



Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 12:26 PM JST

PDB ID : 8YGD
EMDB ID : EMD-39244
Title : Rhodobacter blasticus RC-LH1 dimer
Authors : Liu, L.N.; Zhang, Y.Z.; Wang, P.; Christianson, B.M.; Ugurlar, D.
Deposited on : 2024-02-26
Resolution : 2.84 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

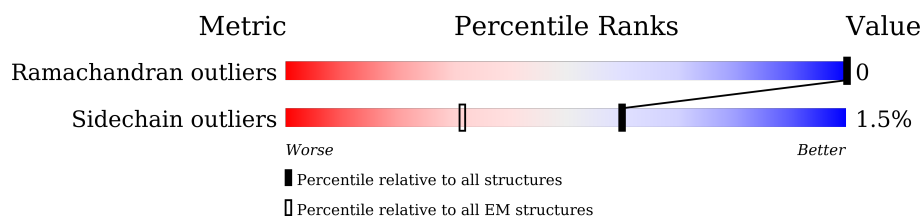
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:










ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 Å.

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



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	0	49	 90% 10%
1	2	49	 14% 76% 20%
1	8	49	 88% 12%
1	B	49	 88% 12%
1	C	49	 27% 82% 6% 12%
1	E	49	 86% 12%
1	G	49	 88% 12%
1	J	49	 88% 12%
1	N	49	 88% 12%

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Mol	Chain	Length	Quality of chain
1	P	49	
1	R	49	
1	T	49	
1	V	49	
1	Z	49	
1	b	49	
2	1	62	
2	3	62	
2	7	62	
2	9	62	
2	A	62	
2	D	62	
2	F	62	
2	I	62	
2	K	62	
2	O	62	
2	Q	62	
2	S	62	
2	U	62	
2	W	62	
2	a	62	
3	H	256	
4	L	282	
5	M	307	
6	X	75	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23255 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	44	Total	C	N	O	S	0	0
			360	241	56	62	1		
1	2	39	Total	C	N	O	S	0	0
			319	213	51	54	1		
1	8	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	B	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	C	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	E	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	G	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	J	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	N	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	P	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	R	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	T	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	V	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	Z	41	Total	C	N	O	S	0	0
			338	228	53	56	1		
1	b	36	Total	C	N	O	S	0	0
			300	201	48	50	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	49	Total	C	N	O	S	0	0
			412	283	65	63	1		
2	3	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	7	44	Total	C	N	O	S	0	0
			379	262	60	55	2		
2	9	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	A	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	D	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	F	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	I	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	K	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	O	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	Q	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	S	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	U	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	W	51	Total	C	N	O	S	0	0
			432	295	71	65	1		
2	a	48	Total	C	N	O	S	0	0
			401	274	64	62	1		

- Molecule 3 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	254	Total	C	N	O	S	0	0
			1980	1259	347	366	8		

- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	281	Total	C	N	O	S	0	0
			2231	1503	349	370	9		

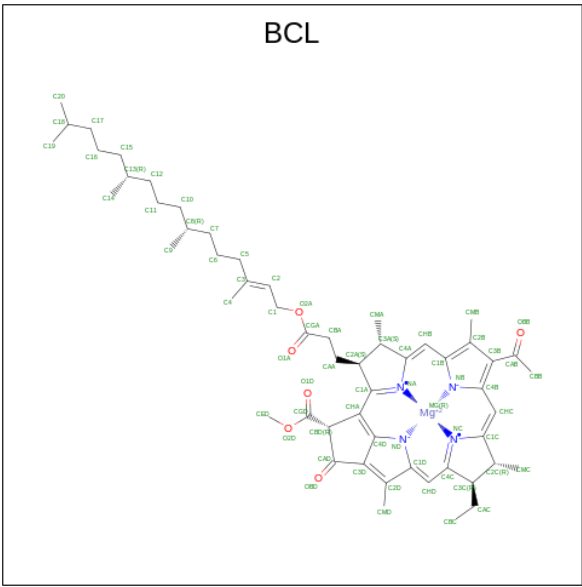
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	304	Total	C	N	O	S	0	0
			2432	1622	394	405	11		

- Molecule 6 is a protein called 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	60	Total	C	N	O	S	0	0
			451	298	74	77	2		

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



Mol	Chain	Residues	Atoms					AltConf
7	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
7	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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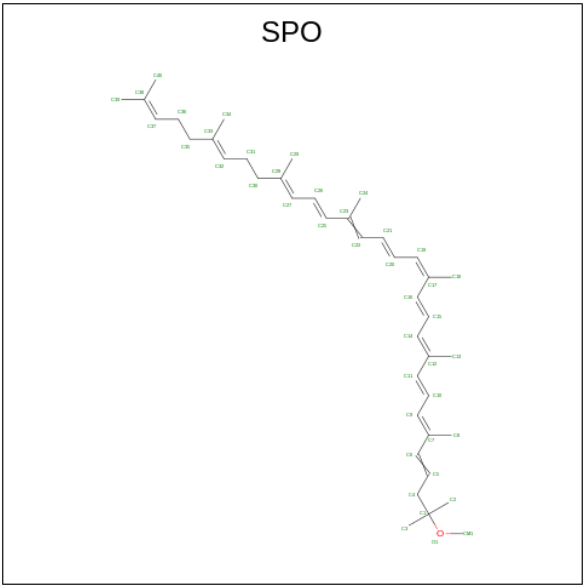
Mol	Chain	Residues	Atoms					AltConf
7	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	C	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 63	C 52	Mg 1	N 4	O 6	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	S	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
7	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	0	1	Total	C	O	0
			42	41	1	
8	0	1	Total	C	O	0
			42	41	1	
8	2	1	Total	C	O	0
			42	41	1	
8	2	1	Total	C	O	0
			42	41	1	
8	2	1	Total	C	O	0
			42	41	1	

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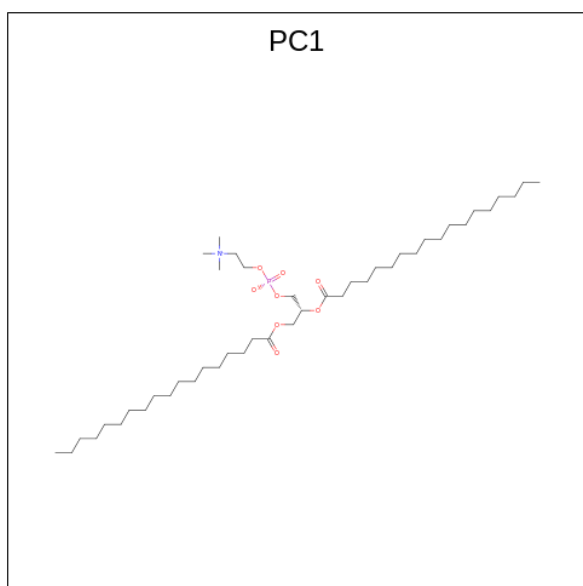
Mol	Chain	Residues	Atoms			AltConf
8	3	1	Total	C	O	0
			42	41	1	
8	8	1	Total	C	O	0
			39	38	1	
8	9	1	Total	C	O	0
			42	41	1	
8	A	1	Total	C	O	0
			42	41	1	
8	D	1	Total	C	O	0
			42	41	1	
8	D	1	Total	C	O	0
			42	41	1	
8	E	1	Total	C	O	0
			42	41	1	
8	F	1	Total	C	O	0
			42	41	1	
8	I	1	Total	C	O	0
			42	41	1	
8	J	1	Total	C	O	0
			42	41	1	
8	K	1	Total	C	O	0
			42	41	1	
8	M	1	Total	C	O	0
			42	41	1	
8	N	1	Total	C	O	0
			42	41	1	
8	O	1	Total	C	O	0
			42	41	1	
8	P	1	Total	C	O	0
			42	41	1	
8	R	1	Total	C	O	0
			42	41	1	
8	R	1	Total	C	O	0
			42	41	1	
8	S	1	Total	C	O	0
			42	41	1	
8	S	1	Total	C	O	0
			42	41	1	
8	T	1	Total	C	O	0
			42	41	1	
8	U	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
8	U	1	Total	C	O	0
			42	41	1	
8	W	1	Total	C	O	0
			42	41	1	
8	Z	1	Total	C	O	0
			42	41	1	

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



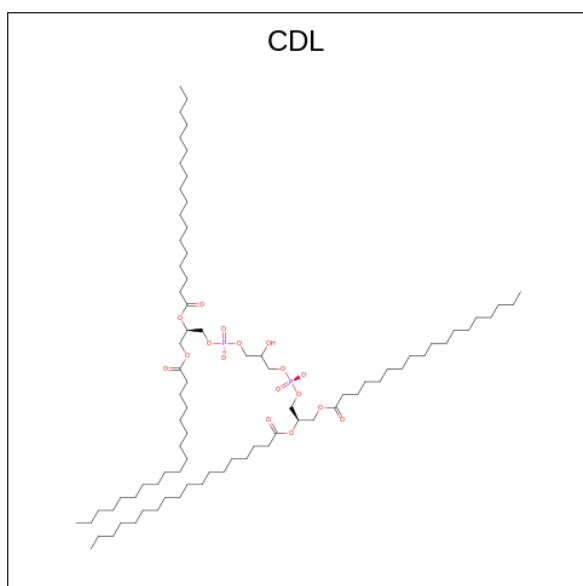
Mol	Chain	Residues	Atoms					AltConf
9	9	1	Total	C	N	O	P	0
			45	35	1	8	1	
9	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	F	1	Total	C	N	O	P	0
			37	27	1	8	1	
9	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
9	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
9	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
9	M	1	Total	C	N	O	P	0
			35	25	1	8	1	

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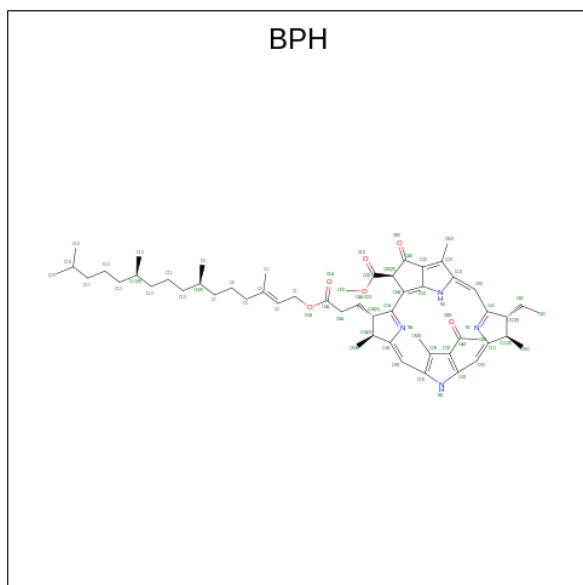
Mol	Chain	Residues	Atoms					AltConf
9	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
9	M	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	W	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



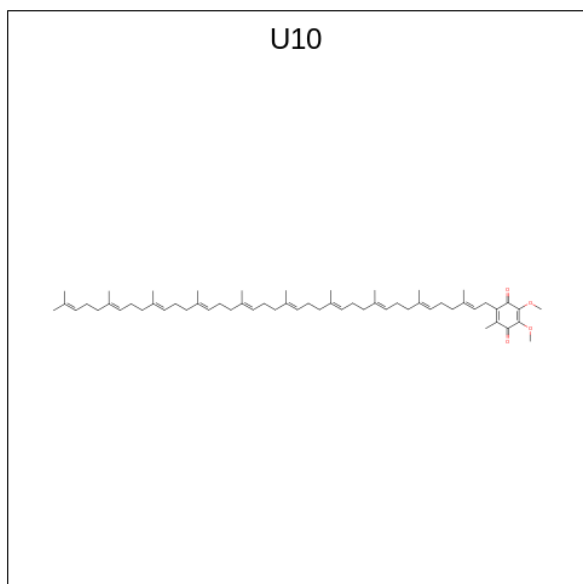
Mol	Chain	Residues	Atoms				AltConf
10	F	1	Total	C	O	P	0
			78	59	17	2	
10	M	1	Total	C	O	P	0
			100	81	17	2	
10	M	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 11 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	L	1	Total	C	N	O	0
			62	52	4	6	
11	L	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			43	39	4	

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Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			43	39	4	
12	L	1	Total	C	O	0
			48	44	4	
12	L	1	Total	C	O	0
			19	15	4	
12	L	1	Total	C	O	0
			38	34	4	
12	M	1	Total	C	O	0
			48	44	4	
12	X	1	Total	C	O	0
			48	44	4	


- Molecule 13 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

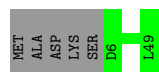
Mol	Chain	Residues	Atoms		AltConf
13	M	1	Total	Fe	0
			1	1	

3 Residue-property plots [i](#)


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

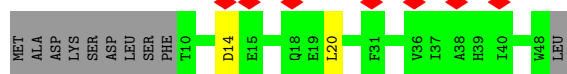
- Molecule 1: Antenna pigment protein beta chain

Chain 0: 




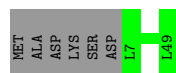
- Molecule 1: Antenna pigment protein beta chain

Chain 2: 



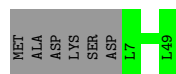
- Molecule 1: Antenna pigment protein beta chain

Chain 8: 




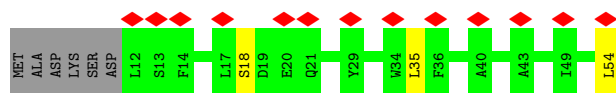
- Molecule 1: Antenna pigment protein beta chain

Chain B: 




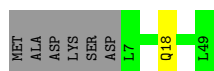
- Molecule 1: Antenna pigment protein beta chain

Chain C: 




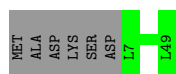
- Molecule 1: Antenna pigment protein beta chain

Chain E:  86% 12%




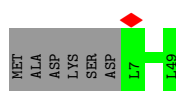
- Molecule 1: Antenna pigment protein beta chain

Chain G:  88% 12%




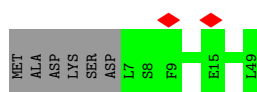
- Molecule 1: Antenna pigment protein beta chain

Chain J:  88% 12%




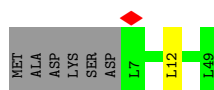
- Molecule 1: Antenna pigment protein beta chain

Chain N:  88% 12%




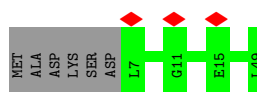
- Molecule 1: Antenna pigment protein beta chain

Chain P:  86% 12%




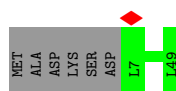
- Molecule 1: Antenna pigment protein beta chain

Chain R:  88% 12% 6%

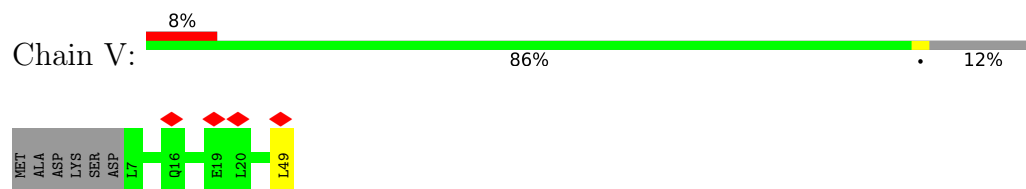


- Molecule 1: Antenna pigment protein beta chain

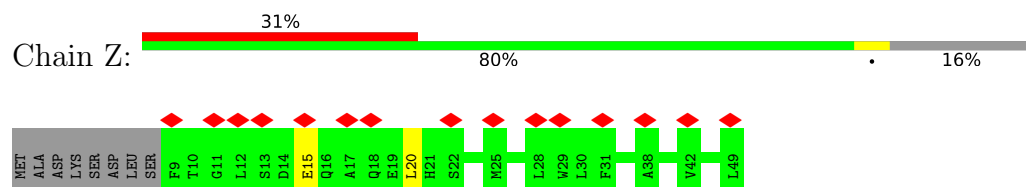
Chain T:  88% 12%



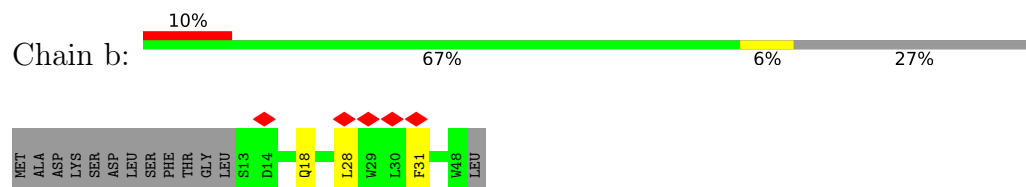
- Molecule 1: Antenna pigment protein beta chain



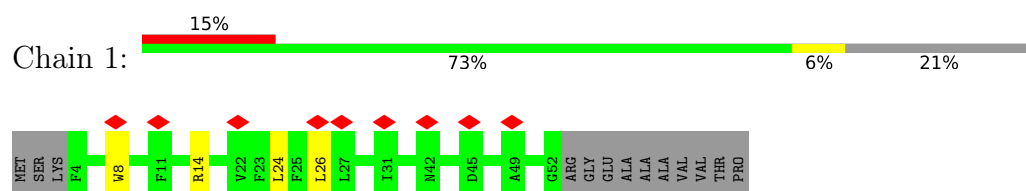
- Molecule 1: Antenna pigment protein beta chain



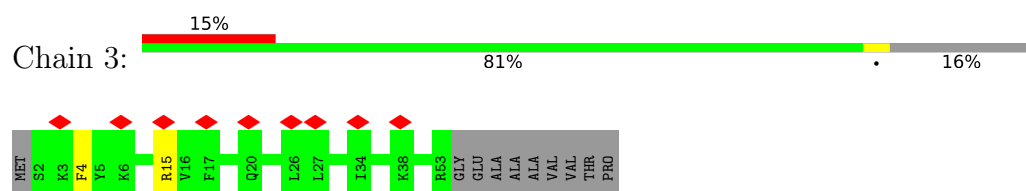
- Molecule 1: Antenna pigment protein beta chain



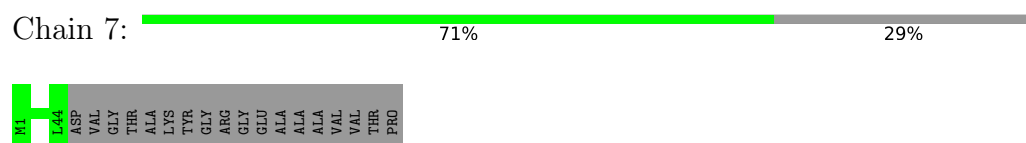
- Molecule 2: Antenna pigment protein alpha chain



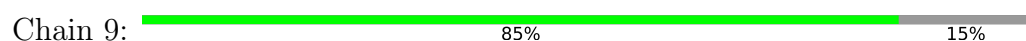
- Molecule 2: Antenna pigment protein alpha chain

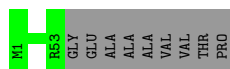


- Molecule 2: Antenna pigment protein alpha chain



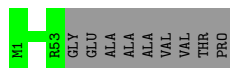
- Molecule 2: Antenna pigment protein alpha chain





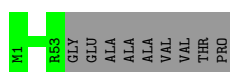
- Molecule 2: Antenna pigment protein alpha chain

Chain A:
85% 15%



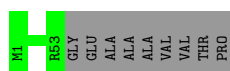
- Molecule 2: Antenna pigment protein alpha chain

Chain D:
85% 15%



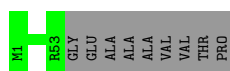
- Molecule 2: Antenna pigment protein alpha chain

Chain F:
85% 15%



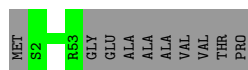
- Molecule 2: Antenna pigment protein alpha chain

Chain I:
85% 15%



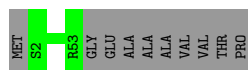
- Molecule 2: Antenna pigment protein alpha chain

Chain K:
84% 16%



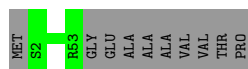
- Molecule 2: Antenna pigment protein alpha chain

Chain O:
84% 16%

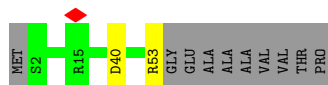
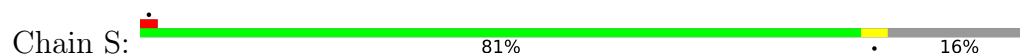


- Molecule 2: Antenna pigment protein alpha chain

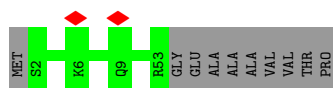
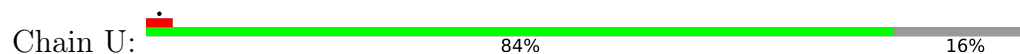
Chain Q:
84% 16%



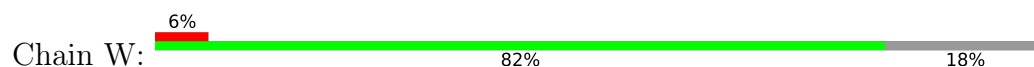
- Molecule 2: Antenna pigment protein alpha chain



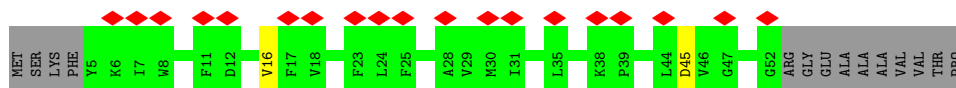
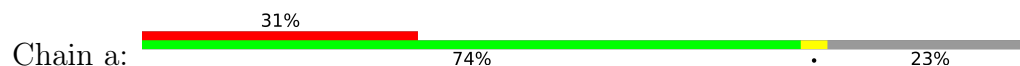
- Molecule 2: Antenna pigment protein alpha chain



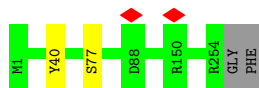
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 3: Photosynthetic reaction center subunit H



- Molecule 4: Reaction center protein L chain




- Molecule 5: Reaction center protein M chain

Chain M:  98% ..



- Molecule 6: 1-deoxy-D-xylulose-5-phosphate synthase

Chain X:  80% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	9149	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.177	Depositor
Minimum map value	-0.768	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	237.824, 237.824, 237.824	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.929, 0.929, 0.929	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.64	0/372	0.47	0/510
1	2	0.52	0/330	0.65	0/453
1	8	0.61	0/364	0.58	0/499
1	B	0.61	0/364	0.49	0/499
1	C	0.49	0/364	0.69	0/499
1	E	0.61	0/364	0.53	0/499
1	G	0.57	0/364	0.50	0/499
1	J	0.53	0/364	0.49	0/499
1	N	0.45	0/364	0.54	0/499
1	P	0.46	0/364	0.47	0/499
1	R	0.44	0/364	0.44	0/499
1	T	0.40	0/364	0.48	0/499
1	V	0.58	0/364	0.72	0/499
1	Z	0.50	0/350	0.70	0/480
1	b	0.50	0/311	0.63	0/427
2	1	0.44	0/426	0.55	0/579
2	3	0.48	0/452	0.67	0/612
2	7	0.72	0/392	0.49	0/531
2	9	0.70	0/460	0.55	0/622
2	A	0.69	0/460	0.54	0/622
2	D	0.68	0/460	0.57	0/622
2	F	0.67	0/460	0.58	0/622
2	I	0.61	0/460	0.60	0/622
2	K	0.55	0/452	0.54	0/612
2	O	0.51	0/452	0.53	0/612
2	Q	0.53	0/452	0.50	0/612
2	S	0.54	0/452	0.62	0/612
2	U	0.47	0/452	0.60	0/612
2	W	0.54	0/446	0.69	0/604
2	a	0.58	0/414	0.73	0/563
3	H	0.61	0/2030	0.58	0/2757
4	L	0.74	0/2317	0.61	0/3172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	M	0.76	0/2525	0.62	1/3453 (0.0%)
6	X	0.62	0/463	0.61	0/636
All	All	0.62	0/19392	0.59	1/26436 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	266	HIS	CB-CA-C	5.12	120.64	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	40	TYR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
1	2	37/49 (76%)	35 (95%)	2 (5%)	0	100	100
1	8	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	B	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	C	41/49 (84%)	38 (93%)	3 (7%)	0	100	100
1	E	41/49 (84%)	41 (100%)	0	0	100	100
1	G	41/49 (84%)	41 (100%)	0	0	100	100
1	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	N	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	P	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	R	41/49 (84%)	41 (100%)	0	0	100	100
1	T	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	V	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	Z	39/49 (80%)	37 (95%)	2 (5%)	0	100	100
1	b	34/49 (69%)	34 (100%)	0	0	100	100
2	1	47/62 (76%)	46 (98%)	1 (2%)	0	100	100
2	3	50/62 (81%)	49 (98%)	1 (2%)	0	100	100
2	7	42/62 (68%)	41 (98%)	1 (2%)	0	100	100
2	9	51/62 (82%)	50 (98%)	1 (2%)	0	100	100
2	A	51/62 (82%)	49 (96%)	2 (4%)	0	100	100
2	D	51/62 (82%)	49 (96%)	2 (4%)	0	100	100
2	F	51/62 (82%)	49 (96%)	2 (4%)	0	100	100
2	I	51/62 (82%)	50 (98%)	1 (2%)	0	100	100
2	K	50/62 (81%)	48 (96%)	2 (4%)	0	100	100
2	O	50/62 (81%)	47 (94%)	3 (6%)	0	100	100
2	Q	50/62 (81%)	46 (92%)	4 (8%)	0	100	100
2	S	50/62 (81%)	46 (92%)	4 (8%)	0	100	100
2	U	50/62 (81%)	49 (98%)	1 (2%)	0	100	100
2	W	49/62 (79%)	48 (98%)	1 (2%)	0	100	100
2	a	46/62 (74%)	46 (100%)	0	0	100	100
3	H	252/256 (98%)	235 (93%)	17 (7%)	0	100	100
4	L	279/282 (99%)	262 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	302/307 (98%)	291 (96%)	11 (4%)	0	100	100
6	X	58/75 (77%)	55 (95%)	3 (5%)	0	100	100
All	All	2233/2585 (86%)	2143 (96%)	90 (4%)	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	0	38/42 (90%)	38 (100%)	0	100	100
1	2	33/42 (79%)	31 (94%)	2 (6%)	15	31
1	8	37/42 (88%)	37 (100%)	0	100	100
1	B	37/42 (88%)	37 (100%)	0	100	100
1	C	37/42 (88%)	34 (92%)	3 (8%)	9	20
1	E	37/42 (88%)	36 (97%)	1 (3%)	40	65
1	G	37/42 (88%)	37 (100%)	0	100	100
1	J	37/42 (88%)	37 (100%)	0	100	100
1	N	37/42 (88%)	37 (100%)	0	100	100
1	P	37/42 (88%)	36 (97%)	1 (3%)	40	65
1	R	37/42 (88%)	37 (100%)	0	100	100
1	T	37/42 (88%)	37 (100%)	0	100	100
1	V	37/42 (88%)	36 (97%)	1 (3%)	40	65
1	Z	35/42 (83%)	33 (94%)	2 (6%)	17	34
1	b	31/42 (74%)	28 (90%)	3 (10%)	6	13
2	1	43/52 (83%)	39 (91%)	4 (9%)	7	15
2	3	46/52 (88%)	44 (96%)	2 (4%)	25	48
2	7	41/52 (79%)	41 (100%)	0	100	100
2	9	47/52 (90%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	47/52 (90%)	47 (100%)	0	100	100
2	D	47/52 (90%)	47 (100%)	0	100	100
2	F	47/52 (90%)	47 (100%)	0	100	100
2	I	47/52 (90%)	47 (100%)	0	100	100
2	K	46/52 (88%)	46 (100%)	0	100	100
2	O	46/52 (88%)	46 (100%)	0	100	100
2	Q	46/52 (88%)	46 (100%)	0	100	100
2	S	46/52 (88%)	44 (96%)	2 (4%)	25	48
2	U	46/52 (88%)	46 (100%)	0	100	100
2	W	45/52 (86%)	45 (100%)	0	100	100
2	a	42/52 (81%)	40 (95%)	2 (5%)	21	43
3	H	207/208 (100%)	206 (100%)	1 (0%)	86	94
4	L	223/224 (100%)	219 (98%)	4 (2%)	54	76
5	M	237/239 (99%)	236 (100%)	1 (0%)	89	95
6	X	47/59 (80%)	47 (100%)	0	100	100
All	All	1940/2140 (91%)	1911 (98%)	29 (2%)	60	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	8	TRP
2	1	14	ARG
2	1	24	LEU
2	1	26	LEU
1	2	14	ASP
1	2	20	LEU
2	3	4	PHE
2	3	15	ARG
1	C	18	SER
1	C	35	LEU
1	C	54	LEU
1	E	18	GLN
3	H	77	SER
4	L	224	SER
4	L	248	CYS
4	L	252	THR
4	L	273	TRP

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Mol	Chain	Res	Type
5	M	262	MET
1	P	12	LEU
2	S	40	ASP
2	S	53	ARG
1	V	49	LEU
1	Z	15	GLU
1	Z	20	LEU
2	a	16	VAL
2	a	45	ASP
1	b	18	GLN
1	b	28	LEU
1	b	31	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	18	GLN
2	7	20	GLN
2	9	20	GLN
1	C	23	GLN
2	F	20	GLN
2	F	32	HIS
1	N	16	GLN
2	O	32	HIS
2	Q	9	GLN
1	R	18	GLN
1	T	21	HIS
2	U	20	GLN
1	V	21	HIS
1	Z	16	GLN
1	b	39	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 1 is monoatomic - leaving 86 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	BCL	A	101	-	64,74,74	1.17	3 (4%)	78,115,115	1.15	8 (10%)
10	CDL	M	408	-	77,77,99	0.34	0	83,89,111	0.41	0
7	BCL	b	101	-	59,69,74	1.16	2 (3%)	72,109,115	1.58	15 (20%)
7	BCL	J	102	-	64,74,74	1.14	6 (9%)	78,115,115	1.23	11 (14%)
12	U10	X	101	-	48,48,63	0.28	0	58,61,79	0.78	2 (3%)
7	BCL	E	101	-	64,74,74	1.10	5 (7%)	78,115,115	1.17	10 (12%)
10	CDL	M	407	-	99,99,99	0.32	0	105,111,111	0.44	0
8	SPO	K	102	-	40,41,41	1.10	2 (5%)	47,50,50	2.60	16 (34%)
7	BCL	a	101	-	54,64,74	1.03	3 (5%)	66,103,115	1.33	9 (13%)
9	PC1	M	402	-	34,34,53	1.15	2 (5%)	40,42,61	0.99	2 (5%)
8	SPO	R	102	-	40,41,41	0.88	0	47,50,50	1.84	12 (25%)
8	SPO	M	406	-	40,41,41	0.40	0	47,50,50	0.59	1 (2%)
7	BCL	8	102	-	64,74,74	1.16	5 (7%)	78,115,115	1.18	10 (12%)
8	SPO	R	101	-	40,41,41	0.22	0	47,50,50	0.50	1 (2%)
7	BCL	3	102	-	64,74,74	1.05	5 (7%)	78,115,115	1.24	11 (14%)
7	BCL	1	101	-	54,64,74	1.26	3 (5%)	66,103,115	1.26	11 (16%)
8	SPO	S	103	-	40,41,41	0.30	0	47,50,50	0.78	2 (4%)
7	BCL	B	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.23	11 (14%)
7	BCL	L	302	-	61,71,74	1.11	5 (8%)	74,111,115	1.25	10 (13%)
8	SPO	E	102	-	40,41,41	1.13	4 (10%)	47,50,50	2.13	15 (31%)
7	BCL	Q	101	-	64,74,74	1.09	3 (4%)	78,115,115	1.17	8 (10%)
8	SPO	P	101	-	40,41,41	0.25	0	47,50,50	0.66	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	3	101	-	64,74,74	1.01	4 (6%)	78,115,115	1.28	13 (16%)
9	PC1	L	305	-	35,35,53	0.35	0	41,43,61	0.37	0
12	U10	L	307	-	48,48,63	0.24	0	58,61,79	0.60	1 (1%)
7	BCL	1	102	-	59,69,74	1.19	4 (6%)	72,109,115	1.20	9 (12%)
7	BCL	U	101	-	64,74,74	1.05	4 (6%)	78,115,115	1.16	9 (11%)
11	BPH	L	311	-	41,60,70	1.10	3 (7%)	40,89,101	1.02	4 (10%)
8	SPO	U	103	-	40,41,41	0.19	0	47,50,50	0.50	0
9	PC1	W	103	-	31,31,53	0.36	0	37,39,61	0.49	0
7	BCL	T	101	-	64,74,74	1.04	5 (7%)	78,115,115	1.28	10 (12%)
8	SPO	O	102	-	40,41,41	0.97	2 (5%)	47,50,50	1.67	11 (23%)
9	PC1	9	103	-	44,44,53	0.32	0	50,52,61	0.50	0
12	U10	L	310	-	38,38,63	0.21	0	46,49,79	0.50	1 (2%)
8	SPO	Z	101	-	40,41,41	0.22	0	47,50,50	0.71	1 (2%)
7	BCL	F	104	-	64,74,74	1.15	4 (6%)	78,115,115	1.23	10 (12%)
7	BCL	V	101	-	64,74,74	1.09	4 (6%)	78,115,115	1.20	11 (14%)
8	SPO	2	102	-	40,41,41	0.97	2 (5%)	47,50,50	2.04	15 (31%)
8	SPO	D	101	-	40,41,41	0.28	0	47,50,50	0.63	1 (2%)
7	BCL	K	101	-	64,74,74	1.14	3 (4%)	78,115,115	1.20	12 (15%)
8	SPO	W	101	-	40,41,41	1.03	3 (7%)	47,50,50	1.63	10 (21%)
7	BCL	L	301	-	64,74,74	1.12	5 (7%)	78,115,115	1.26	10 (12%)
9	PC1	M	409	-	44,44,53	0.30	0	50,52,61	0.39	0
8	SPO	N	101	-	40,41,41	0.30	0	47,50,50	0.66	2 (4%)
7	BCL	9	101	-	64,74,74	1.06	3 (4%)	78,115,115	1.20	9 (11%)
11	BPH	L	303	-	48,67,70	1.03	3 (6%)	48,97,101	1.02	3 (6%)
7	BCL	I	101	-	64,74,74	1.12	3 (4%)	78,115,115	1.20	8 (10%)
12	U10	L	304	-	43,43,63	0.24	0	52,55,79	0.52	1 (1%)
8	SPO	2	101	-	40,41,41	0.25	0	47,50,50	0.91	3 (6%)
8	SPO	J	101	-	40,41,41	0.28	0	47,50,50	0.63	2 (4%)
7	BCL	S	102	-	64,74,74	0.97	3 (4%)	78,115,115	1.20	9 (11%)
8	SPO	9	102	-	40,41,41	0.40	0	47,50,50	0.69	2 (4%)
7	BCL	L	309	-	64,74,74	1.13	4 (6%)	78,115,115	1.17	9 (11%)
7	BCL	W	102	-	64,74,74	1.15	4 (6%)	78,115,115	1.20	10 (12%)
8	SPO	D	103	-	40,41,41	0.23	0	47,50,50	0.64	1 (2%)
7	BCL	O	101	-	64,74,74	1.21	4 (6%)	78,115,115	1.16	10 (12%)
7	BCL	7	101	-	59,69,74	1.17	4 (6%)	72,109,115	1.26	10 (13%)
7	BCL	M	403	-	64,74,74	1.19	4 (6%)	78,115,115	1.19	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	U10	M	405	-	48,48,63	0.32	0	58,61,79	0.56	1 (1%)
7	BCL	D	102	-	64,74,74	1.12	3 (4%)	78,115,115	1.19	10 (12%)
12	U10	L	308	-	19,19,63	0.33	0	23,26,79	0.73	1 (4%)
10	CDL	F	101	-	77,77,99	1.06	4 (5%)	83,89,111	1.05	7 (8%)
7	BCL	R	103	-	64,74,74	1.08	5 (7%)	78,115,115	1.20	11 (14%)
8	SPO	F	105	-	40,41,41	0.85	1 (2%)	47,50,50	1.53	6 (12%)
8	SPO	T	102	-	40,41,41	0.84	0	47,50,50	1.64	10 (21%)
8	SPO	O	102	-	40,41,41	1.02	3 (7%)	47,50,50	2.40	13 (27%)
8	SPO	A	102	-	40,41,41	0.38	0	47,50,50	0.57	1 (2%)
8	SPO	O	103	-	40,41,41	0.83	2 (5%)	47,50,50	2.63	17 (36%)
8	SPO	2	103	-	40,41,41	0.92	1 (2%)	47,50,50	2.08	15 (31%)
12	U10	L	306	-	43,43,63	0.21	0	52,55,79	0.55	1 (1%)
9	PC1	M	410	-	31,31,53	0.36	0	37,39,61	0.35	0
8	SPO	8	101	-	37,38,41	0.40	0	43,46,50	0.88	2 (4%)
7	BCL	C	101	-	64,74,74	1.04	6 (9%)	78,115,115	1.18	10 (12%)
9	PC1	H	301	-	46,46,53	1.00	2 (4%)	52,54,61	1.00	2 (3%)
7	BCL	P	102	-	64,74,74	1.14	4 (6%)	78,115,115	1.17	10 (12%)
9	PC1	M	401	-	39,39,53	0.34	0	45,47,61	0.33	0
7	BCL	F	102	-	64,74,74	1.09	3 (4%)	78,115,115	1.14	9 (11%)
8	SPO	U	102	-	40,41,41	0.19	0	47,50,50	0.48	0
8	SPO	I	102	-	40,41,41	1.22	3 (7%)	47,50,50	2.37	14 (29%)
9	PC1	A	103	-	31,31,53	1.24	2 (6%)	37,39,61	1.32	5 (13%)
8	SPO	S	101	-	40,41,41	1.09	2 (5%)	47,50,50	2.13	15 (31%)
7	BCL	O	101	-	59,69,74	1.21	5 (8%)	72,109,115	1.33	11 (15%)
7	BCL	N	102	-	64,74,74	1.09	2 (3%)	78,115,115	1.21	11 (14%)
8	SPO	3	103	-	40,41,41	1.03	2 (5%)	47,50,50	1.91	15 (31%)
9	PC1	F	103	-	36,36,53	0.35	0	42,44,61	0.35	0
9	PC1	A	104	-	31,31,53	0.38	0	37,39,61	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	A	101	-	-	11/37/137/137	-
10	CDL	M	408	-	-	20/88/88/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	b	101	-	-	20/31/131/137	-
7	BCL	J	102	-	-	21/37/137/137	-
12	U10	X	101	-	-	18/45/69/87	0/1/1/1
7	BCL	E	101	-	-	25/37/137/137	-
10	CDL	M	407	-	-	39/110/110/110	-
8	SPO	K	102	-	-	11/47/47/47	-
7	BCL	a	101	-	-	15/25/125/137	-
9	PC1	M	402	-	-	14/38/38/57	-
8	SPO	R	102	-	-	11/47/47/47	-
8	SPO	M	406	-	-	8/47/47/47	-
7	BCL	8	102	-	-	20/37/137/137	-
8	SPO	R	101	-	-	4/47/47/47	-
7	BCL	3	102	-	-	16/37/137/137	-
7	BCL	1	101	-	-	11/25/125/137	-
8	SPO	S	103	-	-	17/47/47/47	-
7	BCL	B	101	-	-	19/37/137/137	-
7	BCL	L	302	-	-	10/34/134/137	-
8	SPO	E	102	-	-	10/47/47/47	-
7	BCL	Q	101	-	-	16/37/137/137	-
8	SPO	P	101	-	-	4/47/47/47	-
7	BCL	3	101	-	-	18/37/137/137	-
9	PC1	L	305	-	-	13/39/39/57	-
12	U10	L	307	-	-	12/45/69/87	0/1/1/1
7	BCL	1	102	-	-	19/31/131/137	-
7	BCL	U	101	-	-	18/37/137/137	-
11	BPH	L	311	-	-	7/25/93/105	0/5/6/6
8	SPO	U	103	-	-	10/47/47/47	-
9	PC1	W	103	-	-	16/35/35/57	-
7	BCL	T	101	-	-	15/37/137/137	-
8	SPO	O	102	-	-	4/47/47/47	-
9	PC1	9	103	-	-	21/48/48/57	-
12	U10	L	310	-	-	10/33/57/87	0/1/1/1
8	SPO	Z	101	-	-	12/47/47/47	-
7	BCL	F	104	-	-	20/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	V	101	-	-	20/37/137/137	-
8	SPO	2	102	-	-	7/47/47/47	-
8	SPO	D	101	-	-	6/47/47/47	-
7	BCL	K	101	-	-	13/37/137/137	-
8	SPO	W	101	-	-	7/47/47/47	-
7	BCL	L	301	-	-	4/37/137/137	-
9	PC1	M	409	-	-	12/48/48/57	-
8	SPO	N	101	-	-	4/47/47/47	-
7	BCL	9	101	-	-	19/37/137/137	-
11	BPH	L	303	-	-	7/34/102/105	0/5/6/6
7	BCL	I	101	-	-	11/37/137/137	-
12	U10	L	304	-	-	10/39/63/87	0/1/1/1
8	SPO	2	101	-	-	13/47/47/47	-
8	SPO	J	101	-	-	6/47/47/47	-
7	BCL	S	102	-	-	13/37/137/137	-
8	SPO	9	102	-	-	6/47/47/47	-
7	BCL	L	309	-	-	19/37/137/137	-
7	BCL	W	102	-	-	16/37/137/137	-
8	SPO	D	103	-	-	13/47/47/47	-
7	BCL	O	101	-	-	14/37/137/137	-
7	BCL	7	101	-	-	8/31/131/137	-
7	BCL	M	403	-	-	17/37/137/137	-
12	U10	M	405	-	-	5/45/69/87	0/1/1/1
7	BCL	D	102	-	-	15/37/137/137	-
12	U10	L	308	-	-	1/11/35/87	0/1/1/1
10	CDL	F	101	-	-	34/88/88/110	-
7	BCL	R	103	-	-	27/37/137/137	-
8	SPO	F	105	-	-	3/47/47/47	-
8	SPO	T	102	-	-	3/47/47/47	-
8	SPO	0	102	-	-	14/47/47/47	-
8	SPO	A	102	-	-	8/47/47/47	-
8	SPO	0	103	-	-	15/47/47/47	-
8	SPO	2	103	-	-	11/47/47/47	-
12	U10	L	306	-	-	14/39/63/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	M	410	-	-	8/35/35/57	-
8	SPO	8	101	-	-	6/44/44/47	-
7	BCL	C	101	-	-	23/37/137/137	-
9	PC1	H	301	-	-	20/50/50/57	-
7	BCL	P	102	-	-	21/37/137/137	-
9	PC1	M	401	-	-	11/43/43/57	-
7	BCL	F	102	-	-	23/37/137/137	-
8	SPO	U	102	-	-	5/47/47/47	-
8	SPO	I	102	-	-	5/47/47/47	-
9	PC1	A	103	-	-	8/35/35/57	-
8	SPO	S	101	-	-	6/47/47/47	-
7	BCL	0	101	-	-	15/31/131/137	-
7	BCL	N	102	-	-	16/37/137/137	-
8	SPO	3	103	-	-	11/47/47/47	-
9	PC1	F	103	-	-	13/40/40/57	-
9	PC1	A	104	-	-	10/35/35/57	-

