:SPO:H10	4:b9:25:PHE:HE1	1.76	0.50
3:H:190:LEU:HB2	3:H:233:ILE:HD13	1.93	0.50
4:F:6:LYS:HD3	13:I:102:SPO:H393	1.92	0.50
1:l:66:VAL:HB	1:l:148:TYR:HB2	1.94	0.50
4:3:31:ILE:HG12	13:3:102:SPO:H31	1.92	0.50
3:h:190:LEU:HB2	3:h:233:ILE:HD13	1.93	0.50
2:m:155:TRP:NE1	2:m:281:GLY:HA3	2.27	0.50
13:a:102:SPO:H311	4:b9:7:ILE:HD13	1.94	0.50
4:k:20:GLN:HG2	8:o:101:BCL:H101	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:THR:OG1	4:D:40:SER:O	2.23	0.49
13:A:102:SPO:H311	4:9:7:ILE:HD13	1.94	0.49
8:p:101:BCL:H52	13:r:103:SPO:H242	1.93	0.49
2:m:237:GLN:HB2	2:m:262:MET:HG2	1.94	0.49
5:r:41:ALA:HB1	13:r:103:SPO:H81	1.94	0.49
2:M:121:PHE:HZ	4:Q:30:MET:HE2	1.77	0.49
2:M:155:TRP:NE1	2:M:281:GLY:HA3	2.27	0.49
2:M:233:ARG:NH2	3:H:230:GLU:OE1	2.46	0.49
2:m:76:TYR:CD1	4:s:37:SER:HB3	2.47	0.49
4:f:43:TRP:CD2	8:f:101:BCL:H2C	2.48	0.49
1:L:66:VAL:HB	1:L:148:TYR:HB2	1.93	0.49
4:I:43:TRP:CD2	8:I:101:BCL:H2C	2.48	0.49
1:l:151:TRP:HZ2	11:h:301:PC1:H341	1.77	0.49
1:l:190:HIS:HA	10:l:304:U10:O2	2.11	0.49
3:h:168:TRP:HB2	3:h:178:PHE:HB2	1.95	0.49
4:o:6:LYS:HB3	13:r:101:SPO:H402	1.94	0.49
2:m:15:PRO:O	3:h:174:GLN:NE2	2.46	0.49
2:m:121:PHE:HZ	4:q:30:MET:HE2	1.77	0.49
3:H:156:CYS:SG	3:H:209:SER:OG	2.64	0.49
10:m:407:U10:H162	7:y:44:ALA:HA	1.95	0.49
2:M:15:PRO:O	3:H:174:GLN:NE2	2.46	0.49
2:M:199:ASN:HB3	2:M:202:HIS:HB3	1.94	0.49
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.95	0.49
4:K:20:GLN:HG2	8:O:101:BCL:H101	1.93	0.49
4:O:6:LYS:HB3	13:R:101:SPO:H402	1.94	0.49
5:2:43:TYR:HE2	5:2:49:PHE:H	1.58	0.49
11:l:306:PC1:H241	6:x:33:TRP:HB3	1.95	0.49
4:i:43:TRP:CD2	8:i:101:BCL:H2C	2.48	0.49
4:b1:23:PHE:HE1	7:y:16:VAL:HG11	1.78	0.49
8:N:102:BCL:HMB2	8:N:102:BCL:H102	1.95	0.49
1:l:127:ALA:HB2	1:l:241:VAL:HG13	1.94	0.49
13:u:102:SPO:H362	13:u:102:SPO:H341	1.48	0.49
2:M:76:TYR:CD1	4:S:37:SER:HB3	2.47	0.48
13:5:103:SPO:H361	13:5:103:SPO:H341	1.52	0.48
1:L:127:ALA:HB2	1:L:241:VAL:HG13	1.94	0.48
8:N:102:BCL:HBC3	8:N:102:BCL:HHD	1.94	0.48
4:1:23:PHE:HE1	7:Y:16:VAL:HG11	1.78	0.48
13:f:103:SPO:H361	13:f:103:SPO:H341	1.49	0.48
8:n:102:BCL:H102	8:n:102:BCL:HMB2	1.95	0.48
4:F:43:TRP:CD2	8:F:101:BCL:H2C	2.48	0.48
13:S:102:SPO:H362	13:S:102:SPO:H341	1.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:q:7:ILE:HA	13:s:102:SPO:H352	1.96	0.48
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.48	0.48
2:M:300:ASN:OD1	2:M:307:ASN:ND2	2.47	0.48
13:B:102:SPO:H361	13:B:102:SPO:H341	1.63	0.48
8:Q:101:BCL:H41	13:R:103:SPO:H351	1.95	0.48
1:l:146:PHE:HB3	1:l:156:TRP:CD2	2.48	0.48
8:q:101:BCL:H41	13:r:103:SPO:H351	1.96	0.48
4:D:48:ALA:HA	4:D:53:ARG:HB2	1.95	0.48
4:Q:7:ILE:HB	13:S:102:SPO:H32	1.95	0.48
4:q:43:TRP:CD2	8:q:101:BCL:H2C	2.49	0.48
1:L:146:PHE:HB3	1:L:156:TRP:CD2	2.48	0.48
2:M:249:ALA:HB1	2:M:259:ASN:HD22	1.79	0.48
3:H:53:GLN:H	11:A:105:PC1:H142	1.78	0.48
4:U:46:ILE:HD11	5:V:45:TRP:HZ2	1.79	0.48
1:l:277:GLY:O	2:m:87:ARG:NH2	2.45	0.48
2:m:233:ARG:NH2	3:h:230:GLU:OE1	2.46	0.48
8:L:307:BCL:H171	2:M:179:ILE:HD11	1.95	0.48
4:Q:43:TRP:CD2	8:Q:101:BCL:H2C	2.49	0.48
4:l:12:ASP:HB3	4:l:15:ARG:HG3	1.95	0.48
1:l:173:HIS:CE1	1:l:177:ILE:HD11	2.48	0.48
3:h:53:GLN:H	11:a:105:PC1:H142	1.78	0.48
13:n:103:SPO:H362	8:o:101:BCL:H41	1.96	0.48
2:m:300:ASN:OD1	2:m:307:ASN:ND2	2.47	0.48
11:L:306:PC1:H241	6:X:33:TRP:HB3	1.95	0.48
13:N:103:SPO:H362	8:O:101:BCL:H41	1.96	0.48
8:l:307:BCL:H171	2:m:179:ILE:HD11	1.95	0.48
4:d:48:ALA:HA	4:d:53:ARG:HB2	1.95	0.48
8:q:101:BCL:H121	8:q:101:BCL:H8	1.78	0.48
4:u:46:ILE:HD11	5:v:45:TRP:HZ2	1.79	0.47
4:D:6:LYS:HD3	13:F:102:SPO:H393	1.97	0.47
13:R:103:SPO:H5	13:R:103:SPO:H21A	1.63	0.47
6:X:21:LEU:HD11	3:h:255:MET:HG2	1.95	0.47
2:m:249:ALA:HB1	2:m:259:ASN:HD22	1.79	0.47
4:q:7:ILE:HB	13:s:102:SPO:H32	1.95	0.47
4:q:20:GLN:HE22	8:s:101:BCL:H91	1.79	0.47
2:M:122:MET:HG2	2:M:157:TRP:HZ2	1.80	0.47
10:M:407:U10:H162	7:Y:44:ALA:HA	1.95	0.47
4:D:43:TRP:CD2	8:D:103:BCL:H2C	2.49	0.47
4:I:24:LEU:HB2	8:I:101:BCL:H42	1.97	0.47
5:P:32:SER:HB2	8:P:101:BCL:H42	1.95	0.47
5:p:32:SER:HB2	8:p:101:BCL:H42	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:LYS:HB3	13:F:102:SPO:H402	1.96	0.47
4:f:38:THR:OG1	4:f:40:SER:O	2.20	0.47
3:H:187:SER:OG	3:H:189:ARG:NH1	2.47	0.47
4:A:22:VAL:HG11	11:A:103:PC1:H382	1.96	0.47
13:N:103:SPO:H22	8:O:101:BCL:O1D	2.15	0.47
4:Q:7:ILE:HA	13:S:102:SPO:H352	1.96	0.47
4:Q:20:GLN:HE22	8:S:101:BCL:H91	1.79	0.47
4:7:43:TRP:CE3	8:7:101:BCL:H2C	2.50	0.47
1:l:151:TRP:CZ2	11:h:301:PC1:H341	2.49	0.47
4:a:22:VAL:HG11	11:a:103:PC1:H382	1.96	0.47
4:d:6:LYS:HD3	13:f:102:SPO:H393	1.97	0.47
4:d:15:ARG:HB3	11:d:102:PC1:H11	1.96	0.47
4:d:20:GLN:HE22	5:e:24:TYR:HE1	1.63	0.47
4:d:43:TRP:CD2	8:d:103:BCL:H2C	2.49	0.47
4:i:24:LEU:HB2	8:i:101:BCL:H42	1.97	0.47
13:v:102:SPO:H362	13:v:102:SPO:H341	1.79	0.47
4:b1:12:ASP:HB3	4:b1:15:ARG:HG3	1.95	0.47
2:M:123:PHE:HA	2:M:157:TRP:HH2	1.80	0.47
3:H:68:HIS:NE2	3:H:124:ASP:O	2.42	0.47
8:s:101:BCL:H121	8:s:101:BCL:H8	1.75	0.47
4:6:43:TRP:CE3	8:6:101:BCL:H2C	2.50	0.47
1:L:151:TRP:CZ2	11:H:301:PC1:H341	2.49	0.47
1:L:227:LEU:HB2	3:H:175:MET:HE1	1.97	0.47
4:D:15:ARG:HB3	11:D:102:PC1:H11	1.96	0.47
13:J:102:SPO:H341	13:J:102:SPO:H361	1.53	0.47
2:m:294:TRP:O	2:m:298:GLY:N	2.46	0.47
4:d:6:LYS:HB3	13:f:102:SPO:H402	1.96	0.47
2:M:108:PRO:HD2	2:M:111:GLU:HB2	1.97	0.47
8:J:101:BCL:H92	8:J:101:BCL:H62	1.71	0.47
1:l:168:HIS:NE2	8:l:301:BCL:OBB	2.33	0.47
2:m:122:MET:HG2	2:m:157:TRP:HZ2	1.80	0.46
3:h:181:VAL:HG21	3:h:191:LEU:HD12	1.98	0.46
10:M:404:U10:H28	10:M:404:U10:H322	1.76	0.46
3:H:220:LYS:N	3:H:229:GLU:OE2	2.44	0.46
11:d:102:PC1:H151	4:f:15:ARG:HD3	1.98	0.46
13:n:103:SPO:H361	13:n:103:SPO:H341	1.64	0.46
13:n:103:SPO:H22	8:o:101:BCL:O1D	2.15	0.46
1:l:227:LEU:HB2	3:h:175:MET:HE1	1.97	0.46
9:m:403:BPB:H6	9:m:403:BPB:H4	1.78	0.46
8:a:101:BCL:HHH	5:b:42:VAL:HG21	1.97	0.46
5:b:41:ALA:HB2	13:b:102:SPO:H32A	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:54:GLY:HA3	11:H:302:PC1:H153	1.97	0.46
13:V:102:SPO:H362	13:V:102:SPO:H341	1.79	0.46
13:3:103:SPO:H341	13:3:103:SPO:H361	1.52	0.46
8:g:101:BCL:H143	8:g:101:BCL:HBB2	1.98	0.46
4:i:41:TYR:CE1	8:j:101:BCL:HBC1	2.51	0.46
8:A:101:BCL:HHC	8:A:101:BCL:OBB	2.16	0.46
8:A:101:BCL:HHD	5:B:42:VAL:HG21	1.97	0.46
8:S:101:BCL:HHC	8:S:101:BCL:OBB	2.16	0.46
13:9:102:SPO:H341	13:9:102:SPO:H361	1.50	0.46
1:l:62:GLN:HB3	1:l:151:TRP:HD1	1.81	0.46
2:m:108:PRO:HD2	2:m:111:GLU:HB2	1.97	0.46
3:H:181:VAL:HG21	3:H:191:LEU:HD12	1.98	0.46
7:Y:25:PHE:HB2	7:Y:35:GLY:HA2	1.98	0.46
3:h:187:SER:OG	3:h:189:ARG:NH1	2.47	0.46
5:b8:23:VAL:HG21	6:x:19:LEU:HD23	1.98	0.46
8:l:307:BCL:H172	13:m:405:SPO:H133	1.98	0.46
11:a:105:PC1:H151	4:d:15:ARG:HA	1.98	0.46
5:c:35:ALA:O	5:c:39:HIS:ND1	2.31	0.46
1:L:171:PRO:HG2	10:L:305:U10:H212	1.98	0.46
11:D:102:PC1:H151	4:F:15:ARG:HD3	1.98	0.46
5:V:46:ARG:HG3	4:W:53:ARG:NH2	2.31	0.46
2:m:123:PHE:HA	2:m:157:TRP:HH2	1.80	0.46
4:o:43:TRP:CE2	8:o:101:BCL:HHC	2.51	0.46
5:B:41:ALA:HB2	13:B:102:SPO:H32A	1.97	0.46
4:O:43:TRP:CE2	8:O:101:BCL:HHC	2.51	0.46
3:h:54:GLY:HA3	11:h:302:PC1:H153	1.97	0.46
2:M:174:ALA:O	2:M:185:TRP:NE1	2.48	0.45
4:I:41:TYR:CE1	8:J:101:BCL:HBC1	2.51	0.45
8:d:103:BCL:H121	8:d:103:BCL:H8	1.73	0.45
5:j:21:HIS:HE1	8:k:101:BCL:H193	1.81	0.45
8:p:101:BCL:H143	13:r:103:SPO:H16	1.98	0.45
13:u:102:SPO:H362	5:v:20:LEU:HG	1.98	0.45
4:D:20:GLN:HE22	5:E:24:TYR:HE1	1.63	0.45
8:P:101:BCL:H143	13:R:103:SPO:H16	1.98	0.45
8:P:101:BCL:HBC3	8:P:101:BCL:HHD	1.98	0.45
5:b:24:TYR:CE2	8:d:103:BCL:H171	2.51	0.45
13:b:102:SPO:H361	13:b:102:SPO:H341	1.63	0.45
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.51	0.45
10:M:407:U10:H1M1	10:M:407:U10:H103	1.98	0.45
11:A:105:PC1:H151	4:D:15:ARG:HA	1.98	0.45
5:B:24:TYR:CE2	8:D:103:BCL:H171	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:174:ALA:O	2:m:185:TRP:NE1	2.48	0.45
5:v:46:ARG:HG3	4:w:53:ARG:NH2	2.31	0.45
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.99	0.45
5:N:48:TRP:CD2	8:N:102:BCL:H2C	2.52	0.45
13:R:104:SPO:H351	8:S:101:BCL:H41	1.98	0.45
8:s:101:BCL:OBB	8:s:101:BCL:HHC	2.16	0.45
8:B:101:BCL:H62	8:B:101:BCL:H92	1.71	0.45
2:M:294:TRP:O	2:M:298:GLY:N	2.46	0.45
3:H:21:TRP:HZ2	11:H:301:PC1:H331	1.82	0.45
4:9:27:LEU:O	4:9:31:ILE:HG13	2.17	0.45
2:m:202:HIS:CE1	2:m:206:ILE:HD11	2.51	0.45
5:j:48:TRP:CD2	8:j:101:BCL:H2C	2.52	0.45
8:j:101:BCL:H92	8:j:101:BCL:H62	1.71	0.45
8:n:102:BCL:HBB2	8:n:102:BCL:H122	1.98	0.45
8:p:101:BCL:HBC3	8:p:101:BCL:HHD	1.98	0.45
1:L:47:ILE:HG21	4:9:30:MET:HG3	1.99	0.45
1:L:62:GLN:HB3	1:L:151:TRP:HD1	1.81	0.45
4:D:31:ILE:HG12	13:D:104:SPO:H31	1.98	0.45
13:O:102:SPO:H361	13:O:102:SPO:H341	1.54	0.45
5:C:49:PHE:HB3	13:3:103:SPO:H6	1.99	0.45
5:8:23:VAL:HG21	6:X:19:LEU:HD23	1.98	0.45
1:l:230:HIS:HE1	2:m:234:GLU:OE2	1.86	0.45
4:f:10:ILE:HG23	4:i:14:ARG:HG2	1.99	0.45
4:i:43:TRP:CE3	8:i:101:BCL:H2C	2.52	0.45
7:y:25:PHE:HB2	7:y:35:GLY:HA2	1.98	0.45
8:L:302:BCL:H161	9:L:303:BPB:H15A	1.99	0.45
8:G:101:BCL:H143	8:G:101:BCL:HBB2	1.98	0.45
4:I:43:TRP:CE3	8:I:101:BCL:H2C	2.52	0.45
5:J:21:HIS:HE1	8:K:101:BCL:H193	1.81	0.45
8:Q:101:BCL:H121	8:Q:101:BCL:H8	1.78	0.45
3:h:5:THR:HG22	3:h:11:ASP:HB3	1.99	0.45
14:h:303:CDL:H782	4:f:29:VAL:HG11	1.99	0.45
4:a:51:TYR:OH	5:b0:49:PHE:O	2.23	0.45
8:d:103:BCL:HHC	8:d:103:BCL:OBB	2.16	0.45
13:r:104:SPO:H351	8:s:101:BCL:H41	1.98	0.45
13:R:103:SPO:H361	13:R:103:SPO:H341	1.51	0.45
2:m:275:LEU:HD23	2:m:278:LEU:HD23	1.98	0.45
5:n:48:TRP:CD2	8:n:102:BCL:H2C	2.52	0.45
8:b0:101:BCL:H62	8:b0:101:BCL:H92	1.70	0.45
1:L:62:GLN:NE2	11:H:301:PC1:H321	2.32	0.45
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:164:ARG:NH1	2:M:173:GLU:HB3	2.32	0.45
4:d:31:ILE:HG12	13:d:104:SPO:H31	1.98	0.45
8:R:102:BCL:H92	8:R:102:BCL:H62	1.73	0.44
4:S:38:THR:OG1	4:S:40:SER:O	2.24	0.44
1:l:182:THR:HG23	8:l:307:BCL:H42	1.99	0.44
13:b9:102:SPO:H341	5:b0:20:LEU:HD12	1.98	0.44
8:L:307:BCL:H172	13:M:405:SPO:H133	1.98	0.44
5:C:35:ALA:O	5:C:39:HIS:ND1	2.31	0.44
1:l:171:PRO:HG2	10:l:305:U10:H212	1.98	0.44
3:h:21:TRP:HZ2	11:h:301:PC1:H331	1.82	0.44
4:f:20:GLN:NE2	13:f:103:SPO:H392	2.32	0.44
4:f:46:ILE:HD11	5:g:45:TRP:HZ2	1.83	0.44
5:p:49:PHE:O	4:q:51:TYR:OH	2.22	0.44
2:M:275:LEU:HD23	2:M:278:LEU:HD23	1.98	0.44
11:A:105:PC1:H133	11:A:105:PC1:H111	1.75	0.44
4:F:20:GLN:NE2	13:F:103:SPO:H392	2.32	0.44
1:l:47:ILE:HG21	4:b9:30:MET:HG3	1.99	0.44
2:M:200:PRO:HB2	3:H:17:ILE:HD13	2.00	0.44
13:J:102:SPO:H10	5:N:45:TRP:HB2	2.00	0.44
13:U:102:SPO:H362	5:V:20:LEU:HG	1.98	0.44
8:a:101:BCL:HHC	8:a:101:BCL:OBB	2.16	0.44
5:b:39:HIS:CE1	8:b:101:BCL:H91	2.53	0.44
5:B:39:HIS:CE1	8:B:101:BCL:H91	2.53	0.44
4:o:34:ILE:O	4:o:37:SER:OG	2.30	0.44
8:q:101:BCL:OBB	8:q:101:BCL:HHC	2.18	0.44
1:L:105:VAL:O	1:L:109:ARG:HG3	2.17	0.44
3:H:5:THR:HG22	3:H:11:ASP:HB3	1.99	0.44
4:A:51:TYR:HB2	4:A:53:ARG:NE	2.33	0.44
4:I:11:PHE:HB3	4:I:16:VAL:HG21	1.99	0.44
13:I:102:SPO:H26	13:I:102:SPO:H241	1.89	0.44
2:m:164:ARG:NH1	2:m:173:GLU:HB3	2.32	0.44
10:m:407:U10:H1M1	10:m:407:U10:H103	1.98	0.44
8:b:101:BCL:H92	8:b:101:BCL:H62	1.71	0.44
1:L:271:TRP:HB2	11:L:308:PC1:H221	2.00	0.44
8:N:102:BCL:HBB2	8:N:102:BCL:H122	1.99	0.44
5:0:25:MET:SD	5:0:28:LEU:HD23	2.58	0.44
1:l:9:TYR:OH	2:m:246:GLU:OE1	2.31	0.44
1:l:62:GLN:NE2	11:h:301:PC1:H321	2.32	0.44
2:m:200:PRO:HB2	3:h:17:ILE:HD13	2.00	0.44
3:h:112:ALA:HB2	3:h:239:GLY:HA3	1.99	0.44
4:F:10:ILE:HG23	4:I:14:ARG:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:48:TRP:CD2	8:J:101:BCL:H2C	2.52	0.44
5:N:42:VAL:HG11	8:N:102:BCL:HBC1	2.00	0.44
6:X:22:TRP:O	6:X:26:GLN:HG2	2.18	0.44
5:n:46:ARG:HG2	4:o:53:ARG:NH2	2.33	0.44
5:r:31:PHE:HE1	8:r:102:BCL:HBA1	1.82	0.44
2:M:103:LEU:HD11	2:M:166:ILE:HA	2.00	0.44
2:M:301:HIS:NE2	3:H:14:SER:OG	2.50	0.44
2:M:302:GLY:HA3	11:H:301:PC1:H141	2.00	0.44
8:A:101:BCL:H121	8:A:101:BCL:H8	1.89	0.44
4:D:33:LEU:O	4:D:37:SER:OG	2.34	0.44
8:D:103:BCL:HHC	8:D:103:BCL:OBB	2.16	0.44
13:9:102:SPO:H341	5:0:20:LEU:HD12	1.98	0.44
2:m:32:VAL:HG22	2:m:49:PRO:HD3	1.99	0.44
8:c:102:BCL:H61	8:c:102:BCL:H2	1.81	0.44
4:b9:27:LEU:O	4:b9:31:ILE:HG13	2.17	0.44
1:L:182:THR:HG23	8:L:307:BCL:H42	1.99	0.43
14:H:303:CDL:H782	4:F:29:VAL:HG11	1.99	0.43
8:3:101:BCL:H61	13:3:103:SPO:H343	2.01	0.43
4:1:4:PHE:HB3	5:2:21:HIS:CE1	2.53	0.43
1:l:62:GLN:HB3	1:l:151:TRP:CD1	2.53	0.43
5:c:49:PHE:HB3	13:5:103:SPO:H6	1.99	0.43
4:b1:33:LEU:HD22	7:y:27:PHE:CG	2.53	0.43
2:M:24:VAL:HG11	2:M:29:ARG:HH21	1.83	0.43
4:F:46:ILE:HD11	5:G:45:TRP:HZ2	1.82	0.43
8:V:101:BCL:H192	8:V:101:BCL:H162	1.83	0.43
1:l:54:VAL:HG13	4:a:37:SER:HA	2.00	0.43
1:l:105:VAL:O	1:l:109:ARG:HG3	2.17	0.43
8:l:302:BCL:H161	9:l:303:BPB:H15A	1.99	0.43
3:h:7:PHE:CZ	4:f:34:ILE:HG12	2.53	0.43
3:h:37:ARG:HA	3:h:76:PRO:HG3	2.00	0.43
4:i:11:PHE:HB3	4:i:16:VAL:HG21	1.99	0.43
8:i:101:BCL:H121	8:i:101:BCL:H8	1.89	0.43
6:x:22:TRP:O	6:x:26:GLN:HG2	2.18	0.43
2:M:215:LEU:HD11	2:M:265:ILE:HD11	2.01	0.43
13:I:103:SPO:HM12	13:I:103:SPO:H41	1.88	0.43
5:R:31:PHE:HE1	8:R:102:BCL:HBA1	1.82	0.43
1:l:269:LEU:HB2	1:l:272:TRP:NE1	2.34	0.43
10:m:404:U10:H28	10:m:404:U10:H322	1.76	0.43
13:A:102:SPO:H362	13:A:102:SPO:H341	1.71	0.43
8:C:102:BCL:HMA1	8:3:101:BCL:HMA3	2.01	0.43
2:m:103:LEU:HD11	2:m:166:ILE:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:39:HIS:CD2	8:g:101:BCL:H111	2.53	0.43
5:j:48:TRP:O	4:k:47:SER:OG	2.37	0.43
13:j:102:SPO:H10	5:n:45:TRP:HB2	2.00	0.43
13:j:102:SPO:H26	13:j:102:SPO:H241	1.92	0.43
8:6:101:BCL:HHD	5:b8:42:VAL:HG21	2.00	0.43
10:L:305:U10:H121	10:L:305:U10:H101	1.82	0.43
5:T:31:PHE:CE2	8:T:101:BCL:HBA1	2.52	0.43
13:C:101:SPO:H26	13:C:101:SPO:H241	1.88	0.43
2:m:80:TRP:CH2	4:s:34:ILE:HG12	2.54	0.43
3:h:175:MET:HE3	3:h:177:ARG:HH21	1.84	0.43
4:a:27:LEU:O	4:a:31:ILE:HG13	2.18	0.43
5:n:42:VAL:HG11	8:n:102:BCL:HBC1	2.00	0.43
4:s:43:TRP:CD2	8:s:101:BCL:H2C	2.54	0.43
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.34	0.43
5:J:48:TRP:O	4:K:47:SER:OG	2.37	0.43
1:l:271:TRP:HB2	11:l:308:PC1:H221	2.00	0.43
13:s:102:SPO:H341	13:s:102:SPO:H362	1.51	0.43
8:c:102:BCL:HMA1	8:5:101:BCL:HMA3	2.01	0.43
4:5:31:ILE:O	4:5:35:LEU:HG	2.18	0.43
5:b0:25:MET:SD	5:b0:28:LEU:HD23	2.58	0.43
8:E:101:BCL:C2B	8:E:101:BCL:H112	2.49	0.43
5:N:46:ARG:HG2	4:O:53:ARG:NH2	2.33	0.43
13:R:104:SPO:H362	13:R:104:SPO:H341	1.81	0.43
4:1:33:LEU:HD22	7:Y:27:PHE:CG	2.53	0.43
4:d:43:TRP:CE3	8:d:103:BCL:H2C	2.54	0.43
4:b1:4:PHE:HB3	5:4:21:HIS:CE1	2.53	0.43
8:b9:101:BCL:HHD	5:b0:42:VAL:HG21	2.00	0.43
4:A:27:LEU:O	4:A:31:ILE:HG13	2.18	0.43
13:U:102:SPO:H26	13:U:102:SPO:H241	1.86	0.43
1:l:42:ALA:HA	9:l:303:BPB:H7	2.01	0.43
8:u:101:BCL:H122	8:u:101:BCL:H8	1.76	0.43
9:M:403:BPB:H6	9:M:403:BPB:H4	1.78	0.43
8:Q:101:BCL:OBB	8:Q:101:BCL:HHC	2.18	0.43
1:l:255:TRP:NE1	1:l:257:ASP:O	2.52	0.43
5:r:42:VAL:HG22	13:r:103:SPO:H133	2.01	0.43
13:c:101:SPO:H26	13:c:101:SPO:H241	1.88	0.43
13:c:101:SPO:HM11	4:5:29:VAL:HG13	2.01	0.43
3:H:37:ARG:HA	3:H:76:PRO:HG3	2.00	0.43
3:H:54:GLY:H	11:A:105:PC1:H121	1.84	0.43
3:H:175:MET:HE3	3:H:177:ARG:HH21	1.84	0.43
4:F:43:TRP:CE3	8:F:101:BCL:H2C	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:43:TRP:CD2	8:S:101:BCL:H2C	2.54	0.43
5:Z:35:ALA:O	5:Z:39:HIS:ND1	2.48	0.43
2:m:24:VAL:HG11	2:m:29:ARG:HH21	1.83	0.43
4:a:51:TYR:HB2	4:a:53:ARG:NE	2.33	0.43
8:b:101:BCL:H62	8:b:101:BCL:H2	1.87	0.43
1:L:255:TRP:NE1	1:L:257:ASP:O	2.52	0.42
3:H:7:PHE:CZ	4:F:34:ILE:HG12	2.53	0.42
5:E:7:LEU:HD22	5:G:12:LEU:HD11	2.01	0.42
8:S:101:BCL:H121	8:S:101:BCL:H8	1.75	0.42
4:3:31:ILE:O	4:3:35:LEU:HG	2.18	0.42
8:7:101:BCL:HH2	5:8:42:VAL:HG21	2.00	0.42
8:5:101:BCL:H61	13:5:103:SPO:H343	2.00	0.42
5:4:14:ASP:OD1	5:4:15:GLU:N	2.52	0.42
1:L:54:VAL:HG13	4:A:37:SER:HA	2.00	0.42
1:L:207:ARG:HA	1:L:207:ARG:HD3	1.89	0.42
4:D:43:TRP:CE3	8:D:103:BCL:H2C	2.54	0.42
5:G:39:HIS:CD2	8:G:101:BCL:H111	2.53	0.42
4:O:43:TRP:CD2	8:O:101:BCL:H2C	2.54	0.42
13:7:102:SPO:H26	13:7:102:SPO:H241	1.86	0.42
4:A:41:TYR:HE1	5:B:46:ARG:HB3	1.85	0.42
2:m:301:HIS:NE2	3:h:14:SER:OG	2.50	0.42
5:b:39:HIS:CD2	8:b:101:BCL:H91	2.55	0.42
5:e:7:LEU:HD22	5:g:12:LEU:HD11	2.01	0.42
2:M:68:PHE:HZ	4:S:30:MET:HB2	1.85	0.42
2:M:80:TRP:CH2	4:S:34:ILE:HG12	2.54	0.42
13:C:101:SPO:HM11	4:3:29:VAL:HG13	2.01	0.42
8:0:101:BCL:H62	8:0:101:BCL:H92	1.70	0.42
2:m:275:LEU:HA	2:m:278:LEU:HB3	2.02	0.42
13:i:102:SPO:H31	8:k:101:BCL:HBB2	2.01	0.42
1:L:42:ALA:HA	9:L:303:BPB:H7	2.01	0.42
1:L:59:TRP:CG	11:D:101:PC1:H231	2.54	0.42
5:R:38:ALA:O	5:R:42:VAL:HG23	2.19	0.42
8:9:101:BCL:HH2	5:0:42:VAL:HG21	2.00	0.42
2:m:302:GLY:HA3	11:h:301:PC1:H141	2.00	0.42
5:z:35:ALA:O	5:z:39:HIS:ND1	2.48	0.42
1:L:62:GLN:HB3	1:L:151:TRP:CD1	2.54	0.42
2:M:275:LEU:HA	2:M:278:LEU:HB3	2.02	0.42
4:A:14:ARG:NH2	11:A:103:PC1:H142	2.35	0.42
8:f:101:BCL:H121	8:f:101:BCL:H8	1.89	0.42
4:o:43:TRP:CD2	8:o:101:BCL:H2C	2.54	0.42
5:r:38:ALA:O	5:r:42:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:168:HIS:HE2	8:L:301:BCL:HHC	1.85	0.42
1:L:206:MET:O	3:H:67:PRO:HG3	2.20	0.42
5:R:42:VAL:HG22	13:R:103:SPO:H133	2.01	0.42
3:h:83:ARG:HH22	3:h:108:GLY:C	2.25	0.42
4:6:27:LEU:O	4:6:31:ILE:HG13	2.20	0.42
2:M:28:ASN:HB2	2:M:51:TYR:CE2	2.55	0.42
2:M:130:TRP:NE1	2:M:147:ALA:O	2.47	0.42
13:I:102:SPO:H31	8:K:101:BCL:HBB2	2.01	0.42
13:R:104:SPO:H26	13:R:104:SPO:H241	1.94	0.42
5:2:14:ASP:OD1	5:2:15:GLU:N	2.52	0.42
1:l:60:ASN:ND2	1:l:63:LEU:HG	2.35	0.42
1:l:206:MET:O	3:h:67:PRO:HG3	2.19	0.42
4:i:32:HIS:CE1	8:i:101:BCL:NA	2.88	0.42
13:F:103:SPO:H341	13:F:103:SPO:H361	1.49	0.42
4:a:14:ARG:NH2	11:a:103:PC1:H142	2.35	0.42
5:t:31:PHE:CE2	8:t:101:BCL:HBA1	2.52	0.42
13:5:103:SPO:H31	13:5:103:SPO:H5	1.72	0.42
2:M:282:ILE:O	2:M:286:LEU:HG	2.20	0.42
5:B:39:HIS:CD2	8:B:101:BCL:H91	2.55	0.42
4:S:9:MET:HE1	5:T:14:ASP:HA	2.02	0.42
4:7:27:LEU:O	4:7:31:ILE:HG13	2.20	0.42
1:l:175:ILE:HD11	10:l:305:U10:H13	2.02	0.42
8:l:301:BCL:CGA	8:l:302:BCL:HBC1	2.50	0.42
11:l:308:PC1:H231	11:l:308:PC1:H322	2.01	0.42
3:h:55:PRO:O	11:d:102:PC1:H232	2.20	0.42
8:e:101:BCL:C2B	8:e:101:BCL:H112	2.49	0.42
4:i:43:TRP:HA	4:i:46:ILE:HB	2.02	0.42
9:L:303:BPB:H6A	9:L:303:BPB:H10A	1.88	0.41
13:S:102:SPO:H362	5:T:20:LEU:HG	2.02	0.41
8:C:102:BCL:H61	8:C:102:BCL:H2	1.81	0.41
1:l:59:TRP:CG	11:d:101:PC1:H231	2.54	0.41
4:a:41:TYR:HE1	5:b:46:ARG:HB3	1.85	0.41
4:f:43:TRP:CE3	8:f:101:BCL:H2C	2.54	0.41
13:i:103:SPO:HM12	13:i:103:SPO:H41	1.88	0.41
8:j:101:BCL:H112	8:j:101:BCL:C2B	2.50	0.41
13:o:102:SPO:H21A	8:q:101:BCL:HBB2	2.02	0.41
4:s:9:MET:HE1	5:t:14:ASP:HA	2.02	0.41
5:t:49:PHE:OXT	4:u:50:LYS:NZ	2.36	0.41
3:H:55:PRO:O	11:D:102:PC1:H232	2.20	0.41
4:A:15:ARG:HE	11:A:105:PC1:P	2.43	0.41
4:I:3:LYS:HA	4:I:5:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:102:SPO:H362	13:U:102:SPO:H341	1.48	0.41
2:m:28:ASN:HB2	2:m:51:TYR:CE2	2.55	0.41
2:m:68:PHE:HZ	4:s:30:MET:HB2	1.85	0.41
2:m:215:LEU:HD11	2:m:265:ILE:HD11	2.00	0.41
3:h:220:LYS:N	3:h:229:GLU:OE2	2.44	0.41
2:M:75:TRP:HE1	13:M:405:SPO:H22A	1.86	0.41
8:D:103:BCL:H8	8:D:103:BCL:H121	1.73	0.41
4:7:36:LEU:O	4:7:42:ASN:ND2	2.54	0.41
10:l:305:U10:H101	10:l:305:U10:H121	1.82	0.41
3:h:52:ASN:ND2	11:a:104:PC1:H153	2.33	0.41
4:i:3:LYS:HA	4:i:5:TYR:CE1	2.55	0.41
3:H:52:ASN:HB2	11:A:105:PC1:H112	2.03	0.41
8:W:101:BCL:H121	8:W:101:BCL:H8	1.95	0.41
1:l:117:ILE:HD11	2:m:222:THR:HA	2.02	0.41
3:h:54:GLY:H	11:a:105:PC1:H121	1.84	0.41
11:h:301:PC1:H332	11:h:301:PC1:H361	1.83	0.41
13:r:103:SPO:H21A	13:r:103:SPO:H5	1.63	0.41
8:t:101:BCL:H91	8:t:101:BCL:H112	1.84	0.41
13:6:102:SPO:H26	13:6:102:SPO:H241	1.86	0.41
2:M:164:ARG:HD2	2:M:284:ILE:HG22	2.02	0.41
2:M:278:LEU:HD13	14:M:406:CDL:H771	2.02	0.41
13:M:405:SPO:H403	4:Q:33:LEU:HD21	2.02	0.41
8:9:101:BCL:OBB	8:9:101:BCL:HHC	2.21	0.41
4:a:15:ARG:HE	11:a:105:PC1:P	2.43	0.41
11:a:105:PC1:H133	11:a:105:PC1:H111	1.75	0.41
8:r:102:BCL:H92	8:r:102:BCL:H62	1.73	0.41
13:s:102:SPO:H362	5:t:20:LEU:HG	2.02	0.41
6:x:27:MET:HE2	6:x:27:MET:HB3	1.92	0.41
1:L:9:TYR:OH	2:M:246:GLU:OE1	2.31	0.41
11:L:308:PC1:H231	11:L:308:PC1:H322	2.01	0.41
3:H:83:ARG:HH22	3:H:108:GLY:C	2.25	0.41
13:A:102:SPO:H26	13:A:102:SPO:H241	1.85	0.41
4:F:35:LEU:HD11	8:G:101:BCL:HHD	2.01	0.41
4:I:32:HIS:CE1	8:I:101:BCL:NA	2.88	0.41
4:Q:40:SER:HB2	5:R:46:ARG:HH12	1.85	0.41
8:3:101:BCL:HED3	13:3:103:SPO:H27	2.03	0.41
4:1:31:ILE:O	4:1:35:LEU:HG	2.21	0.41
4:9:48:ALA:HA	4:9:53:ARG:HB2	2.03	0.41
1:l:38:THR:HG21	1:l:100:TRP:HE3	1.86	0.41
1:l:179:PHE:CE1	10:l:304:U10:H23	2.55	0.41
4:i:7:ILE:HD12	13:n:101:SPO:H311	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5:101:BCL:HED3	13:5:103:SPO:H27	2.03	0.41
4:6:36:LEU:O	4:6:42:ASN:ND2	2.54	0.41
2:M:24:VAL:HG11	2:M:29:ARG:NH2	2.36	0.41
4:I:43:TRP:CZ2	8:I:101:BCL:HHC	2.56	0.41
4:I:43:TRP:HA	4:I:46:ILE:HB	2.02	0.41
3:h:14:SER:HA	3:h:17:ILE:HG22	2.03	0.41
5:b8:49:PHE:O	4:b9:51:TYR:OH	2.25	0.41
1:L:14:GLY:HA2	1:L:109:ARG:NH1	2.36	0.41
11:H:301:PC1:H261	14:H:303:CDL:H352	2.03	0.41
4:F:38:THR:OG1	4:F:40:SER:O	2.20	0.41
1:l:14:GLY:HA2	1:l:109:ARG:NH1	2.36	0.41
2:m:73:TRP:NE1	2:m:77:GLN:OE1	2.54	0.41
2:m:278:LEU:HD13	14:m:406:CDL:H771	2.02	0.41
2:m:282:ILE:O	2:m:286:LEU:HG	2.20	0.41
13:m:405:SPO:H403	4:q:33:LEU:HD21	2.02	0.41
4:q:40:SER:HB2	5:r:46:ARG:HH12	1.85	0.41
4:b1:23:PHE:CE1	7:y:16:VAL:HG11	2.56	0.41
4:b1:31:ILE:O	4:b1:35:LEU:HG	2.21	0.41
8:4:101:BCL:H62	8:4:101:BCL:H41	1.83	0.41
1:L:226:THR:O	1:L:230:HIS:ND1	2.46	0.41
2:M:235:LEU:HD23	2:M:235:LEU:HA	1.83	0.41
11:A:104:PC1:H133	11:A:104:PC1:H112	1.87	0.41
4:I:7:ILE:HD12	13:N:101:SPO:H311	2.03	0.41
13:N:101:SPO:H26	13:N:101:SPO:H241	1.88	0.41
13:O:102:SPO:H21A	8:Q:101:BCL:HBB2	2.02	0.41
1:l:201:GLU:OE1	1:l:204:LYS:NZ	2.46	0.41
1:l:218:ASP:O	2:m:132:ARG:NH2	2.54	0.41
1:l:269:LEU:HD23	1:l:269:LEU:HA	1.94	0.41
2:m:75:TRP:HE1	13:m:405:SPO:H22A	1.86	0.41
4:a:36:LEU:O	4:a:42:ASN:ND2	2.54	0.41
4:a:41:TYR:OH	5:b:46:ARG:O	2.22	0.41
4:d:27:LEU:O	4:d:31:ILE:HG13	2.21	0.41
4:f:35:LEU:HD11	8:g:101:BCL:HHD	2.01	0.41
13:6:102:SPO:C27	5:b8:27:GLY:HA3	2.51	0.41
13:b9:102:SPO:H361	5:b0:20:LEU:HD12	2.03	0.41
13:b0:102:SPO:H5	13:b0:102:SPO:H9	1.91	0.41
1:L:230:HIS:HE1	2:M:234:GLU:OE2	1.86	0.41
8:L:301:BCL:CGA	8:L:302:BCL:HBC1	2.50	0.41
13:3:103:SPO:H31	13:3:103:SPO:H5	1.72	0.41
4:1:27:LEU:O	4:1:31:ILE:HG13	2.21	0.41
13:7:102:SPO:C27	5:8:27:GLY:HA3	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:101:BCL:H102	8:8:101:BCL:H142	2.03	0.41
13:9:102:SPO:H361	5:0:20:LEU:HD12	2.03	0.41
1:l:150:ILE:HD11	11:h:301:PC1:H291	2.03	0.41
8:b:101:BCL:HMA1	8:d:103:BCL:HMA1	2.03	0.41
5:t:43:TYR:OH	8:t:101:BCL:H18	2.21	0.41
1:L:179:PHE:CE1	10:L:304:U10:H23	2.55	0.40
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.56	0.40
11:h:301:PC1:H261	14:h:303:CDL:H352	2.03	0.40
13:f:102:SPO:H26	13:f:102:SPO:H241	1.87	0.40
13:r:104:SPO:H362	13:r:104:SPO:H341	1.81	0.40
4:b1:4:PHE:HD1	4:b1:4:PHE:HA	1.76	0.40
1:L:189:LEU:HD22	1:L:216:PHE:HZ	1.86	0.40
1:L:218:ASP:O	2:M:132:ARG:NH2	2.54	0.40
14:M:406:CDL:H142	14:M:406:CDL:H111	1.84	0.40
13:O:102:SPO:H241	13:O:102:SPO:H26	1.84	0.40
13:3:102:SPO:H26	13:3:102:SPO:H241	1.85	0.40
1:l:168:HIS:HE2	8:l:301:BCL:HHC	1.85	0.40
8:l:307:BCL:H61	8:l:307:BCL:H102	1.97	0.40
2:m:130:TRP:NE1	2:m:147:ALA:O	2.47	0.40
13:o:102:SPO:H26	13:o:102:SPO:H241	1.84	0.40
8:u:101:BCL:H112	8:u:101:BCL:H72	1.89	0.40
13:M:405:SPO:H361	13:M:405:SPO:H341	1.66	0.40
5:T:43:TYR:OH	8:T:101:BCL:H18	2.21	0.40
8:U:101:BCL:H112	8:U:101:BCL:H72	1.89	0.40
4:W:11:PHE:HD1	4:W:11:PHE:HA	1.77	0.40
4:i:43:TRP:CZ2	8:i:101:BCL:HHC	2.56	0.40
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.86	0.40
1:L:175:ILE:HD11	10:L:305:U10:H13	2.02	0.40
2:M:155:TRP:HB2	14:M:406:CDL:H792	2.04	0.40
3:H:60:LYS:HE3	3:H:60:LYS:HB2	1.89	0.40
4:A:36:LEU:O	4:A:42:ASN:ND2	2.54	0.40
4:D:27:LEU:O	4:D:31:ILE:HG13	2.21	0.40
8:G:101:BCL:HBB2	8:G:101:BCL:H121	2.02	0.40
1:l:189:LEU:HD22	1:l:216:PHE:HZ	1.86	0.40
2:m:24:VAL:HG11	2:m:29:ARG:NH2	2.36	0.40
2:m:182:HIS:CD2	13:m:405:SPO:H181	2.57	0.40
8:g:101:BCL:HBB2	8:g:101:BCL:H121	2.02	0.40
13:r:103:SPO:H361	13:r:103:SPO:H341	1.51	0.40
8:b9:101:BCL:OBB	8:b9:101:BCL:HHC	2.21	0.40
14:M:406:CDL:H602	14:M:406:CDL:H571	1.88	0.40
8:J:101:BCL:H112	8:J:101:BCL:C2B	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:103:SPO:H26	13:N:103:SPO:H241	1.96	0.40
5:8:39:HIS:CD2	8:8:101:BCL:H91	2.57	0.40
1:l:180:PHE:CD2	1:l:240:ALA:HB1	2.56	0.40
10:l:305:U10:H72	10:l:305:U10:H1M3	1.91	0.40
13:a:102:SPO:H26	13:a:102:SPO:H241	1.85	0.40
13:a:102:SPO:H362	13:a:102:SPO:H341	1.71	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%)	273 (98%)	6 (2%)	0	100	100
1	l	279/282 (99%)	273 (98%)	6 (2%)	0	100	100
2	M	305/308 (99%)	297 (97%)	8 (3%)	0	100	100
2	m	305/308 (99%)	297 (97%)	8 (3%)	0	100	100
3	H	256/260 (98%)	252 (98%)	4 (2%)	0	100	100
3	h	256/260 (98%)	252 (98%)	4 (2%)	0	100	100
4	1	51/58 (88%)	49 (96%)	2 (4%)	0	100	100
4	3	52/58 (90%)	52 (100%)	0	0	100	100
4	5	52/58 (90%)	52 (100%)	0	0	100	100
4	6	46/58 (79%)	45 (98%)	1 (2%)	0	100	100
4	7	46/58 (79%)	45 (98%)	1 (2%)	0	100	100
4	9	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	A	53/58 (91%)	53 (100%)	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	52/58 (90%)	52 (100%)	0	0	100	100
4	K	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	O	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	Q	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	S	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	U	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	W	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	a	53/58 (91%)	53 (100%)	0	0	100	100
4	b1	51/58 (88%)	49 (96%)	2 (4%)	0	100	100
4	b9	52/58 (90%)	51 (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%)	52 (100%)	0	0	100	100
4	k	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	o	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	q	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	s	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	u	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	w	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
5	0	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	2	38/49 (78%)	38 (100%)	0	0	100	100
5	4	38/49 (78%)	38 (100%)	0	0	100	100
5	8	42/49 (86%)	42 (100%)	0	0	100	100
5	B	42/49 (86%)	42 (100%)	0	0	100	100
5	C	41/49 (84%)	41 (100%)	0	0	100	100
5	E	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	G	41/49 (84%)	41 (100%)	0	0	100	100
5	J	40/49 (82%)	40 (100%)	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
5	b	42/49 (86%)	42 (100%)	0	0	100	100
5	b0	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	b8	42/49 (86%)	42 (100%)	0	0	100	100
5	c	41/49 (84%)	41 (100%)	0	0	100	100
5	e	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	g	41/49 (84%)	41 (100%)	0	0	100	100
5	j	40/49 (82%)	40 (100%)	0	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	50/82 (61%)	50 (100%)	0	0	100	100
6	x	50/82 (61%)	50 (100%)	0	0	100	100
7	Y	49/53 (92%)	49 (100%)	0	0	100	100
7	y	49/53 (92%)	49 (100%)	0	0	100	100
All	All	4462/4966 (90%)	4394 (98%)	68 (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%)	219 (100%)	1 (0%)	81	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l	220/221 (100%)	219 (100%)	1 (0%)	81	93
2	M	240/241 (100%)	237 (99%)	3 (1%)	61	86
2	m	240/241 (100%)	237 (99%)	3 (1%)	61	86
3	H	207/208 (100%)	207 (100%)	0	100	100
3	h	207/208 (100%)	207 (100%)	0	100	100
4	1	48/51 (94%)	47 (98%)	1 (2%)	47	77
4	3	49/51 (96%)	49 (100%)	0	100	100
4	5	49/51 (96%)	49 (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%)	49 (100%)	0	100	100
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%)	47 (98%)	1 (2%)	47	77
4	a	49/51 (96%)	49 (100%)	0	100	100
4	b1	48/51 (94%)	47 (98%)	1 (2%)	47	77
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%)	49 (100%)	0	100	100
4	q	49/51 (96%)	49 (100%)	0	100	100
4	s	49/51 (96%)	49 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	u	48/51 (94%)	48 (100%)	0	100	100
4	w	48/51 (94%)	47 (98%)	1 (2%)	47	77
5	0	35/40 (88%)	35 (100%)	0	100	100
5	2	33/40 (82%)	33 (100%)	0	100	100
5	4	33/40 (82%)	33 (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	35/40 (88%)	35 (100%)	0	100	100
5	E	35/40 (88%)	34 (97%)	1 (3%)	37	71
5	G	35/40 (88%)	35 (100%)	0	100	100
5	J	34/40 (85%)	34 (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%)	34 (100%)	0	100	100
5	b	36/40 (90%)	36 (100%)	0	100	100
5	b0	35/40 (88%)	35 (100%)	0	100	100
5	b8	36/40 (90%)	36 (100%)	0	100	100
5	c	35/40 (88%)	35 (100%)	0	100	100
5	e	35/40 (88%)	34 (97%)	1 (3%)	37	71
5	g	35/40 (88%)	35 (100%)	0	100	100
5	j	34/40 (85%)	34 (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%)	34 (100%)	0	100	100
6	X	40/66 (61%)	40 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	x	40/66 (61%)	40 (100%)	0	100	100
7	Y	35/37 (95%)	35 (100%)	0	100	100
7	y	35/37 (95%)	35 (100%)	0	100	100
All	All	3808/4094 (93%)	3794 (100%)	14 (0%)	81	94

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

Mol	Chain	Res	Type
1	L	235	LEU
2	M	182	HIS
2	M	216	PHE
2	M	274	VAL
5	E	7	LEU
4	W	11	PHE
4	l	29	VAL
1	l	235	LEU
2	m	182	HIS
2	m	216	PHE
2	m	274	VAL
5	e	7	LEU
4	w	11	PHE
4	b1	29	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	258	GLN
2	M	307	ASN
5	E	16	GLN
4	F	42	ASN
5	J	16	GLN
5	P	18	GLN
4	3	52	ASN
5	2	21	HIS
4	7	20	GLN
4	7	42	ASN
2	m	307	ASN
5	e	16	GLN
4	f	42	ASN
5	j	16	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	p	18	GLN
4	5	52	ASN
5	4	21	HIS
4	6	20	GLN
4	6	42	ASN
5	b8	16	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 152 ligands modelled in this entry, 2 are monoatomic - leaving 150 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	$\# Z > 2$
10	U10	l	304	-	38,38,63	2.69	11 (28%)	46,49,79	1.67	12 (26%)
8	BCL	l	302	1	66,71,74	1.13	8 (12%)	79,111,115	1.43	8 (10%)
8	BCL	F	101	4	69,74,74	1.11	5 (7%)	83,115,115	1.49	10 (12%)
8	BCL	E	101	5	69,74,74	1.11	5 (7%)	83,115,115	1.40	8 (9%)
10	U10	l	305	-	43,43,63	2.68	13 (30%)	52,55,79	1.71	13 (25%)
11	PC1	D	101	-	39,39,53	0.56	0	45,47,61	0.67	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	U10	M	404	-	48,48,63	2.67	14 (29%)	58,61,79	1.69	14 (24%)
8	BCL	5	101	4	69,74,74	1.12	6 (8%)	83,115,115	1.46	9 (10%)
8	BCL	k	101	4	69,74,74	1.11	6 (8%)	83,115,115	1.50	12 (14%)
8	BCL	j	101	5	64,69,74	1.13	5 (7%)	77,109,115	1.46	9 (11%)
9	BPB	m	403	-	47,60,70	1.67	3 (6%)	44,89,101	2.32	10 (22%)
11	PC1	A	105	-	35,35,53	0.54	0	41,43,61	0.64	1 (2%)
13	SPO	u	102	-	40,41,41	0.19	0	47,50,50	0.37	0
8	BCL	S	101	4	69,74,74	1.12	5 (7%)	83,115,115	1.55	12 (14%)
10	U10	m	407	-	38,38,63	2.69	12 (31%)	46,49,79	1.66	11 (23%)
8	BCL	p	101	5	64,69,74	1.14	4 (6%)	77,109,115	1.46	8 (10%)
13	SPO	e	102	-	40,41,41	0.24	0	47,50,50	0.28	0
13	SPO	m	405	-	40,41,41	0.30	0	47,50,50	0.38	0
8	BCL	T	101	5	69,74,74	1.12	5 (7%)	83,115,115	1.50	9 (10%)
13	SPO	F	102	-	40,41,41	0.18	0	47,50,50	0.33	0
13	SPO	U	102	-	40,41,41	0.19	0	47,50,50	0.37	0
8	BCL	e	101	5	69,74,74	1.11	5 (7%)	83,115,115	1.40	8 (9%)
13	SPO	f	103	-	40,41,41	0.27	0	47,50,50	0.44	0
13	SPO	5	102	-	40,41,41	0.19	0	47,50,50	0.29	0
8	BCL	U	101	4	69,74,74	1.12	7 (10%)	83,115,115	1.47	11 (13%)
11	PC1	h	302	-	33,33,53	0.56	0	39,41,61	0.71	1 (2%)
8	BCL	D	103	4	69,74,74	1.13	6 (8%)	83,115,115	1.52	13 (15%)
13	SPO	j	102	-	40,41,41	0.17	0	47,50,50	0.33	0
13	SPO	I	102	-	40,41,41	0.15	0	47,50,50	0.31	0
13	SPO	M	405	-	40,41,41	0.30	0	47,50,50	0.38	0
8	BCL	r	102	5	69,74,74	1.11	5 (7%)	83,115,115	1.43	10 (12%)
11	PC1	L	306	-	38,38,53	0.57	0	44,46,61	0.59	1 (2%)
8	BCL	O	101	4	69,74,74	1.09	6 (8%)	83,115,115	1.53	11 (13%)
13	SPO	i	102	-	40,41,41	0.15	0	47,50,50	0.31	0
13	SPO	R	104	-	40,41,41	0.21	0	47,50,50	0.28	0
8	BCL	W	101	4	69,74,74	1.12	5 (7%)	83,115,115	1.44	8 (9%)
10	U10	m	404	-	48,48,63	2.68	14 (29%)	58,61,79	1.69	14 (24%)
11	PC1	L	308	-	31,31,53	0.60	0	37,39,61	0.75	1 (2%)
9	BPB	M	403	-	47,60,70	1.68	3 (6%)	44,89,101	2.32	10 (22%)
8	BCL	i	101	4	69,74,74	1.08	5 (7%)	83,115,115	1.51	11 (13%)
8	BCL	B	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.45	10 (12%)
9	BPB	l	303	-	57,70,70	1.52	4 (7%)	56,101,101	2.16	10 (17%)
8	BCL	o	101	4	69,74,74	1.09	6 (8%)	83,115,115	1.52	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	SPO	3	103	-	40,41,41	0.18	0	47,50,50	0.36	0
8	BCL	v	101	5	69,74,74	1.13	5 (7%)	83,115,115	1.45	11 (13%)
8	BCL	b8	101	5	64,69,74	1.14	5 (7%)	77,109,115	1.58	11 (14%)
8	BCL	b	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.45	10 (12%)
14	CDL	m	406	-	75,75,99	1.05	8 (10%)	81,87,111	1.25	6 (7%)
13	SPO	0	102	-	40,41,41	0.18	0	47,50,50	0.47	0
8	BCL	Q	101	4	69,74,74	1.10	5 (7%)	83,115,115	1.52	12 (14%)
13	SPO	c	101	-	40,41,41	0.19	0	47,50,50	0.30	0
8	BCL	4	101	5	59,64,74	1.19	5 (8%)	71,103,115	1.50	7 (9%)
11	PC1	d	102	-	36,36,53	0.58	0	42,44,61	0.68	1 (2%)
13	SPO	r	103	-	40,41,41	0.31	0	47,50,50	0.45	0
11	PC1	H	301	-	41,41,53	0.54	0	47,49,61	0.65	0
11	PC1	d	101	-	39,39,53	0.56	0	45,47,61	0.67	1 (2%)
13	SPO	R	101	-	40,41,41	0.22	0	47,50,50	0.32	0
8	BCL	L	302	1	66,71,74	1.13	7 (10%)	79,111,115	1.43	8 (10%)
11	PC1	l	308	-	31,31,53	0.60	0	37,39,61	0.76	1 (2%)
13	SPO	V	102	-	40,41,41	0.28	0	47,50,50	0.47	0
8	BCL	w	101	4	69,74,74	1.12	5 (7%)	83,115,115	1.44	8 (9%)
13	SPO	A	102	-	40,41,41	0.18	0	47,50,50	0.35	0
8	BCL	9	101	4	59,64,74	1.18	5 (8%)	71,103,115	1.58	11 (15%)
13	SPO	3	102	-	40,41,41	0.19	0	47,50,50	0.29	0
8	BCL	2	101	5	59,64,74	1.19	5 (8%)	71,103,115	1.50	7 (9%)
13	SPO	b	102	-	40,41,41	0.23	0	47,50,50	0.28	0
8	BCL	a	101	4	69,74,74	1.11	6 (8%)	83,115,115	1.50	13 (15%)
8	BCL	1	101	4	54,59,74	1.23	5 (9%)	65,97,115	1.61	10 (15%)
10	U10	L	304	-	38,38,63	2.69	12 (31%)	46,49,79	1.67	12 (26%)
13	SPO	v	103	-	40,41,41	0.24	0	47,50,50	0.39	0
8	BCL	J	101	5	64,69,74	1.13	5 (7%)	77,109,115	1.46	9 (11%)
8	BCL	L	307	2	69,74,74	1.10	6 (8%)	83,115,115	1.48	8 (9%)
8	BCL	8	101	5	64,69,74	1.14	5 (7%)	77,109,115	1.58	11 (14%)
11	PC1	A	103	-	44,44,53	0.54	0	50,52,61	0.66	1 (2%)
8	BCL	f	101	4	69,74,74	1.11	5 (7%)	83,115,115	1.49	10 (12%)
8	BCL	b0	101	5	64,69,74	1.14	5 (7%)	77,109,115	1.56	11 (14%)
11	PC1	H	302	-	33,33,53	0.56	0	39,41,61	0.71	1 (2%)
8	BCL	z	101	5	60,65,74	1.18	5 (8%)	72,104,115	1.47	9 (12%)
13	SPO	9	102	-	40,41,41	0.27	0	47,50,50	0.34	0
8	BCL	L	301	1	69,74,74	1.13	6 (8%)	83,115,115	1.44	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	7	101	4	64,69,74	1.14	6 (9%)	77,109,115	1.46	8 (10%)
8	BCL	3	101	4	69,74,74	1.12	6 (8%)	83,115,115	1.46	9 (10%)
8	BCL	I	101	4	69,74,74	1.08	5 (7%)	83,115,115	1.50	11 (13%)
13	SPO	i	103	-	40,41,41	0.20	0	47,50,50	0.30	0
8	BCL	K	101	4	69,74,74	1.10	6 (8%)	83,115,115	1.50	11 (13%)
11	PC1	a	105	-	35,35,53	0.55	0	41,43,61	0.64	1 (2%)
13	SPO	O	102	-	40,41,41	0.18	0	47,50,50	0.35	0
13	SPO	D	104	-	40,41,41	0.23	0	47,50,50	0.33	0
14	CDL	h	303	-	62,62,99	1.15	8 (12%)	68,74,111	1.24	6 (8%)
13	SPO	J	102	-	40,41,41	0.17	0	47,50,50	0.33	0
8	BCL	N	102	5	64,69,74	1.14	4 (6%)	77,109,115	1.45	8 (10%)
8	BCL	0	101	5	64,69,74	1.14	5 (7%)	77,109,115	1.55	11 (14%)
8	BCL	l	301	1	69,74,74	1.13	6 (8%)	83,115,115	1.44	11 (13%)
13	SPO	r	101	-	40,41,41	0.22	0	47,50,50	0.31	0
13	SPO	R	103	-	40,41,41	0.31	0	47,50,50	0.45	0
13	SPO	d	104	-	40,41,41	0.23	0	47,50,50	0.33	0
14	CDL	M	406	-	75,75,99	1.05	8 (10%)	81,87,111	1.25	6 (7%)
8	BCL	G	101	5	69,74,74	1.11	5 (7%)	83,115,115	1.43	9 (10%)
13	SPO	b9	102	-	40,41,41	0.27	0	47,50,50	0.34	0
8	BCL	n	102	5	64,69,74	1.14	4 (6%)	77,109,115	1.45	8 (10%)
8	BCL	Z	101	5	60,65,74	1.18	5 (8%)	72,104,115	1.47	9 (12%)
8	BCL	V	101	5	69,74,74	1.13	5 (7%)	83,115,115	1.45	11 (13%)
13	SPO	s	102	-	40,41,41	0.22	0	47,50,50	0.35	0
11	PC1	A	104	-	30,30,53	0.61	0	36,38,61	0.70	1 (2%)
13	SPO	S	102	-	40,41,41	0.21	0	47,50,50	0.34	0
13	SPO	b0	102	-	40,41,41	0.18	0	47,50,50	0.47	0
13	SPO	B	102	-	40,41,41	0.23	0	47,50,50	0.28	0
13	SPO	N	103	-	40,41,41	0.17	0	47,50,50	0.36	0
8	BCL	s	101	4	69,74,74	1.12	5 (7%)	83,115,115	1.55	12 (14%)
11	PC1	h	301	-	41,41,53	0.54	0	47,49,61	0.65	0
13	SPO	v	102	-	40,41,41	0.29	0	47,50,50	0.47	0
11	PC1	D	102	-	36,36,53	0.58	0	42,44,61	0.68	1 (2%)
13	SPO	E	102	-	40,41,41	0.24	0	47,50,50	0.28	0
13	SPO	n	101	-	40,41,41	0.16	0	47,50,50	0.30	0
8	BCL	b9	101	4	59,64,74	1.18	5 (8%)	71,103,115	1.58	11 (15%)
13	SPO	C	101	-	40,41,41	0.19	0	47,50,50	0.30	0
8	BCL	P	101	5	64,69,74	1.14	4 (6%)	77,109,115	1.46	8 (10%)
10	U10	M	407	-	38,38,63	2.69	12 (31%)	46,49,79	1.66	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	SPO	f	102	-	40,41,41	0.17	0	47,50,50	0.33	0
13	SPO	n	103	-	40,41,41	0.16	0	47,50,50	0.36	0
8	BCL	q	101	4	69,74,74	1.10	5 (7%)	83,115,115	1.52	12 (14%)
8	BCL	d	103	4	69,74,74	1.13	6 (8%)	83,115,115	1.52	13 (15%)
8	BCL	6	101	4	64,69,74	1.14	5 (7%)	77,109,115	1.46	7 (9%)
8	BCL	l	307	2	69,74,74	1.10	6 (8%)	83,115,115	1.48	8 (9%)
8	BCL	t	101	5	69,74,74	1.11	5 (7%)	83,115,115	1.50	10 (12%)
13	SPO	a	102	-	40,41,41	0.18	0	47,50,50	0.35	0
13	SPO	I	103	-	40,41,41	0.20	0	47,50,50	0.30	0
8	BCL	c	102	5	64,69,74	1.15	5 (7%)	77,109,115	1.48	11 (14%)
13	SPO	F	103	-	40,41,41	0.27	0	47,50,50	0.45	0
9	BPB	L	303	-	57,70,70	1.52	4 (7%)	56,101,101	2.16	10 (17%)
14	CDL	H	303	-	62,62,99	1.15	8 (12%)	68,74,111	1.25	6 (8%)
8	BCL	g	101	5	69,74,74	1.11	5 (7%)	83,115,115	1.43	9 (10%)
13	SPO	5	103	-	40,41,41	0.18	0	47,50,50	0.35	0
13	SPO	N	101	-	40,41,41	0.15	0	47,50,50	0.30	0
8	BCL	m	402	2	69,74,74	1.14	7 (10%)	83,115,115	1.49	11 (13%)
8	BCL	C	102	5	64,69,74	1.15	5 (7%)	77,109,115	1.48	11 (14%)
13	SPO	o	102	-	40,41,41	0.18	0	47,50,50	0.34	0
13	SPO	6	102	-	40,41,41	0.19	0	47,50,50	0.39	0
11	PC1	l	306	-	38,38,53	0.57	0	44,46,61	0.59	1 (2%)
13	SPO	r	104	-	40,41,41	0.21	0	47,50,50	0.28	0
11	PC1	a	103	-	44,44,53	0.54	0	50,52,61	0.66	1 (2%)
10	U10	L	305	-	43,43,63	2.68	13 (30%)	52,55,79	1.71	13 (25%)
8	BCL	A	101	4	69,74,74	1.11	5 (7%)	83,115,115	1.50	13 (15%)
8	BCL	M	402	2	69,74,74	1.14	7 (10%)	83,115,115	1.50	11 (13%)
8	BCL	R	102	5	69,74,74	1.11	5 (7%)	83,115,115	1.42	10 (12%)
8	BCL	b1	101	4	54,59,74	1.23	5 (9%)	65,97,115	1.61	10 (15%)
13	SPO	V	103	-	40,41,41	0.25	0	47,50,50	0.40	0
8	BCL	u	101	4	69,74,74	1.12	7 (10%)	83,115,115	1.48	11 (13%)
13	SPO	7	102	-	40,41,41	0.19	0	47,50,50	0.38	0
11	PC1	a	104	-	30,30,53	0.60	0	36,38,61	0.70	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	U10	l	304	-	-	10/33/57/87	0/1/1/1
8	BCL	l	302	1	-	1/38/134/137	-
8	BCL	F	101	4	-	3/41/137/137	-
8	BCL	E	101	5	-	4/41/137/137	-
10	U10	l	305	-	-	10/39/63/87	0/1/1/1
11	PC1	D	101	-	-	18/43/43/57	-
10	U10	M	404	-	-	11/45/69/87	0/1/1/1
8	BCL	5	101	4	-	1/41/137/137	-
8	BCL	k	101	4	-	2/41/137/137	-
8	BCL	j	101	5	-	7/35/131/137	-
9	BPB	m	403	-	-	5/25/93/105	0/5/6/6
11	PC1	A	105	-	-	18/39/39/57	-
13	SPO	u	102	-	-	8/47/47/47	-
8	BCL	S	101	4	-	5/41/137/137	-
10	U10	m	407	-	-	11/33/57/87	0/1/1/1
8	BCL	p	101	5	-	9/35/131/137	-
13	SPO	e	102	-	-	15/47/47/47	-
13	SPO	m	405	-	-	8/47/47/47	-
8	BCL	T	101	5	-	4/41/137/137	-
13	SPO	F	102	-	-	9/47/47/47	-
13	SPO	U	102	-	-	8/47/47/47	-
8	BCL	e	101	5	-	4/41/137/137	-
13	SPO	f	103	-	-	12/47/47/47	-
13	SPO	5	102	-	-	10/47/47/47	-
8	BCL	U	101	4	-	1/41/137/137	-
11	PC1	h	302	-	-	11/37/37/57	-
8	BCL	D	103	4	-	2/41/137/137	-
13	SPO	j	102	-	-	10/47/47/47	-
13	SPO	I	102	-	-	13/47/47/47	-
13	SPO	M	405	-	-	8/47/47/47	-
8	BCL	r	102	5	-	8/41/137/137	-
11	PC1	L	306	-	-	14/42/42/57	-
8	BCL	O	101	4	-	1/41/137/137	-
13	SPO	i	102	-	-	13/47/47/47	-
13	SPO	R	104	-	-	11/47/47/47	-
8	BCL	W	101	4	-	1/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	U10	m	404	-	-	11/45/69/87	0/1/1/1
11	PC1	L	308	-	-	17/35/35/57	-
9	BPB	M	403	-	-	5/25/93/105	0/5/6/6
8	BCL	i	101	4	-	2/41/137/137	-
8	BCL	B	101	5	-	6/41/137/137	-
9	BPB	l	303	-	-	6/37/105/105	0/5/6/6
8	BCL	o	101	4	-	1/41/137/137	-
13	SPO	3	103	-	-	13/47/47/47	-
8	BCL	v	101	5	-	8/41/137/137	-
8	BCL	b8	101	5	-	7/35/131/137	-
8	BCL	b	101	5	-	6/41/137/137	-
14	CDL	m	406	-	-	35/86/86/110	-
13	SPO	0	102	-	-	8/47/47/47	-
8	BCL	Q	101	4	-	3/41/137/137	-
13	SPO	c	101	-	-	11/47/47/47	-
8	BCL	4	101	5	-	4/29/125/137	-
11	PC1	d	102	-	-	19/40/40/57	-
13	SPO	r	103	-	-	21/47/47/47	-
11	PC1	H	301	-	-	7/45/45/57	-
11	PC1	d	101	-	-	18/43/43/57	-
13	SPO	R	101	-	-	12/47/47/47	-
8	BCL	L	302	1	-	1/38/134/137	-
11	PC1	l	308	-	-	17/35/35/57	-
13	SPO	V	102	-	-	9/47/47/47	-
8	BCL	w	101	4	-	1/41/137/137	-
13	SPO	A	102	-	-	9/47/47/47	-
8	BCL	9	101	4	-	1/29/125/137	-
13	SPO	3	102	-	-	10/47/47/47	-
8	BCL	2	101	5	-	4/29/125/137	-
13	SPO	b	102	-	-	14/47/47/47	-
8	BCL	a	101	4	-	3/41/137/137	-
8	BCL	1	101	4	-	1/23/119/137	-
10	U10	L	304	-	-	10/33/57/87	0/1/1/1
13	SPO	v	103	-	-	10/47/47/47	-
8	BCL	J	101	5	-	7/35/131/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	L	307	2	-	4/41/137/137	-
8	BCL	8	101	5	-	7/35/131/137	-
11	PC1	A	103	-	-	20/48/48/57	-
8	BCL	f	101	4	-	3/41/137/137	-
8	BCL	b0	101	5	-	4/35/131/137	-
11	PC1	H	302	-	-	11/37/37/57	-
8	BCL	z	101	5	-	2/31/127/137	-
13	SPO	9	102	-	-	14/47/47/47	-
8	BCL	L	301	1	-	1/41/137/137	-
8	BCL	7	101	4	-	3/35/131/137	-
8	BCL	3	101	4	-	1/41/137/137	-
8	BCL	I	101	4	-	2/41/137/137	-
13	SPO	i	103	-	-	12/47/47/47	-
8	BCL	K	101	4	-	2/41/137/137	-
11	PC1	a	105	-	-	18/39/39/57	-
13	SPO	O	102	-	-	8/47/47/47	-
13	SPO	D	104	-	-	7/47/47/47	-
14	CDL	h	303	-	-	27/73/73/110	-
13	SPO	J	102	-	-	10/47/47/47	-
8	BCL	N	102	5	-	6/35/131/137	-
8	BCL	0	101	5	-	4/35/131/137	-
8	BCL	l	301	1	-	1/41/137/137	-
13	SPO	r	101	-	-	13/47/47/47	-
13	SPO	R	103	-	-	21/47/47/47	-
13	SPO	d	104	-	-	7/47/47/47	-
14	CDL	M	406	-	-	35/86/86/110	-
8	BCL	G	101	5	-	9/41/137/137	-
13	SPO	b9	102	-	-	14/47/47/47	-
8	BCL	n	102	5	-	6/35/131/137	-
8	BCL	Z	101	5	-	2/31/127/137	-
8	BCL	V	101	5	-	7/41/137/137	-
13	SPO	s	102	-	-	8/47/47/47	-
11	PC1	A	104	-	-	17/34/34/57	-
13	SPO	S	102	-	-	8/47/47/47	-
13	SPO	b0	102	-	-	8/47/47/47	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SPO	B	102	-	-	14/47/47/47	-
13	SPO	N	103	-	-	10/47/47/47	-
8	BCL	s	101	4	-	5/41/137/137	-
11	PC1	h	301	-	-	7/45/45/57	-
13	SPO	v	102	-	-	9/47/47/47	-
11	PC1	D	102	-	-	19/40/40/57	-
13	SPO	E	102	-	-	15/47/47/47	-
13	SPO	n	101	-	-	8/47/47/47	-
8	BCL	b9	101	4	-	1/29/125/137	-
13	SPO	C	101	-	-	11/47/47/47	-
8	BCL	P	101	5	-	9/35/131/137	-
10	U10	M	407	-	-	11/33/57/87	0/1/1/1
13	SPO	f	102	-	-	9/47/47/47	-
13	SPO	n	103	-	-	10/47/47/47	-
8	BCL	q	101	4	-	3/41/137/137	-
8	BCL	d	103	4	-	2/41/137/137	-
8	BCL	6	101	4	-	3/35/131/137	-
8	BCL	l	307	2	-	4/41/137/137	-
8	BCL	t	101	5	-	4/41/137/137	-
13	SPO	a	102	-	-	9/47/47/47	-
13	SPO	I	103	-	-	12/47/47/47	-
8	BCL	c	102	5	-	7/35/131/137	-
13	SPO	F	103	-	-	12/47/47/47	-
9	BPB	L	303	-	-	6/37/105/105	0/5/6/6
14	CDL	H	303	-	-	27/73/73/110	-
8	BCL	g	101	5	-	9/41/137/137	-
13	SPO	5	103	-	-	13/47/47/47	-
13	SPO	N	101	-	-	8/47/47/47	-
8	BCL	m	402	2	-	2/41/137/137	-
8	BCL	C	102	5	-	7/35/131/137	-
13	SPO	o	102	-	-	8/47/47/47	-
13	SPO	6	102	-	-	11/47/47/47	-
11	PC1	l	306	-	-	14/42/42/57	-
13	SPO	r	104	-	-	11/47/47/47	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PC1	a	103	-	-	20/48/48/57	-
10	U10	L	305	-	-	10/39/63/87	0/1/1/1
8	BCL	A	101	4	-	3/41/137/137	-
8	BCL	M	402	2	-	2/41/137/137	-
8	BCL	R	102	5	-	8/41/137/137	-
8	BCL	b1	101	4	-	1/23/119/137	-
13	SPO	V	103	-	-	10/47/47/47	-
8	BCL	u	101	4	-	1/41/137/137	-
13	SPO	7	102	-	-	11/47/47/47	-
11	PC1	a	104	-	-	17/34/34/57	-

All (490) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	303	BPB	CAC-C3C	8.72	1.55	1.33
9	l	303	BPB	CAC-C3C	8.71	1.55	1.33
9	M	403	BPB	CAC-C3C	8.51	1.55	1.33
9	m	403	BPB	CAC-C3C	8.50	1.55	1.33
10	L	305	U10	C13-C14	6.08	1.47	1.33
10	l	305	U10	C13-C14	6.08	1.47	1.33
10	l	304	U10	C23-C24	6.04	1.47	1.33
10	l	305	U10	C8-C9	6.03	1.47	1.33
10	L	304	U10	C23-C24	6.03	1.47	1.33
10	m	407	U10	C8-C9	6.02	1.47	1.33
10	m	407	U10	C23-C24	6.02	1.47	1.33
10	M	407	U10	C8-C9	6.01	1.47	1.33
10	L	305	U10	C8-C9	6.00	1.47	1.33
10	M	407	U10	C23-C24	6.00	1.47	1.33
10	m	407	U10	C13-C14	5.99	1.47	1.33
10	M	407	U10	C13-C14	5.99	1.47	1.33
10	L	305	U10	C28-C29	5.98	1.47	1.33
10	l	304	U10	C13-C14	5.97	1.47	1.33
10	l	305	U10	C23-C24	5.97	1.47	1.33
10	l	305	U10	C28-C29	5.97	1.47	1.33
10	L	304	U10	C13-C14	5.97	1.47	1.33
10	l	305	U10	C18-C19	5.97	1.47	1.33
10	L	305	U10	C23-C24	5.96	1.47	1.33
10	L	305	U10	C18-C19	5.95	1.47	1.33
10	l	304	U10	C18-C19	5.94	1.47	1.33
10	L	304	U10	C18-C19	5.94	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	407	U10	C18-C19	5.93	1.47	1.33
10	m	407	U10	C18-C19	5.91	1.47	1.33
10	m	404	U10	C28-C29	5.90	1.47	1.33
10	M	404	U10	C28-C29	5.89	1.47	1.33
10	m	404	U10	C33-C34	5.89	1.47	1.33
10	m	404	U10	C18-C19	5.87	1.47	1.33
10	M	404	U10	C18-C19	5.86	1.47	1.33
10	M	404	U10	C33-C34	5.86	1.47	1.33
10	L	304	U10	C8-C9	5.84	1.47	1.33
10	l	304	U10	C8-C9	5.82	1.46	1.33
10	m	404	U10	C23-C24	5.79	1.46	1.33
10	M	404	U10	C23-C24	5.78	1.46	1.33
10	m	404	U10	C8-C9	5.78	1.46	1.33
10	M	404	U10	C8-C9	5.78	1.46	1.33
10	m	404	U10	C13-C14	5.76	1.46	1.33
10	M	404	U10	C13-C14	5.73	1.46	1.33
10	m	404	U10	O3-C3	-5.61	1.23	1.36
10	M	404	U10	O3-C3	-5.59	1.23	1.36
10	m	404	U10	O4-C4	-5.58	1.23	1.36
10	M	404	U10	O4-C4	-5.57	1.23	1.36
10	l	304	U10	O3-C3	-5.51	1.23	1.36
10	L	304	U10	O3-C3	-5.49	1.23	1.36
10	m	407	U10	O4-C4	-5.46	1.23	1.36
10	M	407	U10	O4-C4	-5.44	1.23	1.36
10	l	304	U10	O4-C4	-5.43	1.23	1.36
10	L	304	U10	O4-C4	-5.43	1.23	1.36
10	L	305	U10	O3-C3	-5.42	1.23	1.36
10	m	407	U10	O3-C3	-5.42	1.23	1.36
10	l	305	U10	O3-C3	-5.42	1.23	1.36
10	M	407	U10	O3-C3	-5.42	1.23	1.36
10	L	305	U10	O4-C4	-5.30	1.23	1.36
10	l	305	U10	O4-C4	-5.29	1.23	1.36
10	l	304	U10	C28-C29	5.24	1.47	1.32
10	L	304	U10	C28-C29	5.24	1.47	1.32
10	l	305	U10	C33-C34	5.24	1.47	1.32
10	m	404	U10	C38-C39	5.24	1.47	1.32
10	M	404	U10	C38-C39	5.23	1.47	1.32
10	L	305	U10	C33-C34	5.22	1.47	1.32
10	m	407	U10	C28-C29	5.22	1.47	1.32
10	M	407	U10	C28-C29	5.21	1.47	1.32
8	T	101	BCL	MG-NA	4.82	2.17	2.06
8	t	101	BCL	MG-NA	4.81	2.17	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	r	102	BCL	MG-NA	4.80	2.17	2.06
8	R	102	BCL	MG-NA	4.80	2.17	2.06
8	m	402	BCL	MG-NA	4.79	2.17	2.06
8	M	402	BCL	MG-NA	4.78	2.17	2.06
8	W	101	BCL	MG-NA	4.76	2.17	2.06
8	7	101	BCL	MG-NA	4.76	2.17	2.06
8	6	101	BCL	MG-NA	4.76	2.17	2.06
8	5	101	BCL	MG-NA	4.75	2.17	2.06
8	3	101	BCL	MG-NA	4.74	2.17	2.06
8	U	101	BCL	MG-NA	4.72	2.17	2.06
8	w	101	BCL	MG-NA	4.72	2.17	2.06
8	q	101	BCL	MG-NA	4.72	2.17	2.06
8	L	301	BCL	MG-NA	4.71	2.17	2.06
8	u	101	BCL	MG-NA	4.71	2.17	2.06
8	Q	101	BCL	MG-NA	4.70	2.17	2.06
8	n	102	BCL	MG-NA	4.70	2.17	2.06
8	v	101	BCL	MG-NA	4.70	2.17	2.06
8	N	102	BCL	MG-NA	4.69	2.17	2.06
8	l	301	BCL	MG-NA	4.69	2.17	2.06
8	V	101	BCL	MG-NA	4.69	2.17	2.06
8	b0	101	BCL	MG-NA	4.68	2.17	2.06
8	2	101	BCL	MG-NA	4.67	2.17	2.06
8	z	101	BCL	MG-NA	4.67	2.17	2.06
8	e	101	BCL	MG-NA	4.66	2.17	2.06
8	b1	101	BCL	MG-NA	4.66	2.17	2.06
8	P	101	BCL	MG-NA	4.65	2.17	2.06
8	p	101	BCL	MG-NA	4.65	2.17	2.06
8	4	101	BCL	MG-NA	4.65	2.17	2.06
8	s	101	BCL	MG-NA	4.65	2.17	2.06
8	0	101	BCL	MG-NA	4.65	2.17	2.06
8	Z	101	BCL	MG-NA	4.65	2.17	2.06
8	1	101	BCL	MG-NA	4.65	2.17	2.06
8	E	101	BCL	MG-NA	4.64	2.17	2.06
8	S	101	BCL	MG-NA	4.64	2.17	2.06
8	J	101	BCL	MG-NA	4.63	2.17	2.06
8	j	101	BCL	MG-NA	4.63	2.17	2.06
8	8	101	BCL	MG-NA	4.61	2.17	2.06
8	g	101	BCL	MG-NA	4.58	2.17	2.06
8	C	102	BCL	MG-NA	4.57	2.17	2.06
8	G	101	BCL	MG-NA	4.57	2.17	2.06
8	b8	101	BCL	MG-NA	4.57	2.17	2.06
8	c	102	BCL	MG-NA	4.57	2.17	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b9	101	BCL	MG-NA	4.56	2.17	2.06
8	9	101	BCL	MG-NA	4.55	2.17	2.06
8	b	101	BCL	MG-NA	4.55	2.17	2.06
8	B	101	BCL	MG-NA	4.54	2.17	2.06
8	f	101	BCL	MG-NA	4.52	2.17	2.06
8	F	101	BCL	MG-NA	4.51	2.17	2.06
8	k	101	BCL	MG-NA	4.50	2.17	2.06
8	K	101	BCL	MG-NA	4.49	2.16	2.06
8	A	101	BCL	MG-NA	4.49	2.16	2.06
8	a	101	BCL	MG-NA	4.46	2.16	2.06
8	D	103	BCL	MG-NA	4.44	2.16	2.06
8	d	103	BCL	MG-NA	4.44	2.16	2.06
8	l	302	BCL	MG-NA	4.40	2.16	2.06
8	o	101	BCL	MG-NA	4.39	2.16	2.06
8	L	302	BCL	MG-NA	4.37	2.16	2.06
8	l	307	BCL	MG-NA	4.37	2.16	2.06
8	O	101	BCL	MG-NA	4.37	2.16	2.06
8	L	307	BCL	MG-NA	4.36	2.16	2.06
8	i	101	BCL	MG-NA	4.29	2.16	2.06
8	I	101	BCL	MG-NA	4.26	2.16	2.06
9	M	403	BPB	CBD-CGD	-4.05	1.47	1.52
9	m	403	BPB	CBD-CGD	-4.02	1.47	1.52
9	L	303	BPB	CBD-CGD	-3.80	1.47	1.52
9	l	303	BPB	CBD-CGD	-3.78	1.47	1.52
10	M	404	U10	C4-C5	-3.49	1.38	1.48
8	v	101	BCL	MG-NC	3.49	2.14	2.06
10	m	404	U10	C4-C5	-3.49	1.38	1.48
8	V	101	BCL	MG-NC	3.46	2.14	2.06
10	m	404	U10	C3-C2	-3.46	1.38	1.48
10	M	404	U10	C3-C2	-3.46	1.38	1.48
8	r	102	BCL	MG-NC	3.46	2.14	2.06
8	R	102	BCL	MG-NC	3.46	2.14	2.06
10	l	304	U10	C3-C2	-3.44	1.39	1.48
8	w	101	BCL	MG-NC	3.43	2.14	2.06
10	L	304	U10	C3-C2	-3.43	1.39	1.48
8	W	101	BCL	MG-NC	3.40	2.14	2.06
8	T	101	BCL	MG-NC	3.39	2.14	2.06
8	t	101	BCL	MG-NC	3.39	2.14	2.06
8	5	101	BCL	MG-NC	3.37	2.14	2.06
8	P	101	BCL	MG-NC	3.37	2.14	2.06
8	p	101	BCL	MG-NC	3.37	2.14	2.06
8	Z	101	BCL	MG-NC	3.37	2.14	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	z	101	BCL	MG-NC	3.36	2.14	2.06
8	3	101	BCL	MG-NC	3.35	2.14	2.06
8	1	101	BCL	MG-NC	3.33	2.14	2.06
10	L	304	U10	C4-C5	-3.32	1.39	1.48
10	l	304	U10	C4-C5	-3.31	1.39	1.48
8	b1	101	BCL	MG-NC	3.31	2.14	2.06
8	u	101	BCL	MG-NC	3.31	2.14	2.06
8	c	102	BCL	MG-NC	3.31	2.14	2.06
8	0	101	BCL	MG-NC	3.31	2.14	2.06
8	U	101	BCL	MG-NC	3.30	2.14	2.06
8	b0	101	BCL	MG-NC	3.29	2.14	2.06
8	n	102	BCL	MG-NC	3.28	2.14	2.06
8	N	102	BCL	MG-NC	3.28	2.14	2.06
8	C	102	BCL	MG-NC	3.28	2.14	2.06
8	G	101	BCL	MG-NC	3.25	2.14	2.06
10	M	407	U10	C4-C5	-3.25	1.39	1.48
8	Q	101	BCL	MG-NC	3.24	2.14	2.06
8	q	101	BCL	MG-NC	3.24	2.14	2.06
8	g	101	BCL	MG-NC	3.24	2.14	2.06
8	F	101	BCL	MG-NC	3.22	2.13	2.06
10	l	305	U10	C4-C5	-3.22	1.39	1.48
10	l	305	U10	C3-C2	-3.22	1.39	1.48
10	m	407	U10	C4-C5	-3.21	1.39	1.48
8	6	101	BCL	MG-NC	3.21	2.13	2.06
8	7	101	BCL	MG-NC	3.20	2.13	2.06
10	M	407	U10	C3-C2	-3.20	1.39	1.48
10	m	407	U10	C3-C2	-3.20	1.39	1.48
8	f	101	BCL	MG-NC	3.20	2.13	2.06
10	L	305	U10	C3-C2	-3.19	1.39	1.48
8	s	101	BCL	MG-NC	3.19	2.13	2.06
10	L	305	U10	C4-C5	-3.19	1.39	1.48
8	4	101	BCL	MG-NC	3.18	2.13	2.06
8	S	101	BCL	MG-NC	3.17	2.13	2.06
8	L	301	BCL	MG-NC	3.17	2.13	2.06
8	l	301	BCL	MG-NC	3.17	2.13	2.06
8	k	101	BCL	MG-NC	3.16	2.13	2.06
8	2	101	BCL	MG-NC	3.16	2.13	2.06
8	b8	101	BCL	MG-NC	3.16	2.13	2.06
8	K	101	BCL	MG-NC	3.16	2.13	2.06
8	a	101	BCL	MG-NC	3.16	2.13	2.06
8	8	101	BCL	MG-NC	3.15	2.13	2.06
8	E	101	BCL	MG-NC	3.14	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	101	BCL	MG-NC	3.14	2.13	2.06
8	A	101	BCL	MG-NC	3.13	2.13	2.06
8	B	101	BCL	MG-NC	3.13	2.13	2.06
8	d	103	BCL	MG-NC	3.13	2.13	2.06
8	b	101	BCL	MG-NC	3.12	2.13	2.06
8	D	103	BCL	MG-NC	3.10	2.13	2.06
8	j	101	BCL	MG-NC	3.10	2.13	2.06
8	J	101	BCL	MG-NC	3.09	2.13	2.06
8	9	101	BCL	MG-NC	3.06	2.13	2.06
8	b9	101	BCL	MG-NC	3.06	2.13	2.06
9	M	403	BPB	C3D-CAD	-2.95	1.41	1.47
9	L	303	BPB	C3D-CAD	-2.93	1.41	1.47
9	l	303	BPB	C3D-CAD	-2.93	1.41	1.47
9	m	403	BPB	C3D-CAD	-2.92	1.41	1.47
8	M	402	BCL	MG-NC	2.87	2.13	2.06
8	m	402	BCL	C3B-C4B	2.84	1.46	1.41
8	m	402	BCL	MG-NC	2.84	2.13	2.06
8	M	402	BCL	C3B-C4B	2.83	1.46	1.41
8	O	101	BCL	MG-NC	2.80	2.12	2.06
8	l	307	BCL	MG-NC	2.78	2.12	2.06
8	L	307	BCL	MG-NC	2.78	2.12	2.06
8	o	101	BCL	MG-NC	2.78	2.12	2.06
8	L	302	BCL	MG-NC	2.75	2.12	2.06
10	l	304	U10	C6-C5	-2.74	1.39	1.46
10	m	407	U10	C6-C5	-2.73	1.39	1.46
8	l	302	BCL	MG-NC	2.73	2.12	2.06
8	I	101	BCL	MG-NC	2.73	2.12	2.06
10	L	304	U10	C6-C5	-2.73	1.39	1.46
10	m	404	U10	C6-C5	-2.73	1.39	1.46
10	M	407	U10	C6-C5	-2.72	1.39	1.46
10	M	404	U10	C6-C5	-2.71	1.39	1.46
8	i	101	BCL	MG-NC	2.70	2.12	2.06
8	a	101	BCL	C3B-C4B	2.66	1.46	1.41
8	A	101	BCL	C3B-C4B	2.65	1.46	1.41
14	m	406	CDL	OA6-CA4	-2.63	1.40	1.46
8	d	103	BCL	C3B-C4B	2.63	1.45	1.41
8	L	301	BCL	C3B-C4B	2.63	1.45	1.41
14	M	406	CDL	OA6-CA4	-2.63	1.40	1.46
8	l	301	BCL	C3B-C4B	2.62	1.45	1.41
10	L	305	U10	C6-C5	-2.62	1.39	1.46
8	L	301	BCL	O1A-CGA	-2.61	1.14	1.22
8	D	103	BCL	C3B-C4B	2.60	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	301	BCL	O1A-CGA	-2.60	1.14	1.22
10	l	305	U10	C6-C5	-2.59	1.39	1.46
14	h	303	CDL	OB6-CB4	-2.59	1.40	1.46
8	s	101	BCL	C3B-C4B	2.59	1.45	1.41
14	H	303	CDL	OB6-CB4	-2.58	1.40	1.46
8	S	101	BCL	C3B-C4B	2.57	1.45	1.41
14	h	303	CDL	OA6-CA4	-2.56	1.40	1.46
14	H	303	CDL	OA6-CA4	-2.56	1.40	1.46
8	c	102	BCL	C3B-C4B	2.55	1.45	1.41
8	0	101	BCL	C3B-C4B	2.54	1.45	1.41
14	M	406	CDL	OB6-CB4	-2.54	1.40	1.46
8	b0	101	BCL	C3B-C4B	2.54	1.45	1.41
8	g	101	BCL	C3B-C4B	2.53	1.45	1.41
14	m	406	CDL	OB6-CB4	-2.53	1.40	1.46
8	C	102	BCL	C3B-C4B	2.51	1.45	1.41
8	V	101	BCL	C3B-C4B	2.50	1.45	1.41
8	v	101	BCL	C3B-C4B	2.49	1.45	1.41
8	G	101	BCL	C3B-C4B	2.49	1.45	1.41
8	Q	101	BCL	C3B-C4B	2.48	1.45	1.41
8	q	101	BCL	C3B-C4B	2.47	1.45	1.41
8	b8	101	BCL	C3B-C4B	2.47	1.45	1.41
14	M	406	CDL	OB8-CB7	2.45	1.40	1.33
8	8	101	BCL	C3B-C4B	2.45	1.45	1.41
14	m	406	CDL	OB8-CB7	2.42	1.40	1.33
14	H	303	CDL	OA8-CA7	2.42	1.40	1.33
14	h	303	CDL	OA8-CA7	2.41	1.40	1.33
8	N	102	BCL	C3B-C4B	2.41	1.45	1.41
8	f	101	BCL	C3B-C4B	2.41	1.45	1.41
10	M	404	U10	C1-C2	-2.40	1.38	1.47
10	m	404	U10	C1-C2	-2.40	1.38	1.47
8	3	101	BCL	C3B-C4B	2.40	1.45	1.41
8	k	101	BCL	C3B-C4B	2.40	1.45	1.41
14	M	406	CDL	OA8-CA7	2.39	1.40	1.33
8	5	101	BCL	C3B-C4B	2.39	1.45	1.41
14	m	406	CDL	OA8-CA7	2.39	1.40	1.33
8	w	101	BCL	C3B-C4B	2.39	1.45	1.41
8	n	102	BCL	C3B-C4B	2.39	1.45	1.41
8	U	101	BCL	C3B-C4B	2.38	1.45	1.41
8	l	302	BCL	C3D-C4D	-2.38	1.38	1.44
8	u	101	BCL	C3B-C4B	2.38	1.45	1.41
8	b1	101	BCL	C3B-C4B	2.38	1.45	1.41
8	1	101	BCL	C3B-C4B	2.38	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	303	CDL	OB8-CB7	2.37	1.40	1.33
14	h	303	CDL	OB8-CB7	2.37	1.40	1.33
8	K	101	BCL	C3B-C4B	2.37	1.45	1.41
8	L	302	BCL	C3D-C4D	-2.37	1.38	1.44
8	b9	101	BCL	C3B-C4B	2.36	1.45	1.41
8	T	101	BCL	C3B-C4B	2.36	1.45	1.41
8	F	101	BCL	C3B-C4B	2.35	1.45	1.41
8	L	307	BCL	C1D-C2D	-2.35	1.40	1.45
8	O	101	BCL	C3B-C4B	2.35	1.45	1.41
8	t	101	BCL	C3B-C4B	2.35	1.45	1.41
8	M	402	BCL	C3D-C4D	-2.35	1.38	1.44
8	W	101	BCL	C3B-C4B	2.35	1.45	1.41
8	m	402	BCL	C3D-C4D	-2.34	1.38	1.44
8	o	101	BCL	C3B-C4B	2.34	1.45	1.41
8	l	307	BCL	C1D-C2D	-2.33	1.40	1.45
10	L	305	U10	C1-C2	-2.33	1.38	1.47
8	l	307	BCL	C3D-C4D	-2.33	1.38	1.44
10	l	305	U10	C1-C2	-2.32	1.38	1.47
8	9	101	BCL	C3B-C4B	2.32	1.45	1.41
10	L	304	U10	C1-C2	-2.31	1.39	1.47
8	L	307	BCL	C3D-C4D	-2.30	1.39	1.44
8	P	101	BCL	C3B-C4B	2.30	1.45	1.41
8	B	101	BCL	C3B-C4B	2.30	1.45	1.41
8	b	101	BCL	C3D-C4D	-2.29	1.39	1.44
10	l	304	U10	C1-C2	-2.29	1.39	1.47
8	i	101	BCL	C3B-C4B	2.29	1.45	1.41
8	p	101	BCL	C3B-C4B	2.29	1.45	1.41
8	b	101	BCL	C3B-C4B	2.28	1.45	1.41
8	B	101	BCL	C3D-C4D	-2.28	1.39	1.44
8	I	101	BCL	C3B-C4B	2.26	1.45	1.41
8	k	101	BCL	C1D-C2D	-2.26	1.40	1.45
8	l	301	BCL	C1D-C2D	-2.26	1.40	1.45
9	L	303	BPB	C3B-C4B	2.25	1.45	1.41
8	L	301	BCL	C1D-C2D	-2.25	1.40	1.45
8	K	101	BCL	C1D-C2D	-2.24	1.40	1.45
10	M	407	U10	C1-C2	-2.24	1.39	1.47
10	m	407	U10	C1-C2	-2.24	1.39	1.47
8	d	103	BCL	C3D-C4D	-2.24	1.39	1.44
9	l	303	BPB	C3B-C4B	2.24	1.45	1.41
8	L	302	BCL	C1D-C2D	-2.23	1.40	1.45
8	4	101	BCL	CHD-C1D	2.23	1.42	1.38
8	l	302	BCL	C1D-C2D	-2.23	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	g	101	BCL	C1D-C2D	-2.22	1.40	1.45
8	2	101	BCL	CHD-C1D	2.22	1.42	1.38
8	j	101	BCL	C3B-C4B	2.22	1.45	1.41
8	G	101	BCL	C1D-C2D	-2.22	1.40	1.45
8	G	101	BCL	C3D-C4D	-2.22	1.39	1.44
8	S	101	BCL	C3D-C4D	-2.20	1.39	1.44
10	M	407	U10	C6-C1	2.20	1.39	1.35
8	l	307	BCL	C3B-C4B	2.20	1.45	1.41
8	J	101	BCL	C3B-C4B	2.20	1.45	1.41
8	D	103	BCL	C3D-C4D	-2.20	1.39	1.44
14	h	303	CDL	OB8-CB6	-2.19	1.40	1.45
8	s	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	E	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	R	102	BCL	C3B-C4B	2.19	1.45	1.41
8	Z	101	BCL	C3B-C4B	2.19	1.45	1.41
8	g	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	E	101	BCL	C3B-C4B	2.19	1.45	1.41
8	L	307	BCL	C3B-C4B	2.19	1.45	1.41
8	O	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	i	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	c	102	BCL	C1D-C2D	-2.18	1.41	1.45
8	e	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	W	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	I	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	o	101	BCL	C3D-C4D	-2.18	1.39	1.44
8	R	102	BCL	C3D-C4D	-2.18	1.39	1.44
10	m	407	U10	C6-C1	2.18	1.39	1.35
8	e	101	BCL	C3B-C4B	2.18	1.45	1.41
14	H	303	CDL	OB8-CB6	-2.17	1.40	1.45
8	N	102	BCL	C3D-C4D	-2.17	1.39	1.44
8	r	102	BCL	C3D-C4D	-2.17	1.39	1.44
8	n	102	BCL	C3D-C4D	-2.17	1.39	1.44
8	w	101	BCL	C3D-C4D	-2.17	1.39	1.44
10	L	305	U10	C6-C1	2.17	1.39	1.35
8	t	101	BCL	C3D-C4D	-2.17	1.39	1.44
8	m	402	BCL	C1D-C2D	-2.16	1.41	1.45
8	r	102	BCL	C3B-C4B	2.16	1.45	1.41
8	C	102	BCL	C3D-C4D	-2.16	1.39	1.44
8	c	102	BCL	C3D-C4D	-2.16	1.39	1.44
8	8	101	BCL	C3D-C4D	-2.16	1.39	1.44
8	8	101	BCL	C1D-C2D	-2.16	1.41	1.45
8	z	101	BCL	C3B-C4B	2.16	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	101	BCL	C3D-C4D	-2.15	1.39	1.44
8	b8	101	BCL	C3D-C4D	-2.15	1.39	1.44
8	C	102	BCL	C1D-C2D	-2.15	1.41	1.45
8	T	101	BCL	C3D-C4D	-2.15	1.39	1.44
8	Q	101	BCL	C3D-C4D	-2.15	1.39	1.44
8	b1	101	BCL	C3D-C4D	-2.15	1.39	1.44
10	l	305	U10	C6-C1	2.15	1.39	1.35
14	M	406	CDL	OA8-CA6	-2.14	1.40	1.45
8	P	101	BCL	C3D-C4D	-2.14	1.39	1.44
8	k	101	BCL	C3D-C4D	-2.14	1.39	1.44
8	b	101	BCL	C1D-C2D	-2.14	1.41	1.45
8	o	101	BCL	C1D-C2D	-2.14	1.41	1.45
8	7	101	BCL	CHD-C1D	2.14	1.42	1.38
8	O	101	BCL	C1D-C2D	-2.13	1.41	1.45
8	b8	101	BCL	C1D-C2D	-2.13	1.41	1.45
8	0	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	A	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	2	101	BCL	C3B-C4B	2.13	1.45	1.41
8	M	402	BCL	C1D-C2D	-2.13	1.41	1.45
8	v	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	b0	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	q	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	V	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	Z	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	S	101	BCL	C1D-C2D	-2.13	1.41	1.45
8	F	101	BCL	C3D-C4D	-2.12	1.39	1.44
8	5	101	BCL	C3D-C4D	-2.12	1.39	1.44
8	b1	101	BCL	CHD-C1D	2.12	1.42	1.38
8	u	101	BCL	O1A-CGA	-2.12	1.16	1.22
8	b0	101	BCL	C1D-C2D	-2.12	1.41	1.45
8	6	101	BCL	CHD-C1D	2.12	1.42	1.38
8	0	101	BCL	C1D-C2D	-2.12	1.41	1.45
8	1	101	BCL	C3D-C4D	-2.12	1.39	1.44
8	R	102	BCL	C1D-C2D	-2.11	1.41	1.45
8	a	101	BCL	C3D-C4D	-2.11	1.39	1.44
8	L	302	BCL	C3B-C4B	2.11	1.45	1.41
8	U	101	BCL	O1A-CGA	-2.11	1.16	1.22
8	d	103	BCL	C1D-C2D	-2.11	1.41	1.45
8	D	103	BCL	C1D-C2D	-2.11	1.41	1.45
8	F	101	BCL	C1D-C2D	-2.11	1.41	1.45
10	m	404	U10	C6-C1	2.11	1.39	1.35
8	l	302	BCL	C3B-C4B	2.11	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	s	101	BCL	C1D-C2D	-2.11	1.41	1.45
14	M	406	CDL	OB6-CB5	2.11	1.40	1.34
8	1	101	BCL	CHD-C1D	2.10	1.42	1.38
14	M	406	CDL	OA6-CA5	2.10	1.40	1.34
8	3	101	BCL	C3D-C4D	-2.10	1.39	1.44
8	4	101	BCL	C3B-C4B	2.10	1.44	1.41
14	h	303	CDL	OA6-CA5	2.10	1.40	1.34
8	B	101	BCL	C1D-C2D	-2.10	1.41	1.45
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	z	101	BCL	C3D-C4D	-2.10	1.39	1.44
14	m	406	CDL	OA8-CA6	-2.10	1.40	1.45
8	5	101	BCL	CHD-C1D	2.10	1.42	1.38
8	K	101	BCL	C3D-C4D	-2.10	1.39	1.44
8	2	101	BCL	C3D-C4D	-2.10	1.39	1.44
14	H	303	CDL	OA6-CA5	2.10	1.40	1.34
8	j	101	BCL	C3D-C4D	-2.10	1.39	1.44
8	e	101	BCL	C1D-C2D	-2.10	1.41	1.45
14	m	406	CDL	OA6-CA5	2.10	1.40	1.34
8	J	101	BCL	C1D-C2D	-2.09	1.41	1.45
8	j	101	BCL	C1D-C2D	-2.09	1.41	1.45
8	4	101	BCL	C3D-C4D	-2.09	1.39	1.44
8	f	101	BCL	C3D-C4D	-2.09	1.39	1.44
8	J	101	BCL	C3D-C4D	-2.09	1.39	1.44
10	M	404	U10	C6-C1	2.09	1.39	1.35
14	H	303	CDL	OB6-CB5	2.09	1.40	1.34
8	o	101	BCL	CHD-C1D	2.09	1.42	1.38
8	Z	101	BCL	CHD-C1D	2.09	1.42	1.38
8	r	102	BCL	C1D-C2D	-2.08	1.41	1.45
14	m	406	CDL	OB6-CB5	2.08	1.40	1.34
8	l	302	BCL	O1A-CGA	-2.08	1.16	1.22
8	d	103	BCL	O1A-CGA	-2.08	1.16	1.22
14	h	303	CDL	OB6-CB5	2.08	1.40	1.34
8	U	101	BCL	C3D-C4D	-2.08	1.39	1.44
8	q	101	BCL	C1D-C2D	-2.08	1.41	1.45
8	f	101	BCL	C1D-C2D	-2.08	1.41	1.45
8	L	302	BCL	CHD-C1D	2.08	1.42	1.38
8	Q	101	BCL	C1D-C2D	-2.08	1.41	1.45
8	E	101	BCL	C1D-C2D	-2.08	1.41	1.45
8	L	301	BCL	C3D-C4D	-2.08	1.39	1.44
8	O	101	BCL	CHD-C1D	2.07	1.42	1.38
8	6	101	BCL	C3B-C4B	2.07	1.44	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	101	BCL	C1D-C2D	-2.07	1.41	1.45
8	9	101	BCL	C3D-C4D	-2.07	1.39	1.44
8	z	101	BCL	CHD-C1D	2.07	1.42	1.38
8	b9	101	BCL	C3D-C4D	-2.07	1.39	1.44
8	L	302	BCL	O1A-CGA	-2.07	1.16	1.22
8	u	101	BCL	C1D-C2D	-2.07	1.41	1.45
8	D	103	BCL	O1A-CGA	-2.07	1.16	1.22
8	t	101	BCL	C1D-C2D	-2.06	1.41	1.45
8	7	101	BCL	C3B-C4B	2.06	1.44	1.41
8	U	101	BCL	C1D-C2D	-2.06	1.41	1.45
8	V	101	BCL	C1D-C2D	-2.06	1.41	1.45
8	v	101	BCL	C1D-C2D	-2.05	1.41	1.45
8	l	301	BCL	C3D-C4D	-2.05	1.39	1.44
8	l	302	BCL	CHD-C1D	2.05	1.42	1.38
8	w	101	BCL	CHD-C1D	2.05	1.42	1.38
14	M	406	CDL	OB8-CB6	-2.05	1.40	1.45
8	9	101	BCL	CHD-C1D	2.05	1.42	1.38
8	a	101	BCL	C1D-C2D	-2.05	1.41	1.45
8	A	101	BCL	C1D-C2D	-2.04	1.41	1.45
8	K	101	BCL	O1A-CGA	-2.04	1.16	1.22
8	I	101	BCL	C1D-C2D	-2.04	1.41	1.45
8	5	101	BCL	C1D-C2D	-2.04	1.41	1.45
14	H	303	CDL	OA8-CA6	-2.04	1.40	1.45
8	b9	101	BCL	CHD-C1D	2.04	1.42	1.38
8	k	101	BCL	O1A-CGA	-2.04	1.16	1.22
14	m	406	CDL	OB8-CB6	-2.03	1.40	1.45
8	U	101	BCL	CHD-C1D	2.03	1.42	1.38
8	6	101	BCL	C3D-C4D	-2.03	1.39	1.44
8	M	402	BCL	CHD-C1D	2.03	1.42	1.38
8	3	101	BCL	C1D-C2D	-2.03	1.41	1.45
8	m	402	BCL	CHD-C1D	2.03	1.42	1.38
8	l	307	BCL	CBD-CGD	-2.02	1.46	1.52
8	7	101	BCL	C3D-C4D	-2.02	1.39	1.44
8	7	101	BCL	C1D-C2D	-2.02	1.41	1.45
8	M	402	BCL	CBD-CGD	-2.02	1.46	1.52
8	m	402	BCL	CBD-CGD	-2.02	1.46	1.52
8	W	101	BCL	CHD-C1D	2.02	1.42	1.38
8	u	101	BCL	CHD-C1D	2.02	1.42	1.38
14	h	303	CDL	OA8-CA6	-2.02	1.40	1.45
8	l	302	BCL	CBD-CGD	-2.01	1.46	1.52
8	i	101	BCL	C1D-C2D	-2.01	1.41	1.45
10	L	304	U10	C6-C1	2.00	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	101	BCL	O1A-CGA	-2.00	1.16	1.22
8	L	307	BCL	CBD-CGD	-2.00	1.46	1.52

All (819) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	303	BPB	C4D-CHA-CBD	-10.84	103.61	108.52
9	l	303	BPB	C4D-CHA-CBD	-10.82	103.62	108.52
9	M	403	BPB	C4D-CHA-CBD	-10.73	103.66	108.52
9	m	403	BPB	C4D-CHA-CBD	-10.71	103.67	108.52
8	T	101	BCL	CHD-C1D-ND	-5.66	119.25	124.45
8	t	101	BCL	CHD-C1D-ND	-5.59	119.32	124.45
8	R	102	BCL	CHD-C1D-ND	-5.52	119.38	124.45
8	r	102	BCL	CHD-C1D-ND	-5.50	119.40	124.45
8	v	101	BCL	CHD-C1D-ND	-5.46	119.44	124.45
8	V	101	BCL	CHD-C1D-ND	-5.43	119.46	124.45
8	L	307	BCL	CHD-C1D-ND	-5.41	119.48	124.45
8	p	101	BCL	CHD-C1D-ND	-5.41	119.49	124.45
8	b9	101	BCL	C4D-CHA-C1A	5.39	127.81	121.25
8	l	307	BCL	CHD-C1D-ND	-5.39	119.50	124.45
8	P	101	BCL	CHD-C1D-ND	-5.39	119.50	124.45
8	m	402	BCL	C4D-CHA-C1A	5.37	127.79	121.25
8	M	402	BCL	C4D-CHA-C1A	5.37	127.78	121.25
8	9	101	BCL	C4D-CHA-C1A	5.34	127.75	121.25
8	O	101	BCL	CHD-C1D-ND	-5.32	119.56	124.45
8	f	101	BCL	CHD-C1D-ND	-5.31	119.57	124.45
8	l	307	BCL	C4D-CHA-C1A	5.31	127.71	121.25
8	L	307	BCL	C4D-CHA-C1A	5.31	127.71	121.25
8	L	302	BCL	CHD-C1D-ND	-5.30	119.58	124.45
8	8	101	BCL	C1-C2-C3	5.30	135.21	126.04
8	b8	101	BCL	C1-C2-C3	5.30	135.21	126.04
8	F	101	BCL	CHD-C1D-ND	-5.30	119.59	124.45
8	7	101	BCL	C4D-CHA-C1A	5.30	127.69	121.25
8	d	103	BCL	C4D-CHA-C1A	5.29	127.69	121.25
8	i	101	BCL	CHD-C1D-ND	-5.29	119.59	124.45
8	I	101	BCL	CHD-C1D-ND	-5.29	119.60	124.45
8	l	302	BCL	CHD-C1D-ND	-5.28	119.60	124.45
8	6	101	BCL	C4D-CHA-C1A	5.28	127.68	121.25
8	A	101	BCL	C4D-CHA-C1A	5.28	127.68	121.25
8	o	101	BCL	CHD-C1D-ND	-5.28	119.60	124.45
8	z	101	BCL	CHD-C1D-ND	-5.28	119.60	124.45
8	b	101	BCL	C4D-CHA-C1A	5.27	127.66	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	101	BCL	C4D-CHA-C1A	5.26	127.65	121.25
8	D	103	BCL	C4D-CHA-C1A	5.26	127.65	121.25
8	s	101	BCL	C4D-CHA-C1A	5.25	127.64	121.25
8	N	102	BCL	CHD-C1D-ND	-5.25	119.63	124.45
8	Z	101	BCL	CHD-C1D-ND	-5.25	119.63	124.45
8	U	101	BCL	C4D-CHA-C1A	5.24	127.62	121.25
8	a	101	BCL	C4D-CHA-C1A	5.23	127.62	121.25
8	k	101	BCL	CHD-C1D-ND	-5.23	119.65	124.45
8	B	101	BCL	C4D-CHA-C1A	5.23	127.61	121.25
8	I	101	BCL	C4D-CHA-C1A	5.23	127.61	121.25
8	n	102	BCL	CHD-C1D-ND	-5.23	119.65	124.45
8	u	101	BCL	C4D-CHA-C1A	5.23	127.61	121.25
8	G	101	BCL	CHD-C1D-ND	-5.22	119.66	124.45
8	o	101	BCL	C4D-CHA-C1A	5.22	127.60	121.25
8	S	101	BCL	C4D-CHA-C1A	5.21	127.59	121.25
8	e	101	BCL	CHD-C1D-ND	-5.21	119.67	124.45
8	g	101	BCL	CHD-C1D-ND	-5.20	119.67	124.45
8	O	101	BCL	C4D-CHA-C1A	5.20	127.58	121.25
8	Z	101	BCL	C4D-CHA-C1A	5.19	127.56	121.25
8	z	101	BCL	C4D-CHA-C1A	5.19	127.56	121.25
8	f	101	BCL	C4D-CHA-C1A	5.19	127.56	121.25
8	E	101	BCL	CHD-C1D-ND	-5.18	119.69	124.45
8	K	101	BCL	CHD-C1D-ND	-5.18	119.69	124.45
8	F	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
8	3	101	BCL	C4D-CHA-C1A	5.18	127.55	121.25
8	D	103	BCL	CHD-C1D-ND	-5.17	119.71	124.45
8	5	101	BCL	C4D-CHA-C1A	5.16	127.53	121.25
8	b1	101	BCL	C4D-CHA-C1A	5.16	127.52	121.25
8	d	103	BCL	CHD-C1D-ND	-5.16	119.72	124.45
8	t	101	BCL	C4D-CHA-C1A	5.15	127.52	121.25
8	N	102	BCL	C4D-CHA-C1A	5.15	127.52	121.25
8	T	101	BCL	C4D-CHA-C1A	5.14	127.50	121.25
8	w	101	BCL	C4D-CHA-C1A	5.13	127.50	121.25
8	1	101	BCL	C4D-CHA-C1A	5.13	127.49	121.25
8	W	101	BCL	C4D-CHA-C1A	5.13	127.49	121.25
8	L	302	BCL	C4D-CHA-C1A	5.12	127.48	121.25
8	l	302	BCL	C4D-CHA-C1A	5.12	127.48	121.25
8	j	101	BCL	CHD-C1D-ND	-5.12	119.75	124.45
8	n	102	BCL	C4D-CHA-C1A	5.12	127.48	121.25
8	c	102	BCL	CHD-C1D-ND	-5.11	119.76	124.45
8	J	101	BCL	C4D-CHA-C1A	5.11	127.47	121.25
8	j	101	BCL	C4D-CHA-C1A	5.11	127.46	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	4	101	BCL	CHD-C1D-ND	-5.11	119.76	124.45
8	G	101	BCL	C4D-CHA-C1A	5.10	127.46	121.25
8	C	102	BCL	CHD-C1D-ND	-5.10	119.77	124.45
8	J	101	BCL	CHD-C1D-ND	-5.10	119.77	124.45
8	g	101	BCL	C4D-CHA-C1A	5.08	127.43	121.25
8	2	101	BCL	CHD-C1D-ND	-5.07	119.80	124.45
8	b8	101	BCL	C4D-CHA-C1A	5.05	127.40	121.25
8	1	101	BCL	CHD-C1D-ND	-5.04	119.82	124.45
8	8	101	BCL	C4D-CHA-C1A	5.04	127.38	121.25
8	A	101	BCL	CHD-C1D-ND	-5.03	119.83	124.45
8	l	301	BCL	CHD-C1D-ND	-5.03	119.83	124.45
8	c	102	BCL	C4D-CHA-C1A	5.03	127.37	121.25
8	a	101	BCL	CHD-C1D-ND	-5.03	119.84	124.45
8	b1	101	BCL	CHD-C1D-ND	-5.02	119.84	124.45
8	p	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
8	9	101	BCL	CHD-C1D-ND	-5.02	119.84	124.45
8	k	101	BCL	C4D-CHA-C1A	5.02	127.36	121.25
8	q	101	BCL	C4D-CHA-C1A	5.01	127.35	121.25
8	P	101	BCL	C4D-CHA-C1A	5.01	127.35	121.25
8	L	301	BCL	CHD-C1D-ND	-5.01	119.85	124.45
8	K	101	BCL	C4D-CHA-C1A	5.00	127.34	121.25
8	V	101	BCL	C4D-CHA-C1A	5.00	127.34	121.25
8	b	101	BCL	CHD-C1D-ND	-5.00	119.86	124.45
8	v	101	BCL	C4D-CHA-C1A	5.00	127.34	121.25
8	Q	101	BCL	C4D-CHA-C1A	4.99	127.33	121.25
8	C	102	BCL	C4D-CHA-C1A	4.99	127.33	121.25
8	B	101	BCL	CHD-C1D-ND	-4.99	119.87	124.45
8	8	101	BCL	CHD-C1D-ND	-4.98	119.88	124.45
8	b9	101	BCL	CHD-C1D-ND	-4.97	119.88	124.45
8	u	101	BCL	CHD-C1D-ND	-4.97	119.89	124.45
8	E	101	BCL	C4D-CHA-C1A	4.96	127.28	121.25
8	w	101	BCL	CHD-C1D-ND	-4.95	119.90	124.45
8	S	101	BCL	CHD-C1D-ND	-4.95	119.90	124.45
8	0	101	BCL	C4D-CHA-C1A	4.94	127.27	121.25
8	b8	101	BCL	CHD-C1D-ND	-4.94	119.92	124.45
8	e	101	BCL	C4D-CHA-C1A	4.94	127.26	121.25
8	s	101	BCL	CHD-C1D-ND	-4.93	119.92	124.45
8	b0	101	BCL	C4D-CHA-C1A	4.93	127.25	121.25
8	W	101	BCL	CHD-C1D-ND	-4.92	119.94	124.45
8	b0	101	BCL	CHD-C1D-ND	-4.91	119.94	124.45
8	U	101	BCL	CHD-C1D-ND	-4.91	119.94	124.45
9	M	403	BPB	C4D-ND-C1D	-4.90	103.84	108.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	r	102	BCL	C4D-CHA-C1A	4.90	127.21	121.25
8	R	102	BCL	C4D-CHA-C1A	4.88	127.19	121.25
8	7	101	BCL	CHD-C1D-ND	-4.88	119.97	124.45
8	6	101	BCL	CHD-C1D-ND	-4.87	119.97	124.45
8	M	402	BCL	CHD-C1D-ND	-4.87	119.98	124.45
9	m	403	BPB	C4D-ND-C1D	-4.87	103.88	108.83
8	0	101	BCL	CHD-C1D-ND	-4.87	119.98	124.45
8	m	402	BCL	CHD-C1D-ND	-4.86	119.99	124.45
10	m	407	U10	C7-C8-C9	-4.82	118.77	126.79
8	3	101	BCL	CHD-C1D-ND	-4.82	120.02	124.45
8	q	101	BCL	CHD-C1D-ND	-4.82	120.03	124.45
8	Q	101	BCL	CHD-C1D-ND	-4.81	120.03	124.45
9	l	303	BPB	C4D-ND-C1D	-4.81	103.93	108.83
9	L	303	BPB	C4D-ND-C1D	-4.81	103.94	108.83
8	5	101	BCL	CHD-C1D-ND	-4.80	120.05	124.45
9	L	303	BPB	CBC-CAC-C3C	-4.79	113.98	126.70
9	l	303	BPB	CBC-CAC-C3C	-4.79	113.99	126.70
10	M	407	U10	C7-C8-C9	-4.79	118.82	126.79
8	L	301	BCL	C4D-CHA-C1A	4.77	127.06	121.25
8	l	301	BCL	C4D-CHA-C1A	4.75	127.03	121.25
8	4	101	BCL	C4D-CHA-C1A	4.52	126.75	121.25
8	2	101	BCL	C4D-CHA-C1A	4.50	126.72	121.25
9	m	403	BPB	CBC-CAC-C3C	-4.36	115.14	126.70
9	M	403	BPB	CBC-CAC-C3C	-4.35	115.15	126.70
14	m	406	CDL	OB6-CB5-C51	4.28	120.72	111.50
14	M	406	CDL	OB6-CB5-C51	4.28	120.72	111.50
8	O	101	BCL	C1D-ND-C4D	-4.16	103.38	106.33
8	o	101	BCL	C4A-NA-C1A	4.15	108.57	106.71
8	O	101	BCL	C4A-NA-C1A	4.14	108.57	106.71
8	l	302	BCL	C1D-ND-C4D	-4.11	103.42	106.33
8	o	101	BCL	C1D-ND-C4D	-4.11	103.42	106.33
8	L	302	BCL	C1D-ND-C4D	-4.09	103.43	106.33
8	i	101	BCL	C1D-ND-C4D	-4.05	103.46	106.33
8	s	101	BCL	C4A-NA-C1A	4.05	108.53	106.71
14	h	303	CDL	OA6-CA5-C11	4.04	120.21	111.50
14	H	303	CDL	OA6-CA5-C11	4.04	120.21	111.50
8	m	402	BCL	C4A-NA-C1A	4.04	108.52	106.71
8	I	101	BCL	C1D-ND-C4D	-4.03	103.47	106.33
8	M	402	BCL	C4A-NA-C1A	4.03	108.52	106.71
10	l	305	U10	C7-C8-C9	-4.03	120.09	126.79
10	L	305	U10	C7-C8-C9	-4.02	120.11	126.79
8	3	101	BCL	C4A-NA-C1A	3.98	108.49	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	m	406	CDL	OA6-CA5-C11	3.98	120.07	111.50
14	M	406	CDL	OA6-CA5-C11	3.96	120.04	111.50
8	5	101	BCL	C4A-NA-C1A	3.96	108.48	106.71
8	S	101	BCL	C4A-NA-C1A	3.94	108.48	106.71
8	9	101	BCL	C4A-NA-C1A	3.88	108.45	106.71
8	K	101	BCL	C4A-NA-C1A	3.85	108.44	106.71
14	H	303	CDL	OB6-CB5-C51	3.83	119.75	111.50
14	h	303	CDL	OB6-CB5-C51	3.82	119.74	111.50
8	b9	101	BCL	C4A-NA-C1A	3.82	108.42	106.71
8	1	101	BCL	C4A-NA-C1A	3.82	108.42	106.71
8	k	101	BCL	C4A-NA-C1A	3.79	108.41	106.71
8	l	307	BCL	C4A-NA-C1A	3.79	108.41	106.71
8	b1	101	BCL	C4A-NA-C1A	3.78	108.41	106.71
8	i	101	BCL	C4A-NA-C1A	3.78	108.41	106.71
10	l	304	U10	C7-C8-C9	-3.76	120.53	126.79
8	2	101	BCL	C1-C2-C3	3.76	132.55	126.04
8	6	101	BCL	C4A-NA-C1A	3.75	108.39	106.71
10	L	304	U10	C7-C8-C9	-3.75	120.54	126.79
8	k	101	BCL	C1D-ND-C4D	-3.75	103.67	106.33
8	4	101	BCL	C1-C2-C3	3.75	132.52	126.04
8	L	307	BCL	C4A-NA-C1A	3.73	108.38	106.71
8	Q	101	BCL	C1-C2-C3	-3.73	119.59	126.04
8	7	101	BCL	C4A-NA-C1A	3.73	108.38	106.71
8	Q	101	BCL	C4A-NA-C1A	3.72	108.38	106.71
8	K	101	BCL	C1D-ND-C4D	-3.71	103.70	106.33
8	q	101	BCL	C1-C2-C3	-3.70	119.64	126.04
8	W	101	BCL	C4A-NA-C1A	3.70	108.37	106.71
8	4	101	BCL	C1D-ND-C4D	-3.70	103.71	106.33
8	q	101	BCL	C4A-NA-C1A	3.69	108.36	106.71
8	p	101	BCL	C4A-NA-C1A	3.68	108.36	106.71
8	l	307	BCL	C1D-ND-C4D	-3.68	103.72	106.33
8	1	101	BCL	C1D-ND-C4D	-3.68	103.72	106.33
8	U	101	BCL	C4A-NA-C1A	3.67	108.36	106.71
8	L	307	BCL	C1D-ND-C4D	-3.67	103.73	106.33
8	I	101	BCL	C4A-NA-C1A	3.66	108.35	106.71
8	2	101	BCL	C1D-ND-C4D	-3.65	103.74	106.33
8	P	101	BCL	C4A-NA-C1A	3.65	108.35	106.71
8	9	101	BCL	C1D-ND-C4D	-3.65	103.74	106.33
8	b1	101	BCL	C1D-ND-C4D	-3.64	103.75	106.33
8	u	101	BCL	C4A-NA-C1A	3.64	108.34	106.71
8	d	103	BCL	C1D-ND-C4D	-3.63	103.75	106.33
8	b9	101	BCL	C1D-ND-C4D	-3.62	103.76	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	103	BCL	C1D-ND-C4D	-3.60	103.78	106.33
8	b0	101	BCL	C6-C7-C8	-3.60	104.27	115.92
8	a	101	BCL	C4A-NA-C1A	3.60	108.33	106.71
8	0	101	BCL	C6-C7-C8	-3.60	104.29	115.92
8	A	101	BCL	C4A-NA-C1A	3.59	108.32	106.71
8	w	101	BCL	C4A-NA-C1A	3.59	108.32	106.71
8	S	101	BCL	C1D-ND-C4D	-3.56	103.80	106.33
8	w	101	BCL	C1D-ND-C4D	-3.56	103.81	106.33
8	s	101	BCL	C1D-ND-C4D	-3.55	103.81	106.33
8	7	101	BCL	C1D-ND-C4D	-3.52	103.83	106.33
8	A	101	BCL	C1D-ND-C4D	-3.51	103.84	106.33
8	p	101	BCL	C1D-ND-C4D	-3.51	103.84	106.33
8	W	101	BCL	C1D-ND-C4D	-3.50	103.85	106.33
8	l	301	BCL	C1D-ND-C4D	-3.49	103.85	106.33
8	j	101	BCL	C1D-ND-C4D	-3.49	103.85	106.33
8	P	101	BCL	C1D-ND-C4D	-3.49	103.85	106.33
8	a	101	BCL	C1D-ND-C4D	-3.49	103.86	106.33
8	F	101	BCL	C4A-NA-C1A	3.48	108.27	106.71
8	E	101	BCL	C1D-ND-C4D	-3.47	103.87	106.33
8	L	301	BCL	C1D-ND-C4D	-3.47	103.87	106.33
8	T	101	BCL	C1D-ND-C4D	-3.47	103.87	106.33
8	J	101	BCL	C1D-ND-C4D	-3.47	103.87	106.33
8	6	101	BCL	C1D-ND-C4D	-3.46	103.87	106.33
8	f	101	BCL	C4A-NA-C1A	3.46	108.26	106.71
8	e	101	BCL	C1D-ND-C4D	-3.45	103.88	106.33
8	5	101	BCL	C1D-ND-C4D	-3.45	103.88	106.33
8	r	102	BCL	C1D-ND-C4D	-3.45	103.89	106.33
10	m	404	U10	C27-C28-C29	-3.45	119.36	127.66
8	F	101	BCL	C1-C2-C3	-3.45	120.08	126.04
8	f	101	BCL	C1-C2-C3	-3.44	120.09	126.04
10	M	404	U10	C27-C28-C29	-3.44	119.39	127.66
8	R	102	BCL	C1D-ND-C4D	-3.43	103.90	106.33
8	3	101	BCL	C1D-ND-C4D	-3.43	103.90	106.33
8	M	402	BCL	C1D-ND-C4D	-3.42	103.90	106.33
8	Q	101	BCL	C1D-ND-C4D	-3.41	103.91	106.33
8	t	101	BCL	C1D-ND-C4D	-3.41	103.91	106.33
10	l	305	U10	C17-C18-C19	-3.41	119.46	127.66
8	u	101	BCL	C1D-ND-C4D	-3.41	103.92	106.33
9	M	403	BPB	C3D-C4D-ND	3.40	112.36	107.72
10	L	305	U10	C17-C18-C19	-3.40	119.48	127.66
8	V	101	BCL	C1D-ND-C4D	-3.39	103.92	106.33
8	f	101	BCL	C1D-ND-C4D	-3.39	103.93	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	m	402	BCL	C1D-ND-C4D	-3.39	103.93	106.33
8	z	101	BCL	C1D-ND-C4D	-3.38	103.93	106.33
9	m	403	BPB	C3D-C4D-ND	3.38	112.32	107.72
8	F	101	BCL	C1D-ND-C4D	-3.38	103.94	106.33
8	q	101	BCL	C1D-ND-C4D	-3.37	103.94	106.33
9	l	303	BPB	C3D-C4D-ND	3.37	112.31	107.72
8	Z	101	BCL	C1D-ND-C4D	-3.36	103.94	106.33
8	v	101	BCL	C1D-ND-C4D	-3.36	103.94	106.33
8	n	102	BCL	C1D-ND-C4D	-3.36	103.95	106.33
9	L	303	BPB	C3D-C4D-ND	3.36	112.30	107.72
8	N	102	BCL	C1D-ND-C4D	-3.35	103.95	106.33
8	n	102	BCL	C4A-NA-C1A	3.35	108.21	106.71
8	U	101	BCL	C1D-ND-C4D	-3.35	103.96	106.33
8	J	101	BCL	C4A-NA-C1A	3.34	108.21	106.71
10	l	305	U10	C22-C23-C24	-3.34	119.62	127.66
8	C	102	BCL	C1D-ND-C4D	-3.34	103.96	106.33
10	m	407	U10	C22-C23-C24	-3.33	119.63	127.66
8	c	102	BCL	C1D-ND-C4D	-3.33	103.97	106.33
8	j	101	BCL	C4A-NA-C1A	3.33	108.20	106.71
10	L	305	U10	C22-C23-C24	-3.33	119.64	127.66
10	M	407	U10	C22-C23-C24	-3.33	119.65	127.66
8	N	102	BCL	C4A-NA-C1A	3.33	108.20	106.71
8	G	101	BCL	C1D-ND-C4D	-3.32	103.97	106.33
8	E	101	BCL	C4A-NA-C1A	3.32	108.20	106.71
9	M	403	BPB	OBD-CAD-CBD	-3.32	120.95	125.82
8	g	101	BCL	C1D-ND-C4D	-3.30	103.99	106.33
8	4	101	BCL	C2A-C1A-CHA	3.28	129.60	123.86
8	e	101	BCL	C4A-NA-C1A	3.28	108.18	106.71
9	m	403	BPB	OBD-CAD-CBD	-3.28	121.01	125.82
8	8	101	BCL	C1D-ND-C4D	-3.27	104.01	106.33
8	2	101	BCL	C2A-C1A-CHA	3.27	129.58	123.86
8	b8	101	BCL	C1D-ND-C4D	-3.27	104.01	106.33
8	t	101	BCL	C4A-NA-C1A	3.27	108.17	106.71
10	m	404	U10	C32-C33-C34	-3.25	119.83	127.66
8	T	101	BCL	C4A-NA-C1A	3.25	108.17	106.71
8	b0	101	BCL	C1D-ND-C4D	-3.25	104.03	106.33
10	M	404	U10	C32-C33-C34	-3.25	119.84	127.66
8	4	101	BCL	CHA-C1A-NA	-3.22	119.03	126.40
8	2	101	BCL	CHA-C1A-NA	-3.20	119.07	126.40
8	m	402	BCL	CHA-C1A-NA	-3.20	119.07	126.40
8	0	101	BCL	C1D-ND-C4D	-3.20	104.06	106.33
8	M	402	BCL	CHA-C1A-NA	-3.19	119.09	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	101	BCL	CAB-C3B-C2B	3.19	133.12	128.34
9	L	303	BPB	OBD-CAD-CBD	-3.19	121.15	125.82
9	l	303	BPB	OBD-CAD-CBD	-3.18	121.15	125.82
10	l	305	U10	C15-C14-C16	3.18	120.62	115.27
10	M	404	U10	C25-C24-C26	3.18	120.62	115.27
10	L	305	U10	C15-C14-C16	3.18	120.61	115.27
8	o	101	BCL	C1-C2-C3	-3.17	120.55	126.04
10	m	404	U10	C25-C24-C26	3.17	120.61	115.27
8	q	101	BCL	CAB-C3B-C2B	3.17	133.09	128.34
8	3	101	BCL	CHA-C1A-NA	-3.15	119.17	126.40
10	L	304	U10	C12-C13-C14	-3.15	120.08	127.66
8	b	101	BCL	C1D-ND-C4D	-3.15	104.10	106.33
8	O	101	BCL	C1-C2-C3	-3.15	120.60	126.04
10	l	304	U10	C12-C13-C14	-3.14	120.10	127.66
8	5	101	BCL	CHA-C1A-NA	-3.14	119.21	126.40
8	b	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
8	B	101	BCL	C1D-ND-C4D	-3.13	104.11	106.33
8	0	101	BCL	CHA-C1A-NA	-3.12	119.25	126.40
8	D	103	BCL	C4A-NA-C1A	3.11	108.11	106.71
8	B	101	BCL	CHA-C1A-NA	-3.11	119.27	126.40
8	w	101	BCL	CHA-C1A-NA	-3.10	119.29	126.40
8	s	101	BCL	CAB-C3B-C2B	3.10	132.99	128.34
8	r	102	BCL	C4A-NA-C1A	3.10	108.10	106.71
8	6	101	BCL	CHA-C1A-NA	-3.10	119.30	126.40
8	b0	101	BCL	CHA-C1A-NA	-3.10	119.30	126.40
10	M	404	U10	C35-C34-C36	3.10	120.49	115.27
10	m	404	U10	C35-C34-C36	3.10	120.49	115.27
8	W	101	BCL	CHA-C1A-NA	-3.10	119.30	126.40
8	d	103	BCL	C4A-NA-C1A	3.10	108.10	106.71
8	s	101	BCL	CHA-C1A-NA	-3.10	119.31	126.40
8	q	101	BCL	CHA-C1A-NA	-3.10	119.31	126.40
8	S	101	BCL	CAB-C3B-C2B	3.10	132.98	128.34
8	7	101	BCL	CHA-C1A-NA	-3.09	119.31	126.40
8	S	101	BCL	CHA-C1A-NA	-3.09	119.31	126.40
8	b9	101	BCL	CHA-C1A-NA	-3.09	119.31	126.40
10	m	407	U10	C25-C24-C26	3.09	120.47	115.27
8	A	101	BCL	CHA-C1A-NA	-3.09	119.32	126.40
8	R	102	BCL	C4A-NA-C1A	3.09	108.09	106.71
8	9	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
8	Q	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
10	M	407	U10	C25-C24-C26	3.08	120.45	115.27
10	m	404	U10	C12-C13-C14	-3.08	120.25	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	101	BCL	CHA-C1A-NA	-3.07	119.37	126.40
8	b8	101	BCL	CHA-C1A-NA	-3.07	119.37	126.40
8	U	101	BCL	CHA-C1A-NA	-3.07	119.37	126.40
8	a	101	BCL	CHA-C1A-NA	-3.07	119.37	126.40
10	M	404	U10	C12-C13-C14	-3.07	120.28	127.66
8	8	101	BCL	CHA-C1A-NA	-3.07	119.38	126.40
8	u	101	BCL	CHA-C1A-NA	-3.07	119.38	126.40
8	O	101	BCL	CHA-C1A-NA	-3.06	119.38	126.40
8	E	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
8	b0	101	BCL	C4A-NA-C1A	3.06	108.08	106.71
8	b1	101	BCL	CHA-C1A-NA	-3.06	119.40	126.40
8	9	101	BCL	CAB-C3B-C2B	3.06	132.92	128.34
8	a	101	BCL	CAB-C3B-C2B	3.06	132.92	128.34
8	o	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
8	b9	101	BCL	CAB-C3B-C2B	3.05	132.91	128.34
10	M	407	U10	C20-C19-C21	3.05	120.40	115.27
8	z	101	BCL	CHA-C1A-NA	-3.05	119.42	126.40
8	Z	101	BCL	CHA-C1A-NA	-3.05	119.42	126.40
8	1	101	BCL	CHA-C1A-NA	-3.04	119.42	126.40
10	m	407	U10	C20-C19-C21	3.04	120.39	115.27
8	L	302	BCL	CHA-C1A-NA	-3.04	119.43	126.40
8	A	101	BCL	CAB-C3B-C2B	3.04	132.89	128.34
8	l	302	BCL	CHA-C1A-NA	-3.04	119.44	126.40
10	m	404	U10	C22-C23-C24	-3.04	120.35	127.66
8	j	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
8	G	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
8	b8	101	BCL	C2A-C1A-CHA	3.03	129.16	123.86
8	g	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
8	J	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
8	d	103	BCL	CHA-C1A-NA	-3.03	119.46	126.40
8	k	101	BCL	CHA-C1A-NA	-3.03	119.47	126.40
10	M	404	U10	C22-C23-C24	-3.03	120.38	127.66
8	D	103	BCL	CHA-C1A-NA	-3.02	119.49	126.40
10	l	305	U10	C10-C9-C11	3.02	120.35	115.27
8	k	101	BCL	CAB-C3B-C2B	3.01	132.85	128.34
10	m	404	U10	C17-C18-C19	-3.01	120.41	127.66
8	8	101	BCL	C2A-C1A-CHA	3.01	129.13	123.86
10	M	407	U10	C15-C14-C16	3.01	120.33	115.27
10	M	404	U10	C17-C18-C19	-3.01	120.42	127.66
8	K	101	BCL	CHA-C1A-NA	-3.01	119.52	126.40
8	L	307	BCL	CHA-C1A-NA	-3.00	119.53	126.40
8	T	101	BCL	CHA-C1A-NA	-3.00	119.53	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	t	101	BCL	CHA-C1A-NA	-2.99	119.55	126.40
8	I	101	BCL	CHA-C1A-NA	-2.99	119.56	126.40
8	N	102	BCL	CHA-C1A-NA	-2.98	119.57	126.40
8	i	101	BCL	CHA-C1A-NA	-2.98	119.57	126.40
10	L	305	U10	C10-C9-C11	2.98	120.28	115.27
8	l	307	BCL	CHA-C1A-NA	-2.98	119.57	126.40
8	K	101	BCL	CAB-C3B-C2B	2.98	132.80	128.34
8	p	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
10	m	407	U10	C15-C14-C16	2.98	120.28	115.27
8	f	101	BCL	CHA-C1A-NA	-2.98	119.58	126.40
8	n	102	BCL	CHA-C1A-NA	-2.98	119.58	126.40
8	C	102	BCL	C4A-NA-C1A	2.97	108.04	106.71
8	L	307	BCL	C2A-C1A-CHA	2.97	129.06	123.86
8	V	101	BCL	CHA-C1A-NA	-2.97	119.59	126.40
8	F	101	BCL	CHA-C1A-NA	-2.97	119.59	126.40
8	l	307	BCL	C2A-C1A-CHA	2.97	129.06	123.86
8	C	102	BCL	C1-C2-C3	2.97	131.18	126.04
8	P	101	BCL	CHA-C1A-NA	-2.97	119.61	126.40
8	R	102	BCL	CHA-C1A-NA	-2.97	119.61	126.40
8	0	101	BCL	C4A-NA-C1A	2.96	108.04	106.71
10	l	304	U10	C17-C18-C19	-2.96	120.52	127.66
8	r	102	BCL	CHA-C1A-NA	-2.96	119.61	126.40
8	c	102	BCL	C1-C2-C3	2.96	131.16	126.04
10	M	404	U10	C30-C29-C31	2.96	120.24	115.27
10	m	404	U10	C15-C14-C16	2.96	120.24	115.27
8	v	101	BCL	CHA-C1A-NA	-2.95	119.63	126.40
10	m	404	U10	C30-C29-C31	2.95	120.24	115.27
10	L	304	U10	C17-C18-C19	-2.95	120.55	127.66
8	L	301	BCL	C4A-NA-C1A	2.95	108.03	106.71
10	L	304	U10	C22-C23-C24	-2.94	120.58	127.66
8	c	102	BCL	CHA-C1A-NA	-2.94	119.66	126.40
8	c	102	BCL	C4A-NA-C1A	2.94	108.03	106.71
8	O	101	BCL	CAB-C3B-C2B	2.94	132.74	128.34
10	M	404	U10	C15-C14-C16	2.93	120.21	115.27
10	l	304	U10	C22-C23-C24	-2.93	120.59	127.66
8	v	101	BCL	C4A-NA-C1A	2.93	108.02	106.71
8	o	101	BCL	CAB-C3B-C2B	2.93	132.73	128.34
8	C	102	BCL	CHA-C1A-NA	-2.93	119.69	126.40
8	l	302	BCL	C4A-NA-C1A	2.93	108.02	106.71
8	d	103	BCL	CAB-C3B-C2B	2.93	132.72	128.34
8	u	101	BCL	CAB-C3B-C2B	2.92	132.72	128.34
8	0	101	BCL	C2A-C1A-CHA	2.92	128.97	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	302	BCL	C4A-NA-C1A	2.92	108.02	106.71
8	U	101	BCL	CAB-C3B-C2B	2.92	132.71	128.34
10	l	305	U10	C25-C24-C26	2.91	120.17	115.27
8	l	301	BCL	C4A-NA-C1A	2.91	108.02	106.71
10	L	305	U10	C25-C24-C26	2.91	120.17	115.27
10	L	304	U10	C10-C9-C11	2.91	120.17	115.27
8	D	103	BCL	CAB-C3B-C2B	2.91	132.70	128.34
8	L	301	BCL	CHA-C1A-NA	-2.91	119.74	126.40
10	m	404	U10	C20-C19-C21	2.91	120.16	115.27
8	b0	101	BCL	C2A-C1A-CHA	2.91	128.94	123.86
8	l	301	BCL	C2A-C1A-CHA	2.90	128.94	123.86
8	L	301	BCL	C2A-C1A-CHA	2.90	128.94	123.86
10	l	304	U10	C10-C9-C11	2.90	120.15	115.27
8	q	101	BCL	C2A-C1A-CHA	2.90	128.93	123.86
8	l	301	BCL	CHA-C1A-NA	-2.90	119.76	126.40
8	L	302	BCL	C2A-C1A-CHA	2.89	128.92	123.86
8	3	101	BCL	CAB-C3B-C2B	2.89	132.67	128.34
8	0	101	BCL	C1-C2-C3	2.89	131.04	126.04
8	b0	101	BCL	C1-C2-C3	2.89	131.03	126.04
10	M	404	U10	C20-C19-C21	2.88	120.12	115.27
8	b	101	BCL	C6-C7-C8	-2.88	106.60	115.92
8	B	101	BCL	C6-C7-C8	-2.88	106.60	115.92
9	L	303	BPB	CMB-C2B-C3B	2.88	130.06	124.68
8	5	101	BCL	CAB-C3B-C2B	2.87	132.65	128.34
9	l	303	BPB	CMB-C2B-C3B	2.87	130.05	124.68
8	l	302	BCL	C2A-C1A-CHA	2.87	128.88	123.86
8	V	101	BCL	C4A-NA-C1A	2.86	107.99	106.71
8	Q	101	BCL	C2A-C1A-CHA	2.86	128.86	123.86
8	b9	101	BCL	C2A-C1A-CHA	2.86	128.86	123.86
10	M	404	U10	C10-C9-C11	2.86	120.08	115.27
8	i	101	BCL	CAB-C3B-C2B	2.85	132.61	128.34
14	M	406	CDL	OB8-CB7-C71	2.85	120.84	111.91
14	m	406	CDL	OB8-CB7-C71	2.85	120.84	111.91
8	I	101	BCL	CAB-C3B-C2B	2.84	132.60	128.34
10	m	404	U10	C10-C9-C11	2.84	120.05	115.27
8	9	101	BCL	C2A-C1A-CHA	2.84	128.83	123.86
9	M	403	BPB	C2D-C1D-ND	2.82	111.47	109.53
8	O	101	BCL	C2A-C1A-CHA	2.82	128.79	123.86
8	s	101	BCL	C2A-C1A-CHA	2.82	128.78	123.86
8	A	101	BCL	C2A-C1A-CHA	2.81	128.77	123.86
8	3	101	BCL	C2A-C1A-CHA	2.80	128.76	123.86
8	S	101	BCL	C2A-C1A-CHA	2.80	128.76	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	m	403	BPB	C2D-C1D-ND	2.80	111.46	109.53
8	a	101	BCL	C2A-C1A-CHA	2.80	128.75	123.86
8	l	301	BCL	CAB-C3B-C2B	2.80	132.53	128.34
8	o	101	BCL	C2A-C1A-CHA	2.80	128.75	123.86
8	G	101	BCL	C4A-NA-C1A	2.79	107.96	106.71
8	5	101	BCL	C2A-C1A-CHA	2.79	128.74	123.86
10	l	305	U10	C20-C19-C21	2.78	119.95	115.27
10	l	304	U10	C25-C24-C26	2.78	119.95	115.27
8	L	301	BCL	CAB-C3B-C2B	2.78	132.50	128.34
8	S	101	BCL	C1-C2-C3	-2.78	121.24	126.04
8	r	102	BCL	C2A-C1A-CHA	2.78	128.71	123.86
10	L	305	U10	C20-C19-C21	2.77	119.93	115.27
8	s	101	BCL	C1-C2-C3	-2.77	121.26	126.04
10	L	305	U10	C30-C29-C31	2.76	119.92	115.27
8	k	101	BCL	C2A-C1A-CHA	2.76	128.69	123.86
8	g	101	BCL	C4A-NA-C1A	2.76	107.95	106.71
10	L	304	U10	C25-C24-C26	2.76	119.91	115.27
14	h	303	CDL	OB8-CB7-C71	2.76	120.56	111.91
10	L	304	U10	C20-C19-C21	2.76	119.91	115.27
8	K	101	BCL	C2A-C1A-CHA	2.76	128.68	123.86
8	i	101	BCL	C2A-C1A-CHA	2.75	128.68	123.86
14	H	303	CDL	OB8-CB7-C71	2.75	120.55	111.91
8	I	101	BCL	C2A-C1A-CHA	2.75	128.67	123.86
8	u	101	BCL	C11-C10-C8	-2.75	107.02	115.92
8	l	101	BCL	CAB-C3B-C2B	2.75	132.46	128.34
8	U	101	BCL	C11-C10-C8	-2.75	107.03	115.92
8	R	102	BCL	C2A-C1A-CHA	2.75	128.66	123.86
10	l	304	U10	C20-C19-C21	2.75	119.89	115.27
8	b	101	BCL	C2A-C1A-CHA	2.75	128.66	123.86
10	l	305	U10	C30-C29-C31	2.74	119.88	115.27
8	V	101	BCL	C2A-C1A-CHA	2.74	128.64	123.86
8	B	101	BCL	C2A-C1A-CHA	2.73	128.64	123.86
8	b1	101	BCL	CAB-C3B-C2B	2.73	132.43	128.34
8	G	101	BCL	C2A-C1A-CHA	2.73	128.63	123.86
8	q	101	BCL	CHC-C4B-NB	-2.72	121.38	124.26
8	m	402	BCL	CAB-C3B-C2B	2.72	132.41	128.34
8	v	101	BCL	C2A-C1A-CHA	2.71	128.60	123.86
8	g	101	BCL	C2A-C1A-CHA	2.71	128.60	123.86
8	m	402	BCL	C2A-C1A-CHA	2.71	128.59	123.86
8	D	103	BCL	C2A-C1A-CHA	2.70	128.58	123.86
8	M	402	BCL	C2A-C1A-CHA	2.70	128.58	123.86
8	W	101	BCL	C2A-C1A-CHA	2.70	128.58	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	402	BCL	CAB-C3B-C2B	2.70	132.38	128.34
8	D	103	BCL	CHC-C4B-NB	-2.70	121.40	124.26
8	Q	101	BCL	CHC-C4B-NB	-2.70	121.40	124.26
8	d	103	BCL	C2A-C1A-CHA	2.69	128.57	123.86
8	f	101	BCL	C2A-C1A-CHA	2.69	128.57	123.86
8	E	101	BCL	C2A-C1A-CHA	2.69	128.56	123.86
8	e	101	BCL	C2A-C1A-CHA	2.69	128.56	123.86
9	L	303	BPB	C2D-C1D-ND	2.69	111.38	109.53
8	z	101	BCL	C2A-C1A-CHA	2.69	128.56	123.86
8	w	101	BCL	C2A-C1A-CHA	2.69	128.56	123.86
8	S	101	BCL	CHC-C4B-NB	-2.68	121.42	124.26
8	s	101	BCL	CHC-C4B-NB	-2.68	121.42	124.26
8	F	101	BCL	C2A-C1A-CHA	2.68	128.54	123.86
10	L	305	U10	C27-C28-C29	-2.68	121.21	127.66
8	d	103	BCL	CHC-C4B-NB	-2.68	121.42	124.26
10	l	305	U10	C27-C28-C29	-2.67	121.22	127.66
8	Z	101	BCL	C2A-C1A-CHA	2.67	128.53	123.86
8	b	101	BCL	C4A-NA-C1A	2.66	107.90	106.71
8	J	101	BCL	C2A-C1A-CHA	2.66	128.50	123.86
9	l	303	BPB	C2D-C1D-ND	2.66	111.36	109.53
8	B	101	BCL	C4A-NA-C1A	2.65	107.90	106.71
8	c	102	BCL	C2A-C1A-CHA	2.65	128.50	123.86
8	j	101	BCL	C2A-C1A-CHA	2.65	128.49	123.86
8	6	101	BCL	C2A-C1A-CHA	2.64	128.48	123.86
8	p	101	BCL	C2A-C1A-CHA	2.64	128.48	123.86
10	l	304	U10	C15-C14-C16	2.64	119.72	115.27
8	1	101	BCL	C2A-C1A-CHA	2.64	128.48	123.86
8	b1	101	BCL	C2A-C1A-CHA	2.64	128.47	123.86
8	C	102	BCL	C2A-C1A-CHA	2.64	128.47	123.86
10	L	304	U10	C15-C14-C16	2.64	119.70	115.27
8	7	101	BCL	C2A-C1A-CHA	2.63	128.47	123.86
8	P	101	BCL	C2A-C1A-CHA	2.63	128.46	123.86
9	l	303	BPB	O2D-CGD-CBD	2.63	114.33	111.00
8	N	102	BCL	C2A-C1A-CHA	2.63	128.46	123.86
14	m	406	CDL	OA8-CA7-C31	2.63	120.15	111.91
14	M	406	CDL	OA8-CA7-C31	2.63	120.15	111.91
9	L	303	BPB	O2D-CGD-CBD	2.62	114.32	111.00
8	D	103	BCL	C11-C10-C8	-2.62	107.44	115.92
8	n	102	BCL	C2A-C1A-CHA	2.62	128.44	123.86
8	d	103	BCL	C11-C10-C8	-2.62	107.45	115.92
8	u	101	BCL	C2A-C1A-CHA	2.62	128.44	123.86
8	w	101	BCL	CAB-C3B-C2B	2.62	132.26	128.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	101	BCL	C2A-C1A-CHA	2.62	128.44	123.86
10	L	304	U10	C1M-C1-C6	-2.61	120.14	124.40
14	H	303	CDL	OA8-CA7-C31	2.61	120.10	111.91
10	l	304	U10	C1M-C1-C6	-2.61	120.15	124.40
10	M	407	U10	C17-C18-C19	-2.60	121.40	127.66
14	h	303	CDL	OA8-CA7-C31	2.60	120.06	111.91
8	k	101	BCL	CHC-C4B-NB	-2.60	121.51	124.26
8	W	101	BCL	CAB-C3B-C2B	2.60	132.23	128.34
8	I	101	BCL	CHC-C4B-NB	-2.59	121.51	124.26
8	i	101	BCL	CHC-C4B-NB	-2.59	121.51	124.26
10	m	407	U10	C17-C18-C19	-2.59	121.42	127.66
8	T	101	BCL	C1-C2-C3	-2.59	121.56	126.04
8	t	101	BCL	C1-C2-C3	-2.59	121.57	126.04
8	K	101	BCL	CHC-C4B-NB	-2.58	121.53	124.26
8	g	101	BCL	CAB-C3B-C2B	2.58	132.20	128.34
8	l	301	BCL	CHC-C4B-NB	-2.57	121.53	124.26
8	z	101	BCL	C4A-NA-C1A	2.57	107.86	106.71
8	G	101	BCL	CAB-C3B-C2B	2.56	132.18	128.34
8	m	402	BCL	CHC-C4B-NB	-2.56	121.55	124.26
8	K	101	BCL	C1-C2-C3	-2.55	121.64	126.04
8	M	402	BCL	CHC-C4B-NB	-2.55	121.56	124.26
8	A	101	BCL	CHC-C4B-NB	-2.55	121.56	124.26
8	k	101	BCL	C1-C2-C3	-2.54	121.65	126.04
8	L	301	BCL	CHC-C4B-NB	-2.54	121.57	124.26
8	Z	101	BCL	C4A-NA-C1A	2.52	107.84	106.71
8	a	101	BCL	CHC-C4B-NB	-2.52	121.59	124.26
9	M	403	BPB	CMB-C2B-C3B	2.51	129.38	124.68
8	m	402	BCL	CMB-C2B-C1B	-2.51	121.54	125.37
8	F	101	BCL	CHC-C4B-NB	-2.51	121.60	124.26
8	f	101	BCL	CHC-C4B-NB	-2.50	121.61	124.26
9	m	403	BPB	CMB-C2B-C3B	2.50	129.35	124.68
10	L	305	U10	C12-C13-C14	-2.49	121.66	127.66
10	l	305	U10	C12-C13-C14	-2.49	121.67	127.66
8	3	101	BCL	CHC-C4B-NB	-2.49	121.62	124.26
11	D	101	PC1	C2-O21-C21	2.49	123.91	117.79
10	m	404	U10	C7-C8-C9	-2.48	122.66	126.79
8	5	101	BCL	CHC-C4B-NB	-2.48	121.63	124.26
11	d	101	PC1	C2-O21-C21	2.48	123.89	117.79
8	b	101	BCL	CHC-C4B-NB	-2.48	121.63	124.26
8	l	307	BCL	CAB-C3B-C2B	2.47	132.04	128.34
8	M	402	BCL	CMB-C2B-C1B	-2.47	121.61	125.37
10	M	404	U10	C7-C8-C9	-2.47	122.68	126.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	l	305	U10	C36-C34-C35	2.47	120.05	114.60
9	m	403	BPB	CMD-C2D-C3D	2.46	129.29	124.68
10	m	407	U10	C31-C29-C30	2.46	120.04	114.60
10	L	305	U10	C36-C34-C35	2.46	120.04	114.60
8	B	101	BCL	CHC-C4B-NB	-2.46	121.65	124.26
8	G	101	BCL	CHC-C4B-NB	-2.45	121.66	124.26
10	M	407	U10	C31-C29-C30	2.45	120.01	114.60
8	o	101	BCL	CHC-C4B-NB	-2.45	121.66	124.26
9	M	403	BPB	CMD-C2D-C3D	2.45	129.26	124.68
8	c	102	BCL	O2A-C1-C2	-2.45	102.20	108.64
8	O	101	BCL	CHC-C4B-NB	-2.45	121.67	124.26
8	L	307	BCL	CAB-C3B-C2B	2.44	132.00	128.34
8	C	102	BCL	O2A-C1-C2	-2.44	102.22	108.64
10	L	304	U10	O2-C2-C3	-2.44	115.75	120.93
8	C	102	BCL	CAB-C3B-C2B	2.44	131.99	128.34
10	m	407	U10	C1M-C1-C6	-2.44	120.42	124.40
8	b	101	BCL	CAB-C3B-C2B	2.44	131.99	128.34
8	c	102	BCL	CAB-C3B-C2B	2.43	131.99	128.34
10	M	407	U10	C1M-C1-C6	-2.43	120.43	124.40
8	D	103	BCL	CMB-C2B-C1B	-2.43	121.67	125.37
8	j	101	BCL	C6-C7-C8	-2.43	108.07	115.92
10	l	304	U10	O2-C2-C3	-2.43	115.78	120.93
8	B	101	BCL	CAB-C3B-C2B	2.42	131.97	128.34
8	J	101	BCL	C6-C7-C8	-2.42	108.09	115.92
8	R	102	BCL	C6-C7-C8	-2.42	108.09	115.92
8	g	101	BCL	CHC-C4B-NB	-2.42	121.69	124.26
8	8	101	BCL	C4A-NA-C1A	2.42	107.79	106.71
8	8	101	BCL	CAB-C3B-C2B	2.42	131.96	128.34
8	d	103	BCL	CMB-C2B-C1B	-2.42	121.69	125.37
8	b8	101	BCL	CAB-C3B-C2B	2.42	131.96	128.34
10	l	305	U10	C1M-C1-C6	-2.41	120.46	124.40
10	m	407	U10	C12-C13-C14	-2.41	121.85	127.66
8	9	101	BCL	CHC-C4B-NB	-2.41	121.71	124.26
8	r	102	BCL	C6-C7-C8	-2.41	108.13	115.92
10	L	305	U10	C1M-C1-C6	-2.41	120.47	124.40
8	t	101	BCL	C2A-C1A-CHA	2.40	128.06	123.86
10	M	407	U10	C12-C13-C14	-2.40	121.88	127.66
8	T	101	BCL	C2A-C1A-CHA	2.40	128.05	123.86
8	0	101	BCL	CAB-C3B-C2B	2.40	131.93	128.34
8	b9	101	BCL	CHC-C4B-NB	-2.40	121.72	124.26
8	f	101	BCL	CAB-C3B-C2B	2.39	131.93	128.34
8	W	101	BCL	CHC-C4B-NB	-2.38	121.73	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	101	BCL	C1-C2-C3	-2.38	121.93	126.04
8	s	101	BCL	CMB-C2B-C1B	-2.37	121.76	125.37
8	t	101	BCL	CAB-C3B-C2B	2.37	131.89	128.34
8	b0	101	BCL	CAB-C3B-C2B	2.37	131.89	128.34
8	M	402	BCL	OBB-CAB-CBB	-2.37	114.48	119.73
8	S	101	BCL	CMB-C2B-C1B	-2.37	121.76	125.37
8	l	101	BCL	CHC-C4B-NB	-2.37	121.75	124.26
8	d	103	BCL	C1-C2-C3	-2.37	121.95	126.04
8	i	101	BCL	C1-C2-C3	-2.37	121.95	126.04
8	m	402	BCL	OBB-CAB-CBB	-2.37	114.48	119.73
9	L	303	BPB	CMD-C2D-C3D	2.37	129.10	124.68
8	r	102	BCL	CHC-C4B-NB	-2.36	121.75	124.26
9	l	303	BPB	CMD-C2D-C3D	2.36	129.10	124.68
8	T	101	BCL	CAB-C3B-C2B	2.36	131.88	128.34
8	D	103	BCL	C1-C2-C3	-2.36	121.96	126.04
8	w	101	BCL	CHC-C4B-NB	-2.36	121.76	124.26
8	F	101	BCL	CAB-C3B-C2B	2.36	131.87	128.34
8	Z	101	BCL	CAB-C3B-C2B	2.36	131.87	128.34
8	b1	101	BCL	CHC-C4B-NB	-2.35	121.77	124.26
10	M	404	U10	C41-C39-C40	2.35	119.80	114.60
11	H	302	PC1	O12-P-O14	2.35	123.86	112.24
8	b8	101	BCL	C4A-NA-C1A	2.35	107.76	106.71
8	u	101	BCL	C1-C2-C3	-2.35	121.98	126.04
9	m	403	BPB	C1-C2-C3	-2.35	121.98	126.04
9	M	403	BPB	C1-C2-C3	-2.35	121.98	126.04
8	R	102	BCL	CHC-C4B-NB	-2.35	121.77	124.26
11	h	302	PC1	O12-P-O14	2.35	123.84	112.24
10	m	404	U10	C41-C39-C40	2.35	119.78	114.60
11	l	308	PC1	O12-P-O14	2.34	123.81	112.24
10	L	304	U10	C31-C29-C30	2.34	119.77	114.60
10	l	304	U10	C31-C29-C30	2.34	119.77	114.60
8	U	101	BCL	C1-C2-C3	-2.33	122.00	126.04
8	0	101	BCL	CHC-C4B-NB	-2.33	121.79	124.26
11	L	308	PC1	O12-P-O14	2.33	123.76	112.24
8	8	101	BCL	CHC-C4B-NB	-2.33	121.79	124.26
8	b8	101	BCL	CAA-CBA-CGA	2.33	120.05	113.25
14	M	406	CDL	OB4-PB2-OB3	-2.32	100.75	112.24
14	m	406	CDL	OB4-PB2-OB3	-2.32	100.76	112.24
8	8	101	BCL	CAA-CBA-CGA	2.32	120.04	113.25
8	z	101	BCL	CAB-C3B-C2B	2.32	131.81	128.34
8	V	101	BCL	CHC-C4B-NB	-2.32	121.81	124.26
8	e	101	BCL	CHC-C4B-NB	-2.32	121.81	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b0	101	BCL	CHC-C4B-NB	-2.32	121.81	124.26
8	L	301	BCL	CMB-C2B-C1B	-2.31	121.84	125.37
8	U	101	BCL	CHC-C4B-NB	-2.31	121.81	124.26
11	D	102	PC1	O12-P-O14	2.30	123.63	112.24
8	v	101	BCL	CHC-C4B-NB	-2.30	121.82	124.26
8	C	102	BCL	CHC-C4B-NB	-2.30	121.82	124.26
8	b8	101	BCL	CHC-C4B-NB	-2.30	121.83	124.26
11	d	102	PC1	O12-P-O14	2.30	123.59	112.24
8	l	301	BCL	CMB-C2B-C1B	-2.29	121.88	125.37
8	M	402	BCL	C4B-C3B-C2B	-2.29	104.67	108.36
8	j	101	BCL	CAB-C3B-C2B	2.29	131.76	128.34
14	H	303	CDL	OB4-PB2-OB3	-2.28	100.95	112.24
8	u	101	BCL	CHC-C4B-NB	-2.28	121.84	124.26
14	H	303	CDL	OA4-PA1-OA3	-2.28	100.97	112.24
14	h	303	CDL	OA4-PA1-OA3	-2.28	100.98	112.24
14	h	303	CDL	OB4-PB2-OB3	-2.28	100.98	112.24
8	m	402	BCL	C4B-C3B-C2B	-2.28	104.70	108.36
8	E	101	BCL	CHC-C4B-NB	-2.27	121.85	124.26
8	A	101	BCL	OBB-CAB-CBB	-2.27	114.70	119.73
8	J	101	BCL	CAB-C3B-C2B	2.27	131.74	128.34
11	l	306	PC1	O12-P-O14	2.27	123.45	112.24
11	L	306	PC1	O12-P-O14	2.27	123.44	112.24
8	l	302	BCL	CHC-C4B-NB	-2.26	121.86	124.26
8	s	101	BCL	C4B-C3B-C2B	-2.26	104.72	108.36
8	A	101	BCL	C1-C2-C3	-2.26	122.14	126.04
8	L	302	BCL	CHC-C4B-NB	-2.26	121.87	124.26
8	c	102	BCL	CHC-C4B-NB	-2.26	121.87	124.26
8	a	101	BCL	C1-C2-C3	-2.25	122.15	126.04
10	M	407	U10	C10-C9-C11	2.25	119.06	115.27
11	a	104	PC1	O12-P-O14	2.25	123.38	112.24
11	A	104	PC1	O12-P-O14	2.25	123.37	112.24
10	m	407	U10	C10-C9-C11	2.25	119.06	115.27
14	M	406	CDL	OA4-PA1-OA3	-2.25	101.12	112.24
8	L	301	BCL	C4B-C3B-C2B	-2.25	104.74	108.36
8	a	101	BCL	OBB-CAB-CBB	-2.25	114.75	119.73
8	V	101	BCL	C6-C5-C3	2.25	119.34	113.45
8	t	101	BCL	CHC-C4B-NB	-2.25	121.88	124.26
8	R	102	BCL	CAB-C3B-C2B	2.24	131.70	128.34
14	m	406	CDL	OA4-PA1-OA3	-2.24	101.15	112.24
8	l	301	BCL	C4B-C3B-C2B	-2.24	104.75	108.36
8	n	102	BCL	CAB-C3B-C2B	2.24	131.70	128.34
8	D	103	BCL	OBB-CAB-CBB	-2.24	114.77	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	101	BCL	C4B-C3B-C2B	-2.24	104.76	108.36
8	N	102	BCL	CAB-C3B-C2B	2.23	131.68	128.34
8	v	101	BCL	C6-C5-C3	2.23	119.29	113.45
11	a	105	PC1	O12-P-O14	2.22	123.24	112.24
8	T	101	BCL	CHC-C4B-NB	-2.22	121.90	124.26
8	d	103	BCL	C4B-C3B-C2B	-2.22	104.79	108.36
11	A	105	PC1	O12-P-O14	2.22	123.20	112.24
8	D	103	BCL	C4B-C3B-C2B	-2.22	104.79	108.36
8	r	102	BCL	CAB-C3B-C2B	2.22	131.66	128.34
8	d	103	BCL	OBb-CAB-CBB	-2.21	114.82	119.73
8	a	101	BCL	C4B-C3B-C2B	-2.21	104.80	108.36
8	L	301	BCL	OBb-CAB-CBB	-2.21	114.83	119.73
8	a	101	BCL	CMB-C2B-C1B	-2.21	122.00	125.37
8	Q	101	BCL	C4B-C3B-C2B	-2.21	104.81	108.36
8	P	101	BCL	CAB-C3B-C2B	2.21	131.65	128.34
8	A	101	BCL	C4B-C3B-C2B	-2.21	104.81	108.36
8	l	301	BCL	OBb-CAB-CBB	-2.20	114.85	119.73
8	A	101	BCL	CMB-C2B-C1B	-2.20	122.01	125.37
8	q	101	BCL	C4B-C3B-C2B	-2.20	104.83	108.36
8	p	101	BCL	CAB-C3B-C2B	2.19	131.63	128.34
8	S	101	BCL	OBb-CAB-CBB	-2.19	114.88	119.73
8	s	101	BCL	OBb-CAB-CBB	-2.18	114.89	119.73
11	A	103	PC1	O12-P-O14	2.17	122.99	112.24
11	a	103	PC1	O12-P-O14	2.17	122.99	112.24
8	V	101	BCL	CAB-C3B-C2B	2.17	131.59	128.34
8	7	101	BCL	C1-C2-C3	2.17	129.79	126.04
8	v	101	BCL	CAB-C3B-C2B	2.17	131.59	128.34
8	z	101	BCL	C1-C2-C3	-2.17	122.30	126.04
8	Z	101	BCL	C1-C2-C3	-2.16	122.30	126.04
8	6	101	BCL	C1-C2-C3	2.16	129.78	126.04
10	L	305	U10	C32-C33-C34	-2.16	120.38	127.75
10	l	305	U10	C32-C33-C34	-2.15	120.40	127.75
8	p	101	BCL	CHC-C4B-NB	-2.15	121.98	124.26
8	n	102	BCL	CHC-C4B-NB	-2.14	121.99	124.26
8	i	101	BCL	C4B-C3B-C2B	-2.13	104.93	108.36
8	Q	101	BCL	OBb-CAB-CBB	-2.13	115.01	119.73
8	O	101	BCL	C2D-C1D-ND	2.13	111.67	110.10
8	e	101	BCL	CAB-C3B-C2B	2.13	131.52	128.34
8	E	101	BCL	CAB-C3B-C2B	2.12	131.52	128.34
8	l	307	BCL	CHC-C4B-NB	-2.12	122.01	124.26
8	q	101	BCL	OBb-CAB-CBB	-2.12	115.03	119.73
8	I	101	BCL	C4B-C3B-C2B	-2.12	104.95	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	101	BCL	CHC-C4B-NB	-2.11	122.02	124.26
8	N	102	BCL	CHC-C4B-NB	-2.11	122.02	124.26
8	k	101	BCL	C4B-C3B-C2B	-2.11	104.97	108.36
8	K	101	BCL	C4B-C3B-C2B	-2.10	104.98	108.36
8	L	307	BCL	CHC-C4B-NB	-2.10	122.03	124.26
8	f	101	BCL	C4B-C3B-C2B	-2.09	104.99	108.36
8	b9	101	BCL	C4B-C3B-C2B	-2.09	105.00	108.36
8	o	101	BCL	C2D-C1D-ND	2.09	111.64	110.10
8	g	101	BCL	C4B-C3B-C2B	-2.09	105.00	108.36
8	G	101	BCL	C4B-C3B-C2B	-2.09	105.00	108.36
8	q	101	BCL	CMB-C2B-C1B	-2.08	122.20	125.37
10	L	304	U10	C27-C28-C29	-2.08	120.64	127.75
8	F	101	BCL	C4B-C3B-C2B	-2.08	105.02	108.36
8	a	101	BCL	C1C-NC-C4C	2.08	107.64	106.71
8	C	102	BCL	C4B-C3B-C2B	-2.07	105.02	108.36
8	J	101	BCL	CHC-C4B-NB	-2.07	122.06	124.26
10	l	304	U10	C27-C28-C29	-2.07	120.67	127.75
8	9	101	BCL	C4B-C3B-C2B	-2.07	105.03	108.36
8	4	101	BCL	CHC-C4B-NB	-2.07	122.07	124.26
8	Q	101	BCL	CMB-C2B-C1B	-2.07	122.22	125.37
8	j	101	BCL	CHC-C4B-NB	-2.06	122.07	124.26
8	V	101	BCL	CMB-C2B-C1B	-2.06	122.23	125.37
8	3	101	BCL	C4B-C3B-C2B	-2.06	105.04	108.36
8	u	101	BCL	C4B-C3B-C2B	-2.06	105.04	108.36
8	c	102	BCL	C4B-C3B-C2B	-2.06	105.04	108.36
8	U	101	BCL	C4B-C3B-C2B	-2.06	105.04	108.36
8	k	101	BCL	C2D-C1D-ND	2.06	111.62	110.10
8	5	101	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
8	O	101	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
8	K	101	BCL	C2D-C1D-ND	2.06	111.62	110.10
8	z	101	BCL	CHC-C4B-NB	-2.06	122.08	124.26
8	o	101	BCL	C4B-C3B-C2B	-2.06	105.05	108.36
8	2	101	BCL	CHC-C4B-NB	-2.05	122.08	124.26
9	l	303	BPB	OBB-CAB-CBB	-2.05	115.55	120.17
8	b8	101	BCL	C4B-C3B-C2B	-2.05	105.06	108.36
9	L	303	BPB	OBB-CAB-CBB	-2.05	115.55	120.17
8	r	102	BCL	CHC-C1C-NC	-2.05	121.68	124.51
8	v	101	BCL	CMB-C2B-C1B	-2.05	122.25	125.37
8	i	101	BCL	C2D-C1D-ND	2.04	111.61	110.10
8	0	101	BCL	C4B-C3B-C2B	-2.04	105.07	108.36
8	b1	101	BCL	C1-C2-C3	-2.04	123.45	126.75
10	M	404	U10	C37-C38-C39	-2.04	120.78	127.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	8	101	BCL	C4B-C3B-C2B	-2.04	105.08	108.36
8	R	102	BCL	CHC-C1C-NC	-2.04	121.69	124.51
10	m	404	U10	C37-C38-C39	-2.04	120.79	127.75
8	I	101	BCL	C2D-C1D-ND	2.03	111.60	110.10
8	V	101	BCL	C4B-C3B-C2B	-2.03	105.09	108.36
8	v	101	BCL	C4B-C3B-C2B	-2.03	105.09	108.36
8	Z	101	BCL	CHC-C4B-NB	-2.03	122.11	124.26
8	L	302	BCL	C2D-C1D-ND	2.03	111.60	110.10
9	M	403	BPB	O2D-CGD-CBD	2.03	113.57	111.00
8	b1	101	BCL	C4B-C3B-C2B	-2.03	105.09	108.36
8	1	101	BCL	C4B-C3B-C2B	-2.03	105.10	108.36
8	l	302	BCL	C2D-C1D-ND	2.03	111.60	110.10
8	9	101	BCL	CMB-C2B-C1B	-2.02	122.28	125.37
8	b9	101	BCL	CMB-C2B-C1B	-2.02	122.28	125.37
9	m	403	BPB	O2D-CGD-CBD	2.02	113.56	111.00
8	b0	101	BCL	C4B-C3B-C2B	-2.02	105.11	108.36
8	A	101	BCL	C1C-NC-C4C	2.02	107.61	106.71
8	1	101	BCL	C1-C2-C3	-2.02	123.49	126.75
10	m	407	U10	C27-C28-C29	-2.01	120.88	127.75
8	7	101	BCL	CHC-C4B-NB	-2.01	122.13	124.26
8	k	101	BCL	CMB-C2B-C1B	-2.01	122.31	125.37
8	b	101	BCL	C4B-C3B-C2B	-2.00	105.14	108.36
10	M	407	U10	C27-C28-C29	-2.00	120.90	127.75
8	9	101	BCL	OBb-CAB-CBB	-2.00	115.29	119.73
8	b9	101	BCL	OBb-CAB-CBB	-2.00	115.29	119.73
8	B	101	BCL	CMB-C2B-C1B	-2.00	122.32	125.37
8	t	101	BCL	C4B-C3B-C2B	-2.00	105.14	108.36