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	0	101	BCL	C4D-ND	-7.13	1.27	1.37
7	M	403	BCL	C4D-ND	-7.02	1.28	1.37
7	A	101	BCL	C4D-ND	-6.93	1.28	1.37
7	P	102	BCL	C4D-ND	-6.83	1.28	1.37
7	B	101	BCL	C4D-ND	-6.67	1.28	1.37
7	b	101	BCL	C4D-ND	-6.61	1.28	1.37
7	L	309	BCL	C4D-ND	-6.51	1.28	1.37
7	F	104	BCL	C4D-ND	-6.47	1.28	1.37
7	8	102	BCL	C4D-ND	-6.47	1.28	1.37
7	J	102	BCL	C4D-ND	-6.45	1.28	1.37
7	9	101	BCL	C4D-ND	-6.41	1.28	1.37
7	7	101	BCL	C4D-ND	-6.38	1.28	1.37
7	N	102	BCL	C4D-ND	-6.35	1.29	1.37
7	E	101	BCL	C4D-ND	-6.34	1.29	1.37
7	I	101	BCL	C4D-ND	-6.33	1.29	1.37
7	V	101	BCL	C4D-ND	-6.20	1.29	1.37
7	K	101	BCL	C4D-ND	-6.19	1.29	1.37
7	R	103	BCL	C4D-ND	-6.18	1.29	1.37
7	Q	101	BCL	C4D-ND	-6.14	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	302	BCL	C4D-ND	-6.05	1.29	1.37
7	D	102	BCL	C4D-ND	-6.02	1.29	1.37
7	T	101	BCL	C4D-ND	-6.01	1.29	1.37
7	F	102	BCL	C4D-ND	-5.97	1.29	1.37
7	W	102	BCL	C4D-ND	-5.91	1.29	1.37
7	1	101	BCL	C4D-ND	-5.83	1.29	1.37
7	U	101	BCL	C4D-ND	-5.81	1.29	1.37
7	L	301	BCL	C4D-ND	-5.80	1.29	1.37
7	O	101	BCL	C4D-ND	-5.68	1.29	1.37
7	C	101	BCL	C4D-ND	-5.54	1.30	1.37
7	a	101	BCL	C4D-ND	-5.53	1.30	1.37
11	L	311	BPH	C3A-C2A	-5.49	1.49	1.54
7	3	102	BCL	C4D-ND	-5.48	1.30	1.37
7	1	102	BCL	C4D-ND	-5.43	1.30	1.37
7	S	102	BCL	C4D-ND	-5.36	1.30	1.37
7	3	101	BCL	C4D-ND	-5.22	1.30	1.37
7	O	101	BCL	C4B-NB	5.22	1.39	1.35
7	1	102	BCL	C4B-NB	4.91	1.39	1.35
11	L	303	BPH	C3A-C2A	-4.79	1.50	1.54
7	1	101	BCL	C4B-NB	4.79	1.39	1.35
7	W	102	BCL	C4B-NB	4.58	1.39	1.35
10	F	101	CDL	OB8-CB7	4.41	1.46	1.33
9	A	103	PC1	O21-C21	4.38	1.46	1.34
9	H	301	PC1	O21-C21	4.31	1.46	1.34
10	F	101	CDL	OA6-CA5	4.31	1.46	1.34
9	M	402	PC1	O21-C21	4.30	1.46	1.34
10	F	101	CDL	OA8-CA7	4.26	1.45	1.33
9	M	402	PC1	O31-C31	4.22	1.45	1.33
7	b	101	BCL	C4B-NB	4.10	1.38	1.35
9	A	103	PC1	O31-C31	4.01	1.45	1.33
9	H	301	PC1	O31-C31	3.94	1.44	1.33
7	F	102	BCL	C4B-NB	3.89	1.38	1.35
10	F	101	CDL	OB6-CB5	3.89	1.45	1.34
7	3	101	BCL	C4B-NB	3.89	1.38	1.35
11	L	303	BPH	C2C-C3C	-3.77	1.51	1.54
7	I	101	BCL	C4B-NB	3.67	1.38	1.35
7	K	101	BCL	C4B-NB	3.65	1.38	1.35
7	S	102	BCL	C4B-NB	3.60	1.38	1.35
7	V	101	BCL	C4B-NB	3.60	1.38	1.35
7	7	101	BCL	C4B-NB	3.58	1.38	1.35
7	3	102	BCL	C4B-NB	3.56	1.38	1.35
7	Q	101	BCL	C4B-NB	3.51	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	101	BCL	C4B-NB	3.48	1.38	1.35
7	B	101	BCL	C4B-NB	3.45	1.38	1.35
7	A	101	BCL	C4B-NB	3.44	1.38	1.35
7	M	403	BCL	C4B-NB	3.43	1.38	1.35
7	8	102	BCL	C4B-NB	3.41	1.38	1.35
7	L	301	BCL	C4B-NB	3.33	1.38	1.35
7	B	101	BCL	MG-NA	-3.32	1.98	2.06
7	D	102	BCL	C4B-NB	3.22	1.38	1.35
7	L	302	BCL	C4B-NB	3.21	1.38	1.35
7	C	101	BCL	C4B-NB	3.21	1.38	1.35
7	N	102	BCL	C4B-NB	3.16	1.38	1.35
8	I	102	SPO	C16-C17	3.11	1.52	1.45
7	F	104	BCL	C1D-C2D	-3.11	1.39	1.45
8	S	101	SPO	C27-C28	3.08	1.37	1.34
7	L	301	BCL	C1D-C2D	-3.00	1.39	1.45
7	E	101	BCL	C1D-C2D	-2.98	1.39	1.45
7	B	101	BCL	C1D-C2D	-2.89	1.39	1.45
7	L	309	BCL	C1D-C2D	-2.87	1.39	1.45
7	F	104	BCL	C4B-NB	2.86	1.37	1.35
7	P	102	BCL	C4B-NB	2.82	1.37	1.35
7	J	102	BCL	C1D-C2D	-2.81	1.39	1.45
7	O	101	BCL	C1D-C2D	-2.80	1.39	1.45
7	W	102	BCL	C1B-NB	2.75	1.37	1.35
7	R	103	BCL	MG-NA	-2.75	1.99	2.06
7	D	102	BCL	C1D-C2D	-2.71	1.40	1.45
7	0	101	BCL	MG-NA	-2.69	1.99	2.06
7	J	102	BCL	MG-NA	-2.68	1.99	2.06
7	K	101	BCL	C1D-C2D	-2.68	1.40	1.45
7	R	103	BCL	C4B-NB	2.65	1.37	1.35
7	1	102	BCL	C1D-C2D	-2.65	1.40	1.45
7	E	101	BCL	C4B-NB	2.64	1.37	1.35
8	I	102	SPO	C11-C12	2.63	1.51	1.45
7	E	101	BCL	MG-NA	-2.59	2.00	2.06
7	9	101	BCL	C4B-NB	2.57	1.37	1.35
7	T	101	BCL	C4B-NB	2.55	1.37	1.35
7	L	309	BCL	MG-NA	-2.55	2.00	2.06
7	J	102	BCL	C4B-NB	2.53	1.37	1.35
7	0	101	BCL	C1D-C2D	-2.49	1.40	1.45
11	L	311	BPH	C2C-C3C	-2.49	1.52	1.54
7	7	101	BCL	C1D-C2D	-2.49	1.40	1.45
8	0	103	SPO	C22-C23	-2.48	1.32	1.35
7	C	101	BCL	MG-NA	-2.48	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	403	BCL	C1D-C2D	-2.43	1.40	1.45
7	V	101	BCL	C1D-C2D	-2.42	1.40	1.45
7	8	102	BCL	MG-NA	-2.41	2.00	2.06
7	F	104	BCL	MG-NA	-2.41	2.00	2.06
8	S	101	SPO	C25-C23	2.41	1.51	1.45
7	R	103	BCL	C1D-C2D	-2.40	1.40	1.45
8	I	102	SPO	C14-C12	2.39	1.39	1.35
8	K	102	SPO	C25-C23	2.37	1.51	1.45
7	L	301	BCL	MG-NA	-2.36	2.00	2.06
8	K	102	SPO	C27-C28	2.34	1.36	1.34
7	8	102	BCL	C1D-C2D	-2.33	1.40	1.45
7	L	302	BCL	MG-NA	-2.32	2.00	2.06
7	3	101	BCL	C3B-C2B	2.31	1.43	1.39
7	a	101	BCL	C3B-C2B	2.31	1.43	1.39
8	W	101	SPO	C27-C28	2.30	1.36	1.34
7	P	102	BCL	MG-NA	-2.30	2.00	2.06
7	C	101	BCL	C1D-C2D	-2.29	1.40	1.45
7	T	101	BCL	MG-NA	-2.29	2.00	2.06
7	3	102	BCL	C3B-C2B	2.29	1.43	1.39
7	I	101	BCL	MG-NA	-2.28	2.00	2.06
7	a	101	BCL	C4B-NB	2.27	1.37	1.35
8	3	103	SPO	C11-C12	2.27	1.50	1.45
7	E	101	BCL	C3B-C2B	2.24	1.43	1.39
7	J	102	BCL	C3B-C2B	2.24	1.43	1.39
7	9	101	BCL	C1D-C2D	-2.23	1.40	1.45
8	2	102	SPO	C6-C7	2.23	1.50	1.45
11	L	303	BPH	C3B-C2B	2.21	1.43	1.39
7	R	103	BCL	C3B-C2B	2.21	1.43	1.39
8	2	103	SPO	C11-C12	2.21	1.50	1.45
7	Q	101	BCL	C1D-C2D	-2.21	1.41	1.45
7	T	101	BCL	C3B-C2B	2.20	1.43	1.39
8	E	102	SPO	C27-C28	2.20	1.36	1.34
8	E	102	SPO	C16-C17	2.19	1.50	1.45
7	T	101	BCL	C1D-C2D	-2.18	1.41	1.45
8	3	103	SPO	C16-C17	2.17	1.50	1.45
7	O	101	BCL	C1B-NB	2.17	1.37	1.35
7	U	101	BCL	C1D-C2D	-2.17	1.41	1.45
7	3	102	BCL	MG-NA	-2.16	2.01	2.06
7	3	102	BCL	C1D-C2D	-2.16	1.41	1.45
8	0	102	SPO	C15-C14	2.16	1.50	1.43
8	W	101	SPO	C25-C23	2.16	1.50	1.45
7	B	101	BCL	C3B-C2B	2.15	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	302	BCL	C1D-C2D	-2.15	1.41	1.45
8	0	102	SPO	C19-C17	2.15	1.38	1.35
8	O	102	SPO	C25-C23	2.13	1.50	1.45
7	J	102	BCL	C1D-ND	-2.12	1.35	1.37
8	2	102	SPO	C16-C17	2.11	1.50	1.45
7	0	101	BCL	C3B-C2B	2.11	1.43	1.39
8	O	102	SPO	C6-C7	2.10	1.50	1.45
7	L	302	BCL	C3B-C2B	2.09	1.43	1.39
7	V	101	BCL	C3B-C2B	2.09	1.43	1.39
8	E	102	SPO	C19-C17	2.09	1.38	1.35
8	E	102	SPO	C25-C23	2.09	1.50	1.45
7	L	309	BCL	C4B-NB	2.08	1.37	1.35
7	P	102	BCL	C1D-C2D	-2.08	1.41	1.45
7	3	101	BCL	C1D-C2D	-2.08	1.41	1.45
8	0	103	SPO	C19-C17	-2.07	1.33	1.35
7	S	102	BCL	C1D-C2D	-2.06	1.41	1.45
7	0	101	BCL	C4B-NB	2.06	1.37	1.35
7	U	101	BCL	C3B-C2B	2.06	1.43	1.39
7	7	101	BCL	MG-NA	-2.05	2.01	2.06
7	W	102	BCL	C3B-C2B	2.05	1.43	1.39
7	1	101	BCL	C1D-C2D	-2.05	1.41	1.45
7	8	102	BCL	C3B-C2B	2.04	1.43	1.39
11	L	311	BPH	C3B-C2B	2.04	1.43	1.39
7	F	102	BCL	C1D-C2D	-2.04	1.41	1.45
7	L	301	BCL	C3B-C2B	2.04	1.43	1.39
8	0	102	SPO	C6-C7	2.03	1.50	1.45
8	W	101	SPO	C11-C12	2.03	1.50	1.45
7	A	101	BCL	C1D-C2D	-2.03	1.41	1.45
7	1	102	BCL	C3B-C2B	2.02	1.43	1.39
7	C	101	BCL	C3C-C4C	2.02	1.54	1.51
7	M	403	BCL	C3B-C2B	2.01	1.43	1.39
7	C	101	BCL	C3B-C2B	2.00	1.43	1.39
8	F	105	SPO	C25-C23	2.00	1.50	1.45

All (579) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	102	SPO	C8-C7-C9	-9.27	109.93	122.92
8	0	103	SPO	C20-C19-C17	-8.78	114.78	127.31
8	0	103	SPO	C20-C21-C22	-6.88	109.38	123.47
8	I	102	SPO	C29-C28-C30	6.57	126.32	115.27
8	K	102	SPO	C10-C9-C7	6.50	136.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2	103	SPO	C8-C7-C9	-6.22	114.21	122.92
8	2	103	SPO	C13-C12-C14	-6.02	114.49	122.92
8	S	101	SPO	C21-C22-C23	5.84	135.65	127.31
8	0	103	SPO	C10-C11-C12	-5.73	110.33	126.42
8	0	102	SPO	C21-C20-C19	5.61	134.97	123.47
8	0	102	SPO	C5-C6-C7	5.19	133.73	125.89
7	O	101	BCL	CAC-C3C-C2C	-5.16	101.38	114.26
8	0	102	SPO	C20-C21-C22	5.12	133.96	123.47
8	E	102	SPO	C21-C20-C19	5.09	133.90	123.47
7	Q	101	BCL	CAC-C3C-C2C	-5.06	101.61	114.26
8	I	102	SPO	C18-C17-C19	-5.02	115.89	122.92
7	b	101	BCL	CAC-C3C-C2C	-4.99	101.80	114.26
7	K	101	BCL	CAC-C3C-C2C	-4.99	101.80	114.26
7	L	302	BCL	CAC-C3C-C2C	-4.97	101.83	114.26
7	a	101	BCL	CAC-C3C-C2C	-4.94	101.92	114.26
7	3	102	BCL	CAC-C3C-C2C	-4.94	101.92	114.26
7	N	102	BCL	CAC-C3C-C2C	-4.90	102.03	114.26
7	9	101	BCL	CAC-C3C-C2C	-4.90	102.03	114.26
7	1	101	BCL	CAC-C3C-C2C	-4.88	102.06	114.26
8	R	102	SPO	C29-C28-C30	4.86	123.45	115.27
7	C	101	BCL	CAC-C3C-C2C	-4.84	102.16	114.26
8	S	101	SPO	C24-C23-C25	4.82	125.67	118.08
7	0	101	BCL	CAC-C3C-C2C	-4.82	102.22	114.26
7	F	102	BCL	CAC-C3C-C2C	-4.80	102.26	114.26
7	D	102	BCL	CAC-C3C-C2C	-4.80	102.27	114.26
8	S	101	SPO	C20-C21-C22	4.80	133.31	123.47
7	A	101	BCL	CAC-C3C-C2C	-4.79	102.28	114.26
7	V	101	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
8	0	102	SPO	C6-C7-C9	4.79	126.28	118.94
7	1	102	BCL	CAC-C3C-C2C	-4.78	102.33	114.26
8	0	102	SPO	C21-C22-C23	-4.77	120.50	127.31
8	E	102	SPO	C8-C7-C9	-4.76	116.25	122.92
8	0	102	SPO	C8-C7-C6	-4.76	110.58	118.08
7	3	101	BCL	CAC-C3C-C2C	-4.75	102.39	114.26
7	W	102	BCL	CAC-C3C-C2C	-4.74	102.41	114.26
7	L	301	BCL	CAC-C3C-C2C	-4.71	102.49	114.26
7	S	102	BCL	CAC-C3C-C2C	-4.70	102.50	114.26
7	L	309	BCL	CAC-C3C-C2C	-4.70	102.51	114.26
7	U	101	BCL	CAC-C3C-C2C	-4.68	102.57	114.26
8	0	102	SPO	C29-C28-C30	4.66	123.11	115.27
7	J	102	BCL	CAC-C3C-C2C	-4.64	102.68	114.26
8	K	102	SPO	C6-C7-C9	4.63	126.05	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	104	BCL	CAC-C3C-C2C	-4.61	102.73	114.26
7	T	101	BCL	CAC-C3C-C2C	-4.61	102.75	114.26
7	8	102	BCL	CAC-C3C-C2C	-4.60	102.78	114.26
7	P	102	BCL	CAC-C3C-C2C	-4.57	102.84	114.26
11	L	303	BPH	C1C-C2C-C3C	-4.55	98.50	102.84
7	R	103	BCL	CAC-C3C-C2C	-4.55	102.89	114.26
8	O	102	SPO	C29-C28-C30	4.52	122.88	115.27
7	7	101	BCL	CAC-C3C-C2C	-4.50	103.03	114.26
7	I	101	BCL	CAC-C3C-C2C	-4.43	103.18	114.26
8	F	105	SPO	C29-C28-C30	4.41	122.70	115.27
8	K	102	SPO	C20-C21-C22	4.40	132.50	123.47
8	K	102	SPO	C21-C20-C19	4.40	132.48	123.47
10	F	101	CDL	OA6-CA5-C11	4.39	120.96	111.50
8	I	102	SPO	C29-C28-C27	-4.39	111.27	122.59
7	M	403	BCL	CAC-C3C-C2C	-4.38	103.31	114.26
8	I	102	SPO	C21-C20-C19	4.36	132.40	123.47
8	2	102	SPO	C20-C19-C17	4.34	133.50	127.31
9	H	301	PC1	O21-C21-C22	4.33	120.83	111.50
8	T	102	SPO	C13-C12-C11	4.32	124.89	118.08
8	I	102	SPO	C21-C22-C23	-4.31	121.16	127.31
8	E	102	SPO	C20-C21-C22	4.29	132.27	123.47
8	2	102	SPO	C24-C23-C25	4.23	124.75	118.08
8	0	102	SPO	C2-C1-C4	4.21	117.32	110.86
7	L	301	BCL	C3D-C4D-ND	-4.21	103.43	110.24
9	A	103	PC1	O21-C21-C22	4.19	120.54	111.50
8	2	102	SPO	C5-C6-C7	4.16	132.18	125.89
7	E	101	BCL	CAC-C3C-C2C	-4.16	103.86	114.26
8	W	101	SPO	C10-C9-C7	4.12	133.20	127.31
8	O	102	SPO	C24-C23-C25	4.12	124.57	118.08
8	I	102	SPO	C15-C14-C12	-4.09	121.47	127.31
8	3	103	SPO	C13-C12-C14	-4.03	117.28	122.92
8	3	103	SPO	C8-C7-C9	-4.02	117.29	122.92
7	B	101	BCL	CAC-C3C-C2C	-3.97	104.34	114.26
7	b	101	BCL	C1D-CHD-C4C	-3.97	117.05	126.62
7	b	101	BCL	CMA-C3A-C4A	-3.93	101.21	111.77
8	I	102	SPO	C20-C19-C17	-3.91	121.73	127.31
8	R	102	SPO	C24-C23-C25	3.91	124.24	118.08
8	S	101	SPO	C21-C20-C19	-3.90	115.49	123.47
8	E	102	SPO	C5-C6-C7	3.85	131.71	125.89
8	3	103	SPO	C18-C17-C19	-3.83	117.55	122.92
8	E	102	SPO	C21-C22-C23	-3.81	121.88	127.31
8	0	102	SPO	C20-C19-C17	-3.81	121.88	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	8	101	SPO	C2-C1-C4	-3.78	105.06	110.86
8	E	102	SPO	C29-C28-C30	3.77	121.61	115.27
8	0	103	SPO	C24-C23-C25	3.76	124.00	118.08
8	2	102	SPO	C18-C17-C16	3.76	124.00	118.08
8	I	102	SPO	C10-C9-C7	-3.75	121.96	127.31
8	2	102	SPO	C21-C20-C19	3.74	131.13	123.47
8	F	105	SPO	C24-C23-C25	3.71	123.93	118.08
8	K	102	SPO	C8-C7-C6	3.69	123.89	118.08
8	W	101	SPO	C24-C23-C25	3.66	123.85	118.08
8	I	102	SPO	C20-C21-C22	3.65	130.94	123.47
8	3	103	SPO	C11-C12-C14	3.64	124.53	118.94
8	0	103	SPO	C5-C6-C7	-3.63	120.40	125.89
8	S	101	SPO	C25-C23-C22	-3.62	113.39	118.94
9	M	402	PC1	O21-C21-C22	3.62	119.29	111.50
8	K	102	SPO	C21-C22-C23	-3.60	122.18	127.31
8	W	101	SPO	C8-C7-C6	3.58	123.72	118.08
8	R	102	SPO	C11-C12-C14	3.56	124.41	118.94
7	0	101	BCL	C1D-ND-C4D	3.55	108.86	106.33
8	K	102	SPO	C5-C6-C7	3.54	131.24	125.89
10	F	101	CDL	OB6-CB5-C51	3.53	119.10	111.50
7	b	101	BCL	C2C-C3C-C4C	-3.52	96.06	101.34
9	A	103	PC1	C11-C12-N	-3.52	104.02	115.78
8	3	103	SPO	C6-C7-C9	3.51	124.32	118.94
7	F	104	BCL	C2A-C3A-C4A	-3.49	96.23	101.87
7	I	101	BCL	CMA-C3A-C4A	-3.48	102.42	111.77
8	2	103	SPO	C21-C20-C19	-3.45	116.42	123.47
12	X	101	U10	C7-C6-C5	-3.44	114.33	118.48
8	0	103	SPO	C18-C17-C19	-3.44	118.10	122.92
7	L	302	BCL	CHC-C1C-NC	3.44	129.27	124.51
8	I	102	SPO	C18-C17-C16	3.44	123.50	118.08
8	O	102	SPO	C5-C6-C7	3.41	131.05	125.89
8	0	103	SPO	C34-C33-C35	3.41	121.01	115.27
7	b	101	BCL	CGD-CBD-CAD	3.41	121.77	110.73
8	T	102	SPO	C24-C23-C25	3.39	123.42	118.08
8	D	101	SPO	C2-C1-C4	-3.36	105.69	110.86
8	E	102	SPO	C20-C19-C17	-3.36	122.52	127.31
7	J	102	BCL	C3D-C4D-ND	-3.35	104.81	110.24
11	L	311	BPH	CMA-C3A-C4A	-3.35	107.03	114.38
7	M	403	BCL	C4D-CHA-C1A	3.34	125.31	121.25
8	T	102	SPO	C8-C7-C6	3.31	123.29	118.08
8	O	102	SPO	C8-C7-C6	3.31	123.29	118.08
8	3	103	SPO	C21-C22-C23	-3.30	122.60	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	101	BCL	C4D-CHA-C1A	3.30	125.26	121.25
7	3	102	BCL	C2A-C3A-C4A	-3.29	96.55	101.87
7	N	102	BCL	C4D-CHA-C1A	3.28	125.25	121.25
7	S	102	BCL	C1D-ND-C4D	3.28	108.67	106.33
7	3	102	BCL	CHC-C1C-NC	3.28	129.04	124.51
8	S	101	SPO	C8-C7-C6	3.26	123.22	118.08
8	W	101	SPO	C6-C7-C9	-3.26	113.94	118.94
8	R	102	SPO	C34-C33-C35	3.25	120.73	115.27
7	0	101	BCL	CMA-C3A-C4A	-3.24	103.05	111.77
8	2	102	SPO	C16-C17-C19	-3.24	113.96	118.94
8	P	101	SPO	C3-C1-C4	-3.24	105.88	110.86
7	B	101	BCL	CHC-C1C-NC	3.23	128.98	124.51
7	B	101	BCL	C2A-C3A-C4A	-3.23	96.65	101.87
7	3	101	BCL	C3D-C4D-ND	-3.23	105.02	110.24
7	b	101	BCL	C1C-NC-C4C	-3.22	105.26	106.71
8	3	103	SPO	C14-C15-C16	3.21	133.24	123.22
8	E	102	SPO	C34-C33-C35	3.20	120.66	115.27
7	P	102	BCL	C4D-CHA-C1A	3.20	125.14	121.25
8	R	102	SPO	C15-C14-C12	-3.19	122.75	127.31
8	2	103	SPO	C13-C12-C11	3.18	123.09	118.08
7	W	102	BCL	CHC-C1C-NC	3.17	128.90	124.51
8	K	102	SPO	C9-C10-C11	3.16	133.07	123.22
7	b	101	BCL	CHC-C1C-NC	3.16	128.88	124.51
7	L	309	BCL	C1D-ND-C4D	3.15	108.58	106.33
8	2	102	SPO	C6-C7-C9	-3.15	114.11	118.94
7	L	309	BCL	CHC-C1C-NC	3.14	128.86	124.51
7	9	101	BCL	C4D-CHA-C1A	3.14	125.07	121.25
7	M	403	BCL	CHC-C1C-NC	3.14	128.86	124.51
10	F	101	CDL	OA8-CA7-C31	3.14	121.76	111.91
8	E	102	SPO	C13-C12-C11	3.14	123.02	118.08
8	2	102	SPO	C20-C21-C22	-3.13	117.07	123.47
7	U	101	BCL	C4D-CHA-C1A	3.12	125.05	121.25
7	I	101	BCL	C1D-ND-C4D	3.12	108.55	106.33
7	Q	101	BCL	C4D-CHA-C1A	3.11	125.03	121.25
7	9	101	BCL	CHC-C1C-NC	3.10	128.80	124.51
7	J	102	BCL	CHC-C1C-NC	3.10	128.80	124.51
8	2	103	SPO	C16-C17-C19	-3.10	114.18	118.94
8	K	102	SPO	C20-C19-C17	-3.10	122.89	127.31
8	Z	101	SPO	C3-C1-C4	-3.08	106.13	110.86
8	W	101	SPO	C9-C10-C11	3.08	132.82	123.22
7	3	101	BCL	CHC-C1C-NC	3.07	128.76	124.51
7	B	101	BCL	C1D-CHD-C4C	-3.07	119.21	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	9	101	BCL	CMA-C3A-C4A	-3.07	103.52	111.77
8	2	102	SPO	C8-C7-C6	3.07	122.92	118.08
7	a	101	BCL	C4D-CHA-C1A	3.07	124.99	121.25
7	L	302	BCL	C1D-ND-C4D	3.06	108.51	106.33
7	J	102	BCL	C4D-CHA-C1A	3.06	124.97	121.25
8	K	102	SPO	C31-C32-C33	-3.06	120.30	127.66
7	I	101	BCL	C4D-CHA-C1A	3.06	124.97	121.25
7	T	101	BCL	C2A-C3A-C4A	-3.05	96.94	101.87
7	F	104	BCL	C4D-CHA-C1A	3.05	124.95	121.25
8	S	101	SPO	C16-C17-C19	-3.04	114.28	118.94
7	E	101	BCL	C4D-CHA-C1A	3.04	124.95	121.25
8	S	101	SPO	C13-C12-C11	3.02	122.83	118.08
7	b	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
7	0	101	BCL	C2A-C3A-C4A	-3.02	97.00	101.87
7	F	102	BCL	CMA-C3A-C4A	-3.01	103.67	111.77
7	3	101	BCL	C4D-CHA-C1A	3.01	124.91	121.25
8	0	103	SPO	C10-C9-C7	-3.01	123.02	127.31
7	W	102	BCL	C2C-C3C-C4C	-3.00	96.84	101.34
8	0	103	SPO	C15-C16-C17	-3.00	117.99	126.42
8	W	101	SPO	C34-C33-C35	3.00	120.32	115.27
7	S	102	BCL	CHC-C1C-NC	2.99	128.65	124.51
8	0	103	SPO	C40-C38-C39	2.99	121.20	114.60
8	0	103	SPO	C8-C7-C6	2.98	122.77	118.08
8	2	103	SPO	C5-C6-C7	2.97	130.39	125.89
8	R	102	SPO	C20-C21-C22	-2.96	117.40	123.47
7	D	102	BCL	C4D-CHA-C1A	2.96	124.85	121.25
7	7	101	BCL	CMA-C3A-C4A	-2.96	103.83	111.77
7	7	101	BCL	C1D-CHD-C4C	-2.96	119.49	126.62
7	C	101	BCL	C4D-CHA-C1A	2.95	124.84	121.25
7	1	102	BCL	C4D-CHA-C1A	2.95	124.84	121.25
7	L	301	BCL	CMA-C3A-C4A	-2.94	103.86	111.77
8	R	102	SPO	C13-C12-C11	-2.94	113.44	118.08
7	P	102	BCL	CMA-C3A-C4A	-2.94	103.86	111.77
8	3	103	SPO	C15-C16-C17	2.93	134.65	126.42
7	O	101	BCL	C4D-CHA-C1A	2.92	124.80	121.25
7	1	102	BCL	CMA-C3A-C4A	-2.91	103.95	111.77
7	C	101	BCL	CMA-C3A-C4A	-2.91	103.96	111.77
7	K	101	BCL	C4D-CHA-C1A	2.91	124.79	121.25
8	E	102	SPO	C24-C23-C22	-2.90	118.87	122.92
8	I	102	SPO	C14-C15-C16	2.89	132.23	123.22
7	R	103	BCL	CMA-C3A-C4A	-2.88	104.02	111.77
7	T	101	BCL	C4D-CHA-C1A	2.88	124.75	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	0	103	SPO	C31-C32-C33	-2.87	120.74	127.66
7	R	103	BCL	C2A-C3A-C4A	-2.87	97.23	101.87
8	S	101	SPO	C15-C14-C12	-2.86	123.22	127.31
7	T	101	BCL	C1D-CHD-C4C	-2.86	119.72	126.62
8	T	102	SPO	C29-C28-C30	2.86	120.08	115.27
8	R	102	SPO	C6-C7-C9	2.86	123.33	118.94
8	0	102	SPO	C31-C32-C33	-2.86	120.78	127.66
8	0	102	SPO	C14-C15-C16	2.86	132.13	123.22
7	A	101	BCL	C4D-CHA-C1A	2.85	124.72	121.25
7	W	102	BCL	C4D-CHA-C1A	2.85	124.72	121.25
7	8	102	BCL	CMA-C3A-C4A	-2.85	104.11	111.77
8	W	101	SPO	C24-C23-C22	-2.85	118.93	122.92
7	7	101	BCL	CHC-C1C-NC	2.85	128.45	124.51
7	W	102	BCL	CMA-C3A-C4A	-2.85	104.12	111.77
7	D	102	BCL	C1D-ND-C4D	2.84	108.36	106.33
8	2	103	SPO	C8-C7-C6	2.84	122.56	118.08
7	L	309	BCL	CMA-C3A-C4A	-2.84	104.14	111.77
7	U	101	BCL	CHC-C1C-NC	2.84	128.44	124.51
7	N	102	BCL	CMA-C3A-C4A	-2.84	104.15	111.77
7	F	102	BCL	CHC-C1C-NC	2.83	128.43	124.51
7	0	101	BCL	C4D-CHA-C1A	2.83	124.69	121.25
7	N	102	BCL	CHC-C1C-NC	2.83	128.42	124.51
8	T	102	SPO	C11-C12-C14	-2.82	114.62	118.94
7	8	102	BCL	C4D-CHA-C1A	2.82	124.68	121.25
7	J	102	BCL	CMA-C3A-C4A	-2.81	104.22	111.77
8	3	103	SPO	C21-C20-C19	2.81	129.23	123.47
8	S	101	SPO	C18-C17-C16	2.80	122.49	118.08
7	T	101	BCL	CHC-C1C-NC	2.80	128.38	124.51
8	2	103	SPO	C21-C22-C23	-2.80	123.32	127.31
7	I	101	BCL	CHC-C1C-NC	2.79	128.37	124.51
7	S	102	BCL	C4D-CHA-C1A	2.79	124.64	121.25
8	2	101	SPO	C21-C20-C19	2.79	129.19	123.47
7	F	104	BCL	C3D-C4D-ND	-2.79	105.72	110.24
7	1	101	BCL	C4D-CHA-C1A	2.79	124.64	121.25
8	0	103	SPO	C27-C26-C25	-2.79	114.52	123.22
7	T	101	BCL	CMA-C3A-C4A	-2.79	104.28	111.77
8	2	103	SPO	C6-C7-C9	2.78	123.20	118.94
8	M	406	SPO	C3-C1-C4	-2.77	106.60	110.86
7	U	101	BCL	CMA-C3A-C4A	-2.77	104.33	111.77
8	9	102	SPO	C2-C1-C4	-2.77	106.61	110.86
7	K	101	BCL	CMA-C3A-C4A	-2.76	104.35	111.77
8	0	103	SPO	C29-C28-C30	2.75	119.91	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	101	BCL	CMA-C3A-C4A	-2.75	104.38	111.77
7	E	101	BCL	C1D-CHD-C4C	-2.75	119.99	126.62
12	X	101	U10	C8-C7-C6	2.75	119.45	112.05
8	2	103	SPO	C24-C23-C25	2.75	122.40	118.08
7	V	101	BCL	C1D-CHD-C4C	-2.73	120.03	126.62
7	a	101	BCL	C4B-CHC-C1C	-2.72	124.73	130.12
7	F	102	BCL	C4D-CHA-C1A	2.72	124.56	121.25
9	A	103	PC1	O31-C31-C32	2.71	120.42	111.91
7	V	101	BCL	C4D-CHA-C1A	2.71	124.55	121.25
8	3	103	SPO	C24-C23-C25	2.71	122.35	118.08
7	3	102	BCL	CMA-C3A-C4A	-2.70	104.51	111.77
7	L	301	BCL	C4D-CHA-C1A	2.70	124.54	121.25
7	F	104	BCL	CMA-C3A-C4A	-2.70	104.53	111.77
8	O	102	SPO	C20-C21-C22	-2.69	117.96	123.47
7	1	102	BCL	C3D-C4D-ND	-2.69	105.88	110.24
8	F	105	SPO	C11-C12-C14	-2.69	114.81	118.94
7	C	101	BCL	CHC-C1C-NC	2.69	128.23	124.51
7	T	101	BCL	C3D-C4D-ND	-2.69	105.89	110.24
10	F	101	CDL	OB8-CB7-C71	2.68	120.33	111.91
7	E	101	BCL	C2A-C3A-C4A	-2.68	97.54	101.87
7	K	101	BCL	C1C-NC-C4C	-2.68	105.50	106.71
8	R	102	SPO	C8-C7-C6	-2.68	113.86	118.08
8	S	101	SPO	C13-C12-C14	-2.67	119.18	122.92
7	0	101	BCL	CHC-C1C-NC	2.67	128.21	124.51
7	J	102	BCL	C3D-C2D-C1D	-2.67	102.19	105.83
7	8	102	BCL	C2A-C3A-C4A	-2.66	97.57	101.87
7	M	403	BCL	C3C-C4C-CHD	-2.66	117.71	123.39
7	a	101	BCL	CHC-C1C-NC	2.66	128.19	124.51
7	b	101	BCL	C3D-C2D-C1D	-2.66	102.21	105.83
7	R	103	BCL	C4D-CHA-C1A	2.65	124.48	121.25
7	S	102	BCL	CMA-C3A-C4A	-2.65	104.65	111.77
7	L	301	BCL	C3D-C2D-C1D	-2.65	102.22	105.83
7	W	102	BCL	C1C-NC-C4C	-2.65	105.52	106.71
7	M	403	BCL	CMA-C3A-C4A	-2.64	104.67	111.77
7	J	102	BCL	C2A-C3A-C4A	-2.64	97.60	101.87
7	A	101	BCL	C1D-ND-C4D	2.64	108.21	106.33
7	V	101	BCL	C3D-C4D-ND	-2.64	105.96	110.24
8	S	101	SPO	C14-C15-C16	2.64	131.46	123.22
7	R	103	BCL	C3D-C4D-ND	-2.64	105.97	110.24
7	b	101	BCL	C3D-C4D-ND	-2.64	105.97	110.24
7	D	102	BCL	CHC-C1C-NC	2.64	128.16	124.51
7	N	102	BCL	C3D-C4D-ND	-2.63	105.97	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	SPO	C2-C1-C4	-2.63	106.81	110.86
8	K	102	SPO	C14-C15-C16	2.63	131.44	123.22
7	K	101	BCL	C1D-CHD-C4C	-2.63	120.27	126.62
7	A	101	BCL	CMA-C3A-C4A	-2.63	104.71	111.77
8	2	102	SPO	C2-C1-C4	2.62	114.88	110.86
7	b	101	BCL	C4D-CHA-C1A	2.62	124.44	121.25
7	1	101	BCL	CHC-C1C-NC	2.62	128.14	124.51
7	L	309	BCL	C4D-CHA-C1A	2.62	124.43	121.25
7	N	102	BCL	CMD-C2D-C1D	2.62	129.32	124.71
7	A	101	BCL	C3C-C4C-CHD	-2.61	117.81	123.39
7	P	102	BCL	C3D-C2D-C1D	-2.61	102.27	105.83
7	F	104	BCL	CHC-C1C-NC	2.61	128.12	124.51
7	L	301	BCL	CMD-C2D-C1D	2.61	129.31	124.71
7	O	101	BCL	CHC-C1C-NC	2.61	128.12	124.51
7	A	101	BCL	CHC-C1C-NC	2.61	128.12	124.51
7	O	101	BCL	CMA-C3A-C4A	-2.58	104.83	111.77
7	7	101	BCL	C3D-C4D-ND	-2.58	106.06	110.24
7	D	102	BCL	CMA-C3A-C4A	-2.58	104.85	111.77
7	1	101	BCL	CMA-C3A-C4A	-2.58	104.85	111.77
7	D	102	BCL	C3C-C4C-CHD	-2.57	117.89	123.39
7	Q	101	BCL	CMA-C3A-C4A	-2.57	104.87	111.77
11	L	303	BPH	CMA-C3A-C4A	-2.57	108.75	114.38
8	F	105	SPO	C24-C23-C22	-2.56	119.33	122.92
7	F	102	BCL	C1D-ND-C4D	2.56	108.15	106.33
8	K	102	SPO	C3-C1-C4	2.56	114.78	110.86
8	8	101	SPO	C3-C1-C4	-2.55	106.94	110.86
8	3	103	SPO	C20-C21-C22	2.54	128.68	123.47
7	E	101	BCL	CMA-C3A-C4A	-2.53	104.97	111.77
7	a	101	BCL	CMD-C2D-C1D	2.53	129.17	124.71
7	C	101	BCL	C2A-C3A-C4A	-2.53	97.79	101.87
7	a	101	BCL	CMA-C3A-C4A	-2.53	104.98	111.77
8	E	102	SPO	C35-C33-C32	-2.53	116.00	121.12
7	V	101	BCL	CHC-C1C-NC	2.53	128.00	124.51
7	E	101	BCL	CHC-C1C-NC	2.52	128.00	124.51
7	L	302	BCL	CMA-C3A-C4A	-2.52	105.01	111.77
7	a	101	BCL	C3D-C2D-C1D	-2.51	102.40	105.83
7	1	101	BCL	CHA-C1A-NA	-2.51	120.65	126.40
7	N	102	BCL	C3D-C2D-C1D	-2.51	102.41	105.83
8	I	102	SPO	C13-C12-C14	-2.51	119.41	122.92
8	2	102	SPO	C25-C23-C22	-2.51	115.10	118.94
7	N	102	BCL	C1-C2-C3	-2.50	121.72	126.04
8	R	102	SPO	C25-C23-C22	-2.50	115.10	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	101	BCL	C4D-CHA-C1A	2.49	124.28	121.25
7	O	101	BCL	C1D-CHD-C4C	-2.49	120.62	126.62
7	1	102	BCL	C1D-CHD-C4C	-2.48	120.63	126.62
8	2	102	SPO	C9-C10-C11	2.48	130.95	123.22
8	D	103	SPO	C2-C1-C4	-2.48	107.06	110.86
8	R	102	SPO	C34-C33-C32	-2.48	117.33	123.68
8	E	102	SPO	C14-C15-C16	2.47	130.94	123.22
8	J	101	SPO	C2-C1-C4	-2.47	107.06	110.86
7	1	102	BCL	C1C-NC-C4C	-2.47	105.60	106.71
7	8	102	BCL	CHC-C1C-NC	2.47	127.92	124.51
7	I	101	BCL	C1D-CHD-C4C	-2.47	120.67	126.62
7	D	102	BCL	C3D-C4D-ND	-2.46	106.25	110.24
7	3	101	BCL	C3D-C2D-C1D	-2.46	102.47	105.83
8	K	102	SPO	C40-C38-C39	2.46	120.04	114.60
8	O	102	SPO	C6-C7-C9	-2.46	115.17	118.94
8	0	102	SPO	C34-C33-C35	2.46	119.41	115.27
7	O	101	BCL	C3D-C4D-ND	-2.46	106.26	110.24
8	2	103	SPO	C14-C15-C16	-2.45	115.57	123.22
7	3	102	BCL	C4D-CHA-C1A	2.45	124.23	121.25
8	0	102	SPO	C3-C1-C4	-2.45	107.10	110.86
7	1	102	BCL	CHC-C1C-NC	2.45	127.90	124.51
7	V	101	BCL	CMA-C3A-C4A	-2.45	105.20	111.77
7	T	101	BCL	CHA-C1A-NA	-2.45	120.80	126.40
7	b	101	BCL	CMD-C2D-C1D	2.44	129.01	124.71
7	P	102	BCL	CMD-C2D-C1D	2.43	129.00	124.71
7	3	101	BCL	CMA-C3A-C4A	-2.43	105.23	111.77
8	E	102	SPO	C8-C7-C6	2.43	121.91	118.08
8	0	103	SPO	C11-C12-C14	-2.43	115.21	118.94
12	L	306	U10	C7-C6-C5	-2.43	115.56	118.48
7	P	102	BCL	CHC-C1C-NC	2.42	127.86	124.51
10	F	101	CDL	OA6-CA5-OA7	-2.41	117.87	123.70
7	L	302	BCL	CGD-CBD-CAD	-2.41	102.94	110.73
7	C	101	BCL	C4B-CHC-C1C	-2.41	125.35	130.12
7	0	101	BCL	C1D-CHD-C4C	-2.40	120.82	126.62
8	N	101	SPO	C3-C1-C4	-2.40	107.18	110.86
12	L	304	U10	C7-C6-C5	-2.39	115.60	118.48
8	O	102	SPO	C3-C1-C4	-2.39	107.19	110.86
8	S	103	SPO	C2-C1-C4	-2.39	107.19	110.86
8	2	102	SPO	C11-C12-C14	-2.38	115.29	118.94
8	O	102	SPO	C31-C32-C33	-2.38	121.93	127.66
7	L	302	BCL	CHA-C1A-NA	-2.38	120.95	126.40
7	3	102	BCL	C3D-C4D-ND	-2.37	106.40	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	101	BCL	C3C-C4C-CHD	-2.37	118.32	123.39
7	7	101	BCL	C3D-C2D-C1D	-2.37	102.59	105.83
8	F	105	SPO	C21-C20-C19	-2.37	118.62	123.47
7	L	301	BCL	CHC-C1C-NC	2.37	127.79	124.51
8	E	102	SPO	C11-C12-C14	-2.37	115.31	118.94
8	0	103	SPO	C25-C23-C22	-2.37	115.31	118.94
7	7	101	BCL	CMD-C2D-C1D	2.36	128.88	124.71
8	3	103	SPO	C15-C14-C12	-2.36	123.94	127.31
7	L	301	BCL	CHA-C1A-NA	-2.36	120.99	126.40
7	K	101	BCL	CHC-C1C-NC	2.36	127.77	124.51
7	T	101	BCL	C3D-C2D-C1D	-2.35	102.62	105.83
7	3	101	BCL	CMD-C2D-C1D	2.35	128.86	124.71
7	Q	101	BCL	CHA-C1A-NA	-2.35	121.01	126.40
7	L	301	BCL	C1D-ND-C4D	2.35	108.01	106.33
11	L	311	BPH	CAC-C3C-C2C	-2.35	108.38	114.26
12	L	308	U10	C7-C6-C5	-2.35	115.65	118.48
7	0	101	BCL	CHA-C1A-NA	-2.35	121.02	126.40
7	3	101	BCL	C2C-C3C-C4C	-2.35	97.83	101.34
8	W	101	SPO	C34-C33-C32	-2.34	117.67	123.68
7	J	102	BCL	C1D-CHD-C4C	-2.34	120.98	126.62
7	F	104	BCL	CHA-C1A-NA	-2.34	121.04	126.40
8	S	103	SPO	C14-C15-C16	2.34	130.51	123.22
7	9	101	BCL	CHA-C1A-NA	-2.33	121.06	126.40
7	O	101	BCL	C3D-C2D-C1D	-2.33	102.65	105.83
7	7	101	BCL	C2C-C3C-C4C	-2.33	97.85	101.34
7	E	101	BCL	C3D-C4D-ND	-2.33	106.47	110.24
7	9	101	BCL	C3C-C4C-CHD	-2.32	118.43	123.39
7	W	102	BCL	C1D-CHD-C4C	-2.32	121.02	126.62
7	Q	101	BCL	CHC-C1C-NC	2.32	127.72	124.51
7	K	101	BCL	CHA-C1A-NA	-2.31	121.10	126.40
8	T	102	SPO	C8-C7-C9	-2.31	119.69	122.92
7	M	403	BCL	C3D-C2D-C1D	-2.31	102.68	105.83
7	P	102	BCL	C3D-C4D-ND	-2.31	106.50	110.24
7	R	103	BCL	CHC-C1C-NC	2.30	127.70	124.51
7	C	101	BCL	C3D-C4D-ND	-2.30	106.51	110.24
7	1	101	BCL	C3D-C2D-C1D	-2.30	102.69	105.83
7	V	101	BCL	CHA-C1A-NA	-2.30	121.13	126.40
8	T	102	SPO	C21-C20-C19	-2.30	118.77	123.47
7	B	101	BCL	C1C-NC-C4C	-2.30	105.67	106.71
7	J	102	BCL	CMD-C2D-C1D	2.29	128.76	124.71
7	8	102	BCL	C3D-C2D-C1D	-2.29	102.70	105.83
7	B	101	BCL	C2C-C3C-C4C	-2.29	97.91	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	102	BCL	CHA-C1A-NA	-2.29	121.16	126.40
12	L	307	U10	C7-C6-C5	-2.28	115.73	118.48
11	L	311	BPH	CMD-C2D-C3D	2.28	128.95	124.68
7	K	101	BCL	C3D-C2D-C1D	-2.28	102.72	105.83
8	S	101	SPO	C15-C16-C17	2.28	132.82	126.42
7	V	101	BCL	C3D-C2D-C1D	-2.28	102.72	105.83
8	K	102	SPO	C39-C38-C37	-2.27	116.08	122.65
7	K	101	BCL	C3D-C4D-ND	-2.27	106.56	110.24
7	K	101	BCL	C2A-C3A-C4A	-2.27	98.20	101.87
7	8	102	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
8	2	103	SPO	C11-C12-C14	2.27	122.42	118.94
7	3	102	BCL	CHA-C1A-NA	-2.26	121.22	126.40
7	9	101	BCL	CMD-C2D-C1D	2.26	128.69	124.71
8	2	102	SPO	C13-C12-C11	2.26	121.63	118.08
7	R	103	BCL	C3D-C2D-C1D	-2.25	102.75	105.83
8	2	101	SPO	C20-C21-C22	2.25	128.09	123.47
7	9	101	BCL	C3D-C2D-C1D	-2.25	102.76	105.83
7	S	102	BCL	CHA-C1A-NA	-2.25	121.25	126.40
7	1	102	BCL	C3D-C2D-C1D	-2.25	102.76	105.83
7	3	101	BCL	CHA-C1A-NA	-2.24	121.26	126.40
9	M	402	PC1	O31-C31-C32	2.23	118.92	111.91
7	3	101	BCL	C1D-CHD-C4C	-2.23	121.24	126.62
7	1	101	BCL	C2A-C3A-C4A	-2.23	98.26	101.87
7	A	101	BCL	CMD-C2D-C1D	2.23	128.64	124.71
7	M	403	BCL	CMD-C2D-C1D	2.23	128.64	124.71
7	3	102	BCL	C3D-C2D-C1D	-2.23	102.79	105.83
7	1	101	BCL	CMD-C2D-C1D	2.23	128.64	124.71
7	A	101	BCL	CHA-C1A-NA	-2.22	121.31	126.40
7	R	103	BCL	C4B-CHC-C1C	-2.22	125.72	130.12
7	1	101	BCL	C3D-C4D-ND	-2.22	106.65	110.24
8	O	102	SPO	C34-C33-C35	2.22	119.00	115.27
7	a	101	BCL	C2A-C3A-C4A	-2.22	98.29	101.87
7	7	101	BCL	CHA-C1A-NA	-2.21	121.34	126.40
7	Q	101	BCL	C3C-C4C-CHD	-2.21	118.68	123.39
7	8	102	BCL	C3C-C4C-CHD	-2.21	118.68	123.39
7	O	101	BCL	CHA-C1A-NA	-2.20	121.35	126.40
7	3	101	BCL	C2A-C3A-C4A	-2.20	98.32	101.87
8	O	102	SPO	C25-C23-C22	-2.20	115.57	118.94
7	3	101	BCL	C1B-CHB-C4A	-2.20	125.77	130.12
7	L	309	BCL	C3C-C4C-CHD	-2.19	118.71	123.39
7	b	101	BCL	C2A-C1A-CHA	2.19	127.69	123.86
8	O	102	SPO	C24-C23-C22	-2.19	119.86	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	102	SPO	C30-C28-C27	-2.19	115.35	121.98
8	W	101	SPO	C20-C21-C22	-2.19	119.00	123.47
7	U	101	BCL	CHA-C1A-NA	-2.19	121.39	126.40
8	9	102	SPO	C3-C1-C4	-2.18	107.50	110.86
7	L	301	BCL	C1D-CHD-C4C	-2.18	121.36	126.62
7	8	102	BCL	CMD-C2D-C1D	2.18	128.56	124.71
7	L	309	BCL	CHA-C1A-NA	-2.18	121.41	126.40
7	S	102	BCL	C3C-C4C-CHD	-2.18	118.74	123.39
7	T	101	BCL	CMD-C2D-C1D	2.17	128.55	124.71
7	L	302	BCL	CMD-C2D-C1D	2.17	128.54	124.71
7	F	104	BCL	C1D-CHD-C4C	-2.17	121.38	126.62
8	S	101	SPO	C10-C9-C7	-2.17	124.22	127.31
7	Q	101	BCL	C3D-C2D-C1D	-2.17	102.87	105.83
8	T	102	SPO	C40-C38-C39	2.17	119.39	114.60
7	Q	101	BCL	CMD-C2D-C1D	2.16	128.53	124.71
7	O	101	BCL	CMD-C2D-C1D	2.16	128.53	124.71
7	P	102	BCL	C1D-CHD-C4C	-2.16	121.41	126.62
7	B	101	BCL	CHA-C1A-NA	-2.16	121.46	126.40
7	I	101	BCL	CHA-C1A-NA	-2.16	121.46	126.40
7	I	101	BCL	CMD-C2D-C1D	2.15	128.51	124.71
7	W	102	BCL	CMD-C2D-C1D	2.15	128.51	124.71
7	E	101	BCL	C4B-CHC-C1C	-2.15	125.86	130.12
7	B	101	BCL	C3D-C4D-ND	-2.15	106.76	110.24
7	F	104	BCL	C3D-C2D-C1D	-2.15	102.90	105.83
11	L	303	BPH	CMD-C2D-C3D	2.15	128.70	124.68
7	3	102	BCL	CMD-C2D-C1D	2.15	128.50	124.71
12	L	310	U10	C7-C6-C5	-2.14	115.90	118.48
8	2	101	SPO	C5-C6-C7	2.14	129.13	125.89
8	2	103	SPO	C34-C33-C35	2.14	118.88	115.27
7	M	403	BCL	CHA-C1A-NA	-2.14	121.50	126.40
11	L	311	BPH	OBD-CAD-CBD	-2.14	122.69	125.82
7	N	102	BCL	C3C-C4C-CHD	-2.13	118.83	123.39
7	R	103	BCL	CMD-C2D-C1D	2.13	128.47	124.71
7	D	102	BCL	CMD-C2D-C1D	2.13	128.47	124.71
7	D	102	BCL	C3D-C2D-C1D	-2.13	102.92	105.83
8	A	102	SPO	C2-C1-C4	-2.13	107.59	110.86
7	J	102	BCL	CHA-C1A-NA	-2.13	121.53	126.40
7	J	102	BCL	C3C-C4C-CHD	-2.13	118.85	123.39
7	3	101	BCL	C1D-ND-C4D	2.12	107.84	106.33
7	3	102	BCL	C1D-ND-C4D	2.12	107.84	106.33
7	E	101	BCL	CHA-C1A-NA	-2.12	121.54	126.40
7	L	309	BCL	C2A-C3A-C4A	-2.12	98.44	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	8	102	BCL	C1-C2-C3	-2.12	122.38	126.04
8	2	103	SPO	C9-C10-C11	2.12	129.82	123.22
7	C	101	BCL	CHA-C1A-NA	-2.12	121.55	126.40
9	A	103	PC1	O12-P-O14	2.12	122.70	112.24
7	U	101	BCL	C3D-C2D-C1D	-2.12	102.94	105.83
7	P	102	BCL	C3C-C4C-CHD	-2.11	118.88	123.39
8	J	101	SPO	C3-C1-C4	-2.11	107.61	110.86
8	F	105	SPO	C30-C28-C27	-2.10	115.61	121.98
7	3	102	BCL	C3C-C4C-CHD	-2.10	118.90	123.39
7	R	103	BCL	CHA-C1A-NA	-2.10	121.58	126.40
7	P	102	BCL	CHA-C1A-NA	-2.10	121.58	126.40
7	N	102	BCL	CHA-C1A-NA	-2.10	121.58	126.40
7	K	101	BCL	CMD-C2D-C1D	2.10	128.41	124.71
7	B	101	BCL	C3D-C2D-C1D	-2.10	102.97	105.83
7	O	101	BCL	C1C-NC-C4C	-2.10	105.76	106.71
7	9	101	BCL	C1D-CHD-C4C	-2.09	121.57	126.62
7	a	101	BCL	CHA-C1A-NA	-2.09	121.61	126.40
7	L	309	BCL	C3D-C4D-ND	-2.09	106.86	110.24
9	A	103	PC1	O31-C31-O32	-2.09	118.33	123.59
7	F	102	BCL	C3C-C4C-CHD	-2.09	118.94	123.39
8	0	103	SPO	C16-C17-C19	2.08	122.14	118.94
8	W	101	SPO	C13-C12-C11	2.08	121.36	118.08
7	U	101	BCL	C3D-C4D-ND	-2.08	106.87	110.24
7	1	102	BCL	CHA-C1A-NA	-2.08	121.64	126.40
8	K	102	SPO	C15-C16-C17	2.08	132.25	126.42
7	E	101	BCL	C3D-C2D-C1D	-2.07	103.00	105.83
7	W	102	BCL	CHA-C1A-NA	-2.07	121.65	126.40
8	S	101	SPO	C34-C33-C35	2.07	118.75	115.27
7	S	102	BCL	CMD-C2D-C1D	2.07	128.36	124.71
7	N	102	BCL	C1D-CHD-C4C	-2.07	121.64	126.62
10	F	101	CDL	CB6-OB8-CB7	2.06	124.77	117.12
8	T	102	SPO	C10-C9-C7	-2.06	124.37	127.31
7	F	102	BCL	C1C-NC-C4C	-2.06	105.78	106.71
7	L	302	BCL	C3C-C4C-CHD	-2.06	119.00	123.39
7	S	102	BCL	C2C-C3C-C4C	-2.05	98.26	101.34
8	2	103	SPO	C18-C17-C16	2.05	121.31	118.08
8	I	102	SPO	C3-C1-C4	-2.05	107.70	110.86
8	3	103	SPO	C16-C17-C19	2.05	122.09	118.94
7	L	302	BCL	C4D-CHA-C1A	2.05	123.74	121.25
7	U	101	BCL	CMD-C2D-C1D	2.05	128.32	124.71
7	W	102	BCL	C3D-C2D-C1D	-2.05	103.04	105.83
9	H	301	PC1	C3-O31-C31	2.05	124.69	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	0	101	BCL	CMD-C2D-C1D	2.04	128.31	124.71
7	V	101	BCL	CMD-C2D-C1D	2.04	128.31	124.71
7	R	103	BCL	C1D-CHD-C4C	-2.04	121.70	126.62
10	F	101	CDL	OA8-CA7-OA9	-2.04	118.45	123.59
8	T	102	SPO	C2-C1-C4	-2.03	107.73	110.86
7	F	102	BCL	C1D-CHD-C4C	-2.03	121.72	126.62
7	C	101	BCL	C3D-C2D-C1D	-2.03	103.06	105.83
7	V	101	BCL	C1C-NC-C4C	-2.03	105.79	106.71
7	1	101	BCL	C3C-C4C-CHD	-2.03	119.06	123.39
7	K	101	BCL	C1D-ND-C4D	2.03	107.77	106.33
7	F	104	BCL	C3C-C4C-CHD	-2.02	119.07	123.39
7	0	101	BCL	C3D-C2D-C1D	-2.02	103.07	105.83
8	3	103	SPO	C31-C32-C33	-2.02	122.79	127.66
7	b	101	BCL	C2A-C3A-C4A	-2.02	98.60	101.87
8	I	102	SPO	C24-C23-C25	2.02	121.26	118.08
7	b	101	BCL	CHD-C1D-ND	-2.02	122.60	124.45
12	M	405	U10	C7-C6-C5	-2.02	116.05	118.48
7	M	403	BCL	C1D-CHD-C4C	-2.02	121.75	126.62
8	E	102	SPO	C24-C23-C25	2.02	121.26	118.08
7	0	101	BCL	C2C-C3C-C4C	-2.02	98.32	101.34
7	1	101	BCL	C1D-CHD-C4C	-2.02	121.76	126.62
7	V	101	BCL	C1-C2-C3	-2.01	122.56	126.04
8	R	101	SPO	C3-C1-C4	-2.01	107.77	110.86
7	C	101	BCL	C1D-ND-C4D	2.01	107.76	106.33
7	L	302	BCL	C3D-C2D-C1D	-2.01	103.09	105.83
8	3	103	SPO	C40-C38-C39	2.01	119.03	114.60
7	F	102	BCL	CHA-C1A-NA	-2.00	121.81	126.40
8	2	102	SPO	C24-C23-C22	-2.00	120.12	122.92

There are no chirality outliers.

All (1131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	0	101	BCL	C1-C2-C3-C4
7	0	101	BCL	C1-C2-C3-C5
7	1	101	BCL	C4C-C3C-CAC-CBC
7	1	101	BCL	CHA-CBD-CGD-O1D
7	1	101	BCL	CHA-CBD-CGD-O2D
7	1	101	BCL	CBD-CGD-O2D-CED
7	1	101	BCL	C1-C2-C3-C4
7	1	101	BCL	C4-C3-C5-C6
7	1	102	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	1	102	BCL	C3A-C2A-CAA-CBA
7	1	102	BCL	C2C-C3C-CAC-CBC
7	1	102	BCL	C4C-C3C-CAC-CBC
7	1	102	BCL	C1-C2-C3-C4
7	3	101	BCL	C4C-C3C-CAC-CBC
7	3	101	BCL	O2A-C1-C2-C3
7	3	102	BCL	C1A-C2A-CAA-CBA
7	3	102	BCL	C2C-C3C-CAC-CBC
7	3	102	BCL	C4C-C3C-CAC-CBC
7	3	102	BCL	C1-C2-C3-C4
7	3	102	BCL	C1-C2-C3-C5
7	3	102	BCL	C2-C3-C5-C6
7	3	102	BCL	C4-C3-C5-C6
7	3	102	BCL	C14-C13-C15-C16
7	8	102	BCL	C2C-C3C-CAC-CBC
7	9	101	BCL	C4C-C3C-CAC-CBC
7	9	101	BCL	C14-C13-C15-C16
7	C	101	BCL	C4C-C3C-CAC-CBC
7	C	101	BCL	C1-C2-C3-C4
7	D	102	BCL	C2C-C3C-CAC-CBC
7	D	102	BCL	CBD-CGD-O2D-CED
7	E	101	BCL	C1-C2-C3-C4
7	E	101	BCL	C1-C2-C3-C5
7	F	102	BCL	C1A-C2A-CAA-CBA
7	F	102	BCL	C3A-C2A-CAA-CBA
7	F	102	BCL	C4C-C3C-CAC-CBC
7	F	102	BCL	C11-C10-C8-C9
7	F	104	BCL	C1A-C2A-CAA-CBA
7	F	104	BCL	C3A-C2A-CAA-CBA
7	F	104	BCL	C2C-C3C-CAC-CBC
7	J	102	BCL	CBA-CGA-O2A-C1
7	J	102	BCL	O1A-CGA-O2A-C1
7	J	102	BCL	C4C-C3C-CAC-CBC
7	J	102	BCL	O2A-C1-C2-C3
7	J	102	BCL	C1-C2-C3-C4
7	K	101	BCL	C1-C2-C3-C4
7	K	101	BCL	C1-C2-C3-C5
7	L	302	BCL	C4C-C3C-CAC-CBC
7	L	302	BCL	C1-C2-C3-C4
7	L	302	BCL	C1-C2-C3-C5
7	L	309	BCL	C4C-C3C-CAC-CBC
7	L	309	BCL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
7	L	309	BCL	C1-C2-C3-C5
7	M	403	BCL	C2C-C3C-CAC-CBC
7	M	403	BCL	C4C-C3C-CAC-CBC
7	M	403	BCL	C1-C2-C3-C4
7	M	403	BCL	C2-C3-C5-C6
7	M	403	BCL	C4-C3-C5-C6
7	N	102	BCL	C4C-C3C-CAC-CBC
7	O	101	BCL	C1-C2-C3-C4
7	O	101	BCL	C1-C2-C3-C5
7	P	102	BCL	C1A-C2A-CAA-CBA
7	P	102	BCL	C4C-C3C-CAC-CBC
7	P	102	BCL	C11-C10-C8-C9
7	P	102	BCL	C11-C12-C13-C14
7	Q	101	BCL	C1A-C2A-CAA-CBA
7	Q	101	BCL	C3A-C2A-CAA-CBA
7	Q	101	BCL	C1-C2-C3-C4
7	Q	101	BCL	C1-C2-C3-C5
7	Q	101	BCL	C14-C13-C15-C16
7	R	103	BCL	C1A-C2A-CAA-CBA
7	R	103	BCL	C2C-C3C-CAC-CBC
7	R	103	BCL	C2-C3-C5-C6
7	R	103	BCL	C4-C3-C5-C6
7	T	101	BCL	C2-C3-C5-C6
7	T	101	BCL	C4-C3-C5-C6
7	U	101	BCL	CBD-CGD-O2D-CED
7	U	101	BCL	C1-C2-C3-C4
7	U	101	BCL	C1-C2-C3-C5
7	W	102	BCL	C1-C2-C3-C4
7	a	101	BCL	C1A-C2A-CAA-CBA
7	a	101	BCL	C3A-C2A-CAA-CBA
7	a	101	BCL	C1-C2-C3-C4
7	a	101	BCL	C1-C2-C3-C5
7	b	101	BCL	C1-C2-C3-C4
8	0	102	SPO	C5-C6-C7-C9
8	0	102	SPO	C10-C11-C12-C14
8	0	102	SPO	C27-C28-C30-C31
8	0	102	SPO	C29-C28-C30-C31
8	0	102	SPO	C33-C35-C36-C37
8	0	103	SPO	C5-C6-C7-C8
8	0	103	SPO	C5-C6-C7-C9
8	0	103	SPO	C12-C14-C15-C16
8	0	103	SPO	C17-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
8	0	103	SPO	C27-C28-C30-C31
8	0	103	SPO	C29-C28-C30-C31
8	2	101	SPO	C1-C4-C5-C6
8	2	101	SPO	C17-C19-C20-C21
8	2	102	SPO	O1-C1-C4-C5
8	2	102	SPO	C2-C1-C4-C5
8	2	102	SPO	C3-C1-C4-C5
8	3	103	SPO	O1-C1-C4-C5
8	A	102	SPO	C3-C1-O1-CM1
8	A	102	SPO	C4-C1-O1-CM1
8	D	101	SPO	C2-C1-O1-CM1
8	D	101	SPO	C4-C1-O1-CM1
8	D	103	SPO	C3-C1-C4-C5
8	D	103	SPO	C30-C31-C32-C33
8	E	102	SPO	C1-C4-C5-C6
8	E	102	SPO	C27-C28-C30-C31
8	E	102	SPO	C29-C28-C30-C31
8	F	105	SPO	C1-C4-C5-C6
8	I	102	SPO	C29-C28-C30-C31
8	J	101	SPO	C1-C4-C5-C6
8	J	101	SPO	C28-C30-C31-C32
8	J	101	SPO	C32-C33-C35-C36
8	J	101	SPO	C34-C33-C35-C36
8	J	101	SPO	C33-C35-C36-C37
8	K	102	SPO	O1-C1-C4-C5
8	K	102	SPO	C2-C1-C4-C5
8	K	102	SPO	C3-C1-C4-C5
8	K	102	SPO	C1-C4-C5-C6
8	N	101	SPO	C30-C31-C32-C33
8	O	102	SPO	C1-C4-C5-C6
8	R	102	SPO	C1-C4-C5-C6
8	R	102	SPO	C5-C6-C7-C8
8	R	102	SPO	C5-C6-C7-C9
8	R	102	SPO	C27-C28-C30-C31
8	R	102	SPO	C29-C28-C30-C31
8	S	101	SPO	C1-C4-C5-C6
8	S	101	SPO	C28-C30-C31-C32
8	S	103	SPO	C4-C1-O1-CM1
8	T	102	SPO	C1-C4-C5-C6
8	U	103	SPO	C5-C6-C7-C9
8	U	103	SPO	C33-C35-C36-C37
8	W	101	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
8	Z	101	SPO	C3-C1-O1-CM1
8	Z	101	SPO	C4-C1-O1-CM1
8	Z	101	SPO	C5-C6-C7-C8
8	Z	101	SPO	C5-C6-C7-C9
9	9	103	PC1	C11-O13-P-O14
9	9	103	PC1	O13-C11-C12-N
9	9	103	PC1	C2-C1-O11-P
9	9	103	PC1	O22-C21-O21-C2
9	9	103	PC1	C22-C21-O21-C2
9	A	103	PC1	C1-O11-P-O14
9	A	103	PC1	O13-C11-C12-N
9	A	104	PC1	C11-O13-P-O11
9	A	104	PC1	C1-O11-P-O12
9	F	103	PC1	C1-O11-P-O14
9	H	301	PC1	C11-O13-P-O12
9	H	301	PC1	C11-O13-P-O14
9	H	301	PC1	O13-C11-C12-N
9	L	305	PC1	C11-O13-P-O12
9	L	305	PC1	C11-O13-P-O14
9	L	305	PC1	C1-O11-P-O14
9	L	305	PC1	O21-C2-C3-O31
9	M	401	PC1	C11-O13-P-O12
9	M	401	PC1	C2-C1-O11-P
9	M	401	PC1	O32-C31-O31-C3
9	M	401	PC1	C32-C31-O31-C3
9	M	402	PC1	C11-O13-P-O11
9	M	402	PC1	C1-O11-P-O12
9	M	402	PC1	C1-O11-P-O14
9	M	402	PC1	C1-O11-P-O13
9	M	409	PC1	C1-O11-P-O14
9	M	410	PC1	C1-O11-P-O14
9	M	410	PC1	O21-C2-C3-O31
9	W	103	PC1	C11-O13-P-O12
9	W	103	PC1	C1-O11-P-O12
10	F	101	CDL	CA2-OA2-PA1-OA3
10	F	101	CDL	OA7-CA5-OA6-CA4
10	F	101	CDL	C11-CA5-OA6-CA4
10	F	101	CDL	CB2-OB2-PB2-OB4
10	F	101	CDL	CB3-OB5-PB2-OB3
10	F	101	CDL	C51-CB5-OB6-CB4
10	M	407	CDL	OA7-CA5-OA6-CA4
10	M	407	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
10	M	407	CDL	OB9-CB7-OB8-CB6
10	M	407	CDL	C71-CB7-OB8-CB6
10	M	408	CDL	OB7-CB5-OB6-CB4
10	M	408	CDL	C51-CB5-OB6-CB4
12	L	304	U10	C31-C32-C33-C34
12	L	306	U10	C18-C19-C21-C22
12	L	306	U10	C20-C19-C21-C22
12	L	306	U10	C24-C26-C27-C28
12	L	307	U10	C14-C16-C17-C18
12	L	307	U10	C28-C29-C31-C32
12	L	307	U10	C30-C29-C31-C32
12	L	307	U10	C29-C31-C32-C33
12	L	310	U10	C12-C11-C9-C8
12	L	310	U10	C12-C11-C9-C10
12	L	310	U10	C14-C16-C17-C18
12	L	310	U10	C24-C26-C27-C28
12	X	101	U10	C1-C6-C7-C8
12	X	101	U10	C5-C6-C7-C8
12	X	101	U10	C15-C14-C16-C17
12	X	101	U10	C24-C26-C27-C28
12	X	101	U10	C26-C27-C28-C29
12	X	101	U10	C29-C31-C32-C33
7	1	101	BCL	O1D-CGD-O2D-CED
7	F	102	BCL	CBD-CGD-O2D-CED
7	a	101	BCL	CBD-CGD-O2D-CED
7	1	102	BCL	O1A-CGA-O2A-C1
7	F	102	BCL	O1D-CGD-O2D-CED
9	H	301	PC1	C2-C3-O31-C31
7	D	102	BCL	O1D-CGD-O2D-CED
7	U	101	BCL	O1D-CGD-O2D-CED
7	1	102	BCL	CBA-CGA-O2A-C1
7	M	403	BCL	CBD-CGD-O2D-CED
7	b	101	BCL	CBD-CGD-O2D-CED
7	C	101	BCL	O1A-CGA-O2A-C1
7	N	102	BCL	O1A-CGA-O2A-C1
7	N	102	BCL	C15-C16-C17-C18
9	A	103	PC1	O22-C21-O21-C2
10	F	101	CDL	OB7-CB5-OB6-CB4
7	0	101	BCL	C3-C5-C6-C7
7	3	101	BCL	C3-C5-C6-C7
7	F	102	BCL	C3-C5-C6-C7
7	F	104	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
7	L	309	BCL	C3-C5-C6-C7
7	S	102	BCL	C3-C5-C6-C7
7	N	102	BCL	CBA-CGA-O2A-C1
7	F	104	BCL	CBD-CGD-O2D-CED
7	L	309	BCL	C4-C3-C5-C6
8	9	102	SPO	C34-C33-C35-C36
8	M	406	SPO	C29-C28-C30-C31
12	L	310	U10	C20-C19-C21-C22
7	1	101	BCL	C2-C3-C5-C6
8	I	102	SPO	C27-C28-C30-C31
8	M	406	SPO	C27-C28-C30-C31
8	W	101	SPO	C32-C33-C35-C36
12	X	101	U10	C13-C14-C16-C17
7	R	103	BCL	CBD-CGD-O2D-CED
7	C	101	BCL	C2A-CAA-CBA-CGA
7	V	101	BCL	C2A-CAA-CBA-CGA
7	a	101	BCL	C2A-CAA-CBA-CGA
7	7	101	BCL	C3-C5-C6-C7
7	D	102	BCL	C3-C5-C6-C7
7	Q	101	BCL	C3-C5-C6-C7
7	1	101	BCL	CBA-CGA-O2A-C1
7	C	101	BCL	CBA-CGA-O2A-C1
7	1	101	BCL	C1-C2-C3-C5
7	1	102	BCL	C1-C2-C3-C5
7	C	101	BCL	C1-C2-C3-C5
7	J	102	BCL	C1-C2-C3-C5
7	b	101	BCL	C1-C2-C3-C5
8	0	103	SPO	C11-C10-C9-C7
8	2	102	SPO	C17-C19-C20-C21
8	K	102	SPO	C11-C10-C9-C7
8	S	101	SPO	C20-C21-C22-C23
8	S	101	SPO	C25-C26-C27-C28
8	W	101	SPO	C11-C10-C9-C7
7	a	101	BCL	O1D-CGD-O2D-CED
7	U	101	BCL	C3-C5-C6-C7
7	b	101	BCL	CBA-CGA-O2A-C1
7	1	101	BCL	O1A-CGA-O2A-C1
9	A	103	PC1	C22-C21-O21-C2
7	3	102	BCL	C10-C11-C12-C13
7	8	102	BCL	C4-C3-C5-C6
8	2	101	SPO	C34-C33-C35-C36
8	E	102	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
8	F	105	SPO	C29-C28-C30-C31
8	O	102	SPO	C29-C28-C30-C31
8	R	102	SPO	C34-C33-C35-C36
12	L	304	U10	C12-C11-C9-C10
12	X	101	U10	C12-C11-C9-C10
12	X	101	U10	C20-C19-C21-C22
12	X	101	U10	C35-C34-C36-C37
7	8	102	BCL	C2-C3-C5-C6
8	2	101	SPO	C32-C33-C35-C36
8	E	102	SPO	C32-C33-C35-C36
8	F	105	SPO	C27-C28-C30-C31
8	O	102	SPO	C27-C28-C30-C31
8	R	102	SPO	C32-C33-C35-C36
12	L	304	U10	C12-C11-C9-C8
12	X	101	U10	C12-C11-C9-C8
12	X	101	U10	C18-C19-C21-C22
12	X	101	U10	C33-C34-C36-C37
7	1	102	BCL	C2A-CAA-CBA-CGA
7	b	101	BCL	C2A-CAA-CBA-CGA
7	b	101	BCL	O1A-CGA-O2A-C1
8	0	103	SPO	C28-C30-C31-C32
8	2	101	SPO	C33-C35-C36-C37
8	2	103	SPO	C28-C30-C31-C32
8	3	103	SPO	C28-C30-C31-C32
8	A	102	SPO	C28-C30-C31-C32
8	A	102	SPO	C33-C35-C36-C37
8	K	102	SPO	C33-C35-C36-C37
8	N	101	SPO	C33-C35-C36-C37
8	P	101	SPO	C33-C35-C36-C37
8	R	101	SPO	C33-C35-C36-C37
8	S	103	SPO	C33-C35-C36-C37
8	T	102	SPO	C28-C30-C31-C32
12	L	304	U10	C14-C16-C17-C18
12	L	304	U10	C19-C21-C22-C23
12	L	304	U10	C29-C31-C32-C33
12	L	306	U10	C19-C21-C22-C23
12	L	307	U10	C9-C11-C12-C13
12	L	307	U10	C24-C26-C27-C28
12	L	310	U10	C19-C21-C22-C23
12	X	101	U10	C14-C16-C17-C18
9	W	103	PC1	C11-C12-N-C15
7	8	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
7	M	403	BCL	O1D-CGD-O2D-CED
7	B	101	BCL	CBA-CGA-O2A-C1
7	N	102	BCL	C5-C6-C7-C8
7	C	101	BCL	CBD-CGD-O2D-CED
7	J	102	BCL	CBD-CGD-O2D-CED
7	P	102	BCL	C10-C11-C12-C13
7	Q	101	BCL	C15-C16-C17-C18
7	S	102	BCL	C15-C16-C17-C18
7	a	101	BCL	C5-C6-C7-C8
10	M	408	CDL	O1-C1-CB2-OB2
7	L	309	BCL	C2-C3-C5-C6
8	9	102	SPO	C32-C33-C35-C36
12	L	310	U10	C18-C19-C21-C22
7	0	101	BCL	C6-C7-C8-C9
7	1	102	BCL	C6-C7-C8-C9
7	3	101	BCL	C11-C12-C13-C14
7	8	102	BCL	C11-C10-C8-C9
7	9	101	BCL	C11-C12-C13-C14
7	B	101	BCL	C6-C7-C8-C9
7	C	101	BCL	C11-C10-C8-C9
7	C	101	BCL	C14-C13-C15-C16
7	J	102	BCL	C6-C7-C8-C9
7	K	101	BCL	C14-C13-C15-C16
7	N	102	BCL	C6-C7-C8-C9
7	N	102	BCL	C11-C12-C13-C14
7	P	102	BCL	C14-C13-C15-C16
7	R	103	BCL	C11-C10-C8-C9
7	V	101	BCL	C11-C10-C8-C9
7	V	101	BCL	C14-C13-C15-C16
7	W	102	BCL	C11-C12-C13-C14
7	W	102	BCL	C14-C13-C15-C16
7	b	101	BCL	O1D-CGD-O2D-CED
7	R	103	BCL	C5-C6-C7-C8
7	W	102	BCL	C10-C11-C12-C13
7	W	102	BCL	C2A-CAA-CBA-CGA
8	0	102	SPO	C5-C6-C7-C8
8	0	102	SPO	C10-C11-C12-C13
8	0	103	SPO	C10-C11-C12-C13
8	0	103	SPO	C24-C23-C25-C26
8	D	103	SPO	C5-C6-C7-C8
8	R	102	SPO	C10-C11-C12-C13
8	U	103	SPO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	U	103	SPO	C10-C11-C12-C13
8	0	103	SPO	C10-C11-C12-C14
8	0	103	SPO	C22-C23-C25-C26
8	D	103	SPO	C5-C6-C7-C9
8	R	102	SPO	C10-C11-C12-C14
8	S	103	SPO	C15-C16-C17-C19
7	E	101	BCL	C8-C10-C11-C12
7	I	101	BCL	C15-C16-C17-C18
7	K	101	BCL	C8-C10-C11-C12
10	F	101	CDL	C31-CA7-OA8-CA6
7	3	102	BCL	C8-C10-C11-C12
7	3	102	BCL	C13-C15-C16-C17
7	J	102	BCL	C8-C10-C11-C12
7	T	101	BCL	C10-C11-C12-C13
7	3	101	BCL	C13-C15-C16-C17
7	E	101	BCL	C10-C11-C12-C13
7	E	101	BCL	C13-C15-C16-C17
7	L	309	BCL	C8-C10-C11-C12
7	V	101	BCL	C5-C6-C7-C8
9	9	103	PC1	C31-C32-C33-C34
7	9	101	BCL	C5-C6-C7-C8
7	C	101	BCL	C10-C11-C12-C13
7	E	101	BCL	C15-C16-C17-C18
7	P	102	BCL	C8-C10-C11-C12
7	R	103	BCL	C13-C15-C16-C17
9	W	103	PC1	C11-C12-N-C14
9	M	410	PC1	C31-C32-C33-C34
7	W	102	BCL	CBD-CGD-O2D-CED
7	1	102	BCL	C5-C6-C7-C8
7	Q	101	BCL	C5-C6-C7-C8
7	V	101	BCL	C8-C10-C11-C12
7	3	101	BCL	C11-C10-C8-C7
7	C	101	BCL	C11-C12-C13-C15
7	E	101	BCL	C12-C13-C15-C16
7	F	104	BCL	C6-C7-C8-C10
7	I	101	BCL	C11-C12-C13-C15
7	L	309	BCL	C11-C10-C8-C7
7	N	102	BCL	C12-C13-C15-C16
8	2	101	SPO	C12-C14-C15-C16
12	M	405	U10	C4-C3-O3-C3M
9	M	401	PC1	C21-C22-C23-C24
7	1	102	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	K	101	BCL	C15-C16-C17-C18
7	M	403	BCL	C10-C11-C12-C13
8	D	103	SPO	C33-C35-C36-C37
8	K	102	SPO	C28-C30-C31-C32
8	P	101	SPO	C28-C30-C31-C32
8	T	102	SPO	C33-C35-C36-C37
8	W	101	SPO	C28-C30-C31-C32
8	Z	101	SPO	C33-C35-C36-C37
12	L	304	U10	C24-C26-C27-C28
12	L	306	U10	C9-C11-C12-C13
12	L	306	U10	C29-C31-C32-C33
12	M	405	U10	C34-C36-C37-C38
7	L	302	BCL	C3-C5-C6-C7
7	1	102	BCL	C10-C11-C12-C13
7	D	102	BCL	C8-C10-C11-C12
7	J	102	BCL	C13-C15-C16-C17
7	B	101	BCL	O1A-CGA-O2A-C1
7	A	101	BCL	C5-C6-C7-C8
7	F	104	BCL	C13-C15-C16-C17
7	b	101	BCL	C5-C6-C7-C8
7	F	104	BCL	O1D-CGD-O2D-CED
7	F	102	BCL	C10-C11-C12-C13
7	O	101	BCL	C15-C16-C17-C18
9	9	103	PC1	C11-O13-P-O11
9	A	103	PC1	C1-O11-P-O13
9	A	104	PC1	C1-O11-P-O13
9	F	103	PC1	C1-O11-P-O13
9	H	301	PC1	C11-O13-P-O11
9	L	305	PC1	C11-O13-P-O11
9	M	401	PC1	C11-O13-P-O11
9	W	103	PC1	C11-O13-P-O11
10	F	101	CDL	CB2-OB2-PB2-OB5
10	M	407	CDL	CA2-OA2-PA1-OA5
10	M	407	CDL	CB2-OB2-PB2-OB5
7	A	101	BCL	C8-C10-C11-C12
7	E	101	BCL	C16-C17-C18-C19
7	O	101	BCL	C16-C17-C18-C20
7	R	103	BCL	CBA-CGA-O2A-C1
7	U	101	BCL	C10-C11-C12-C13
8	0	103	SPO	C25-C26-C27-C28
8	S	103	SPO	C12-C14-C15-C16
9	H	301	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
10	F	101	CDL	C38-C39-C40-C41
10	F	101	CDL	C40-C41-C42-C43
10	M	408	CDL	C83-C84-C85-C86
7	R	103	BCL	O1D-CGD-O2D-CED
7	9	101	BCL	C16-C17-C18-C19
7	a	101	BCL	C6-C7-C8-C9
10	F	101	CDL	CB3-CB4-OB6-CB5
10	F	101	CDL	CA4-CA3-OA5-PA1
10	F	101	CDL	OA9-CA7-OA8-CA6
9	9	103	PC1	C2A-C2B-C2C-C2D
10	F	101	CDL	C79-C80-C81-C82
7	B	101	BCL	C3-C5-C6-C7
8	S	103	SPO	C11-C12-C14-C15
8	S	103	SPO	C16-C17-C19-C20
7	N	102	BCL	C10-C11-C12-C13
7	0	101	BCL	C11-C12-C13-C14
7	1	102	BCL	C11-C12-C13-C15
7	B	101	BCL	C16-C17-C18-C20
10	M	407	CDL	C34-C35-C36-C37
7	F	104	BCL	C11-C10-C8-C9
7	L	302	BCL	C6-C7-C8-C9
7	O	101	BCL	C11-C12-C13-C14
10	M	407	CDL	C71-C72-C73-C74
10	M	408	CDL	C32-C33-C34-C35
10	M	408	CDL	C36-C37-C38-C39
7	8	102	BCL	C2A-CAA-CBA-CGA
8	S	103	SPO	C15-C16-C17-C18
10	M	407	CDL	C62-C63-C64-C65
7	U	101	BCL	C15-C16-C17-C18
10	M	407	CDL	CA5-C11-C12-C13
10	M	408	CDL	C71-C72-C73-C74
9	W	103	PC1	C11-C12-N-C13
7	F	102	BCL	C16-C17-C18-C19
7	F	104	BCL	C16-C17-C18-C19
7	T	101	BCL	C16-C17-C18-C19
7	T	101	BCL	C16-C17-C18-C20
11	L	311	BPH	C6-C7-C8-C9
8	S	101	SPO	C33-C35-C36-C37
10	M	407	CDL	C21-C22-C23-C24
9	9	103	PC1	C2E-C2F-C2G-C2H
10	M	407	CDL	CB5-C51-C52-C53
7	K	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	L	302	BCL	C13-C15-C16-C17
7	0	101	BCL	C3A-C2A-CAA-CBA
7	3	102	BCL	C3A-C2A-CAA-CBA
7	E	101	BCL	C3A-C2A-CAA-CBA
7	N	102	BCL	C3A-C2A-CAA-CBA
7	P	102	BCL	C3A-C2A-CAA-CBA
7	R	103	BCL	C3A-C2A-CAA-CBA
7	T	101	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	C8-C10-C11-C12
9	H	301	PC1	C22-C23-C24-C25
7	E	101	BCL	C16-C17-C18-C20
7	O	101	BCL	C16-C17-C18-C19
7	P	102	BCL	C16-C17-C18-C19
10	M	407	CDL	C54-C55-C56-C57
7	F	104	BCL	C4-C3-C5-C6
7	P	102	BCL	C4-C3-C5-C6
7	W	102	BCL	C4-C3-C5-C6
8	P	101	SPO	C29-C28-C30-C31
7	0	101	BCL	CBA-CGA-O2A-C1
7	F	104	BCL	C2-C3-C5-C6
7	W	102	BCL	C2-C3-C5-C6
8	P	101	SPO	C27-C28-C30-C31
7	R	103	BCL	O1A-CGA-O2A-C1
7	0	101	BCL	C11-C12-C13-C15
7	B	101	BCL	C16-C17-C18-C19
7	F	104	BCL	C16-C17-C18-C20
7	a	101	BCL	C6-C7-C8-C10
10	M	407	CDL	C72-C73-C74-C75
7	D	102	BCL	C15-C16-C17-C18
7	E	101	BCL	C2-C1-O2A-CGA
7	M	403	BCL	C2-C1-O2A-CGA
9	H	301	PC1	C29-C2A-C2B-C2C
7	B	101	BCL	C8-C10-C11-C12
7	L	309	BCL	C15-C16-C17-C18
7	W	102	BCL	C8-C10-C11-C12
7	V	101	BCL	C16-C17-C18-C19
7	7	101	BCL	CBA-CGA-O2A-C1
7	E	101	BCL	CBA-CGA-O2A-C1
7	F	104	BCL	C10-C11-C12-C13
7	N	102	BCL	C13-C15-C16-C17
7	1	102	BCL	C6-C7-C8-C10
7	7	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
7	8	102	BCL	C6-C7-C8-C10
7	A	101	BCL	C2-C3-C5-C6
7	F	102	BCL	C11-C12-C13-C15
7	K	101	BCL	C11-C12-C13-C15
7	L	309	BCL	C12-C13-C15-C16
7	O	101	BCL	C6-C7-C8-C10
7	O	101	BCL	C11-C12-C13-C15
7	P	102	BCL	C2-C3-C5-C6
7	Q	101	BCL	C6-C7-C8-C10
7	Q	101	BCL	C11-C12-C13-C15
7	0	101	BCL	O1A-CGA-O2A-C1
7	9	101	BCL	C8-C10-C11-C12
7	1	102	BCL	C11-C12-C13-C14
7	9	101	BCL	C16-C17-C18-C20
12	L	306	U10	C4-C3-O3-C3M
7	I	101	BCL	CBA-CGA-O2A-C1
7	F	102	BCL	C13-C15-C16-C17
7	L	302	BCL	C8-C10-C11-C12
10	M	407	CDL	C19-C20-C21-C22
10	M	408	CDL	C75-C76-C77-C78
9	L	305	PC1	C31-C32-C33-C34
7	O	101	BCL	C13-C15-C16-C17
7	I	101	BCL	C16-C17-C18-C19
9	A	104	PC1	C21-C22-C23-C24
7	T	101	BCL	CBD-CGD-O2D-CED
9	A	103	PC1	C22-C23-C24-C25
9	M	409	PC1	C27-C28-C29-C2A
9	W	103	PC1	O21-C2-C3-O31
7	C	101	BCL	C16-C17-C18-C20
7	S	102	BCL	C16-C17-C18-C19
7	A	101	BCL	C4-C3-C5-C6
9	A	103	PC1	C21-C22-C23-C24
7	7	101	BCL	C6-C7-C8-C9
7	8	102	BCL	C6-C7-C8-C9
7	8	102	BCL	C11-C12-C13-C14
7	E	101	BCL	C11-C12-C13-C14
7	F	102	BCL	C11-C12-C13-C14
7	F	104	BCL	C6-C7-C8-C9
7	I	101	BCL	C6-C7-C8-C9
7	K	101	BCL	C11-C12-C13-C14
7	L	309	BCL	C11-C10-C8-C9
7	L	309	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
7	O	101	BCL	C6-C7-C8-C9
7	Q	101	BCL	C6-C7-C8-C9
7	Q	101	BCL	C11-C12-C13-C14
7	S	102	BCL	C11-C10-C8-C9
7	V	101	BCL	C11-C12-C13-C14
7	E	101	BCL	O1A-CGA-O2A-C1
7	9	101	BCL	C15-C16-C17-C18
10	M	407	CDL	C51-C52-C53-C54
7	7	101	BCL	O1A-CGA-O2A-C1
7	E	101	BCL	C1A-C2A-CAA-CBA
7	N	102	BCL	C1A-C2A-CAA-CBA
7	T	101	BCL	C1A-C2A-CAA-CBA
10	M	407	CDL	C41-C42-C43-C44
7	L	309	BCL	C5-C6-C7-C8
7	U	101	BCL	C8-C10-C11-C12
10	F	101	CDL	CA3-OA5-PA1-OA2
7	C	101	BCL	O1D-CGD-O2D-CED
7	3	101	BCL	C5-C6-C7-C8
10	F	101	CDL	OA5-CA3-CA4-CA6
7	J	102	BCL	O1D-CGD-O2D-CED
7	F	102	BCL	C16-C17-C18-C20
8	I	102	SPO	C1-C4-C5-C6
8	N	101	SPO	C1-C4-C5-C6
7	F	102	BCL	CBA-CGA-O2A-C1
8	9	102	SPO	C29-C28-C30-C31
7	3	101	BCL	C2C-C3C-CAC-CBC
7	9	101	BCL	C2C-C3C-CAC-CBC
7	C	101	BCL	C2C-C3C-CAC-CBC
7	F	102	BCL	C2C-C3C-CAC-CBC
7	J	102	BCL	C2C-C3C-CAC-CBC
7	N	102	BCL	C2C-C3C-CAC-CBC
7	P	102	BCL	C2C-C3C-CAC-CBC
7	V	101	BCL	C2C-C3C-CAC-CBC
10	M	407	CDL	C16-C17-C18-C19
7	R	103	BCL	C15-C16-C17-C18
8	U	102	SPO	C30-C31-C32-C33
7	I	101	BCL	O1A-CGA-O2A-C1
10	M	408	CDL	C51-C52-C53-C54
9	L	305	PC1	O31-C31-C32-C33
7	W	102	BCL	O1D-CGD-O2D-CED
7	C	101	BCL	C3-C5-C6-C7
8	0	102	SPO	C4-C1-O1-CM1