There are no chirality outliers.

All (1318) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	G	101	BCL	CHA-CBD-CGD-O1D
8	G	101	BCL	CHA-CBD-CGD-O2D
8	N	102	BCL	C4C-C3C-CAC-CBC
8	P	101	BCL	C2C-C3C-CAC-CBC
8	P	101	BCL	C4C-C3C-CAC-CBC
8	S	101	BCL	C4C-C3C-CAC-CBC
8	2	101	BCL	O2A-C1-C2-C3
8	2	101	BCL	C2-C3-C5-C6
8	2	101	BCL	C4-C3-C5-C6
8	7	101	BCL	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	8	101	BCL	O2A-C1-C2-C3
8	g	101	BCL	CHA-CBD-CGD-O1D
8	g	101	BCL	CHA-CBD-CGD-O2D
8	n	102	BCL	C4C-C3C-CAC-CBC
8	p	101	BCL	C2C-C3C-CAC-CBC
8	p	101	BCL	C4C-C3C-CAC-CBC
8	s	101	BCL	C4C-C3C-CAC-CBC
8	4	101	BCL	O2A-C1-C2-C3
8	4	101	BCL	C2-C3-C5-C6
8	4	101	BCL	C4-C3-C5-C6
8	6	101	BCL	O2A-C1-C2-C3
8	b8	101	BCL	O2A-C1-C2-C3
9	L	303	BPB	C2C-C3C-CAC-CBC
9	L	303	BPB	C4C-C3C-CAC-CBC
9	M	403	BPB	C2-C3-C5-C6
9	M	403	BPB	C4-C3-C5-C6
9	M	403	BPB	C4C-C3C-CAC-CBC
9	l	303	BPB	C2C-C3C-CAC-CBC
9	l	303	BPB	C4C-C3C-CAC-CBC
9	m	403	BPB	C2-C3-C5-C6
9	m	403	BPB	C4-C3-C5-C6
9	m	403	BPB	C4C-C3C-CAC-CBC
10	L	305	U10	C17-C18-C19-C20
10	L	305	U10	C17-C18-C19-C21
10	M	407	U10	C12-C13-C14-C15
10	M	407	U10	C12-C13-C14-C16
10	l	305	U10	C17-C18-C19-C20
10	l	305	U10	C17-C18-C19-C21
10	m	407	U10	C12-C13-C14-C15
10	m	407	U10	C12-C13-C14-C16
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	308	PC1	C11-O13-P-O12
11	L	308	PC1	C1-O11-P-O14
11	H	301	PC1	C1-O11-P-O14
11	H	301	PC1	O13-C11-C12-N
11	H	302	PC1	C11-O13-P-O12
11	H	302	PC1	C11-O13-P-O14
11	H	302	PC1	C1-O11-P-O12
11	H	302	PC1	C1-O11-P-O14
11	H	302	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	H	302	PC1	O13-C11-C12-N
11	A	103	PC1	C1-O11-P-O14
11	A	104	PC1	C11-O13-P-O12
11	A	104	PC1	C11-O13-P-O14
11	A	104	PC1	C1-O11-P-O14
11	A	104	PC1	O11-C1-C2-O21
11	A	105	PC1	C11-O13-P-O12
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-O14
11	A	105	PC1	C1-O11-P-O13
11	A	105	PC1	O32-C31-O31-C3
11	D	101	PC1	C11-O13-P-O12
11	D	101	PC1	C11-O13-P-O11
11	D	101	PC1	O13-C11-C12-N
11	D	102	PC1	C11-O13-P-O14
11	D	102	PC1	C1-O11-P-O13
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	308	PC1	C11-O13-P-O12
11	l	308	PC1	C1-O11-P-O14
11	h	301	PC1	C1-O11-P-O14
11	h	301	PC1	O13-C11-C12-N
11	h	302	PC1	C11-O13-P-O12
11	h	302	PC1	C11-O13-P-O14
11	h	302	PC1	C1-O11-P-O12
11	h	302	PC1	C1-O11-P-O14
11	h	302	PC1	C1-O11-P-O13
11	h	302	PC1	O13-C11-C12-N
11	a	103	PC1	C1-O11-P-O14
11	a	104	PC1	C11-O13-P-O12
11	a	104	PC1	C11-O13-P-O14
11	a	104	PC1	C1-O11-P-O14
11	a	104	PC1	O11-C1-C2-O21
11	a	105	PC1	C11-O13-P-O12
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-O14
11	a	105	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	a	105	PC1	O32-C31-O31-C3
11	d	101	PC1	C11-O13-P-O12
11	d	101	PC1	C11-O13-P-O11
11	d	101	PC1	O13-C11-C12-N
11	d	102	PC1	C11-O13-P-O14
11	d	102	PC1	C1-O11-P-O13
13	A	102	SPO	C15-C16-C17-C18
13	B	102	SPO	C2-C1-C4-C5
13	B	102	SPO	C3-C1-C4-C5
13	B	102	SPO	C11-C10-C9-C7
13	B	102	SPO	C10-C11-C12-C13
13	B	102	SPO	C10-C11-C12-C14
13	D	104	SPO	C5-C6-C7-C8
13	D	104	SPO	C5-C6-C7-C9
13	D	104	SPO	C33-C35-C36-C37
13	E	102	SPO	O1-C1-C4-C5
13	E	102	SPO	C2-C1-C4-C5
13	E	102	SPO	C3-C1-C4-C5
13	E	102	SPO	C11-C10-C9-C7
13	E	102	SPO	C10-C11-C12-C13
13	E	102	SPO	C10-C11-C12-C14
13	E	102	SPO	C12-C14-C15-C16
13	F	102	SPO	C5-C6-C7-C8
13	F	102	SPO	C5-C6-C7-C9
13	F	102	SPO	C15-C16-C17-C18
13	F	102	SPO	C33-C35-C36-C37
13	F	103	SPO	C15-C16-C17-C18
13	F	103	SPO	C34-C33-C35-C36
13	I	102	SPO	C5-C6-C7-C8
13	I	102	SPO	C5-C6-C7-C9
13	I	102	SPO	C15-C16-C17-C18
13	I	102	SPO	C15-C16-C17-C19
13	I	102	SPO	C33-C35-C36-C37
13	I	103	SPO	C10-C11-C12-C13
13	I	103	SPO	C10-C11-C12-C14
13	I	103	SPO	C15-C16-C17-C18
13	I	103	SPO	C15-C16-C17-C19
13	N	101	SPO	C5-C6-C7-C8
13	N	101	SPO	C5-C6-C7-C9
13	N	101	SPO	C15-C16-C17-C18
13	N	101	SPO	C15-C16-C17-C19
13	N	103	SPO	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	N	103	SPO	C5-C6-C7-C9
13	O	102	SPO	C15-C16-C17-C18
13	O	102	SPO	C15-C16-C17-C19
13	O	102	SPO	C34-C33-C35-C36
13	O	102	SPO	C33-C35-C36-C37
13	R	101	SPO	C5-C6-C7-C8
13	R	101	SPO	C5-C6-C7-C9
13	R	101	SPO	C10-C11-C12-C13
13	R	101	SPO	C10-C11-C12-C14
13	R	101	SPO	C33-C35-C36-C37
13	R	103	SPO	O1-C1-C4-C5
13	R	103	SPO	C1-C4-C5-C6
13	R	103	SPO	C15-C16-C17-C18
13	R	103	SPO	C15-C16-C17-C19
13	R	103	SPO	C24-C23-C25-C26
13	R	103	SPO	C32-C33-C35-C36
13	R	103	SPO	C34-C33-C35-C36
13	R	103	SPO	C33-C35-C36-C37
13	R	104	SPO	O1-C1-C4-C5
13	R	104	SPO	C2-C1-C4-C5
13	R	104	SPO	C3-C1-C4-C5
13	R	104	SPO	C10-C11-C12-C13
13	R	104	SPO	C10-C11-C12-C14
13	R	104	SPO	C32-C33-C35-C36
13	R	104	SPO	C34-C33-C35-C36
13	S	102	SPO	C32-C33-C35-C36
13	S	102	SPO	C34-C33-C35-C36
13	U	102	SPO	C15-C16-C17-C18
13	U	102	SPO	C32-C33-C35-C36
13	U	102	SPO	C34-C33-C35-C36
13	V	102	SPO	C32-C33-C35-C36
13	V	102	SPO	C34-C33-C35-C36
13	V	103	SPO	C10-C11-C12-C13
13	V	103	SPO	C10-C11-C12-C14
13	V	103	SPO	C24-C23-C25-C26
13	C	101	SPO	C10-C11-C12-C13
13	C	101	SPO	C10-C11-C12-C14
13	C	101	SPO	C33-C35-C36-C37
13	3	102	SPO	C11-C10-C9-C7
13	3	102	SPO	C10-C11-C12-C13
13	3	102	SPO	C33-C35-C36-C37
13	3	103	SPO	C1-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	3	103	SPO	C27-C28-C30-C31
13	3	103	SPO	C29-C28-C30-C31
13	7	102	SPO	C5-C6-C7-C8
13	7	102	SPO	C5-C6-C7-C9
13	7	102	SPO	C10-C11-C12-C13
13	7	102	SPO	C10-C11-C12-C14
13	7	102	SPO	C15-C16-C17-C18
13	7	102	SPO	C15-C16-C17-C19
13	9	102	SPO	C1-C4-C5-C6
13	0	102	SPO	C5-C6-C7-C8
13	0	102	SPO	C5-C6-C7-C9
13	0	102	SPO	C10-C11-C12-C13
13	0	102	SPO	C10-C11-C12-C14
13	a	102	SPO	C15-C16-C17-C18
13	b	102	SPO	C2-C1-C4-C5
13	b	102	SPO	C3-C1-C4-C5
13	b	102	SPO	C11-C10-C9-C7
13	b	102	SPO	C10-C11-C12-C13
13	b	102	SPO	C10-C11-C12-C14
13	d	104	SPO	C5-C6-C7-C8
13	d	104	SPO	C5-C6-C7-C9
13	d	104	SPO	C33-C35-C36-C37
13	e	102	SPO	O1-C1-C4-C5
13	e	102	SPO	C2-C1-C4-C5
13	e	102	SPO	C3-C1-C4-C5
13	e	102	SPO	C11-C10-C9-C7
13	e	102	SPO	C10-C11-C12-C13
13	e	102	SPO	C10-C11-C12-C14
13	e	102	SPO	C12-C14-C15-C16
13	f	102	SPO	C5-C6-C7-C8
13	f	102	SPO	C5-C6-C7-C9
13	f	102	SPO	C15-C16-C17-C18
13	f	102	SPO	C33-C35-C36-C37
13	f	103	SPO	C15-C16-C17-C18
13	f	103	SPO	C34-C33-C35-C36
13	i	102	SPO	C5-C6-C7-C8
13	i	102	SPO	C5-C6-C7-C9
13	i	102	SPO	C15-C16-C17-C18
13	i	102	SPO	C15-C16-C17-C19
13	i	102	SPO	C33-C35-C36-C37
13	i	103	SPO	C10-C11-C12-C13
13	i	103	SPO	C10-C11-C12-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	i	103	SPO	C15-C16-C17-C18
13	i	103	SPO	C15-C16-C17-C19
13	n	101	SPO	C5-C6-C7-C8
13	n	101	SPO	C5-C6-C7-C9
13	n	101	SPO	C15-C16-C17-C18
13	n	101	SPO	C15-C16-C17-C19
13	n	103	SPO	C5-C6-C7-C8
13	n	103	SPO	C5-C6-C7-C9
13	o	102	SPO	C15-C16-C17-C18
13	o	102	SPO	C15-C16-C17-C19
13	o	102	SPO	C34-C33-C35-C36
13	o	102	SPO	C33-C35-C36-C37
13	r	101	SPO	C5-C6-C7-C8
13	r	101	SPO	C5-C6-C7-C9
13	r	101	SPO	C10-C11-C12-C13
13	r	101	SPO	C10-C11-C12-C14
13	r	101	SPO	C33-C35-C36-C37
13	r	103	SPO	O1-C1-C4-C5
13	r	103	SPO	C1-C4-C5-C6
13	r	103	SPO	C15-C16-C17-C18
13	r	103	SPO	C15-C16-C17-C19
13	r	103	SPO	C24-C23-C25-C26
13	r	103	SPO	C32-C33-C35-C36
13	r	103	SPO	C34-C33-C35-C36
13	r	103	SPO	C33-C35-C36-C37
13	r	104	SPO	O1-C1-C4-C5
13	r	104	SPO	C2-C1-C4-C5
13	r	104	SPO	C3-C1-C4-C5
13	r	104	SPO	C10-C11-C12-C13
13	r	104	SPO	C10-C11-C12-C14
13	r	104	SPO	C32-C33-C35-C36
13	r	104	SPO	C34-C33-C35-C36
13	s	102	SPO	C32-C33-C35-C36
13	s	102	SPO	C34-C33-C35-C36
13	u	102	SPO	C15-C16-C17-C18
13	u	102	SPO	C32-C33-C35-C36
13	u	102	SPO	C34-C33-C35-C36
13	v	102	SPO	C32-C33-C35-C36
13	v	102	SPO	C34-C33-C35-C36
13	v	103	SPO	C10-C11-C12-C13
13	v	103	SPO	C10-C11-C12-C14
13	v	103	SPO	C24-C23-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	c	101	SPO	C10-C11-C12-C13
13	c	101	SPO	C10-C11-C12-C14
13	c	101	SPO	C33-C35-C36-C37
13	5	102	SPO	C11-C10-C9-C7
13	5	102	SPO	C10-C11-C12-C13
13	5	102	SPO	C33-C35-C36-C37
13	5	103	SPO	C1-C4-C5-C6
13	5	103	SPO	C27-C28-C30-C31
13	5	103	SPO	C29-C28-C30-C31
13	6	102	SPO	C5-C6-C7-C8
13	6	102	SPO	C5-C6-C7-C9
13	6	102	SPO	C10-C11-C12-C13
13	6	102	SPO	C10-C11-C12-C14
13	6	102	SPO	C15-C16-C17-C18
13	6	102	SPO	C15-C16-C17-C19
13	b9	102	SPO	C1-C4-C5-C6
13	b0	102	SPO	C5-C6-C7-C8
13	b0	102	SPO	C5-C6-C7-C9
13	b0	102	SPO	C10-C11-C12-C13
13	b0	102	SPO	C10-C11-C12-C14
14	M	406	CDL	CA2-OA2-PA1-OA3
14	M	406	CDL	CA2-OA2-PA1-OA4
14	M	406	CDL	CB2-OB2-PB2-OB4
14	M	406	CDL	CB3-OB5-PB2-OB2
14	M	406	CDL	CB3-OB5-PB2-OB3
14	M	406	CDL	CB3-OB5-PB2-OB4
14	H	303	CDL	C11-CA5-OA6-CA4
14	H	303	CDL	CB3-OB5-PB2-OB2
14	H	303	CDL	CB3-OB5-PB2-OB3
14	H	303	CDL	CB3-OB5-PB2-OB4
14	m	406	CDL	CA2-OA2-PA1-OA3
14	m	406	CDL	CA2-OA2-PA1-OA4
14	m	406	CDL	CB2-OB2-PB2-OB4
14	m	406	CDL	CB3-OB5-PB2-OB2
14	m	406	CDL	CB3-OB5-PB2-OB3
14	m	406	CDL	CB3-OB5-PB2-OB4
14	h	303	CDL	C11-CA5-OA6-CA4
14	h	303	CDL	CB3-OB5-PB2-OB2
14	h	303	CDL	CB3-OB5-PB2-OB3
14	h	303	CDL	CB3-OB5-PB2-OB4
11	L	308	PC1	O32-C31-O31-C3
11	l	308	PC1	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	M	406	CDL	OA9-CA7-OA8-CA6
14	H	303	CDL	OB9-CB7-OB8-CB6
14	m	406	CDL	OA9-CA7-OA8-CA6
14	h	303	CDL	OB9-CB7-OB8-CB6
14	H	303	CDL	OA7-CA5-OA6-CA4
14	h	303	CDL	OA7-CA5-OA6-CA4
11	A	105	PC1	C32-C31-O31-C3
11	a	105	PC1	C32-C31-O31-C3
14	M	406	CDL	C31-CA7-OA8-CA6
14	m	406	CDL	C31-CA7-OA8-CA6
10	L	305	U10	C25-C24-C26-C27
10	l	305	U10	C25-C24-C26-C27
13	F	102	SPO	C34-C33-C35-C36
13	I	102	SPO	C34-C33-C35-C36
13	N	103	SPO	C34-C33-C35-C36
13	R	103	SPO	C29-C28-C30-C31
13	V	102	SPO	C29-C28-C30-C31
13	C	101	SPO	C34-C33-C35-C36
13	3	102	SPO	C34-C33-C35-C36
13	f	102	SPO	C34-C33-C35-C36
13	i	102	SPO	C34-C33-C35-C36
13	n	103	SPO	C34-C33-C35-C36
13	r	103	SPO	C29-C28-C30-C31
13	v	102	SPO	C29-C28-C30-C31
13	c	101	SPO	C34-C33-C35-C36
13	5	102	SPO	C34-C33-C35-C36
10	L	305	U10	C23-C24-C26-C27
10	l	305	U10	C23-C24-C26-C27
13	N	103	SPO	C32-C33-C35-C36
13	O	102	SPO	C32-C33-C35-C36
13	R	103	SPO	C27-C28-C30-C31
13	C	101	SPO	C32-C33-C35-C36
13	n	103	SPO	C32-C33-C35-C36
13	o	102	SPO	C32-C33-C35-C36
13	r	103	SPO	C27-C28-C30-C31
13	c	101	SPO	C32-C33-C35-C36
8	B	101	BCL	C2A-CAA-CBA-CGA
8	E	101	BCL	C2A-CAA-CBA-CGA
8	J	101	BCL	C2A-CAA-CBA-CGA
8	R	102	BCL	C2A-CAA-CBA-CGA
8	b	101	BCL	C2A-CAA-CBA-CGA
8	e	101	BCL	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	j	101	BCL	C2A-CAA-CBA-CGA
8	r	102	BCL	C2A-CAA-CBA-CGA
11	L	308	PC1	C32-C31-O31-C3
11	l	308	PC1	C32-C31-O31-C3
14	H	303	CDL	C71-CB7-OB8-CB6
14	h	303	CDL	C71-CB7-OB8-CB6
13	F	103	SPO	C11-C10-C9-C7
13	f	103	SPO	C11-C10-C9-C7
10	l	305	U10	C12-C11-C9-C10
13	M	405	SPO	C34-C33-C35-C36
13	B	102	SPO	C34-C33-C35-C36
13	E	102	SPO	C34-C33-C35-C36
13	J	102	SPO	C34-C33-C35-C36
13	3	103	SPO	C34-C33-C35-C36
13	9	102	SPO	C34-C33-C35-C36
13	m	405	SPO	C34-C33-C35-C36
13	b	102	SPO	C34-C33-C35-C36
13	e	102	SPO	C34-C33-C35-C36
13	j	102	SPO	C34-C33-C35-C36
13	5	103	SPO	C34-C33-C35-C36
13	b9	102	SPO	C34-C33-C35-C36
13	M	405	SPO	C32-C33-C35-C36
13	B	102	SPO	C32-C33-C35-C36
13	E	102	SPO	C32-C33-C35-C36
13	F	102	SPO	C32-C33-C35-C36
13	F	103	SPO	C32-C33-C35-C36
13	J	102	SPO	C32-C33-C35-C36
13	3	103	SPO	C32-C33-C35-C36
13	9	102	SPO	C32-C33-C35-C36
13	m	405	SPO	C32-C33-C35-C36
13	b	102	SPO	C32-C33-C35-C36
13	e	102	SPO	C32-C33-C35-C36
13	f	102	SPO	C32-C33-C35-C36
13	f	103	SPO	C32-C33-C35-C36
13	j	102	SPO	C32-C33-C35-C36
13	5	103	SPO	C32-C33-C35-C36
13	b9	102	SPO	C32-C33-C35-C36
11	L	308	PC1	C22-C23-C24-C25
11	l	308	PC1	C22-C23-C24-C25
10	L	304	U10	C24-C26-C27-C28
10	M	407	U10	C14-C16-C17-C18
10	l	304	U10	C24-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	m	407	U10	C14-C16-C17-C18
13	F	103	SPO	C28-C30-C31-C32
13	J	102	SPO	C28-C30-C31-C32
13	J	102	SPO	C33-C35-C36-C37
13	R	103	SPO	C28-C30-C31-C32
13	U	102	SPO	C33-C35-C36-C37
13	9	102	SPO	C33-C35-C36-C37
13	f	103	SPO	C28-C30-C31-C32
13	j	102	SPO	C28-C30-C31-C32
13	j	102	SPO	C33-C35-C36-C37
13	r	103	SPO	C28-C30-C31-C32
13	u	102	SPO	C33-C35-C36-C37
13	b9	102	SPO	C33-C35-C36-C37
11	L	308	PC1	C22-C21-O21-C2
11	l	308	PC1	C22-C21-O21-C2
11	L	306	PC1	C11-C12-N-C13
11	A	105	PC1	C11-C12-N-C13
11	A	105	PC1	C11-C12-N-C14
11	l	306	PC1	C11-C12-N-C13
11	a	105	PC1	C11-C12-N-C13
11	a	105	PC1	C11-C12-N-C14
11	D	102	PC1	C32-C31-O31-C3
11	d	102	PC1	C32-C31-O31-C3
13	R	103	SPO	C11-C10-C9-C7
13	r	103	SPO	C11-C10-C9-C7
10	M	404	U10	C37-C38-C39-C40
10	m	404	U10	C37-C38-C39-C40
11	L	306	PC1	O21-C2-C3-O31
11	l	306	PC1	O21-C2-C3-O31
10	L	305	U10	C12-C11-C9-C10
13	D	104	SPO	C34-C33-C35-C36
13	d	104	SPO	C34-C33-C35-C36
13	I	102	SPO	C32-C33-C35-C36
13	V	102	SPO	C27-C28-C30-C31
13	3	102	SPO	C32-C33-C35-C36
13	i	102	SPO	C32-C33-C35-C36
13	v	102	SPO	C27-C28-C30-C31
13	5	102	SPO	C32-C33-C35-C36
8	V	101	BCL	C6-C7-C8-C9
8	v	101	BCL	C6-C7-C8-C9
13	E	102	SPO	C15-C16-C17-C18
13	I	103	SPO	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	N	101	SPO	C10-C11-C12-C13
13	N	103	SPO	C10-C11-C12-C13
13	R	103	SPO	C5-C6-C7-C8
13	R	104	SPO	C5-C6-C7-C8
13	S	102	SPO	C10-C11-C12-C13
13	C	101	SPO	C15-C16-C17-C18
13	3	103	SPO	C5-C6-C7-C8
13	9	102	SPO	C5-C6-C7-C8
13	9	102	SPO	C10-C11-C12-C13
13	9	102	SPO	C15-C16-C17-C18
13	e	102	SPO	C15-C16-C17-C18
13	i	103	SPO	C5-C6-C7-C8
13	n	101	SPO	C10-C11-C12-C13
13	n	103	SPO	C10-C11-C12-C13
13	r	103	SPO	C5-C6-C7-C8
13	r	104	SPO	C5-C6-C7-C8
13	s	102	SPO	C10-C11-C12-C13
13	c	101	SPO	C15-C16-C17-C18
13	5	103	SPO	C5-C6-C7-C8
13	b9	102	SPO	C5-C6-C7-C8
13	b9	102	SPO	C10-C11-C12-C13
13	b9	102	SPO	C15-C16-C17-C18
13	E	102	SPO	C15-C16-C17-C19
13	I	103	SPO	C5-C6-C7-C9
13	R	103	SPO	C5-C6-C7-C9
13	R	103	SPO	C22-C23-C25-C26
13	V	103	SPO	C5-C6-C7-C9
13	3	102	SPO	C10-C11-C12-C14
13	3	103	SPO	C5-C6-C7-C9
13	9	102	SPO	C5-C6-C7-C9
13	9	102	SPO	C10-C11-C12-C14
13	9	102	SPO	C15-C16-C17-C19
13	e	102	SPO	C15-C16-C17-C19
13	i	103	SPO	C5-C6-C7-C9
13	r	103	SPO	C5-C6-C7-C9
13	r	103	SPO	C22-C23-C25-C26
13	v	103	SPO	C5-C6-C7-C9
13	5	102	SPO	C10-C11-C12-C14
13	5	103	SPO	C5-C6-C7-C9
13	b9	102	SPO	C5-C6-C7-C9
13	b9	102	SPO	C10-C11-C12-C14
13	b9	102	SPO	C15-C16-C17-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	D	102	PC1	C31-C32-C33-C34
11	d	102	PC1	C31-C32-C33-C34
14	M	406	CDL	CA7-C31-C32-C33
14	m	406	CDL	CA7-C31-C32-C33
11	L	308	PC1	O22-C21-O21-C2
11	l	308	PC1	O22-C21-O21-C2
8	B	101	BCL	C10-C11-C12-C13
8	b	101	BCL	C10-C11-C12-C13
8	D	103	BCL	C11-C10-C8-C7
8	d	103	BCL	C11-C10-C8-C7
11	D	102	PC1	O32-C31-O31-C3
11	d	102	PC1	O32-C31-O31-C3
10	L	304	U10	C14-C16-C17-C18
10	M	404	U10	C24-C26-C27-C28
10	M	407	U10	C24-C26-C27-C28
10	l	304	U10	C14-C16-C17-C18
10	m	404	U10	C24-C26-C27-C28
10	m	407	U10	C24-C26-C27-C28
13	A	102	SPO	C33-C35-C36-C37
13	N	101	SPO	C33-C35-C36-C37
13	N	103	SPO	C28-C30-C31-C32
13	S	102	SPO	C33-C35-C36-C37
13	3	103	SPO	C33-C35-C36-C37
13	a	102	SPO	C33-C35-C36-C37
13	n	101	SPO	C33-C35-C36-C37
13	n	103	SPO	C28-C30-C31-C32
13	s	102	SPO	C33-C35-C36-C37
13	5	103	SPO	C33-C35-C36-C37
11	L	308	PC1	C11-O13-P-O11
11	L	308	PC1	C1-O11-P-O13
11	H	302	PC1	C11-O13-P-O11
11	A	104	PC1	C11-O13-P-O11
11	A	104	PC1	C1-O11-P-O13
11	D	101	PC1	C1-O11-P-O13
11	D	102	PC1	C11-O13-P-O11
11	l	308	PC1	C11-O13-P-O11
11	l	308	PC1	C1-O11-P-O13
11	h	302	PC1	C11-O13-P-O11
11	a	104	PC1	C11-O13-P-O11
11	a	104	PC1	C1-O11-P-O13
11	d	101	PC1	C1-O11-P-O13
11	d	102	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	M	406	CDL	CA2-OA2-PA1-OA5
14	M	406	CDL	CB2-OB2-PB2-OB5
14	m	406	CDL	CA2-OA2-PA1-OA5
14	m	406	CDL	CB2-OB2-PB2-OB5
11	D	101	PC1	C32-C33-C34-C35
11	d	101	PC1	C32-C33-C34-C35
8	R	102	BCL	C4-C3-C5-C6
8	r	102	BCL	C4-C3-C5-C6
11	L	306	PC1	C11-C12-N-C14
11	l	306	PC1	C11-C12-N-C14
13	R	103	SPO	C17-C19-C20-C21
13	r	103	SPO	C17-C19-C20-C21
11	L	306	PC1	C22-C21-O21-C2
11	l	306	PC1	C22-C21-O21-C2
10	M	404	U10	C37-C38-C39-C41
10	m	404	U10	C37-C38-C39-C41
11	L	306	PC1	O22-C21-O21-C2
11	l	306	PC1	O22-C21-O21-C2
8	J	101	BCL	C4-C3-C5-C6
8	j	101	BCL	C4-C3-C5-C6
10	M	407	U10	C12-C11-C9-C10
10	m	407	U10	C12-C11-C9-C10
8	R	102	BCL	C2-C3-C5-C6
8	r	102	BCL	C2-C3-C5-C6
8	S	101	BCL	C11-C10-C8-C9
8	s	101	BCL	C11-C10-C8-C9
11	A	103	PC1	C28-C29-C2A-C2B
11	a	103	PC1	C28-C29-C2A-C2B
13	V	103	SPO	C5-C6-C7-C8
13	v	103	SPO	C5-C6-C7-C8
13	F	102	SPO	C15-C16-C17-C19
13	R	104	SPO	C5-C6-C7-C9
13	U	102	SPO	C15-C16-C17-C19
13	f	102	SPO	C15-C16-C17-C19
13	r	104	SPO	C5-C6-C7-C9
13	u	102	SPO	C15-C16-C17-C19
14	M	406	CDL	C11-CA5-OA6-CA4
14	m	406	CDL	C11-CA5-OA6-CA4
11	L	306	PC1	C21-C22-C23-C24
11	l	306	PC1	C21-C22-C23-C24
11	D	102	PC1	C22-C23-C24-C25
11	d	102	PC1	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	303	CDL	C32-C33-C34-C35
14	M	406	CDL	CA5-C11-C12-C13
14	m	406	CDL	CA5-C11-C12-C13
14	h	303	CDL	C32-C33-C34-C35
11	A	103	PC1	C32-C33-C34-C35
11	a	103	PC1	C32-C33-C34-C35
14	M	406	CDL	C78-C79-C80-C81
14	m	406	CDL	C78-C79-C80-C81
14	M	406	CDL	C34-C35-C36-C37
14	m	406	CDL	C34-C35-C36-C37
14	M	406	CDL	OA7-CA5-OA6-CA4
14	m	406	CDL	OA7-CA5-OA6-CA4
8	C	102	BCL	C4-C3-C5-C6
8	c	102	BCL	C4-C3-C5-C6
10	L	304	U10	C20-C19-C21-C22
10	M	404	U10	C30-C29-C31-C32
10	l	304	U10	C20-C19-C21-C22
10	m	404	U10	C30-C29-C31-C32
8	C	102	BCL	C2-C3-C5-C6
8	c	102	BCL	C2-C3-C5-C6
10	L	304	U10	C13-C14-C16-C17
10	L	304	U10	C18-C19-C21-C22
10	M	404	U10	C28-C29-C31-C32
10	M	407	U10	C12-C11-C9-C8
10	l	304	U10	C13-C14-C16-C17
10	l	304	U10	C18-C19-C21-C22
10	m	404	U10	C28-C29-C31-C32
10	m	407	U10	C12-C11-C9-C8
13	D	104	SPO	C32-C33-C35-C36
13	d	104	SPO	C32-C33-C35-C36
11	A	105	PC1	C22-C21-O21-C2
11	a	105	PC1	C22-C21-O21-C2
11	L	306	PC1	C11-C12-N-C15
11	A	105	PC1	C11-C12-N-C15
11	l	306	PC1	C11-C12-N-C15
11	a	105	PC1	C11-C12-N-C15
10	L	304	U10	C15-C14-C16-C17
10	l	304	U10	C15-C14-C16-C17
8	F	101	BCL	C11-C10-C8-C7
8	J	101	BCL	C2-C3-C5-C6
8	S	101	BCL	C11-C10-C8-C7
8	T	101	BCL	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	f	101	BCL	C11-C10-C8-C7
8	j	101	BCL	C2-C3-C5-C6
8	s	101	BCL	C11-C10-C8-C7
8	t	101	BCL	C2-C3-C5-C6
11	A	105	PC1	O22-C21-O21-C2
11	a	105	PC1	O22-C21-O21-C2
14	H	303	CDL	OB7-CB5-OB6-CB4
14	h	303	CDL	OB7-CB5-OB6-CB4
11	A	103	PC1	C2A-C2B-C2C-C2D
11	a	103	PC1	C2A-C2B-C2C-C2D
8	T	101	BCL	C2A-CAA-CBA-CGA
8	t	101	BCL	C2A-CAA-CBA-CGA
10	M	407	U10	C22-C23-C24-C25
10	m	407	U10	C22-C23-C24-C25
14	M	406	CDL	C31-C32-C33-C34
14	m	406	CDL	C31-C32-C33-C34
11	A	104	PC1	C22-C21-O21-C2
11	a	104	PC1	C22-C21-O21-C2
14	H	303	CDL	C51-CB5-OB6-CB4
14	h	303	CDL	C51-CB5-OB6-CB4
11	A	104	PC1	O22-C21-O21-C2
11	a	104	PC1	O22-C21-O21-C2
8	T	101	BCL	C4-C3-C5-C6
8	t	101	BCL	C4-C3-C5-C6
13	a	102	SPO	C34-C33-C35-C36
10	L	305	U10	C12-C11-C9-C8
10	l	305	U10	C12-C11-C9-C8
8	D	103	BCL	C11-C10-C8-C9
8	F	101	BCL	C11-C10-C8-C9
8	d	103	BCL	C11-C10-C8-C9
8	f	101	BCL	C11-C10-C8-C9
13	A	102	SPO	C5-C6-C7-C8
13	E	102	SPO	C5-C6-C7-C8
13	O	102	SPO	C5-C6-C7-C8
13	S	102	SPO	C5-C6-C7-C8
13	V	102	SPO	C5-C6-C7-C8
13	3	102	SPO	C5-C6-C7-C8
13	a	102	SPO	C5-C6-C7-C8
13	e	102	SPO	C5-C6-C7-C8
13	o	102	SPO	C5-C6-C7-C8
13	s	102	SPO	C5-C6-C7-C8
13	v	102	SPO	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	5	102	SPO	C5-C6-C7-C8
13	A	102	SPO	C5-C6-C7-C9
13	E	102	SPO	C5-C6-C7-C9
13	F	103	SPO	C15-C16-C17-C19
13	O	102	SPO	C5-C6-C7-C9
13	S	102	SPO	C5-C6-C7-C9
13	V	102	SPO	C5-C6-C7-C9
13	3	102	SPO	C5-C6-C7-C9
13	a	102	SPO	C5-C6-C7-C9
13	e	102	SPO	C5-C6-C7-C9
13	f	103	SPO	C15-C16-C17-C19
13	o	102	SPO	C5-C6-C7-C9
13	s	102	SPO	C5-C6-C7-C9
13	v	102	SPO	C5-C6-C7-C9
13	5	102	SPO	C5-C6-C7-C9
11	L	308	PC1	C24-C25-C26-C27
11	l	308	PC1	C24-C25-C26-C27
13	F	103	SPO	C25-C26-C27-C28
13	I	103	SPO	C17-C19-C20-C21
13	J	102	SPO	C11-C10-C9-C7
13	9	102	SPO	C12-C14-C15-C16
13	f	103	SPO	C25-C26-C27-C28
13	i	103	SPO	C17-C19-C20-C21
13	j	102	SPO	C11-C10-C9-C7
13	b9	102	SPO	C12-C14-C15-C16
14	H	303	CDL	C73-C74-C75-C76
14	h	303	CDL	C73-C74-C75-C76
11	L	308	PC1	O11-C1-C2-C3
11	A	104	PC1	O11-C1-C2-C3
11	l	308	PC1	O11-C1-C2-C3
11	a	104	PC1	O11-C1-C2-C3
14	m	406	CDL	C53-C54-C55-C56
14	M	406	CDL	C53-C54-C55-C56
11	D	101	PC1	C21-C22-C23-C24
11	d	101	PC1	C21-C22-C23-C24
13	A	102	SPO	C34-C33-C35-C36
13	I	103	SPO	C34-C33-C35-C36
13	i	103	SPO	C34-C33-C35-C36
8	N	102	BCL	C2C-C3C-CAC-CBC
8	S	101	BCL	C2C-C3C-CAC-CBC
8	n	102	BCL	C2C-C3C-CAC-CBC
8	s	101	BCL	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	M	406	CDL	C51-CB5-OB6-CB4
14	m	406	CDL	C51-CB5-OB6-CB4
11	D	102	PC1	C37-C38-C39-C3A
11	d	102	PC1	C37-C38-C39-C3A
11	L	306	PC1	C1-C2-C3-O31
11	L	308	PC1	C1-C2-C3-O31
11	A	105	PC1	C1-C2-C3-O31
11	l	306	PC1	C1-C2-C3-O31
11	l	308	PC1	C1-C2-C3-O31
11	a	105	PC1	C1-C2-C3-O31
13	B	102	SPO	C33-C35-C36-C37
13	I	102	SPO	C4-C1-O1-CM1
13	V	103	SPO	C33-C35-C36-C37
13	b	102	SPO	C33-C35-C36-C37
13	i	102	SPO	C4-C1-O1-CM1
13	v	103	SPO	C33-C35-C36-C37
11	A	103	PC1	C22-C23-C24-C25
11	a	103	PC1	C22-C23-C24-C25
11	D	102	PC1	C22-C21-O21-C2
11	d	102	PC1	C22-C21-O21-C2
8	v	101	BCL	C10-C11-C12-C13
14	M	406	CDL	CA4-CA3-OA5-PA1
14	m	406	CDL	CA4-CA3-OA5-PA1
11	L	306	PC1	C22-C23-C24-C25
11	l	306	PC1	C22-C23-C24-C25
14	M	406	CDL	OA5-CA3-CA4-OA6
14	m	406	CDL	OA5-CA3-CA4-OA6
8	V	101	BCL	C10-C11-C12-C13
13	I	102	SPO	C2-C1-O1-CM1
13	I	102	SPO	C3-C1-O1-CM1
13	i	102	SPO	C2-C1-O1-CM1
13	i	102	SPO	C3-C1-O1-CM1
11	D	101	PC1	O21-C2-C3-O31
11	d	101	PC1	O21-C2-C3-O31
13	M	405	SPO	C2-C1-C4-C5
13	M	405	SPO	C3-C1-C4-C5
13	R	103	SPO	C2-C1-C4-C5
13	m	405	SPO	C2-C1-C4-C5
13	m	405	SPO	C3-C1-C4-C5
13	r	103	SPO	C2-C1-C4-C5
13	0	102	SPO	C34-C33-C35-C36
13	b0	102	SPO	C34-C33-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	103	PC1	C23-C24-C25-C26
8	Q	101	BCL	C11-C10-C8-C7
8	q	101	BCL	C11-C10-C8-C7
11	a	103	PC1	C23-C24-C25-C26
8	A	101	BCL	C11-C10-C8-C9
8	Q	101	BCL	C11-C10-C8-C9
8	7	101	BCL	C6-C7-C8-C9
8	a	101	BCL	C11-C10-C8-C9
8	q	101	BCL	C11-C10-C8-C9
8	6	101	BCL	C6-C7-C8-C9
13	B	102	SPO	O1-C1-C4-C5
13	3	103	SPO	O1-C1-C4-C5
13	b	102	SPO	O1-C1-C4-C5
13	5	103	SPO	O1-C1-C4-C5
13	U	102	SPO	C5-C6-C7-C8
13	V	102	SPO	C10-C11-C12-C13
13	C	101	SPO	C5-C6-C7-C8
13	u	102	SPO	C5-C6-C7-C8
13	v	102	SPO	C10-C11-C12-C13
13	c	101	SPO	C5-C6-C7-C8
13	A	102	SPO	C15-C16-C17-C19
13	N	103	SPO	C10-C11-C12-C14
13	C	101	SPO	C5-C6-C7-C9
13	C	101	SPO	C15-C16-C17-C19
13	a	102	SPO	C15-C16-C17-C19
13	n	103	SPO	C10-C11-C12-C14
13	c	101	SPO	C5-C6-C7-C9
13	c	101	SPO	C15-C16-C17-C19
11	H	302	PC1	O11-C1-C2-C3
11	D	101	PC1	O11-C1-C2-C3
11	h	302	PC1	O11-C1-C2-C3
11	d	101	PC1	O11-C1-C2-C3
14	M	406	CDL	OA5-CA3-CA4-CA6
14	m	406	CDL	OA5-CA3-CA4-CA6
11	A	103	PC1	C33-C34-C35-C36
11	a	103	PC1	C33-C34-C35-C36
13	F	103	SPO	C29-C28-C30-C31
13	f	103	SPO	C29-C28-C30-C31
14	M	406	CDL	C39-C40-C41-C42
14	m	406	CDL	C39-C40-C41-C42
11	A	103	PC1	C1-C2-C3-O31
11	A	104	PC1	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	D	101	PC1	C1-C2-C3-O31
11	a	103	PC1	C1-C2-C3-O31
11	a	104	PC1	C1-C2-C3-O31
11	d	101	PC1	C1-C2-C3-O31
14	H	303	CDL	CA3-CA4-CA6-OA8
14	h	303	CDL	CA3-CA4-CA6-OA8
11	A	103	PC1	C27-C28-C29-C2A
11	a	103	PC1	C27-C28-C29-C2A
8	8	101	BCL	C8-C10-C11-C12
8	b8	101	BCL	C8-C10-C11-C12
14	H	303	CDL	CB2-OB2-PB2-OB5
14	h	303	CDL	CB2-OB2-PB2-OB5
10	L	304	U10	C12-C13-C14-C15
10	l	304	U10	C12-C13-C14-C15
11	L	308	PC1	O21-C2-C3-O31
11	A	103	PC1	O21-C2-C3-O31
11	D	102	PC1	O21-C2-C3-O31
11	l	308	PC1	O21-C2-C3-O31
11	a	103	PC1	O21-C2-C3-O31
11	d	102	PC1	O21-C2-C3-O31
14	H	303	CDL	OB6-CB4-CB6-OB8
14	h	303	CDL	OB6-CB4-CB6-OB8
8	8	101	BCL	C11-C12-C13-C14
8	b8	101	BCL	C11-C12-C13-C14
13	F	103	SPO	C33-C35-C36-C37
13	f	103	SPO	C33-C35-C36-C37
11	D	102	PC1	O22-C21-O21-C2
11	d	102	PC1	O22-C21-O21-C2
14	M	406	CDL	OB7-CB5-OB6-CB4
14	m	406	CDL	OB7-CB5-OB6-CB4
8	1	101	BCL	C2-C1-O2A-CGA
8	b1	101	BCL	C2-C1-O2A-CGA
13	M	405	SPO	C5-C6-C7-C8
13	m	405	SPO	C5-C6-C7-C8
13	N	101	SPO	C10-C11-C12-C14
13	S	102	SPO	C10-C11-C12-C14
13	V	103	SPO	C22-C23-C25-C26
13	n	101	SPO	C10-C11-C12-C14
13	s	102	SPO	C10-C11-C12-C14
13	v	103	SPO	C22-C23-C25-C26
11	A	105	PC1	O11-C1-C2-C3
11	a	105	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	M	406	CDL	OB5-CB3-CB4-CB6
14	m	406	CDL	OB5-CB3-CB4-CB6
8	A	101	BCL	C11-C10-C8-C7
8	V	101	BCL	C6-C7-C8-C10
8	a	101	BCL	C11-C10-C8-C7
8	v	101	BCL	C6-C7-C8-C10
13	N	103	SPO	C11-C10-C9-C7
13	n	103	SPO	C11-C10-C9-C7
8	L	302	BCL	CAD-CBD-CGD-O2D
8	l	302	BCL	CAD-CBD-CGD-O2D
9	L	303	BPB	CAD-CBD-CGD-O2D
9	M	403	BPB	CAD-CBD-CGD-O2D
9	l	303	BPB	CAD-CBD-CGD-O2D
9	m	403	BPB	CAD-CBD-CGD-O2D
11	D	101	PC1	C22-C23-C24-C25
11	d	101	PC1	C22-C23-C24-C25
10	M	404	U10	C33-C34-C36-C37
10	m	404	U10	C33-C34-C36-C37
10	M	407	U10	C5-C4-O4-C4M
10	m	407	U10	C5-C4-O4-C4M
11	A	105	PC1	O11-C1-C2-O21
11	a	105	PC1	O11-C1-C2-O21
14	H	303	CDL	OA5-CA3-CA4-OA6
14	h	303	CDL	OA5-CA3-CA4-OA6
11	A	105	PC1	O21-C2-C3-O31
11	a	105	PC1	O21-C2-C3-O31
8	B	101	BCL	C4-C3-C5-C6
8	b	101	BCL	C4-C3-C5-C6
10	M	404	U10	C35-C34-C36-C37
10	m	404	U10	C35-C34-C36-C37
11	A	103	PC1	C31-C32-C33-C34
11	a	103	PC1	C31-C32-C33-C34
8	G	101	BCL	C10-C11-C12-C13
8	g	101	BCL	C10-C11-C12-C13
13	B	102	SPO	C5-C6-C7-C8
13	R	101	SPO	C15-C16-C17-C18
13	b	102	SPO	C5-C6-C7-C8
13	r	101	SPO	C15-C16-C17-C18
13	B	102	SPO	C5-C6-C7-C9
13	U	102	SPO	C5-C6-C7-C9
13	V	102	SPO	C10-C11-C12-C14
13	b	102	SPO	C5-C6-C7-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	u	102	SPO	C5-C6-C7-C9
13	v	102	SPO	C10-C11-C12-C14
14	H	303	CDL	C31-CA7-OA8-CA6
13	I	103	SPO	C12-C14-C15-C16
13	i	103	SPO	C12-C14-C15-C16
11	A	103	PC1	C1-O11-P-O13
11	a	103	PC1	C1-O11-P-O13
13	J	102	SPO	C29-C28-C30-C31
13	3	102	SPO	C29-C28-C30-C31
13	5	102	SPO	C29-C28-C30-C31
8	A	101	BCL	C8-C10-C11-C12
8	a	101	BCL	C8-C10-C11-C12
11	A	104	PC1	C2-C1-O11-P
11	A	105	PC1	C2-C1-O11-P
11	a	104	PC1	C2-C1-O11-P
11	a	105	PC1	C2-C1-O11-P
13	A	102	SPO	C32-C33-C35-C36
13	a	102	SPO	C32-C33-C35-C36
11	L	308	PC1	C11-O13-P-O14
11	L	308	PC1	C1-O11-P-O12
11	A	103	PC1	C11-C12-N-C13
11	A	103	PC1	C11-C12-N-C14
11	A	104	PC1	C1-O11-P-O12
11	D	101	PC1	C1-O11-P-O12
11	D	101	PC1	C1-O11-P-O14
11	D	102	PC1	C11-O13-P-O12
11	D	102	PC1	C1-O11-P-O14
11	l	308	PC1	C11-O13-P-O14
11	l	308	PC1	C1-O11-P-O12
11	a	103	PC1	C11-C12-N-C13
11	a	103	PC1	C11-C12-N-C14
11	a	104	PC1	C1-O11-P-O12
11	d	101	PC1	C1-O11-P-O12
11	d	101	PC1	C1-O11-P-O14
11	d	102	PC1	C11-O13-P-O12
11	d	102	PC1	C1-O11-P-O14
14	M	406	CDL	CB2-OB2-PB2-OB3
14	H	303	CDL	CA2-OA2-PA1-OA3
14	H	303	CDL	CB2-OB2-PB2-OB4
14	m	406	CDL	CB2-OB2-PB2-OB3
14	h	303	CDL	CA2-OA2-PA1-OA3
14	h	303	CDL	CB2-OB2-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	h	303	CDL	C31-CA7-OA8-CA6
10	L	305	U10	C29-C31-C32-C33
10	l	305	U10	C29-C31-C32-C33
14	m	406	CDL	C77-C78-C79-C80
14	M	406	CDL	C77-C78-C79-C80
8	8	101	BCL	C11-C12-C13-C15
8	b8	101	BCL	C11-C12-C13-C15
11	H	302	PC1	C12-C11-O13-P
11	A	104	PC1	C12-C11-O13-P
11	D	101	PC1	C12-C11-O13-P
11	h	302	PC1	C12-C11-O13-P
11	a	104	PC1	C12-C11-O13-P
11	d	101	PC1	C12-C11-O13-P
13	V	102	SPO	C1-C4-C5-C6
13	v	102	SPO	C1-C4-C5-C6
8	V	101	BCL	C4-C3-C5-C6
8	v	101	BCL	C4-C3-C5-C6
13	j	102	SPO	C29-C28-C30-C31
11	L	308	PC1	O11-C1-C2-O21
11	H	302	PC1	O11-C1-C2-O21
11	D	101	PC1	O11-C1-C2-O21
11	l	308	PC1	O11-C1-C2-O21
11	h	302	PC1	O11-C1-C2-O21
11	d	101	PC1	O11-C1-C2-O21
14	M	406	CDL	OB5-CB3-CB4-OB6
14	m	406	CDL	OB5-CB3-CB4-OB6
11	A	104	PC1	C32-C33-C34-C35
11	a	104	PC1	C32-C33-C34-C35
14	H	303	CDL	C77-C78-C79-C80
14	h	303	CDL	C77-C78-C79-C80
11	L	308	PC1	O13-C11-C12-N
11	D	102	PC1	O13-C11-C12-N
11	l	308	PC1	O13-C11-C12-N
11	d	102	PC1	O13-C11-C12-N
11	A	104	PC1	O21-C2-C3-O31
11	a	104	PC1	O21-C2-C3-O31
14	H	303	CDL	OA6-CA4-CA6-OA8
14	h	303	CDL	OA6-CA4-CA6-OA8
8	C	102	BCL	C11-C12-C13-C14
8	c	102	BCL	C11-C12-C13-C14
8	B	101	BCL	C2-C3-C5-C6
8	b	101	BCL	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	303	CDL	OA9-CA7-OA8-CA6
14	h	303	CDL	OA9-CA7-OA8-CA6
13	M	405	SPO	C33-C35-C36-C37
13	I	103	SPO	C33-C35-C36-C37
13	m	405	SPO	C33-C35-C36-C37
13	i	103	SPO	C33-C35-C36-C37
13	B	102	SPO	C9-C10-C11-C12
13	E	102	SPO	C9-C10-C11-C12
13	R	104	SPO	C9-C10-C11-C12
13	b	102	SPO	C9-C10-C11-C12
13	e	102	SPO	C9-C10-C11-C12
13	r	104	SPO	C9-C10-C11-C12
8	j	101	BCL	C10-C11-C12-C13
14	M	406	CDL	C40-C41-C42-C43
14	m	406	CDL	C40-C41-C42-C43
8	J	101	BCL	C10-C11-C12-C13
13	I	103	SPO	C32-C33-C35-C36
13	3	102	SPO	C27-C28-C30-C31
13	i	103	SPO	C32-C33-C35-C36
13	5	102	SPO	C27-C28-C30-C31
11	D	101	PC1	C3-C2-O21-C21
11	d	101	PC1	C3-C2-O21-C21
13	A	102	SPO	C17-C19-C20-C21
13	a	102	SPO	C17-C19-C20-C21
11	D	102	PC1	O11-C1-C2-O21
11	d	102	PC1	O11-C1-C2-O21
11	D	101	PC1	O21-C21-C22-C23
13	F	103	SPO	C27-C28-C30-C31
13	0	102	SPO	C32-C33-C35-C36
13	f	103	SPO	C27-C28-C30-C31
13	b0	102	SPO	C32-C33-C35-C36
11	d	101	PC1	O21-C21-C22-C23
8	C	102	BCL	C11-C12-C13-C15
8	c	102	BCL	C11-C12-C13-C15
14	h	303	CDL	CB5-C51-C52-C53
11	D	102	PC1	C1-C2-C3-O31
11	d	102	PC1	C1-C2-C3-O31
14	M	406	CDL	CA3-CA4-CA6-OA8
14	m	406	CDL	CA3-CA4-CA6-OA8
8	V	101	BCL	C2-C3-C5-C6
8	v	101	BCL	C2-C3-C5-C6
14	H	303	CDL	CB5-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	d	102	PC1	C35-C36-C37-C38
13	V	103	SPO	C17-C19-C20-C21
13	7	102	SPO	C11-C10-C9-C7
13	v	103	SPO	C17-C19-C20-C21
13	6	102	SPO	C11-C10-C9-C7
11	D	102	PC1	C35-C36-C37-C38
10	L	304	U10	C5-C4-O4-C4M
10	M	404	U10	C5-C4-O4-C4M
10	l	304	U10	C5-C4-O4-C4M
10	m	404	U10	C5-C4-O4-C4M
13	M	405	SPO	O1-C1-C4-C5
13	I	103	SPO	O1-C1-C4-C5
13	V	103	SPO	O1-C1-C4-C5
13	m	405	SPO	O1-C1-C4-C5
13	i	103	SPO	O1-C1-C4-C5
13	v	103	SPO	O1-C1-C4-C5
13	M	405	SPO	C5-C6-C7-C9
13	R	101	SPO	C15-C16-C17-C19
13	m	405	SPO	C5-C6-C7-C9
13	r	101	SPO	C15-C16-C17-C19
8	P	101	BCL	C10-C11-C12-C13
11	d	102	PC1	C32-C33-C34-C35
13	A	102	SPO	C20-C21-C22-C23
13	B	102	SPO	C25-C26-C27-C28
13	N	103	SPO	C25-C26-C27-C28
13	0	102	SPO	C11-C10-C9-C7
13	a	102	SPO	C20-C21-C22-C23
13	b	102	SPO	C25-C26-C27-C28
13	n	103	SPO	C25-C26-C27-C28
13	b0	102	SPO	C11-C10-C9-C7
11	D	102	PC1	C32-C33-C34-C35
8	F	101	BCL	C8-C10-C11-C12
8	f	101	BCL	C8-C10-C11-C12
8	p	101	BCL	C10-C11-C12-C13
14	M	406	CDL	C52-C53-C54-C55
14	m	406	CDL	C52-C53-C54-C55
14	h	303	CDL	C54-C55-C56-C57
14	H	303	CDL	C54-C55-C56-C57
10	L	305	U10	C5-C4-O4-C4M
10	l	305	U10	C5-C4-O4-C4M
8	7	101	BCL	C8-C10-C11-C12
8	6	101	BCL	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	F	103	SPO	C8-C7-C9-C10
13	J	102	SPO	C8-C7-C9-C10
13	3	103	SPO	C8-C7-C9-C10
13	f	103	SPO	C8-C7-C9-C10
13	j	102	SPO	C8-C7-C9-C10
13	5	103	SPO	C8-C7-C9-C10
11	D	101	PC1	C1-C2-O21-C21
11	d	101	PC1	C1-C2-O21-C21
8	P	101	BCL	C1A-C2A-CAA-CBA
8	p	101	BCL	C1A-C2A-CAA-CBA
11	A	103	PC1	C11-C12-N-C15
11	a	103	PC1	C11-C12-N-C15
13	r	103	SPO	C12-C14-C15-C16
11	D	102	PC1	O11-C1-C2-C3
11	d	102	PC1	O11-C1-C2-C3
14	H	303	CDL	OA5-CA3-CA4-CA6
14	h	303	CDL	OA5-CA3-CA4-CA6
11	H	301	PC1	C29-C2A-C2B-C2C
11	h	301	PC1	C29-C2A-C2B-C2C
10	L	304	U10	C12-C11-C9-C10
10	l	304	U10	C12-C11-C9-C10
13	F	102	SPO	C29-C28-C30-C31
13	f	102	SPO	C29-C28-C30-C31
14	H	303	CDL	O1-C1-CB2-OB2
14	h	303	CDL	O1-C1-CB2-OB2
10	M	407	U10	C27-C28-C29-C31
13	F	103	SPO	C6-C7-C9-C10
13	J	102	SPO	C6-C7-C9-C10
13	3	103	SPO	C6-C7-C9-C10
13	f	103	SPO	C6-C7-C9-C10
13	j	102	SPO	C6-C7-C9-C10
13	5	103	SPO	C6-C7-C9-C10
13	R	103	SPO	C12-C14-C15-C16
10	m	407	U10	C27-C28-C29-C31
13	J	102	SPO	C1-C4-C5-C6
13	N	103	SPO	C1-C4-C5-C6
13	7	102	SPO	C1-C4-C5-C6
13	j	102	SPO	C1-C4-C5-C6
13	n	103	SPO	C1-C4-C5-C6
13	6	102	SPO	C1-C4-C5-C6
11	d	101	PC1	C23-C24-C25-C26
11	D	101	PC1	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	M	407	U10	C9-C11-C12-C13
10	m	407	U10	C9-C11-C12-C13
13	R	101	SPO	C28-C30-C31-C32
13	7	102	SPO	C28-C30-C31-C32
13	r	101	SPO	C28-C30-C31-C32
13	6	102	SPO	C28-C30-C31-C32
14	H	303	CDL	CA2-C1-CB2-OB2
14	h	303	CDL	CA2-C1-CB2-OB2
11	H	301	PC1	C33-C34-C35-C36
11	h	301	PC1	C33-C34-C35-C36
14	M	406	CDL	C76-C77-C78-C79
13	N	101	SPO	C29-C28-C30-C31
13	n	101	SPO	C29-C28-C30-C31
14	m	406	CDL	C76-C77-C78-C79
8	T	101	BCL	CAA-CBA-CGA-O2A
8	t	101	BCL	CAA-CBA-CGA-O2A
11	H	301	PC1	C36-C37-C38-C39
11	h	301	PC1	C36-C37-C38-C39
11	L	306	PC1	O31-C31-C32-C33
11	l	306	PC1	O31-C31-C32-C33
8	L	301	BCL	C2A-CAA-CBA-CGA
8	l	301	BCL	C2A-CAA-CBA-CGA
14	H	303	CDL	CB3-CB4-CB6-OB8
14	h	303	CDL	CB3-CB4-CB6-OB8
13	C	101	SPO	C11-C10-C9-C7
13	9	102	SPO	C20-C21-C22-C23
13	c	101	SPO	C11-C10-C9-C7
13	b9	102	SPO	C20-C21-C22-C23
8	L	307	BCL	C4-C3-C5-C6
8	3	101	BCL	C4-C3-C5-C6
8	l	307	BCL	C4-C3-C5-C6
8	5	101	BCL	C4-C3-C5-C6
13	D	104	SPO	C29-C28-C30-C31
13	d	104	SPO	C29-C28-C30-C31
8	M	402	BCL	C10-C11-C12-C13
8	m	402	BCL	C10-C11-C12-C13
11	A	103	PC1	O11-C1-C2-O21
11	a	103	PC1	O11-C1-C2-O21
11	H	302	PC1	C35-C36-C37-C38
11	h	302	PC1	C35-C36-C37-C38
13	I	102	SPO	C29-C28-C30-C31
13	R	101	SPO	C34-C33-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	S	102	SPO	C29-C28-C30-C31
13	i	102	SPO	C29-C28-C30-C31
13	r	101	SPO	C34-C33-C35-C36
13	s	102	SPO	C29-C28-C30-C31
10	M	404	U10	C34-C36-C37-C38
10	m	404	U10	C34-C36-C37-C38
8	L	307	BCL	C2-C3-C5-C6
8	L	307	BCL	C11-C10-C8-C7
8	l	307	BCL	C2-C3-C5-C6
8	l	307	BCL	C11-C10-C8-C7
13	E	102	SPO	C17-C19-C20-C21
13	R	104	SPO	C25-C26-C27-C28
13	e	102	SPO	C17-C19-C20-C21
13	r	104	SPO	C25-C26-C27-C28
10	M	407	U10	C27-C28-C29-C30
10	m	407	U10	C27-C28-C29-C30
8	K	101	BCL	C4-C3-C5-C6
8	8	101	BCL	C4-C3-C5-C6
8	k	101	BCL	C4-C3-C5-C6
8	b8	101	BCL	C4-C3-C5-C6
8	b9	101	BCL	C4-C3-C5-C6
10	M	404	U10	C25-C24-C26-C27
10	m	404	U10	C25-C24-C26-C27
13	O	102	SPO	C29-C28-C30-C31
13	U	102	SPO	C29-C28-C30-C31
13	C	101	SPO	C29-C28-C30-C31
13	o	102	SPO	C29-C28-C30-C31
13	u	102	SPO	C29-C28-C30-C31
13	c	101	SPO	C29-C28-C30-C31
10	L	304	U10	C12-C11-C9-C8
10	l	304	U10	C12-C11-C9-C8
13	J	102	SPO	C27-C28-C30-C31
13	j	102	SPO	C27-C28-C30-C31
8	N	102	BCL	CAA-CBA-CGA-O2A
8	n	102	BCL	CAA-CBA-CGA-O2A
8	G	101	BCL	C6-C7-C8-C9
8	G	101	BCL	C11-C12-C13-C14
8	g	101	BCL	C6-C7-C8-C9
8	g	101	BCL	C11-C12-C13-C14
8	P	101	BCL	C3A-C2A-CAA-CBA
8	p	101	BCL	C3A-C2A-CAA-CBA
8	U	101	BCL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	P	101	BCL	CAA-CBA-CGA-O2A
8	p	101	BCL	CAA-CBA-CGA-O2A
8	M	402	BCL	CAD-CBD-CGD-O2D
8	m	402	BCL	CAD-CBD-CGD-O2D
13	d	104	SPO	C20-C21-C22-C23
8	u	101	BCL	C10-C11-C12-C13
11	H	301	PC1	O21-C21-C22-C23
11	h	301	PC1	O21-C21-C22-C23
14	M	406	CDL	C12-C11-CA5-OA6
14	m	406	CDL	C12-C11-CA5-OA6
8	9	101	BCL	C4-C3-C5-C6
13	R	101	SPO	C29-C28-C30-C31
13	V	103	SPO	C34-C33-C35-C36
13	r	101	SPO	C29-C28-C30-C31
13	v	103	SPO	C34-C33-C35-C36
8	K	101	BCL	C2-C3-C5-C6
8	k	101	BCL	C2-C3-C5-C6
13	F	102	SPO	C27-C28-C30-C31
13	f	102	SPO	C27-C28-C30-C31
11	A	103	PC1	O21-C21-C22-C23
11	A	104	PC1	O21-C21-C22-C23
11	a	103	PC1	O21-C21-C22-C23
11	a	104	PC1	O21-C21-C22-C23
10	M	404	U10	C29-C31-C32-C33
10	m	404	U10	C29-C31-C32-C33
8	G	101	BCL	O2A-C1-C2-C3
8	N	102	BCL	O2A-C1-C2-C3
8	g	101	BCL	O2A-C1-C2-C3
8	n	102	BCL	O2A-C1-C2-C3
9	L	303	BPB	O2A-C1-C2-C3
9	l	303	BPB	O2A-C1-C2-C3
8	B	101	BCL	CHA-CBD-CGD-O1D
8	B	101	BCL	CHA-CBD-CGD-O2D
8	E	101	BCL	CHA-CBD-CGD-O1D
8	E	101	BCL	CHA-CBD-CGD-O2D
8	J	101	BCL	CHA-CBD-CGD-O1D
8	J	101	BCL	CHA-CBD-CGD-O2D
8	P	101	BCL	CHA-CBD-CGD-O1D
8	P	101	BCL	CHA-CBD-CGD-O2D
8	R	102	BCL	CHA-CBD-CGD-O1D
8	R	102	BCL	CHA-CBD-CGD-O2D
8	V	101	BCL	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	2	101	BCL	CHA-CBD-CGD-O2D
8	0	101	BCL	CHA-CBD-CGD-O1D
8	0	101	BCL	CHA-CBD-CGD-O2D
8	b	101	BCL	CHA-CBD-CGD-O1D
8	b	101	BCL	CHA-CBD-CGD-O2D
8	e	101	BCL	CHA-CBD-CGD-O1D
8	e	101	BCL	CHA-CBD-CGD-O2D
8	j	101	BCL	CHA-CBD-CGD-O1D
8	j	101	BCL	CHA-CBD-CGD-O2D
8	p	101	BCL	CHA-CBD-CGD-O1D
8	p	101	BCL	CHA-CBD-CGD-O2D
8	r	102	BCL	CHA-CBD-CGD-O1D
8	r	102	BCL	CHA-CBD-CGD-O2D
8	v	101	BCL	CHA-CBD-CGD-O2D
8	4	101	BCL	CHA-CBD-CGD-O2D
8	b0	101	BCL	CHA-CBD-CGD-O1D
8	b0	101	BCL	CHA-CBD-CGD-O2D
13	D	104	SPO	C20-C21-C22-C23
13	9	102	SPO	C29-C28-C30-C31
13	b9	102	SPO	C29-C28-C30-C31
13	R	101	SPO	C27-C28-C30-C31
13	r	101	SPO	C27-C28-C30-C31
13	7	102	SPO	C2-C1-O1-CM1
13	6	102	SPO	C2-C1-O1-CM1
8	Z	101	BCL	CAA-CBA-CGA-O2A
8	z	101	BCL	CAA-CBA-CGA-O2A
9	L	303	BPB	CHA-CBD-CGD-O1D
9	M	403	BPB	CHA-CBD-CGD-O2D
9	l	303	BPB	CHA-CBD-CGD-O1D
9	m	403	BPB	CHA-CBD-CGD-O2D
13	R	103	SPO	C3-C1-C4-C5
13	3	103	SPO	C3-C1-C4-C5
13	7	102	SPO	C2-C1-C4-C5
13	r	103	SPO	C3-C1-C4-C5
13	5	103	SPO	C3-C1-C4-C5
13	6	102	SPO	C2-C1-C4-C5
9	L	303	BPB	C10-C11-C12-C13
9	l	303	BPB	C10-C11-C12-C13
8	g	101	BCL	CAA-CBA-CGA-O2A
8	L	307	BCL	C11-C10-C8-C9
8	l	307	BCL	C11-C10-C8-C9
13	9	102	SPO	C11-C10-C9-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	b9	102	SPO	C11-C10-C9-C7
8	G	101	BCL	CAA-CBA-CGA-O2A
10	L	305	U10	C26-C27-C28-C29
10	l	305	U10	C26-C27-C28-C29
13	R	103	SPO	C30-C31-C32-C33
13	r	103	SPO	C30-C31-C32-C33
11	A	104	PC1	O22-C21-C22-C23
11	a	104	PC1	O22-C21-C22-C23
13	r	101	SPO	C24-C23-C25-C26
11	H	301	PC1	O22-C21-C22-C23
11	h	301	PC1	O22-C21-C22-C23
13	0	102	SPO	C29-C28-C30-C31
13	b0	102	SPO	C29-C28-C30-C31
11	A	103	PC1	C35-C36-C37-C38
11	a	103	PC1	C35-C36-C37-C38
8	N	102	BCL	C1A-C2A-CAA-CBA
8	C	102	BCL	C1A-C2A-CAA-CBA
8	n	102	BCL	C1A-C2A-CAA-CBA
8	c	102	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	CAA-CBA-CGA-O1A
8	p	101	BCL	CAA-CBA-CGA-O1A
10	L	305	U10	C16-C17-C18-C19
10	l	305	U10	C16-C17-C18-C19
11	A	103	PC1	O22-C21-C22-C23
11	a	103	PC1	O22-C21-C22-C23
8	W	101	BCL	C4-C3-C5-C6
8	w	101	BCL	C4-C3-C5-C6
8	E	101	BCL	C10-C11-C12-C13
11	A	103	PC1	C1-O11-P-O12
11	a	103	PC1	C1-O11-P-O12
14	M	406	CDL	CA3-OA5-PA1-OA3
14	m	406	CDL	CA3-OA5-PA1-OA3
8	b0	101	BCL	CAA-CBA-CGA-O2A
8	Q	101	BCL	C8-C10-C11-C12
8	q	101	BCL	C8-C10-C11-C12
8	N	102	BCL	CAA-CBA-CGA-O1A
8	0	101	BCL	CAA-CBA-CGA-O2A
8	e	101	BCL	C10-C11-C12-C13
8	n	102	BCL	CAA-CBA-CGA-O1A
14	M	406	CDL	C12-C11-CA5-OA7
14	m	406	CDL	C12-C11-CA5-OA7
8	Z	101	BCL	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	g	101	BCL	CAA-CBA-CGA-O1A
8	z	101	BCL	CAA-CBA-CGA-O1A
8	I	101	BCL	C4-C3-C5-C6
8	i	101	BCL	C4-C3-C5-C6
13	3	103	SPO	C11-C10-C9-C7
13	5	103	SPO	C11-C10-C9-C7
8	J	101	BCL	CAD-CBD-CGD-O1D
8	R	102	BCL	CAD-CBD-CGD-O1D
8	S	101	BCL	CAD-CBD-CGD-O1D
8	0	101	BCL	CAD-CBD-CGD-O1D
8	j	101	BCL	CAD-CBD-CGD-O1D
8	r	102	BCL	CAD-CBD-CGD-O1D
8	s	101	BCL	CAD-CBD-CGD-O1D
8	b0	101	BCL	CAD-CBD-CGD-O1D
8	G	101	BCL	CAA-CBA-CGA-O1A
8	I	101	BCL	C11-C10-C8-C9
8	O	101	BCL	C11-C10-C8-C9
8	i	101	BCL	C11-C10-C8-C9
8	o	101	BCL	C11-C10-C8-C9
8	R	102	BCL	CAA-CBA-CGA-O2A
8	C	102	BCL	CAA-CBA-CGA-O2A
8	r	102	BCL	CAA-CBA-CGA-O2A
8	c	102	BCL	CAA-CBA-CGA-O2A
13	B	102	SPO	C1-C4-C5-C6
13	b	102	SPO	C1-C4-C5-C6
8	8	101	BCL	CAA-CBA-CGA-O2A
8	b8	101	BCL	CAA-CBA-CGA-O2A
8	G	101	BCL	C11-C12-C13-C15
8	g	101	BCL	C11-C12-C13-C15
8	V	101	BCL	CAA-CBA-CGA-O2A
8	v	101	BCL	CAA-CBA-CGA-O2A
13	I	102	SPO	C10-C11-C12-C14
13	R	101	SPO	C22-C23-C25-C26
13	R	103	SPO	C10-C11-C12-C14
13	i	102	SPO	C10-C11-C12-C14
13	r	101	SPO	C22-C23-C25-C26
13	r	103	SPO	C10-C11-C12-C14
8	8	101	BCL	CAA-CBA-CGA-O1A
8	r	102	BCL	CAA-CBA-CGA-O1A
8	b8	101	BCL	CAA-CBA-CGA-O1A
13	I	102	SPO	C28-C30-C31-C32
13	i	102	SPO	C28-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	C	102	BCL	CAA-CBA-CGA-O1A
8	c	102	BCL	CAA-CBA-CGA-O1A
8	R	102	BCL	CAA-CBA-CGA-O1A
8	v	101	BCL	CAA-CBA-CGA-O1A
11	L	306	PC1	O21-C21-C22-C23
11	l	306	PC1	O21-C21-C22-C23