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Mol	Chain	Res	Type	Atoms
8	2	103	SPO	C4-C1-O1-CM1
8	9	102	SPO	C28-C30-C31-C32
8	M	406	SPO	C28-C30-C31-C32
8	U	102	SPO	C4-C1-O1-CM1
8	W	101	SPO	C4-C1-O1-CM1
10	M	407	CDL	C61-C62-C63-C64
7	B	101	BCL	C10-C11-C12-C13
7	L	309	BCL	C10-C11-C12-C13
8	M	406	SPO	C34-C33-C35-C36
7	J	102	BCL	C16-C17-C18-C20
9	H	301	PC1	C32-C31-O31-C3
9	M	409	PC1	O11-C1-C2-O21
7	W	102	BCL	C13-C15-C16-C17
7	U	101	BCL	C13-C15-C16-C17
8	0	102	SPO	C2-C1-O1-CM1
8	2	103	SPO	C3-C1-O1-CM1
8	8	101	SPO	C3-C1-O1-CM1
8	D	101	SPO	C3-C1-O1-CM1
8	D	103	SPO	C2-C1-O1-CM1
8	I	102	SPO	C2-C1-O1-CM1
8	I	102	SPO	C3-C1-O1-CM1
8	S	103	SPO	C3-C1-O1-CM1
8	U	102	SPO	C3-C1-O1-CM1
8	Z	101	SPO	C2-C1-O1-CM1
7	R	103	BCL	C10-C11-C12-C13
7	F	102	BCL	O1A-CGA-O2A-C1
8	0	102	SPO	C2-C1-C4-C5
8	0	102	SPO	C3-C1-C4-C5
8	2	101	SPO	C2-C1-C4-C5
8	3	103	SPO	C2-C1-C4-C5
8	3	103	SPO	C3-C1-C4-C5
8	D	103	SPO	C2-C1-C4-C5
8	D	103	SPO	C29-C28-C30-C31
12	X	101	U10	C25-C24-C26-C27
7	8	102	BCL	C11-C10-C8-C7
7	8	102	BCL	C11-C12-C13-C15
7	9	101	BCL	C11-C10-C8-C7
7	D	102	BCL	C11-C12-C13-C15
7	E	101	BCL	C6-C7-C8-C10
7	F	104	BCL	C11-C10-C8-C7
7	I	101	BCL	C6-C7-C8-C10
7	K	101	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
7	R	103	BCL	C11-C10-C8-C7
7	R	103	BCL	C12-C13-C15-C16
7	S	102	BCL	C11-C10-C8-C7
7	V	101	BCL	C11-C12-C13-C15
8	9	102	SPO	C27-C28-C30-C31
8	M	406	SPO	C32-C33-C35-C36
9	H	301	PC1	O32-C31-O31-C3
7	3	101	BCL	C14-C13-C15-C16
7	9	101	BCL	C11-C10-C8-C9
7	C	101	BCL	C11-C12-C13-C14
7	E	101	BCL	C14-C13-C15-C16
7	F	104	BCL	C14-C13-C15-C16
11	L	303	BPH	C11-C10-C8-C9
8	8	101	SPO	C24-C23-C25-C26
7	R	103	BCL	C8-C10-C11-C12
7	3	102	BCL	CBD-CGD-O2D-CED
7	E	101	BCL	C5-C6-C7-C8
7	Q	101	BCL	C8-C10-C11-C12
8	9	102	SPO	C33-C35-C36-C37
10	M	407	CDL	C52-C53-C54-C55
7	F	102	BCL	C4-C3-C5-C6
7	a	101	BCL	C4-C3-C5-C6
12	L	306	U10	C30-C29-C31-C32
7	F	102	BCL	C2-C3-C5-C6
8	D	103	SPO	C27-C28-C30-C31
12	X	101	U10	C23-C24-C26-C27
7	D	102	BCL	CBA-CGA-O2A-C1
7	A	101	BCL	C3A-C2A-CAA-CBA
7	D	102	BCL	C3A-C2A-CAA-CBA
7	b	101	BCL	C3A-C2A-CAA-CBA
7	F	102	BCL	C15-C16-C17-C18
9	M	402	PC1	C32-C31-O31-C3
9	L	305	PC1	C1-C2-C3-O31
9	W	103	PC1	C1-C2-C3-O31
10	M	407	CDL	CA3-CA4-CA6-OA8
11	L	303	BPH	O2A-C1-C2-C3
7	S	102	BCL	C10-C11-C12-C13
8	A	102	SPO	C34-C33-C35-C36
7	R	103	BCL	C16-C17-C18-C19
11	L	311	BPH	C6-C7-C8-C10
10	M	407	CDL	C73-C74-C75-C76
9	H	301	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
10	F	101	CDL	OA5-CA3-CA4-OA6
7	C	101	BCL	C16-C17-C18-C19
7	V	101	BCL	C16-C17-C18-C20
7	b	101	BCL	CAA-CBA-CGA-O2A
9	9	103	PC1	O21-C2-C3-O31
7	K	101	BCL	CBA-CGA-O2A-C1
7	3	102	BCL	C15-C16-C17-C18
10	F	101	CDL	C76-C77-C78-C79
7	8	102	BCL	C16-C17-C18-C19
7	S	102	BCL	C16-C17-C18-C20
7	b	101	BCL	C11-C12-C13-C14
8	N	101	SPO	C28-C30-C31-C32
8	O	102	SPO	C33-C35-C36-C37
8	U	102	SPO	C28-C30-C31-C32
7	9	101	BCL	C4-C3-C5-C6
11	L	311	BPH	C4-C3-C5-C6
7	I	101	BCL	C2-C1-O2A-CGA
7	R	103	BCL	C2-C1-O2A-CGA
7	3	101	BCL	C11-C10-C8-C9
7	F	102	BCL	C6-C7-C8-C9
7	R	103	BCL	C14-C13-C15-C16
9	A	104	PC1	C2-C1-O11-P
7	L	301	BCL	C16-C17-C18-C19
7	P	102	BCL	C16-C17-C18-C20
7	I	101	BCL	C10-C11-C12-C13
8	S	103	SPO	C10-C11-C12-C14
8	U	103	SPO	C10-C11-C12-C14
7	I	101	BCL	C16-C17-C18-C20
9	L	305	PC1	C33-C34-C35-C36
7	1	102	BCL	C11-C10-C8-C7
7	3	102	BCL	C12-C13-C15-C16
7	9	101	BCL	C6-C7-C8-C10
7	9	101	BCL	C12-C13-C15-C16
7	C	101	BCL	C11-C10-C8-C7
7	D	102	BCL	C6-C7-C8-C10
7	D	102	BCL	C11-C10-C8-C7
7	E	101	BCL	C11-C10-C8-C7
7	F	102	BCL	C6-C7-C8-C10
7	F	102	BCL	C11-C10-C8-C7
7	J	102	BCL	C6-C7-C8-C10
7	P	102	BCL	C11-C10-C8-C7
7	T	101	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
7	V	101	BCL	C11-C10-C8-C7
7	V	101	BCL	C12-C13-C15-C16
8	S	103	SPO	C27-C28-C30-C31
11	L	303	BPH	C11-C10-C8-C7
7	8	102	BCL	C16-C17-C18-C20
7	J	102	BCL	C16-C17-C18-C19
7	T	101	BCL	O1D-CGD-O2D-CED
10	F	101	CDL	C32-C31-CA7-OA8
7	A	101	BCL	C2A-CAA-CBA-CGA
7	J	102	BCL	C15-C16-C17-C18
10	F	101	CDL	C71-C72-C73-C74
7	A	101	BCL	CBD-CGD-O2D-CED
7	3	101	BCL	CAD-CBD-CGD-O2D
7	9	101	BCL	CAD-CBD-CGD-O2D
7	L	302	BCL	CAD-CBD-CGD-O2D
7	Q	101	BCL	CAD-CBD-CGD-O2D
11	L	311	BPH	CAD-CBD-CGD-O2D
8	R	101	SPO	C29-C28-C30-C31
12	L	306	U10	C15-C14-C16-C17
7	9	101	BCL	C2-C3-C5-C6
8	D	101	SPO	C28-C30-C31-C32
9	M	401	PC1	C1-C2-C3-O31
9	M	410	PC1	C1-C2-C3-O31
7	K	101	BCL	O1A-CGA-O2A-C1
9	W	103	PC1	O21-C21-C22-C23
7	R	103	BCL	CHA-CBD-CGD-O1D
7	S	102	BCL	CHA-CBD-CGD-O1D
7	S	102	BCL	CHA-CBD-CGD-O2D
7	U	101	BCL	CHA-CBD-CGD-O1D
7	B	101	BCL	C15-C16-C17-C18
7	D	102	BCL	O1A-CGA-O2A-C1
9	M	402	PC1	O32-C31-O31-C3
9	M	409	PC1	C2C-C2D-C2E-C2F
9	M	401	PC1	O21-C2-C3-O31
9	H	301	PC1	C32-C33-C34-C35
9	9	103	PC1	C25-C26-C27-C28
7	B	101	BCL	C4-C3-C5-C6
8	D	103	SPO	C34-C33-C35-C36
12	L	306	U10	C13-C14-C16-C17
12	L	306	U10	C28-C29-C31-C32
7	D	102	BCL	C11-C10-C8-C9
7	I	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	L	302	BCL	C14-C13-C15-C16
9	9	103	PC1	C2D-C2E-C2F-C2G
8	8	101	SPO	C22-C23-C25-C26
7	b	101	BCL	C1A-C2A-CAA-CBA
9	M	410	PC1	C1-O11-P-O13
10	F	101	CDL	CA2-OA2-PA1-OA5
10	M	407	CDL	CB3-OB5-PB2-OB2
10	M	408	CDL	CA2-OA2-PA1-OA5
7	J	102	BCL	C10-C11-C12-C13
9	9	103	PC1	C11-O13-P-O12
9	A	103	PC1	C1-O11-P-O12
9	A	104	PC1	C11-O13-P-O12
9	F	103	PC1	C1-O11-P-O12
9	M	402	PC1	C11-O13-P-O14
10	F	101	CDL	CA3-OA5-PA1-OA3
10	F	101	CDL	CA3-OA5-PA1-OA4
10	F	101	CDL	CB2-OB2-PB2-OB3
10	M	407	CDL	CA2-OA2-PA1-OA4
10	M	407	CDL	CB2-OB2-PB2-OB3
10	M	407	CDL	CB2-OB2-PB2-OB4
7	M	403	BCL	C8-C10-C11-C12
9	H	301	PC1	O11-C1-C2-C3
10	M	408	CDL	OB5-CB3-CB4-CB6
10	F	101	CDL	C74-C75-C76-C77
12	M	405	U10	C5-C4-O4-C4M
7	M	403	BCL	CAD-CBD-CGD-O1D
9	9	103	PC1	C12-C11-O13-P
9	L	305	PC1	C12-C11-O13-P
9	M	402	PC1	C12-C11-O13-P
9	W	103	PC1	C12-C11-O13-P
8	2	103	SPO	C1-C4-C5-C6
8	U	103	SPO	C1-C4-C5-C6
9	M	402	PC1	C24-C25-C26-C27
9	H	301	PC1	C36-C37-C38-C39
7	3	101	BCL	CBA-CGA-O2A-C1
8	S	103	SPO	C29-C28-C30-C31
7	A	101	BCL	C6-C7-C8-C10
7	E	101	BCL	C2C-C3C-CAC-CBC
7	N	102	BCL	C6-C7-C8-C10
7	Q	101	BCL	C12-C13-C15-C16
7	T	101	BCL	C11-C10-C8-C7
7	V	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
7	b	101	BCL	C11-C10-C8-C7
9	W	103	PC1	O11-C1-C2-O21
10	M	408	CDL	OB5-CB3-CB4-OB6
7	K	101	BCL	C16-C17-C18-C20
7	U	101	BCL	C16-C17-C18-C19
7	E	101	BCL	C3-C5-C6-C7
7	8	102	BCL	C15-C16-C17-C18
9	9	103	PC1	C1-C2-C3-O31
9	A	104	PC1	O13-C11-C12-N
9	F	103	PC1	O13-C11-C12-N
9	M	401	PC1	O13-C11-C12-N
9	M	409	PC1	O13-C11-C12-N
9	W	103	PC1	O13-C11-C12-N
10	M	407	CDL	CB3-CB4-CB6-OB8
10	M	407	CDL	OA6-CA4-CA6-OA8
10	M	407	CDL	OB6-CB4-CB6-OB8
12	L	310	U10	C1-C6-C7-C8
7	M	403	BCL	CAA-CBA-CGA-O2A
7	R	103	BCL	C16-C17-C18-C20
10	F	101	CDL	C41-C42-C43-C44
10	M	407	CDL	C1-CA2-OA2-PA1
8	S	103	SPO	C34-C33-C35-C36
10	M	407	CDL	C40-C41-C42-C43
7	B	101	BCL	C2-C3-C5-C6
7	E	101	BCL	C11-C10-C8-C9
7	M	403	BCL	C14-C13-C15-C16
7	N	102	BCL	C14-C13-C15-C16
7	S	102	BCL	C6-C7-C8-C9
7	S	102	BCL	C14-C13-C15-C16
7	3	102	BCL	O1D-CGD-O2D-CED
8	0	103	SPO	C4-C1-O1-CM1
8	M	406	SPO	C33-C35-C36-C37
8	R	102	SPO	C28-C30-C31-C32
8	S	103	SPO	C28-C30-C31-C32
7	3	101	BCL	O1A-CGA-O2A-C1
7	0	101	BCL	C2A-CAA-CBA-CGA
7	R	103	BCL	C2A-CAA-CBA-CGA
10	M	408	CDL	C73-C74-C75-C76
8	0	102	SPO	C14-C15-C16-C17
8	2	101	SPO	C23-C25-C26-C27
8	2	102	SPO	C9-C10-C11-C12
8	2	103	SPO	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	3	103	SPO	C14-C15-C16-C17
8	E	102	SPO	C14-C15-C16-C17
8	K	102	SPO	C14-C15-C16-C17
8	S	101	SPO	C14-C15-C16-C17
8	S	103	SPO	C14-C15-C16-C17
8	Z	101	SPO	C23-C25-C26-C27
7	A	101	BCL	O1D-CGD-O2D-CED
9	M	402	PC1	C11-C12-N-C14
7	V	101	BCL	C13-C15-C16-C17
7	J	102	BCL	C5-C6-C7-C8
7	J	102	BCL	C4-C3-C5-C6
8	R	101	SPO	C27-C28-C30-C31
12	L	310	U10	C5-C6-C7-C8
9	H	301	PC1	C3-C2-O21-C21
7	b	101	BCL	C11-C12-C13-C15
7	9	101	BCL	C13-C15-C16-C17
8	D	103	SPO	C32-C33-C35-C36
7	B	101	BCL	C2A-CAA-CBA-CGA
7	Q	101	BCL	C2A-CAA-CBA-CGA
8	0	102	SPO	C3-C1-O1-CM1
8	2	101	SPO	C16-C17-C19-C20
8	2	103	SPO	C2-C1-O1-CM1
8	8	101	SPO	C2-C1-O1-CM1
8	A	102	SPO	C2-C1-O1-CM1
8	D	103	SPO	C3-C1-O1-CM1
8	S	103	SPO	C2-C1-O1-CM1
8	U	102	SPO	C2-C1-O1-CM1
8	W	101	SPO	C2-C1-O1-CM1
8	W	101	SPO	C3-C1-O1-CM1
9	M	402	PC1	C27-C28-C29-C2A
9	F	103	PC1	O21-C2-C3-O31
9	9	103	PC1	C1-O11-P-O13
9	H	301	PC1	C1-O11-P-O13
10	F	101	CDL	CB3-OB5-PB2-OB2
10	M	408	CDL	CB3-OB5-PB2-OB2
9	9	103	PC1	C29-C2A-C2B-C2C
8	M	406	SPO	C2-C1-C4-C5
8	U	103	SPO	C3-C1-C4-C5
9	F	103	PC1	C1-C2-C3-O31
8	A	102	SPO	C32-C33-C35-C36
11	L	311	BPH	C2-C3-C5-C6
7	1	102	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
7	9	101	BCL	C6-C7-C8-C9
7	A	101	BCL	C6-C7-C8-C9
7	T	101	BCL	C11-C12-C13-C14
12	L	306	U10	C5-C4-O4-C4M
10	F	101	CDL	C36-C37-C38-C39
7	8	102	BCL	C5-C6-C7-C8
10	F	101	CDL	CA2-C1-CB2-OB2
8	M	406	SPO	C30-C31-C32-C33
7	a	101	BCL	C2-C3-C5-C6
9	M	402	PC1	C11-C12-N-C15
9	W	103	PC1	O11-C1-C2-C3
7	L	301	BCL	C3-C5-C6-C7
8	8	101	SPO	C28-C30-C31-C32
12	L	307	U10	C35-C34-C36-C37
7	V	101	BCL	C2-C3-C5-C6
7	8	102	BCL	C10-C11-C12-C13
10	M	408	CDL	C1-CB2-OB2-PB2
9	L	305	PC1	O32-C31-C32-C33
12	L	308	U10	C5-C4-O4-C4M
7	V	101	BCL	C4-C3-C5-C6
7	O	101	BCL	C14-C13-C15-C16
8	2	103	SPO	C8-C7-C9-C10
8	2	103	SPO	C13-C12-C14-C15
8	3	103	SPO	C8-C7-C9-C10
8	3	103	SPO	C13-C12-C14-C15
8	3	103	SPO	C18-C17-C19-C20
8	E	102	SPO	C8-C7-C9-C10
8	K	102	SPO	C8-C7-C9-C10
7	C	101	BCL	O2A-C1-C2-C3
9	A	104	PC1	C1-C2-O21-C21
9	L	305	PC1	C1-C2-O21-C21
9	W	103	PC1	C1-C2-O21-C21
7	0	101	BCL	C1A-C2A-CAA-CBA
7	8	102	BCL	C1A-C2A-CAA-CBA
7	A	101	BCL	C1A-C2A-CAA-CBA
7	D	102	BCL	C1A-C2A-CAA-CBA
7	U	101	BCL	C1A-C2A-CAA-CBA
7	B	101	BCL	C6-C7-C8-C10
7	L	309	BCL	C11-C12-C13-C15
7	T	101	BCL	C12-C13-C15-C16
7	W	102	BCL	C6-C7-C8-C10
7	W	102	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
7	F	104	BCL	C8-C10-C11-C12
7	L	301	BCL	C16-C17-C18-C20
7	3	101	BCL	C15-C16-C17-C18
10	M	407	CDL	C59-C60-C61-C62
12	M	405	U10	C35-C34-C36-C37
7	J	102	BCL	C2-C3-C5-C6
12	L	307	U10	C33-C34-C36-C37
10	F	101	CDL	O1-C1-CA2-OA2
7	O	101	BCL	CBA-CGA-O2A-C1
12	L	304	U10	C5-C4-O4-C4M
12	L	310	U10	C5-C4-O4-C4M
9	M	402	PC1	C11-C12-N-C13
9	M	410	PC1	C11-C12-N-C13
8	2	103	SPO	C6-C7-C9-C10
8	2	103	SPO	C11-C12-C14-C15
8	3	103	SPO	C6-C7-C9-C10
8	3	103	SPO	C11-C12-C14-C15
8	3	103	SPO	C16-C17-C19-C20
8	E	102	SPO	C6-C7-C9-C10
8	K	102	SPO	C6-C7-C9-C10
8	2	101	SPO	C25-C26-C27-C28
8	Z	101	SPO	C25-C26-C27-C28
12	X	101	U10	C21-C22-C23-C24
12	L	307	U10	C20-C19-C21-C22
7	8	102	BCL	C2-C1-O2A-CGA
7	O	101	BCL	O1A-CGA-O2A-C1
8	2	101	SPO	C35-C36-C37-C38
7	B	101	BCL	C13-C15-C16-C17
7	T	101	BCL	CAA-CBA-CGA-O2A
9	H	301	PC1	C25-C26-C27-C28
7	0	101	BCL	C4-C3-C5-C6
12	L	304	U10	C25-C24-C26-C27
8	K	102	SPO	C5-C6-C7-C9
8	S	103	SPO	C32-C33-C35-C36
10	M	408	CDL	CB5-C51-C52-C53
7	W	102	BCL	C15-C16-C17-C18
12	L	307	U10	C2-C3-O3-C3M
7	1	102	BCL	C4-C3-C5-C6
8	8	101	SPO	C4-C1-O1-CM1
8	D	103	SPO	C4-C1-O1-CM1
7	9	101	BCL	C11-C12-C13-C15
7	F	104	BCL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
7	L	302	BCL	C12-C13-C15-C16
12	L	304	U10	C23-C24-C26-C27
12	L	307	U10	C18-C19-C21-C22
10	M	407	CDL	C38-C39-C40-C41
7	3	101	BCL	C1-C2-C3-C4
7	7	101	BCL	C1-C2-C3-C4
7	F	102	BCL	C1-C2-C3-C4
7	N	102	BCL	C1-C2-C3-C4
7	P	102	BCL	C1-C2-C3-C4
7	V	101	BCL	C1-C2-C3-C4
7	0	101	BCL	CAA-CBA-CGA-O2A
7	M	403	BCL	C16-C17-C18-C19
7	F	104	BCL	CAA-CBA-CGA-O2A
10	M	407	CDL	C35-C36-C37-C38
7	U	101	BCL	C16-C17-C18-C20
7	3	101	BCL	O1D-CGD-O2D-CED
7	E	101	BCL	C4-C3-C5-C6
7	b	101	BCL	C4-C3-C5-C6
8	D	101	SPO	C29-C28-C30-C31
8	Z	101	SPO	C34-C33-C35-C36
12	M	405	U10	C33-C34-C36-C37
9	M	409	PC1	C25-C26-C27-C28
7	8	102	BCL	C14-C13-C15-C16
7	D	102	BCL	C11-C12-C13-C14
7	M	403	BCL	C11-C10-C8-C9
7	R	103	BCL	C11-C12-C13-C14
7	T	101	BCL	C11-C10-C8-C9
7	V	101	BCL	C6-C7-C8-C9
7	b	101	BCL	C11-C10-C8-C9
7	8	102	BCL	C3A-C2A-CAA-CBA
7	B	101	BCL	C3A-C2A-CAA-CBA
11	L	311	BPH	C3A-C2A-CAA-CBA
9	F	103	PC1	O31-C31-C32-C33
7	C	101	BCL	CAD-CBD-CGD-O2D
7	J	102	BCL	CAD-CBD-CGD-O2D
9	L	305	PC1	C3-C2-O21-C21
9	M	409	PC1	C1-C2-O21-C21
9	M	409	PC1	C3-C2-O21-C21
7	L	301	BCL	C2A-CAA-CBA-CGA
7	0	101	BCL	C2-C3-C5-C6
9	9	103	PC1	O21-C21-C22-C23
9	9	103	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
10	M	408	CDL	C32-C31-CA7-OA8
8	U	103	SPO	C15-C16-C17-C19
7	P	102	BCL	O1A-CGA-O2A-C1
7	L	309	BCL	O2A-C1-C2-C3
7	P	102	BCL	O2A-C1-C2-C3
7	S	102	BCL	O2A-C1-C2-C3
11	L	311	BPH	O2A-C1-C2-C3
7	b	101	BCL	CAA-CBA-CGA-O1A
10	M	408	CDL	CA2-C1-CB2-OB2
7	L	309	BCL	CHA-CBD-CGD-O1D
7	L	309	BCL	CHA-CBD-CGD-O2D
7	M	403	BCL	CHA-CBD-CGD-O1D
7	R	103	BCL	CHA-CBD-CGD-O2D
7	U	101	BCL	CHA-CBD-CGD-O2D
7	V	101	BCL	CHA-CBD-CGD-O1D
7	V	101	BCL	CHA-CBD-CGD-O2D
7	a	101	BCL	CHA-CBD-CGD-O1D
7	a	101	BCL	CHA-CBD-CGD-O2D
7	b	101	BCL	CHA-CBD-CGD-O1D
7	b	101	BCL	CHA-CBD-CGD-O2D
7	b	101	BCL	C2-C3-C5-C6
9	M	409	PC1	O11-C1-C2-C3
10	M	407	CDL	C72-C71-CB7-OB8
7	C	101	BCL	C8-C10-C11-C12
9	F	103	PC1	C33-C34-C35-C36
9	H	301	PC1	O22-C21-O21-C2
7	U	101	BCL	O1A-CGA-O2A-C1
9	M	410	PC1	C11-C12-N-C15
8	2	101	SPO	C3-C1-C4-C5
11	L	303	BPH	CHA-CBD-CGD-O1D
11	L	303	BPH	CHA-CBD-CGD-O2D
7	P	102	BCL	CBA-CGA-O2A-C1
7	U	101	BCL	CBA-CGA-O2A-C1
8	2	103	SPO	C34-C33-C35-C36
7	C	101	BCL	C12-C13-C15-C16
7	M	403	BCL	C12-C13-C15-C16
7	U	101	BCL	C6-C7-C8-C10
7	W	102	BCL	C12-C13-C15-C16
7	E	101	BCL	C6-C7-C8-C9
7	L	309	BCL	C11-C12-C13-C14
7	W	102	BCL	C6-C7-C8-C9
7	K	101	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
10	M	408	CDL	C32-C31-CA7-OA9
8	0	103	SPO	C35-C36-C37-C38
8	R	102	SPO	C35-C36-C37-C38
8	2	101	SPO	O1-C1-C4-C5
7	7	101	BCL	C8-C10-C11-C12
9	F	103	PC1	C32-C33-C34-C35
7	E	101	BCL	C2-C3-C5-C6
8	Z	101	SPO	C32-C33-C35-C36
9	9	103	PC1	O22-C21-C22-C23
8	J	101	SPO	C10-C11-C12-C14
10	M	407	CDL	C36-C37-C38-C39
10	F	101	CDL	C53-C54-C55-C56
7	7	101	BCL	C1A-C2A-CAA-CBA
7	B	101	BCL	C1A-C2A-CAA-CBA
10	F	101	CDL	CB2-C1-CA2-OA2
8	R	101	SPO	C35-C36-C37-C38
9	A	104	PC1	C32-C33-C34-C35
7	B	101	BCL	CAA-CBA-CGA-O2A
9	F	103	PC1	C22-C23-C24-C25
9	F	103	PC1	C24-C25-C26-C27
9	M	402	PC1	C25-C26-C27-C28
7	R	103	BCL	CAA-CBA-CGA-O2A
7	0	101	BCL	CAA-CBA-CGA-O1A
9	9	103	PC1	O32-C31-C32-C33
9	H	301	PC1	C1-O11-P-O14
9	M	409	PC1	C1-O11-P-O12
9	W	103	PC1	C1-O11-P-O14
10	M	408	CDL	CB3-OB5-PB2-OB3
12	L	306	U10	C6-C7-C8-C9
9	M	409	PC1	C26-C27-C28-C29
8	E	102	SPO	C28-C30-C31-C32
9	F	103	PC1	O32-C31-C32-C33
10	F	101	CDL	C32-C31-CA7-OA9
12	L	306	U10	C25-C24-C26-C27
12	L	307	U10	C15-C14-C16-C17
8	2	102	SPO	C35-C36-C37-C38
8	E	102	SPO	C35-C36-C37-C38
8	U	103	SPO	C30-C31-C32-C33
7	B	101	BCL	CAD-CBD-CGD-O1D
9	A	104	PC1	C3-C2-O21-C21
9	H	301	PC1	C12-C11-O13-P
9	M	409	PC1	C12-C11-O13-P

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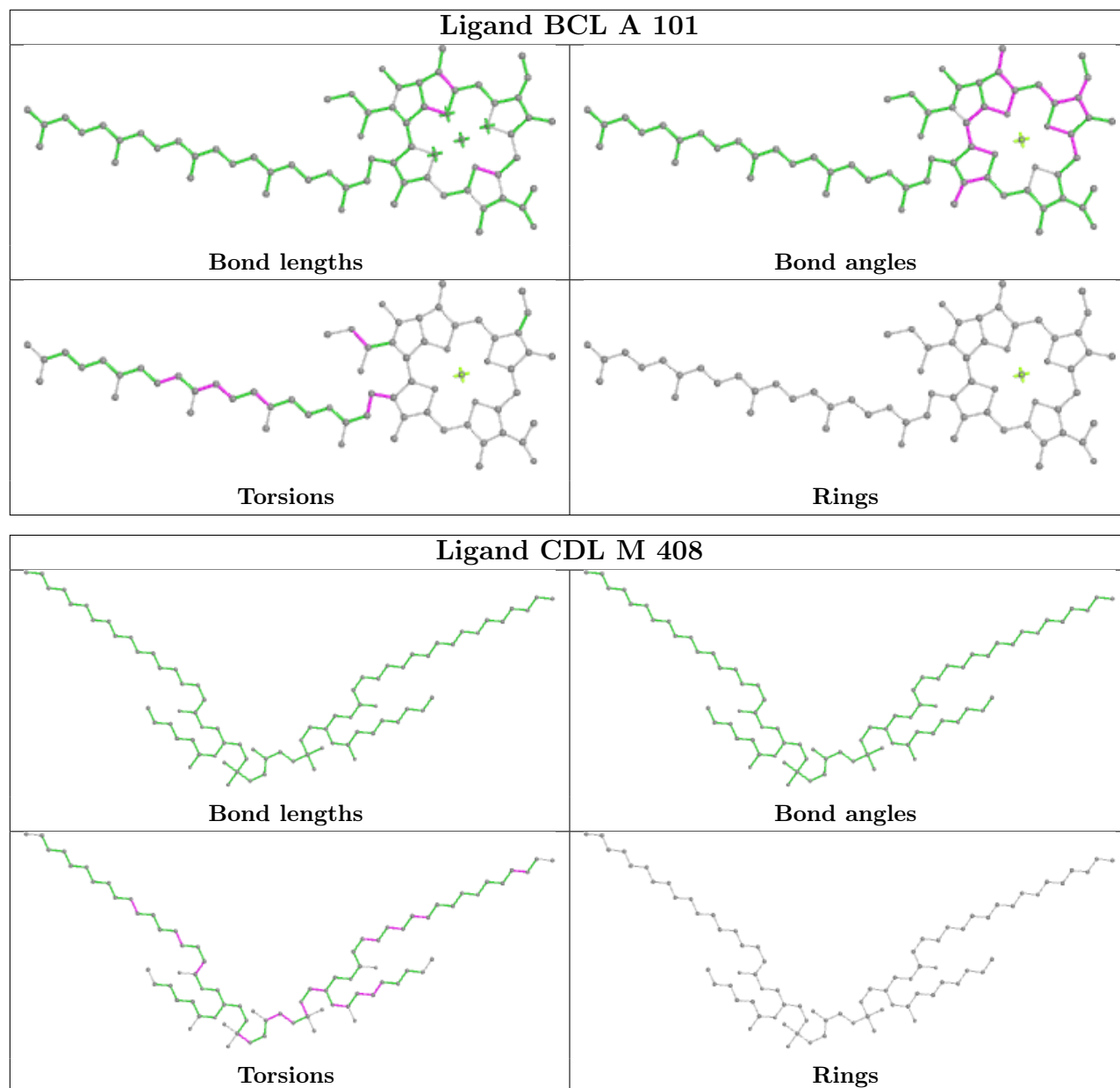
Mol	Chain	Res	Type	Atoms
10	M	407	CDL	CB6-CB4-OB6-CB5
11	L	303	BPH	C6-C7-C8-C9
7	3	101	BCL	CBD-CGD-O2D-CED
9	W	103	PC1	O22-C21-C22-C23
9	M	410	PC1	C11-C12-N-C14
9	M	401	PC1	O21-C21-C22-C23
9	F	103	PC1	C28-C29-C2A-C2B
8	0	102	SPO	C1-C4-C5-C6
8	2	102	SPO	C1-C4-C5-C6
8	A	102	SPO	C1-C4-C5-C6
8	D	101	SPO	C1-C4-C5-C6
8	S	103	SPO	C1-C4-C5-C6
8	Z	101	SPO	C1-C4-C5-C6
7	C	101	BCL	CAA-CBA-CGA-O2A
12	X	101	U10	C11-C12-C13-C14
7	3	101	BCL	C11-C12-C13-C15
7	P	102	BCL	C11-C12-C13-C15
7	P	102	BCL	C12-C13-C15-C16
7	S	102	BCL	C6-C7-C8-C10
7	U	101	BCL	C3A-C2A-CAA-CBA
10	M	407	CDL	OA5-CA3-CA4-OA6
11	L	303	BPH	C6-C7-C8-C10
7	B	101	BCL	CAA-CBA-CGA-O1A
7	a	101	BCL	C3-C5-C6-C7
8	Z	101	SPO	C15-C16-C17-C19
7	R	103	BCL	CAA-CBA-CGA-O1A
10	M	407	CDL	C72-C71-CB7-OB9
7	P	102	BCL	CAA-CBA-CGA-O2A
8	U	103	SPO	C28-C30-C31-C32
9	M	401	PC1	O22-C21-C22-C23

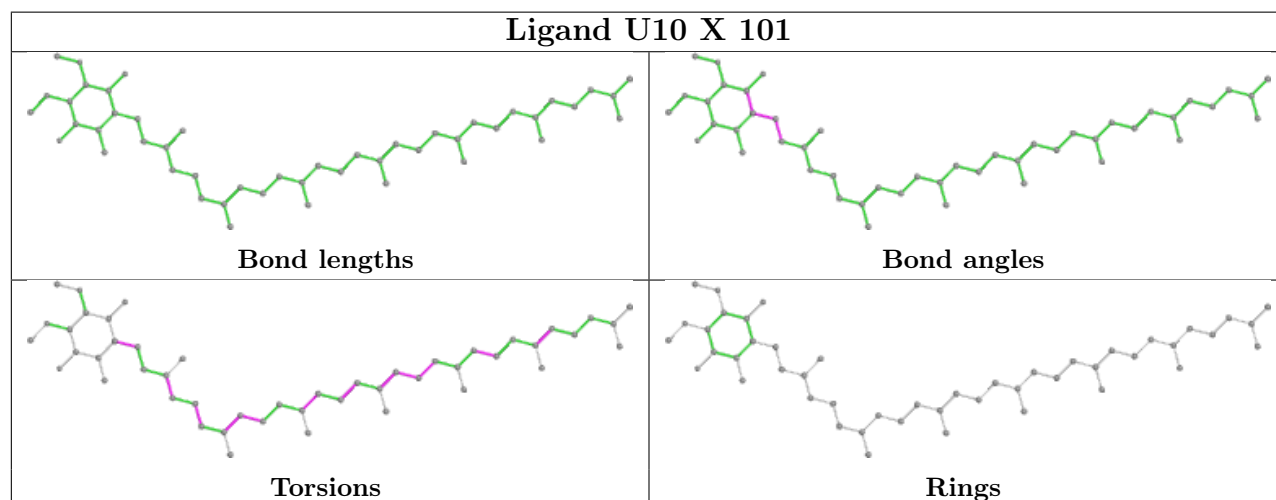
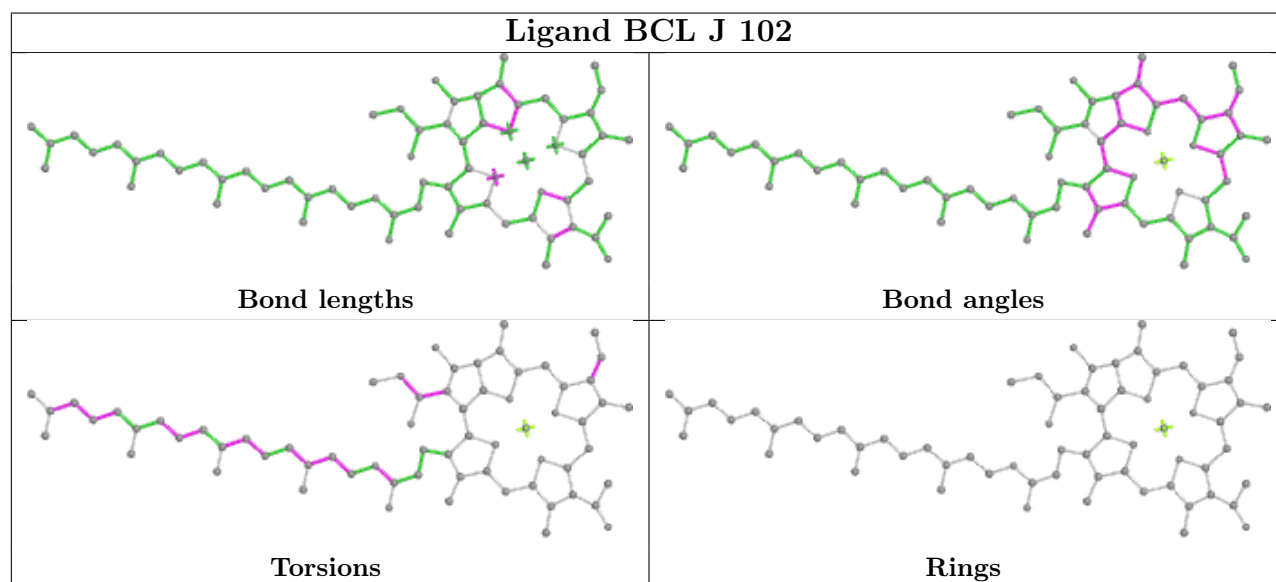
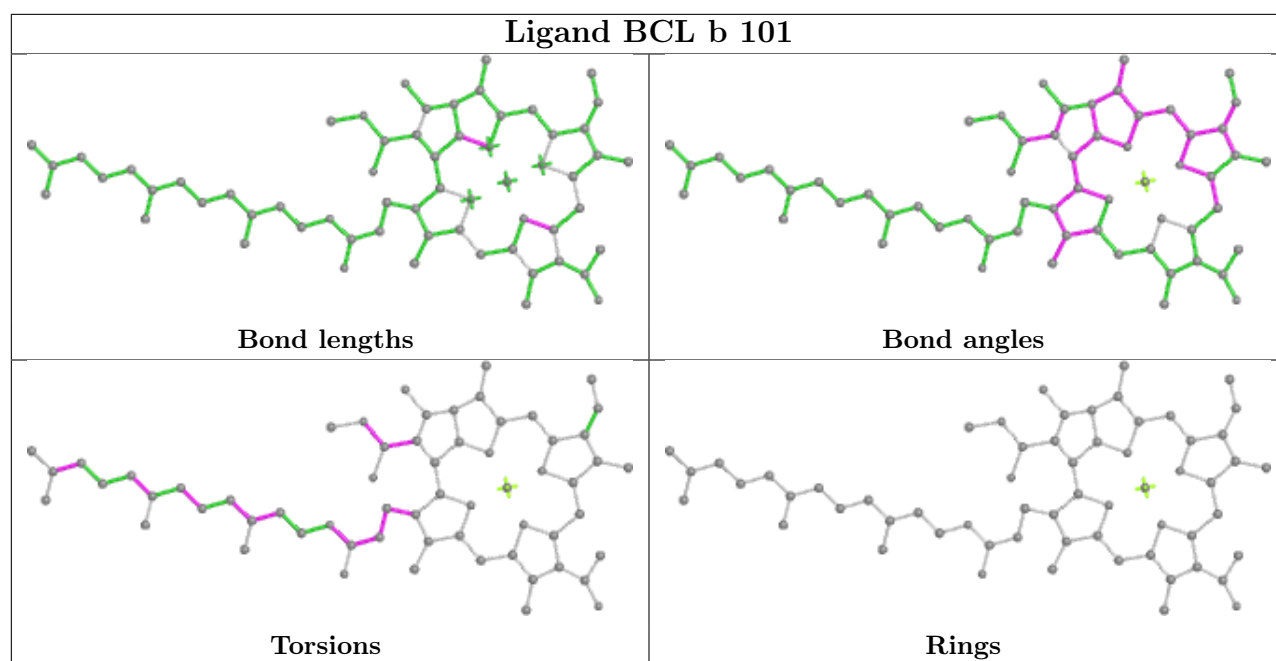
There are no ring outliers.

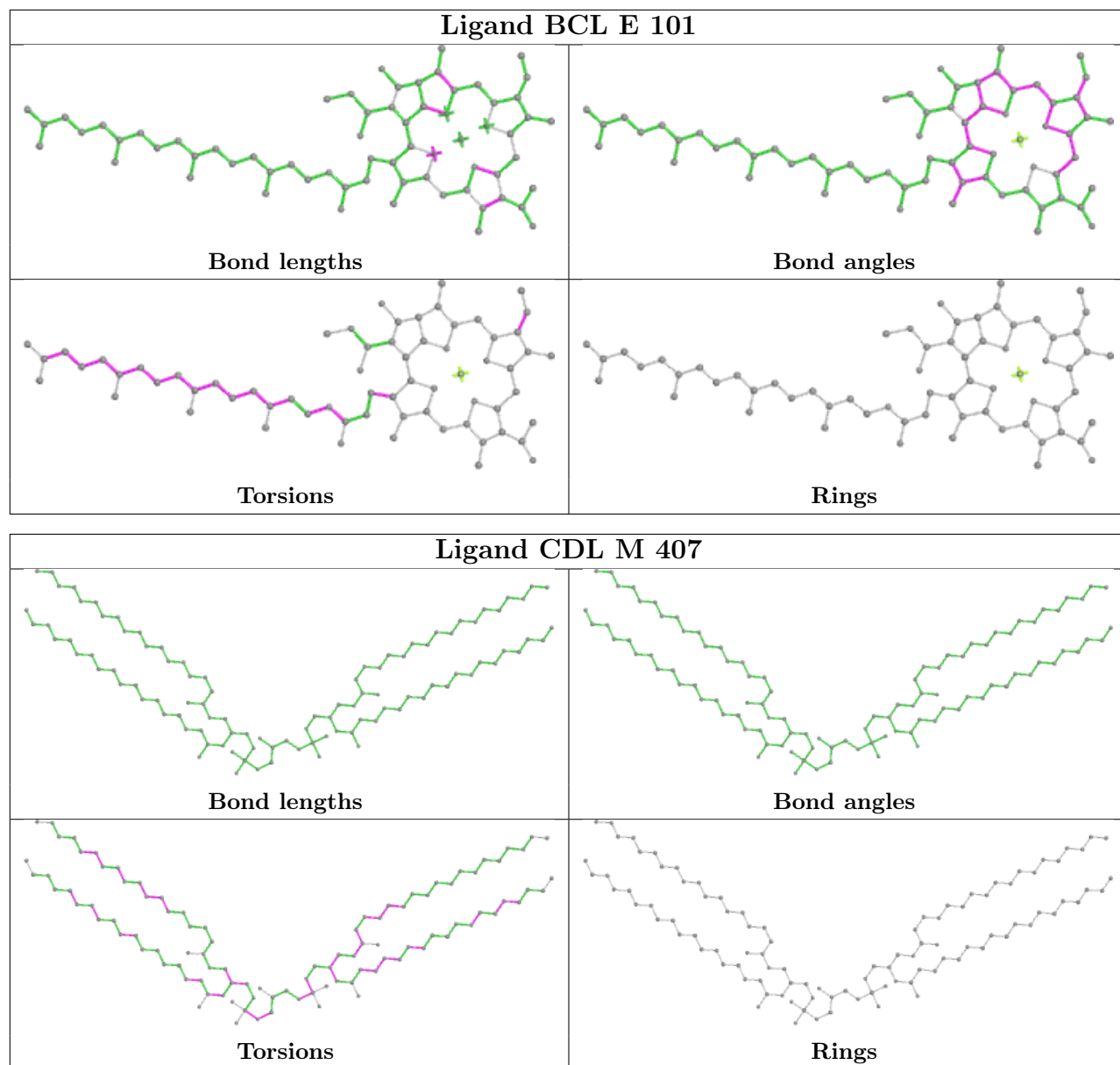
No monomer is involved in short contacts.

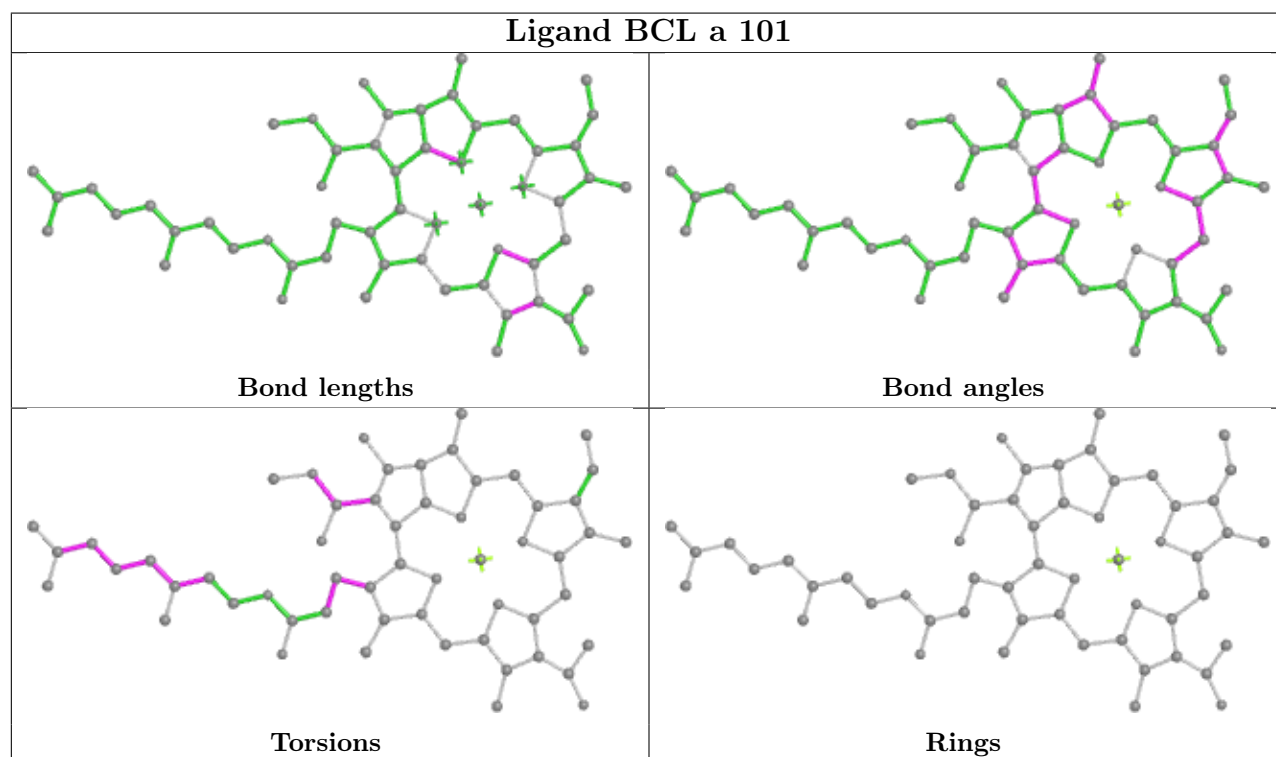
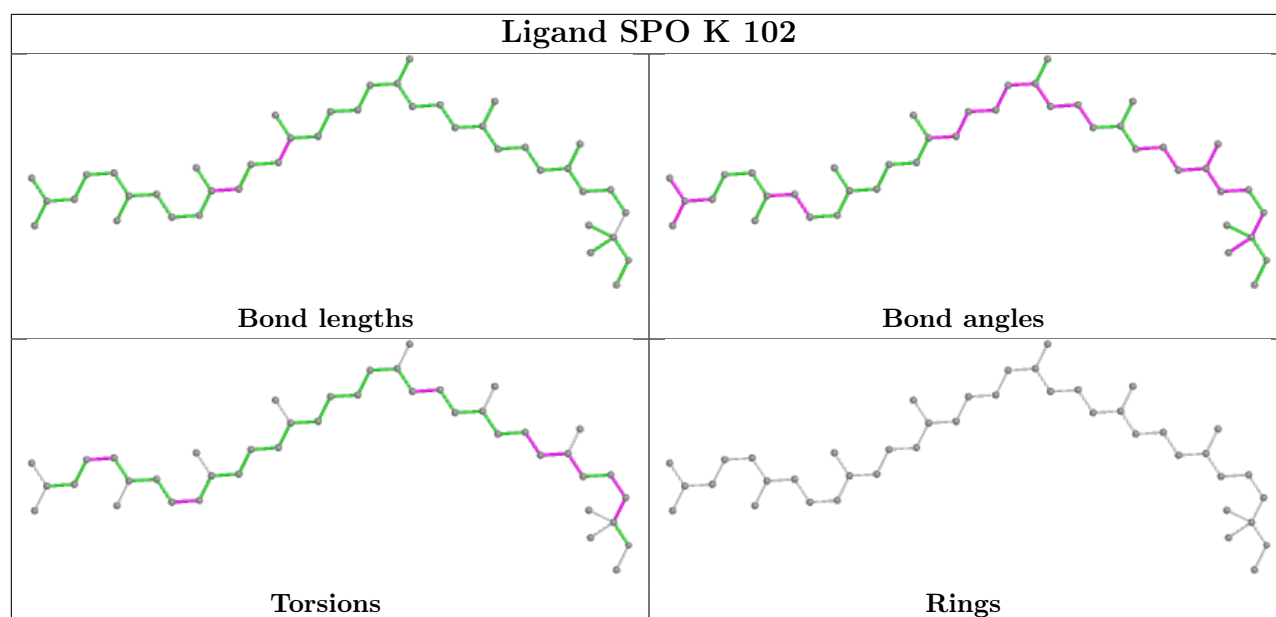
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

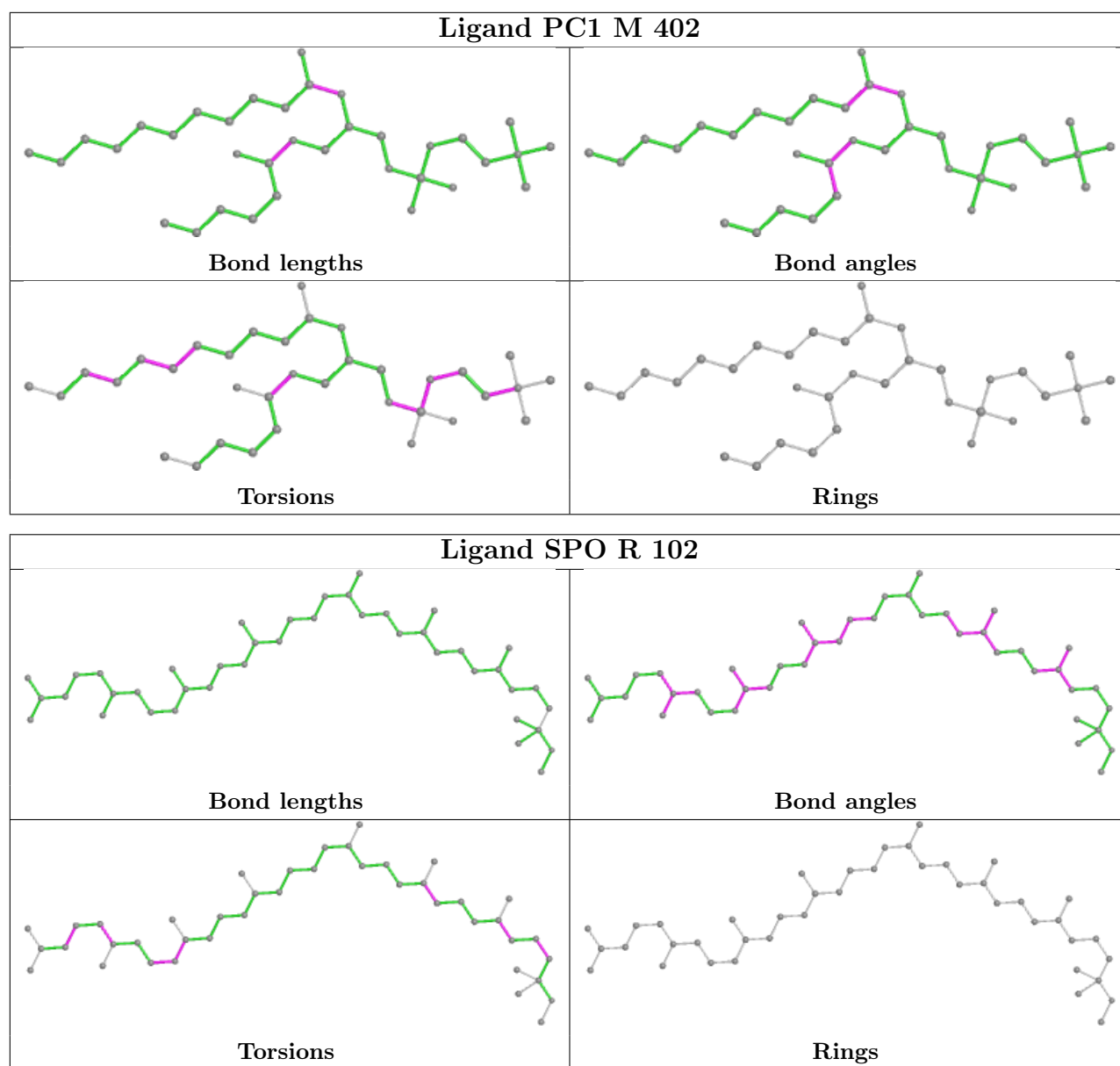
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

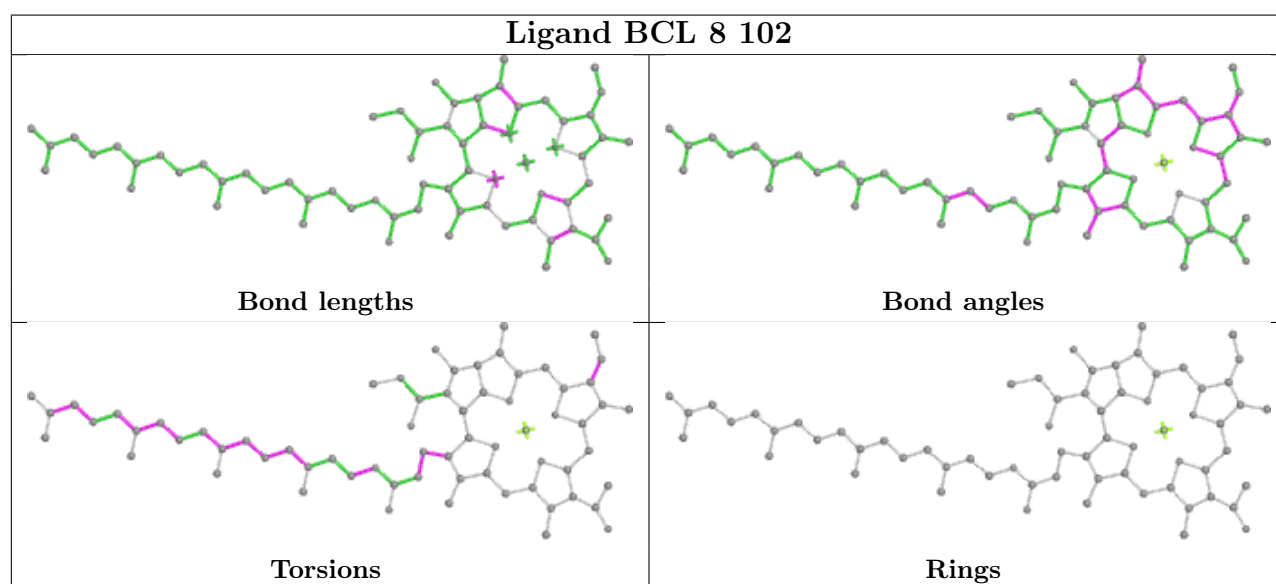
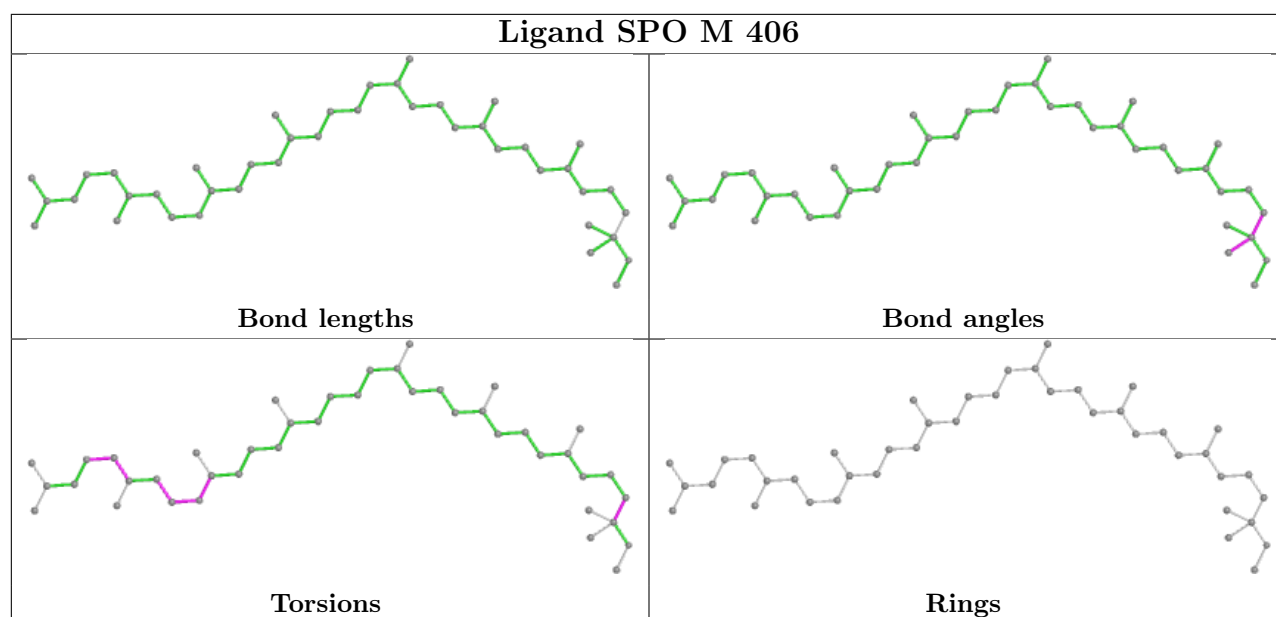