There are no ring outliers.

140 monomers are involved in 426 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	l	304	U10	3	0
8	l	302	BCL	4	0
8	F	101	BCL	4	0
8	E	101	BCL	2	0
10	l	305	U10	6	0
11	D	101	PC1	2	0
10	M	404	U10	1	0
8	5	101	BCL	4	0
8	k	101	BCL	4	0
8	j	101	BCL	5	0
9	m	403	BPB	2	0
11	A	105	PC1	7	0
13	u	102	SPO	2	0
8	S	101	BCL	5	0
10	m	407	U10	2	0
8	p	101	BCL	4	0
13	m	405	SPO	5	0
8	T	101	BCL	3	0
13	F	102	SPO	2	0
13	U	102	SPO	3	0
8	e	101	BCL	2	0
13	f	103	SPO	4	0
13	5	102	SPO	1	0
8	U	101	BCL	1	0
11	h	302	PC1	1	0
8	D	103	BCL	5	0
13	j	102	SPO	4	0
13	I	102	SPO	3	0
13	M	405	SPO	5	0
8	r	102	BCL	3	0
11	L	306	PC1	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	O	101	BCL	10	0
13	i	102	SPO	2	0
13	R	104	SPO	3	0
8	W	101	BCL	2	0
10	m	404	U10	1	0
11	L	308	PC1	3	0
9	M	403	BPB	2	0
8	i	101	BCL	6	0
8	B	101	BCL	3	0
9	l	303	BPB	4	0
8	o	101	BCL	10	0
13	3	103	SPO	5	0
8	v	101	BCL	1	0
8	b	101	BCL	5	0
14	m	406	CDL	1	0
8	Q	101	BCL	6	0
13	c	101	SPO	2	0
8	4	101	BCL	2	0
11	d	102	PC1	5	0
13	r	103	SPO	9	0
11	H	301	PC1	7	0
11	d	101	PC1	2	0
13	R	101	SPO	1	0
8	L	302	BCL	4	0
11	l	308	PC1	3	0
13	V	102	SPO	1	0
8	w	101	BCL	1	0
13	A	102	SPO	4	0
8	9	101	BCL	4	0
13	3	102	SPO	2	0
8	2	101	BCL	1	0
13	b	102	SPO	2	0
8	a	101	BCL	3	0
10	L	304	U10	3	0
8	J	101	BCL	5	0
8	L	307	BCL	3	0
8	8	101	BCL	2	0
11	A	103	PC1	2	0
8	f	101	BCL	5	0
8	b0	101	BCL	2	0
11	H	302	PC1	1	0
13	9	102	SPO	3	0

Continued on next page...

Continued from previous page...

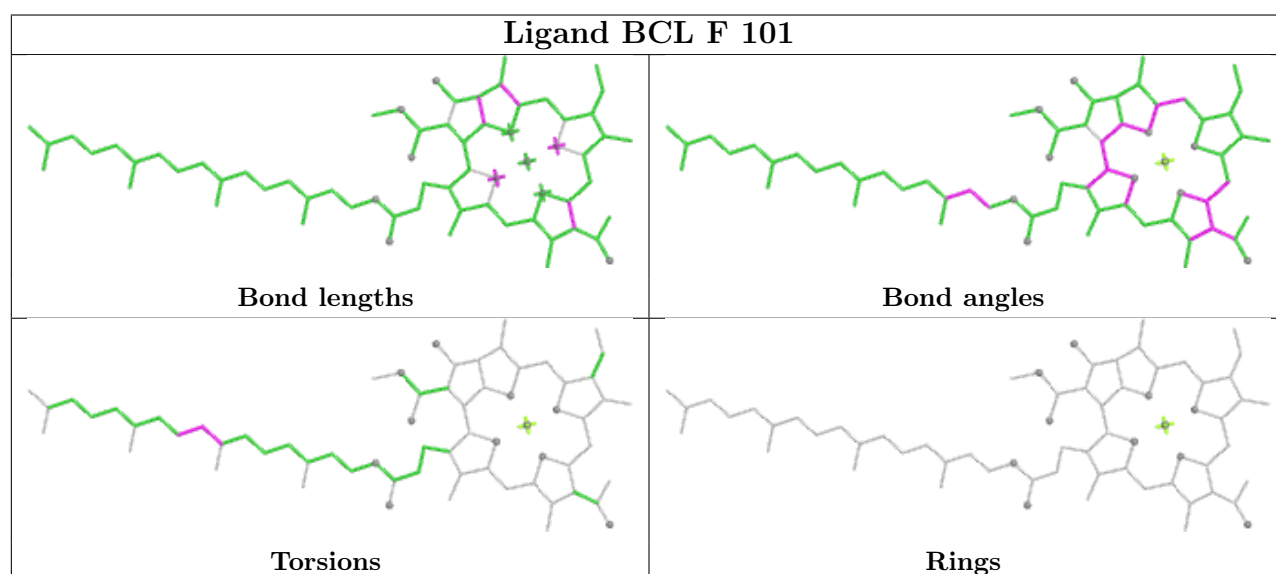
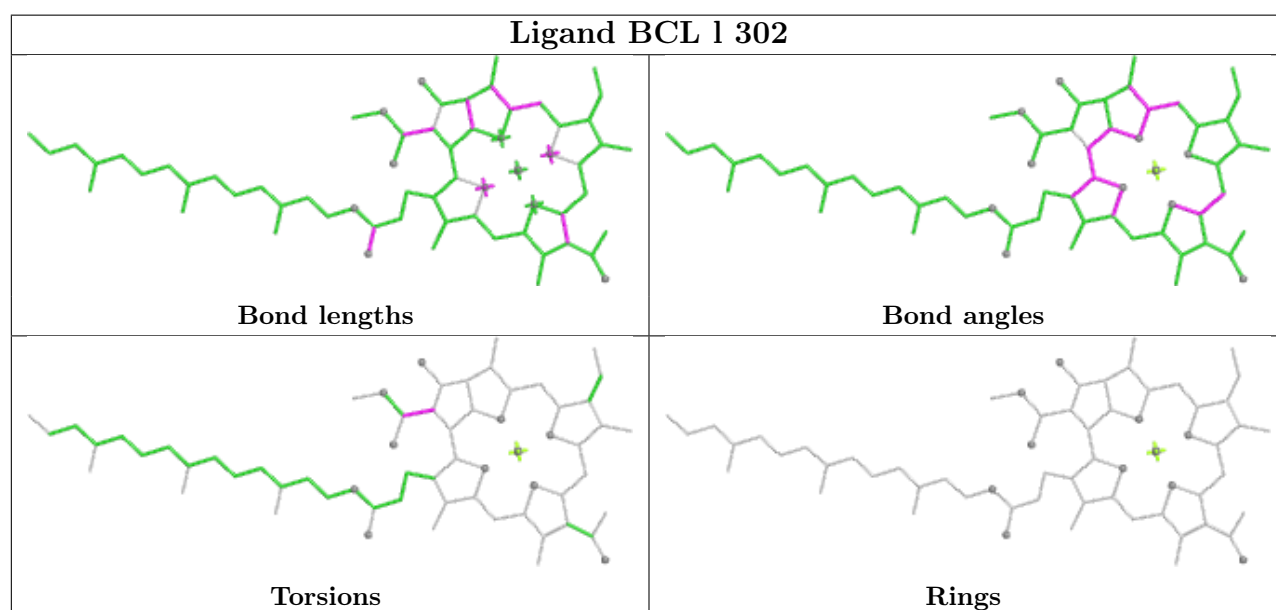
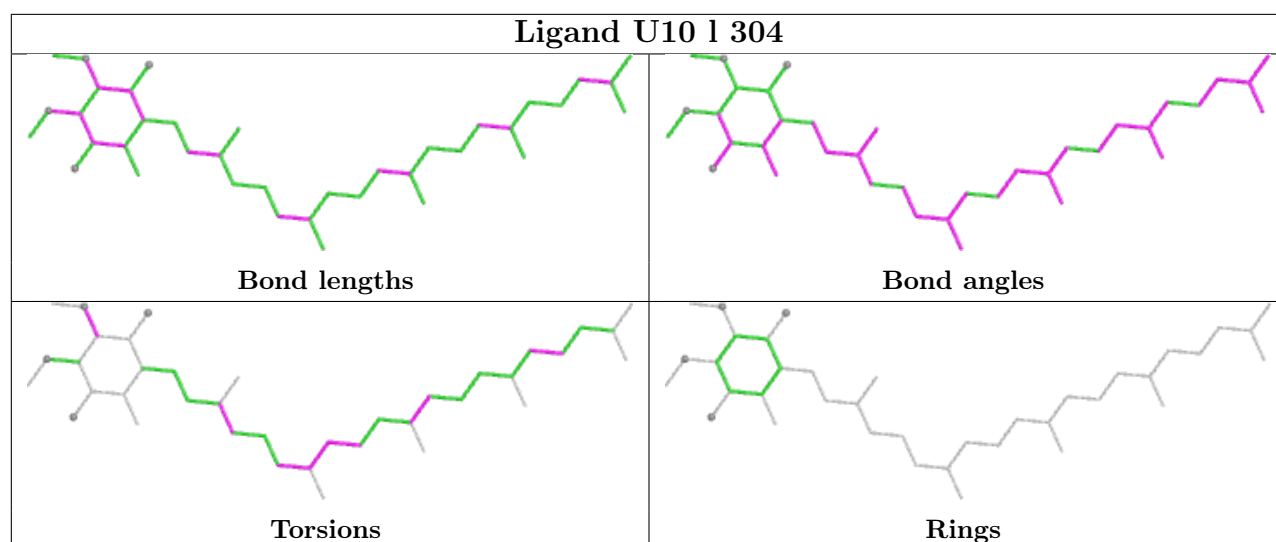
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	301	BCL	4	0
8	7	101	BCL	2	0
8	3	101	BCL	4	0
8	I	101	BCL	5	0
13	i	103	SPO	1	0
8	K	101	BCL	4	0
11	a	105	PC1	6	0
13	O	102	SPO	3	0
13	D	104	SPO	2	0
14	h	303	CDL	2	0
13	J	102	SPO	4	0
8	N	102	BCL	5	0
8	0	101	BCL	2	0
8	l	301	BCL	4	0
13	r	101	SPO	1	0
13	R	103	SPO	9	0
13	d	104	SPO	2	0
14	M	406	CDL	4	0
8	G	101	BCL	5	0
13	b9	102	SPO	2	0
8	n	102	BCL	5	0
8	V	101	BCL	2	0
13	s	102	SPO	4	0
11	A	104	PC1	4	0
13	S	102	SPO	4	0
13	b0	102	SPO	1	0
13	B	102	SPO	2	0
13	N	103	SPO	5	0
8	s	101	BCL	5	0
11	h	301	PC1	9	0
13	v	102	SPO	1	0
11	D	102	PC1	5	0
13	n	101	SPO	1	0
8	b9	101	BCL	4	0
13	C	101	SPO	2	0
8	P	101	BCL	4	0
10	M	407	U10	2	0
13	f	102	SPO	3	0
13	n	103	SPO	5	0
8	q	101	BCL	6	0
8	d	103	BCL	6	0
8	6	101	BCL	2	0

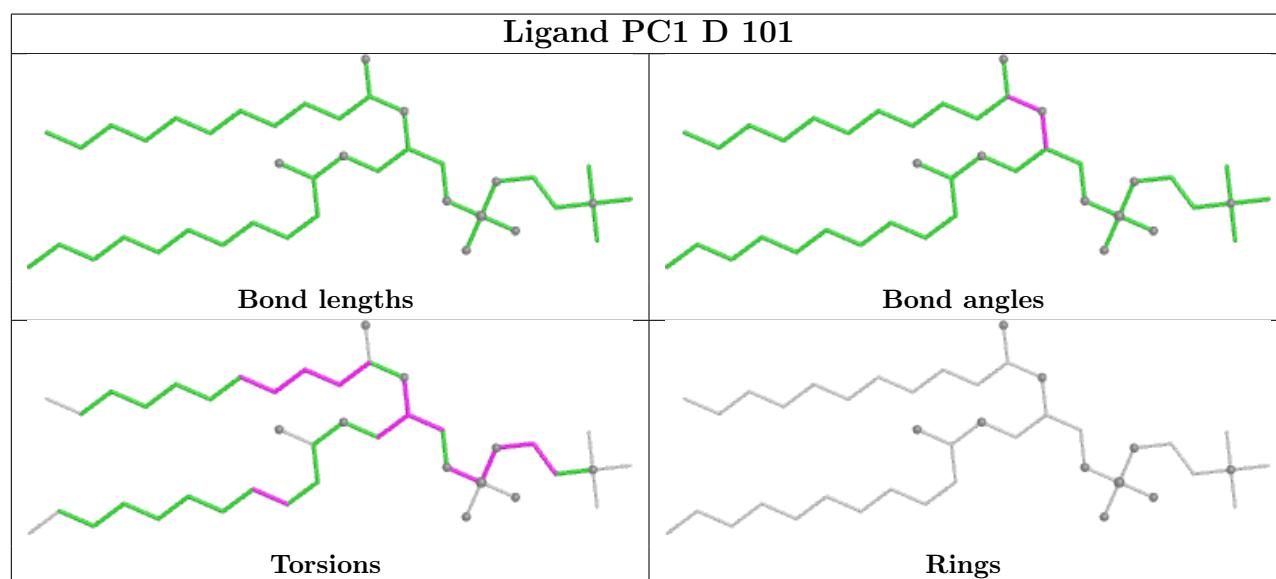
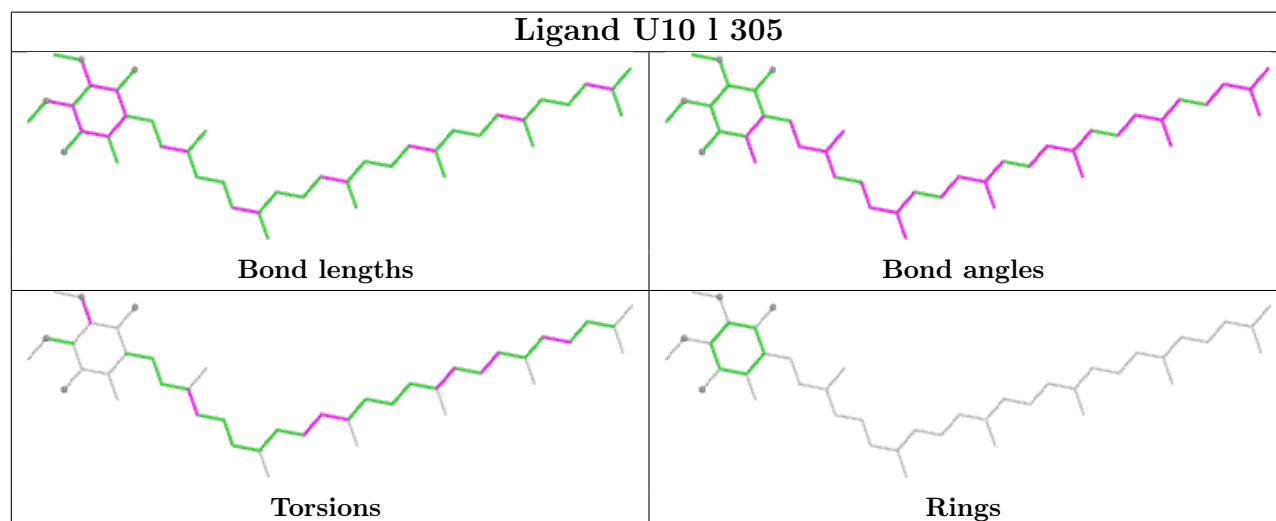
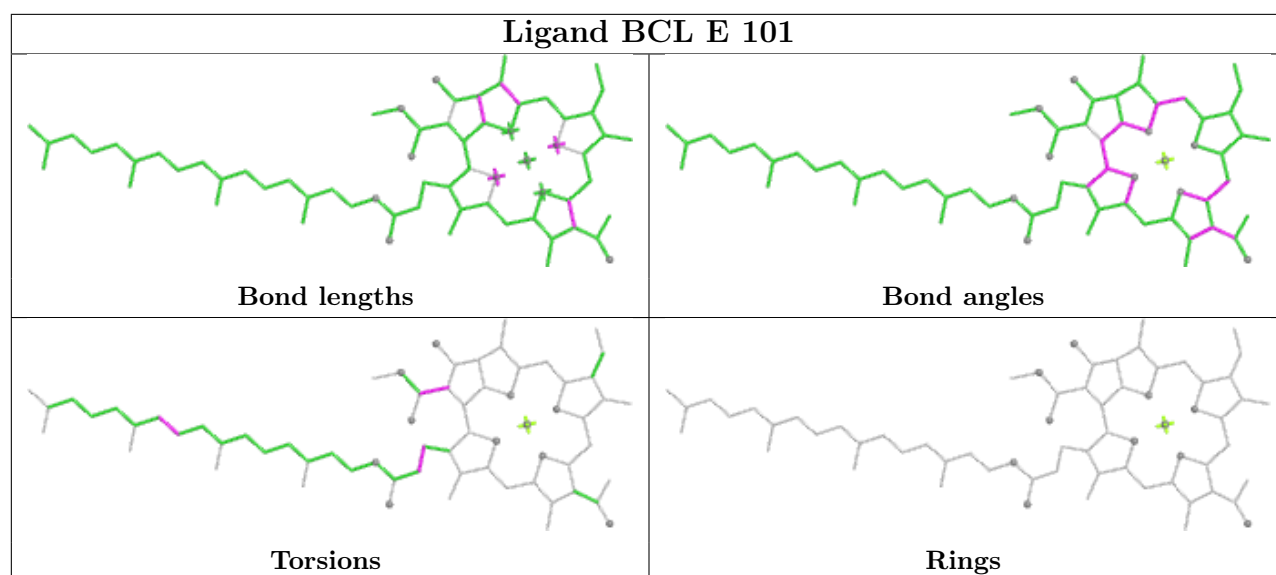
Continued on next page...

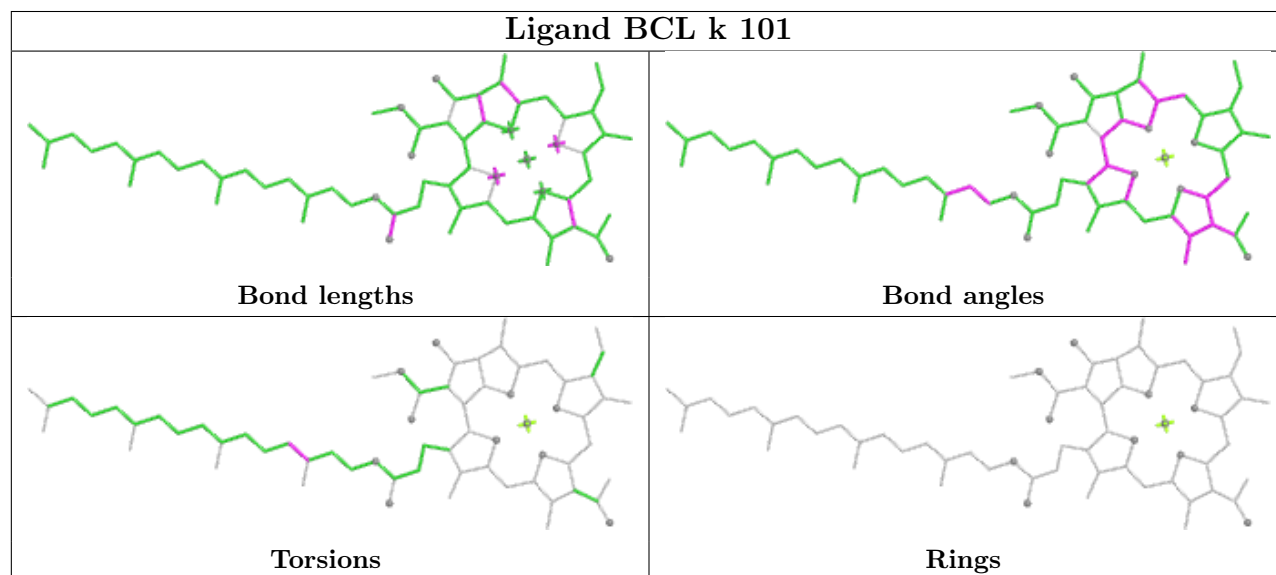
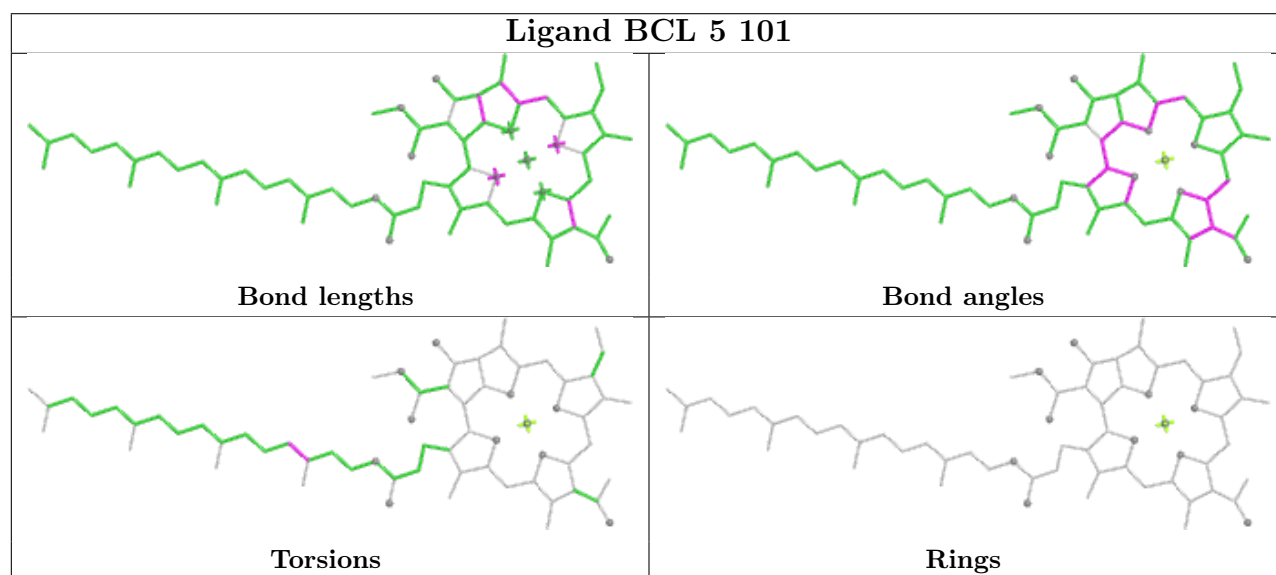
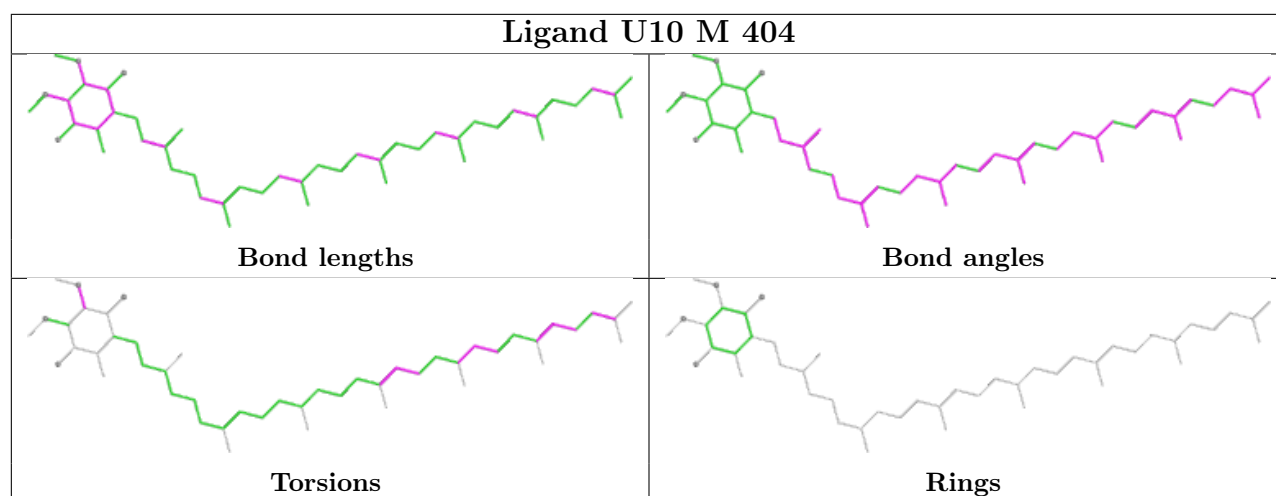
Continued from previous page...

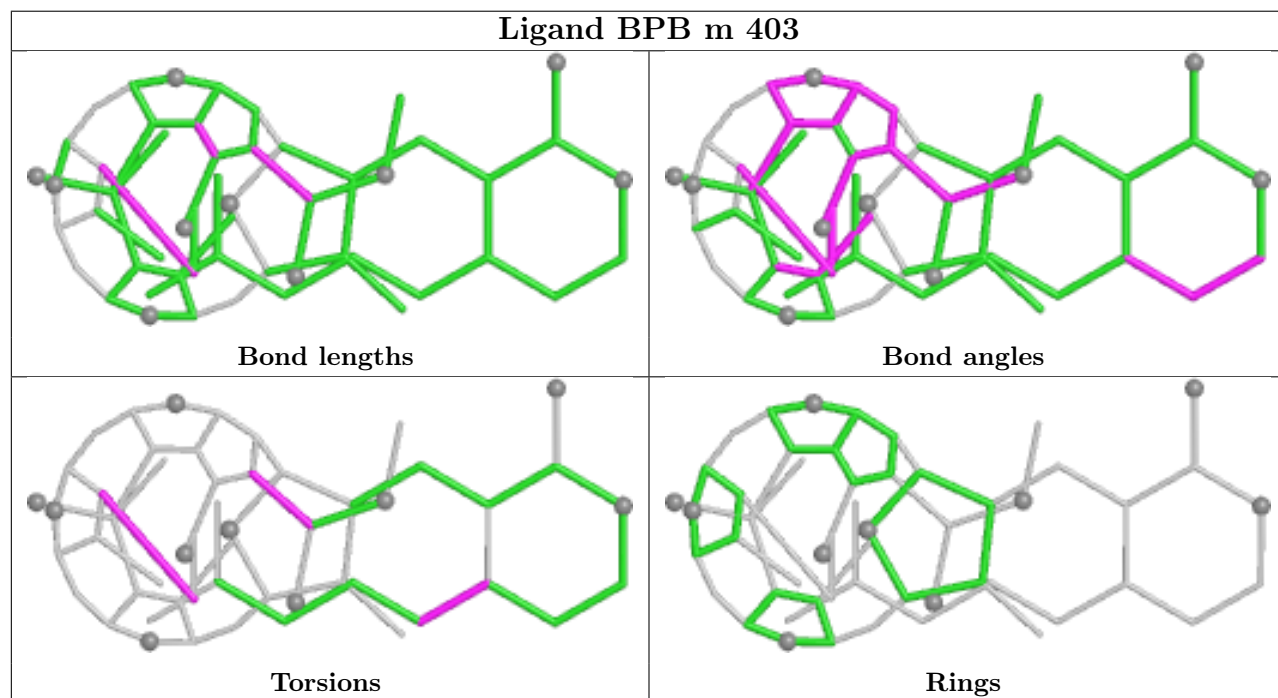
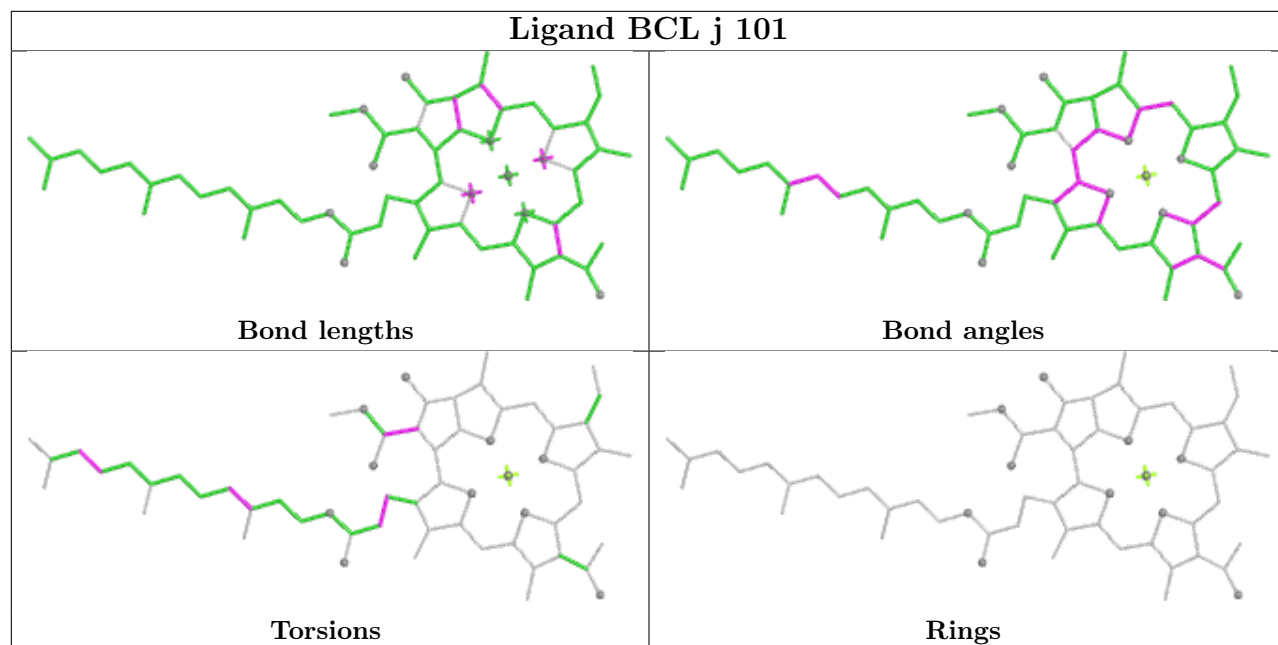
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	l	307	BCL	4	0
8	t	101	BCL	4	0
13	a	102	SPO	4	0
13	I	103	SPO	1	0
8	c	102	BCL	2	0
13	F	103	SPO	4	0
9	L	303	BPB	5	0
14	H	303	CDL	2	0
8	g	101	BCL	5	0
13	5	103	SPO	5	0
13	N	101	SPO	2	0
8	m	402	BCL	1	0
8	C	102	BCL	2	0
13	o	102	SPO	2	0
13	6	102	SPO	5	0
11	l	306	PC1	2	0
13	r	104	SPO	2	0
11	a	103	PC1	2	0
10	L	305	U10	5	0
8	A	101	BCL	4	0
8	M	402	BCL	1	0
8	R	102	BCL	3	0
8	u	101	BCL	2	0
13	7	102	SPO	5	0
11	a	104	PC1	4	0

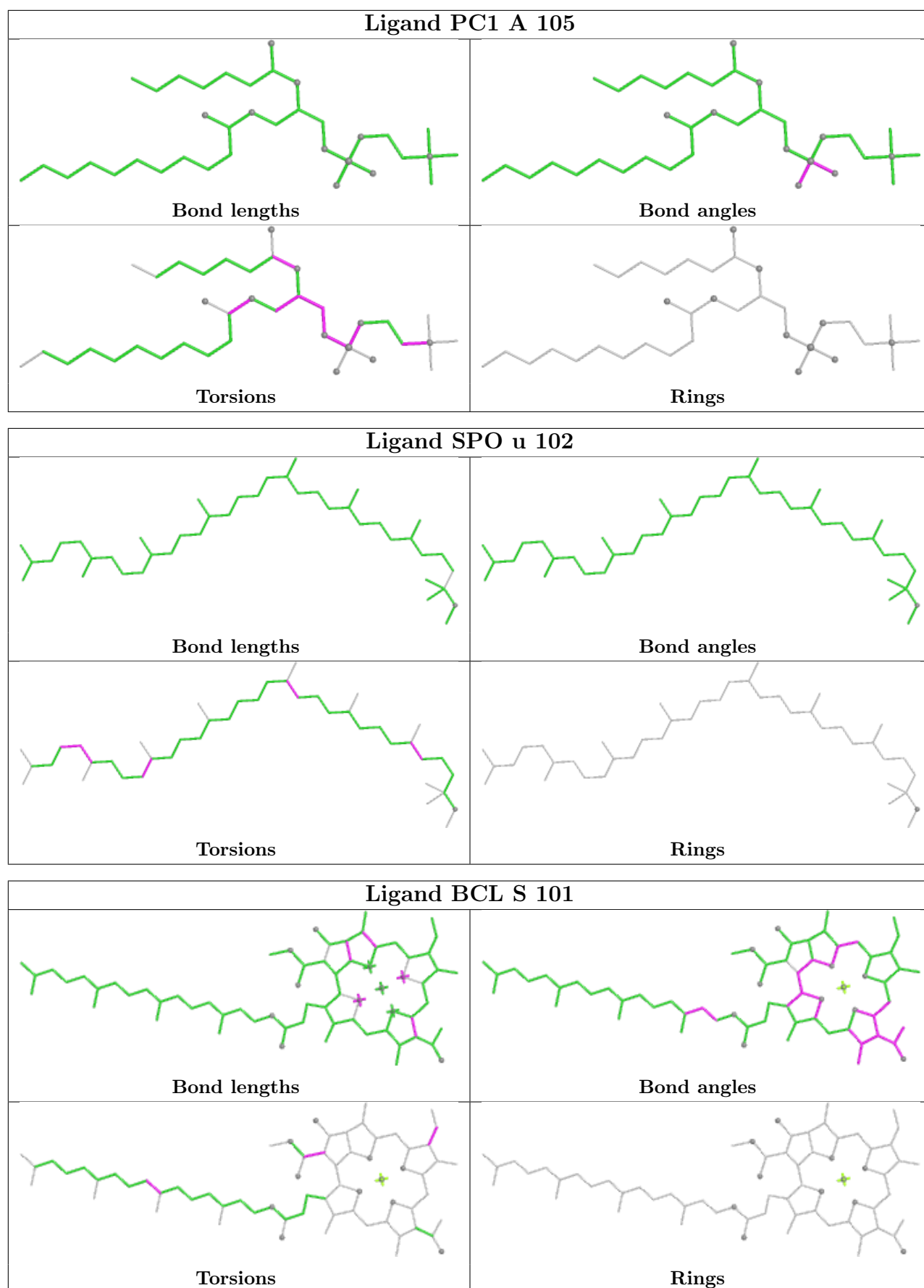
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

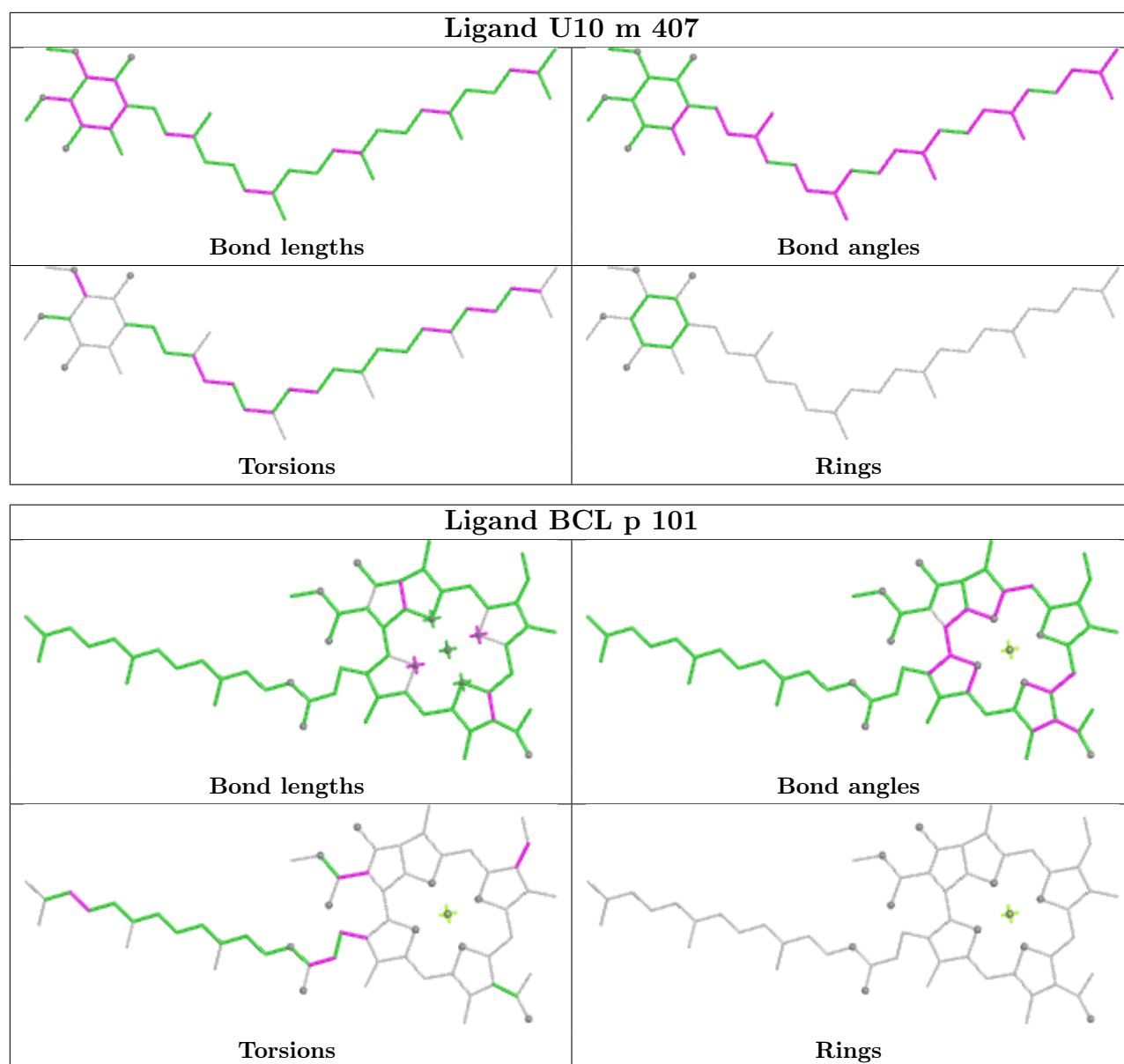


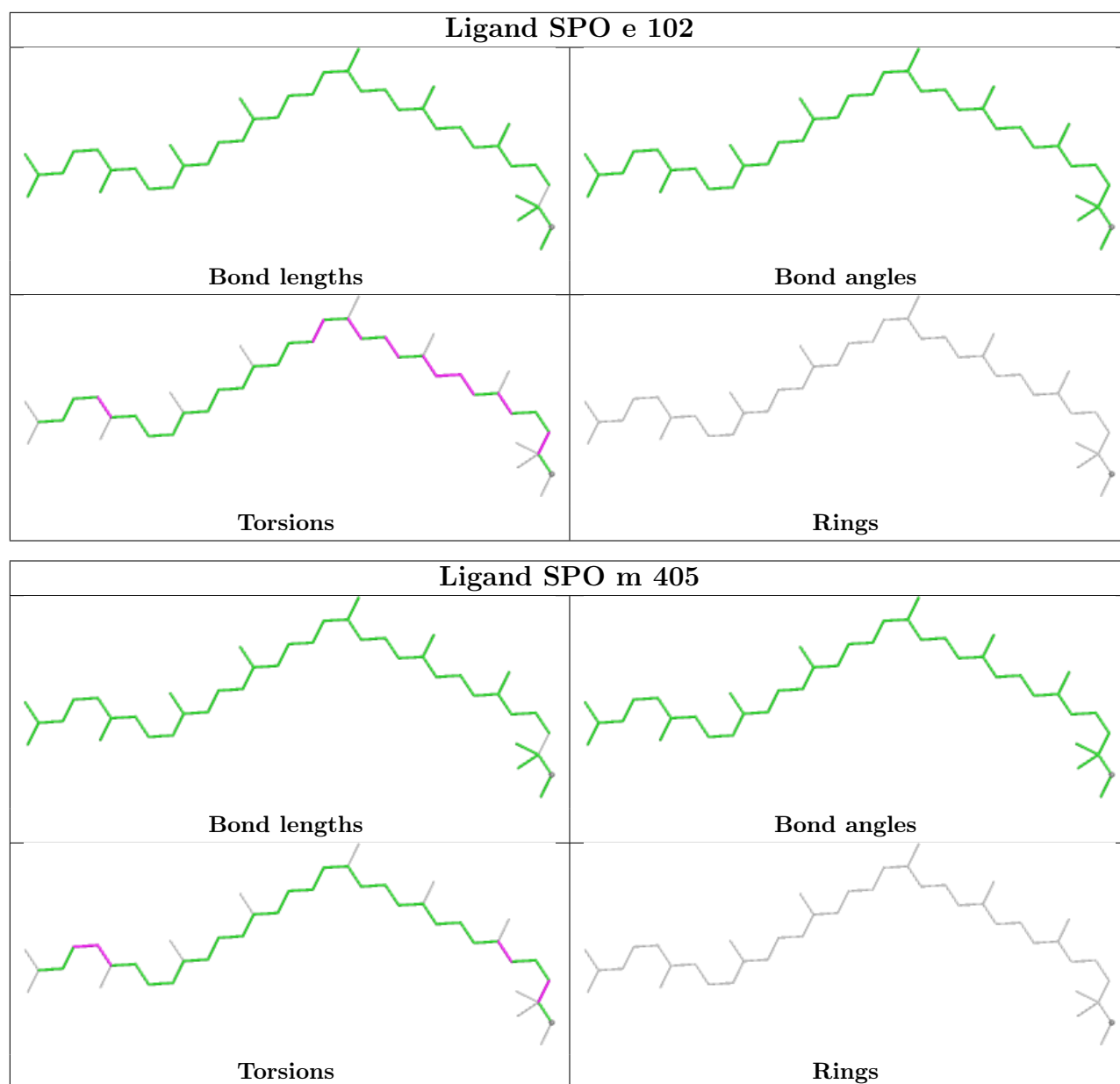


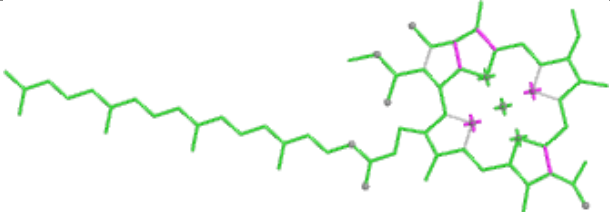
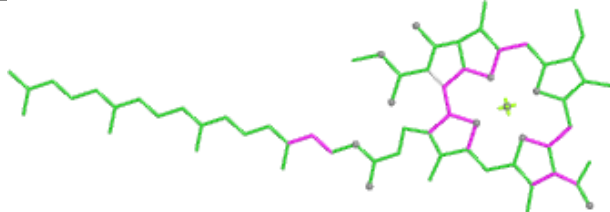
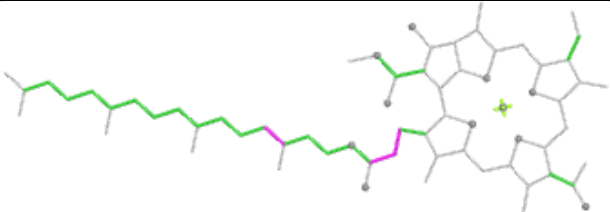
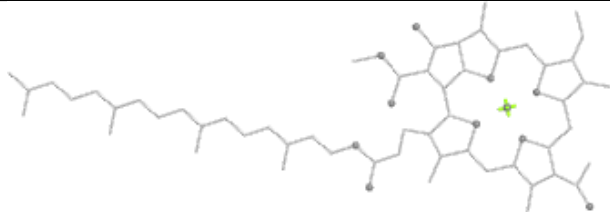
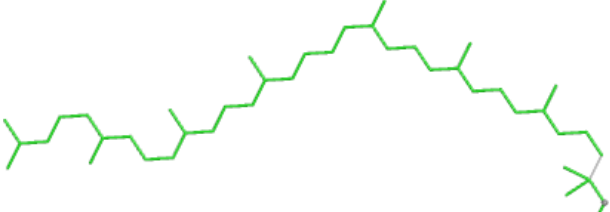
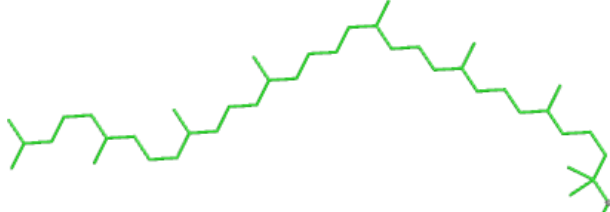
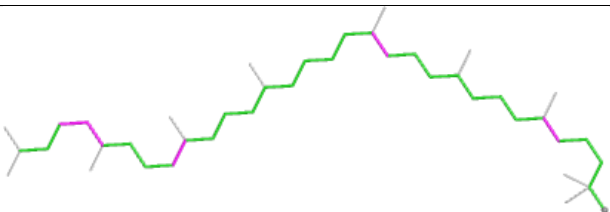
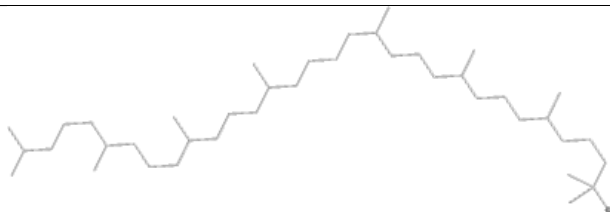