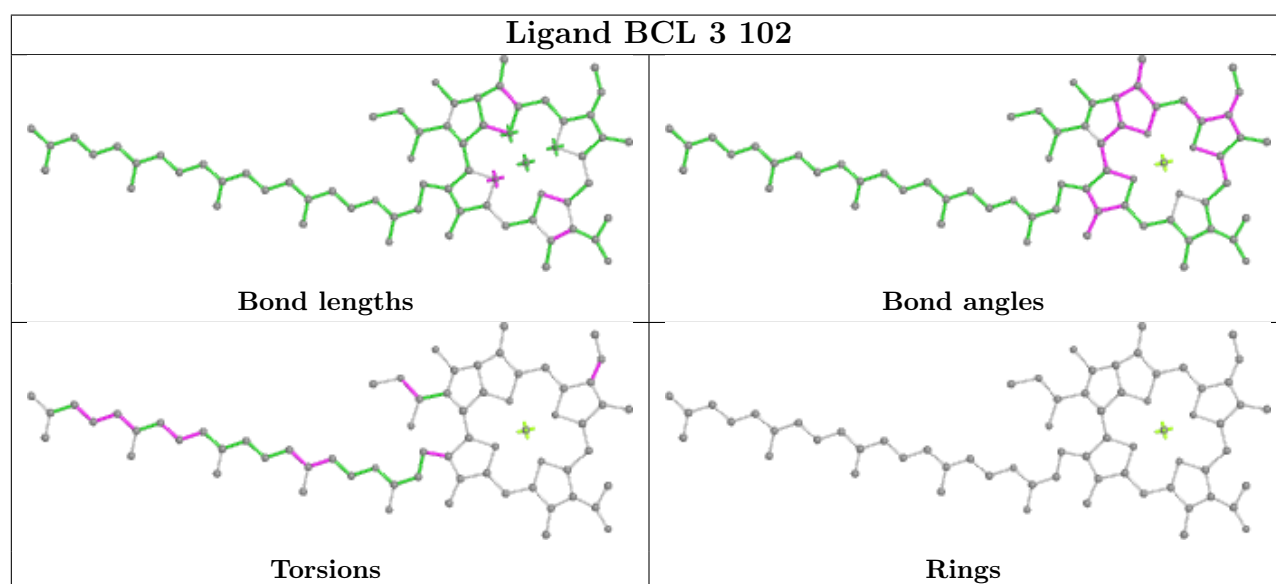
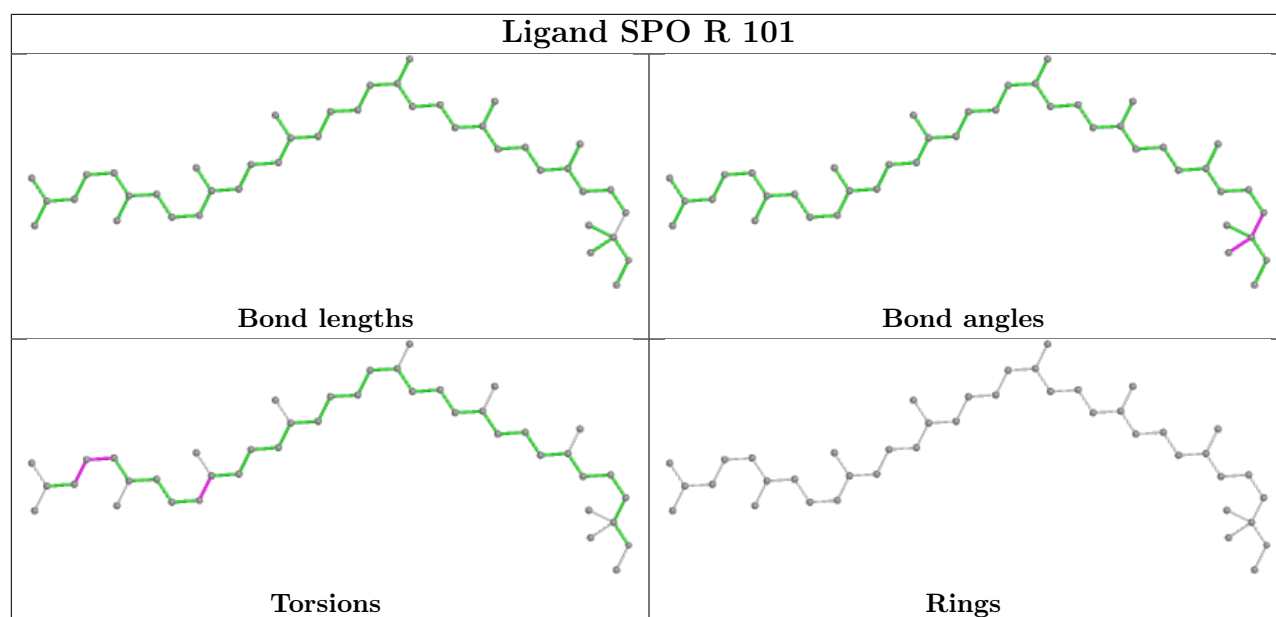


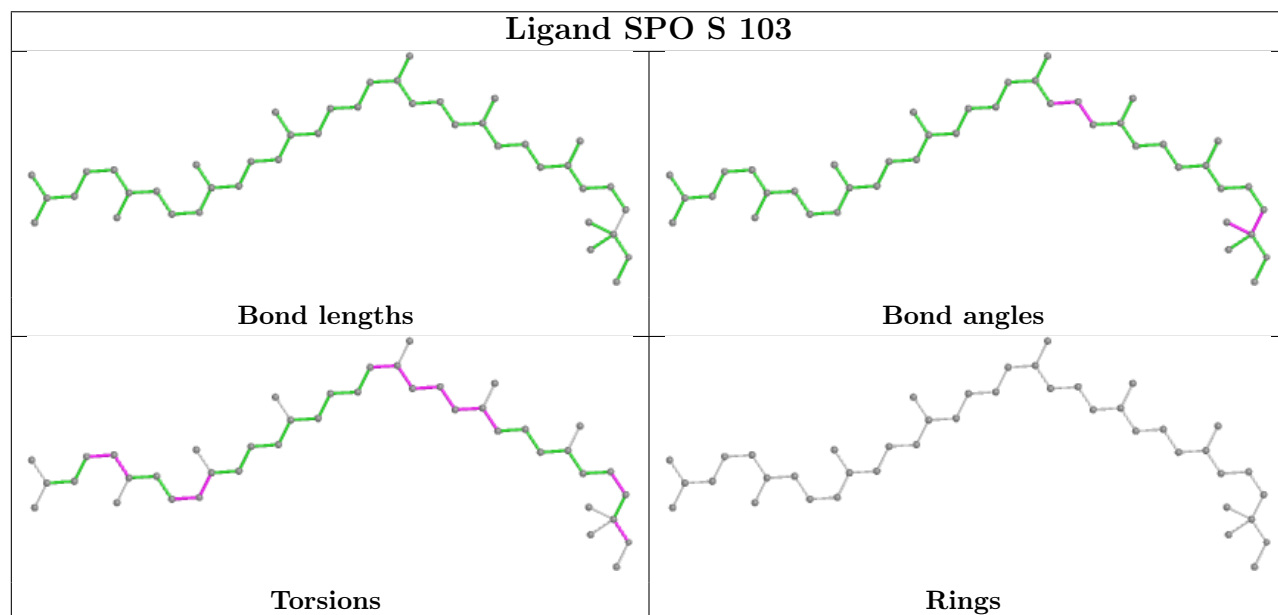
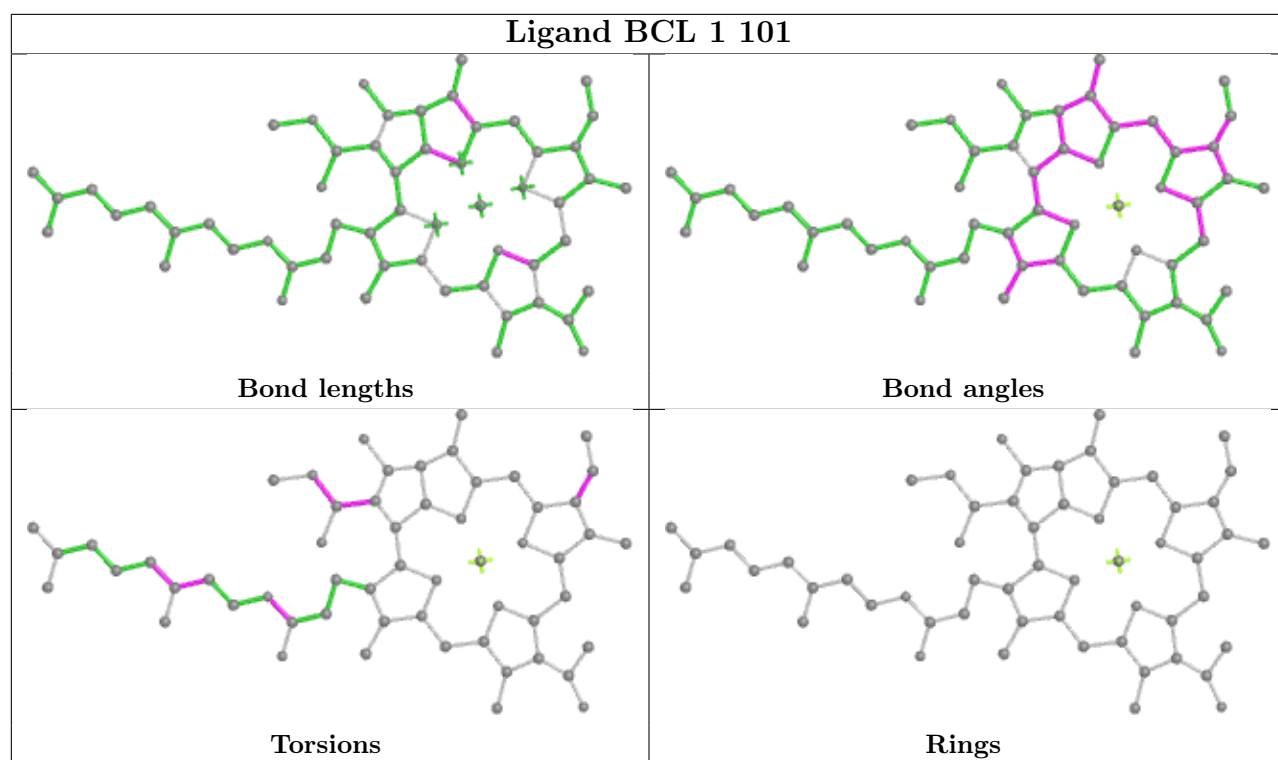


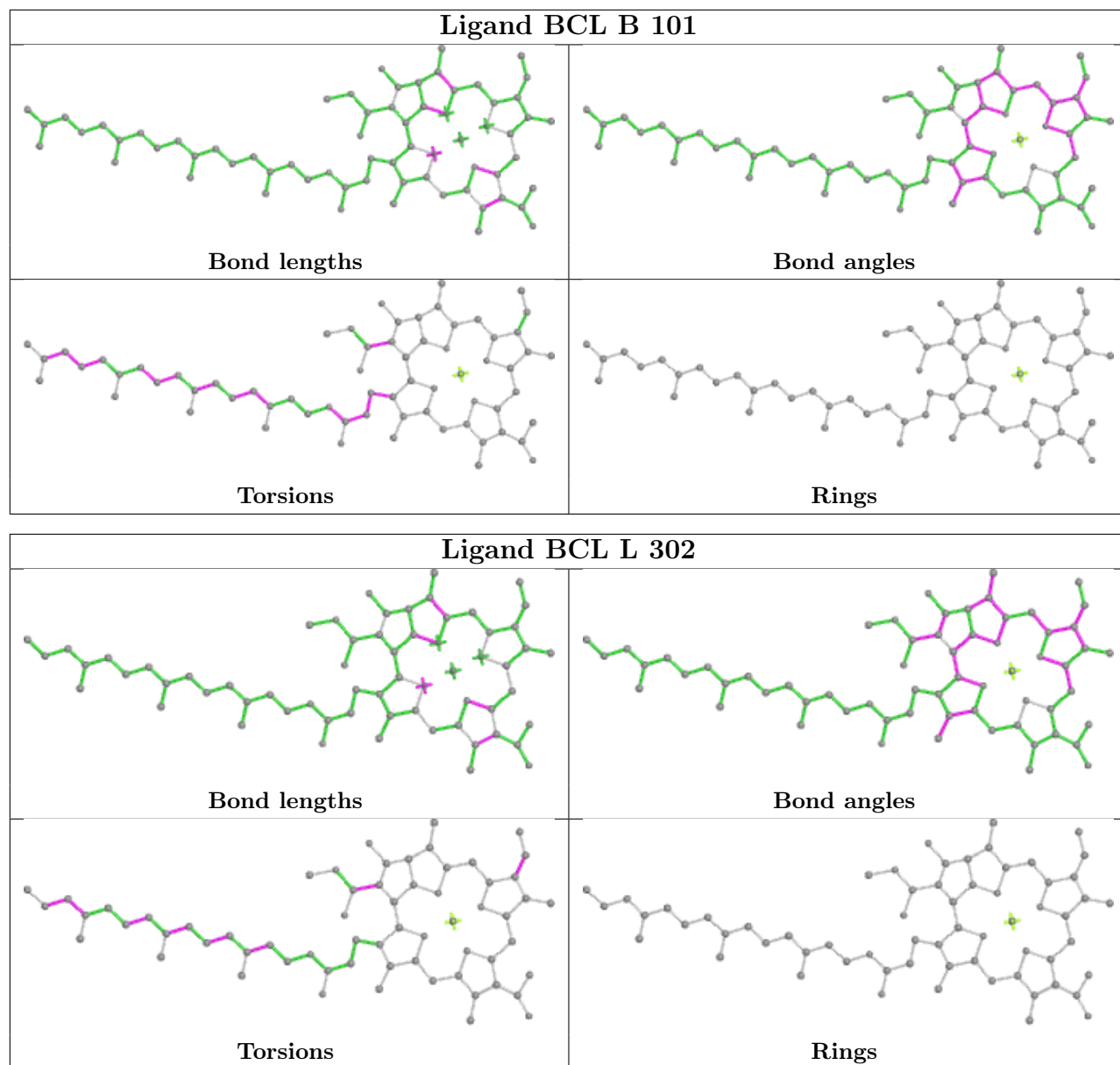


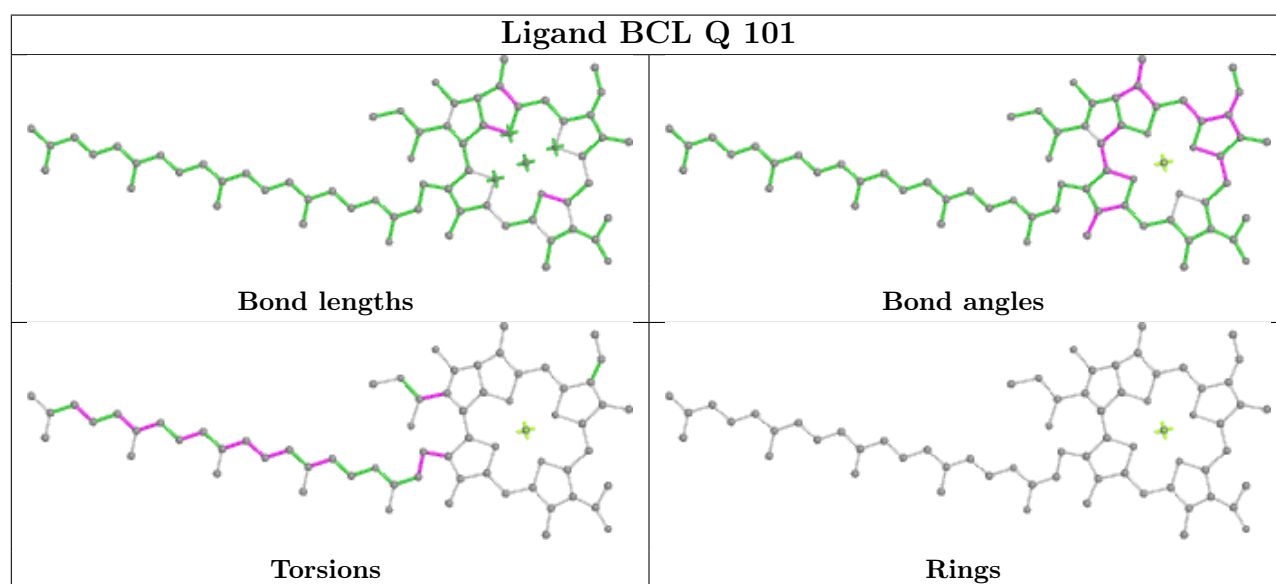
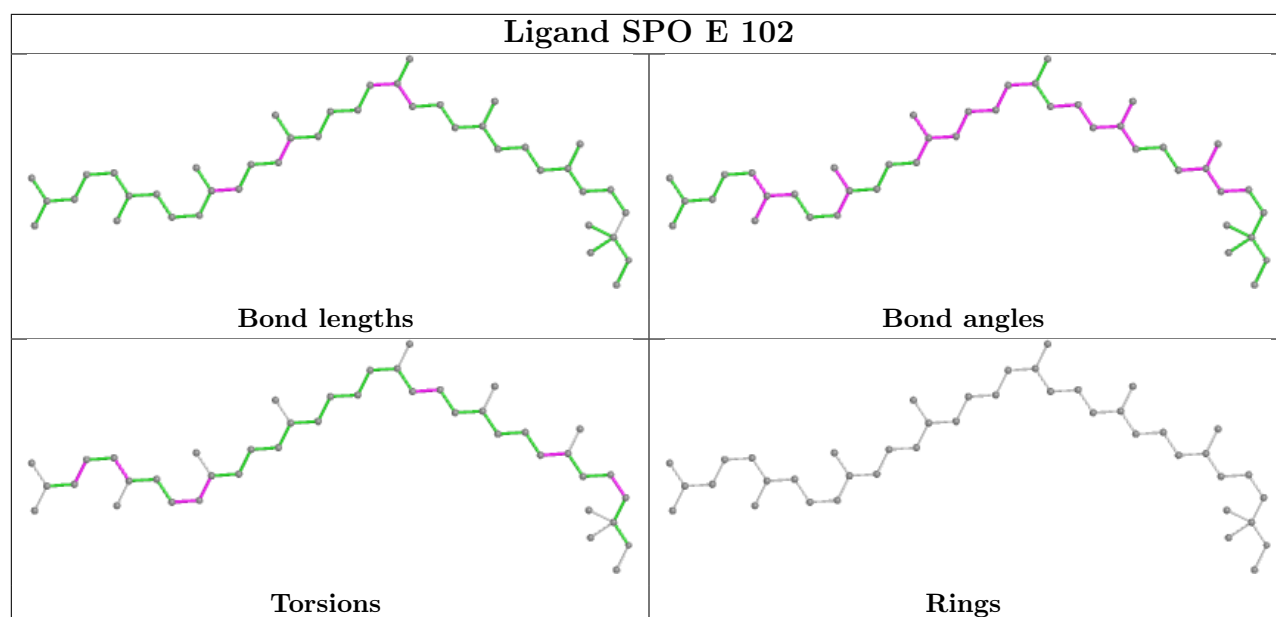


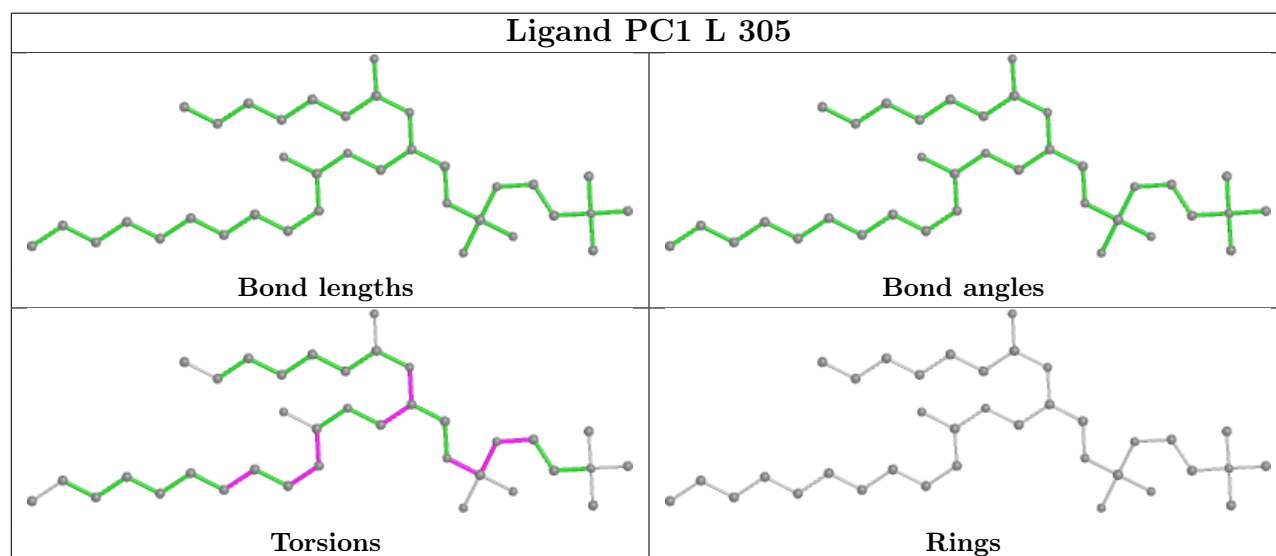
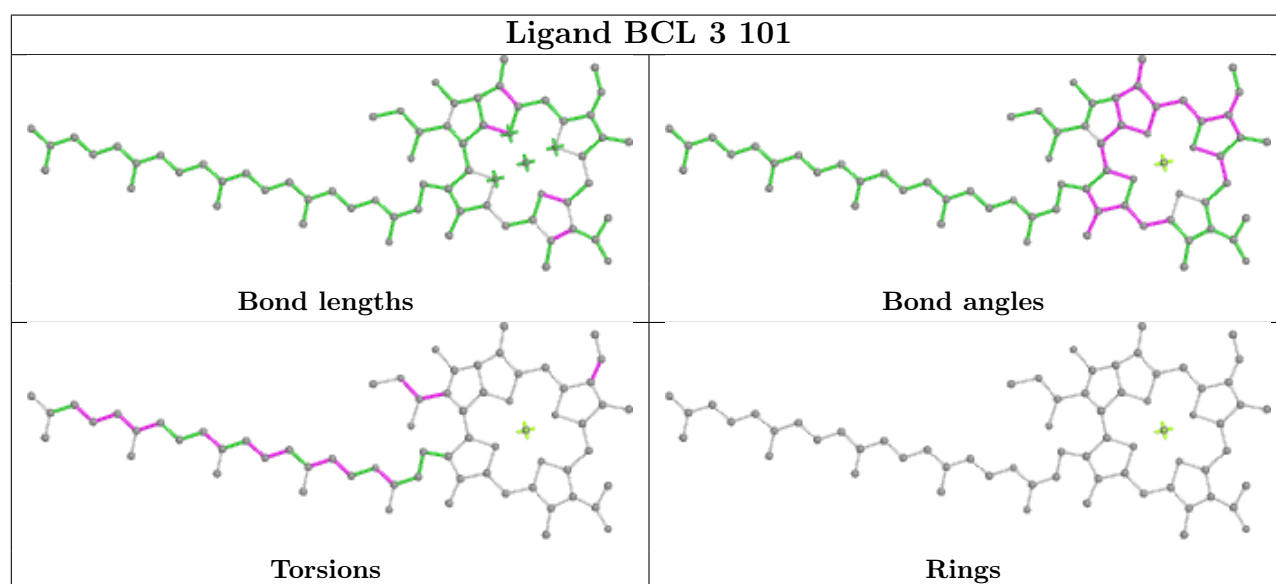
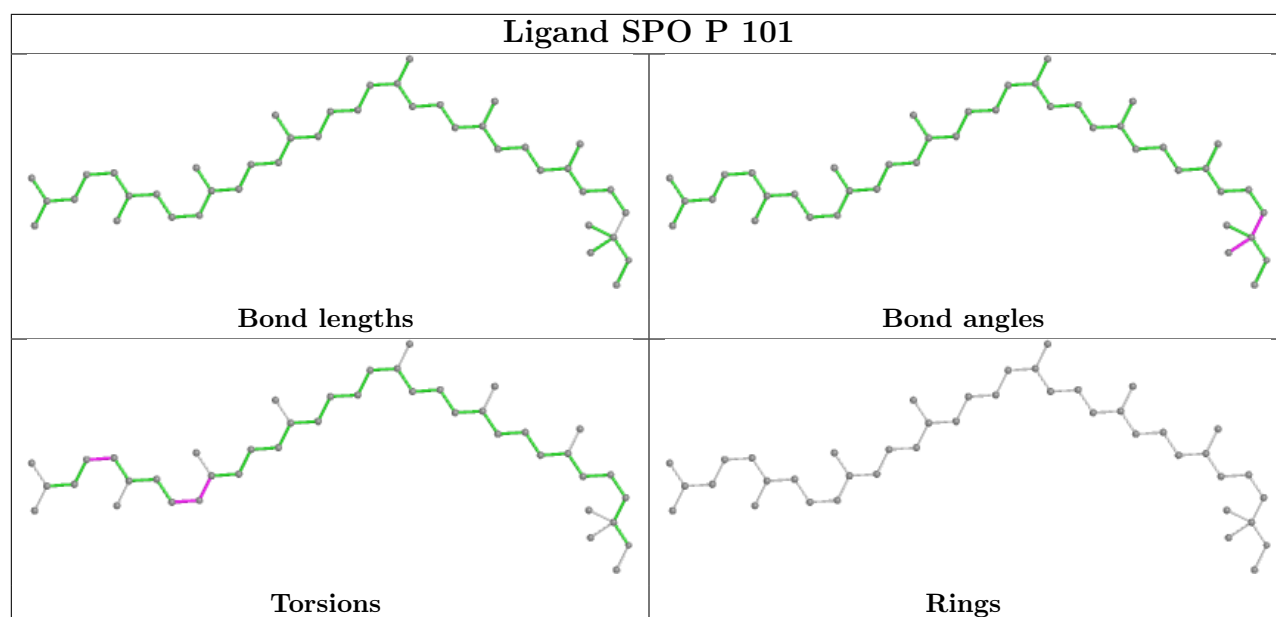


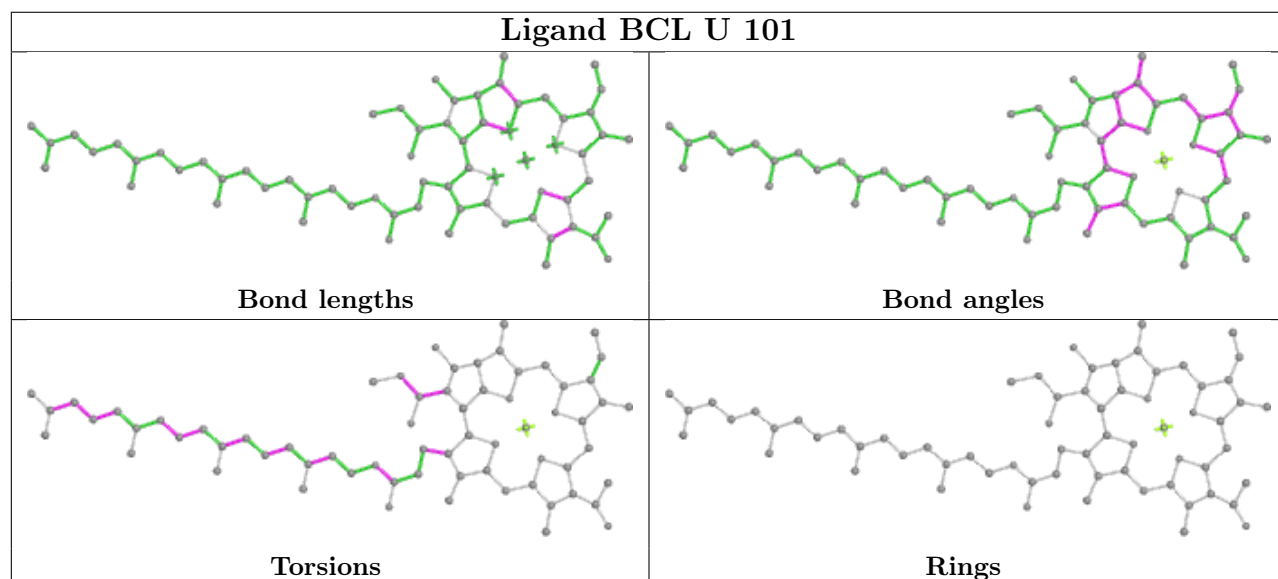
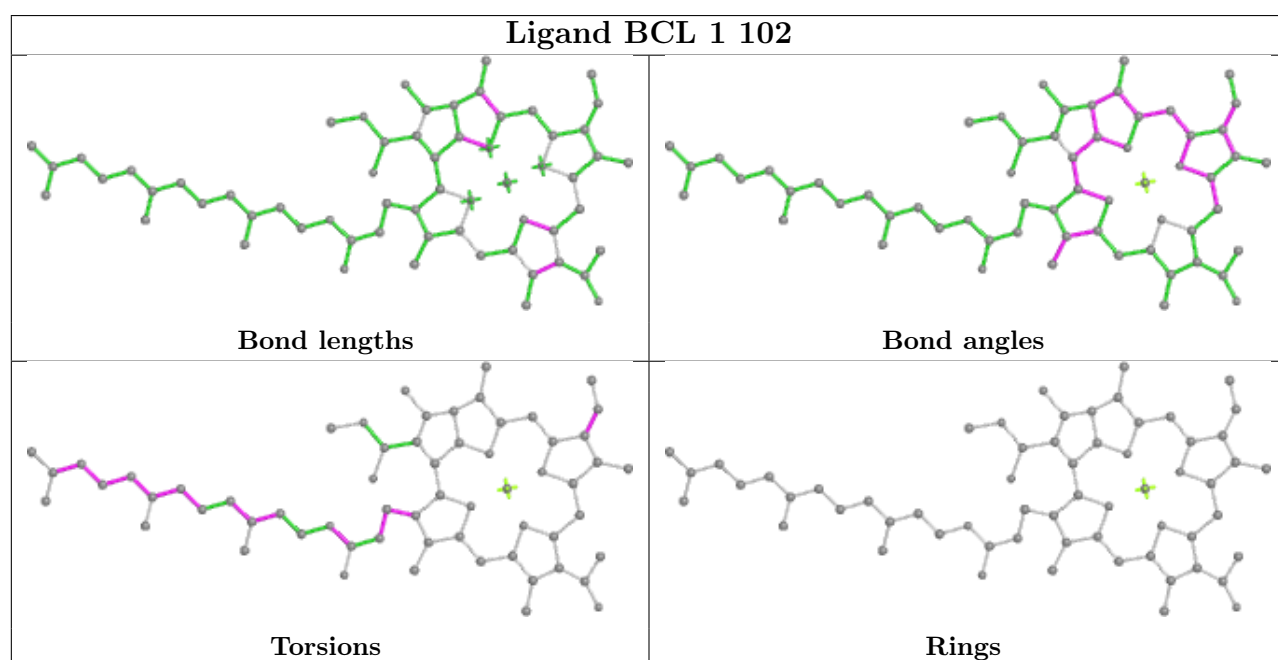
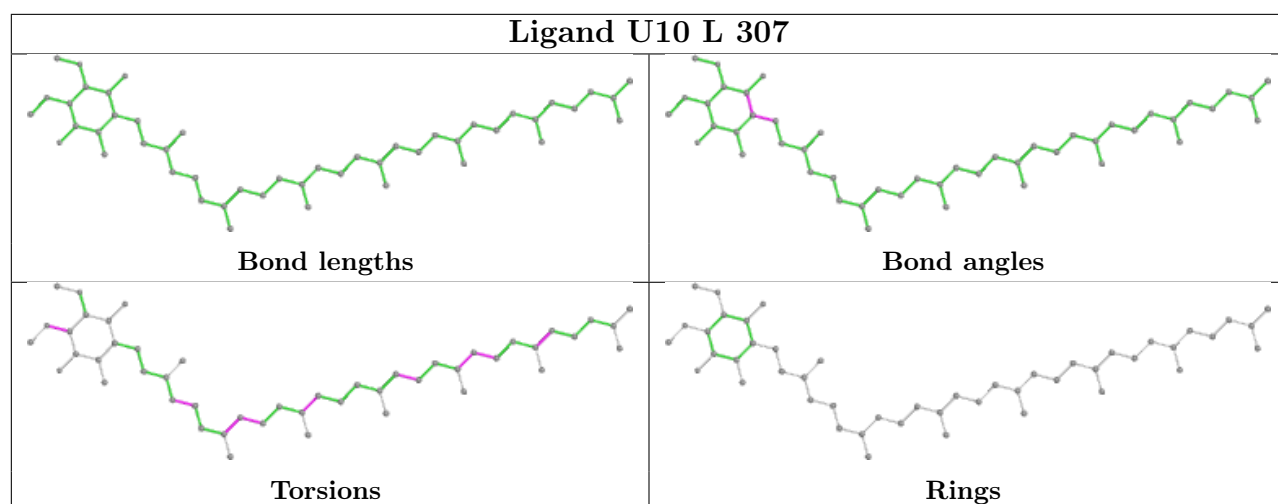




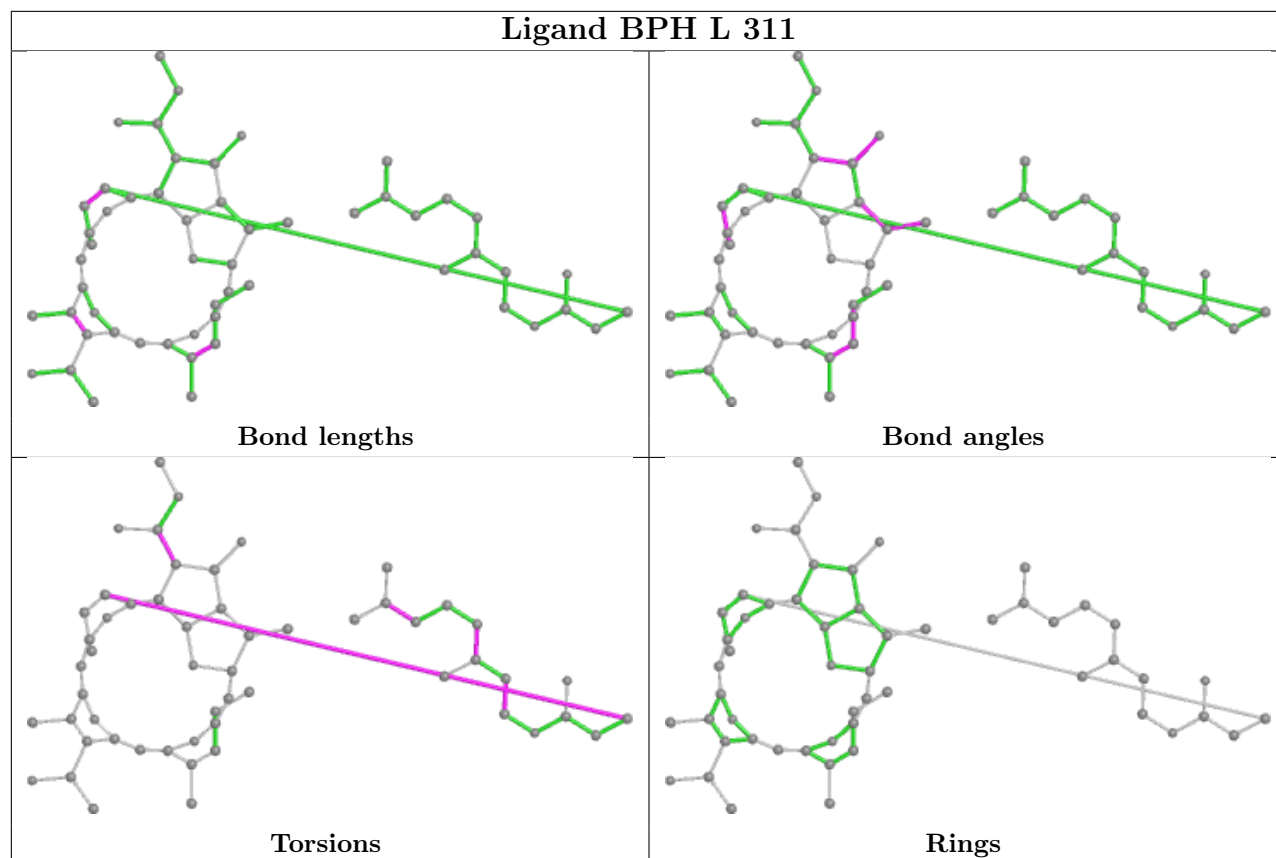




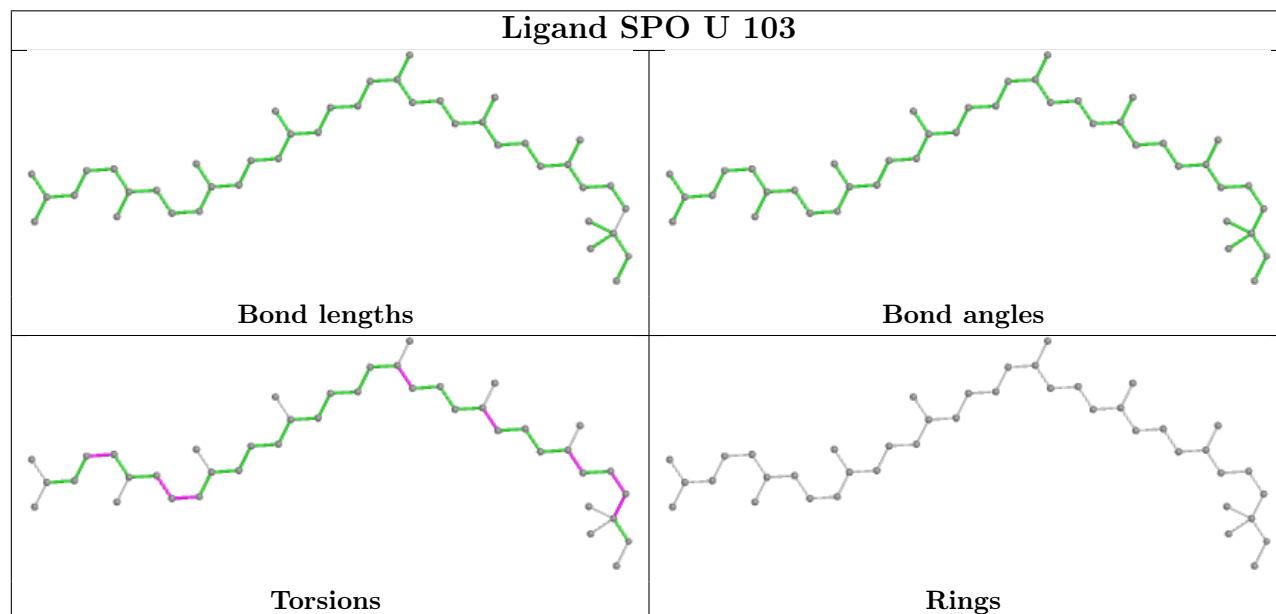


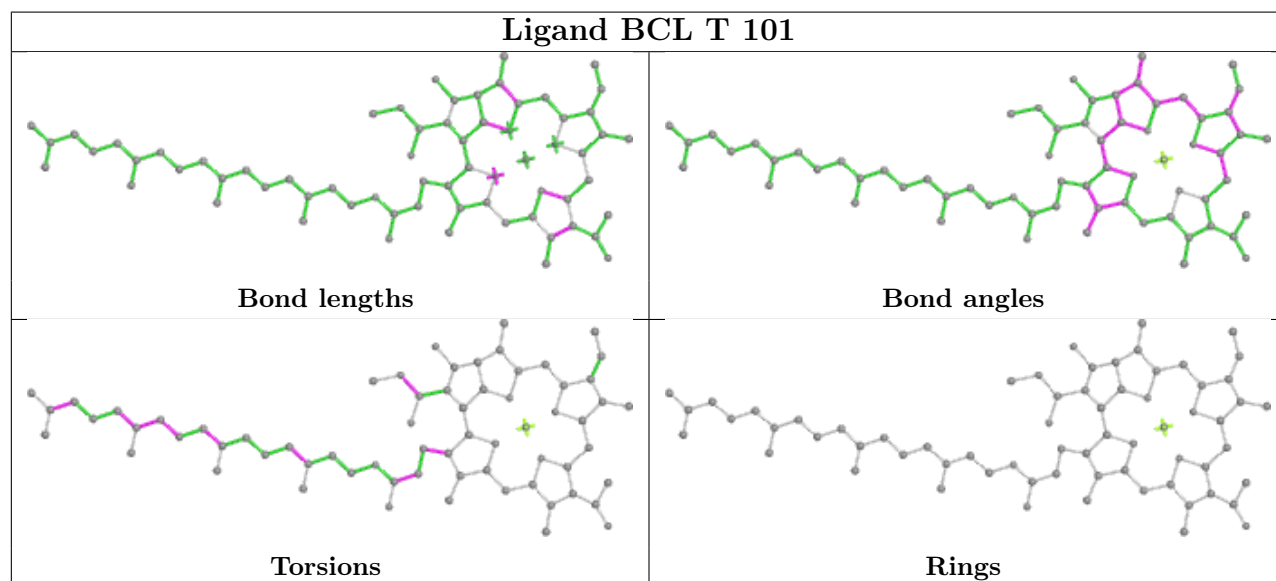
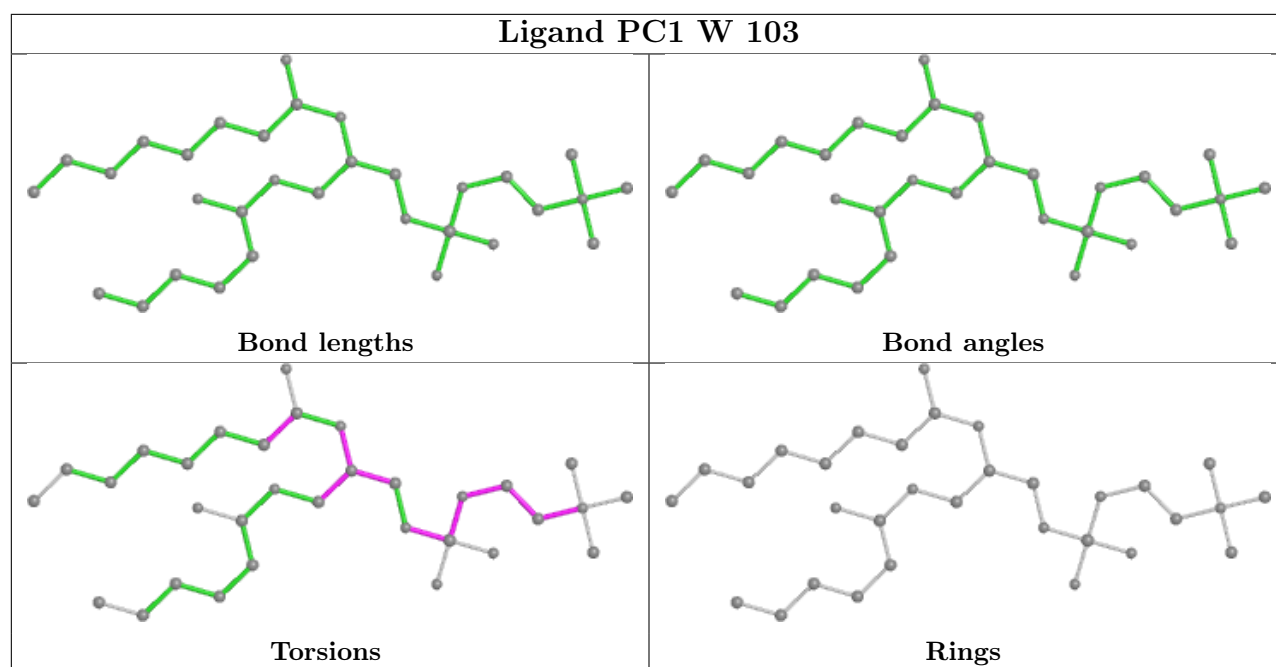


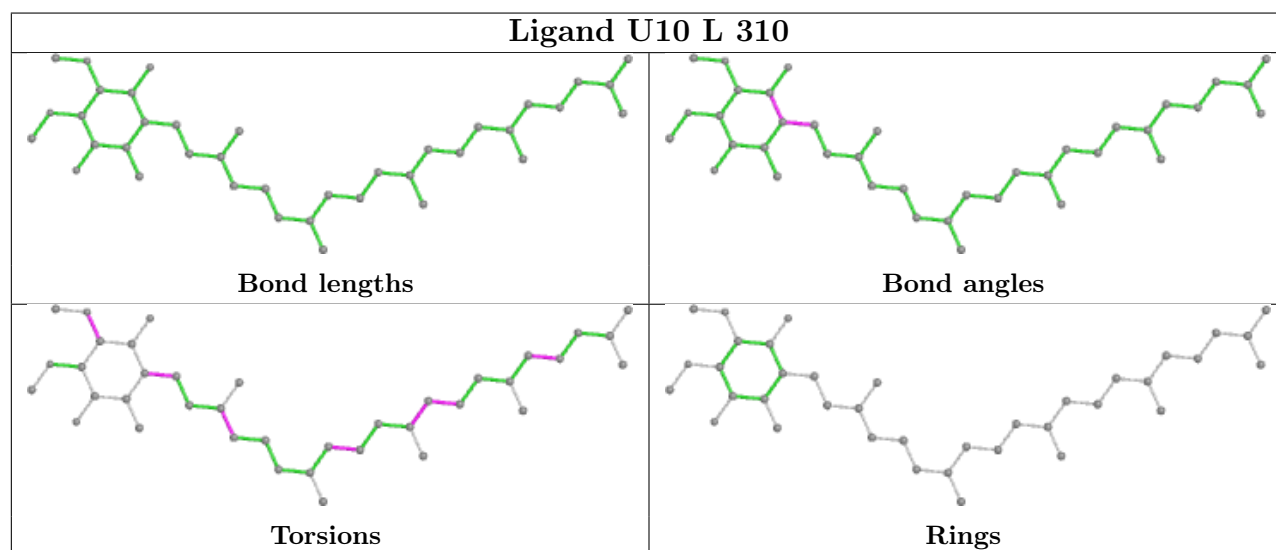
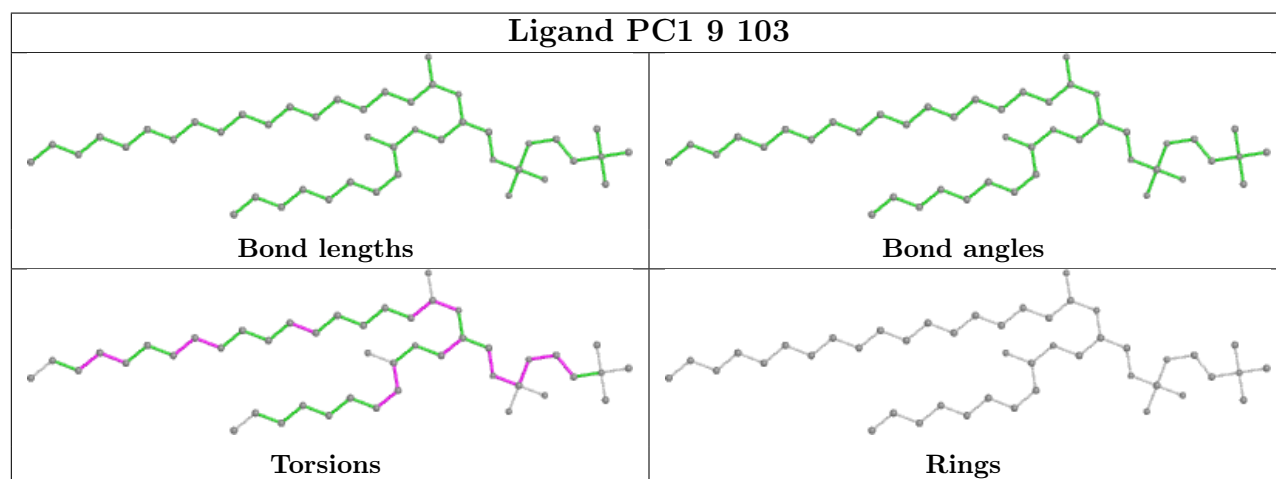
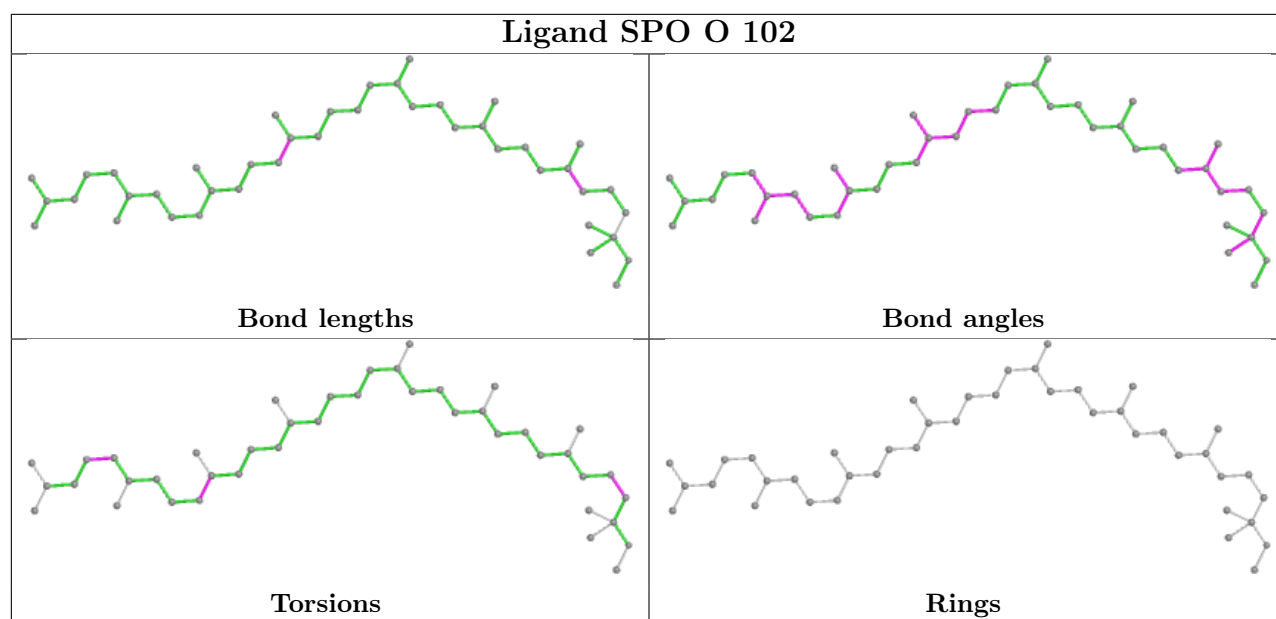
Ligand BPH L 311

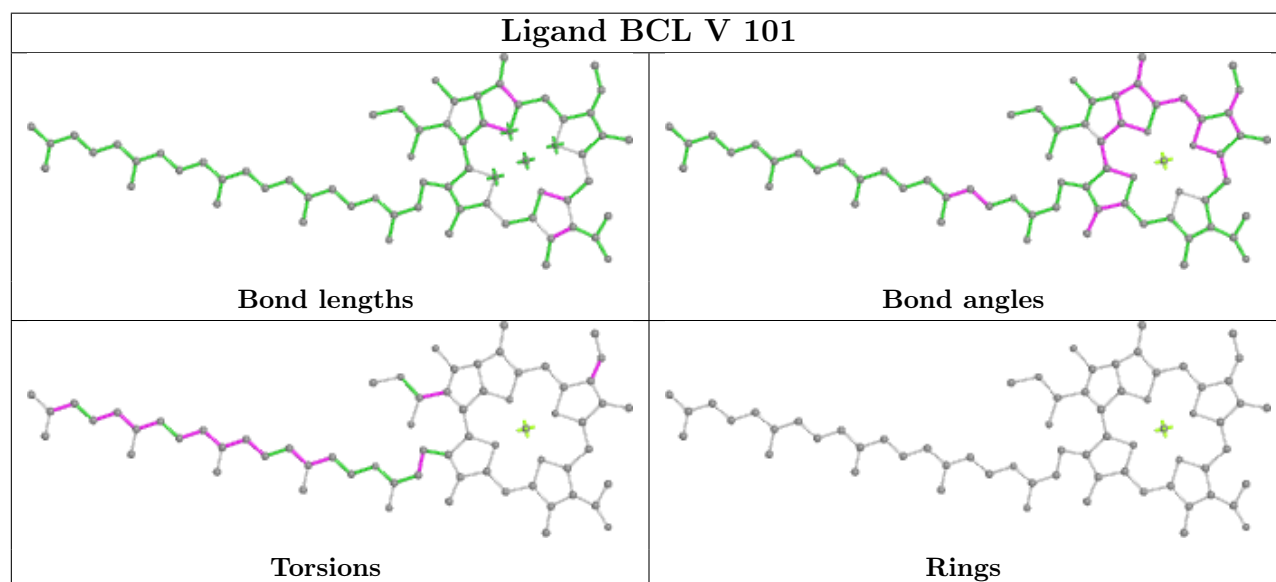
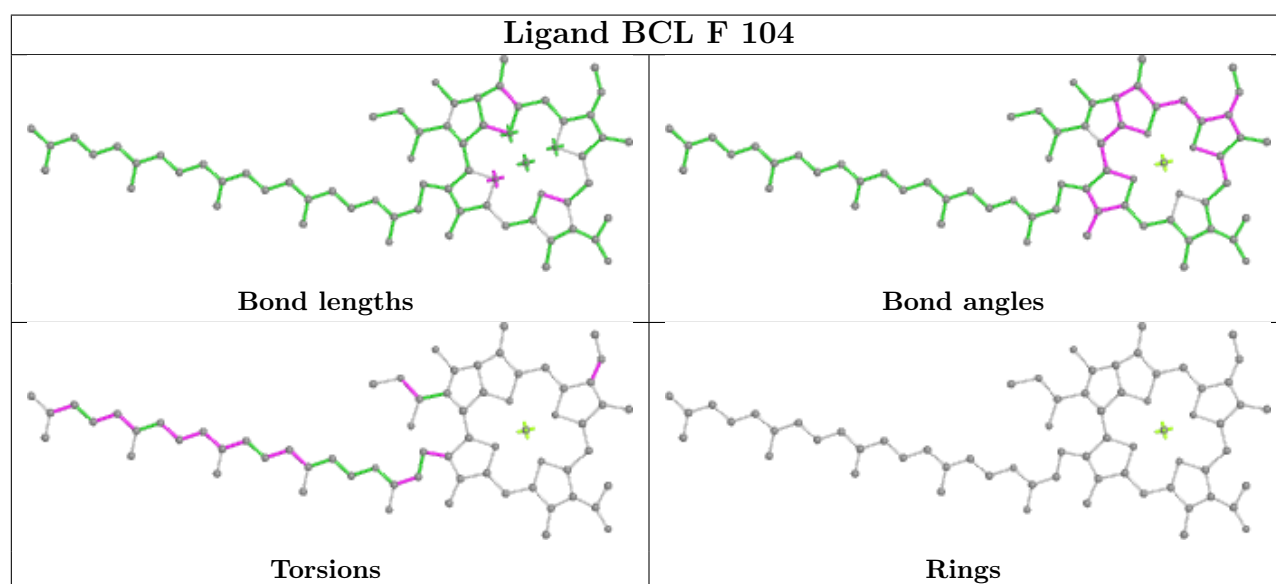
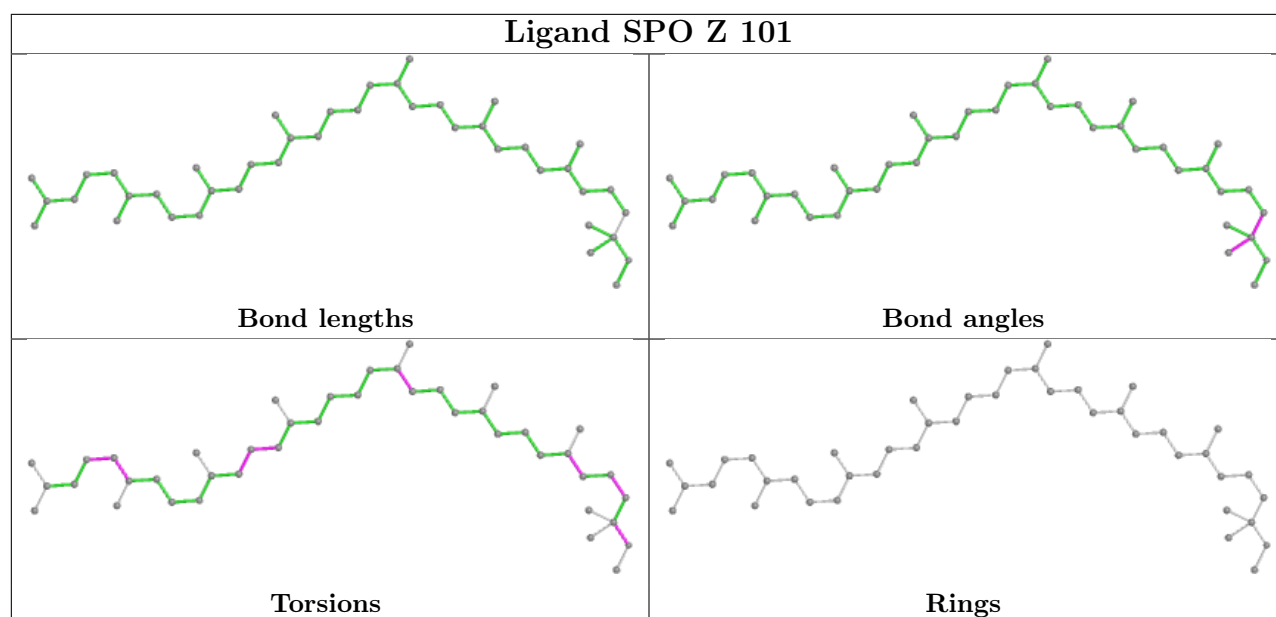


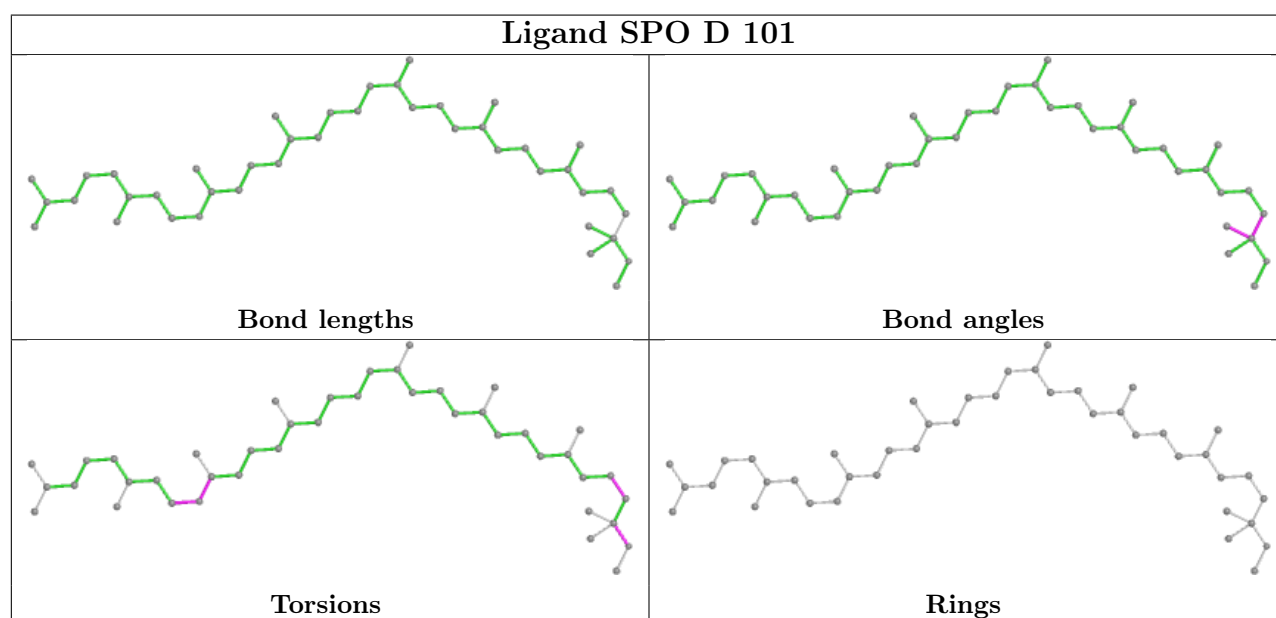
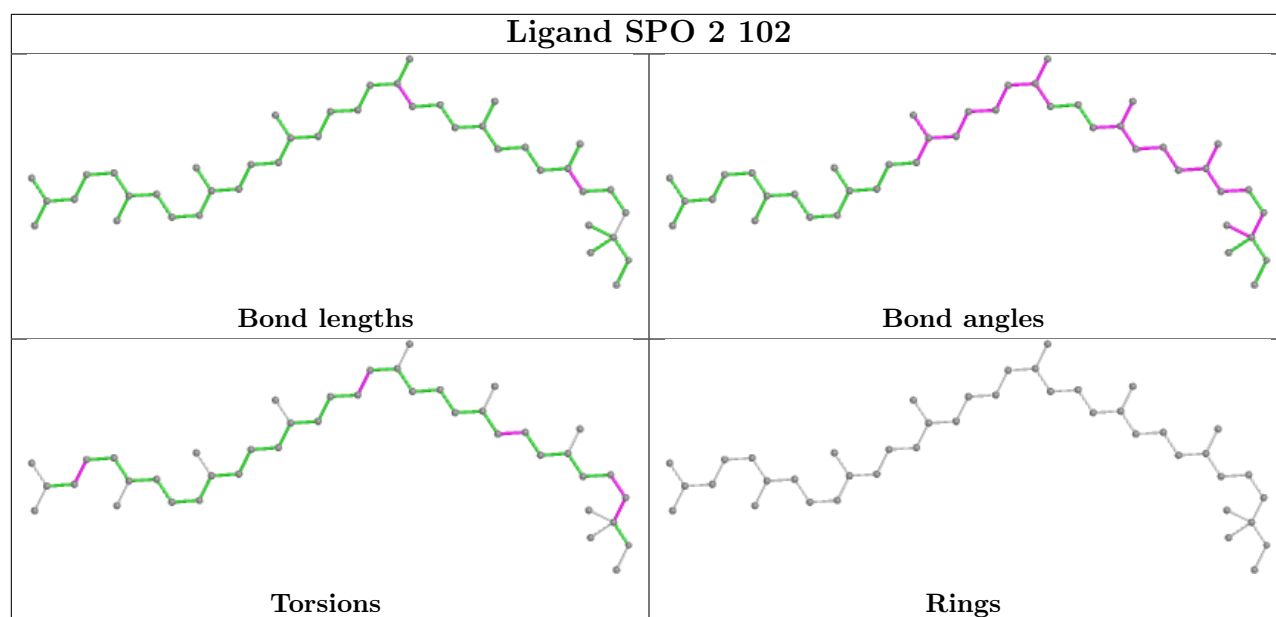
Ligand SPO U 103

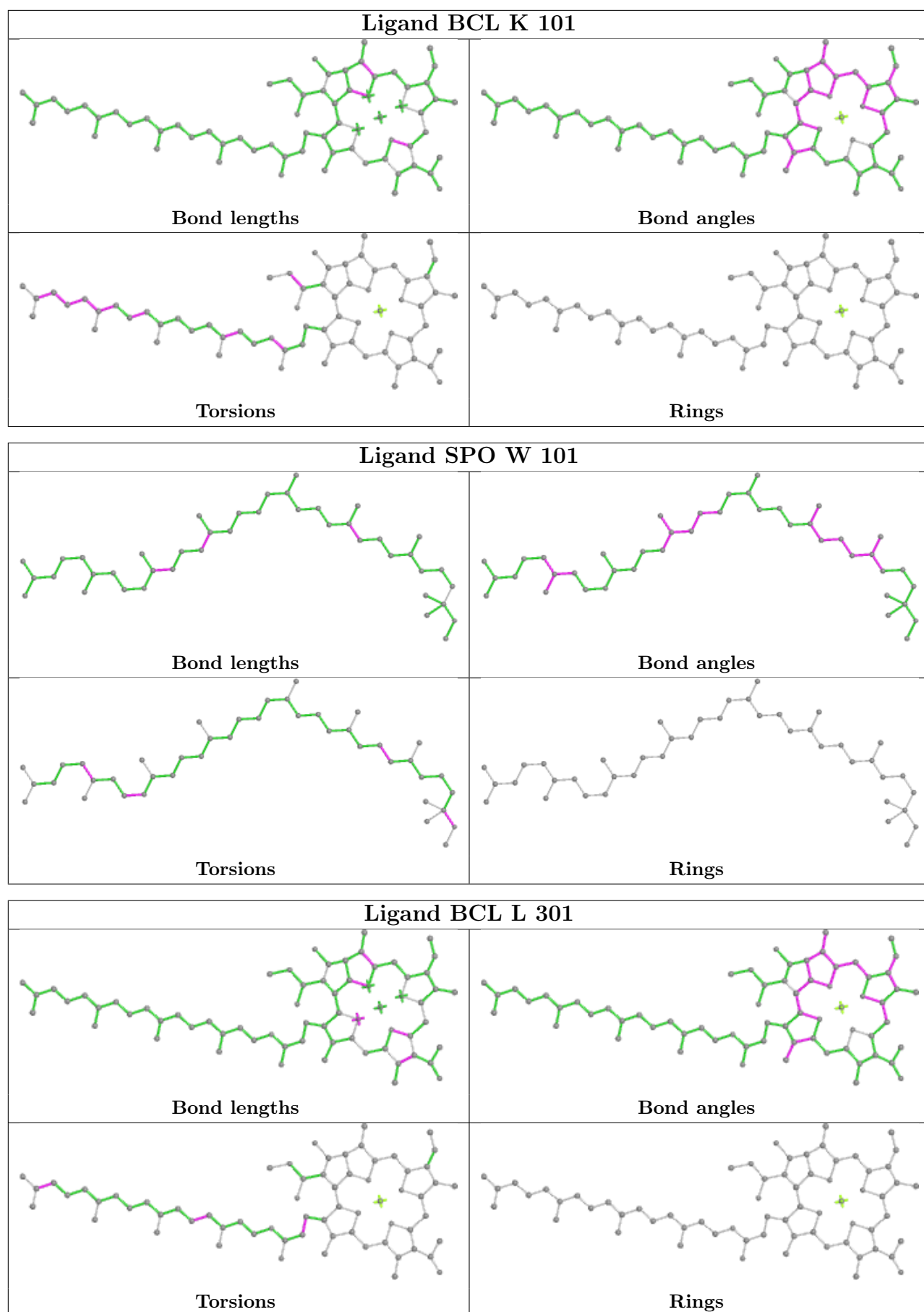


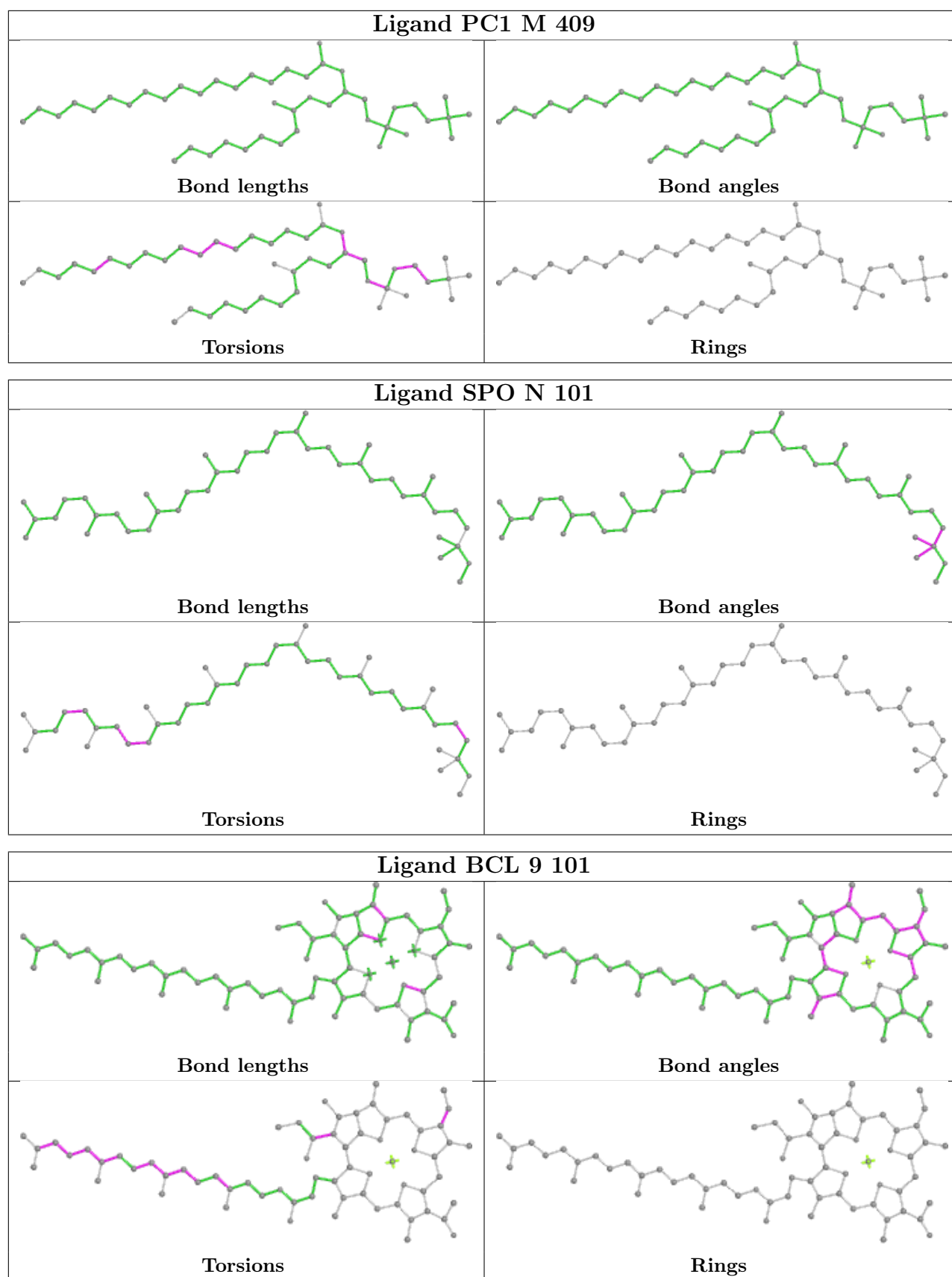




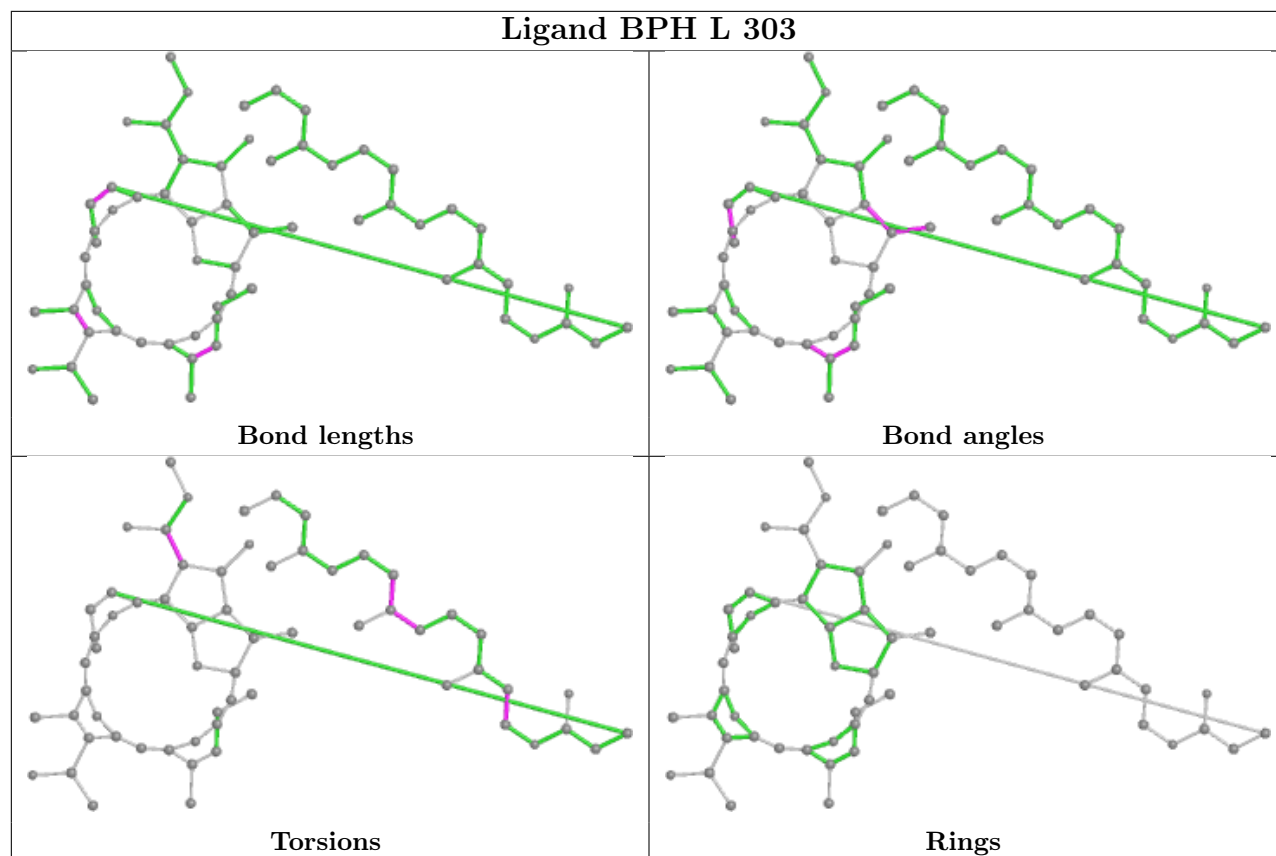




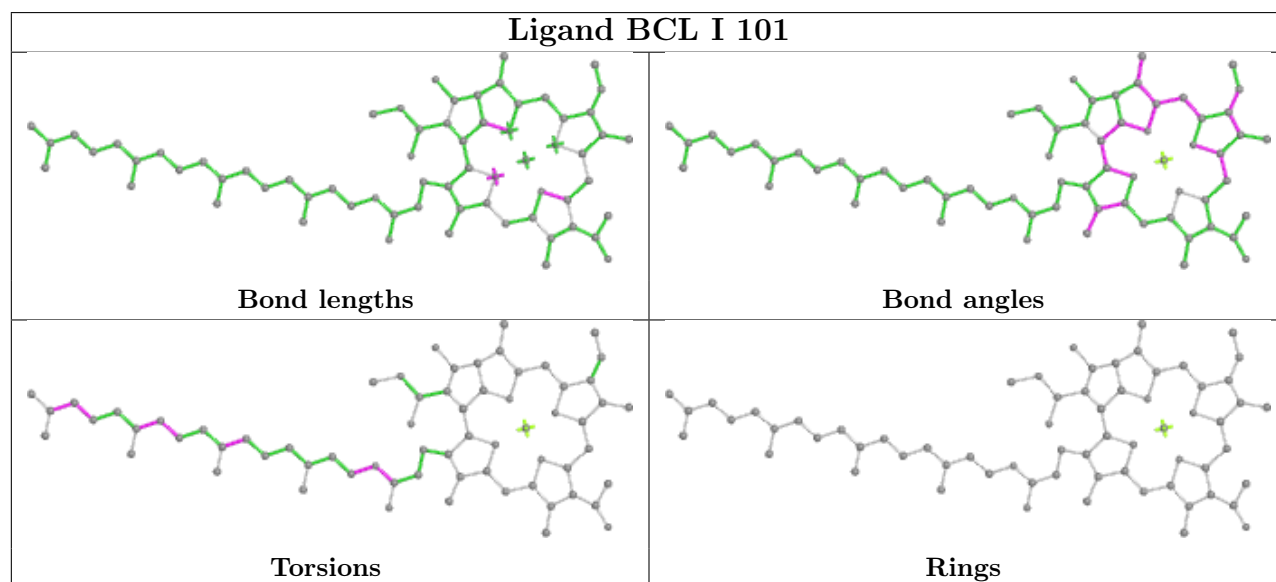


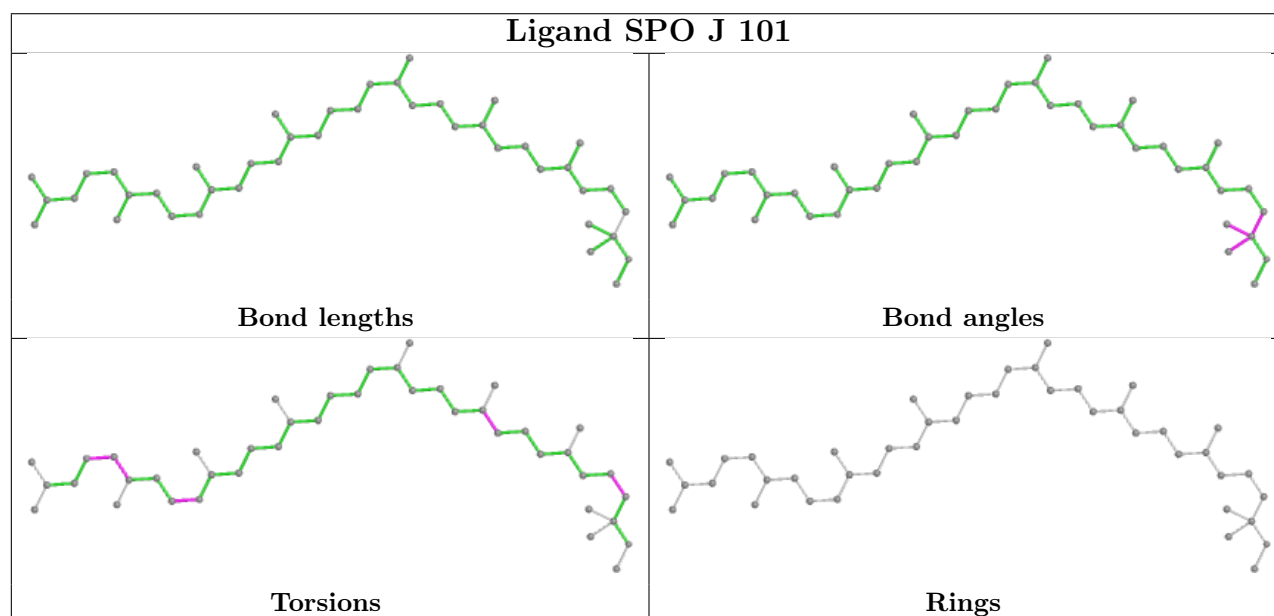
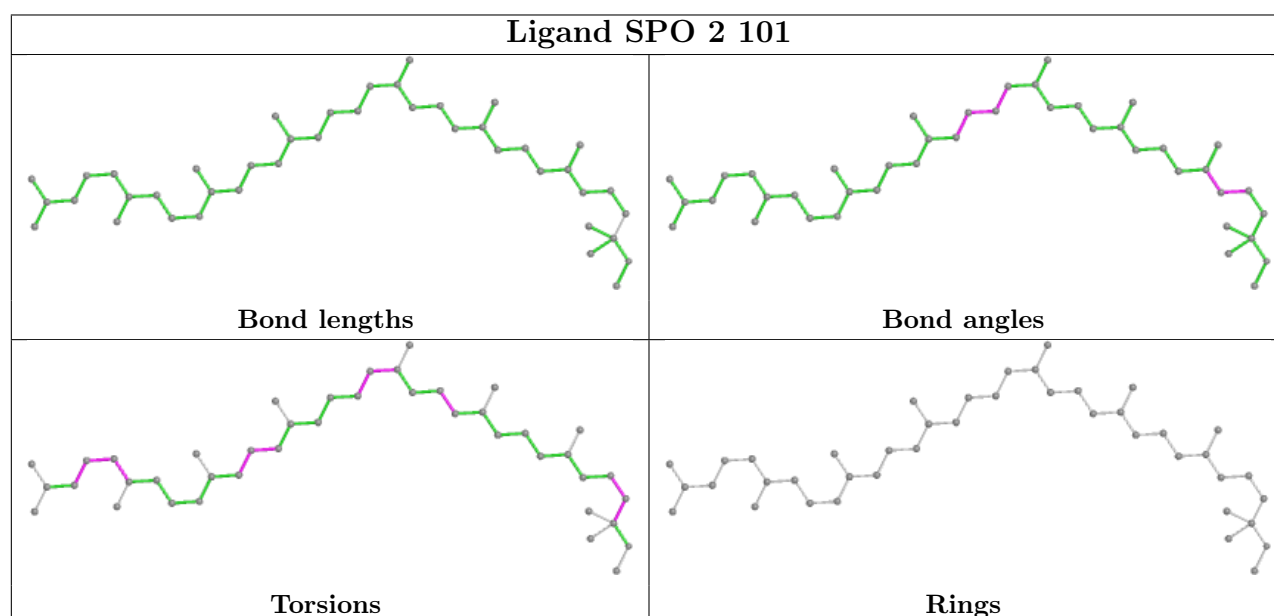
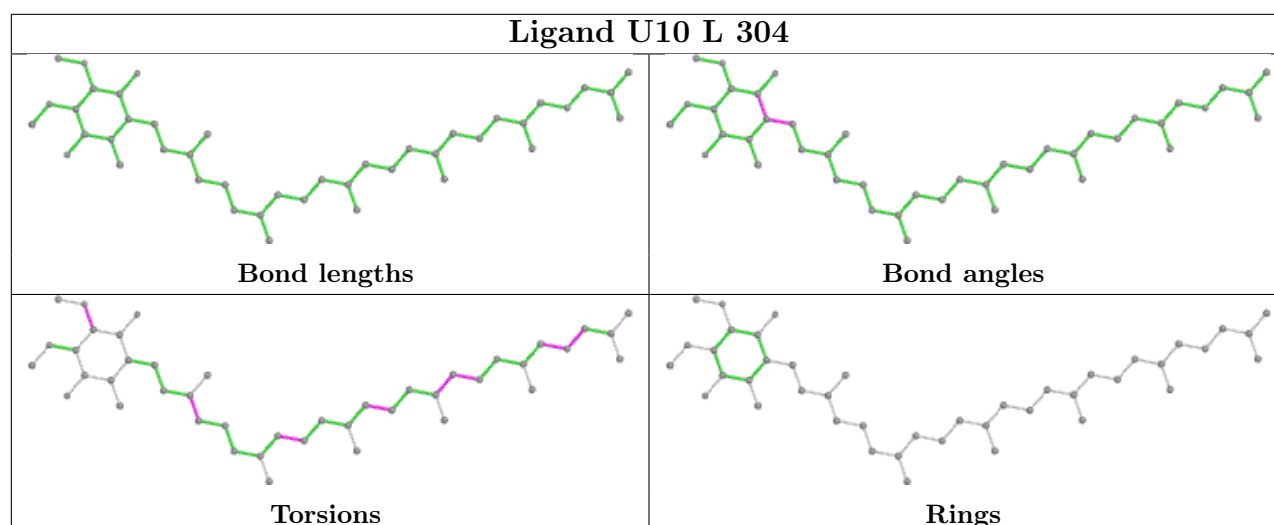


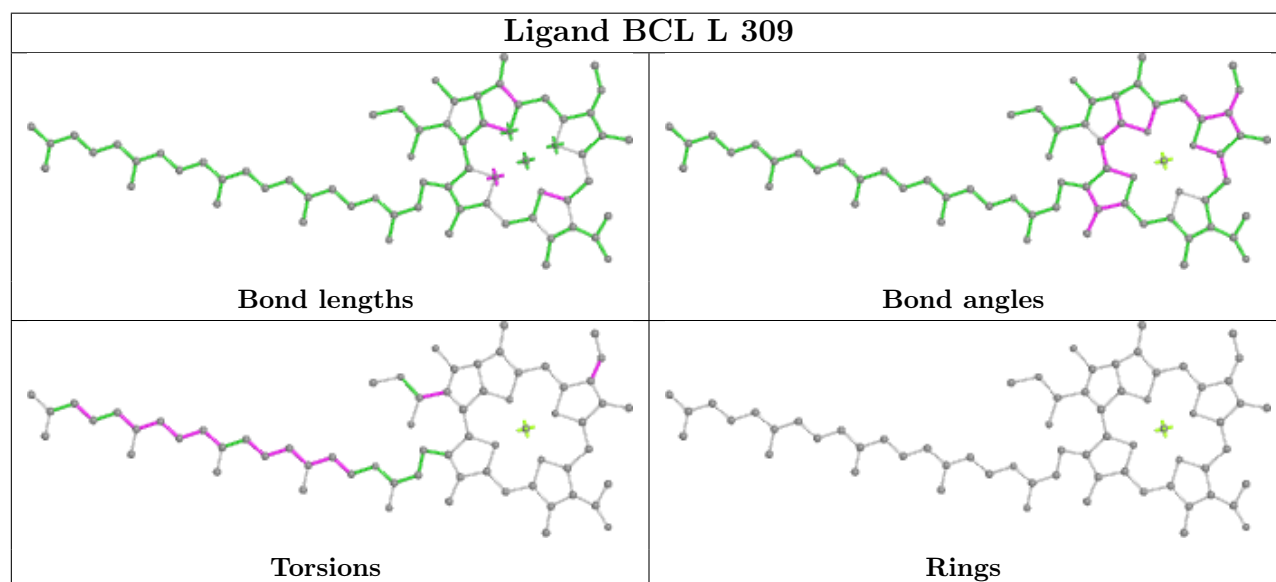
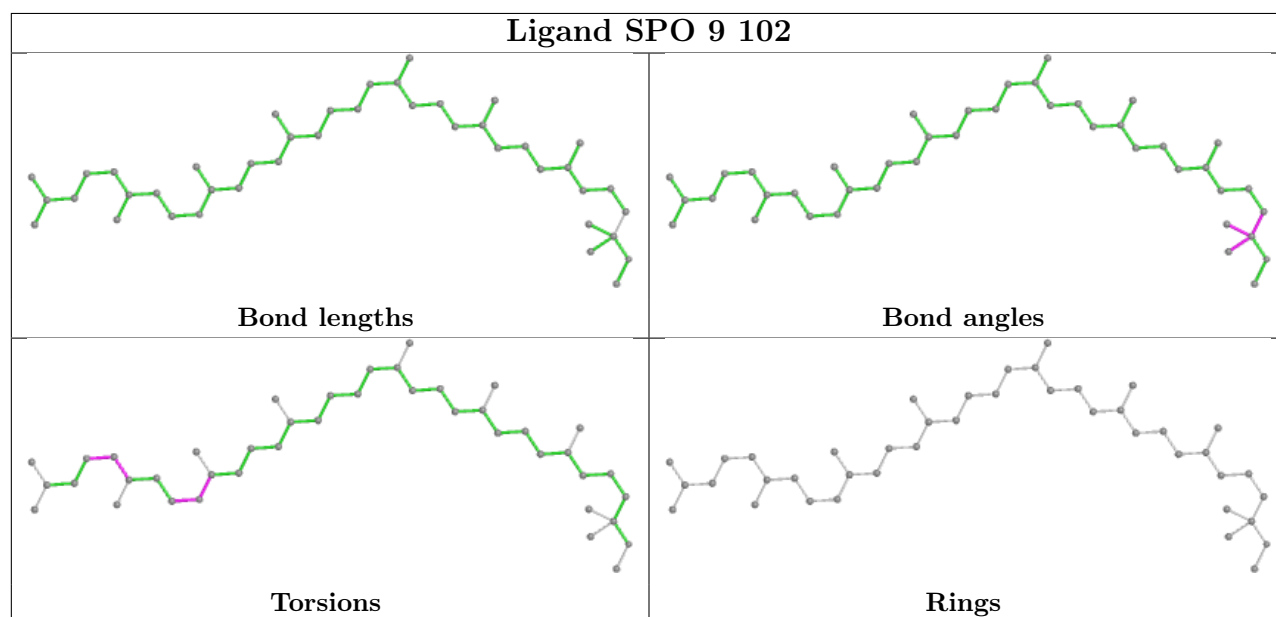
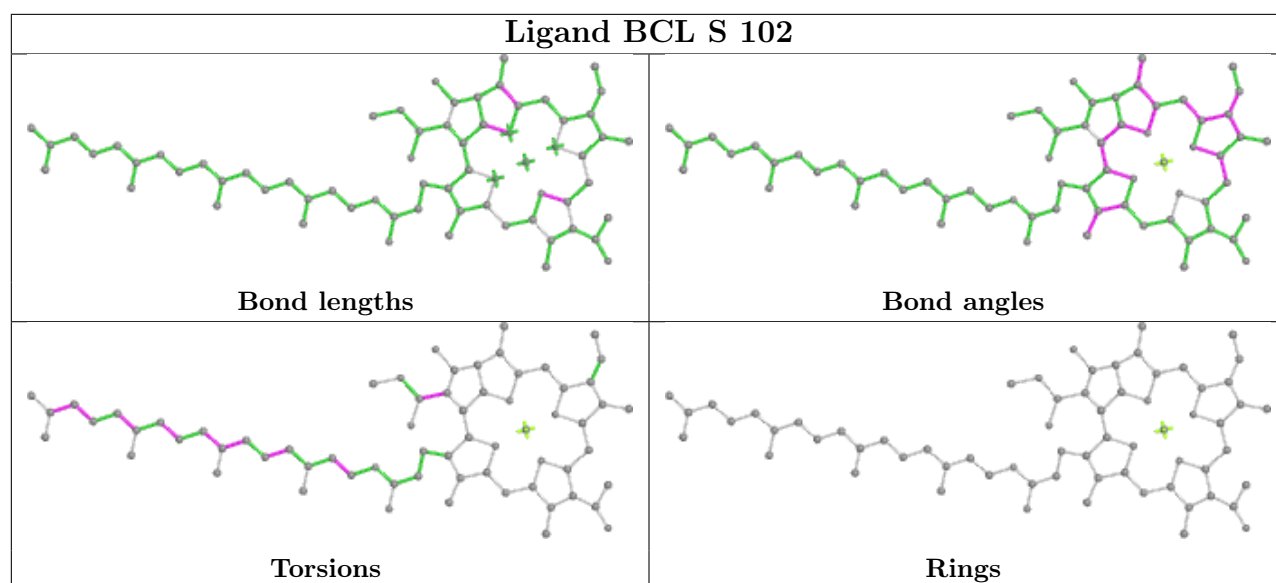
Ligand BPH L 303

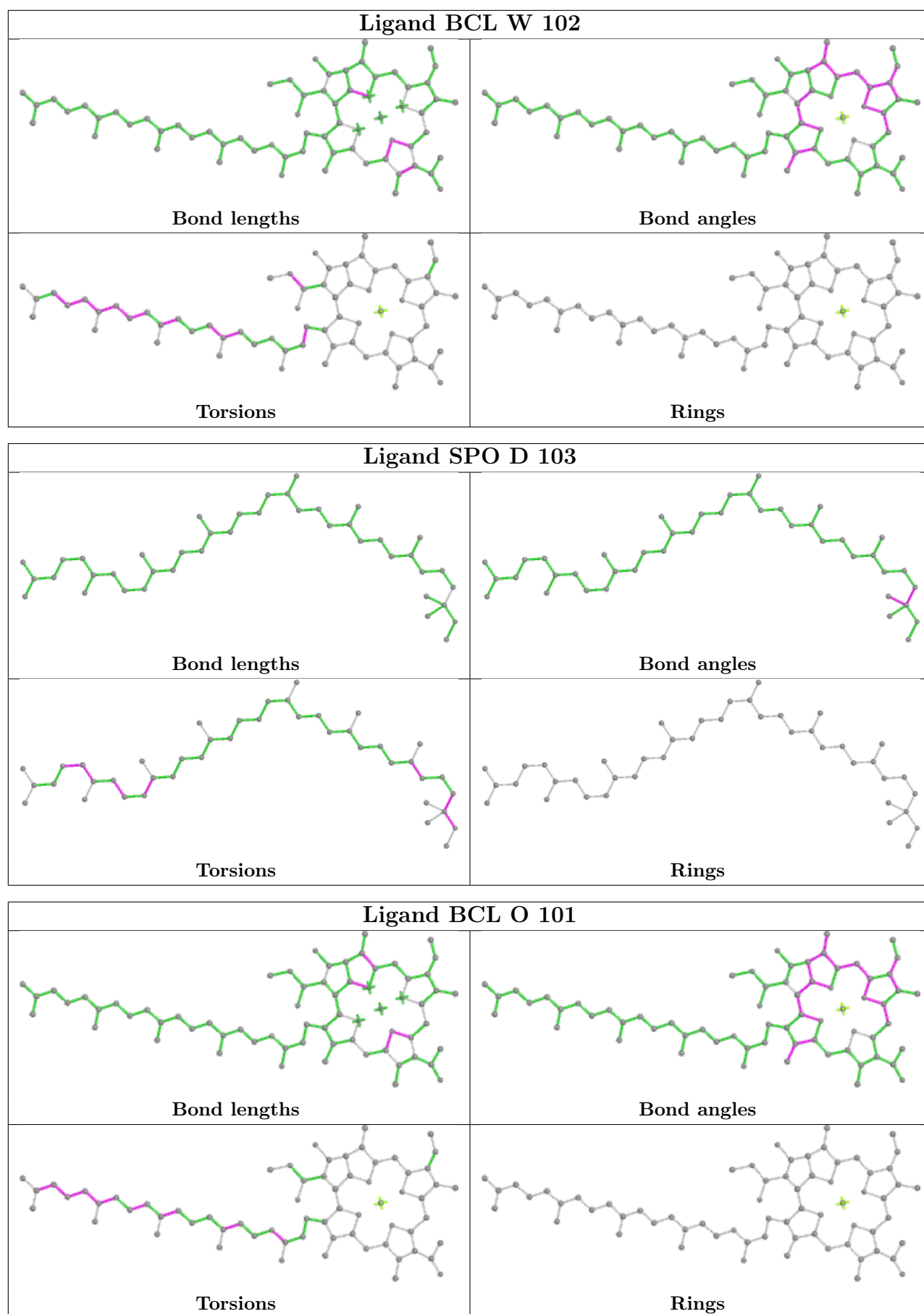


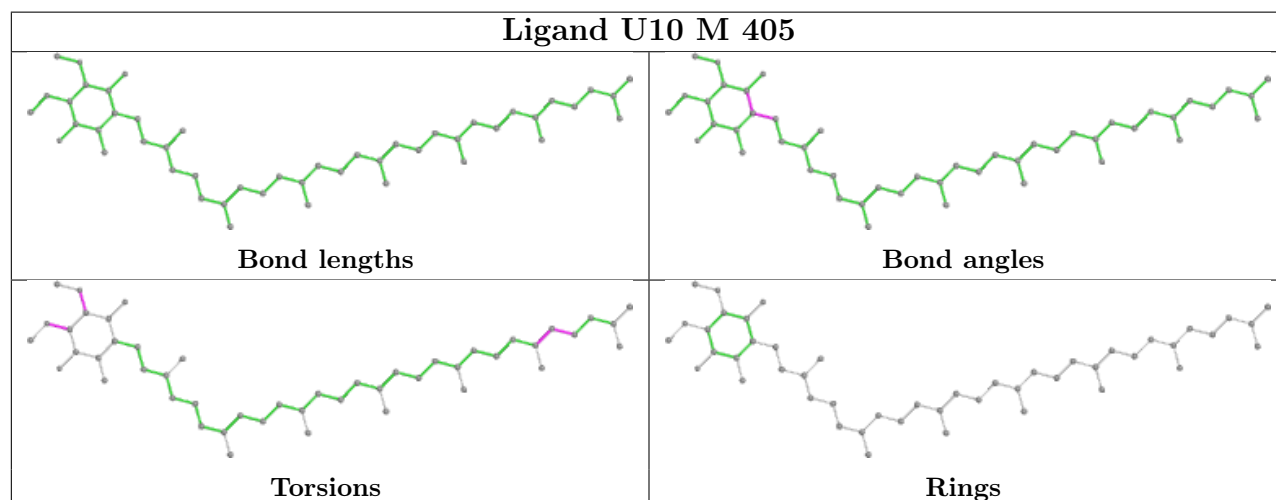
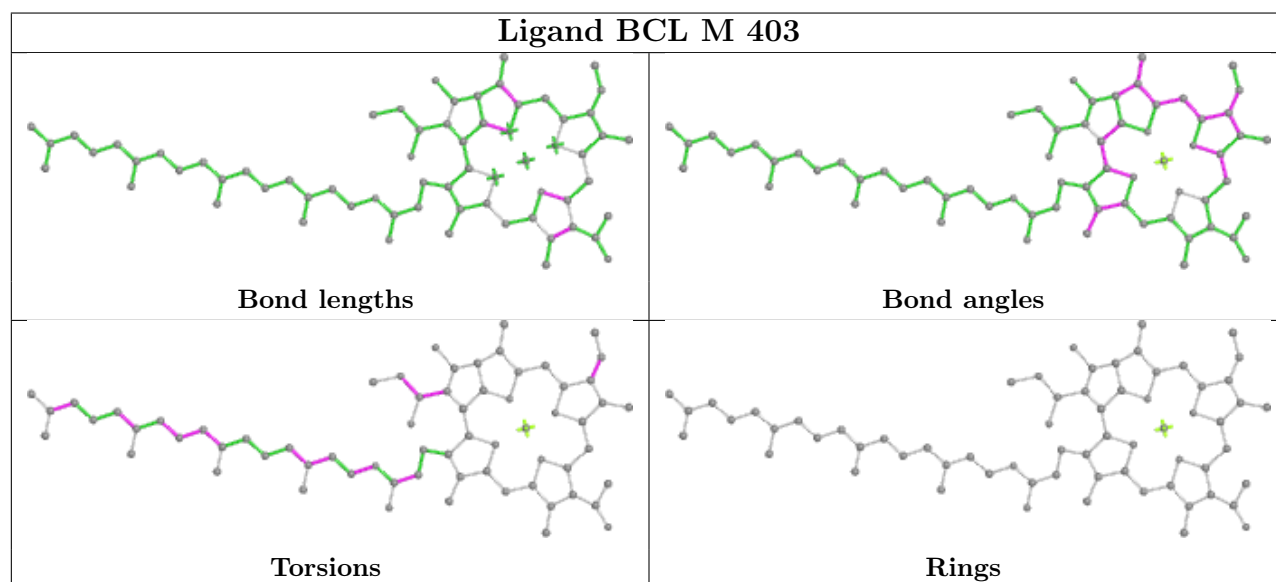
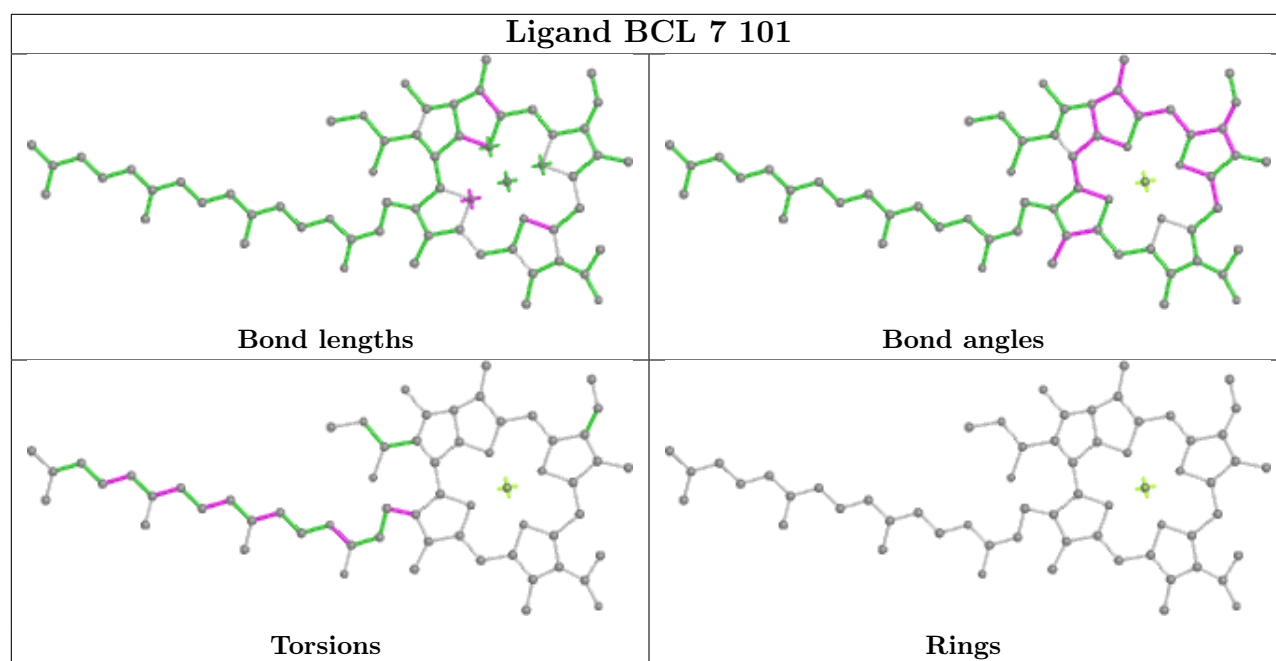
Ligand BCL I 101