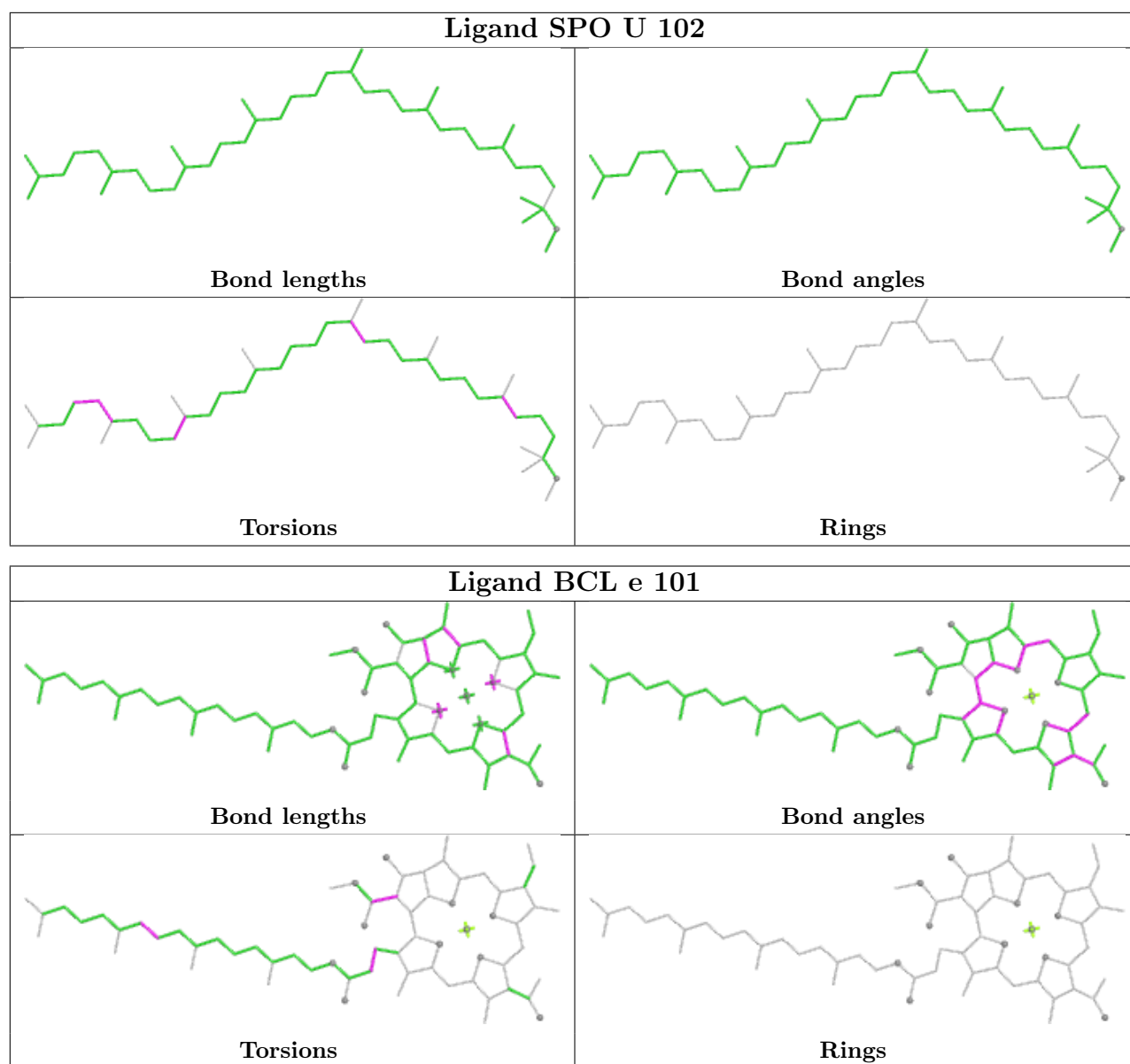


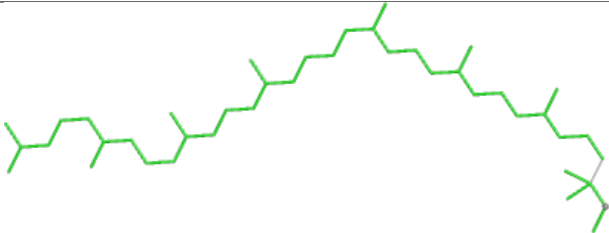
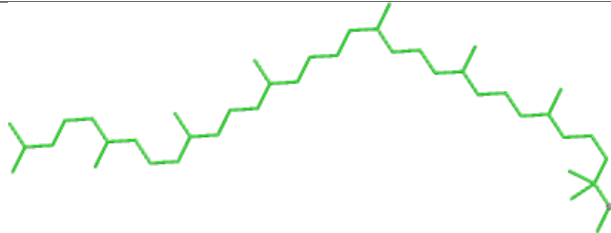
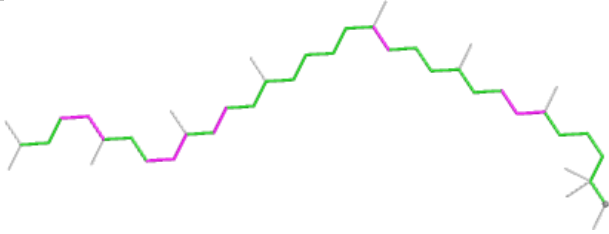
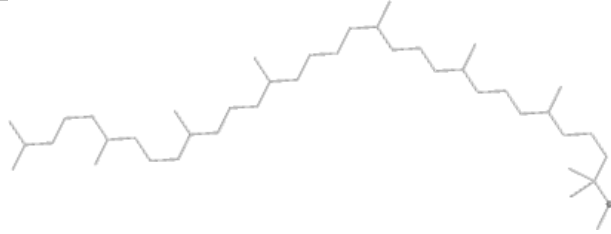


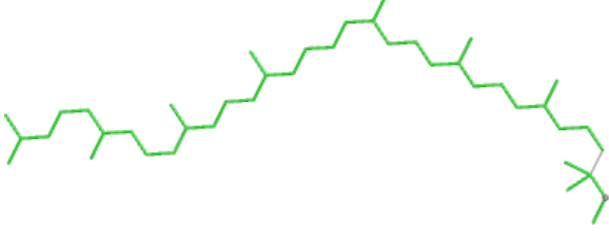
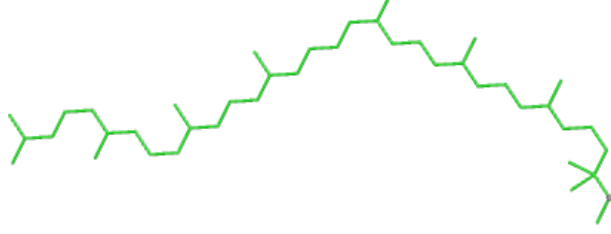
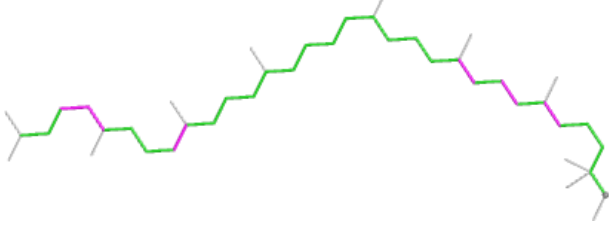
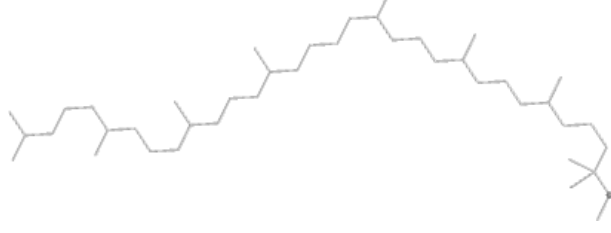


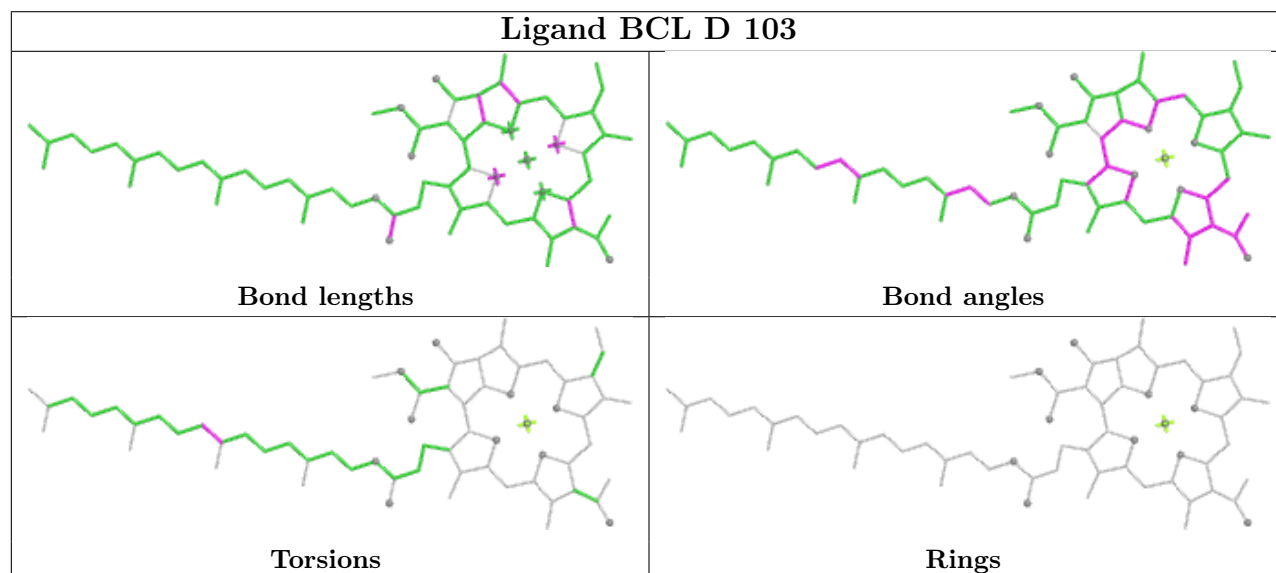
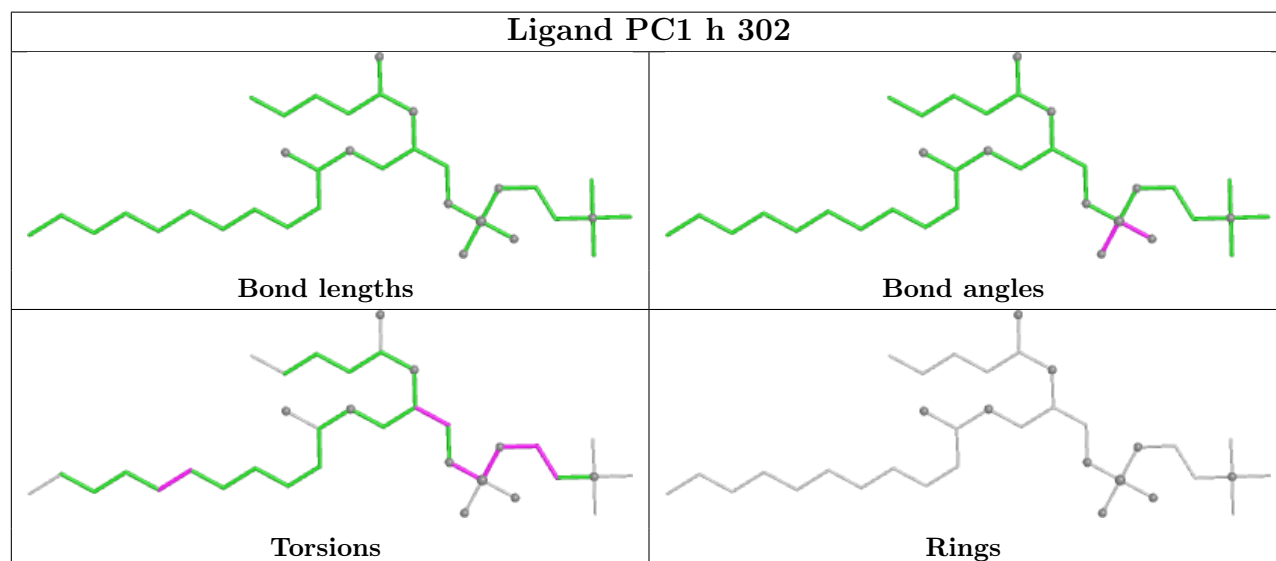
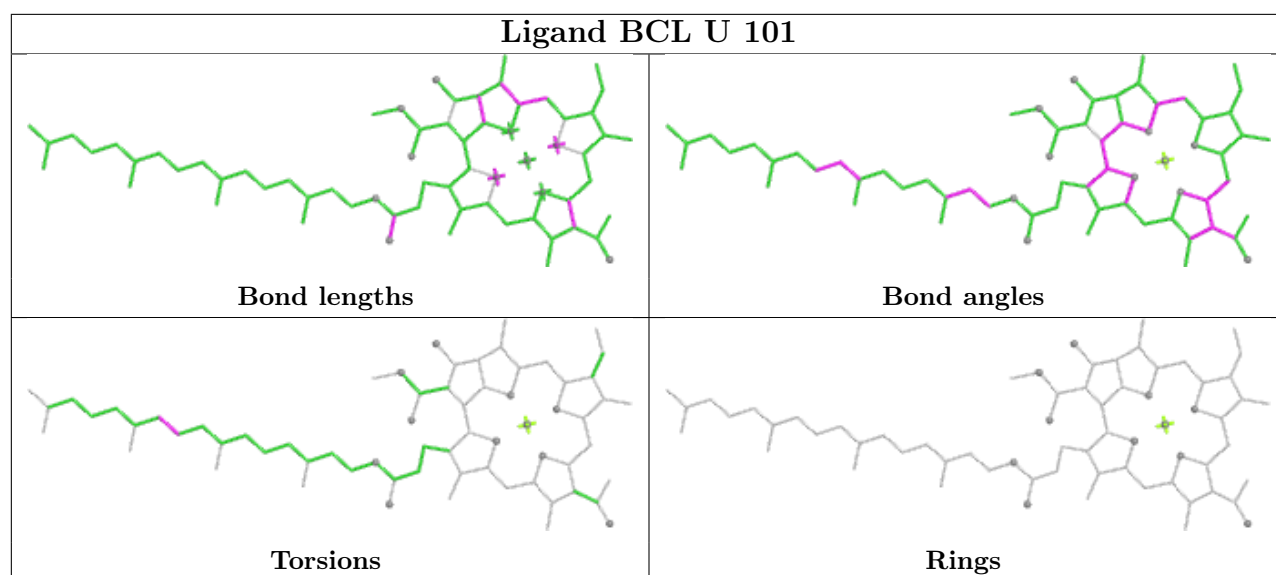


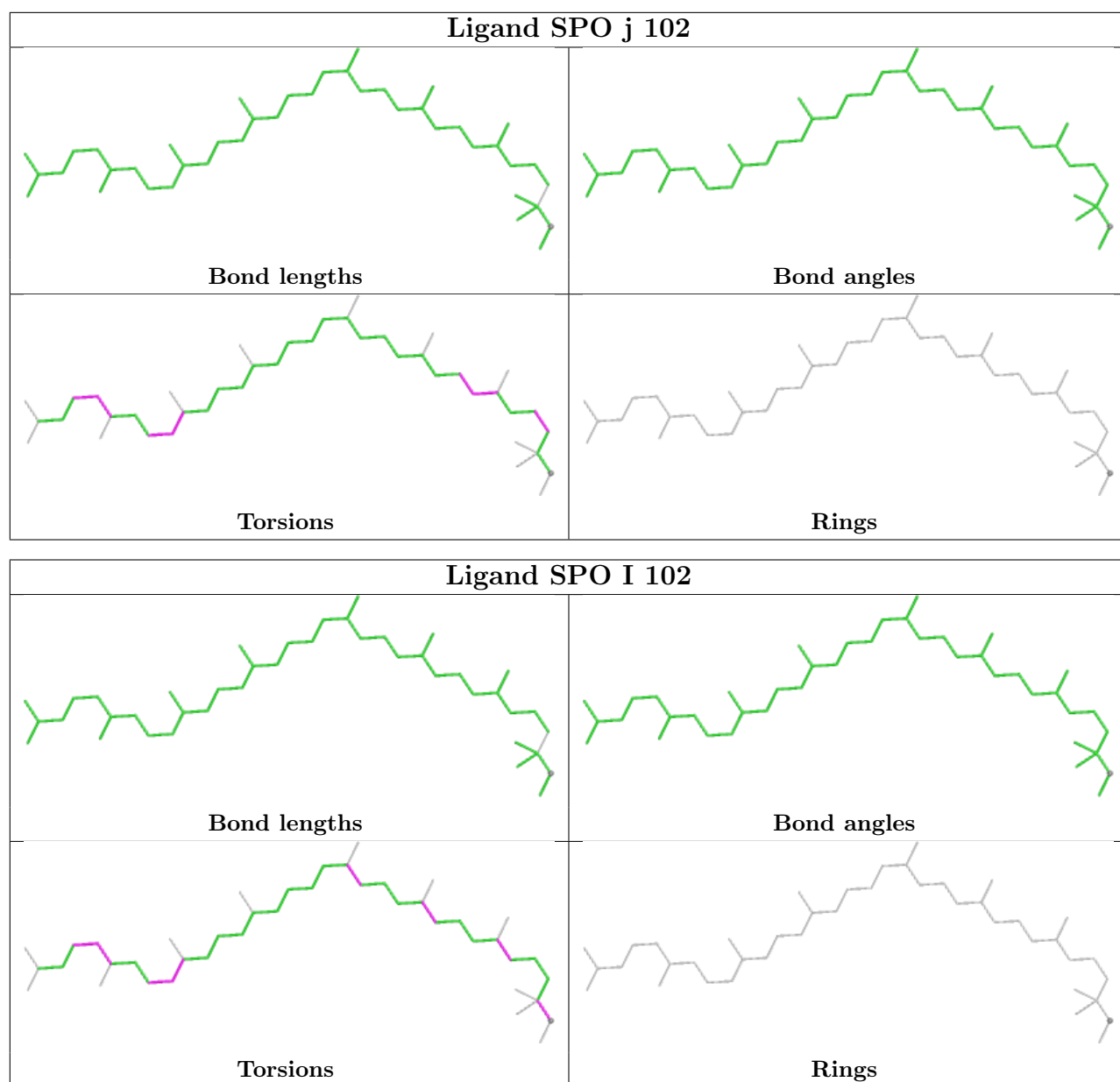
Ligand BCL T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO F 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

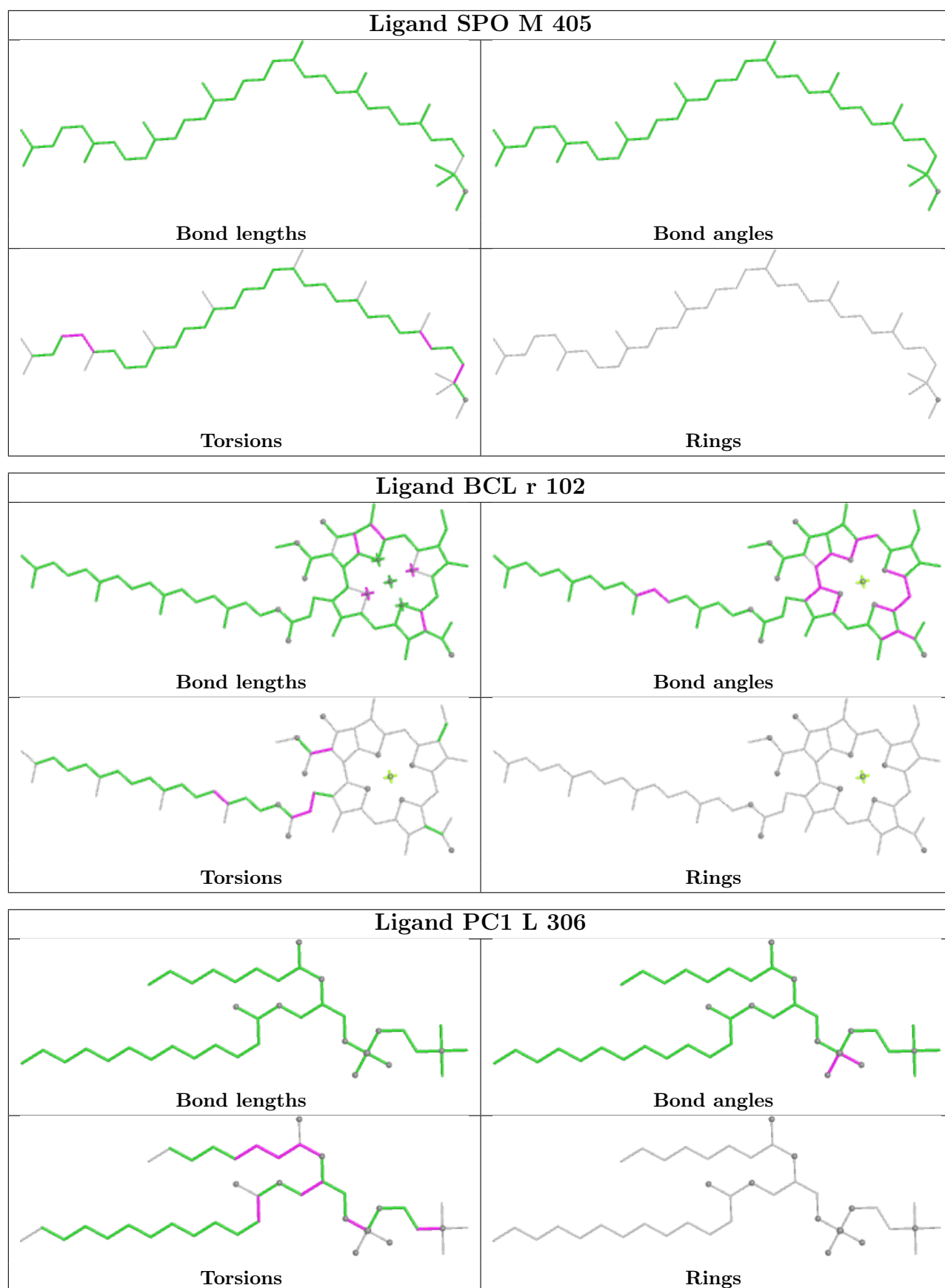


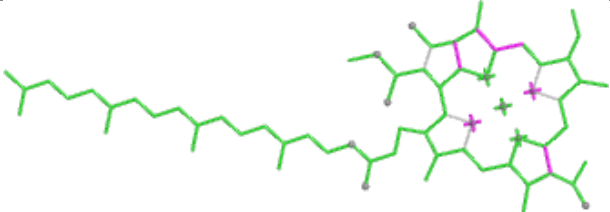
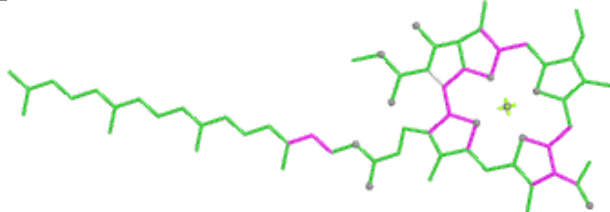
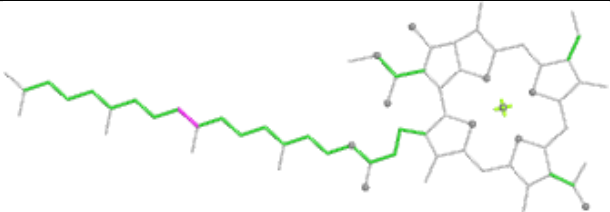
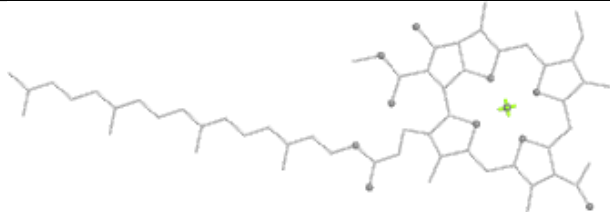
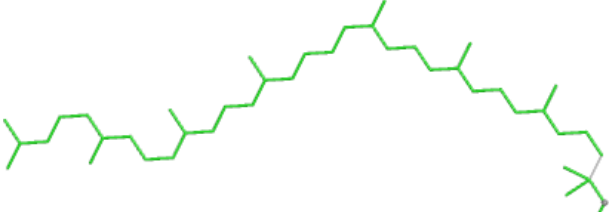
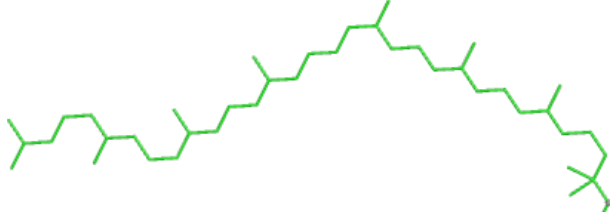
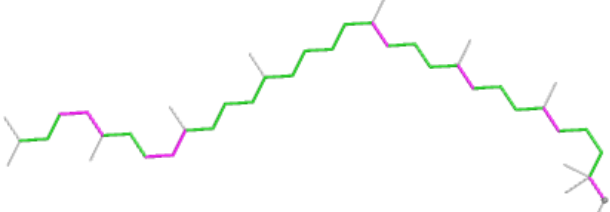
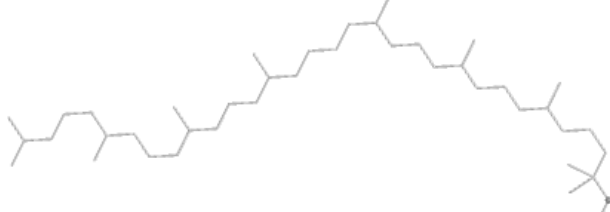
Ligand SPO f 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

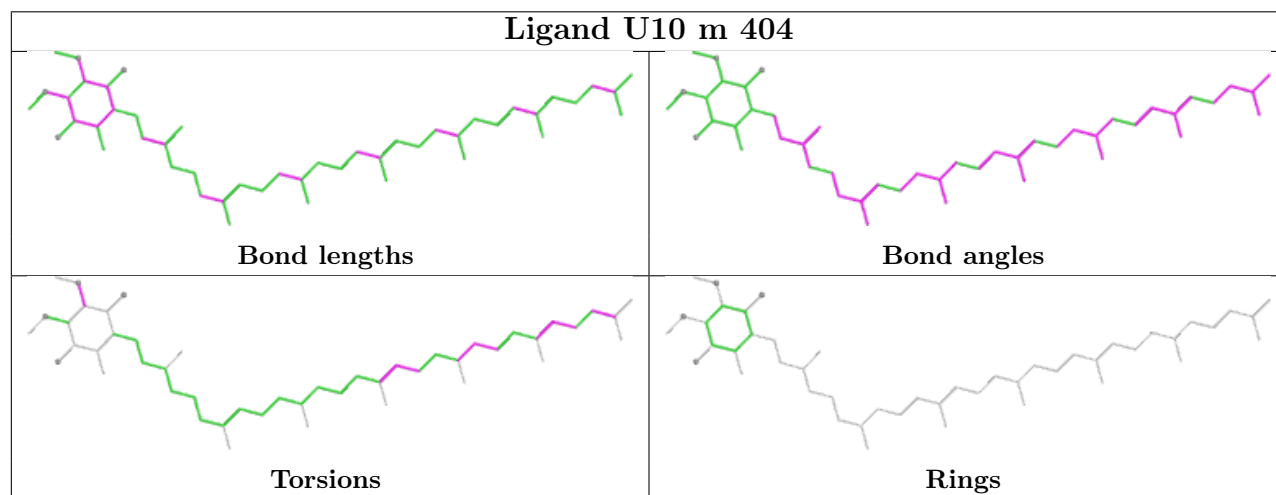
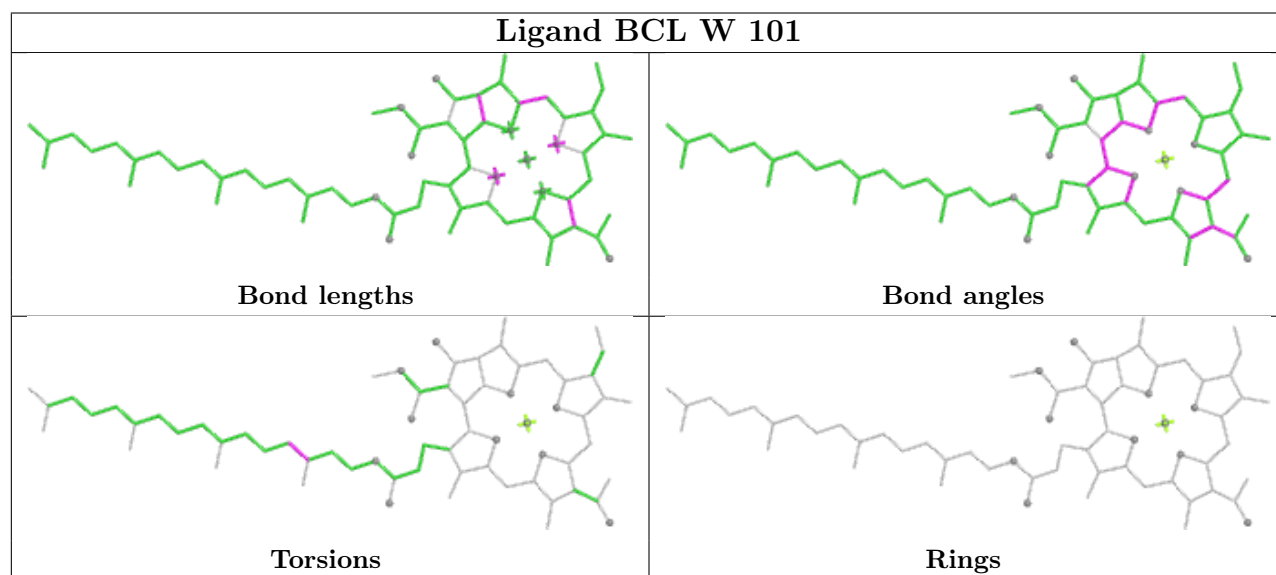
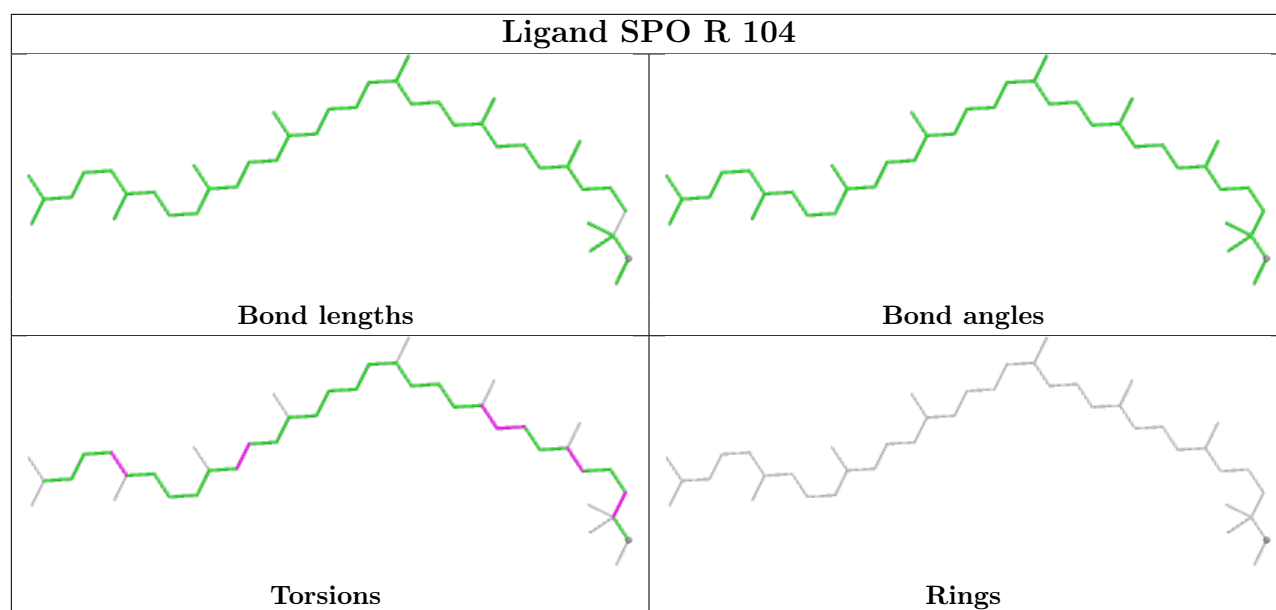
Ligand SPO 5 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

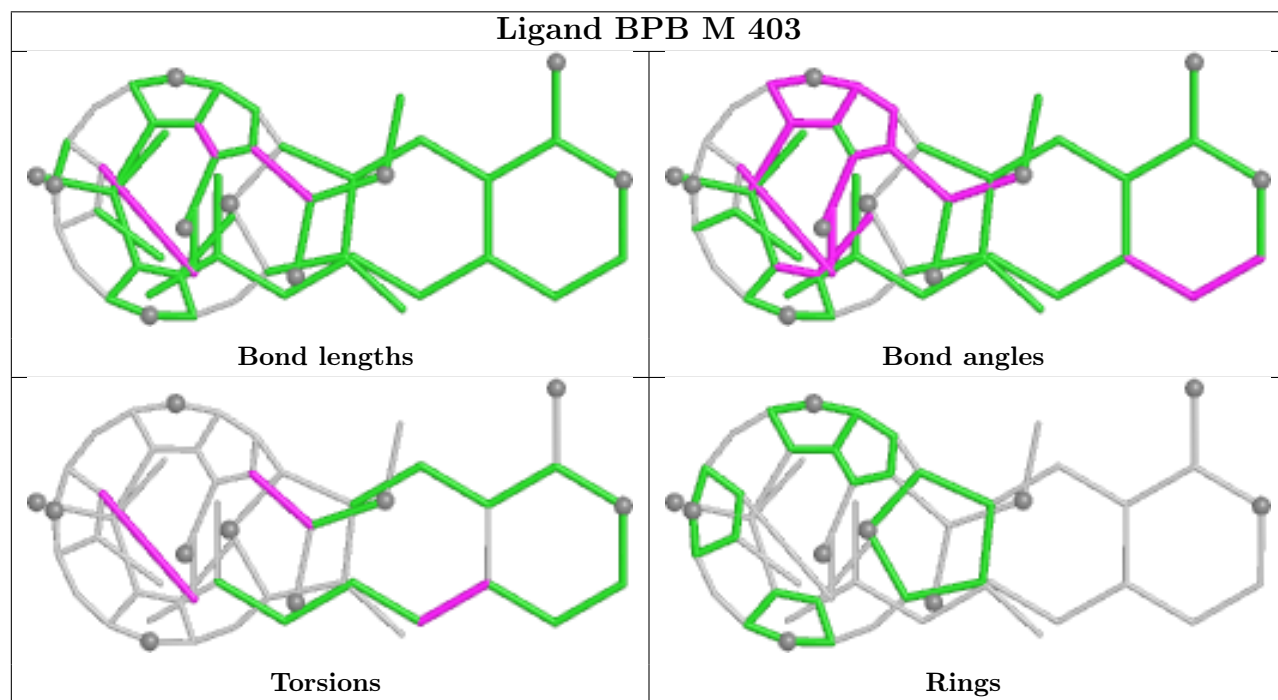
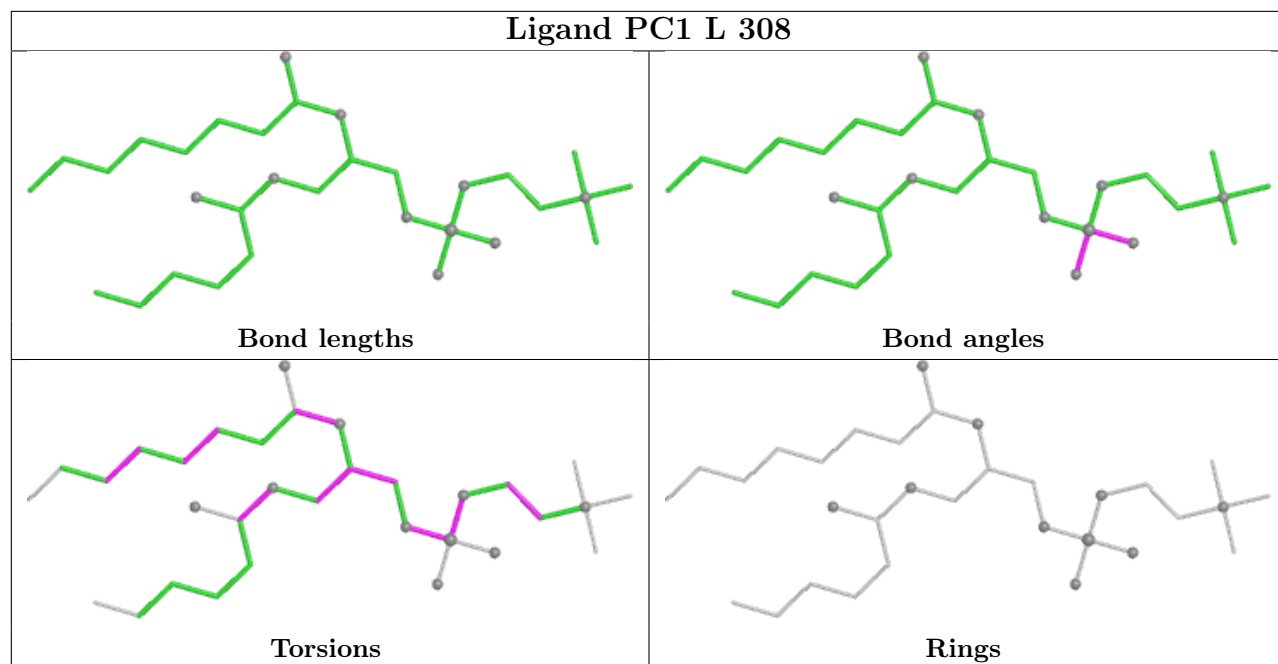


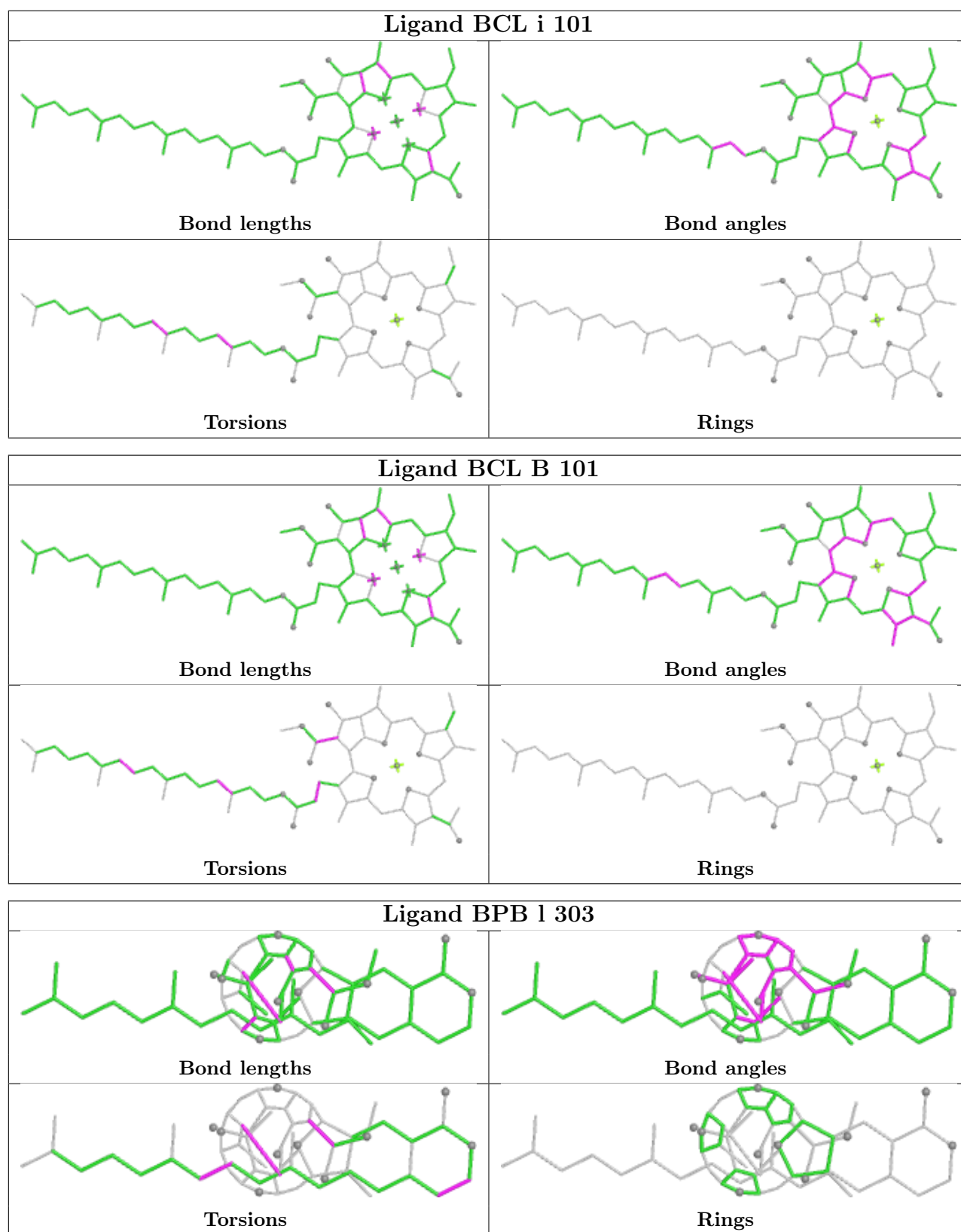


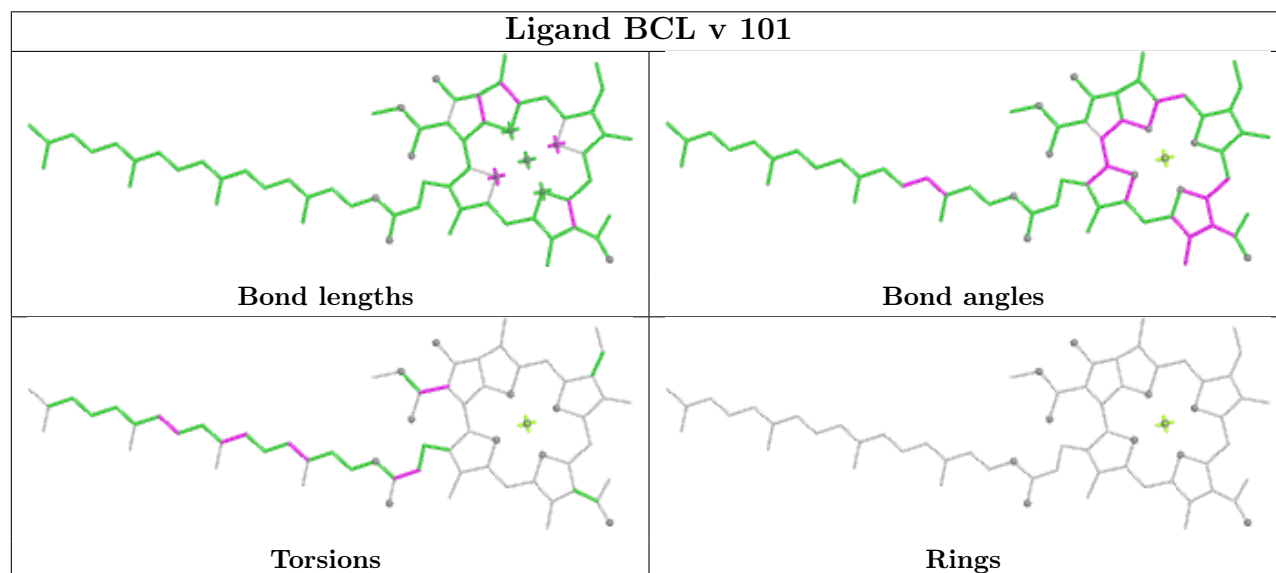
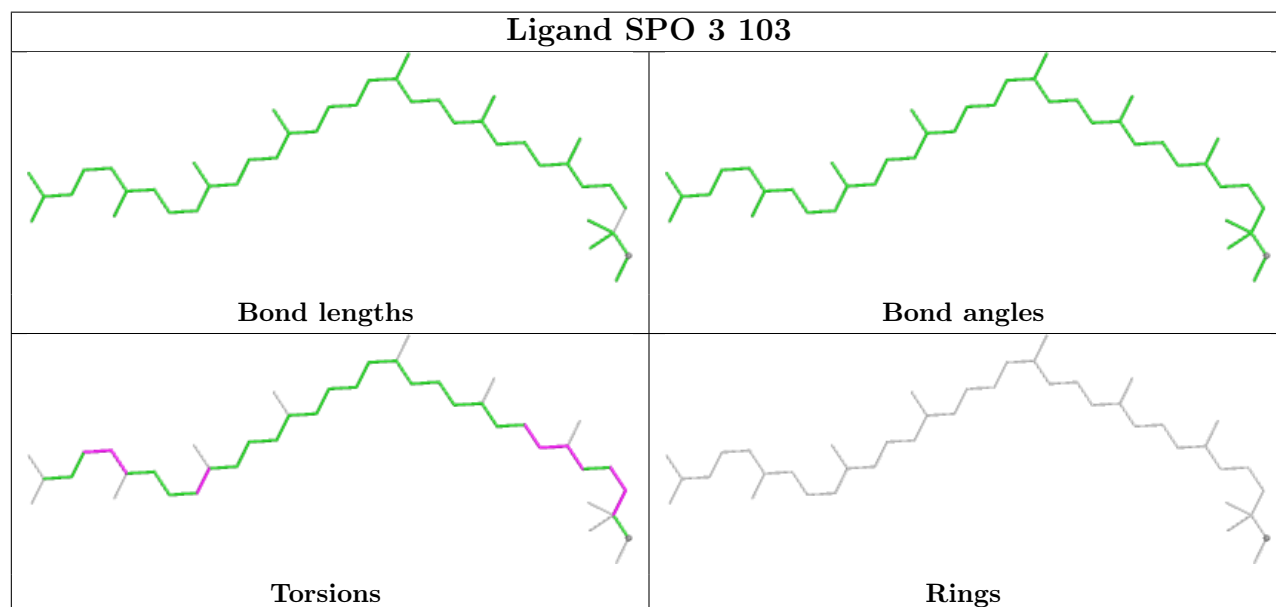
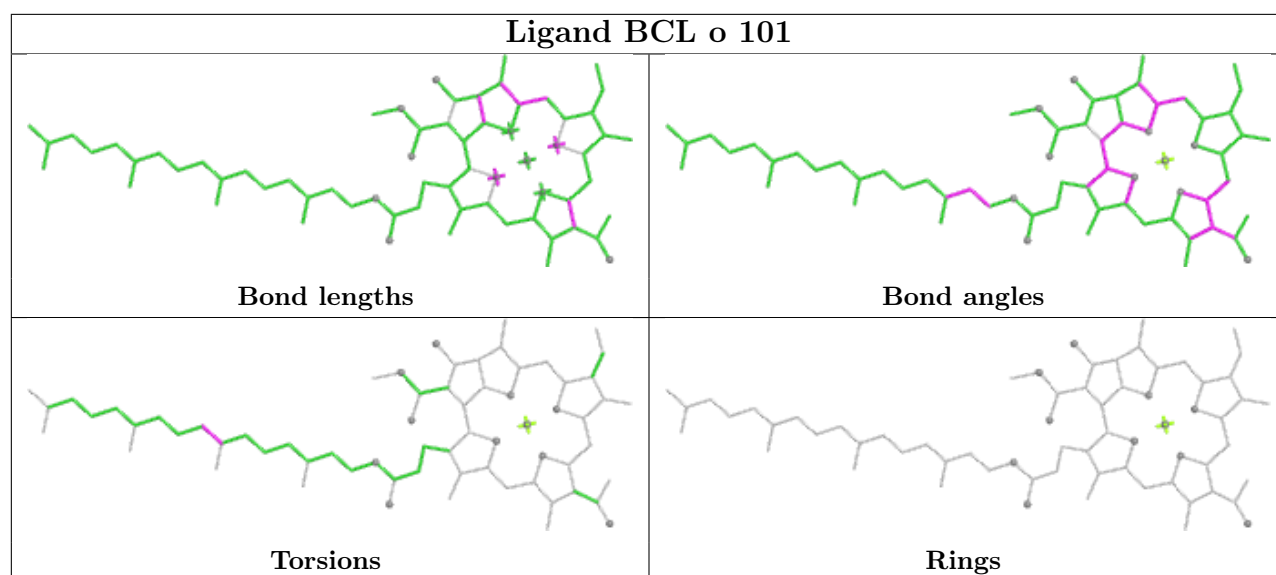


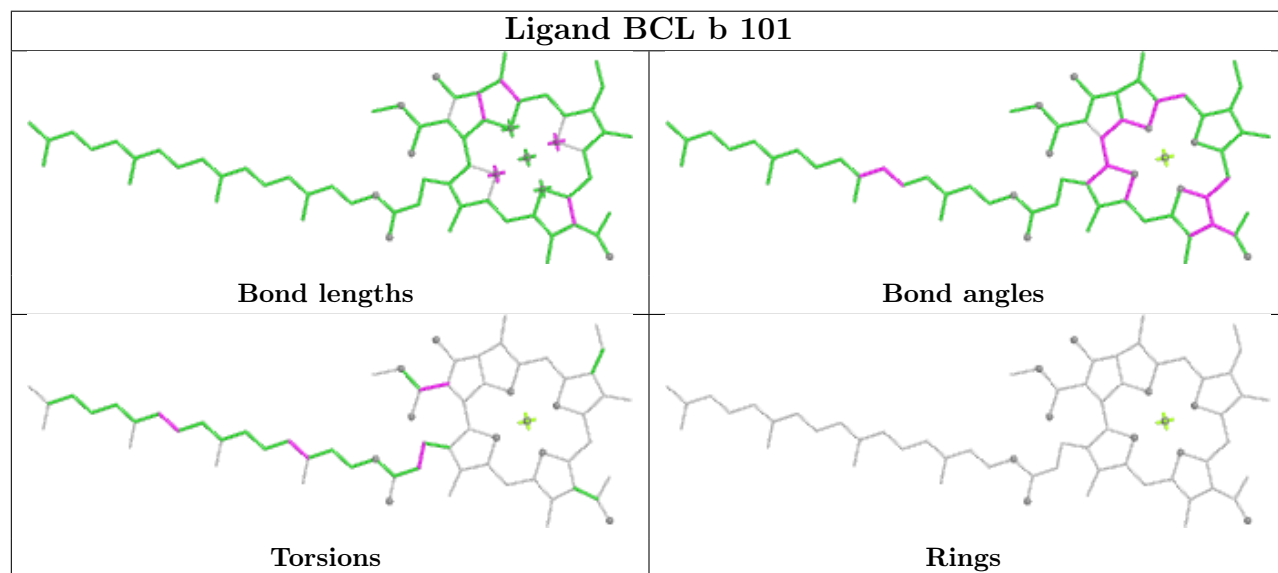
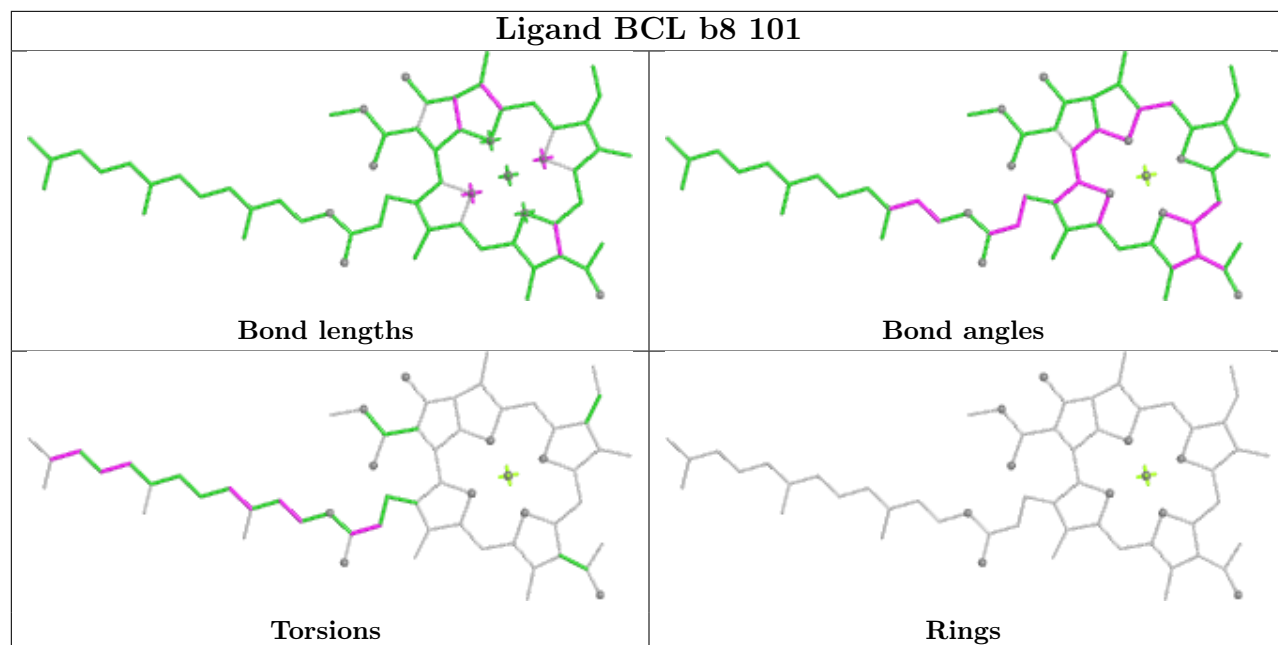
Ligand BCL O 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO i 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

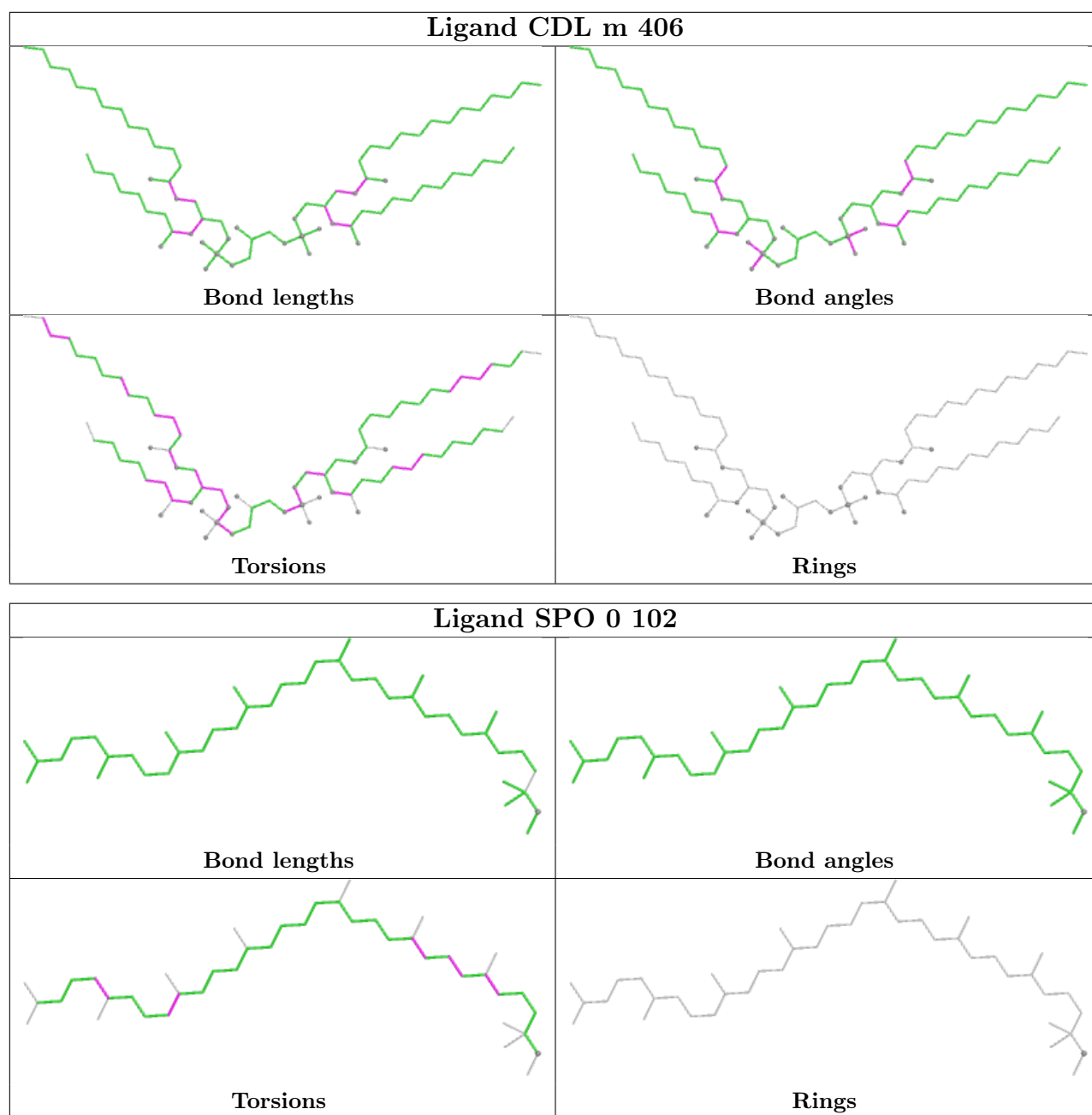


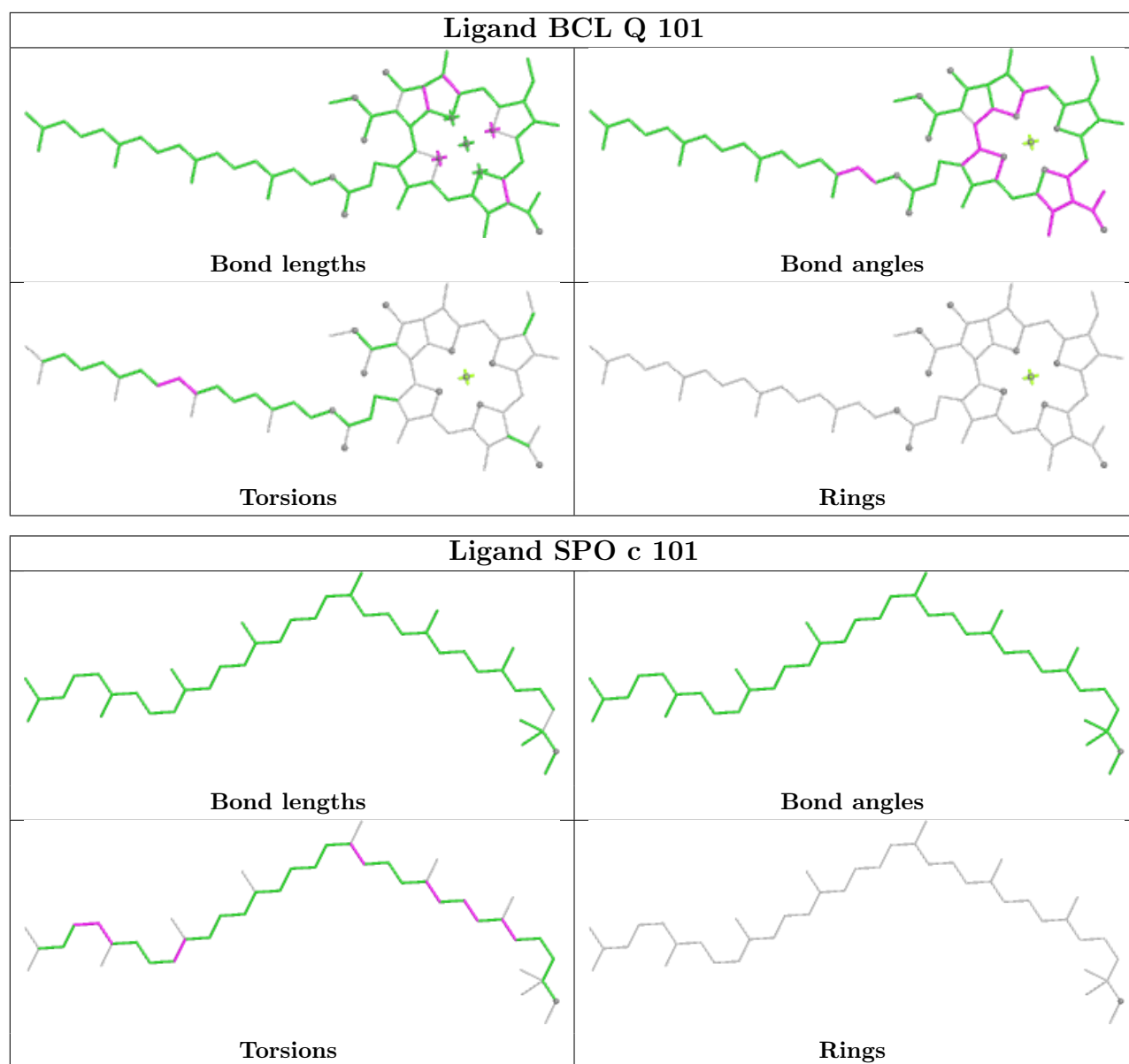


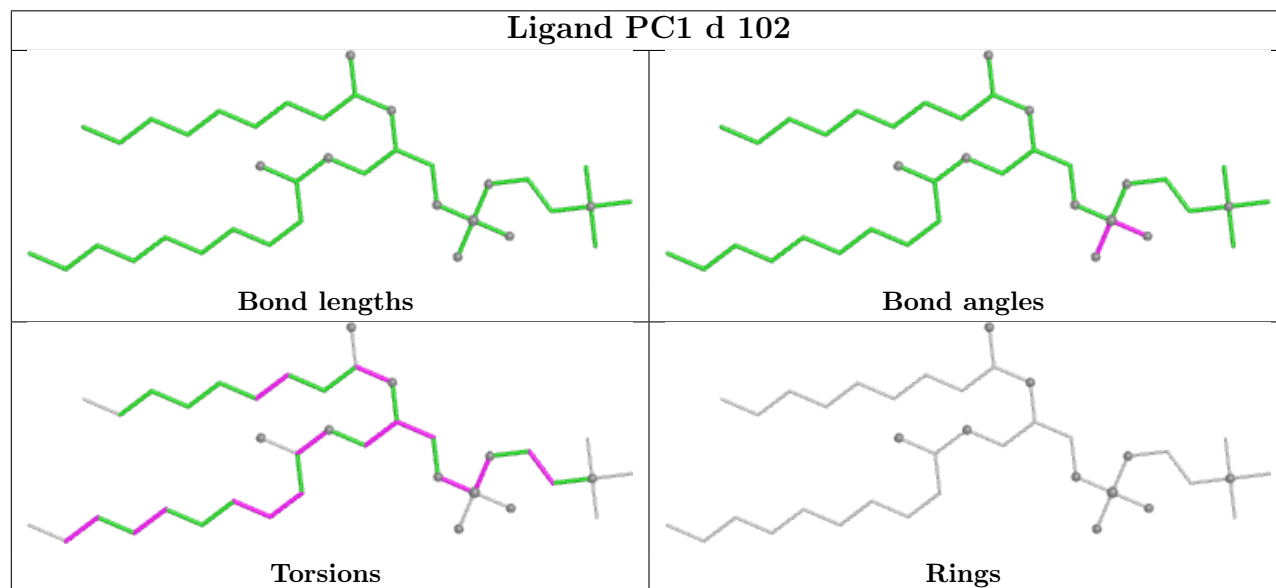
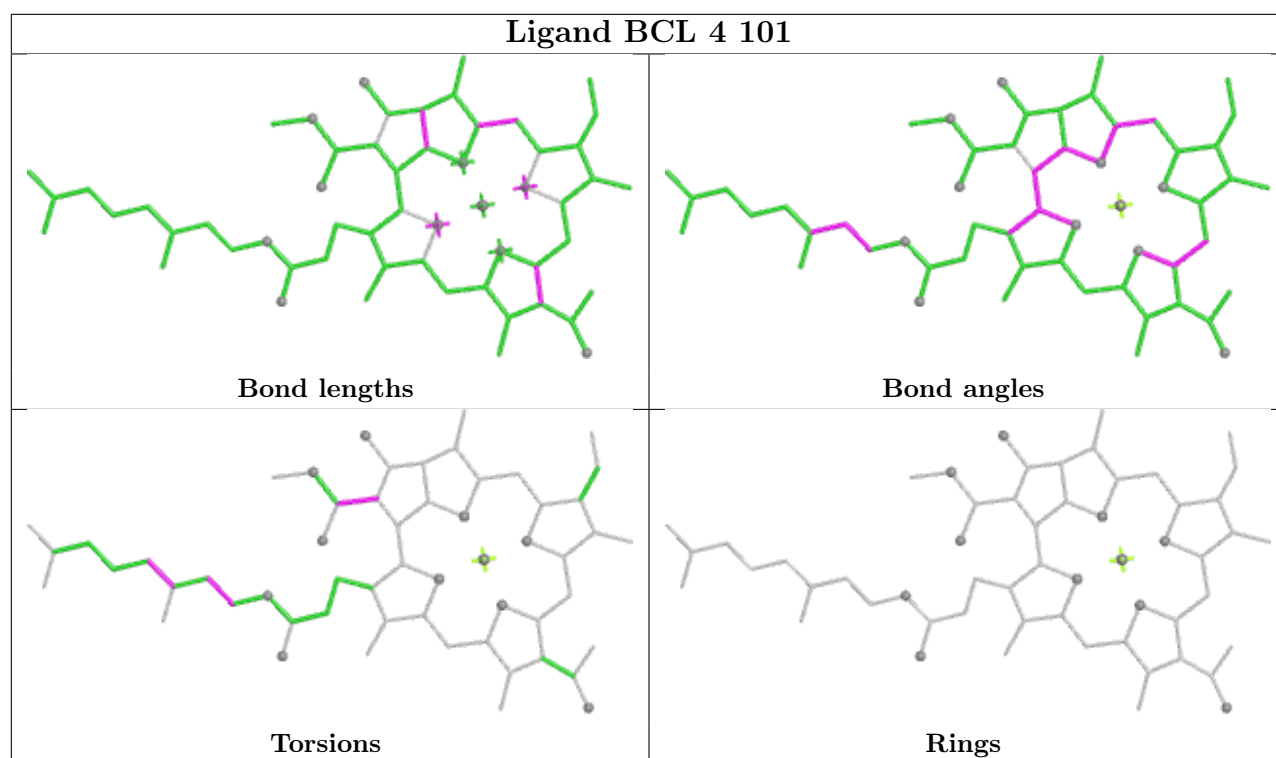


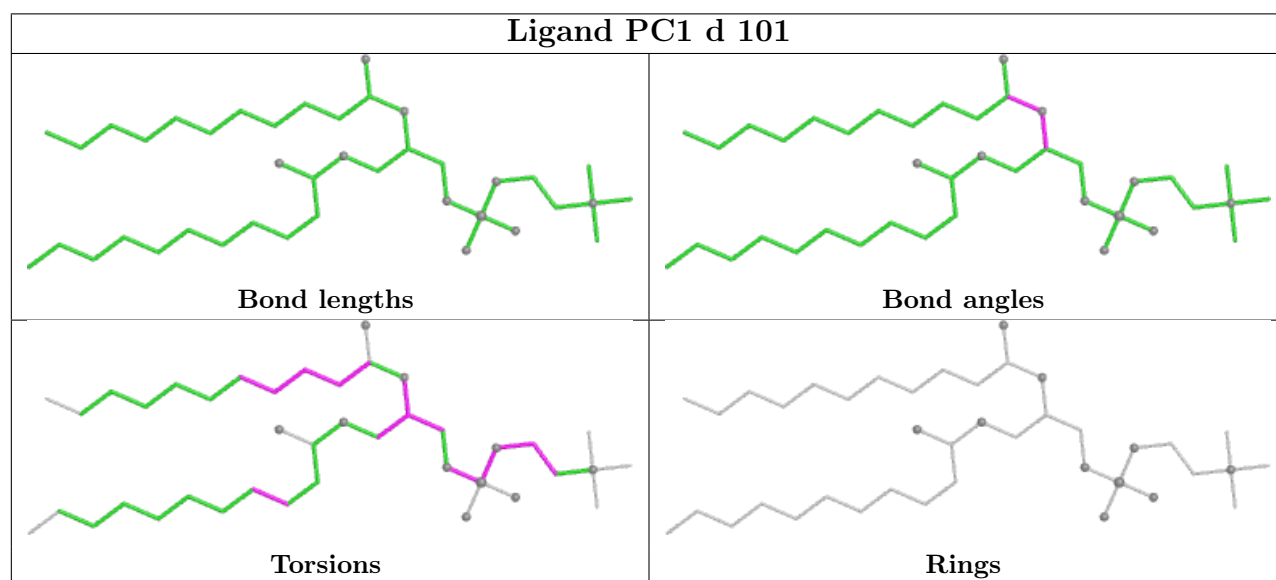
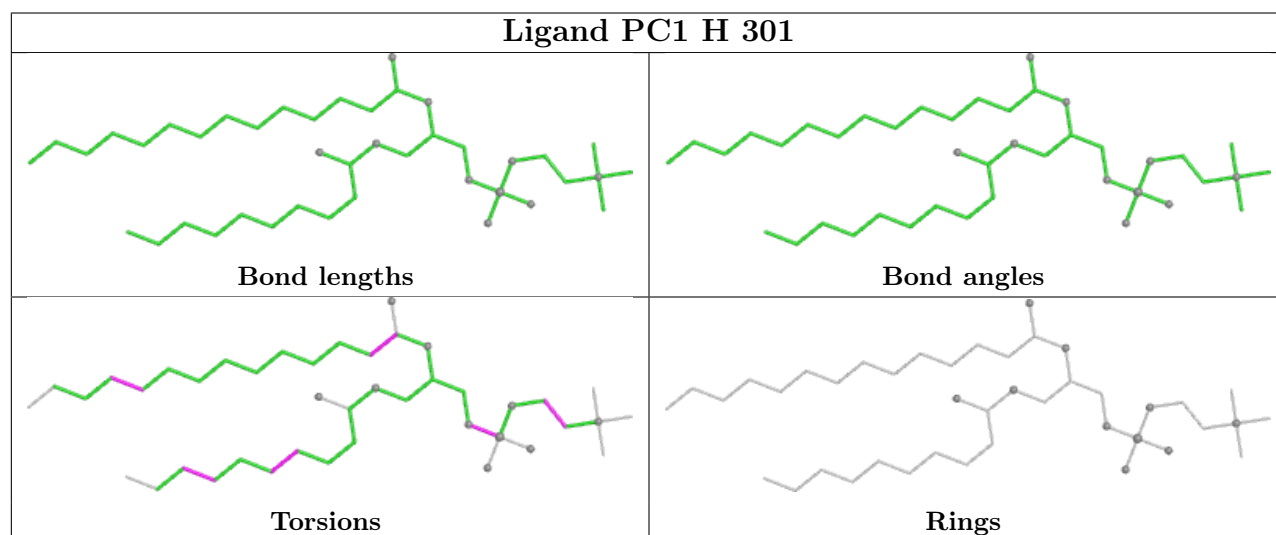
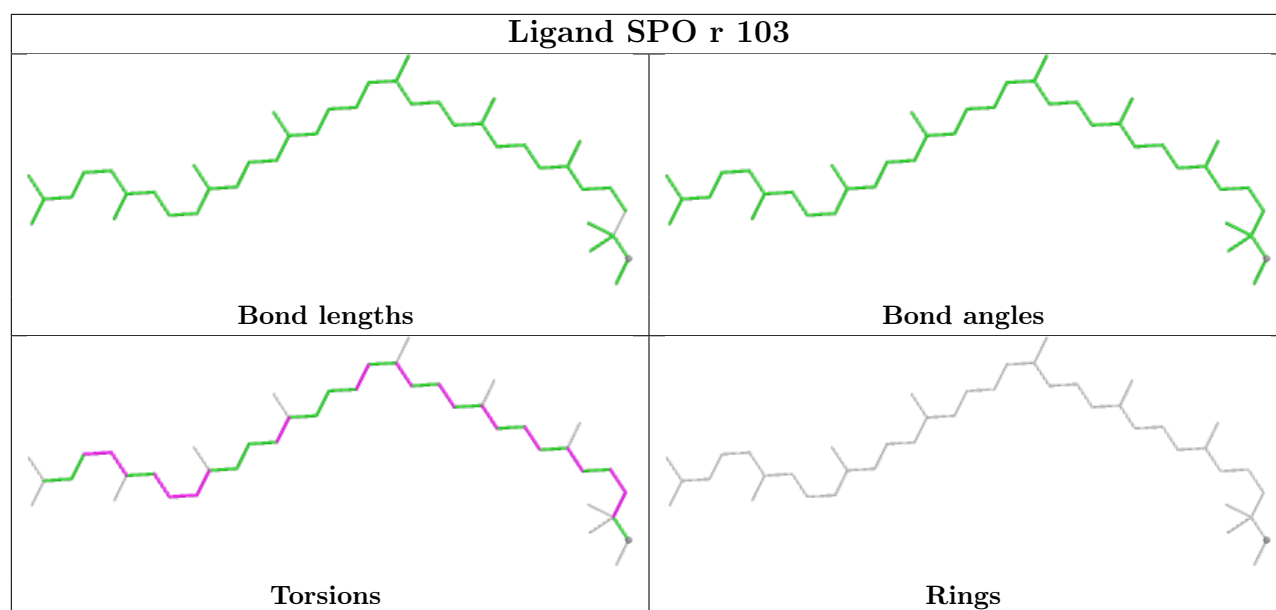


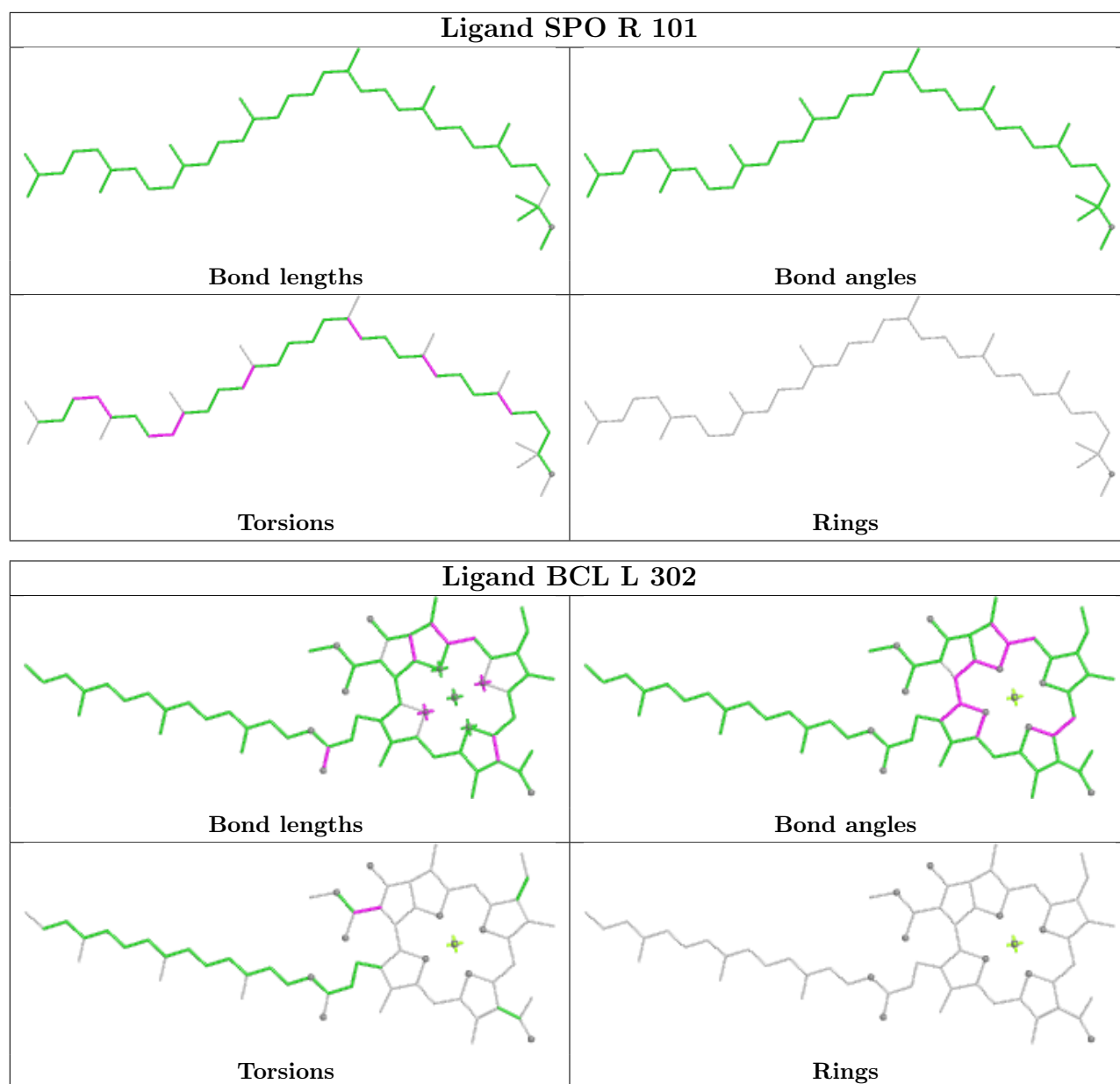


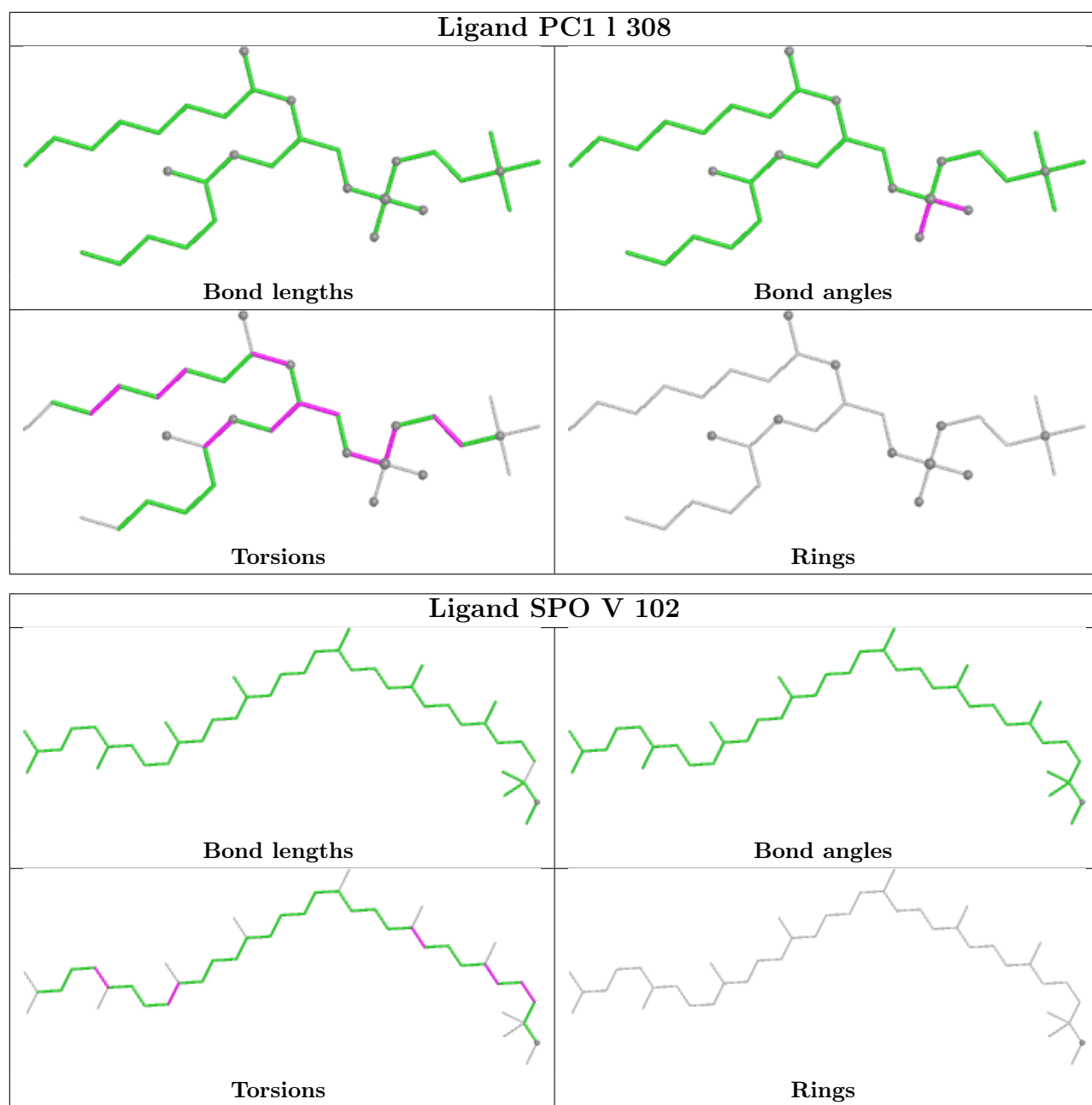


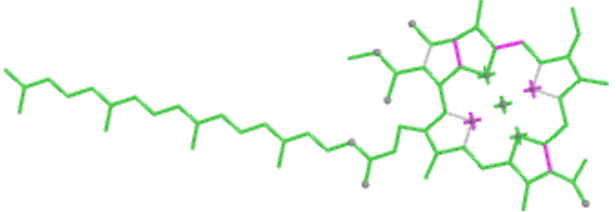
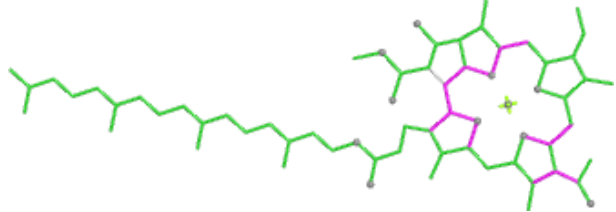
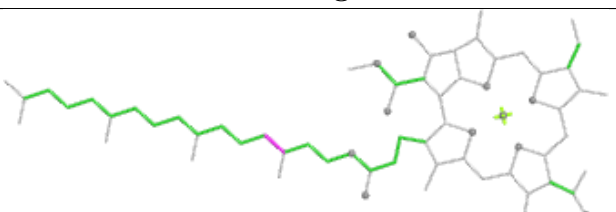
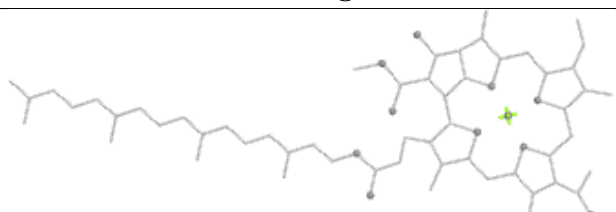
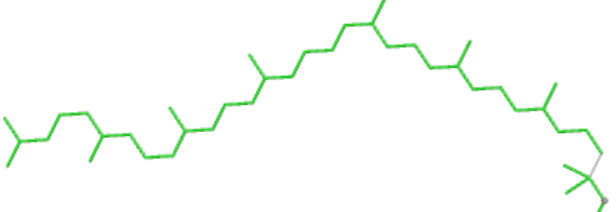
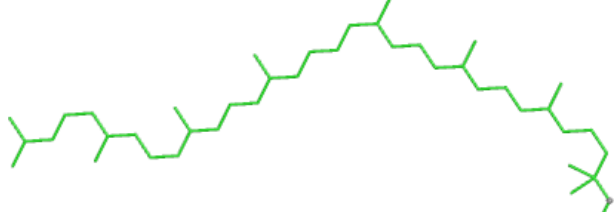
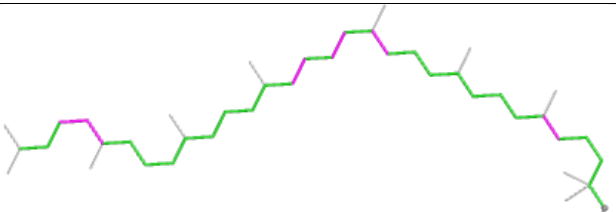
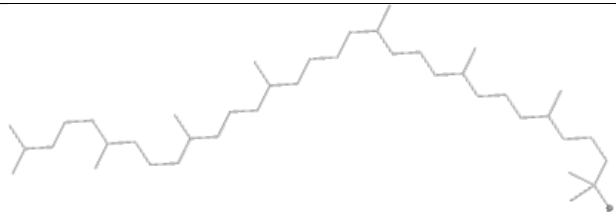


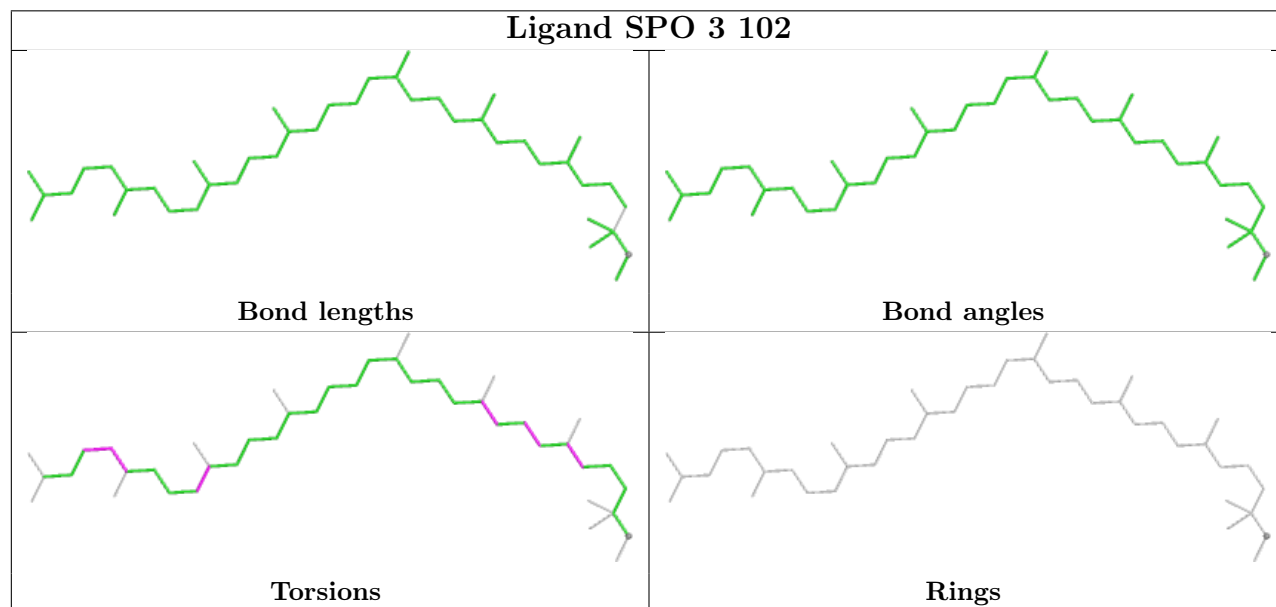
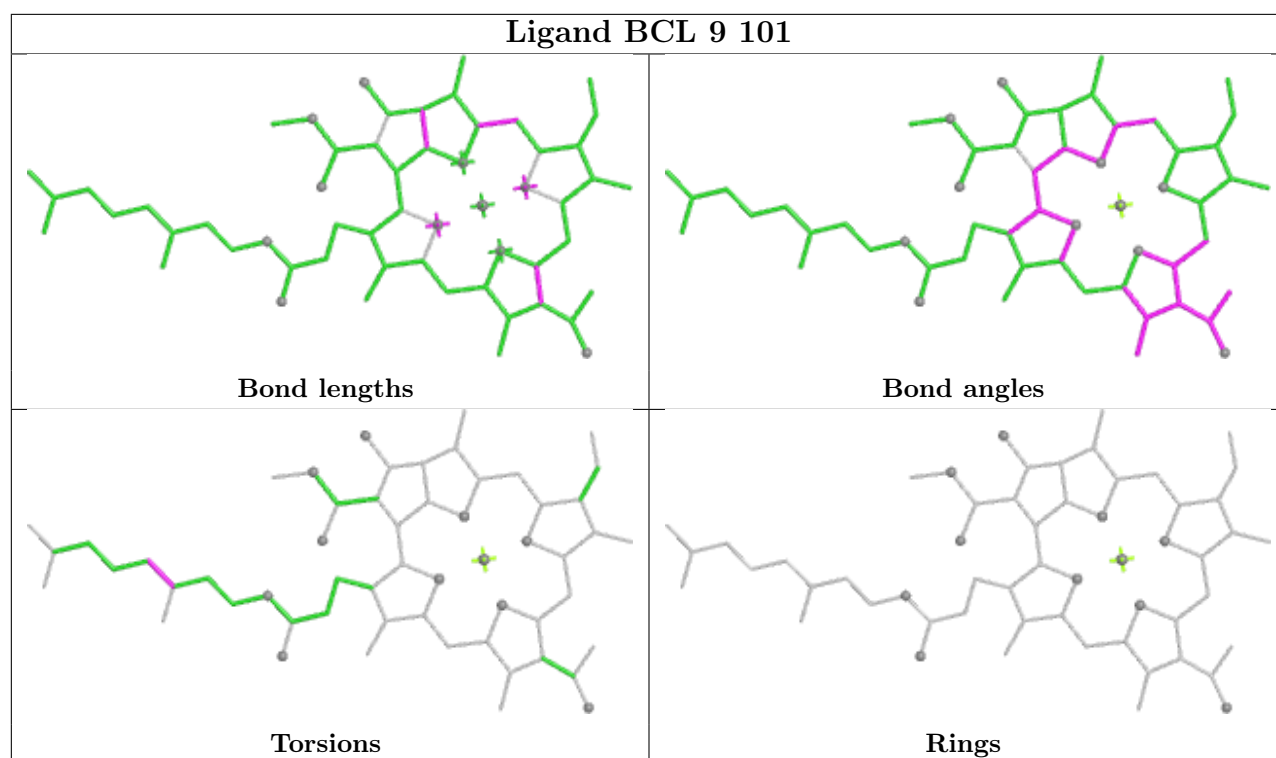


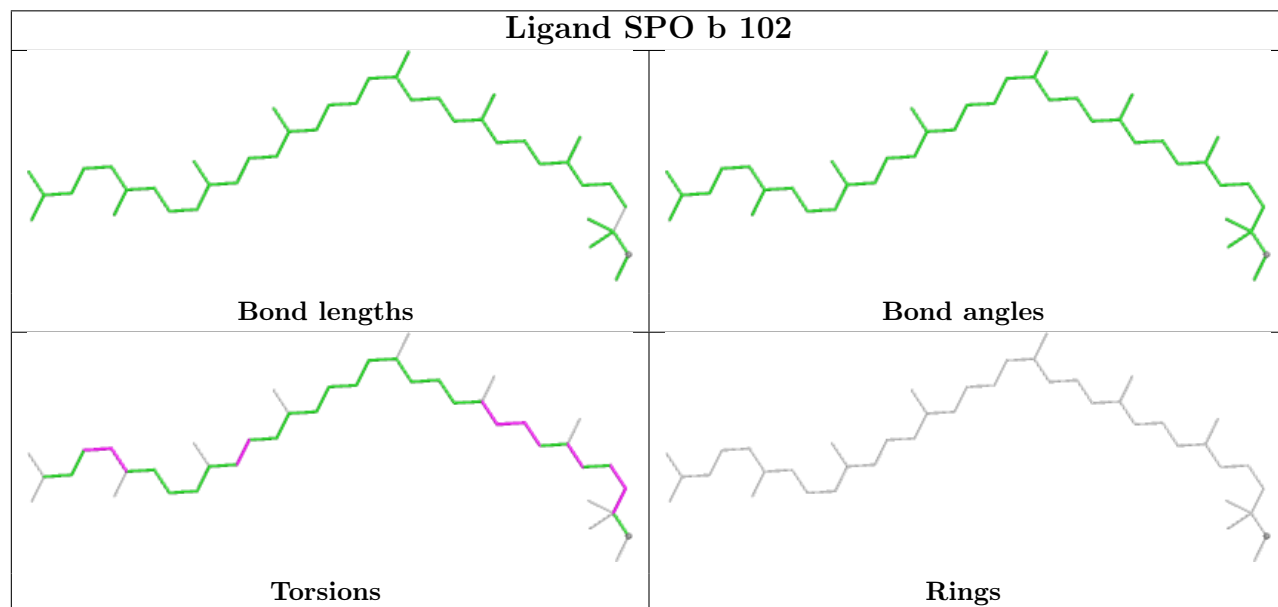
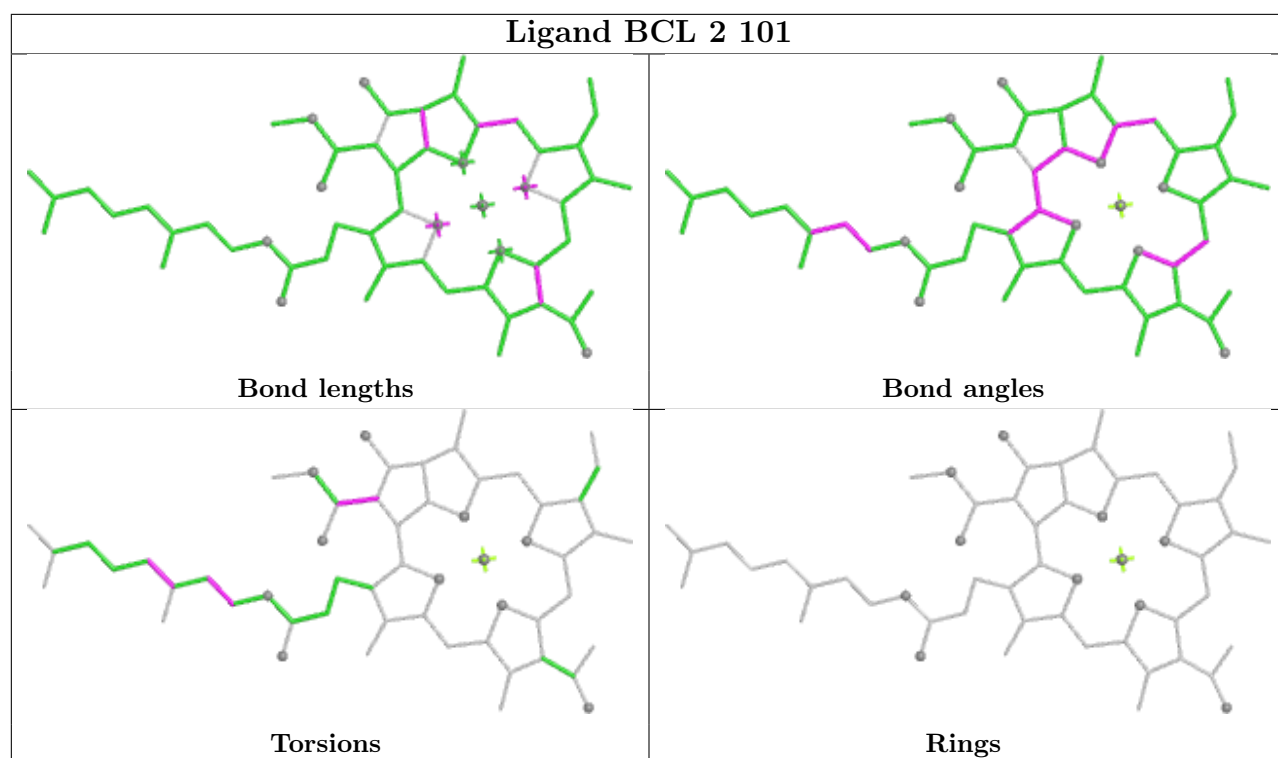


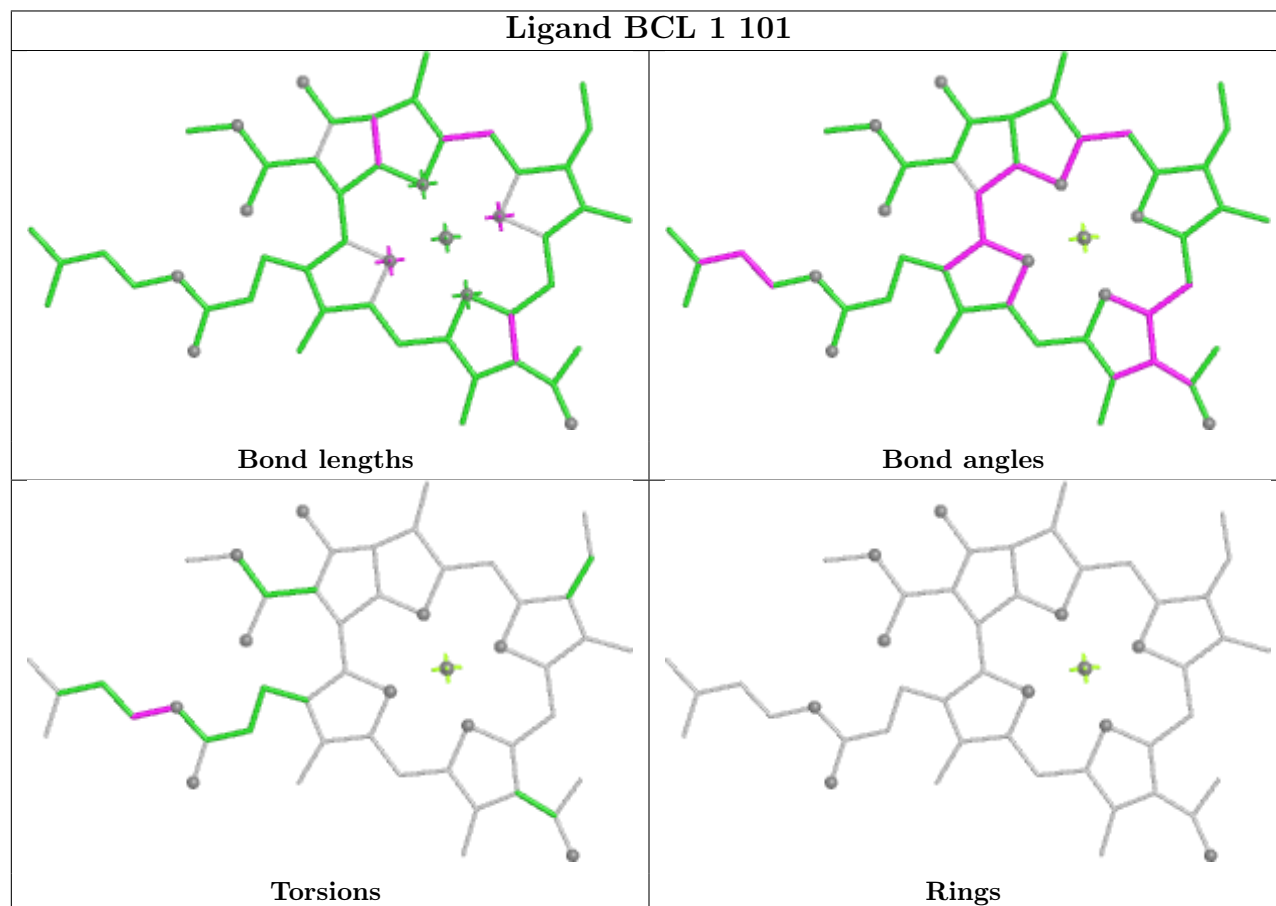
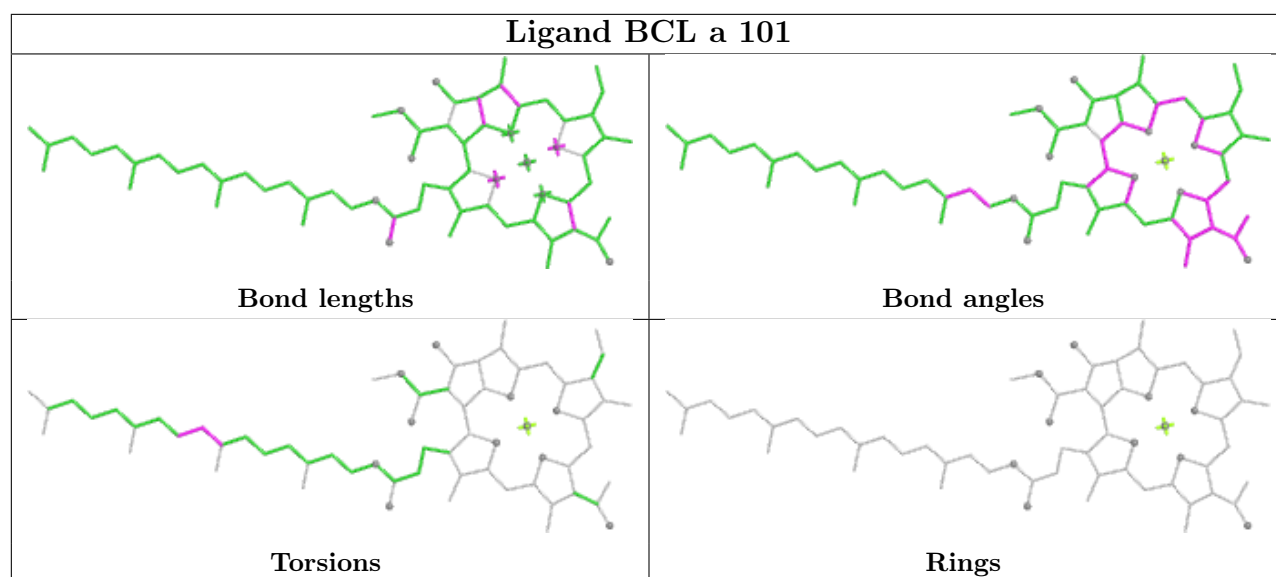


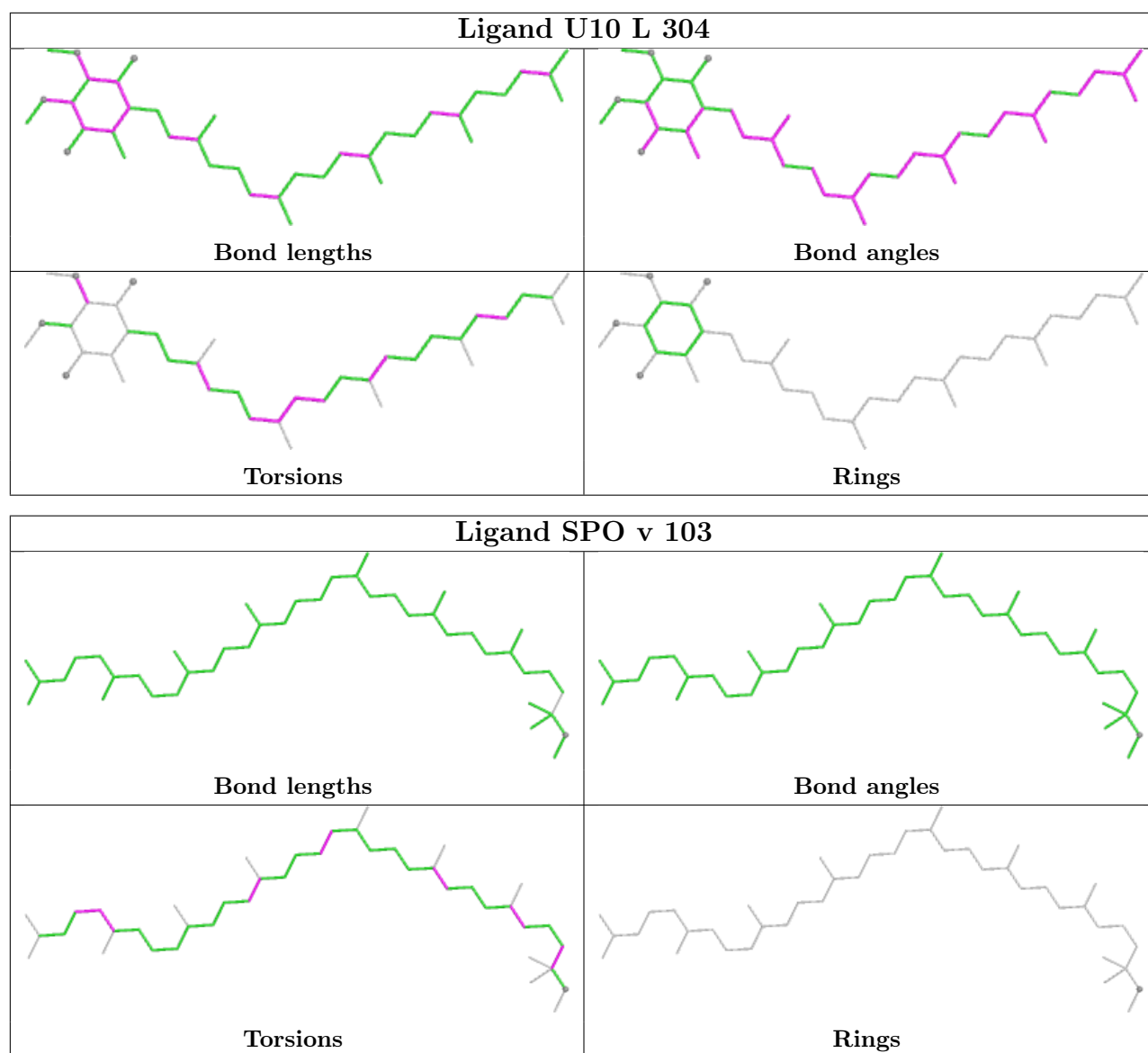


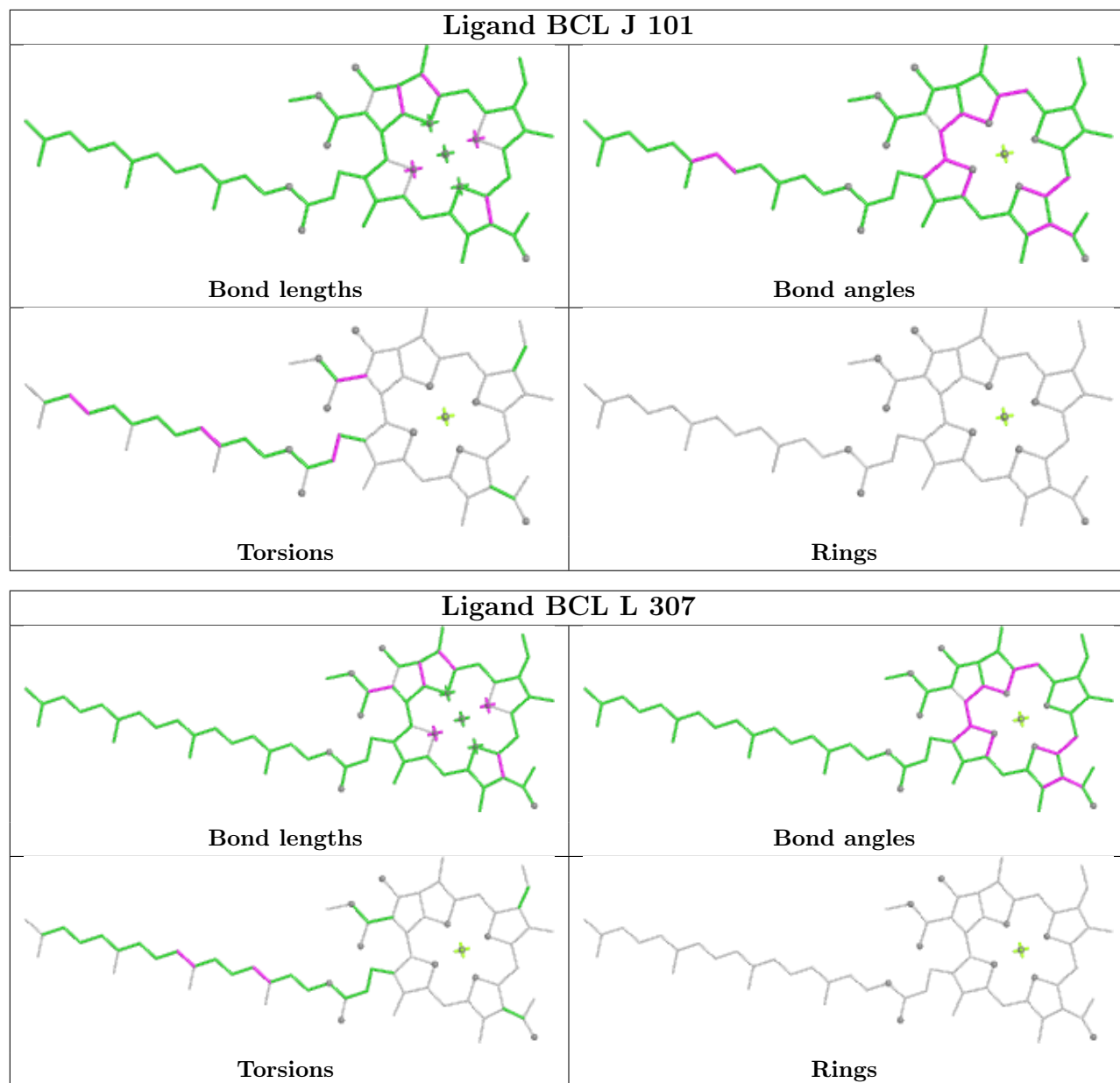
Ligand BCL w 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO A 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

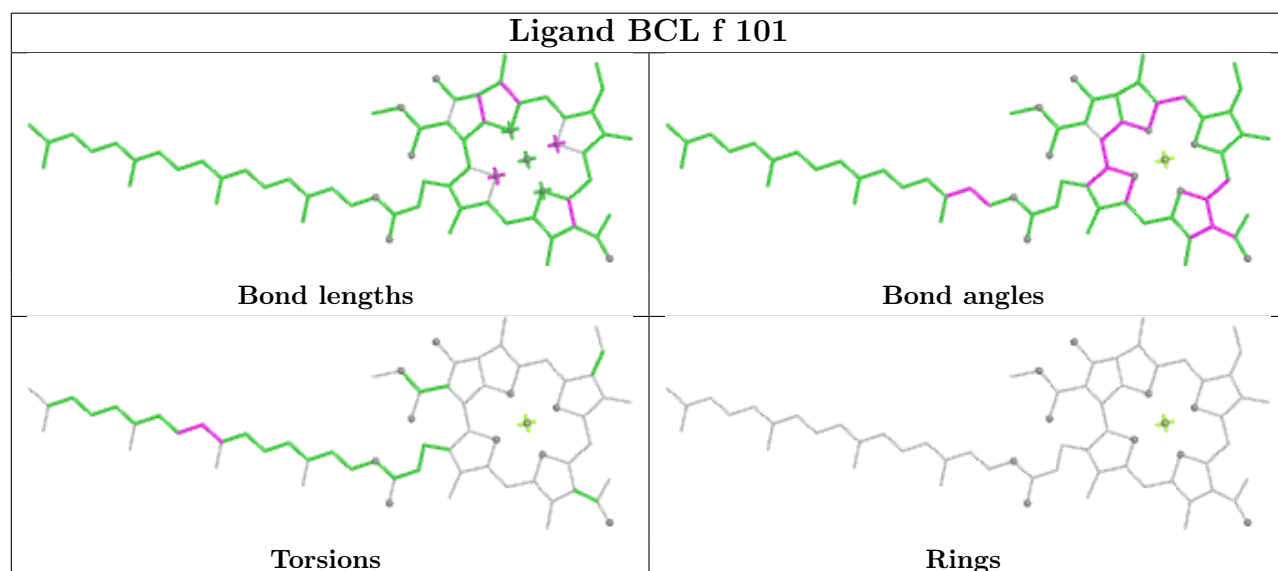
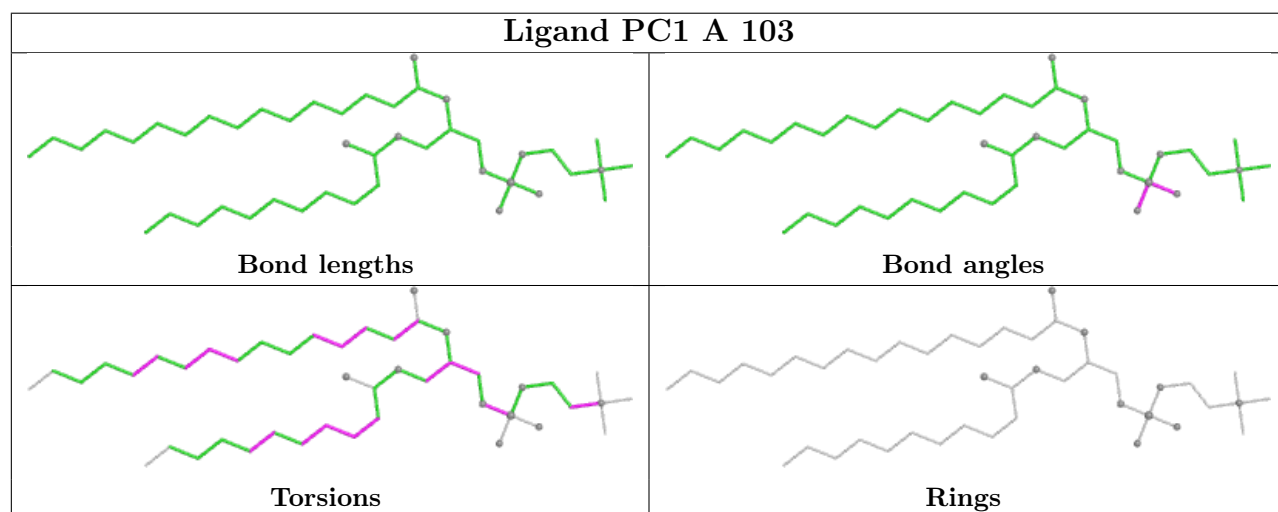
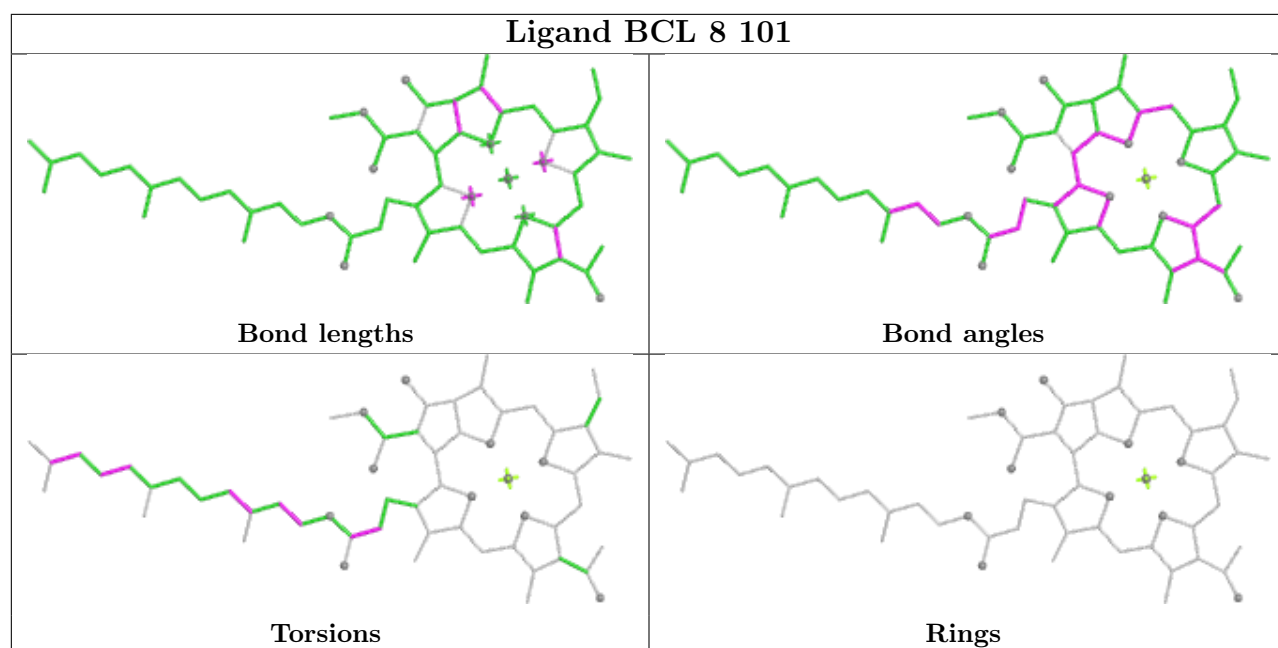


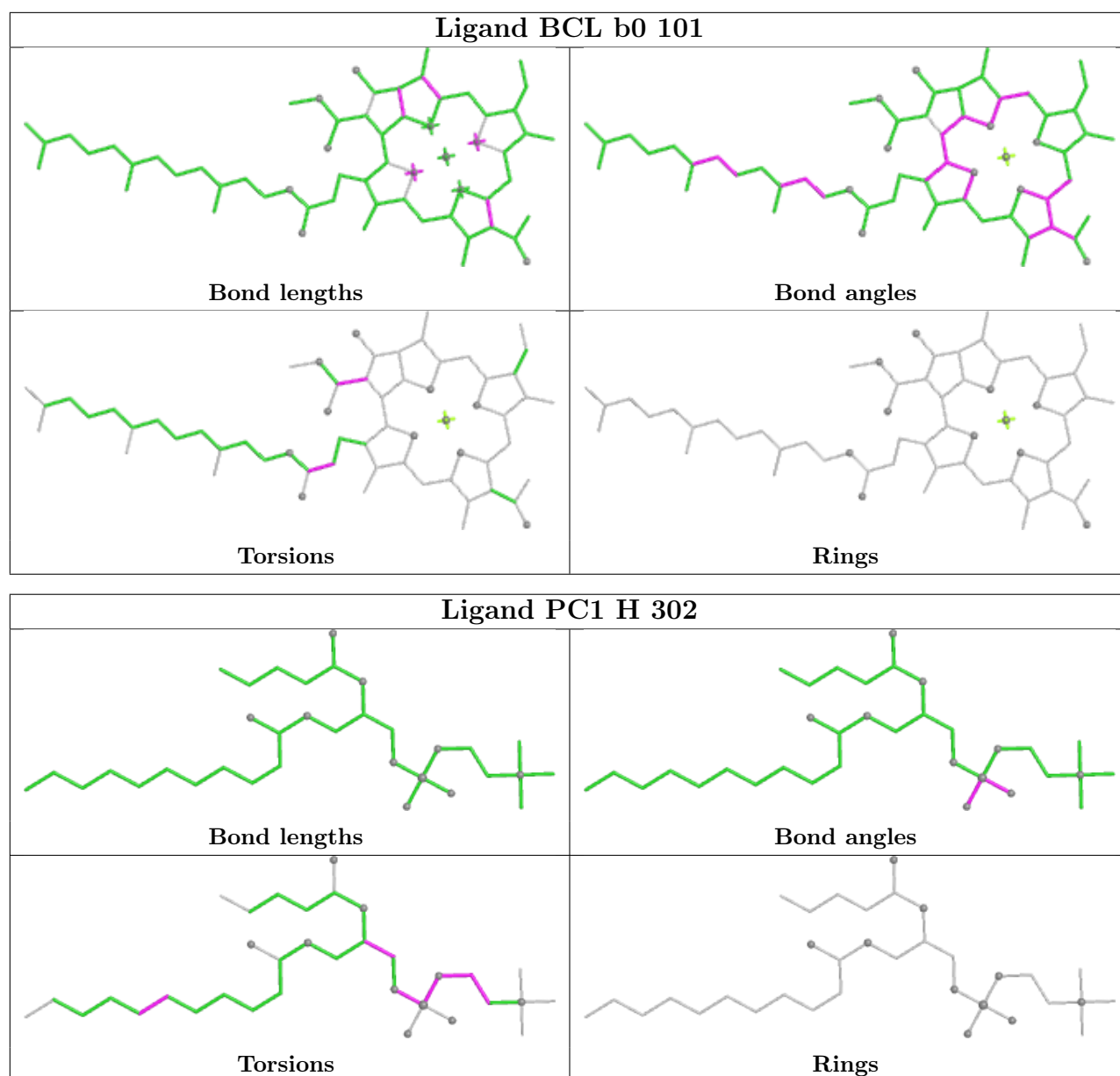


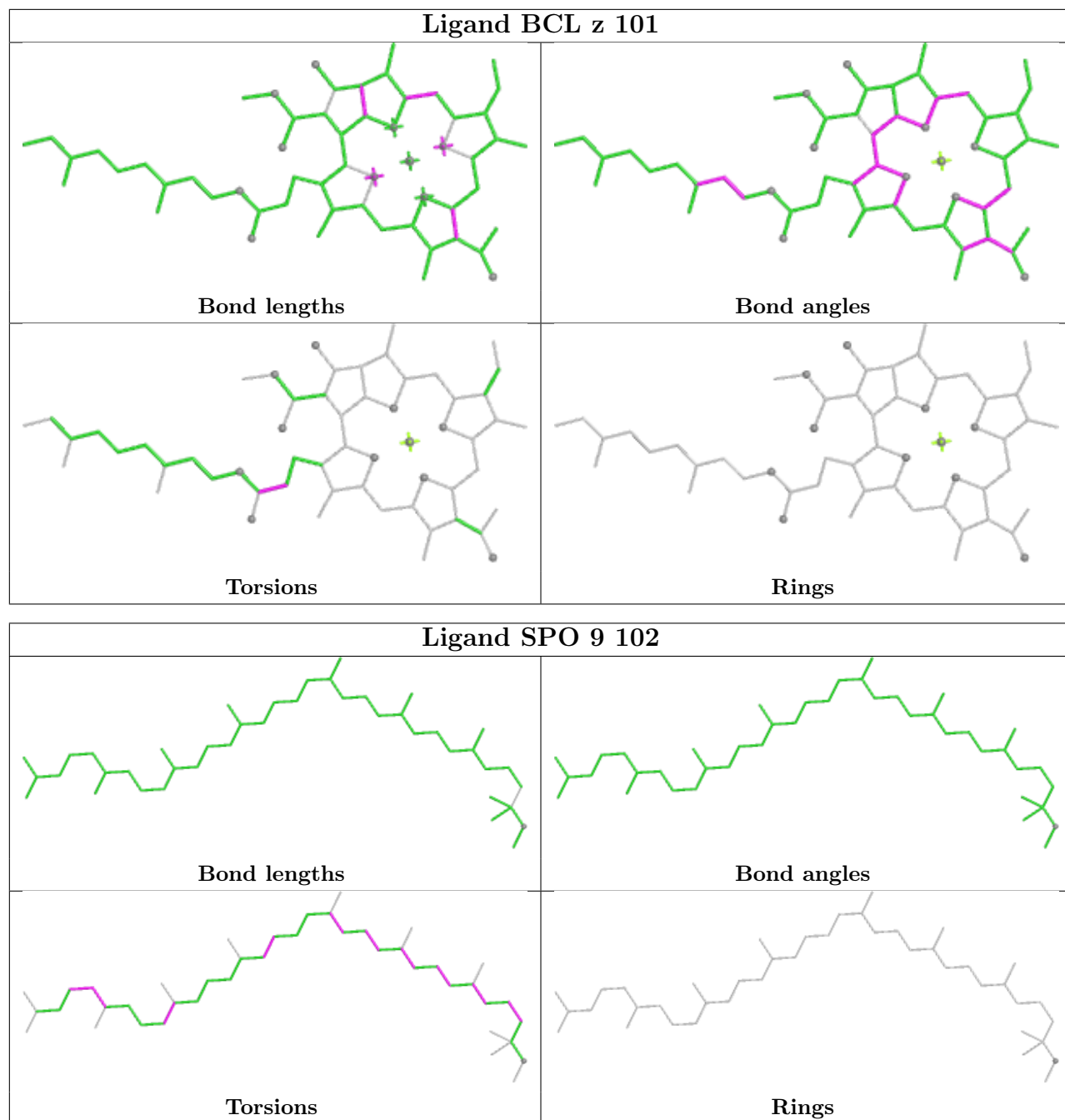


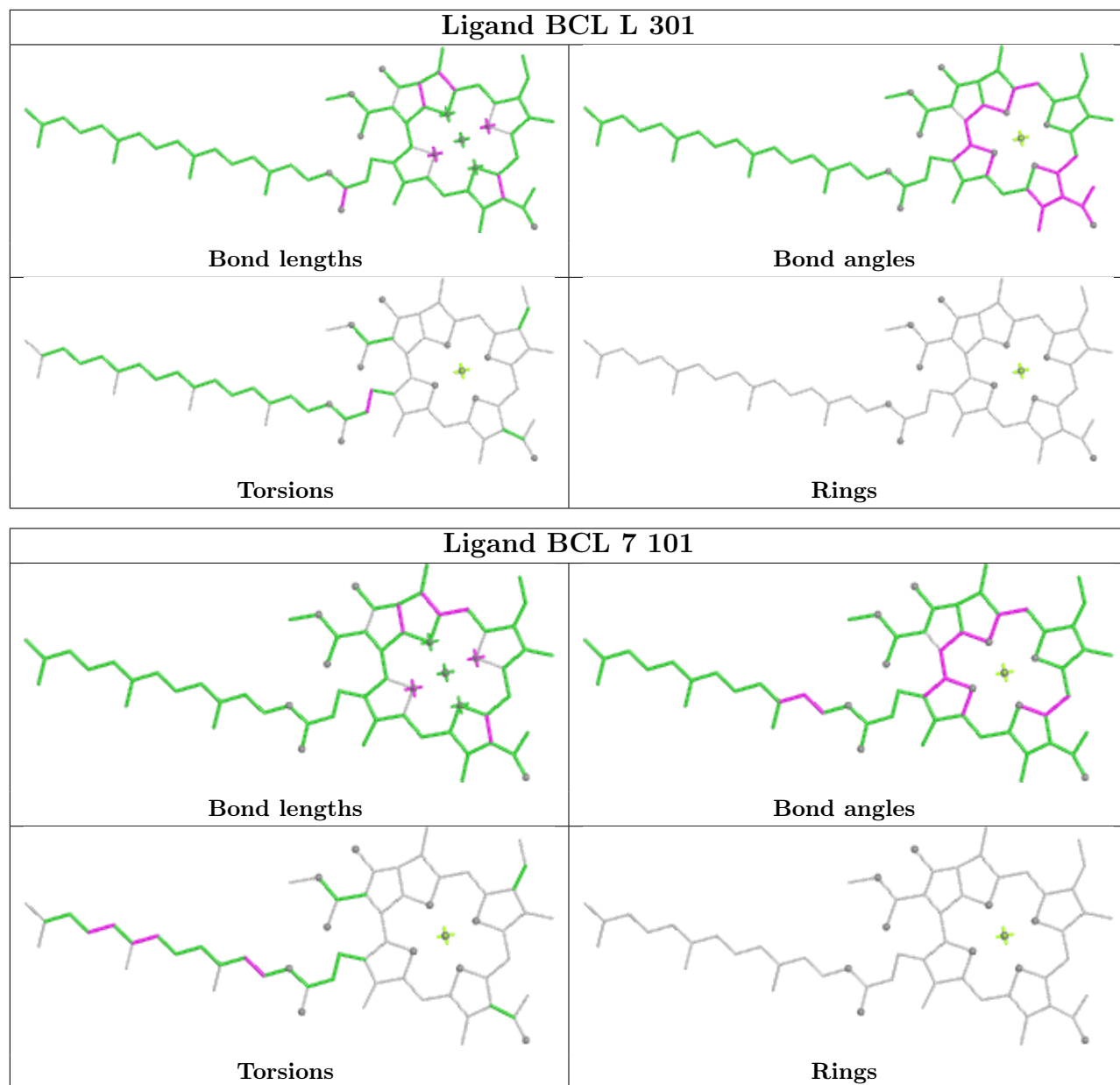


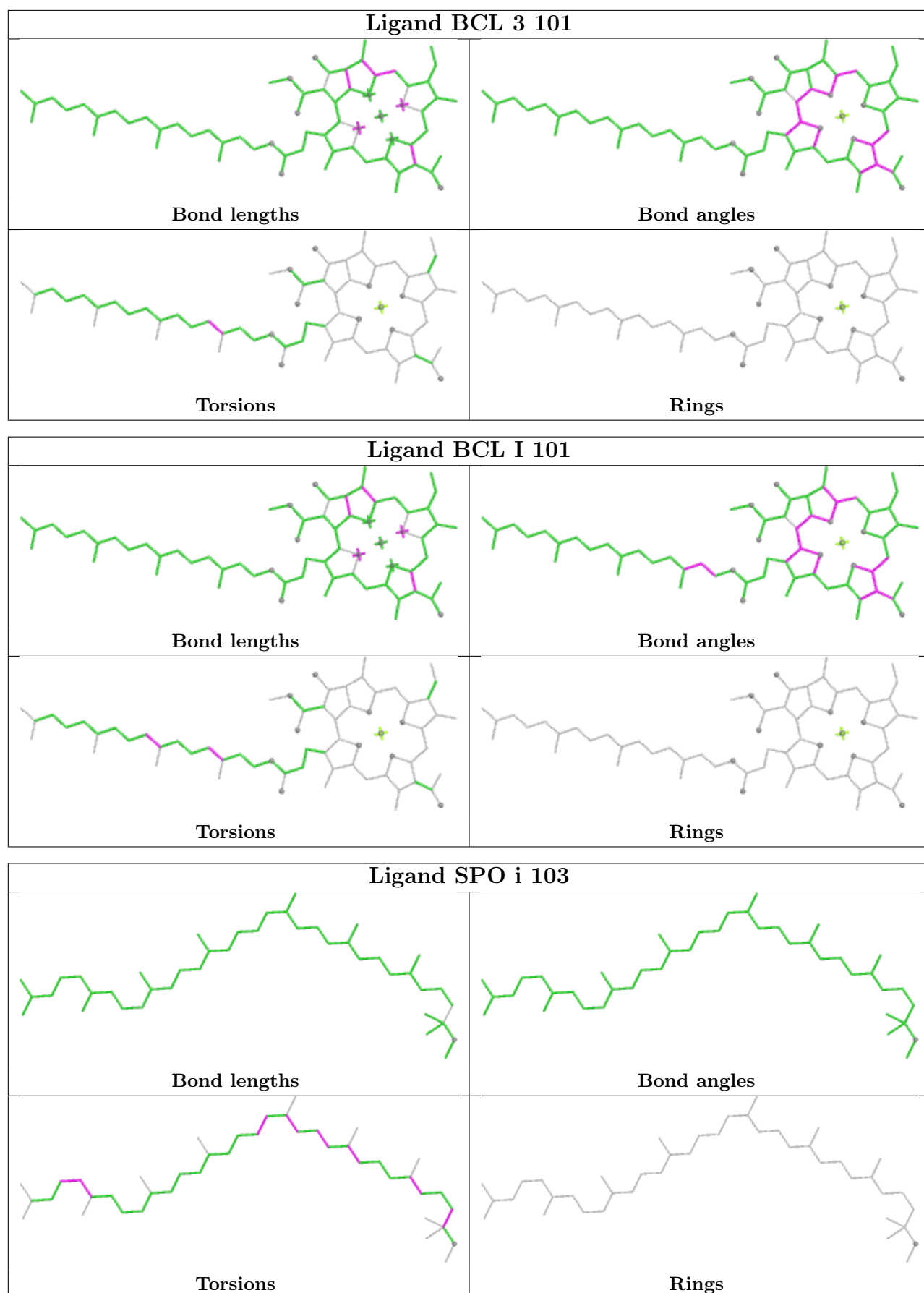


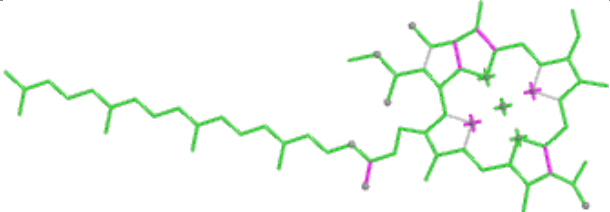
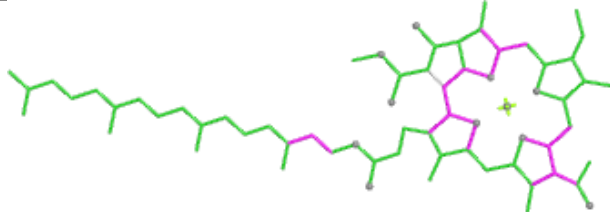
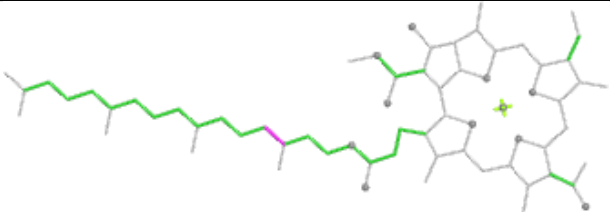
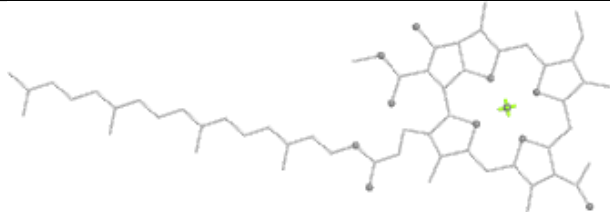
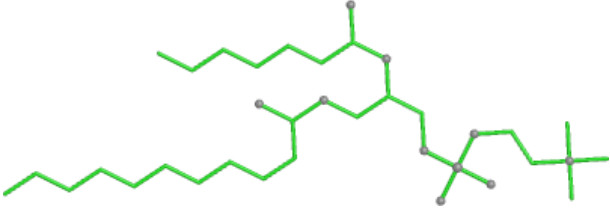
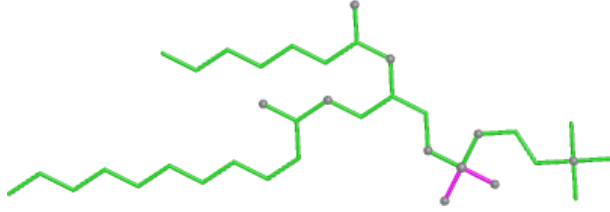
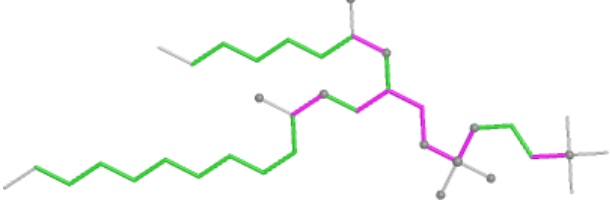
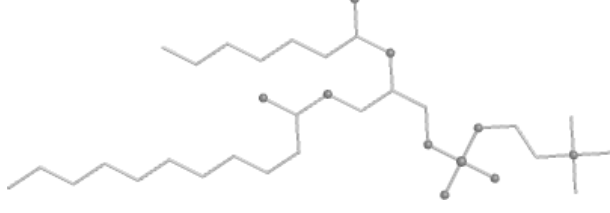
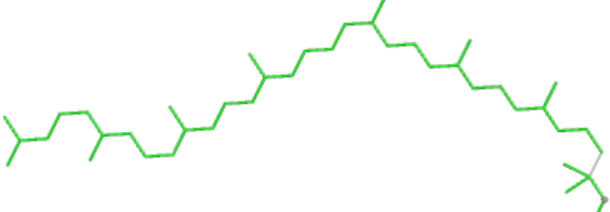
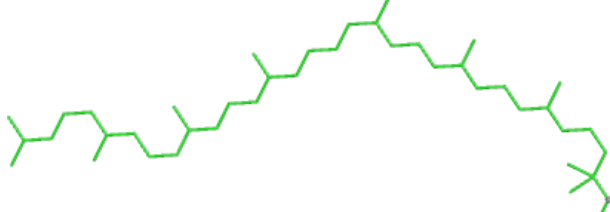
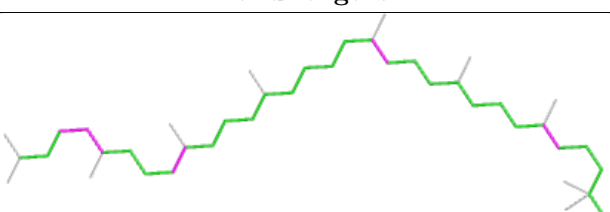
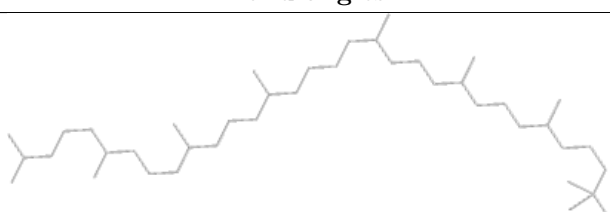


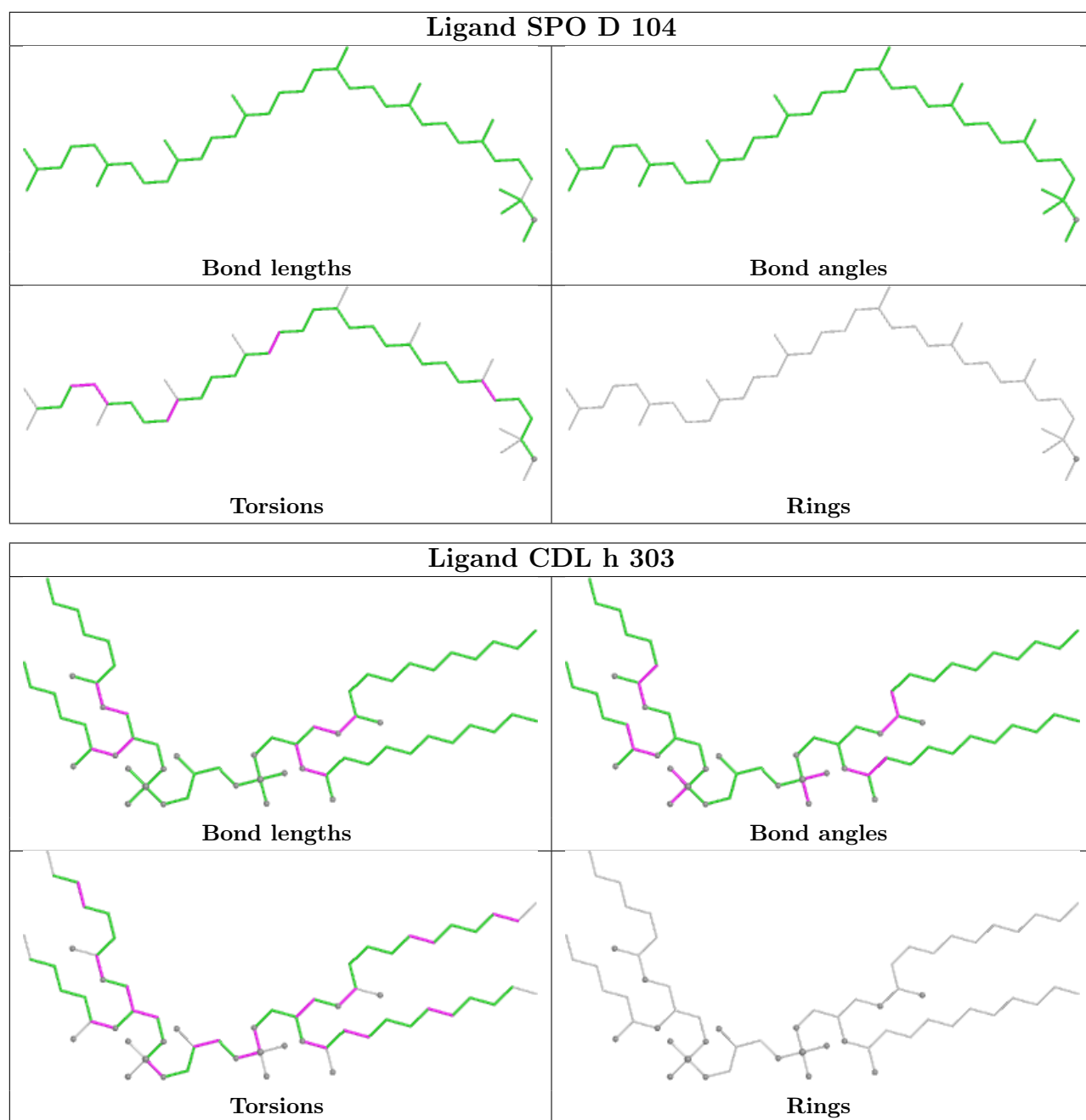


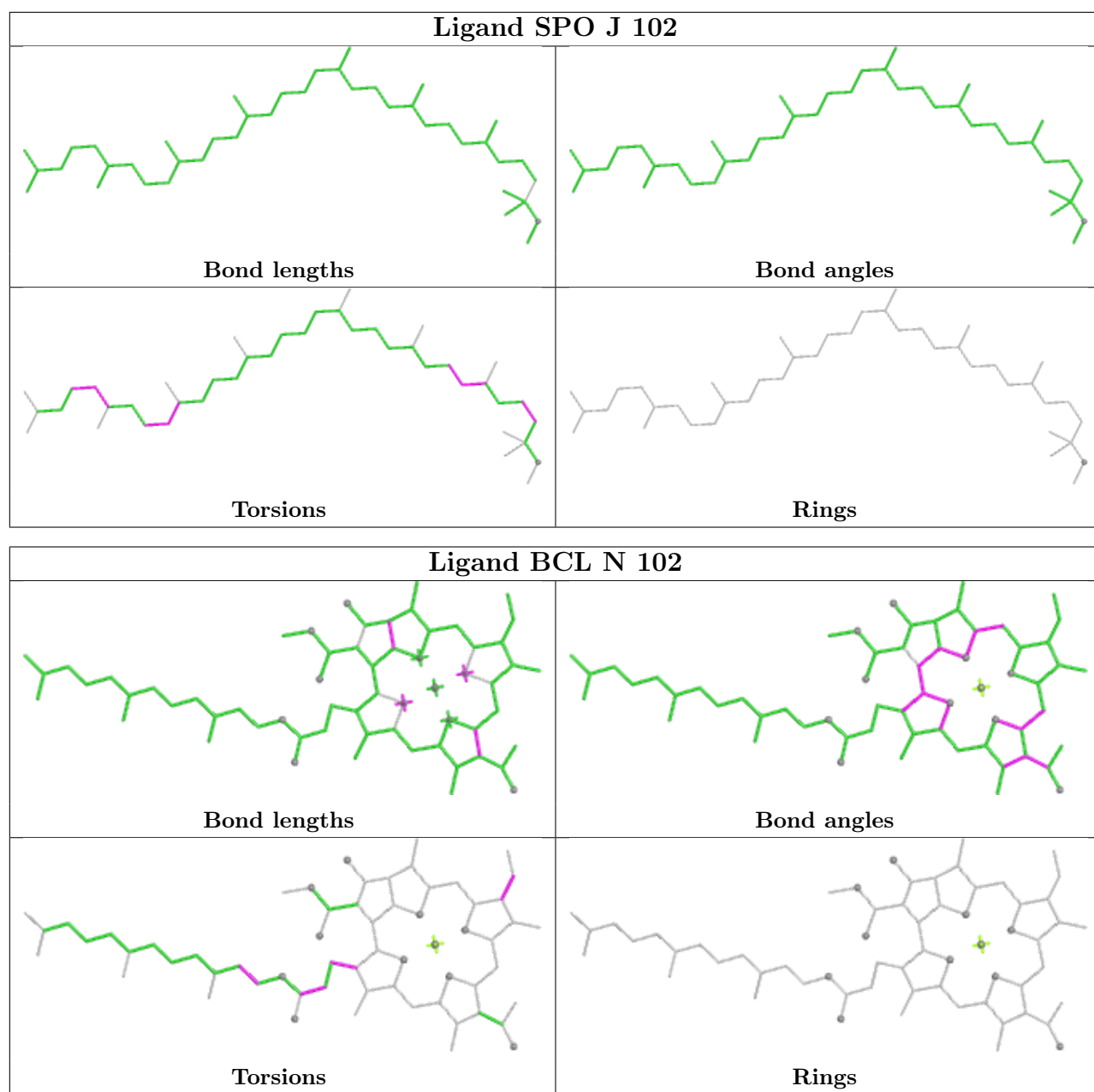


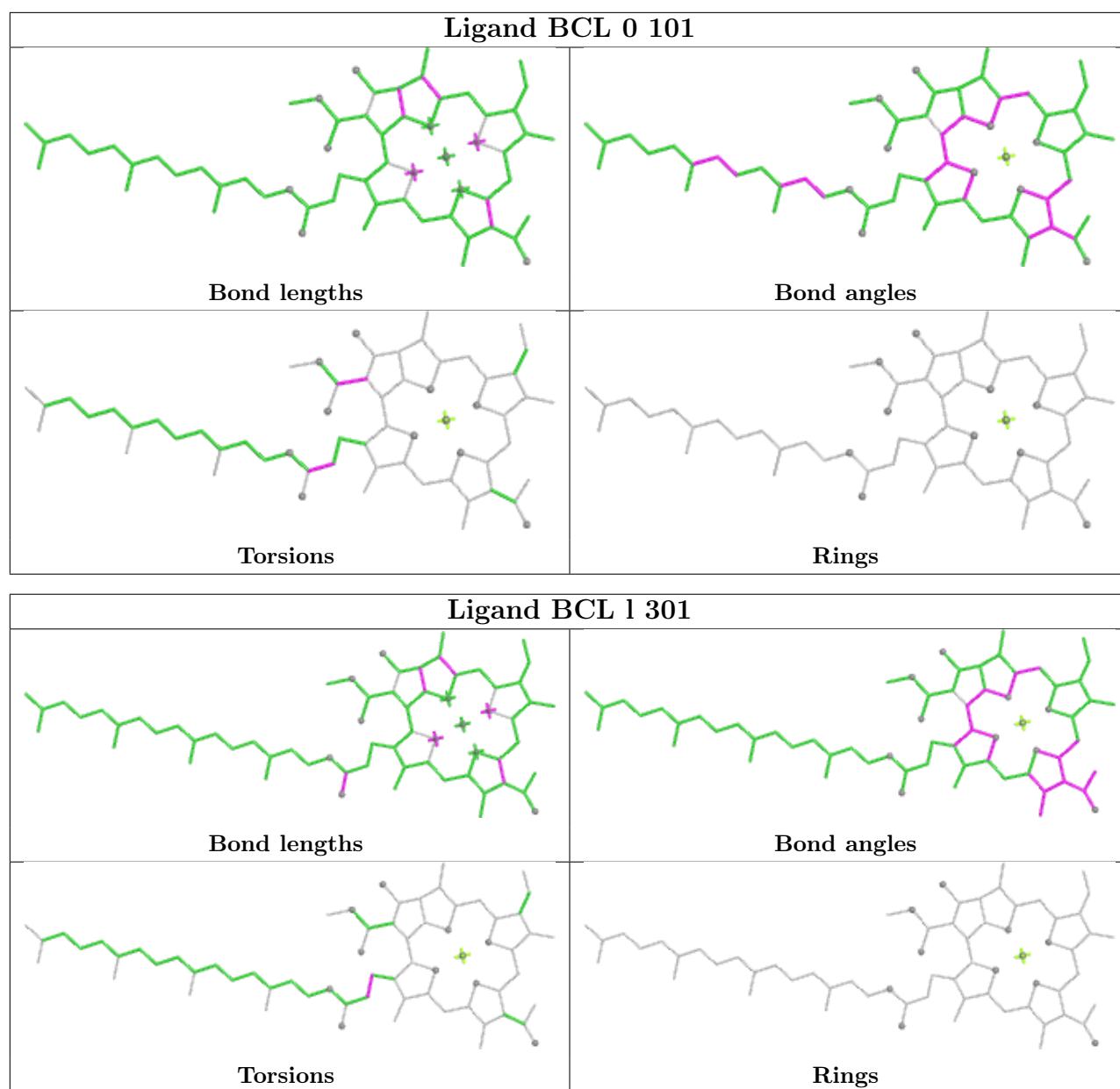


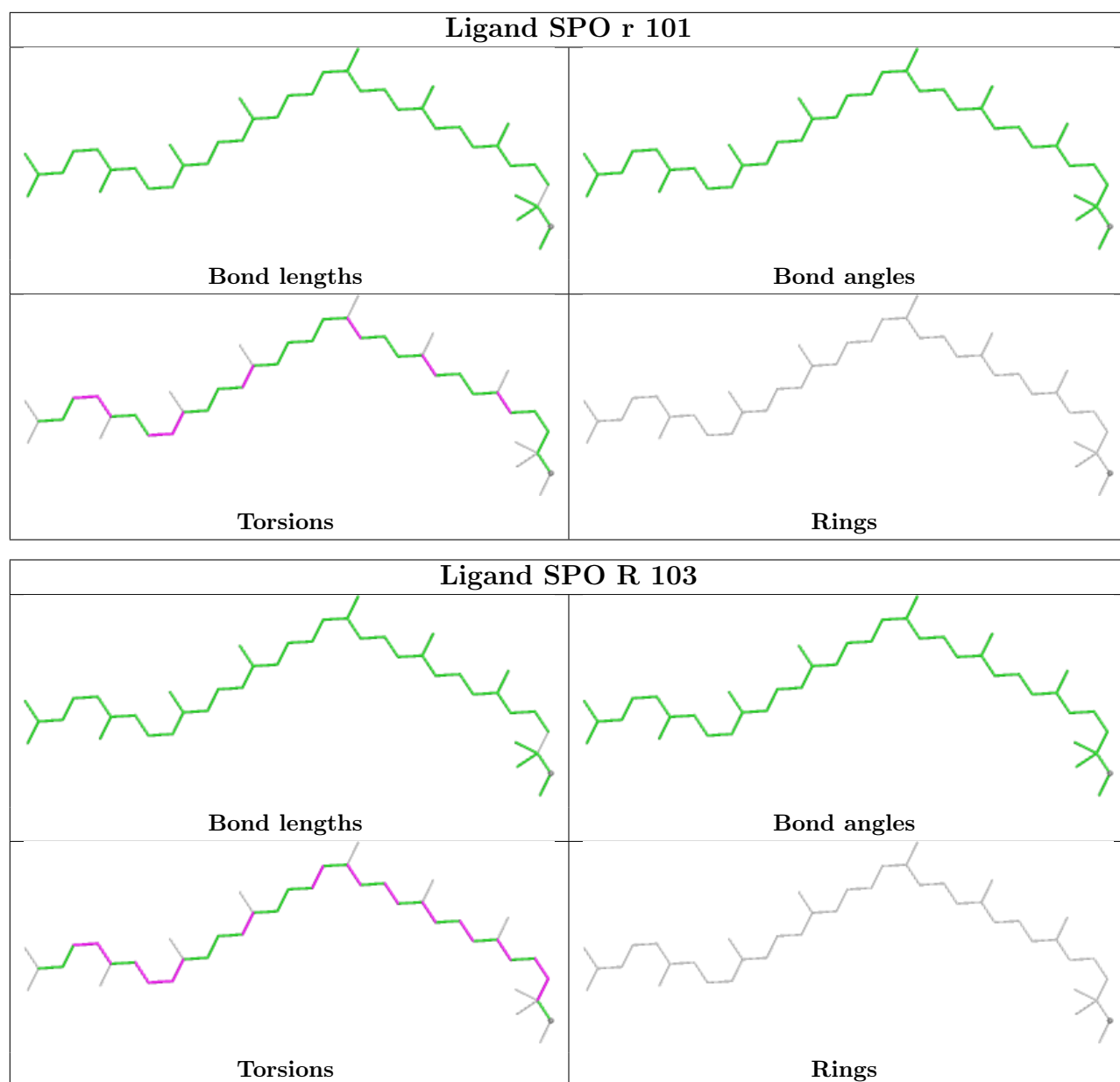


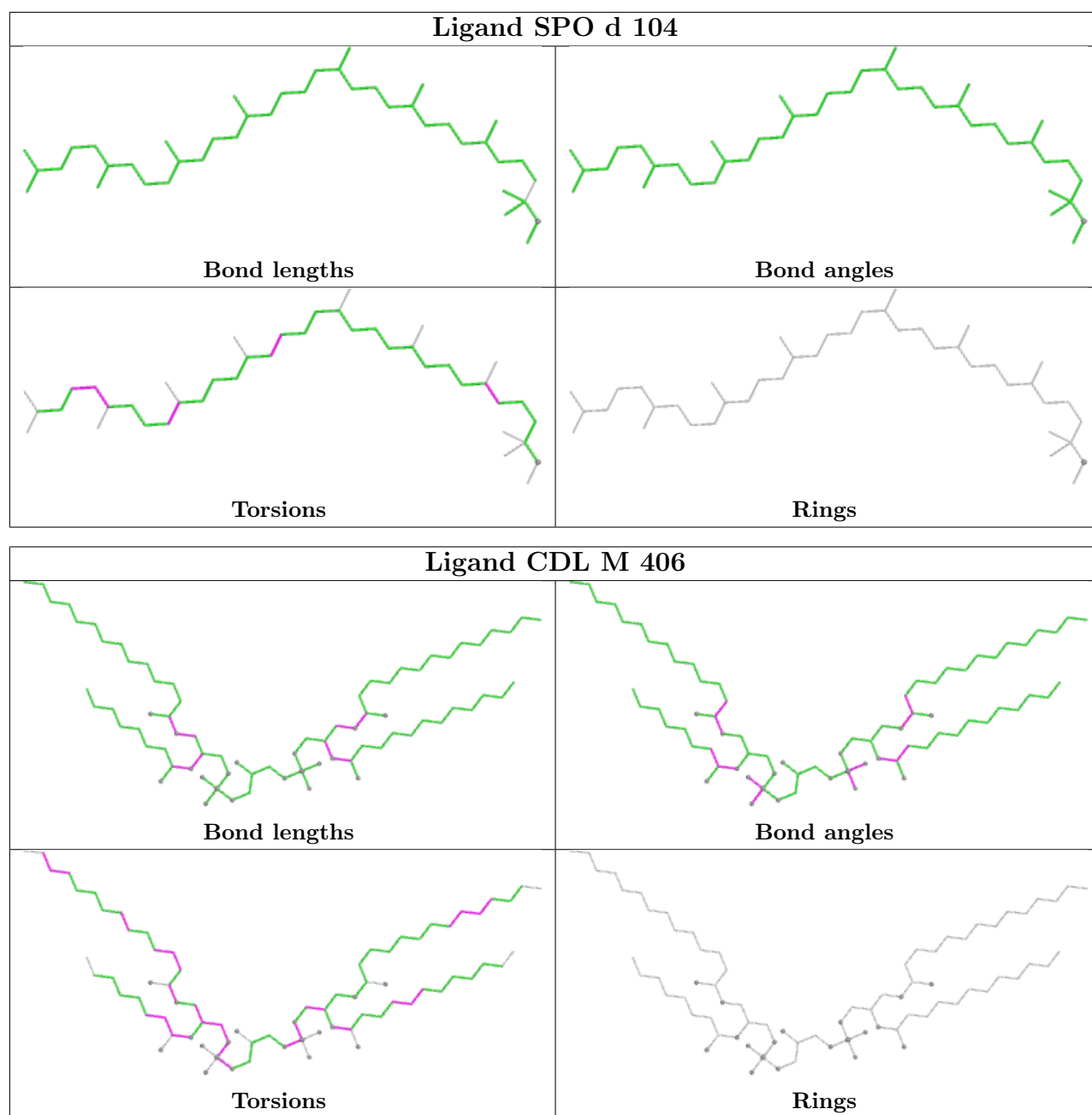
Ligand BCL K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 a 105	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO O 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