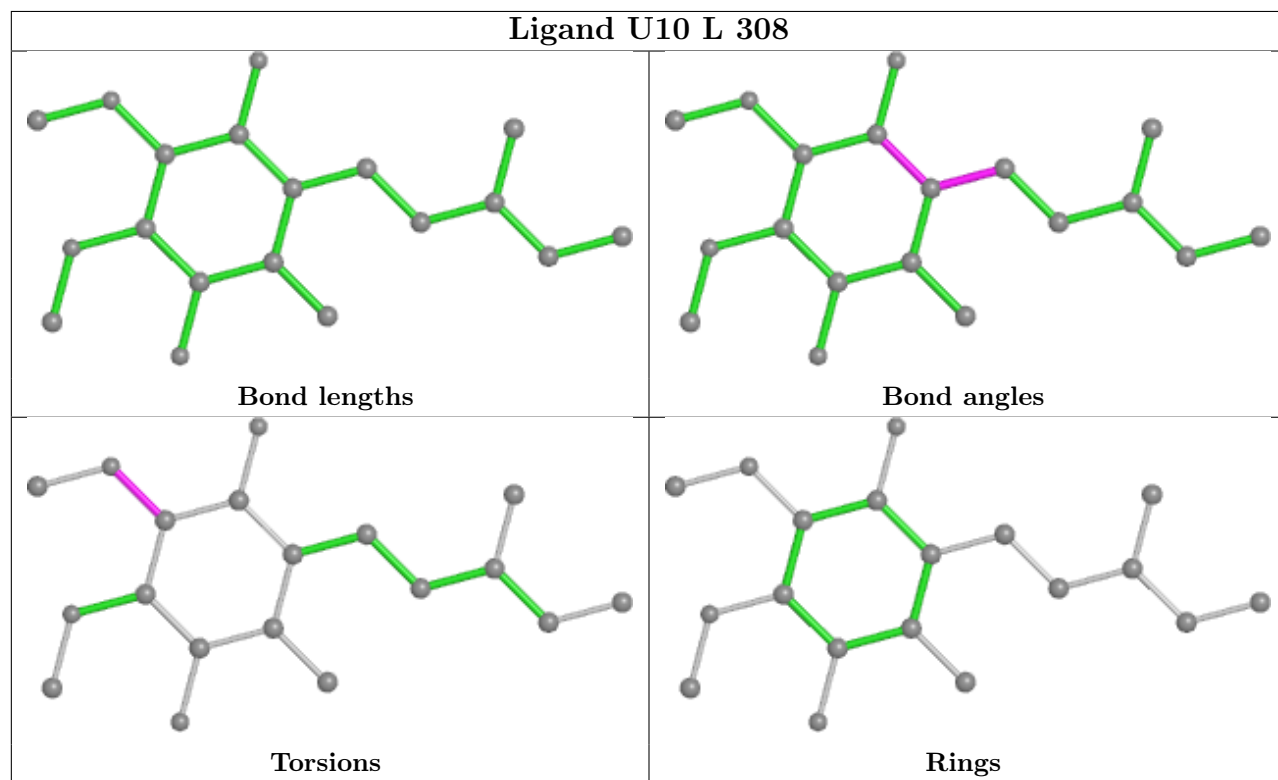
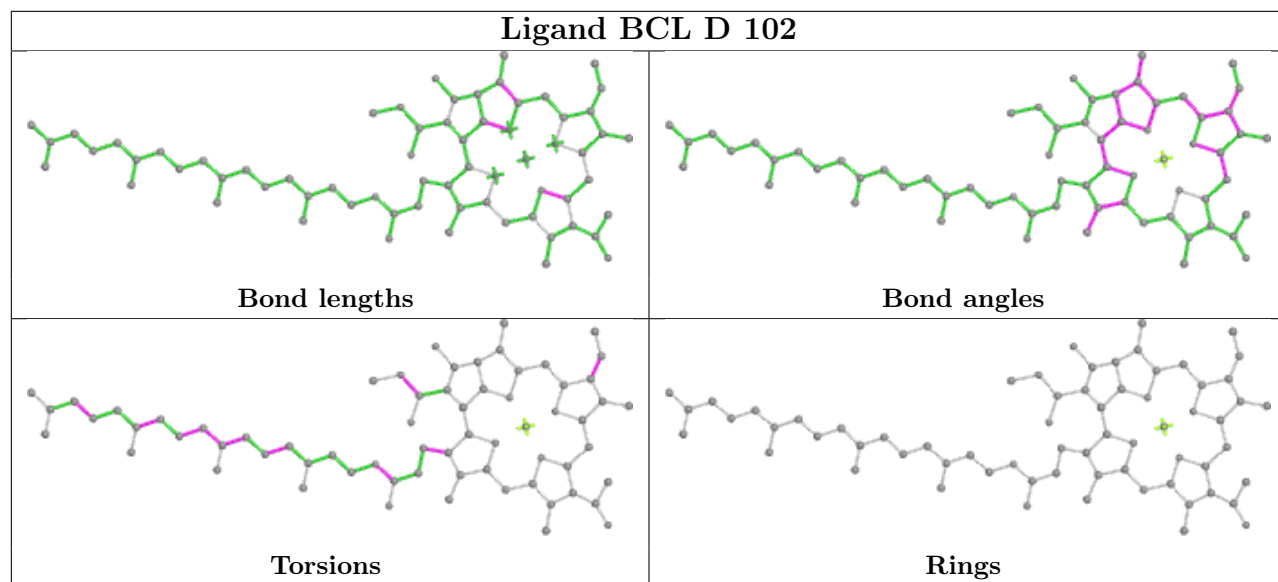


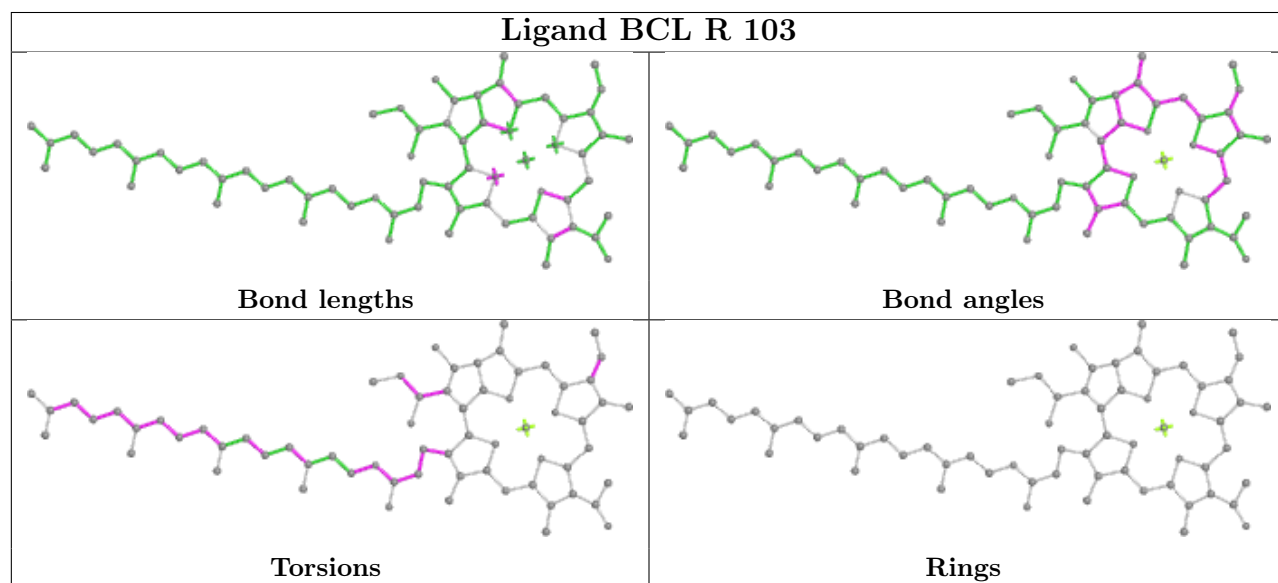
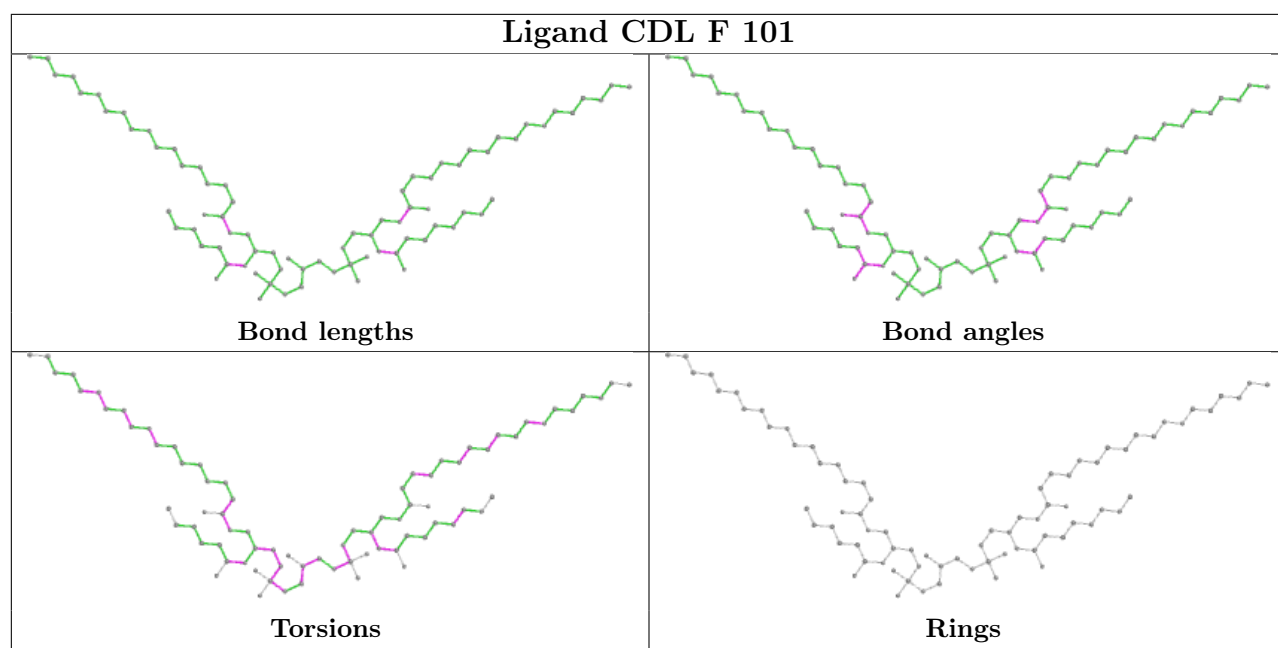


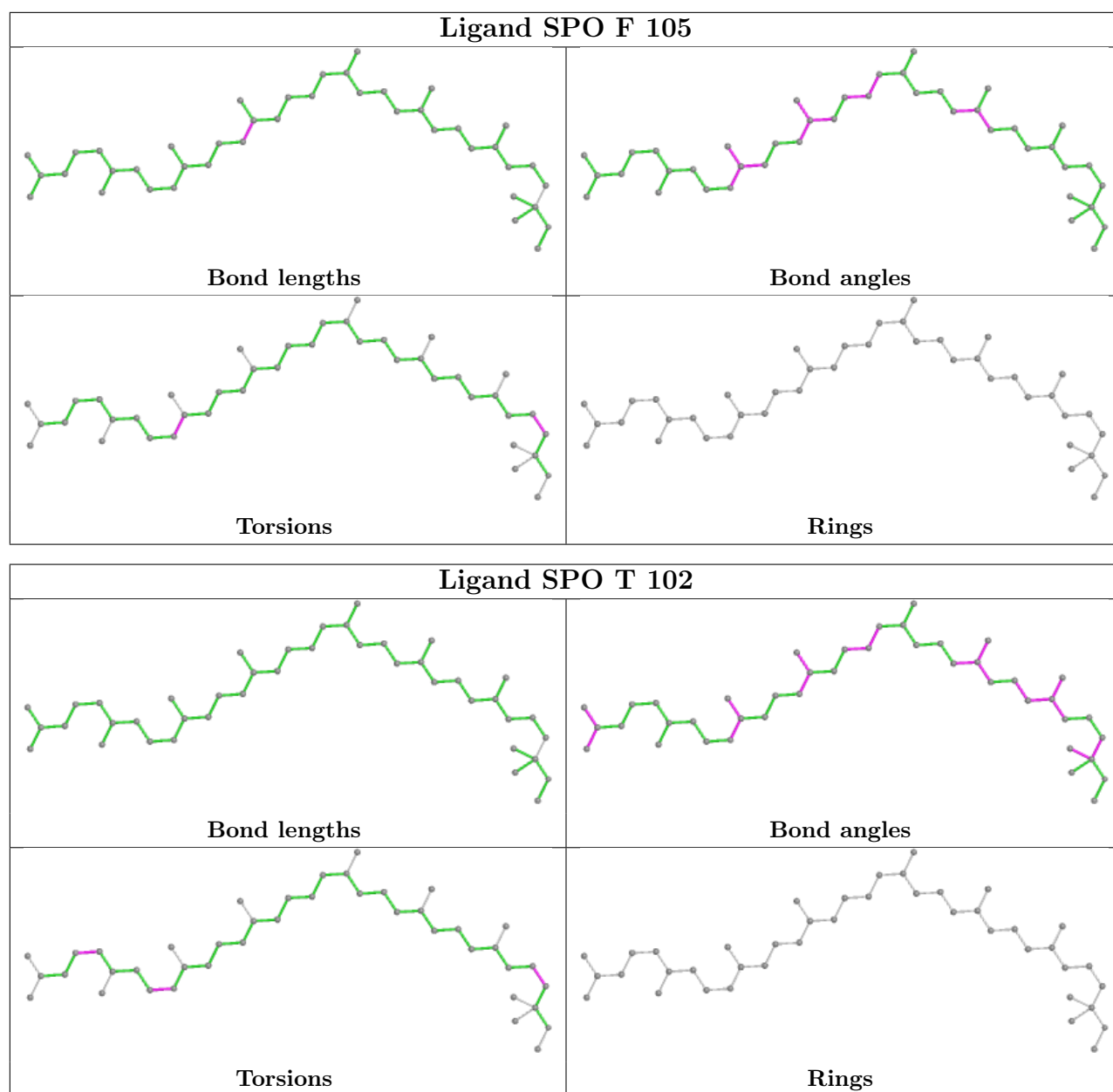


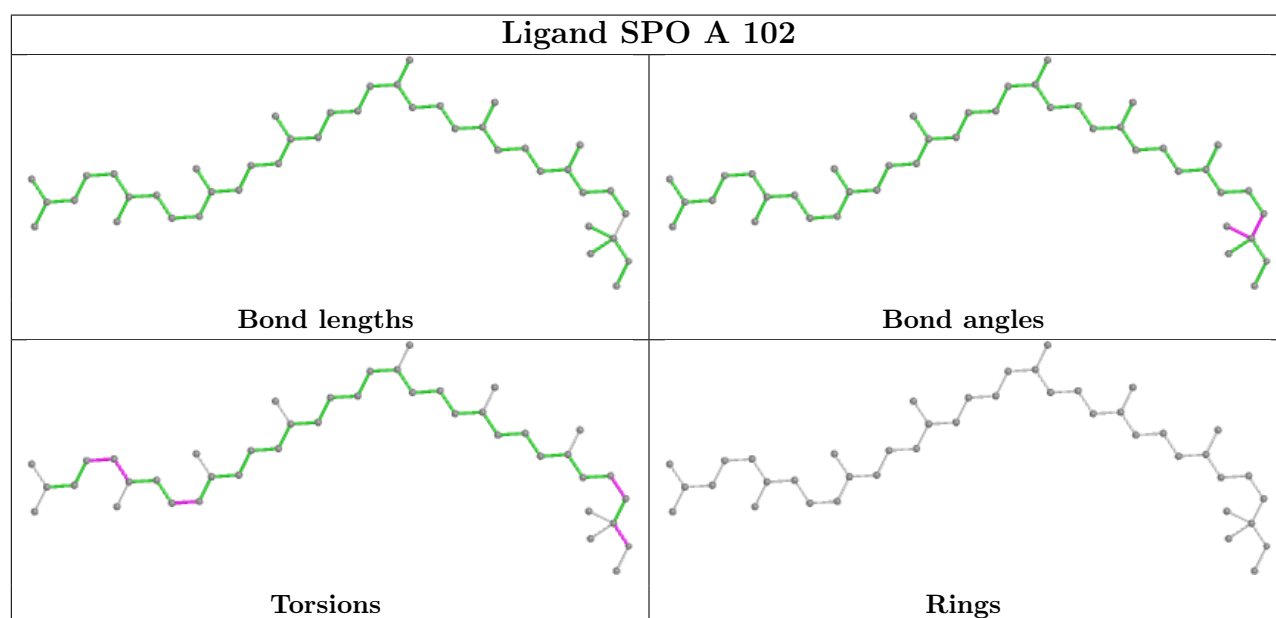
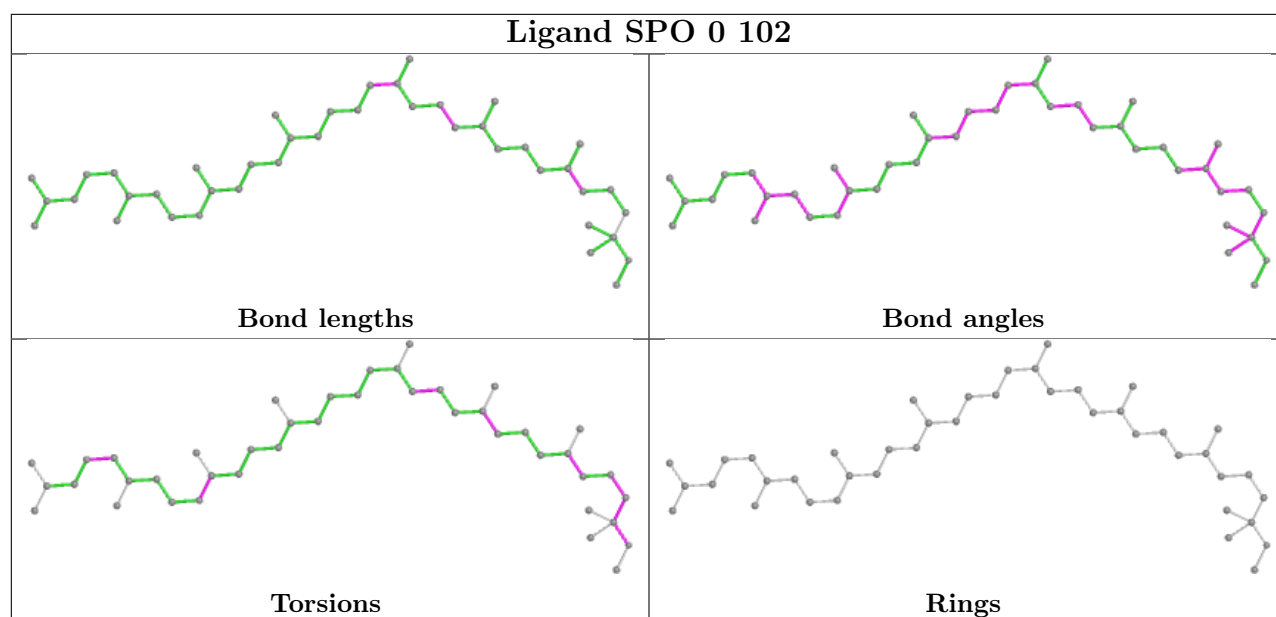


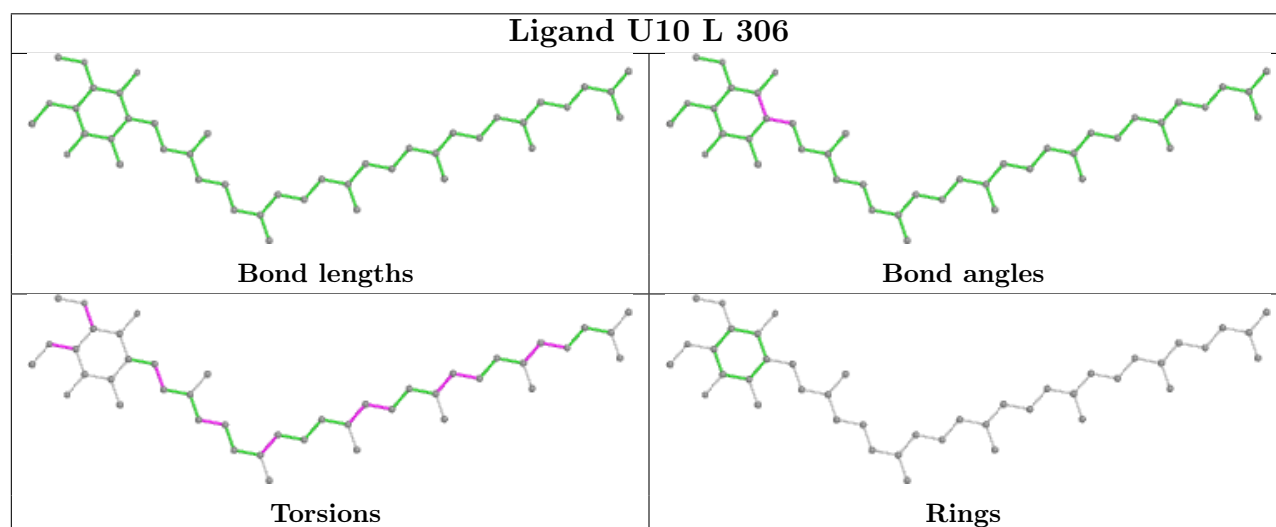
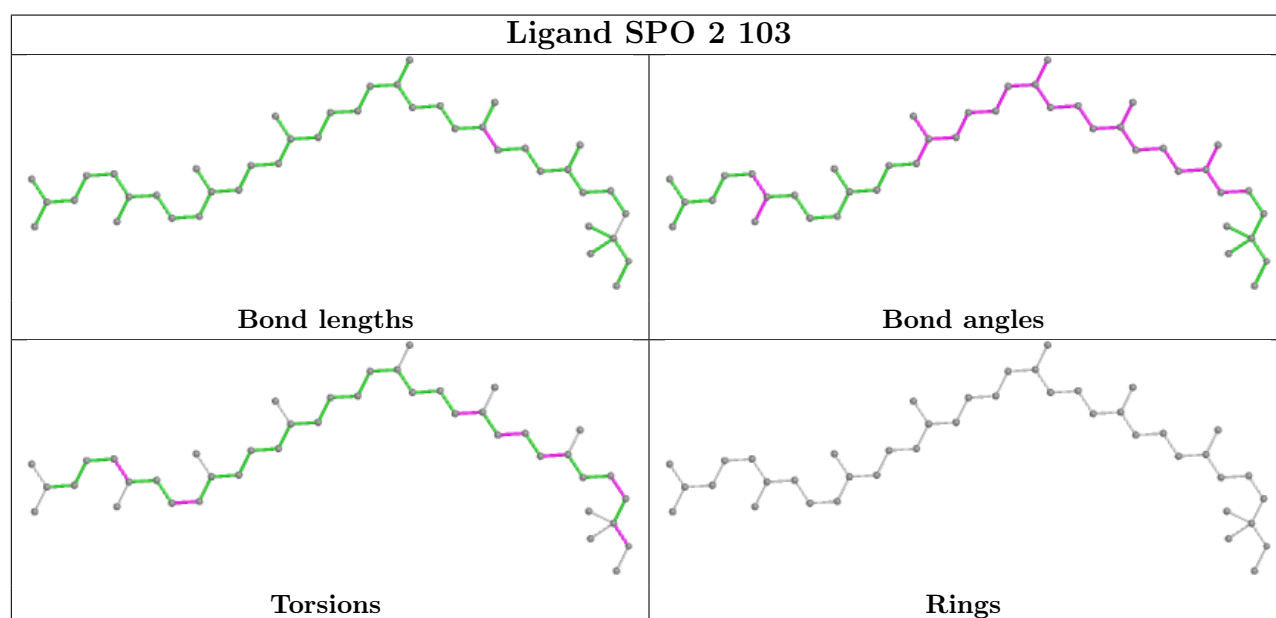
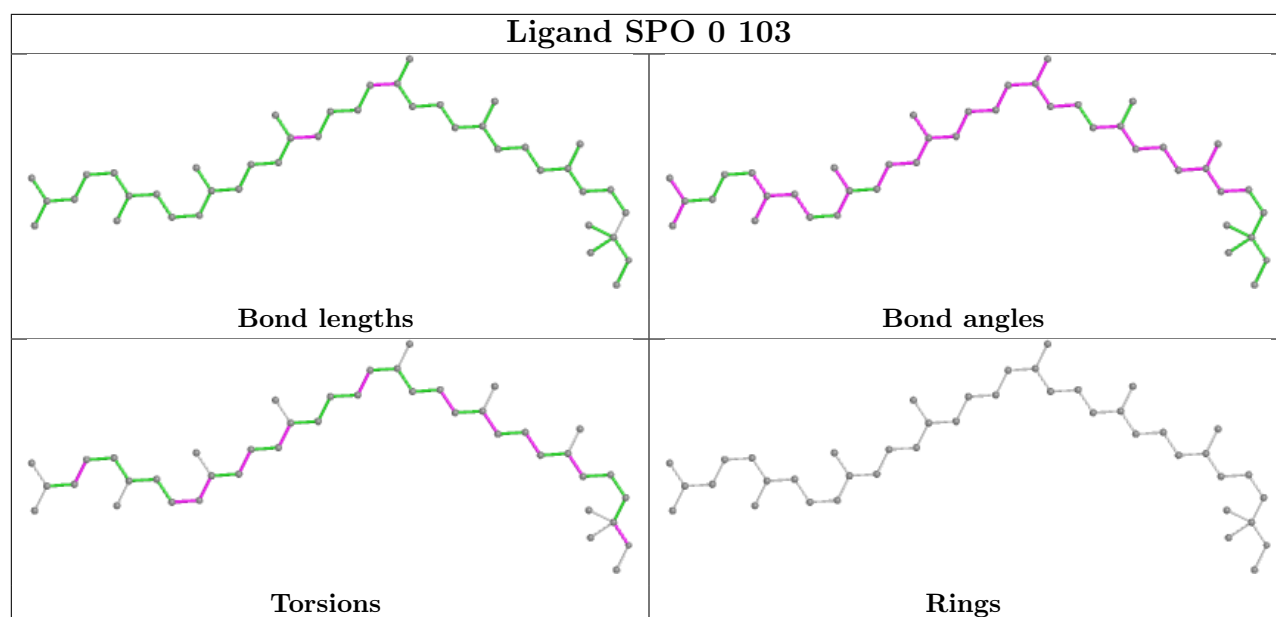


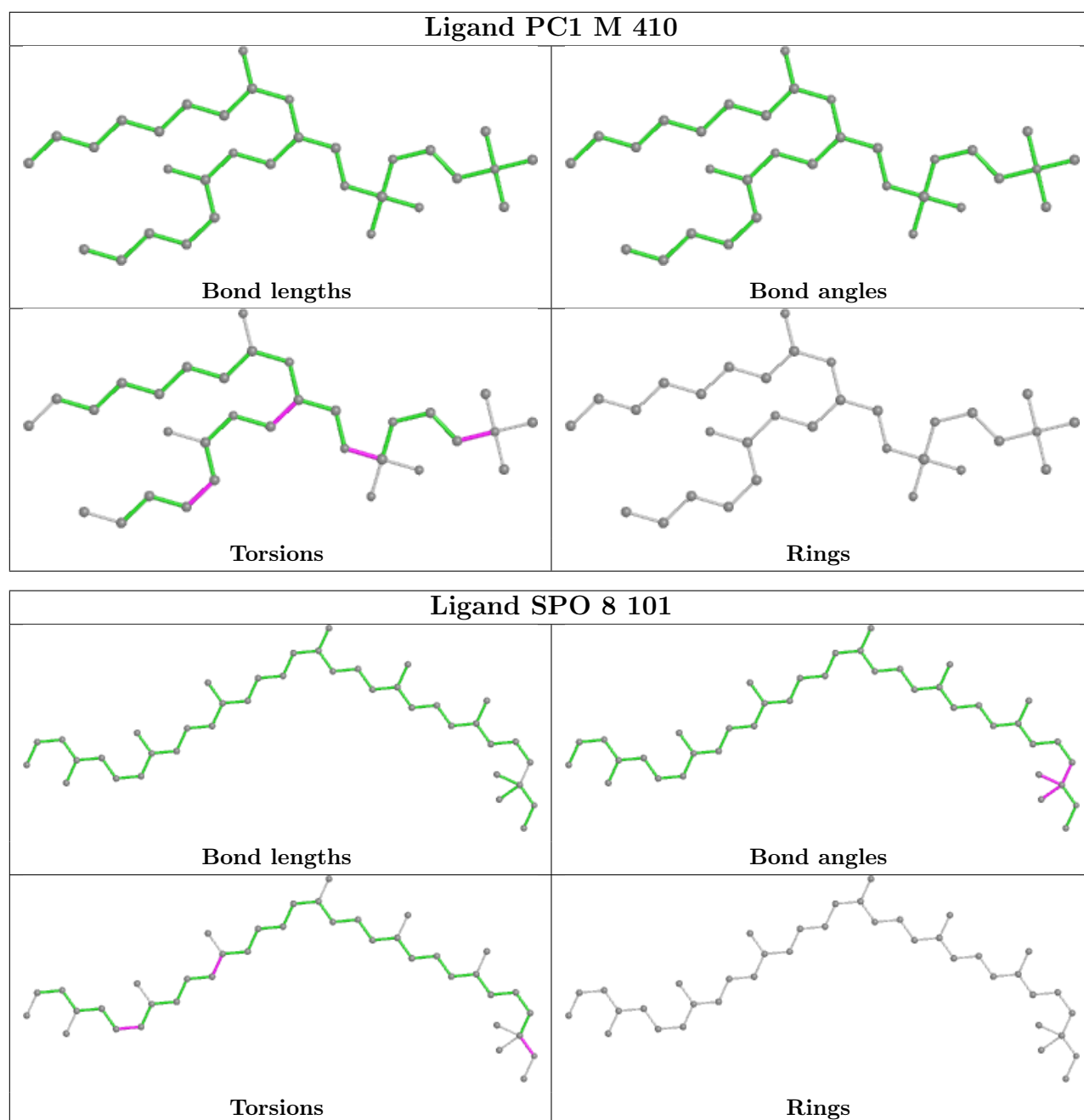


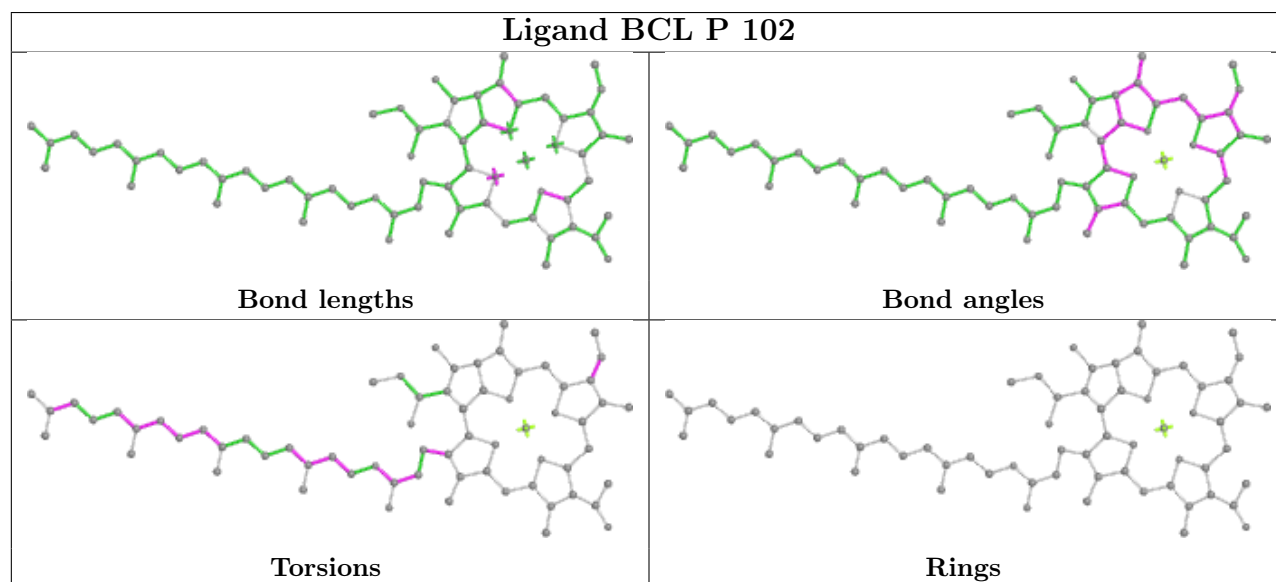
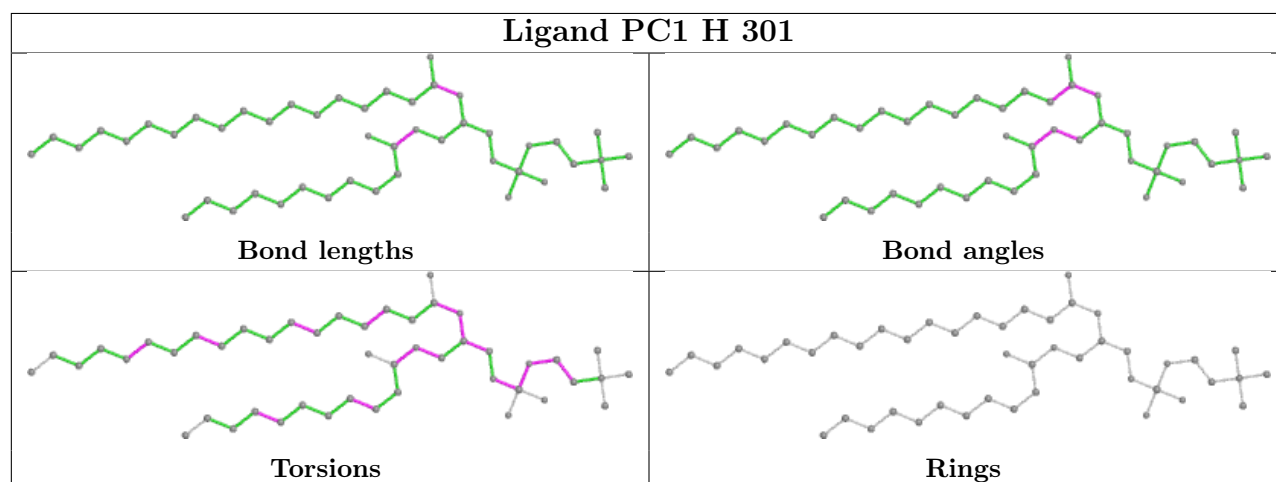
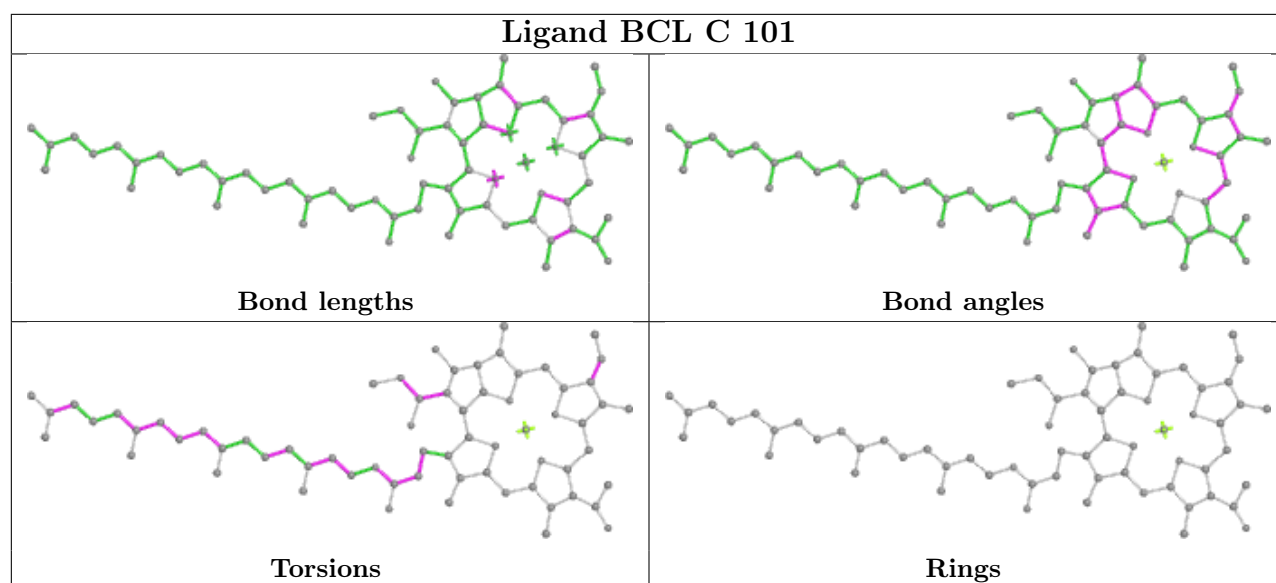


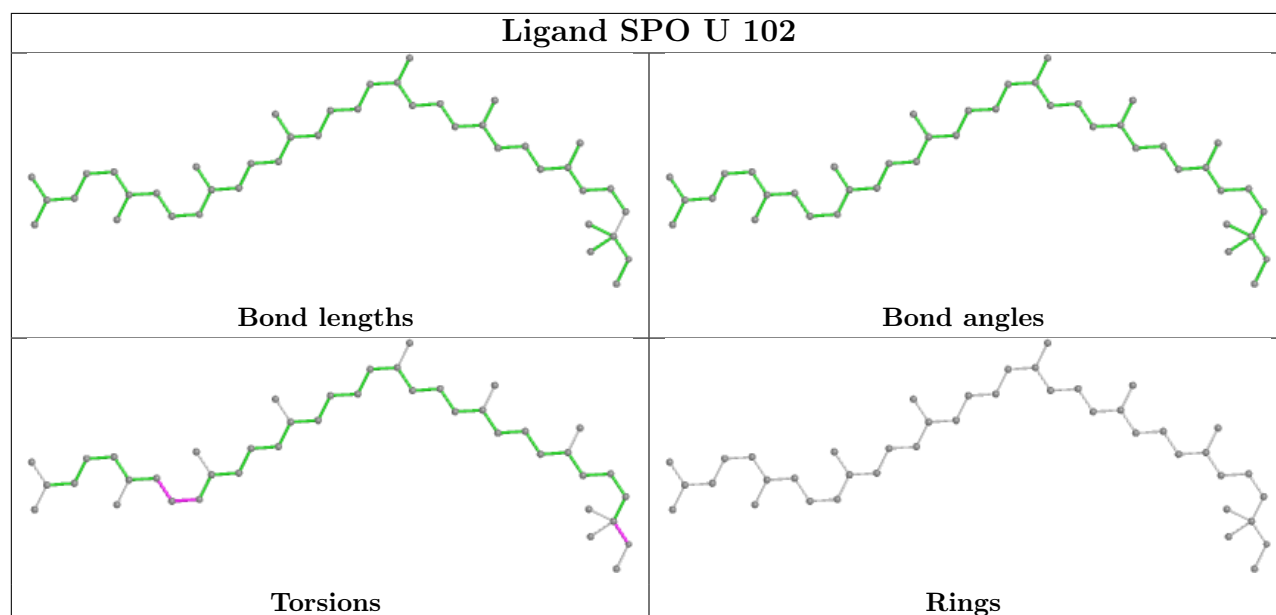
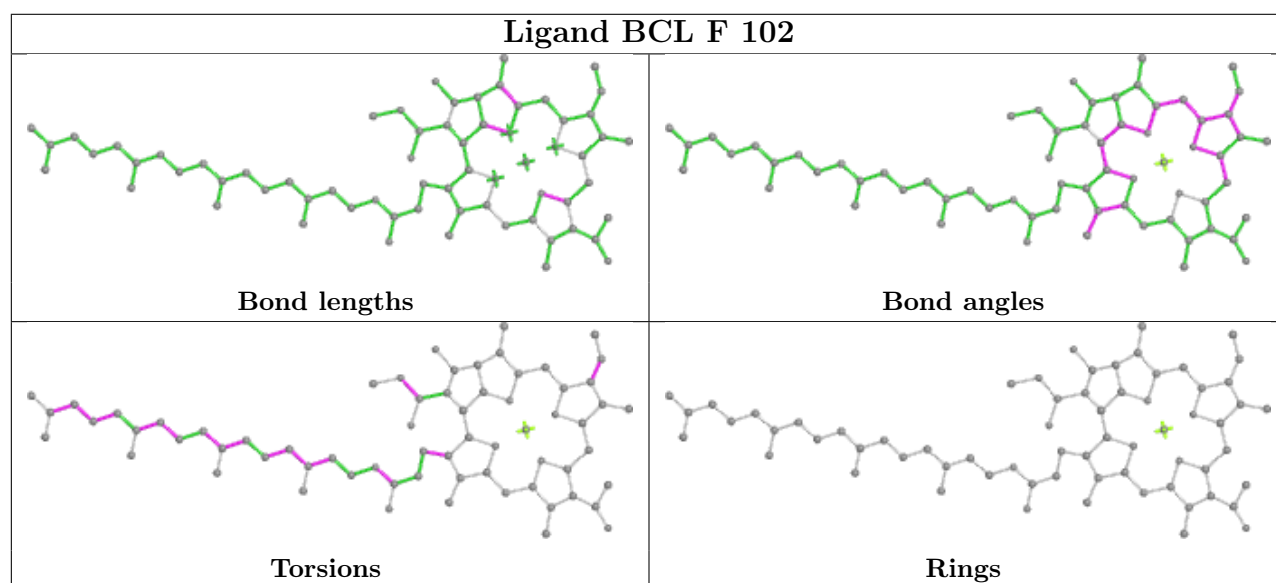
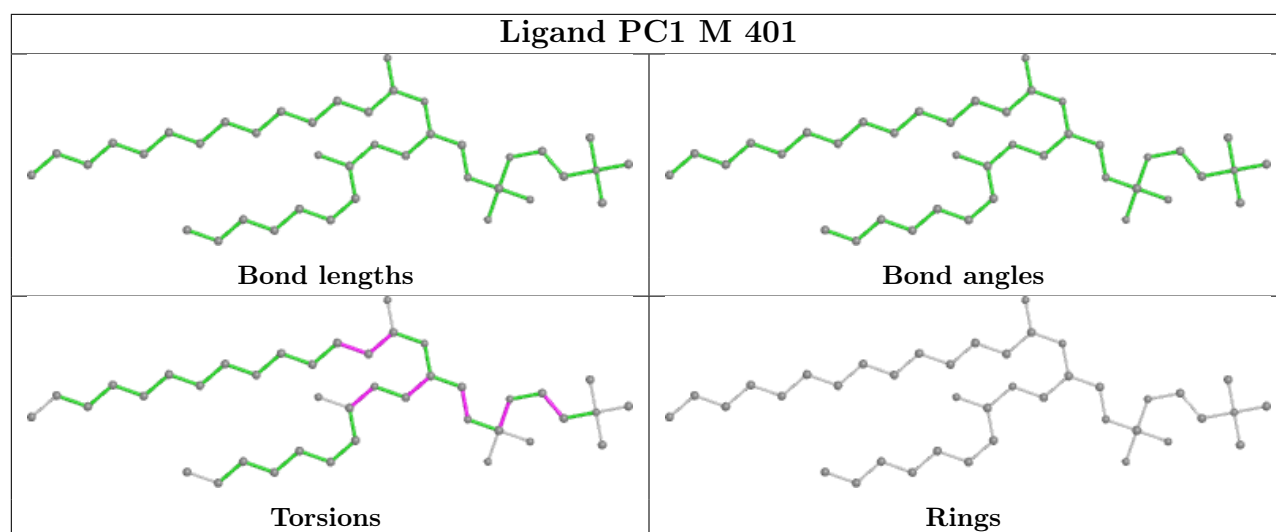