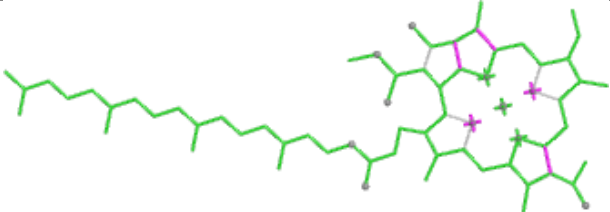
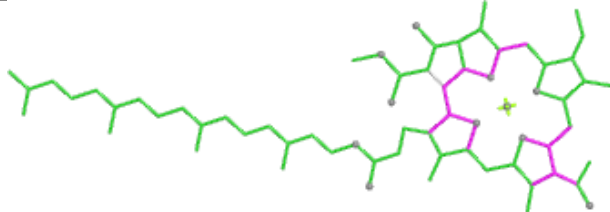
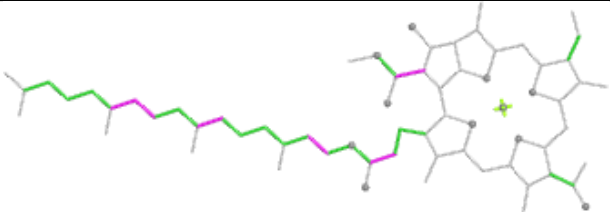
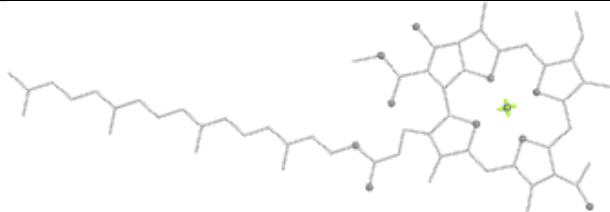
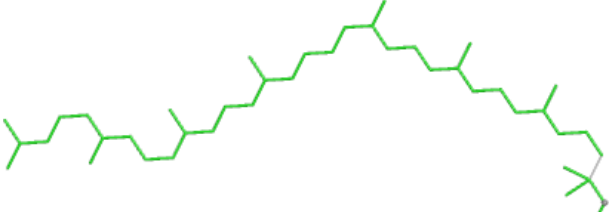
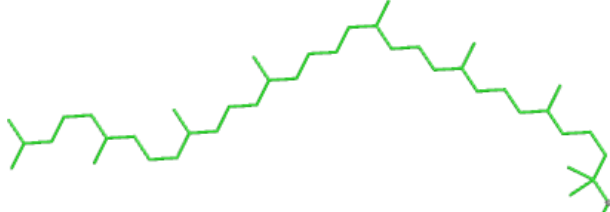
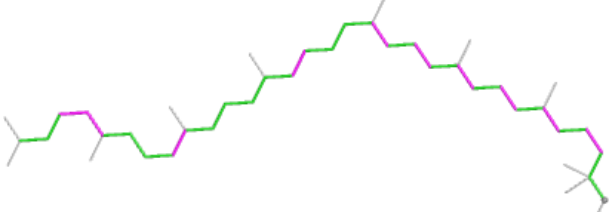
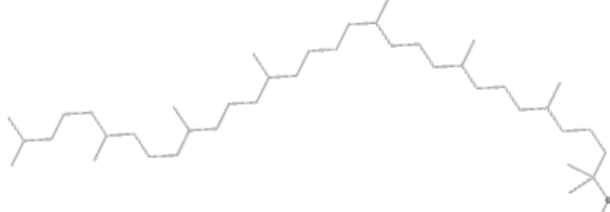


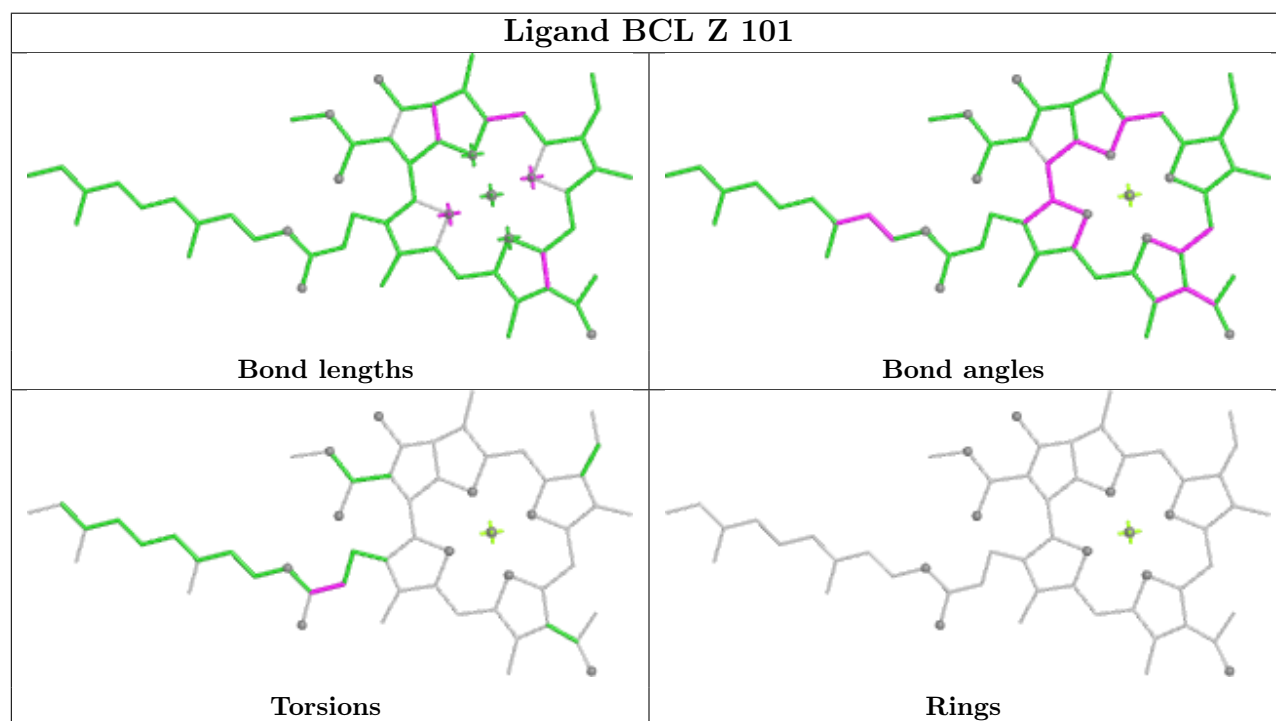
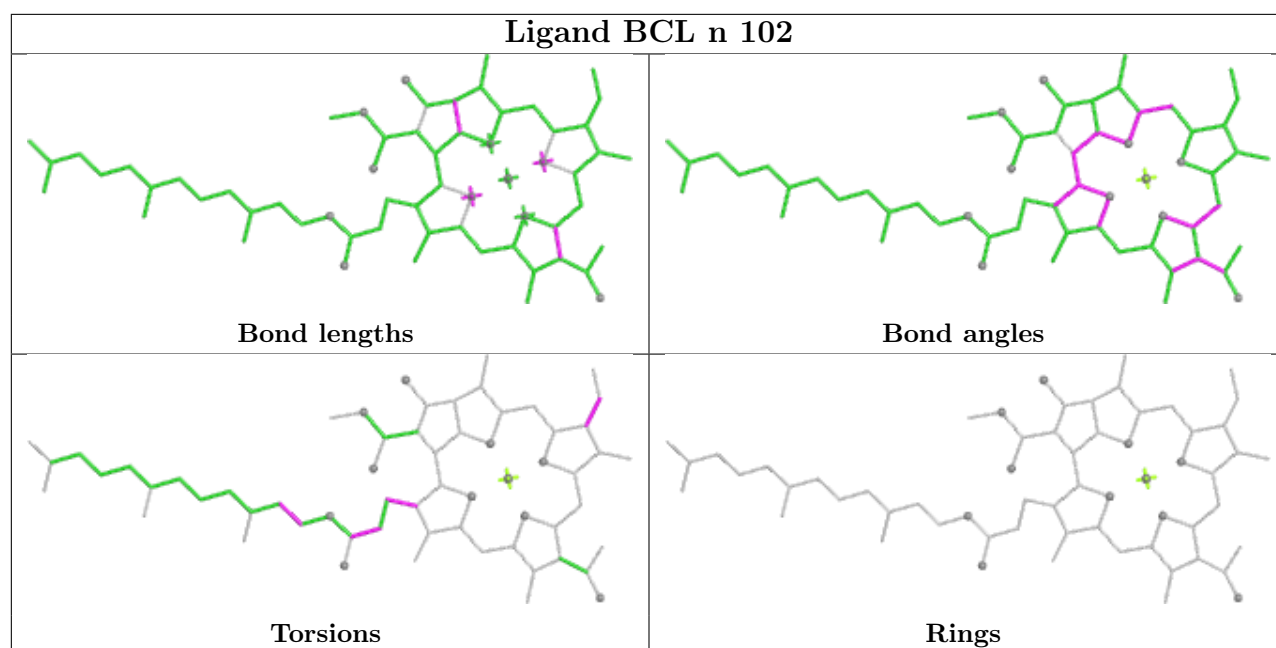


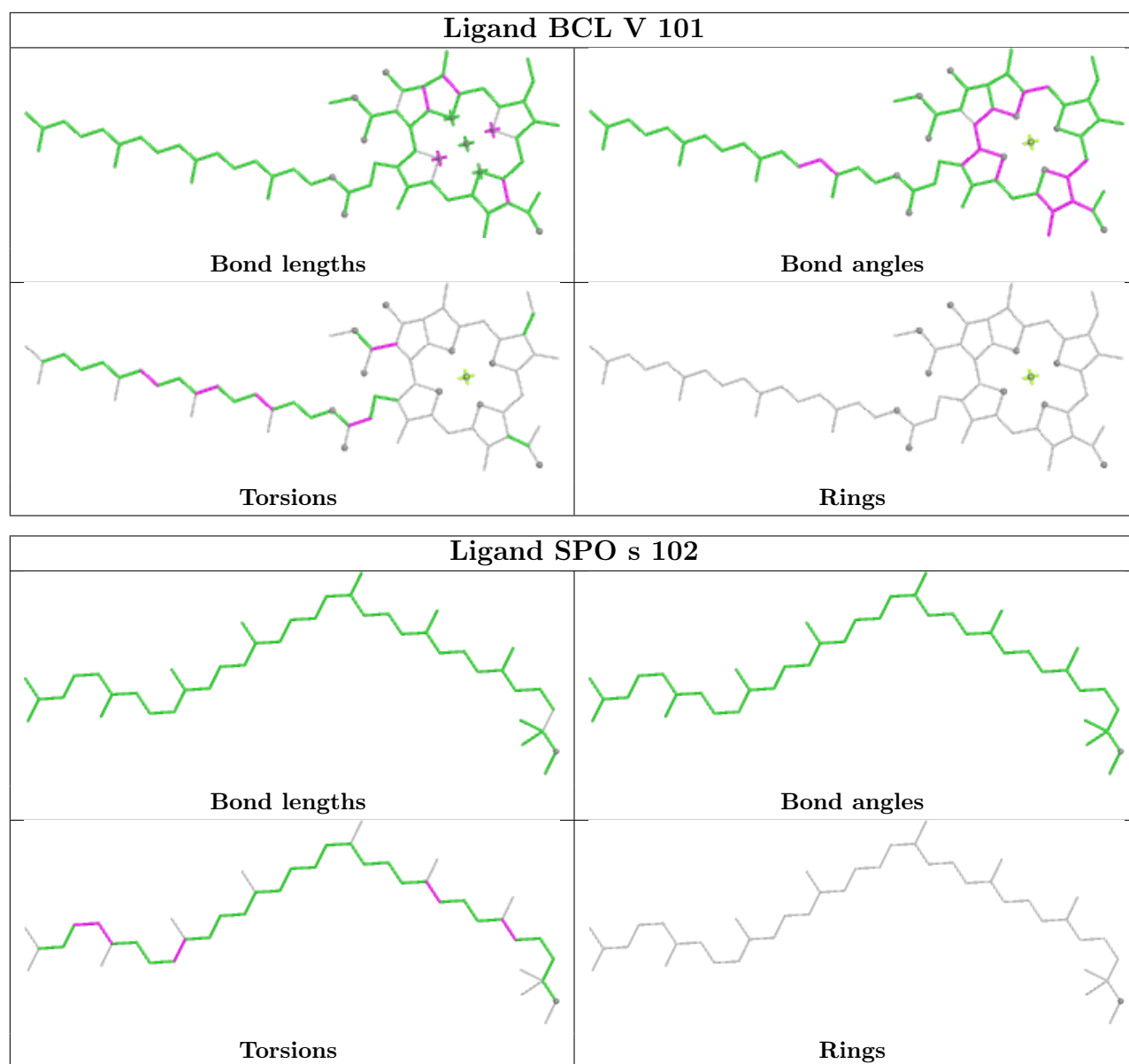


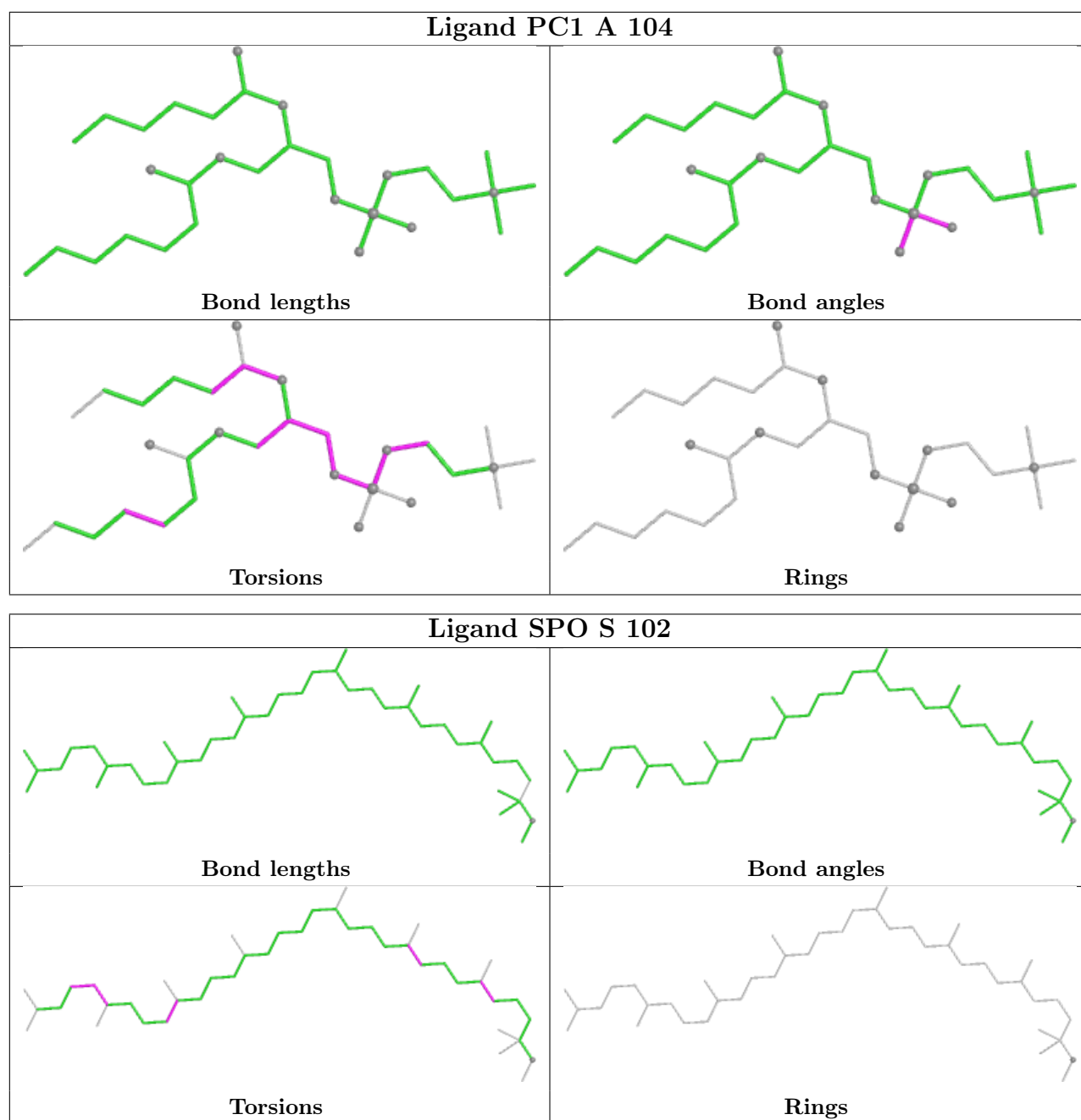


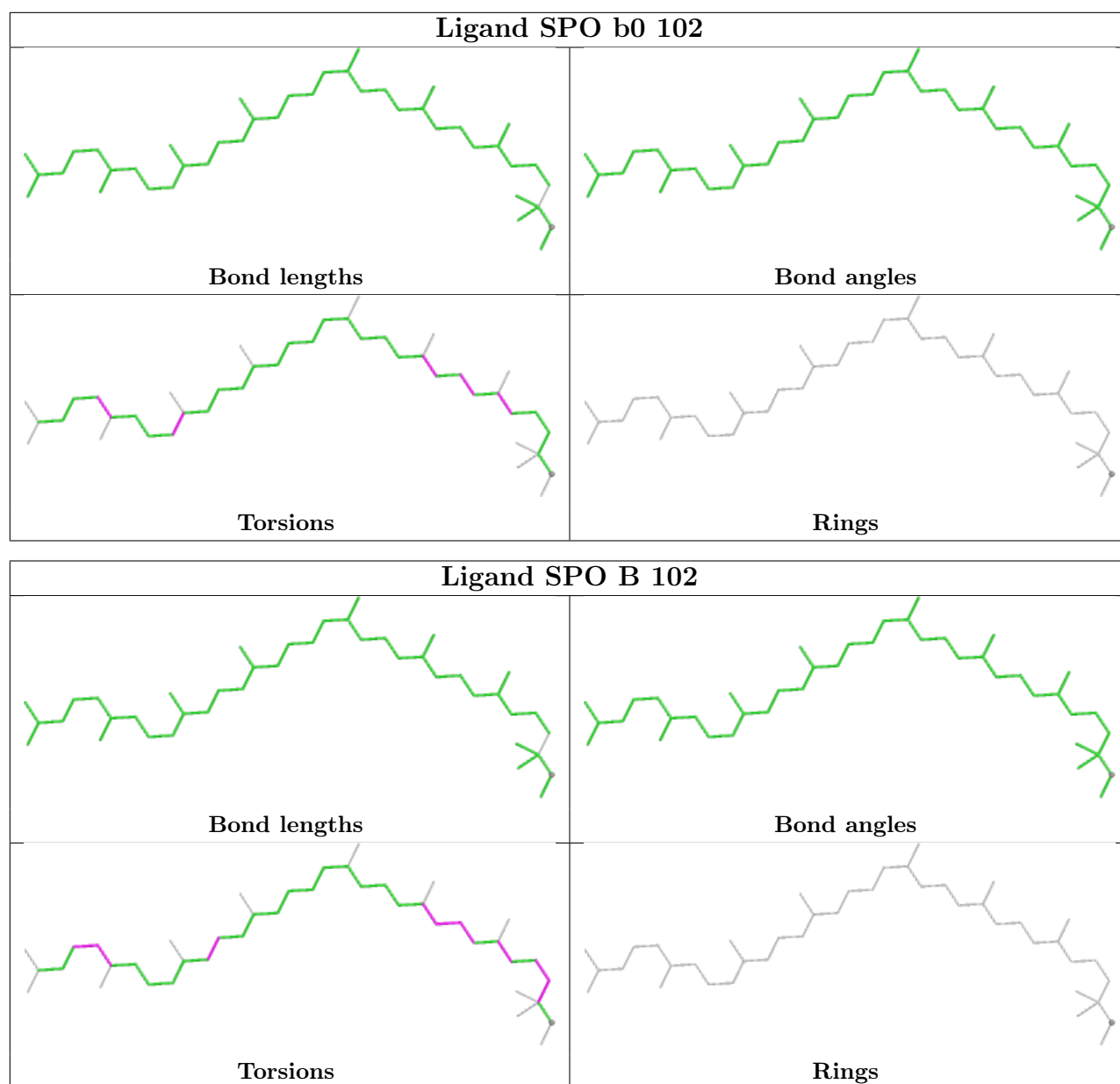


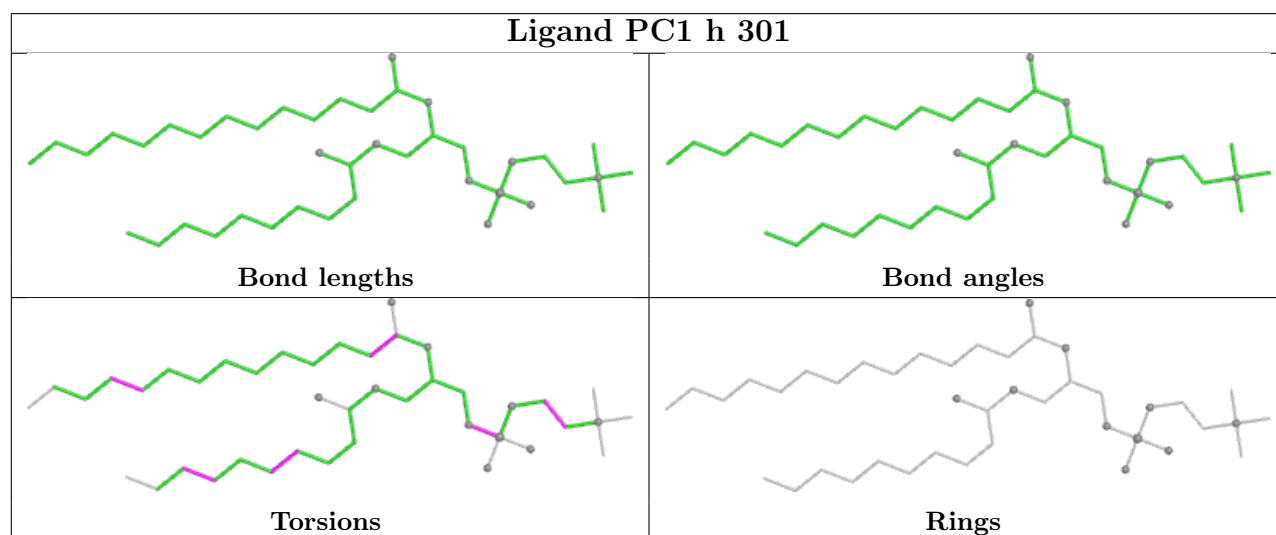
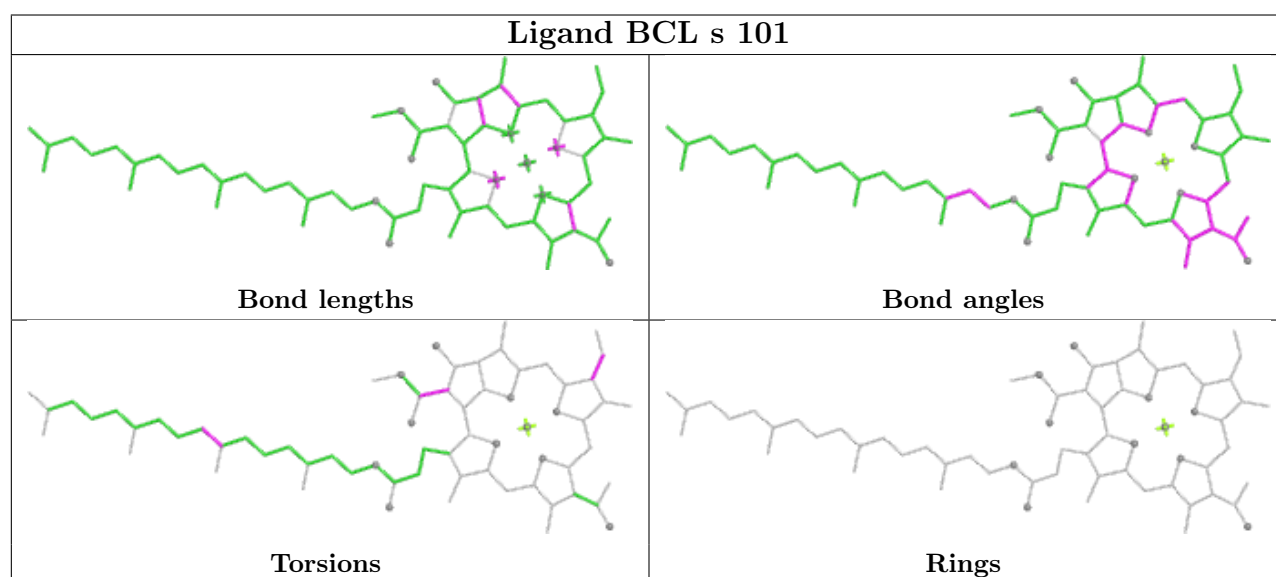
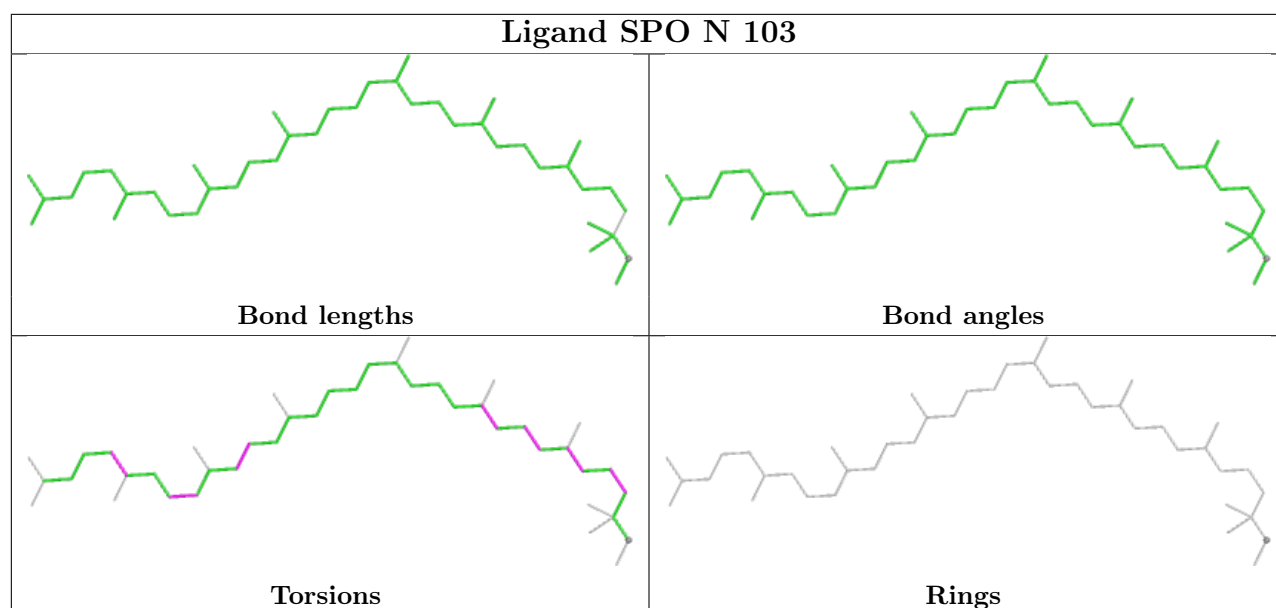
Ligand BCL G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO b9 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

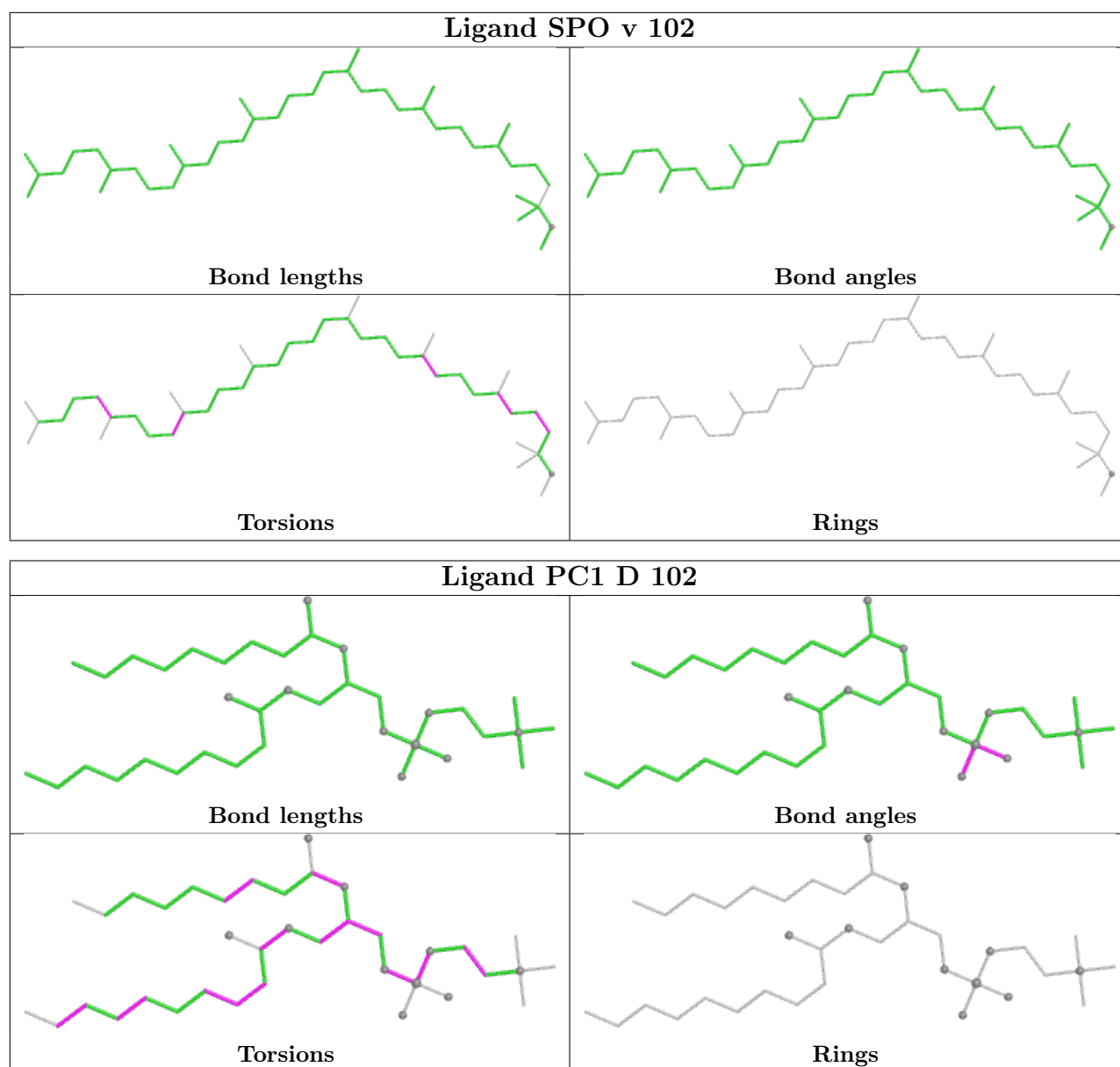


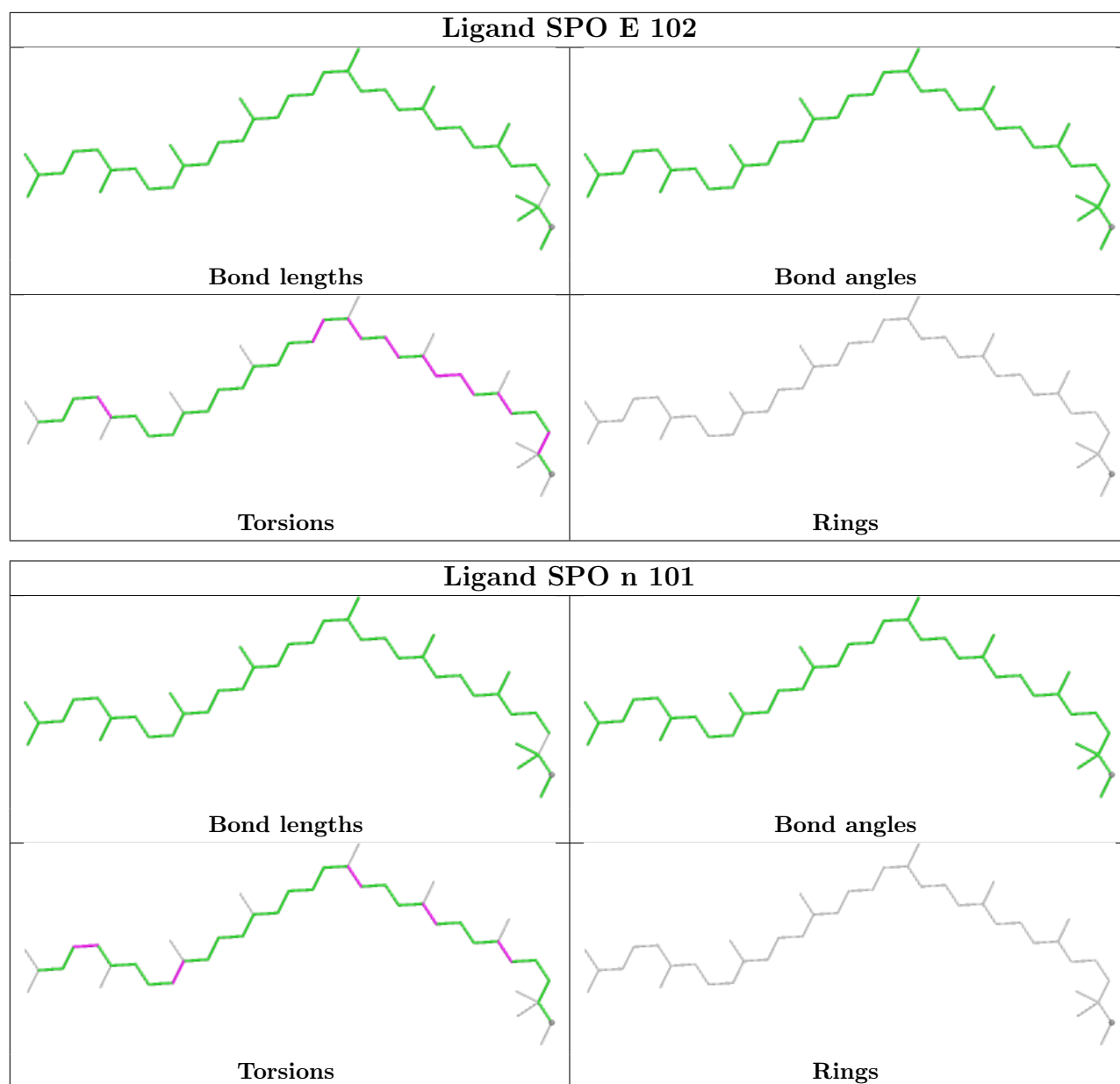


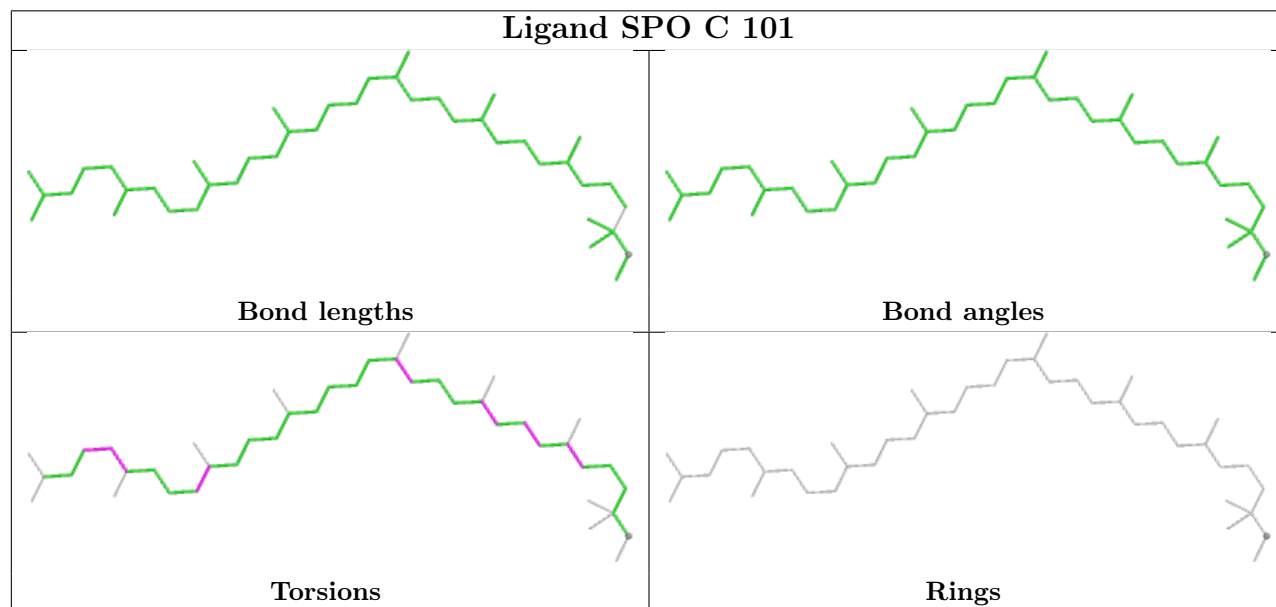
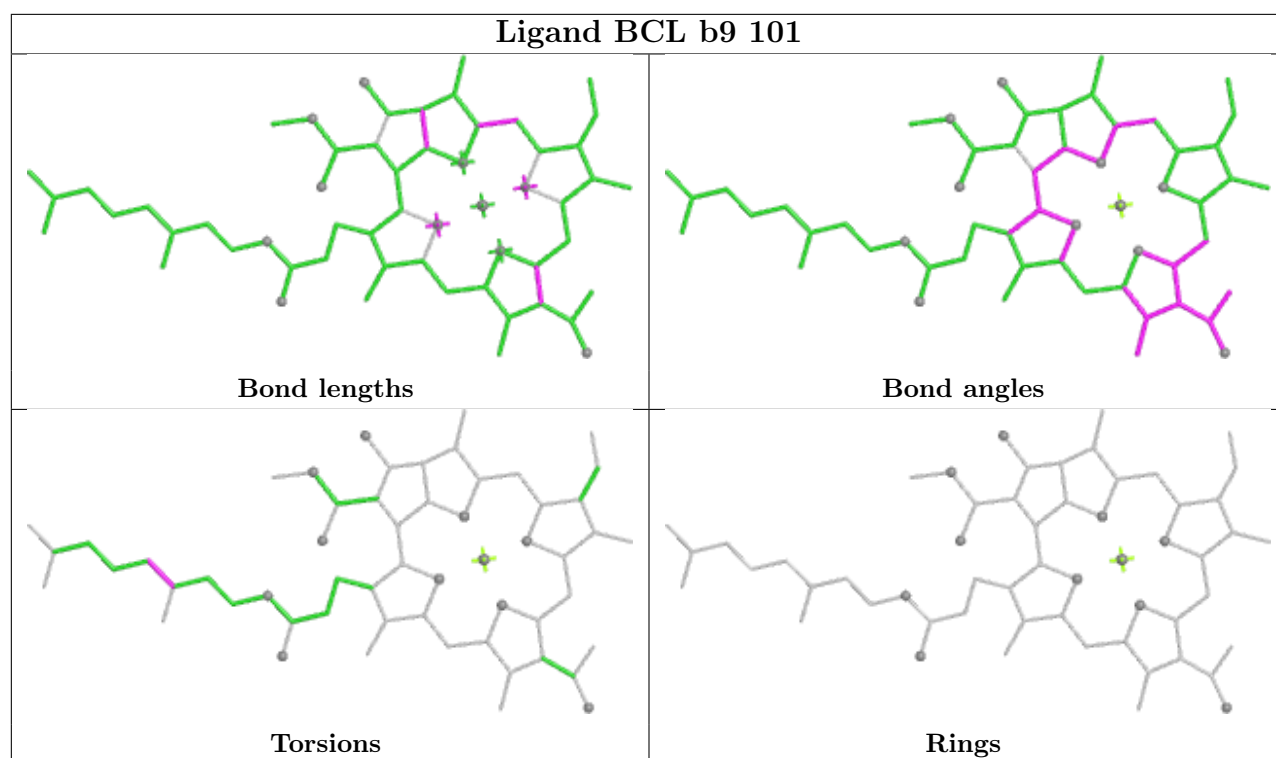


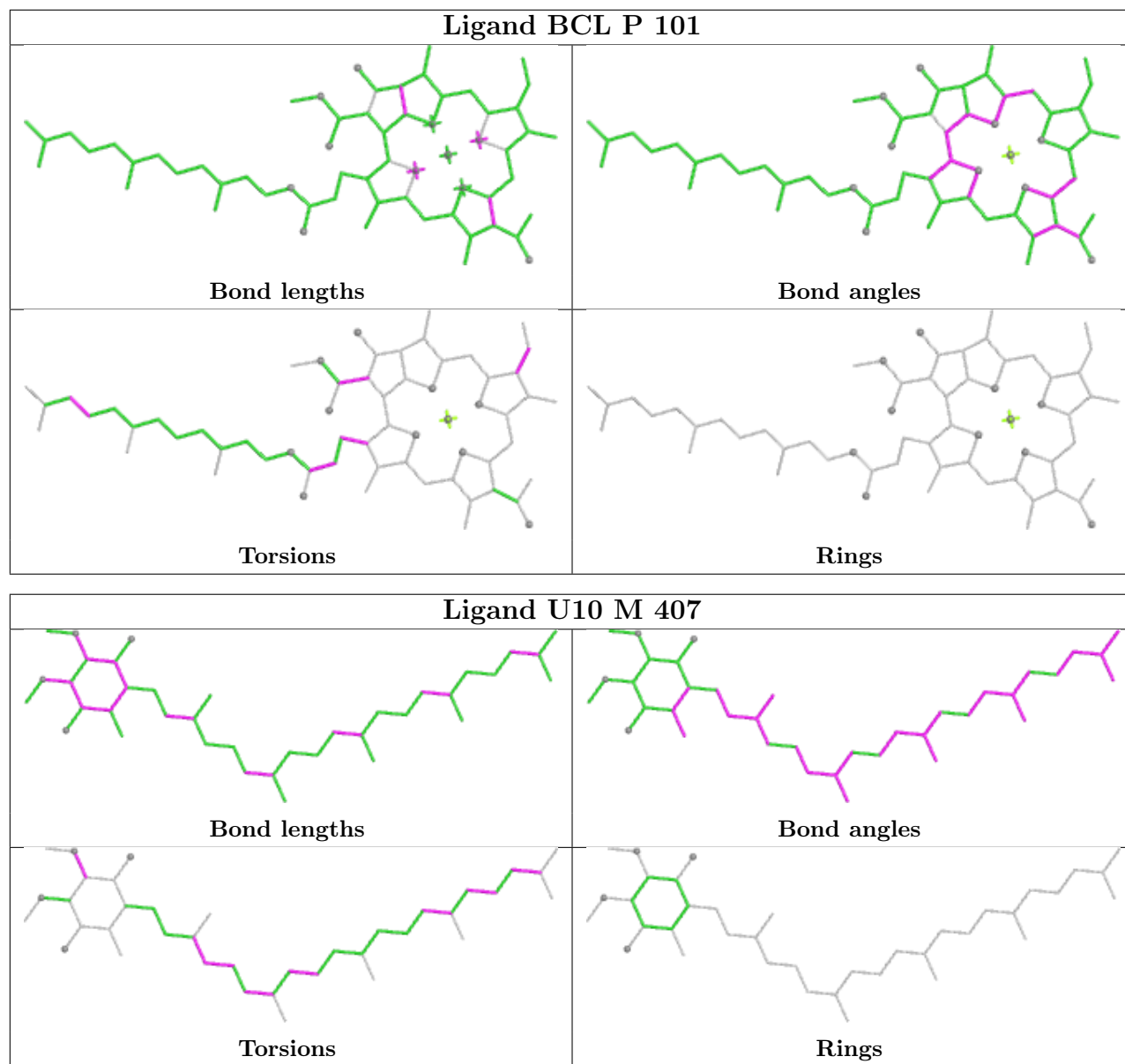


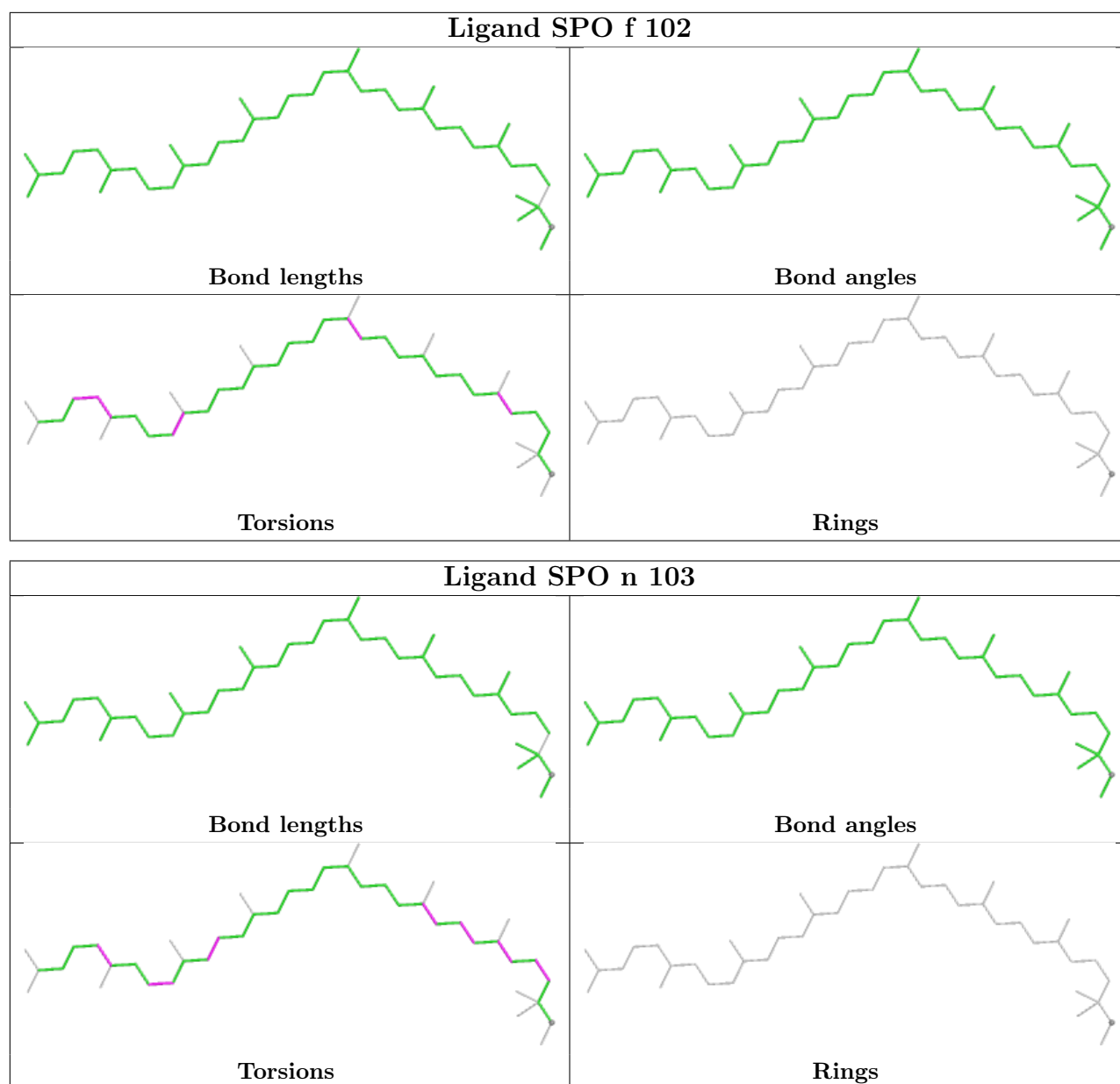


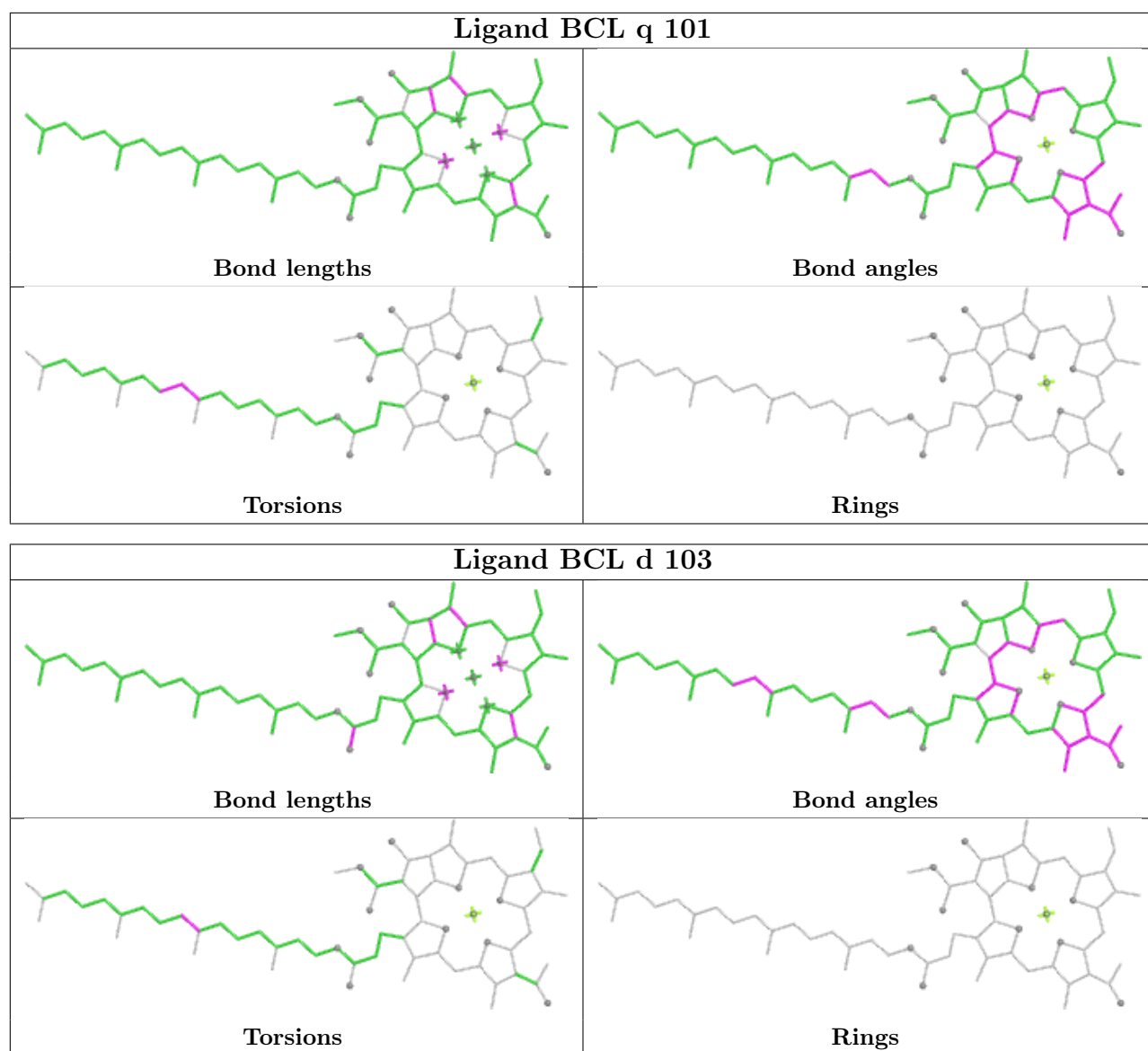


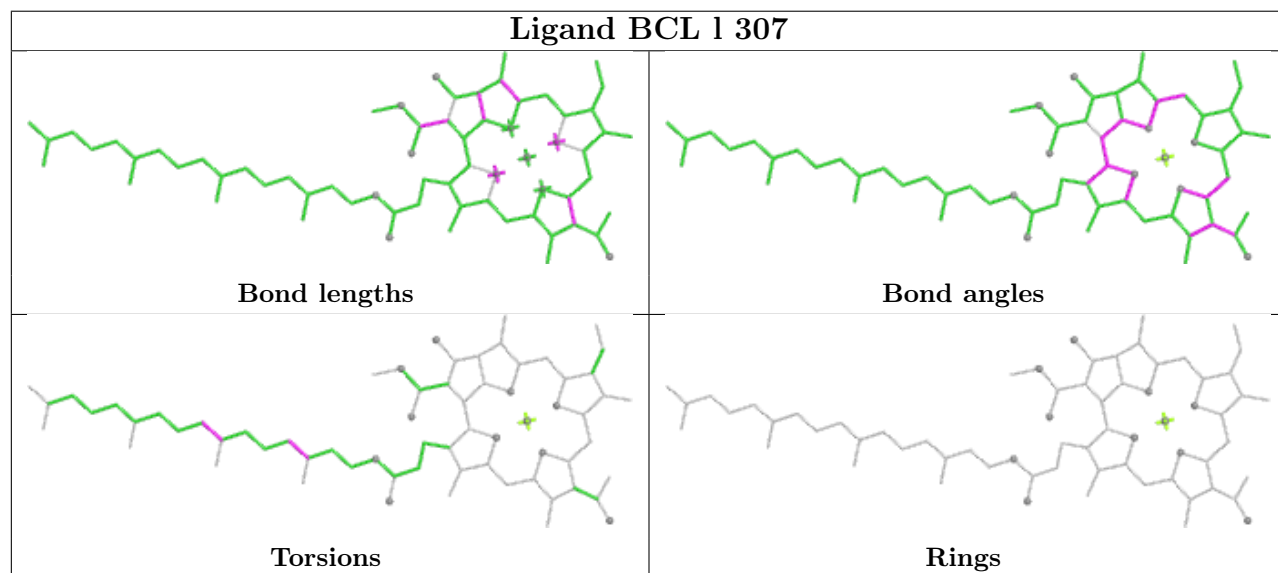
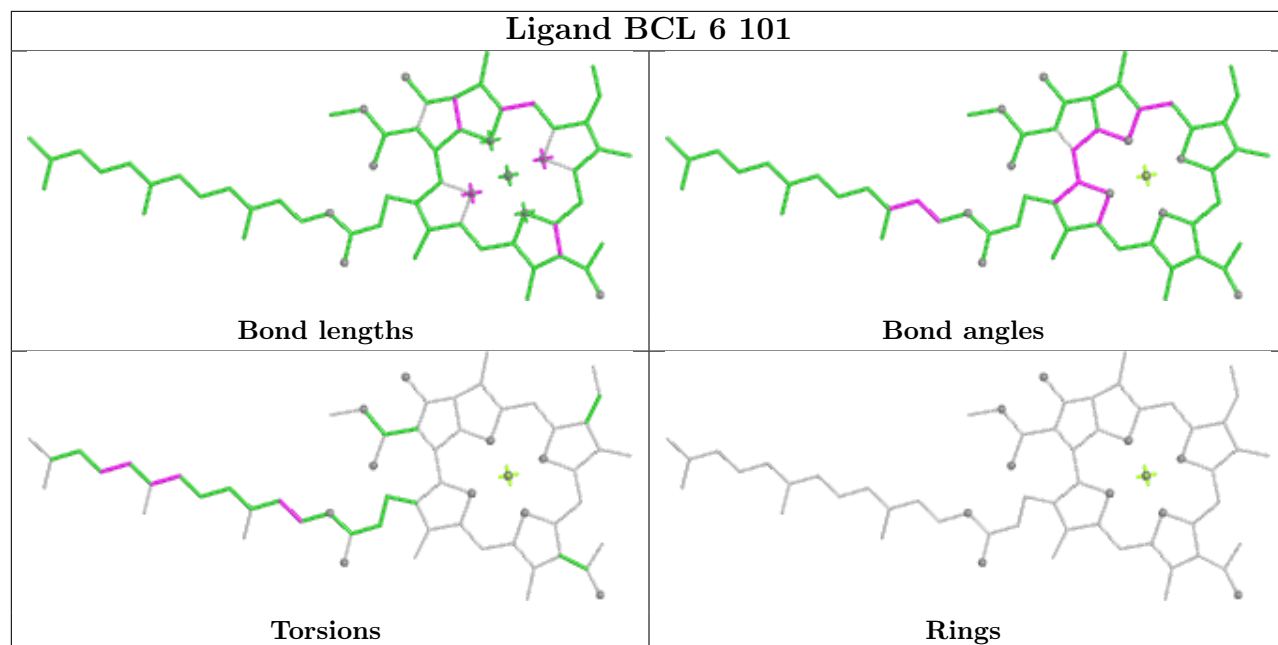


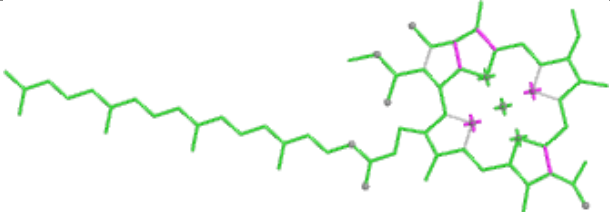
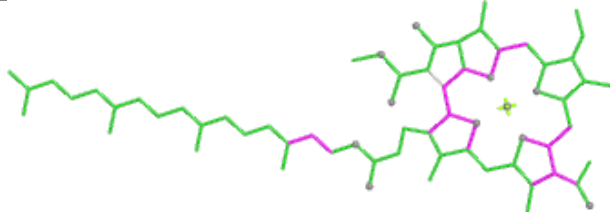
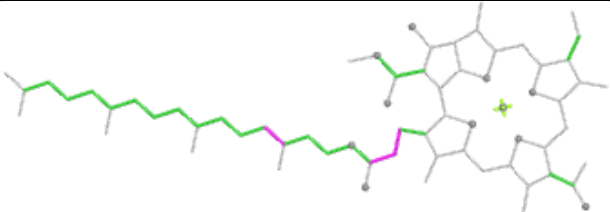
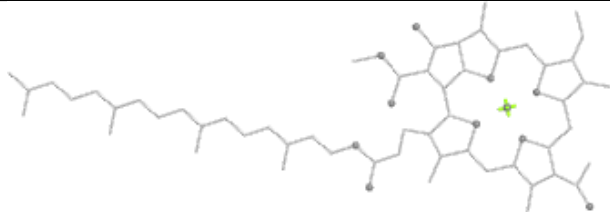
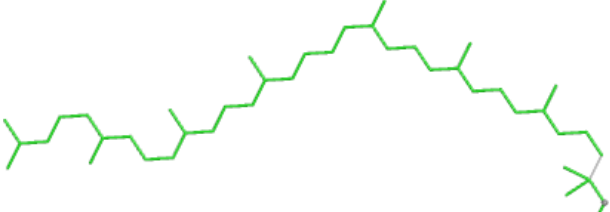
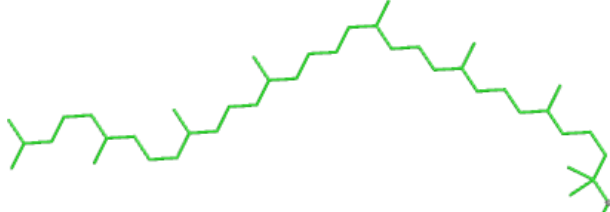
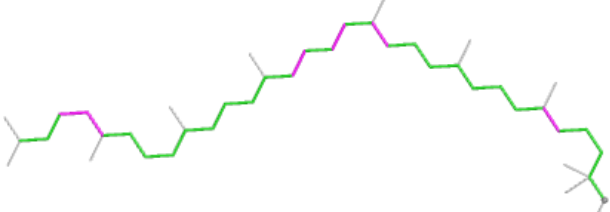
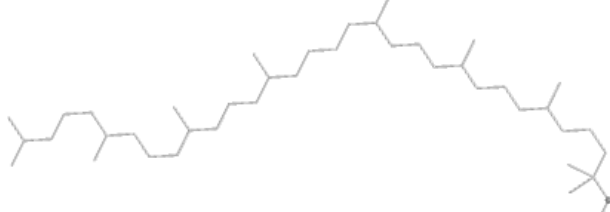


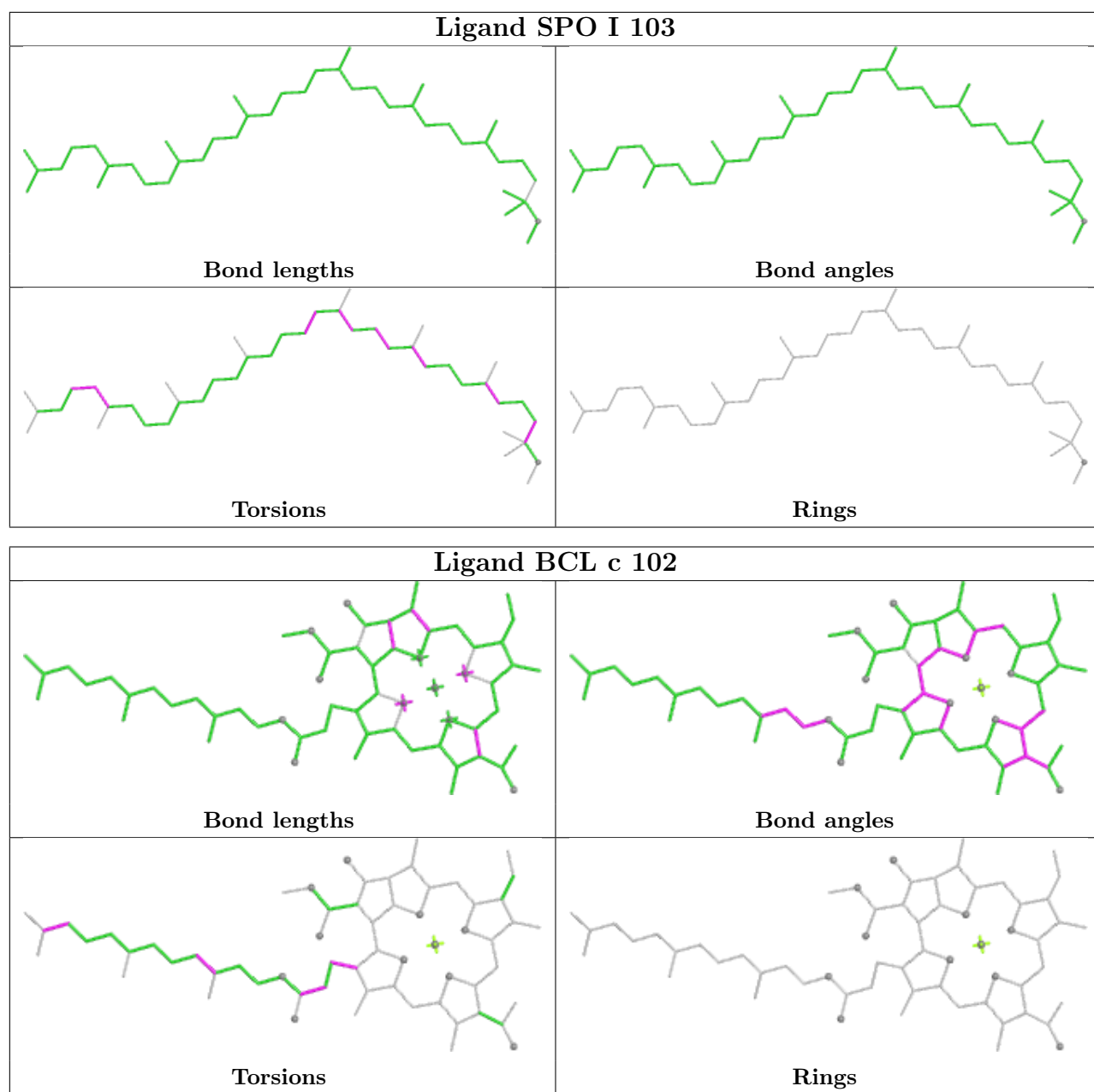


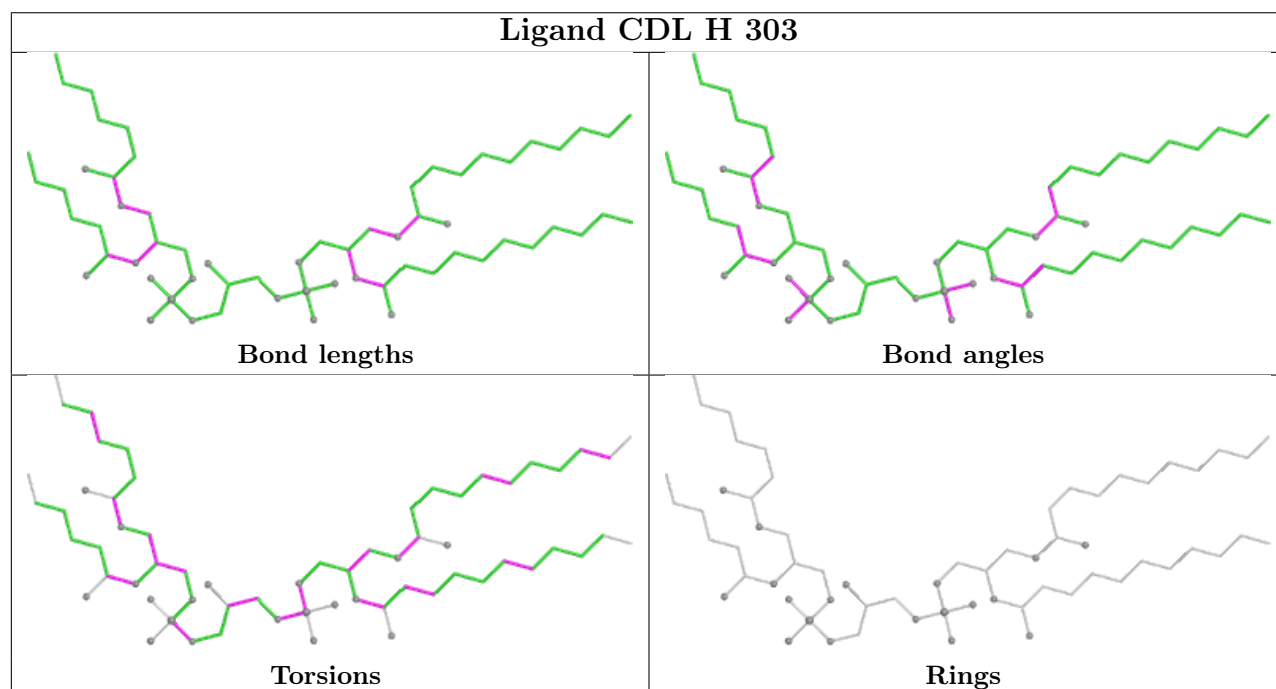
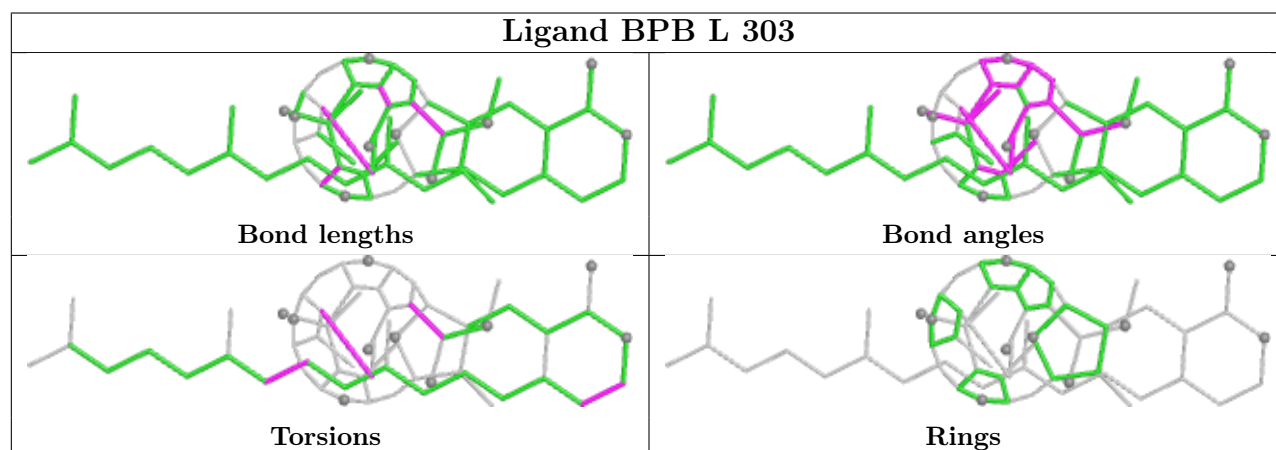
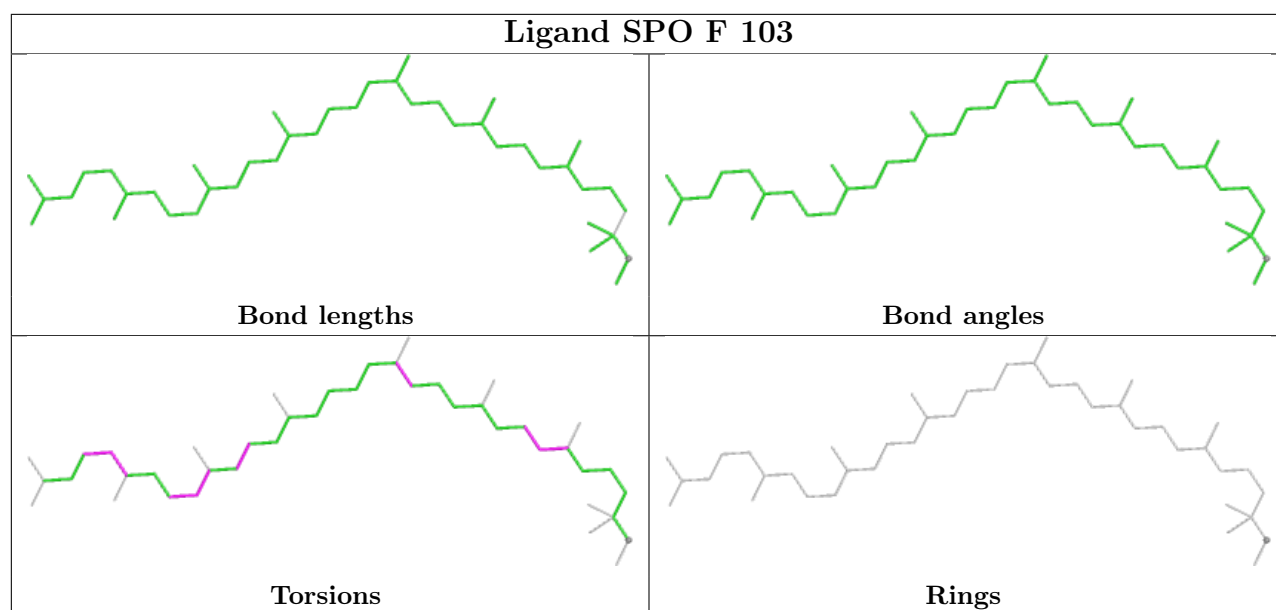


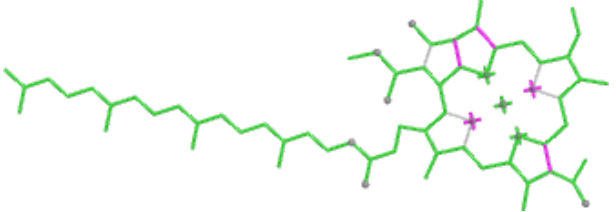
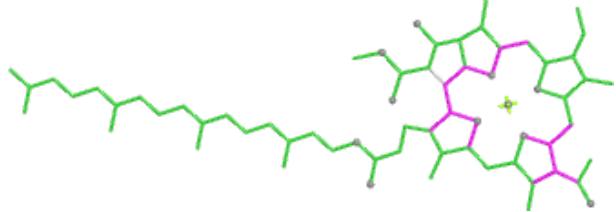
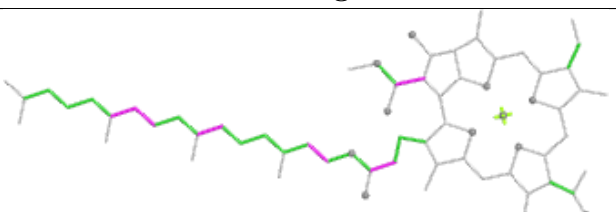
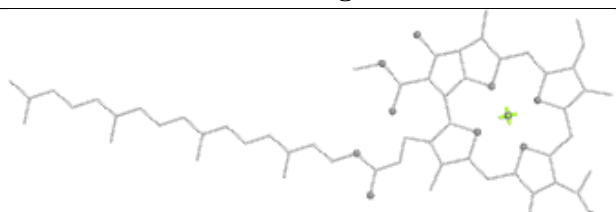
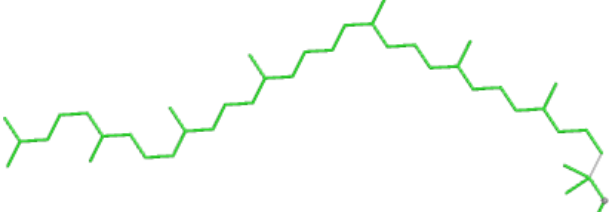
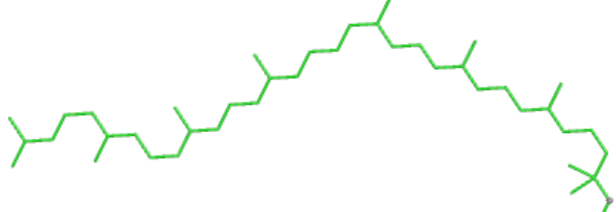
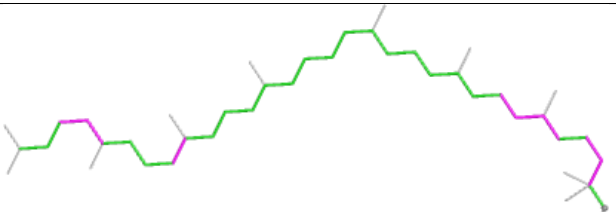
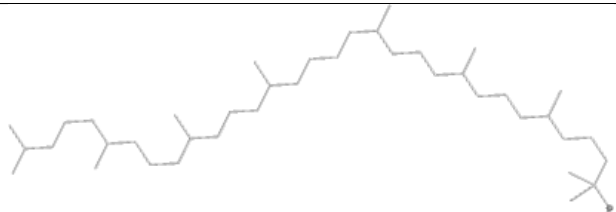


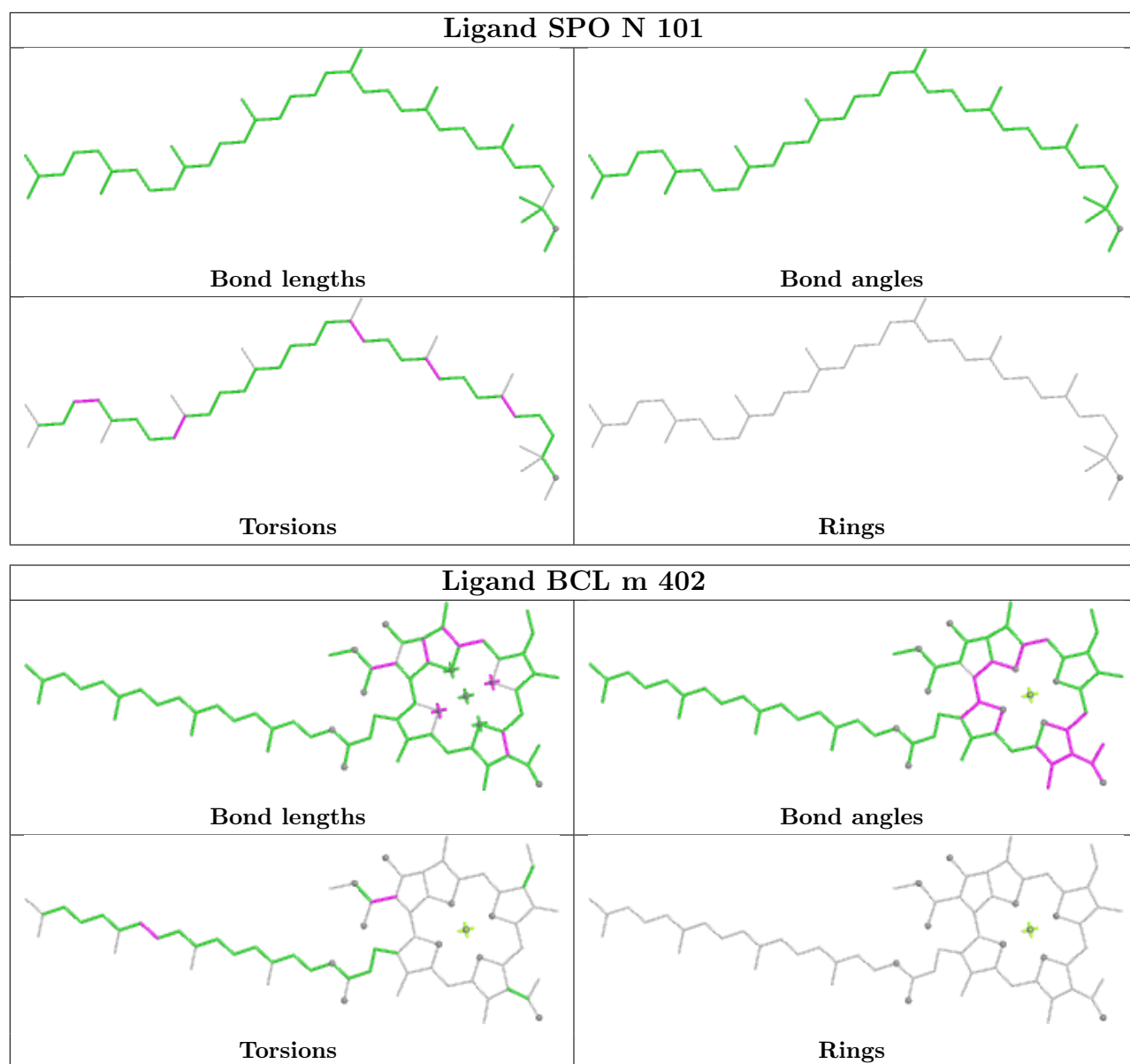


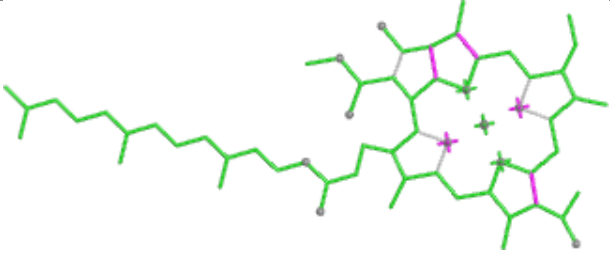
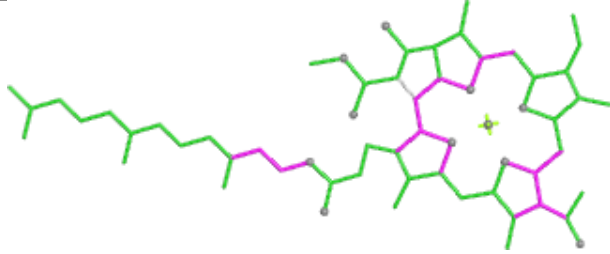
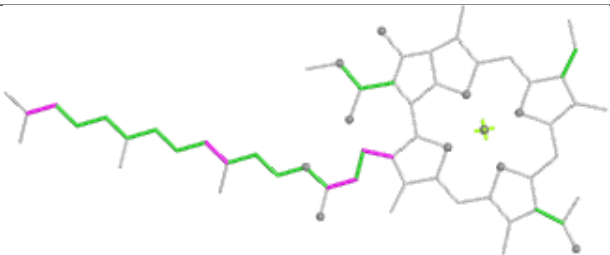
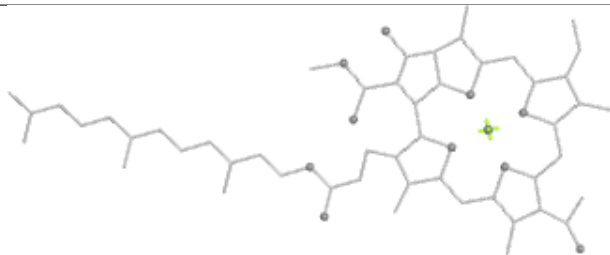
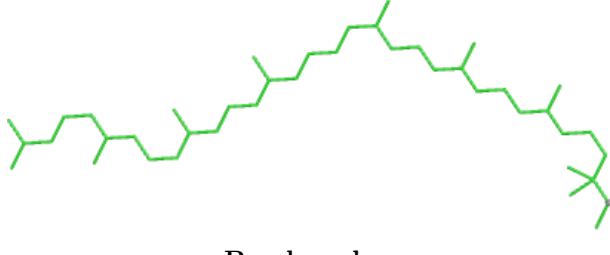
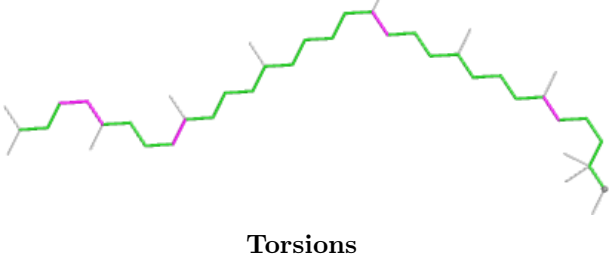
Ligand BCL t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO a 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

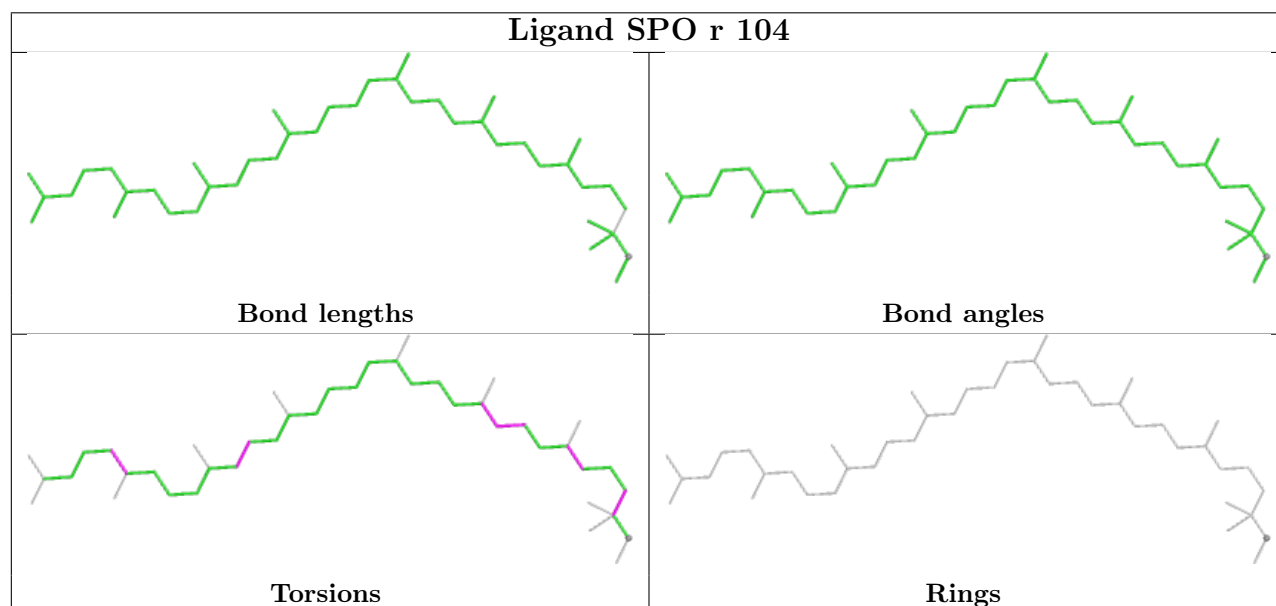
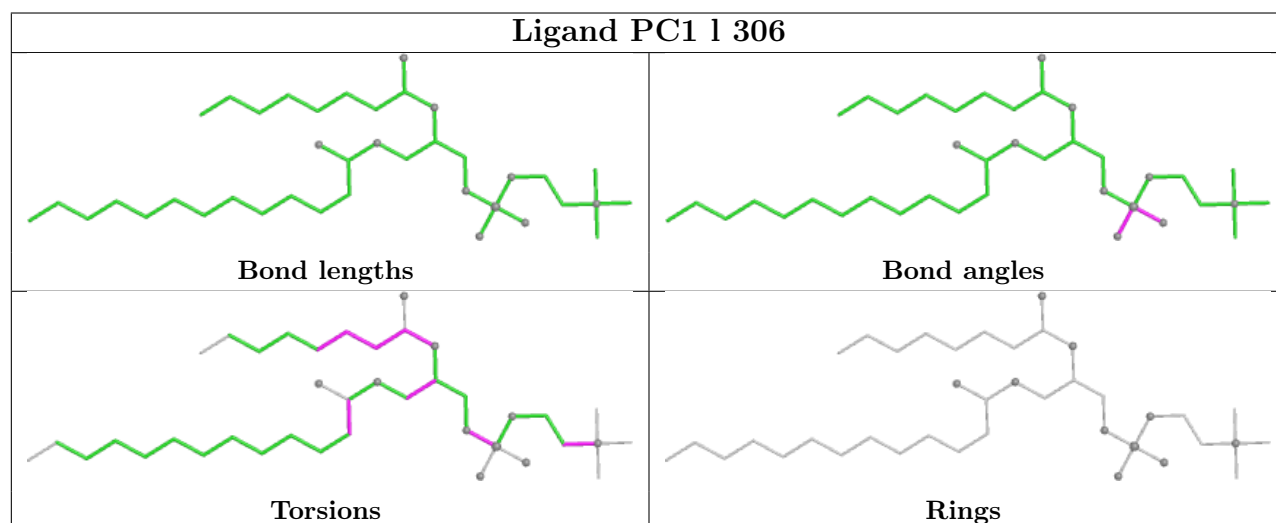
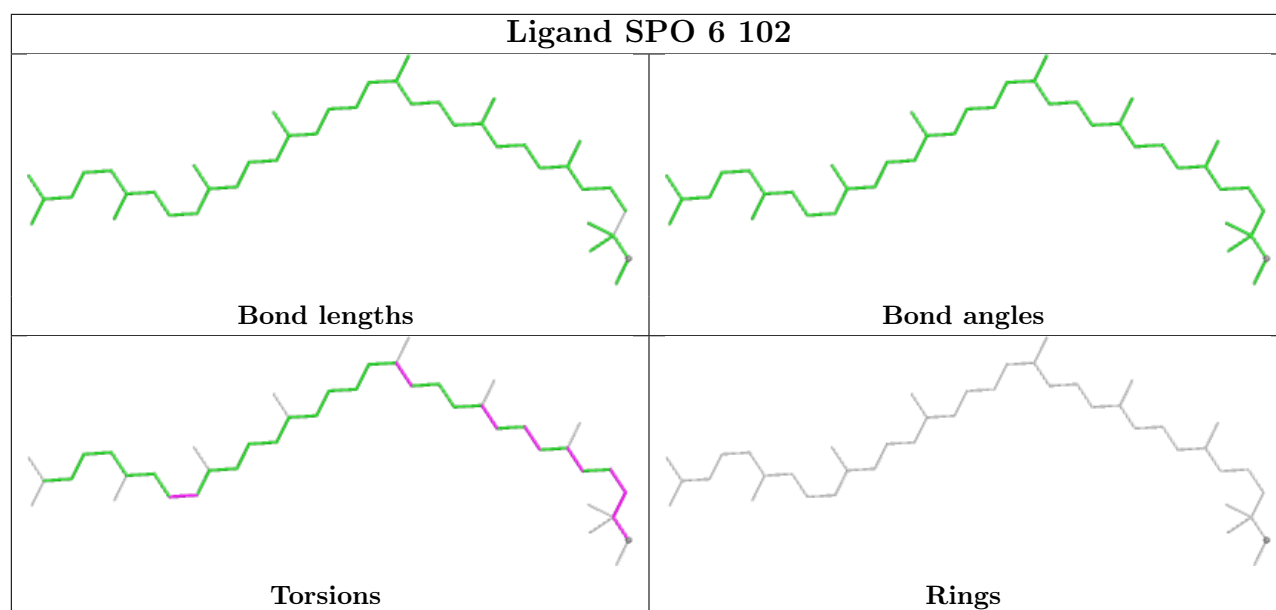


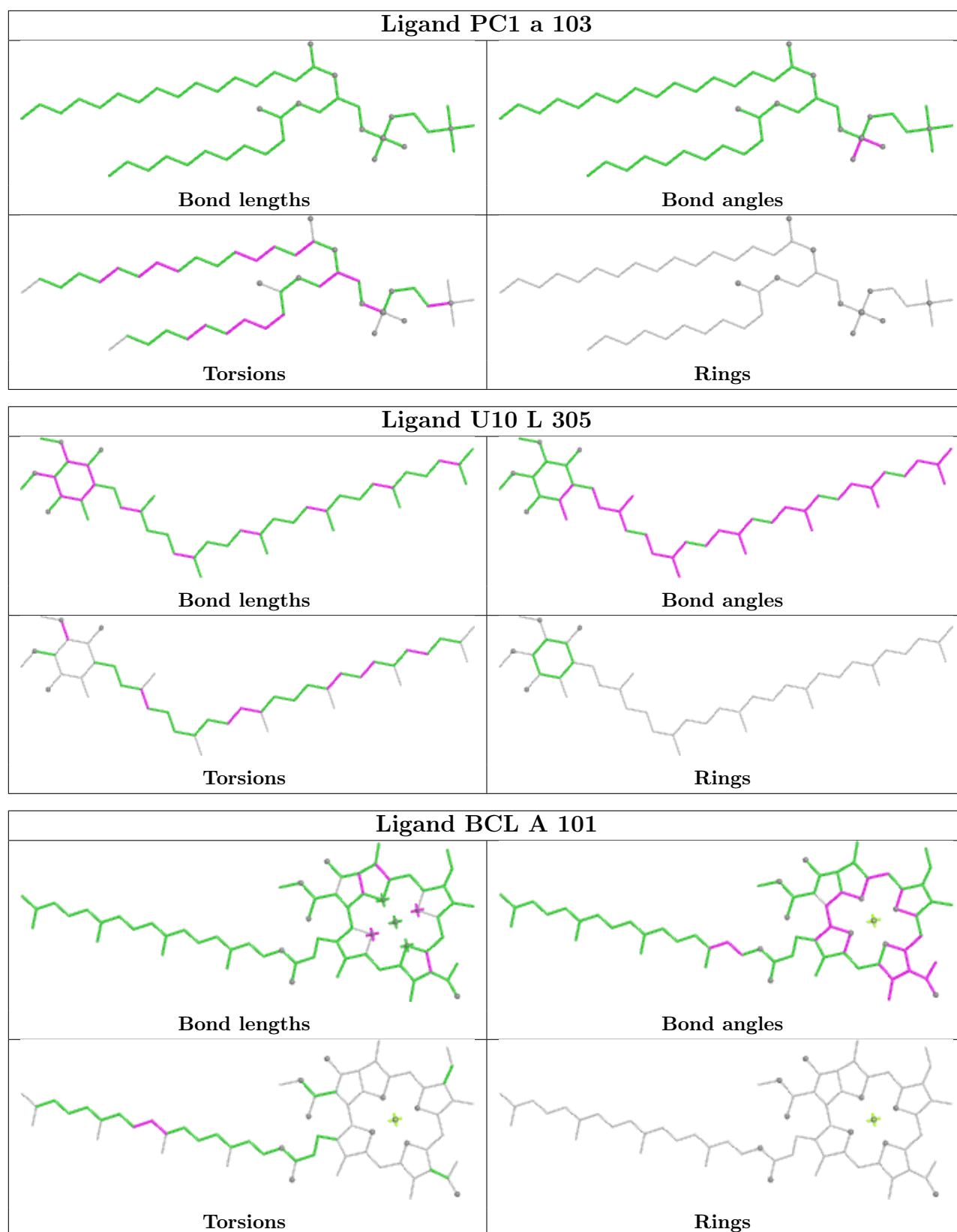


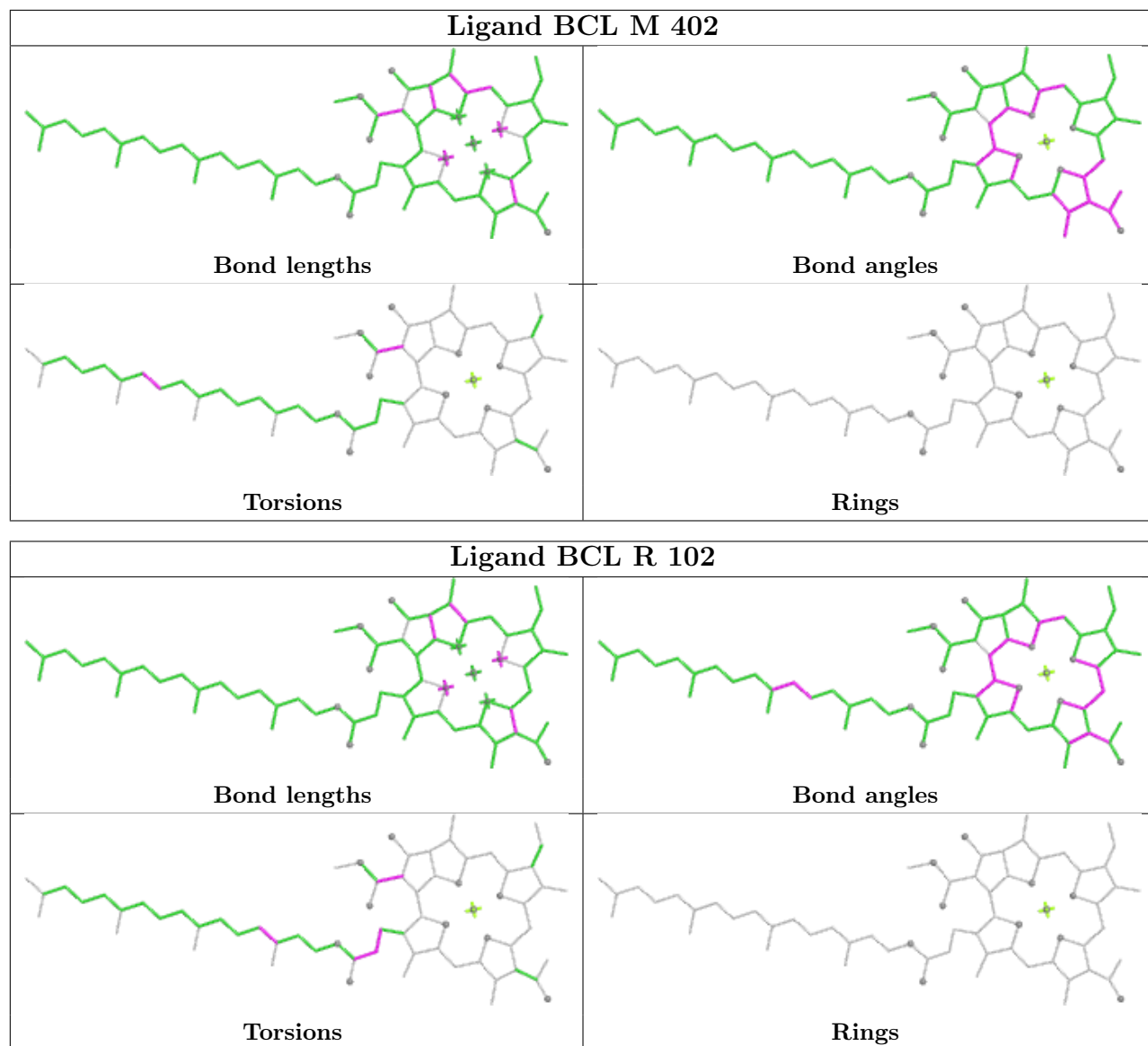
Ligand BCL g 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO 5 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

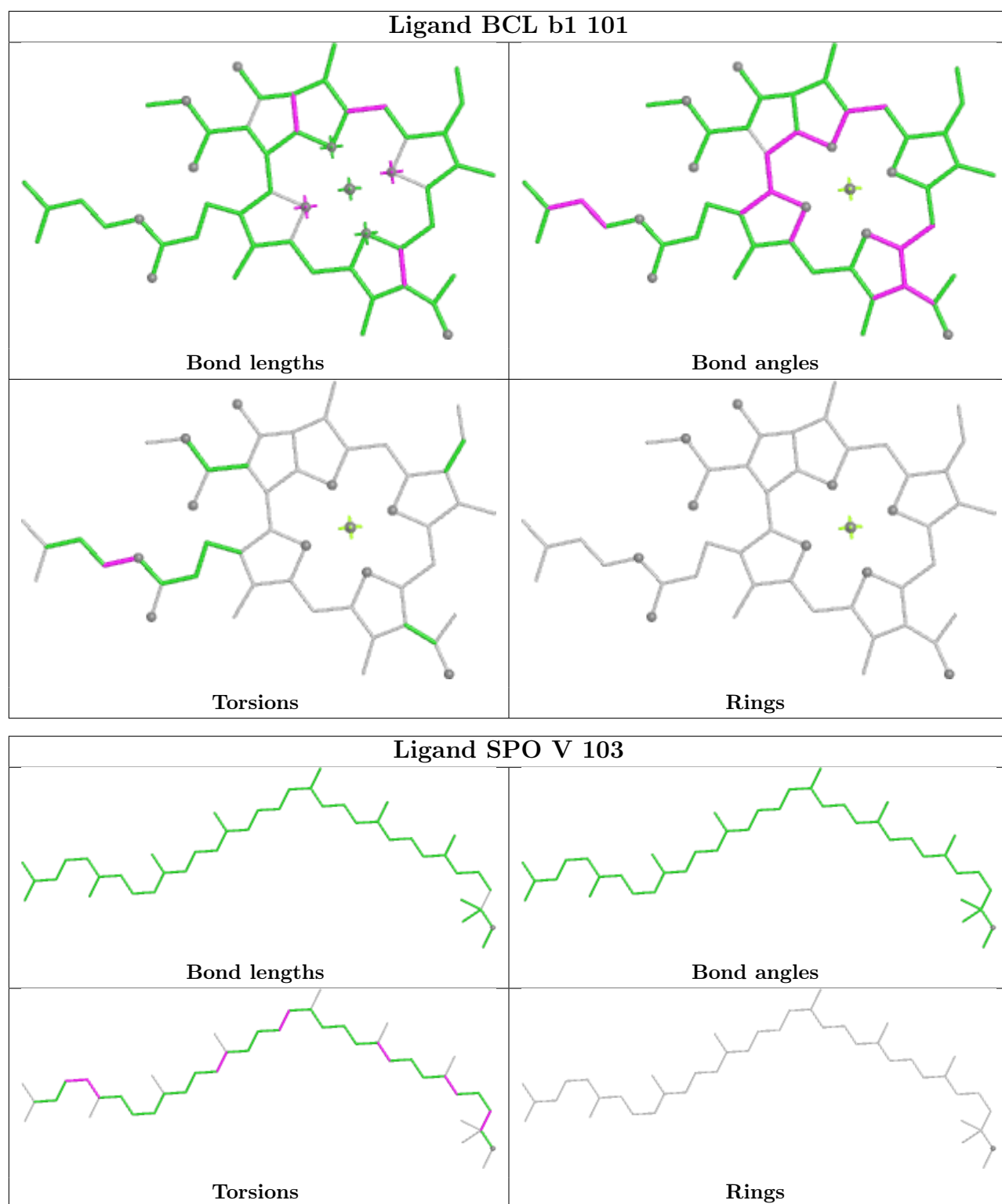


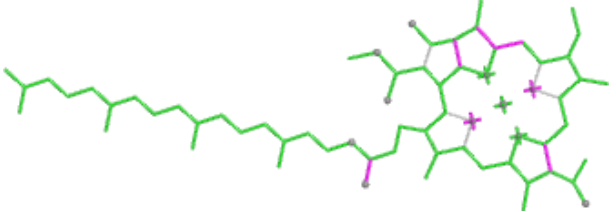
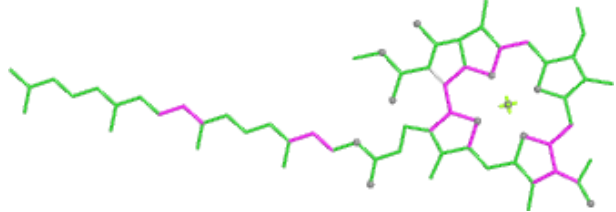
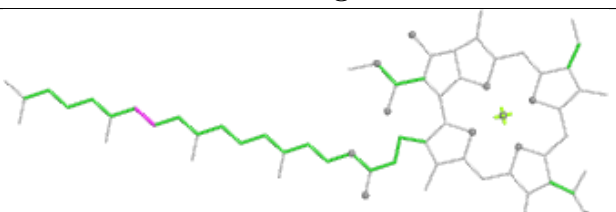
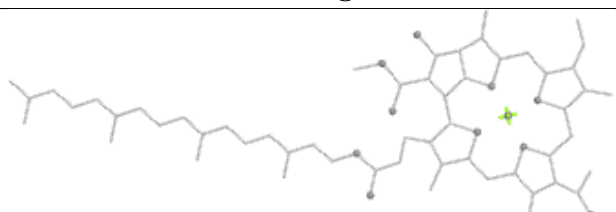
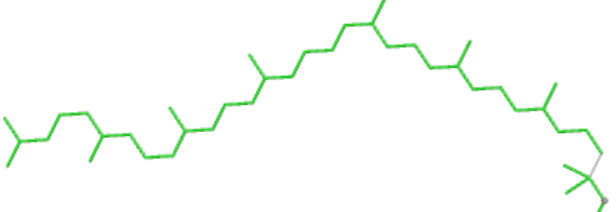
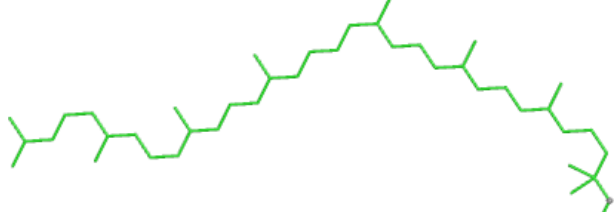
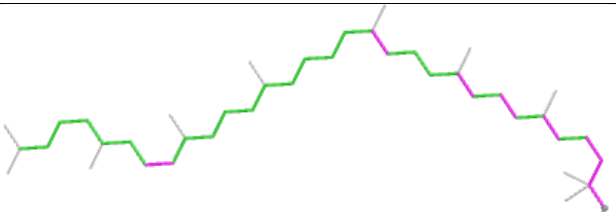
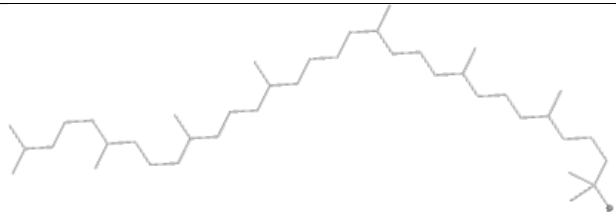
Ligand BCL C 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO o 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

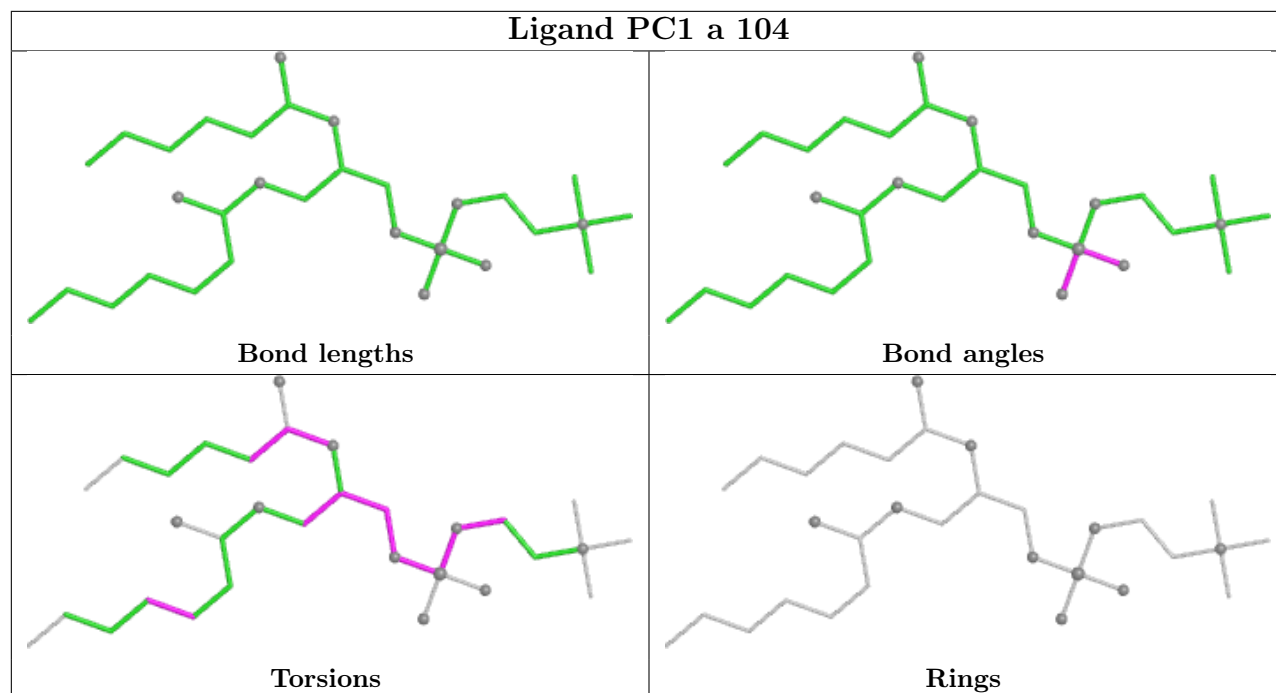








Ligand BCL u 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO 7 102	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

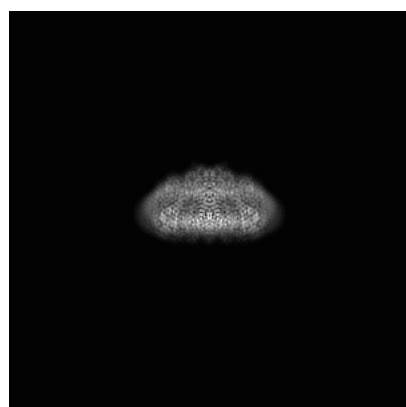
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32059. These allow visual inspection of the internal detail of the map and identification of artifacts.

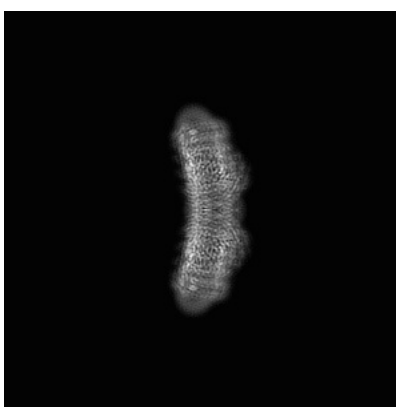
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

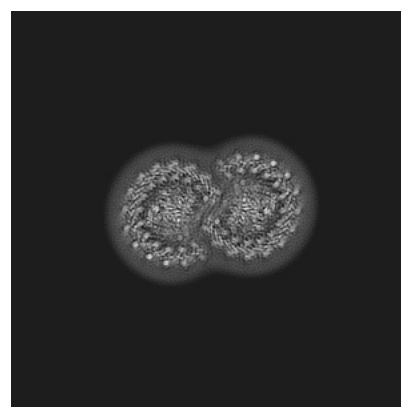
6.1.1 Primary map



X



Y

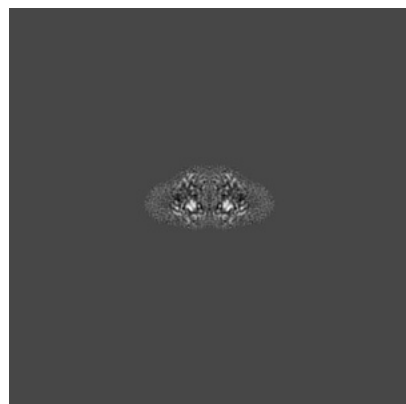


Z

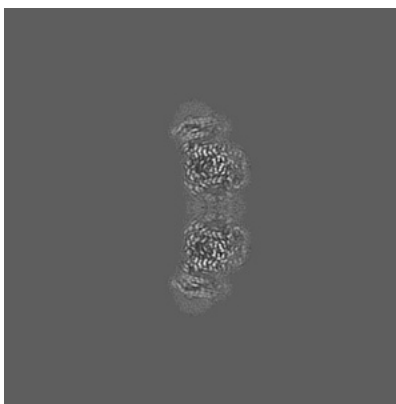
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

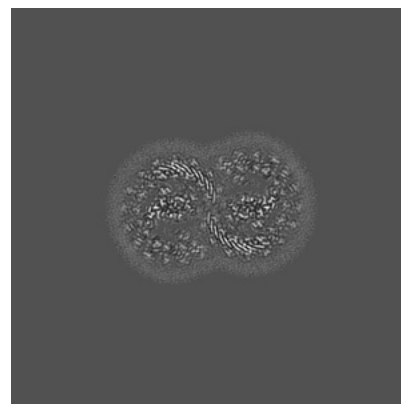
6.2.1 Primary map



X Index: 208



Y Index: 208



Z Index: 208

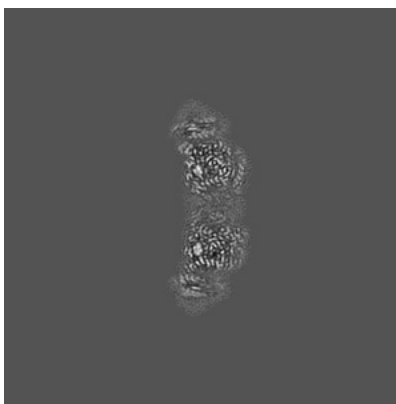
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

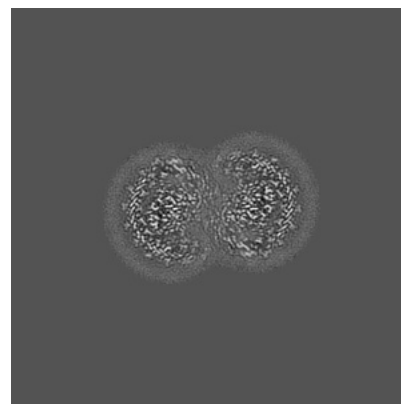
6.3.1 Primary map



X Index: 255



Y Index: 210

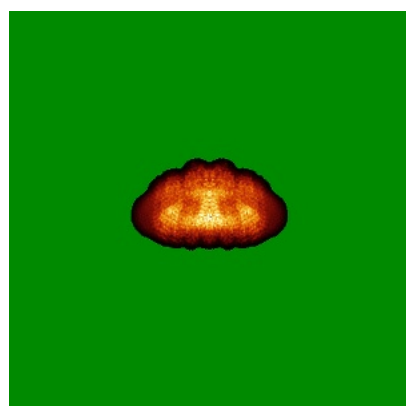


Z Index: 198

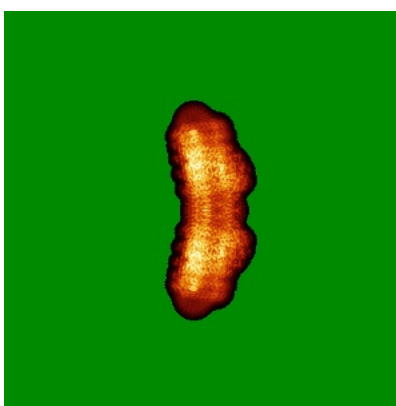
The images above show the largest variance slices of the map in three orthogonal directions.

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

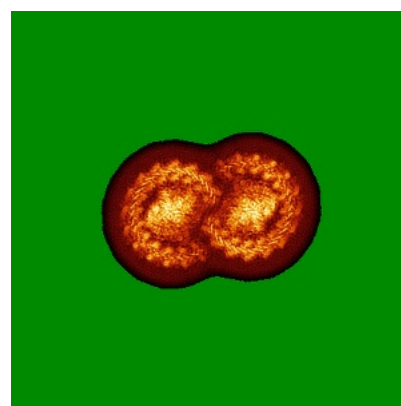
6.4.1 Primary map



X



Y

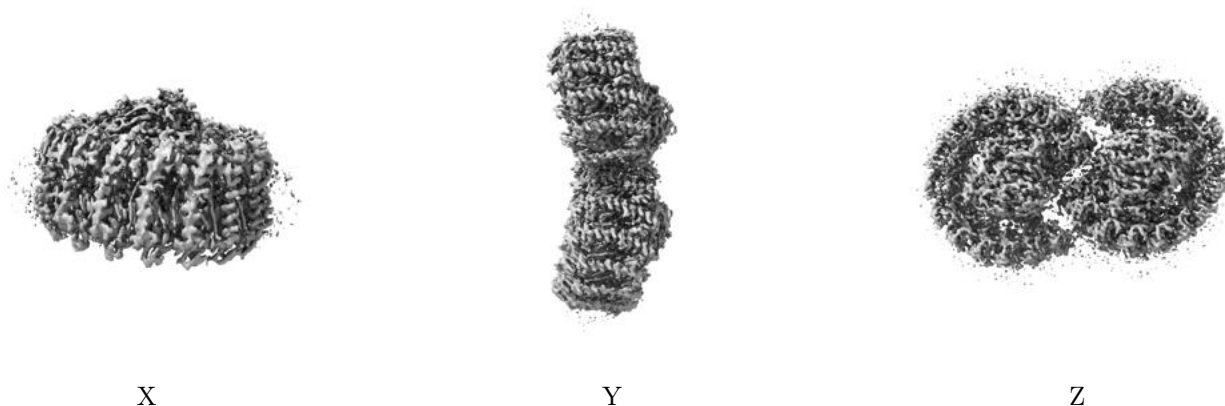


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

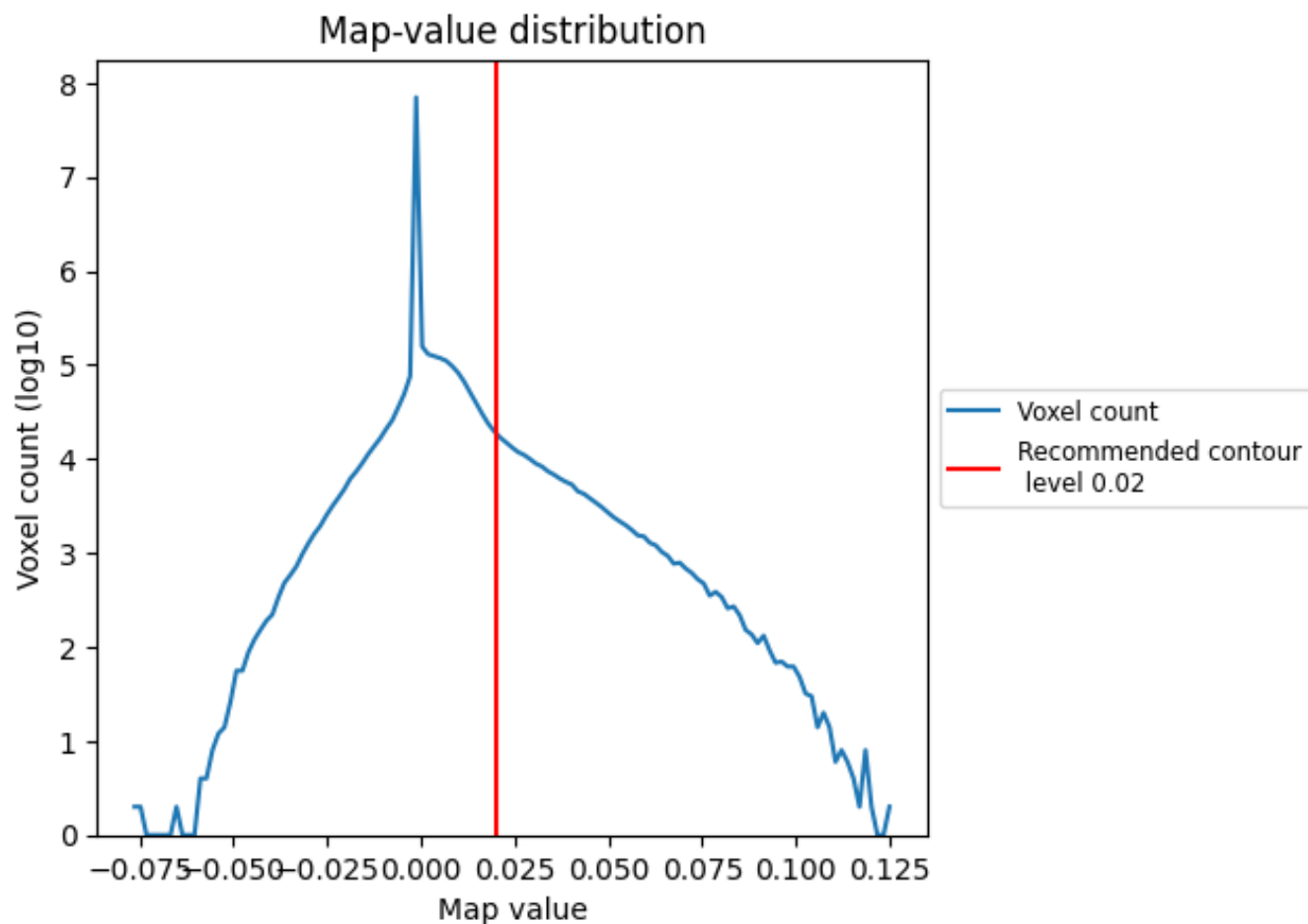
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

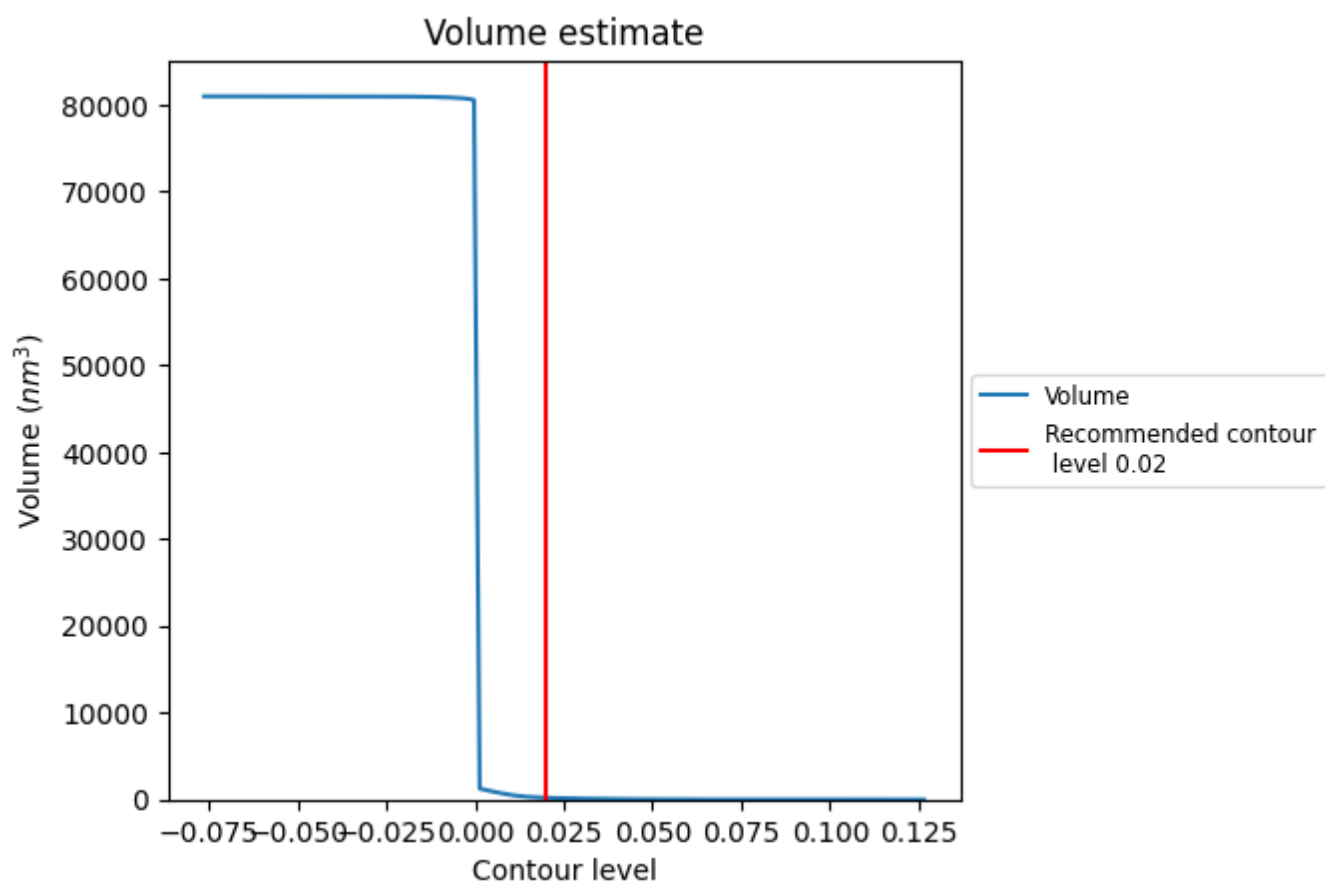
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

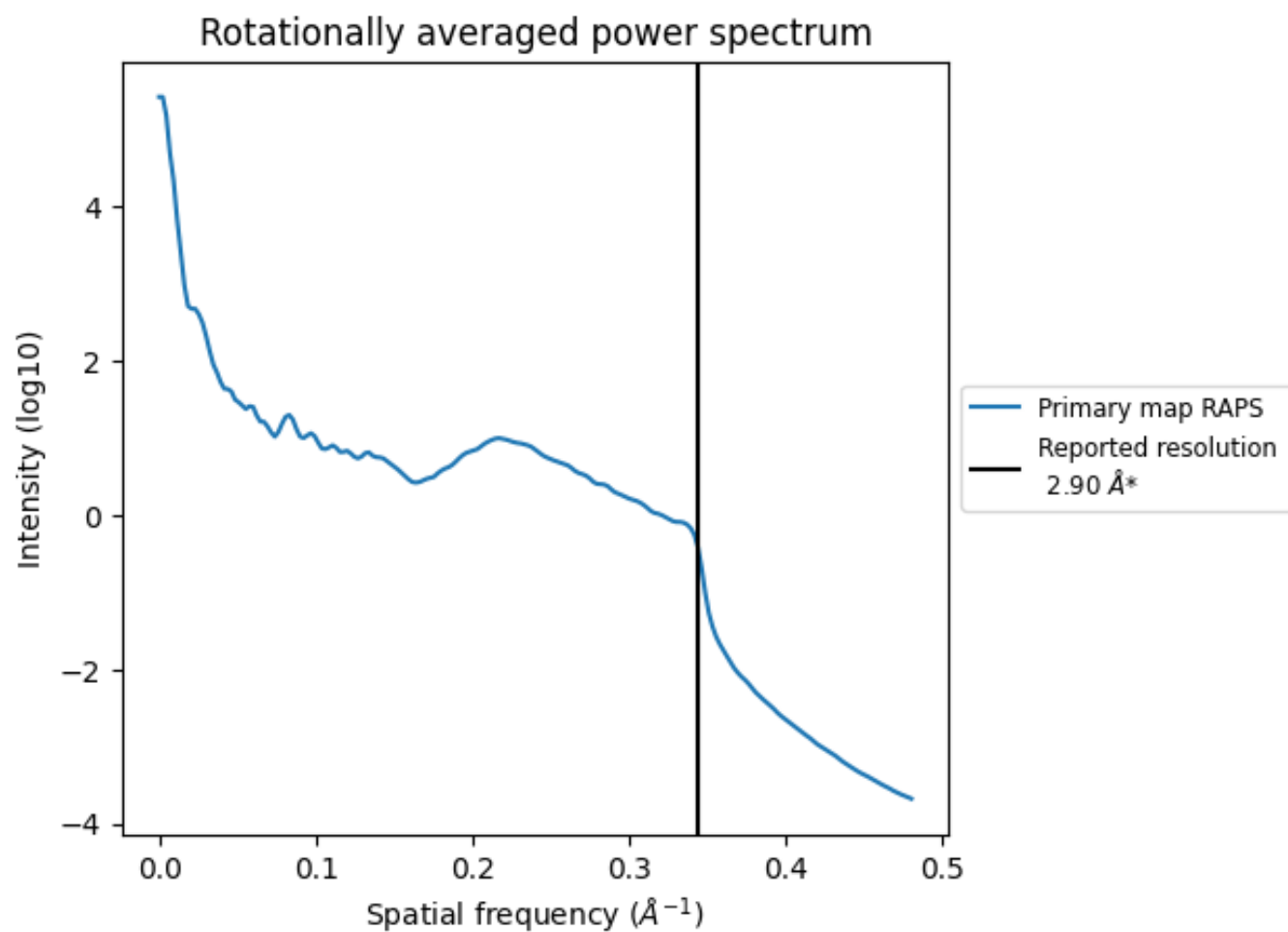
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm^3 ; this corresponds to an approximate mass of 188 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



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

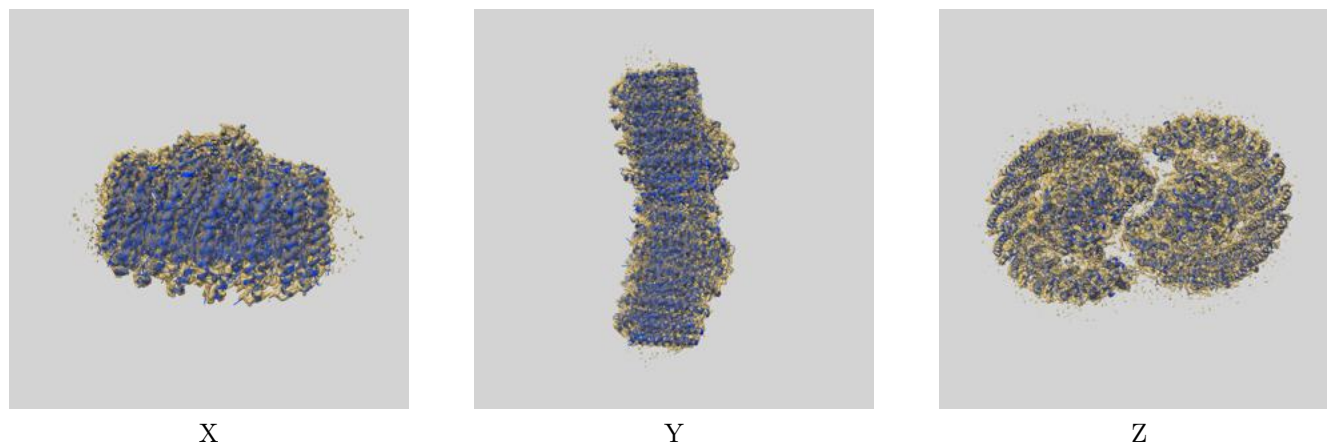
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

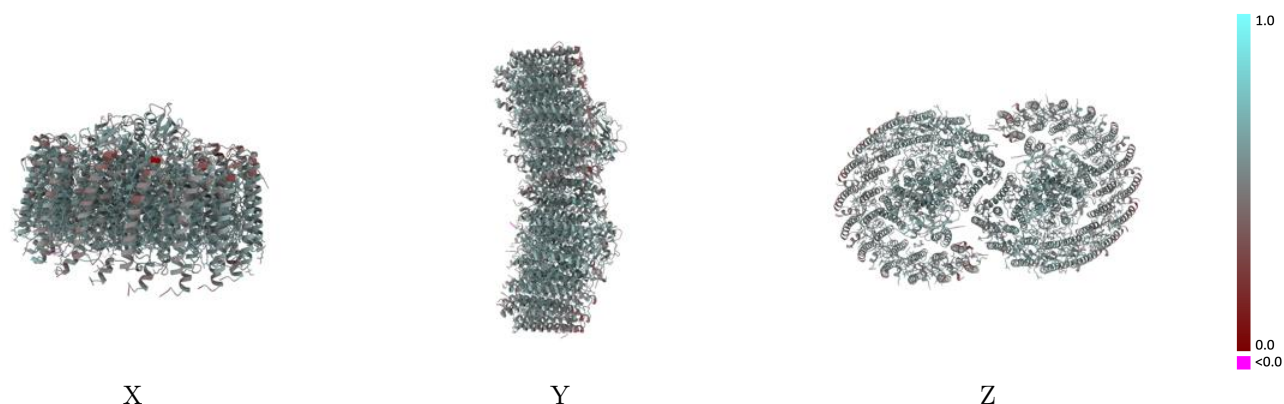
This section contains information regarding the fit between EMDB map EMD-32059 and PDB model 7VOT. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



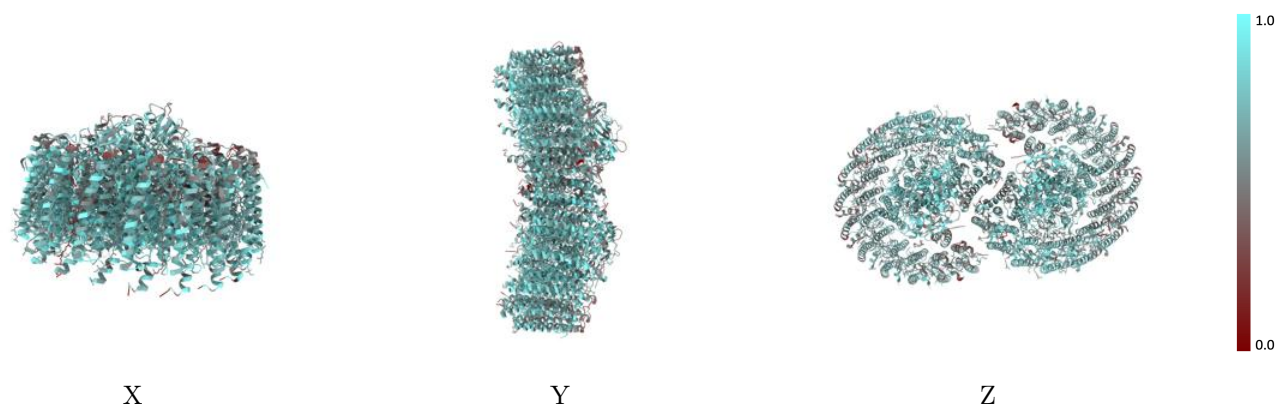
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



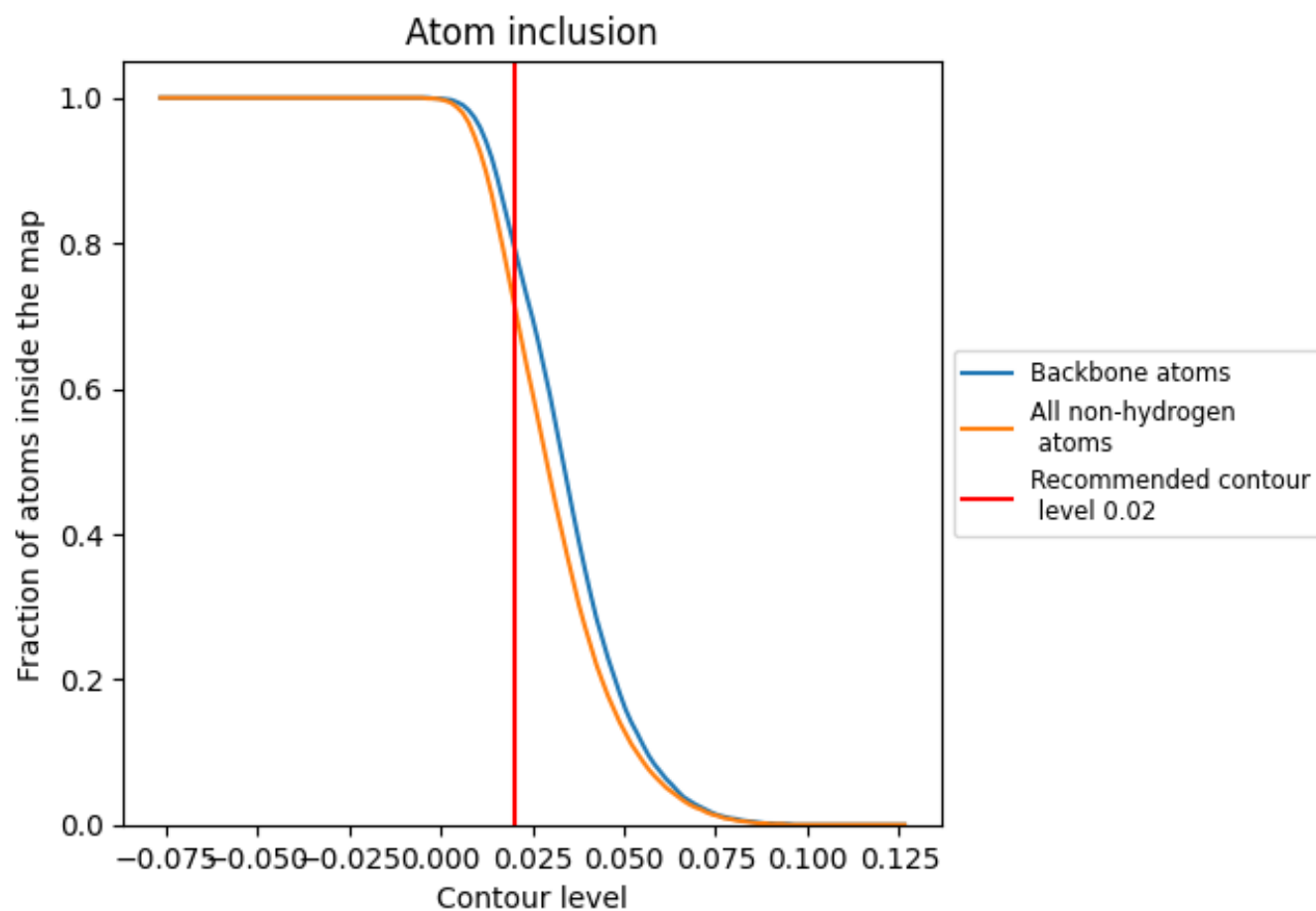
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% 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	 0.7190	 0.5420
0	 0.7520	 0.5420
1	 0.5400	 0.4860
2	 0.5740	 0.4560
3	 0.6340	 0.5180
4	 0.5870	 0.4580
5	 0.6490	 0.5250
6	 0.6960	 0.5410
7	 0.6740	 0.5300
8	 0.6580	 0.5080
9	 0.7490	 0.5570
A	 0.7460	 0.5650
B	 0.7260	 0.5520
C	 0.6750	 0.5260
D	 0.7400	 0.5580
E	 0.7390	 0.5450
F	 0.7430	 0.5490
G	 0.6850	 0.5230
H	 0.6870	 0.5400
I	 0.6680	 0.5250
J	 0.6300	 0.5050
K	 0.6660	 0.5000
L	 0.8120	 0.5840
M	 0.8380	 0.5840
N	 0.6290	 0.4710
O	 0.6390	 0.5040
P	 0.6560	 0.4620
Q	 0.6790	 0.5150
R	 0.6320	 0.5030
S	 0.7140	 0.5400
T	 0.6990	 0.5120
U	 0.7440	 0.5440
V	 0.6930	 0.5230
W	 0.7290	 0.5370
X	 0.6090	 0.5230



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.5750	 0.5260
Z	 0.6200	 0.5010
a	 0.7520	 0.5700
b	 0.7350	 0.5580
b0	 0.7670	 0.5540
b1	 0.5510	 0.4870
b8	 0.6600	 0.5110
b9	 0.7770	 0.5660
c	 0.7110	 0.5360
d	 0.7560	 0.5660
e	 0.7460	 0.5540
f	 0.7460	 0.5550
g	 0.6970	 0.5260
h	 0.6920	 0.5460
i	 0.6810	 0.5300
j	 0.6390	 0.5110
k	 0.6680	 0.5090
l	 0.8170	 0.5840
m	 0.8450	 0.5840
n	 0.6270	 0.4770
o	 0.6300	 0.5120
p	 0.6560	 0.4750
q	 0.6890	 0.5250
r	 0.6410	 0.5170
s	 0.7250	 0.5460
t	 0.7140	 0.5230
u	 0.7650	 0.5520
v	 0.7120	 0.5310
w	 0.7410	 0.5430
x	 0.6160	 0.5280
y	 0.5620	 0.5410
z	 0.6350	 0.5070