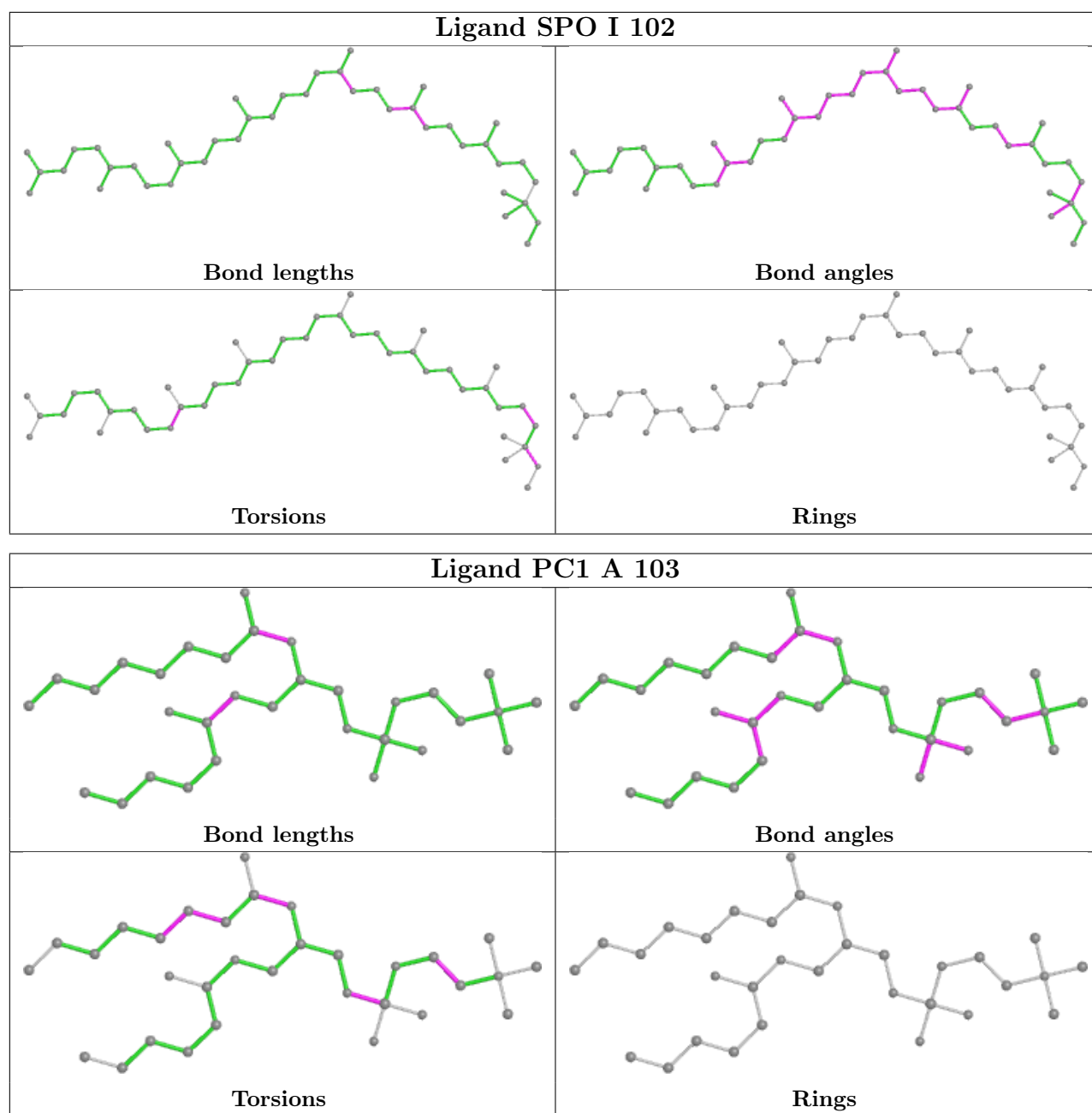


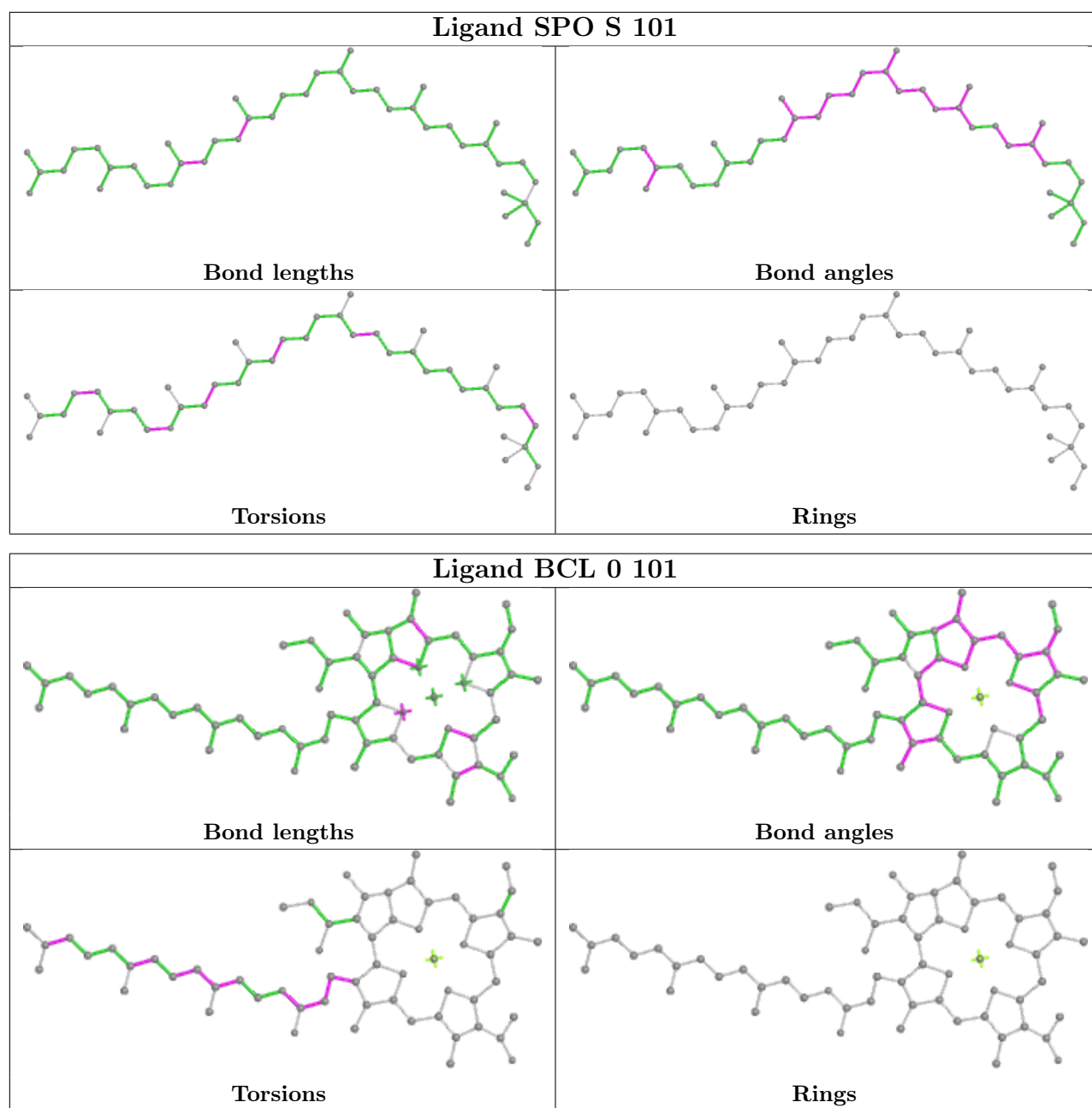


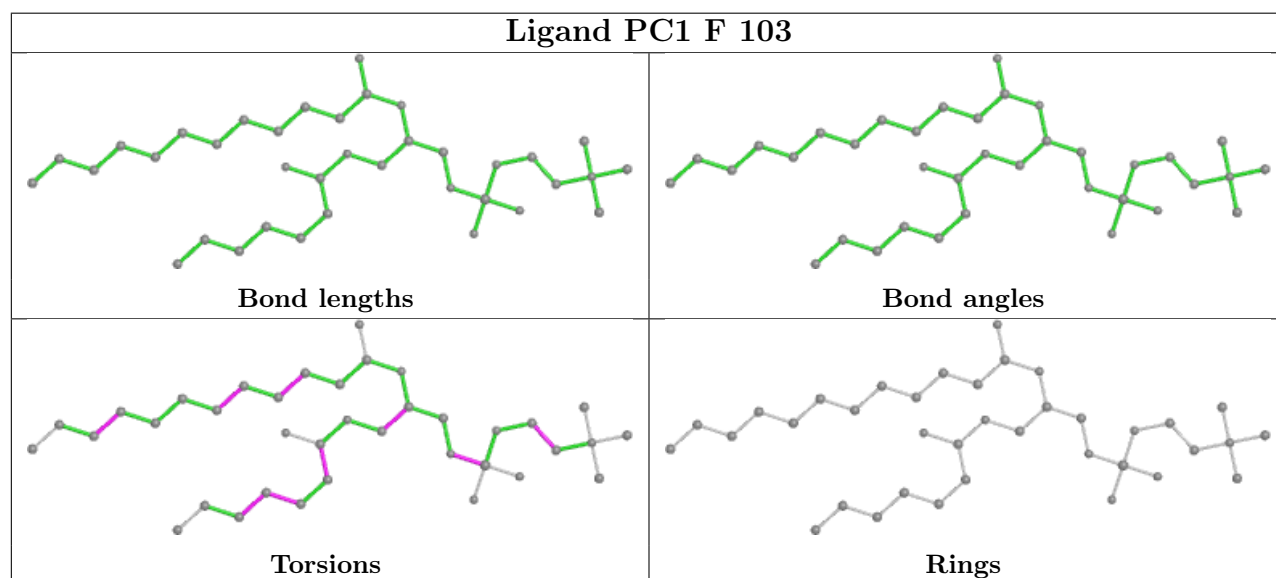
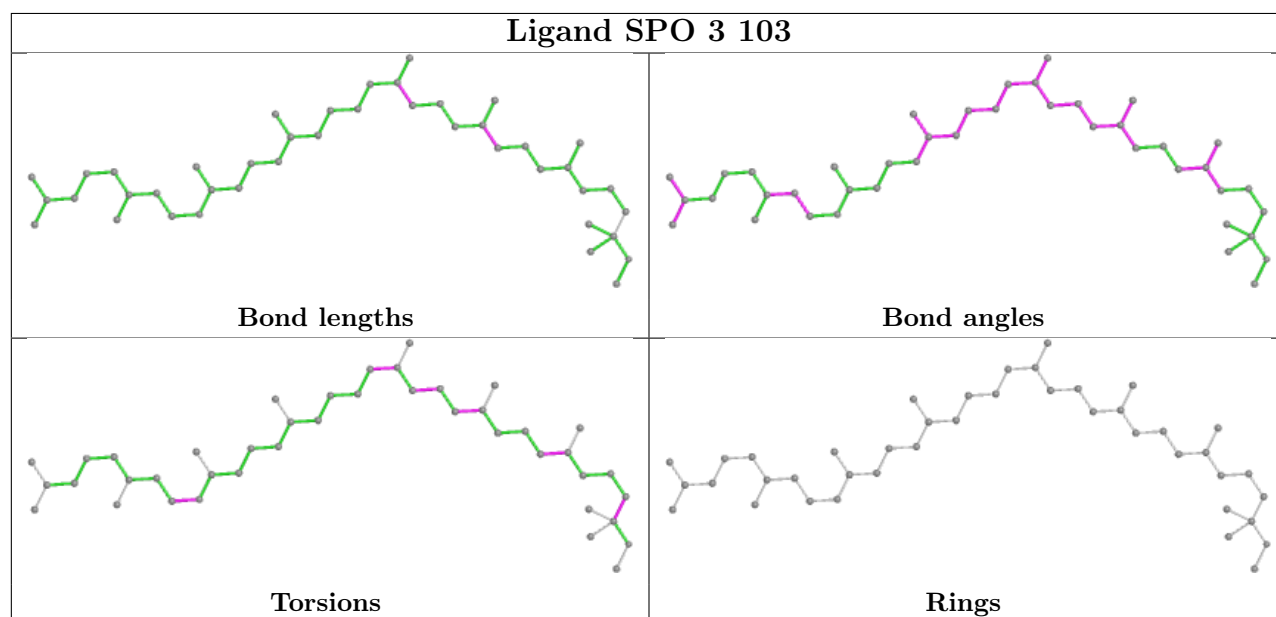
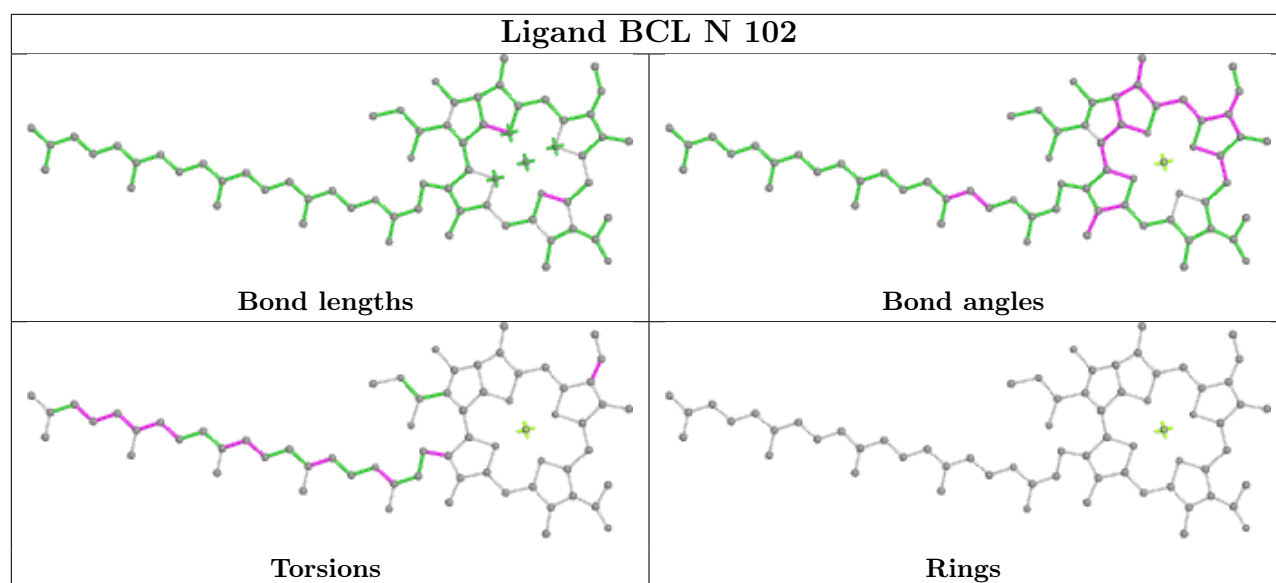


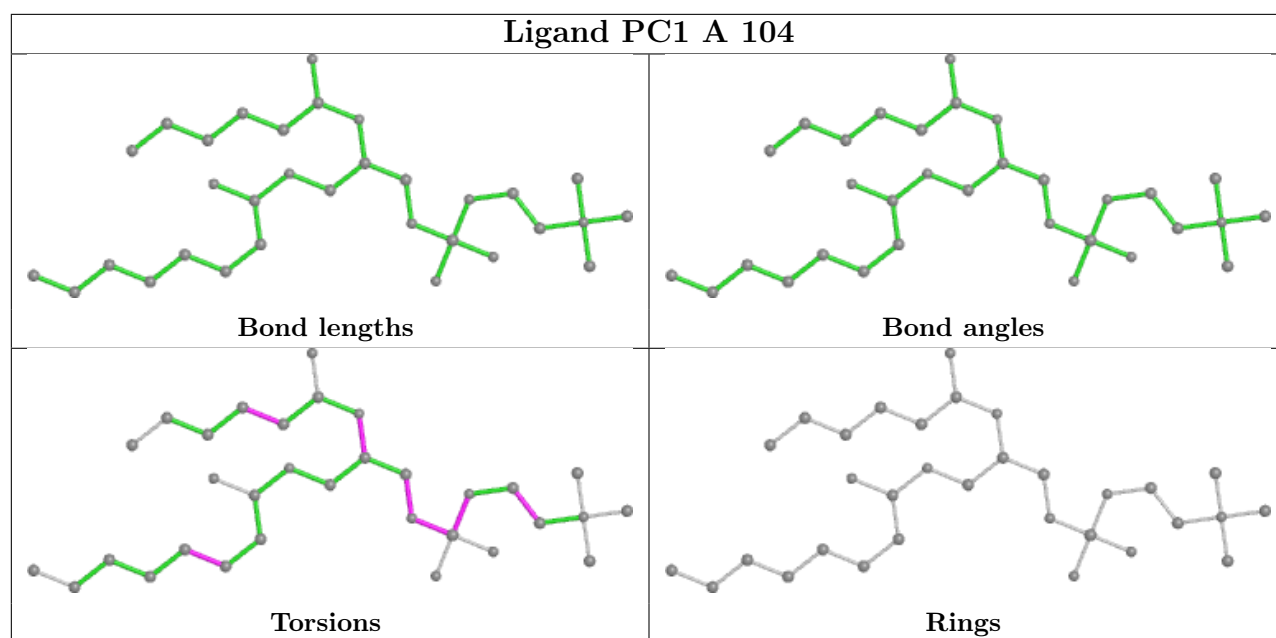












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

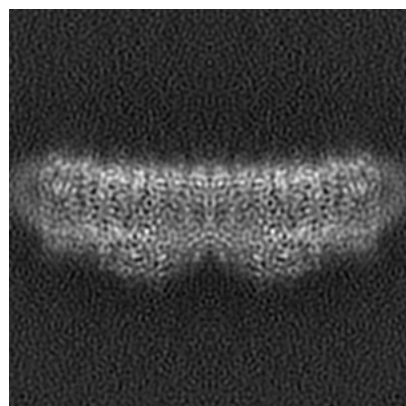
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39244. These allow visual inspection of the internal detail of the map and identification of artifacts.

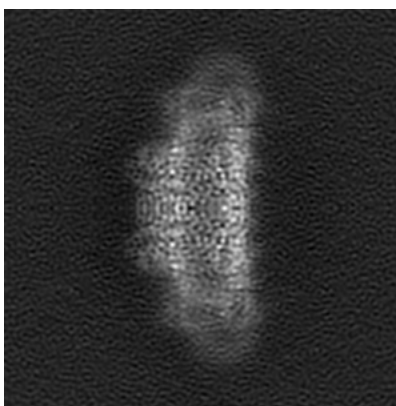
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

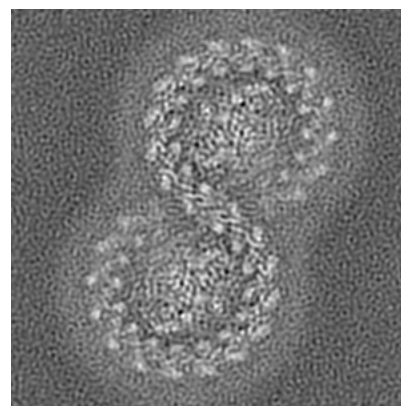
6.1.1 Primary map



X

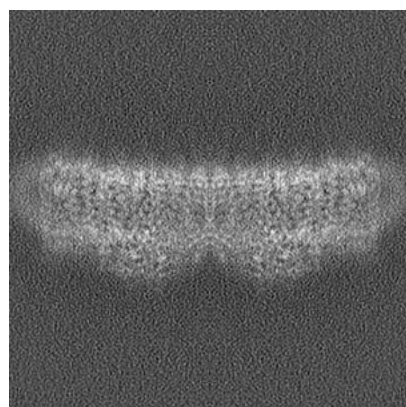


Y

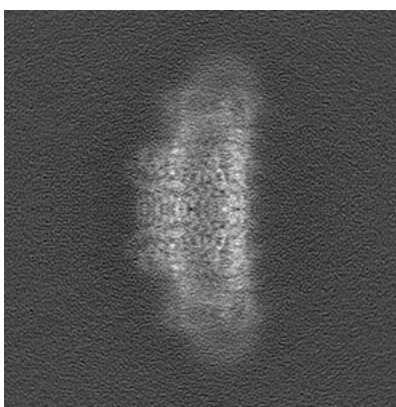


Z

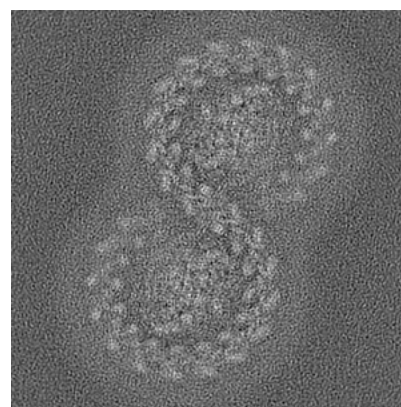
6.1.2 Raw map



X



Y

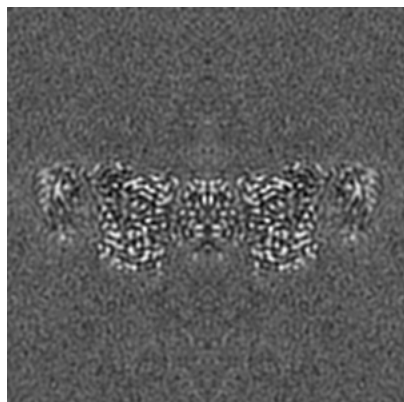


Z

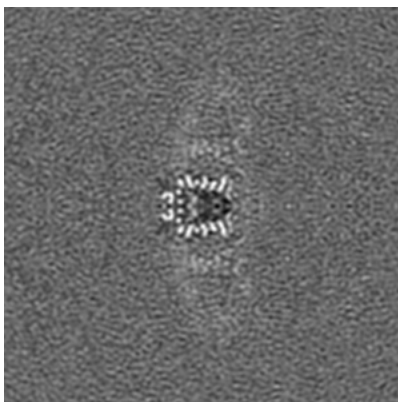
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

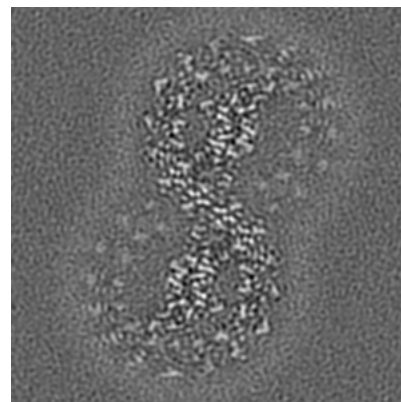
6.2.1 Primary map



X Index: 128

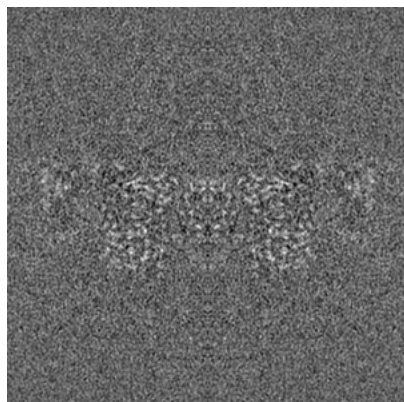


Y Index: 128

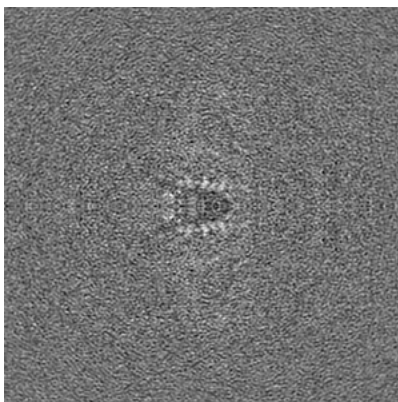


Z Index: 128

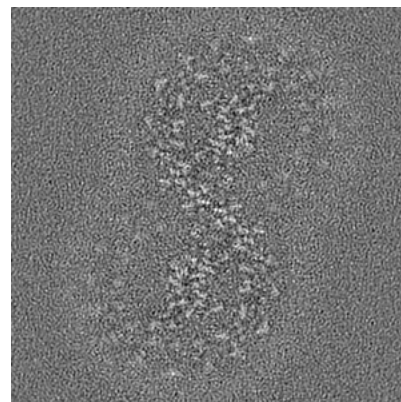
6.2.2 Raw map



X Index: 128



Y Index: 128

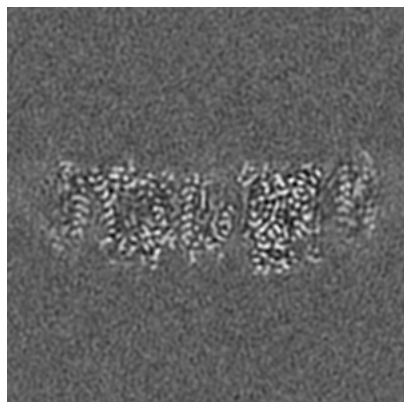


Z Index: 128

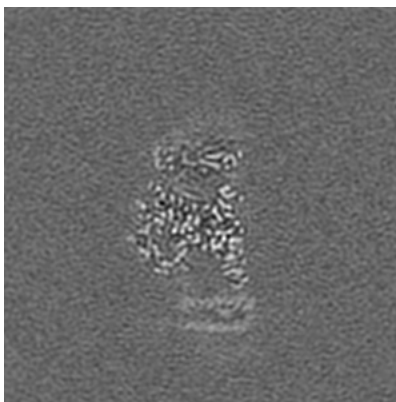
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

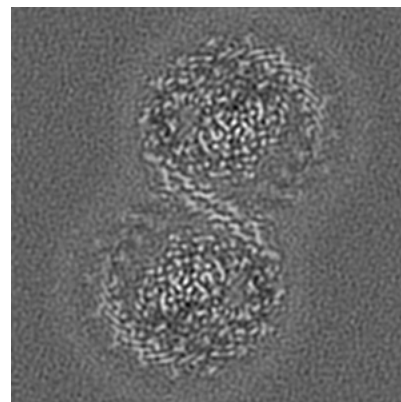
6.3.1 Primary map



X Index: 134

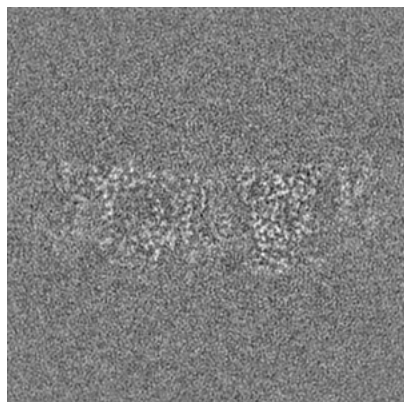


Y Index: 81

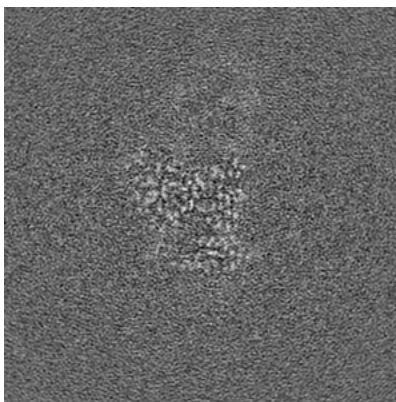


Z Index: 144

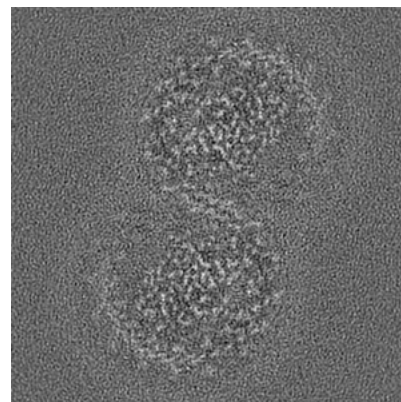
6.3.2 Raw map



X Index: 134



Y Index: 165

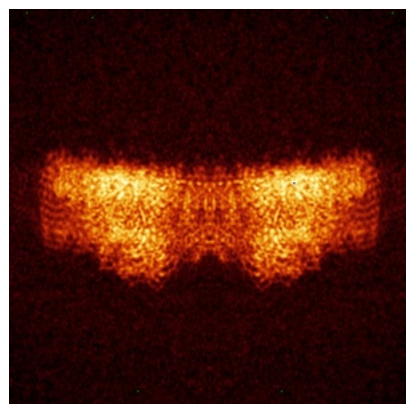


Z Index: 143

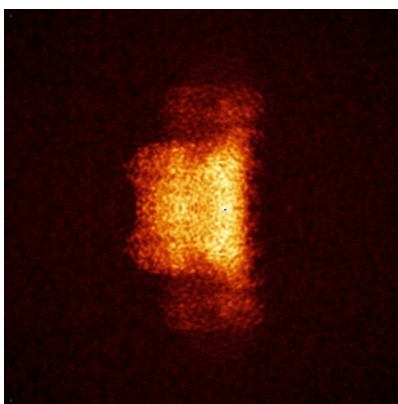
The images above show the largest variance slices of the map in three orthogonal directions.

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

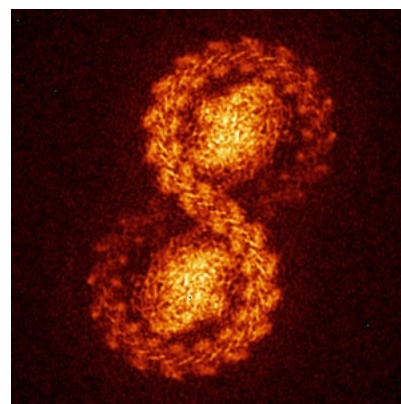
6.4.1 Primary map



X

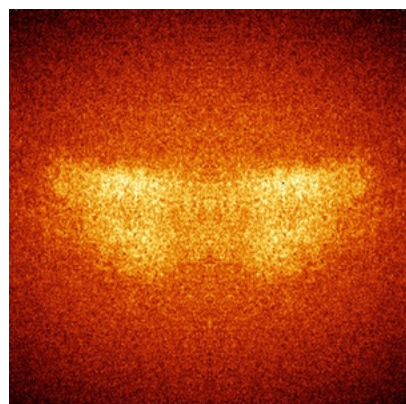


Y

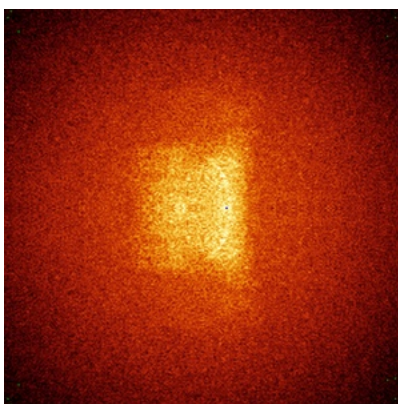


Z

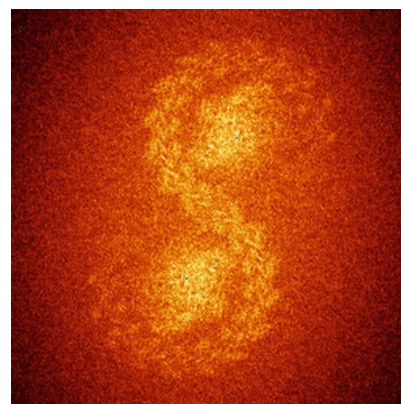
6.4.2 Raw map



X



Y

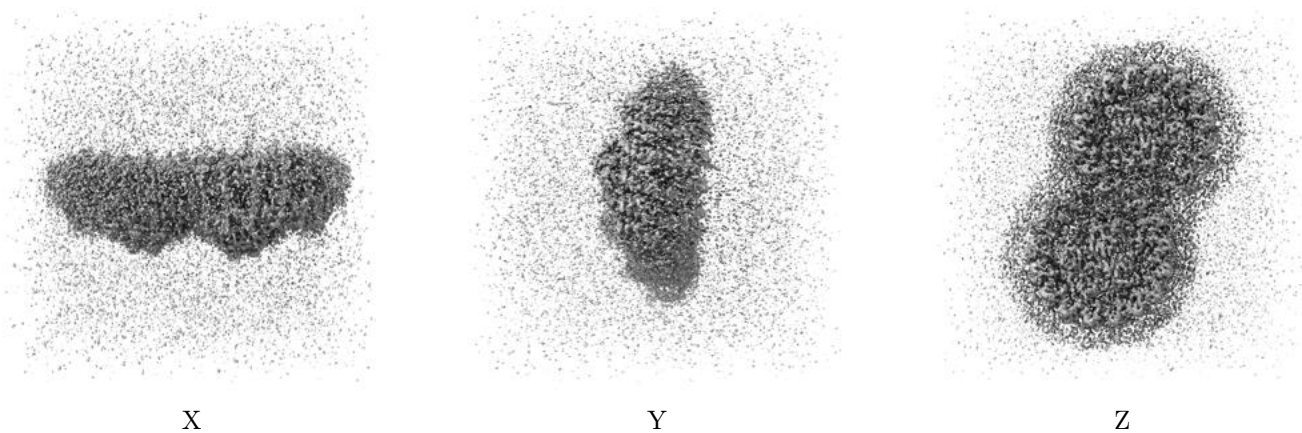


Z

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

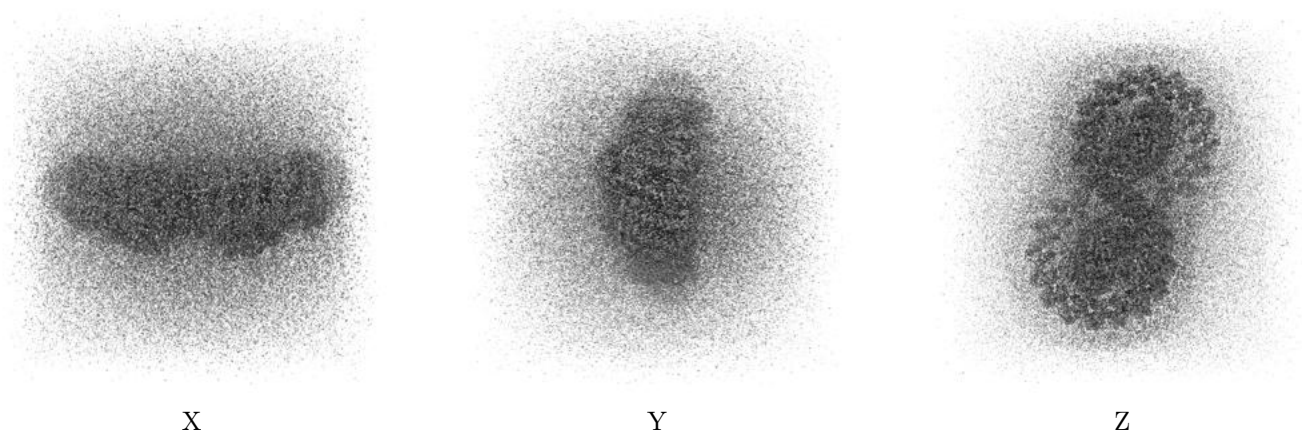
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

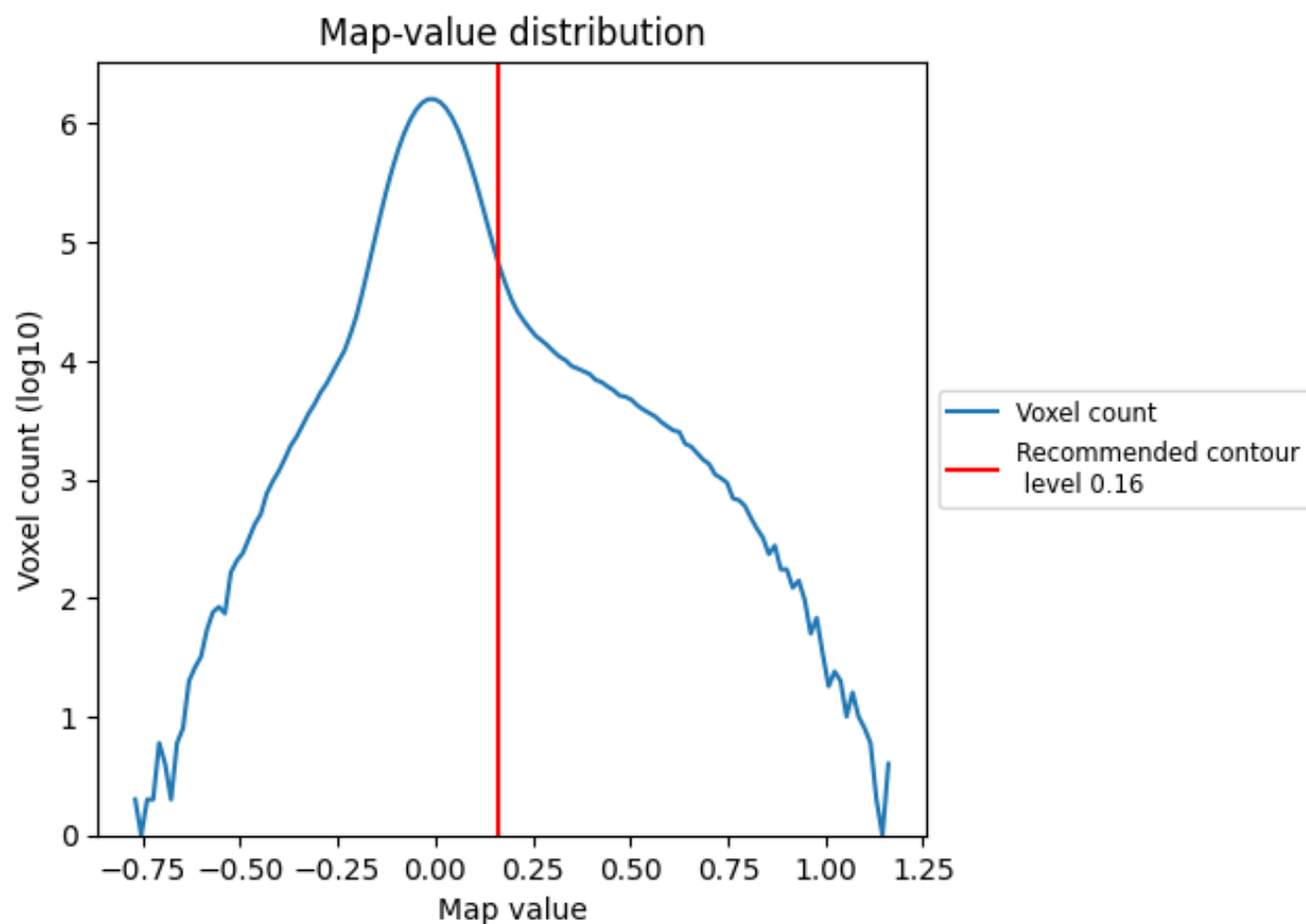
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

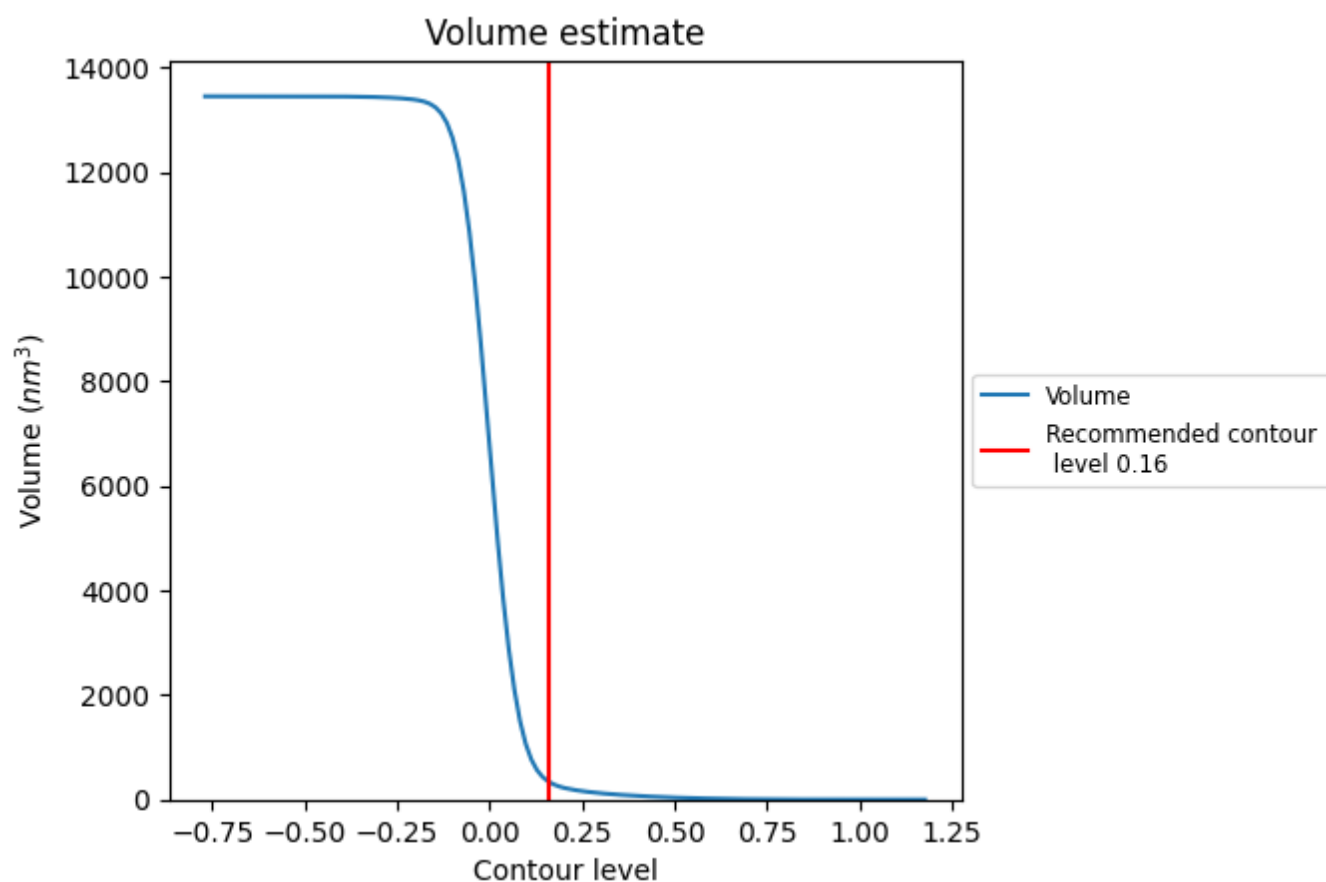
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

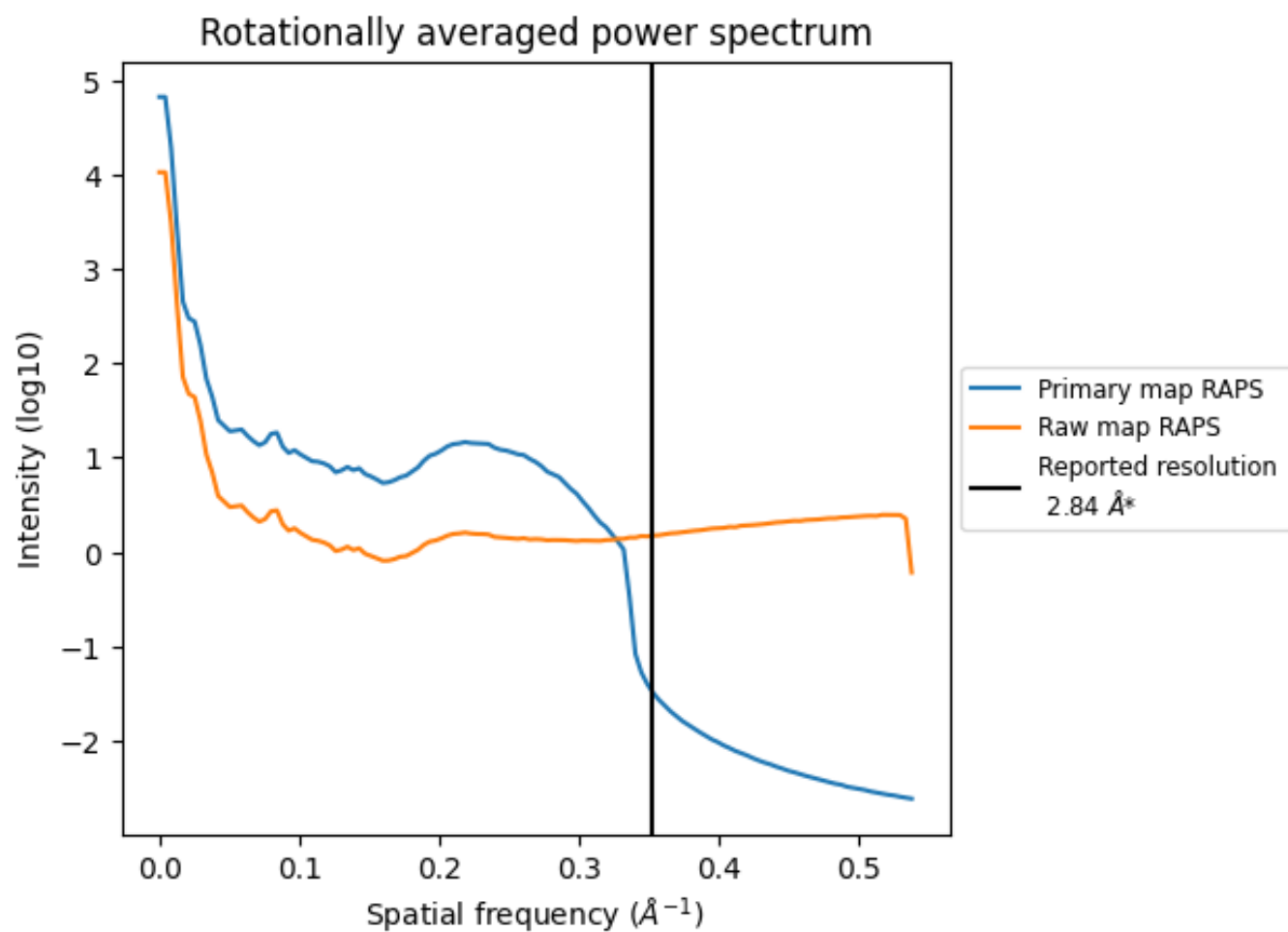
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm^3 ; this corresponds to an approximate mass of 309 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

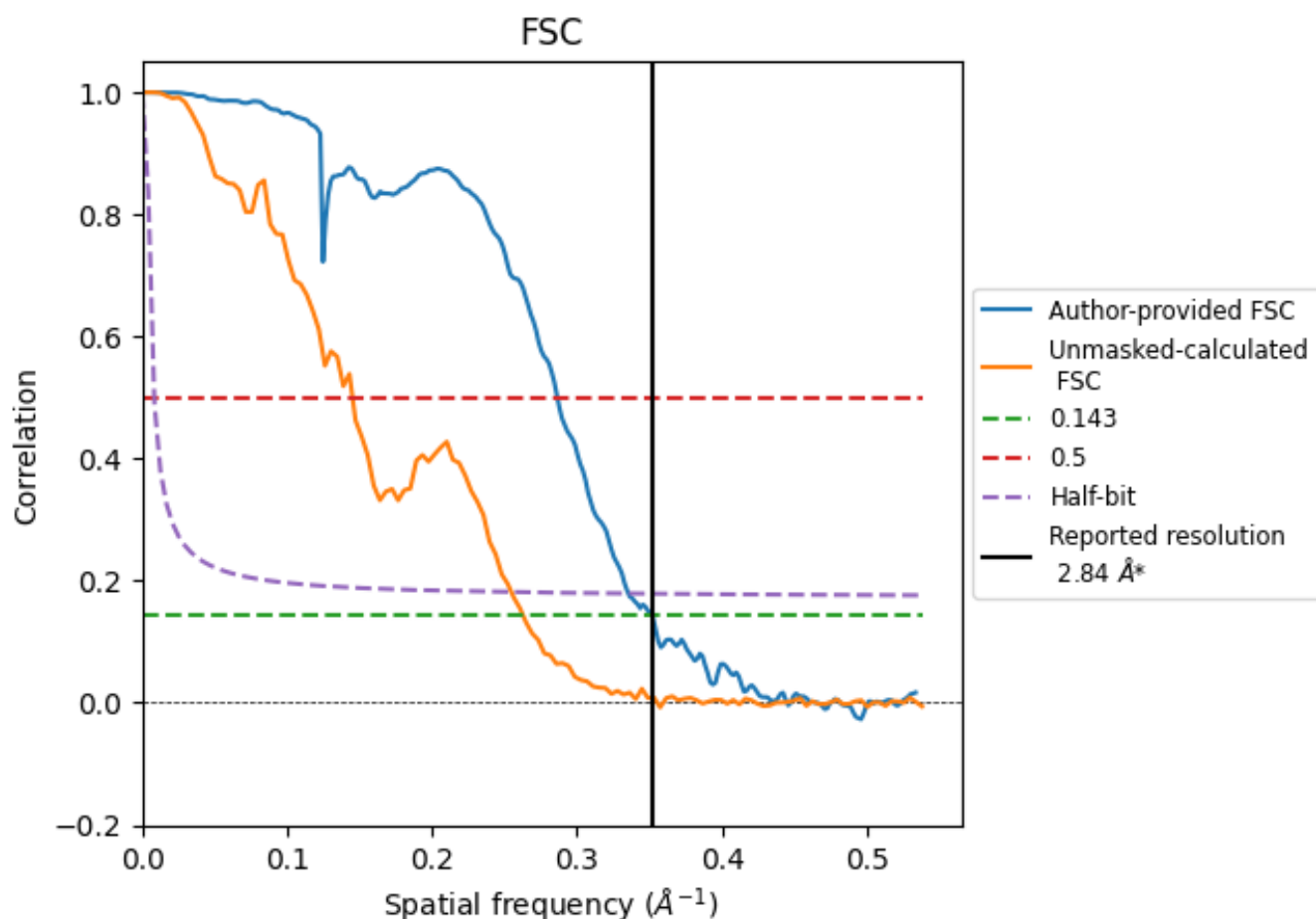


*Reported resolution corresponds to spatial frequency of 0.352 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.352 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.49	2.97
Unmasked-calculated*	3.81	6.89	3.93

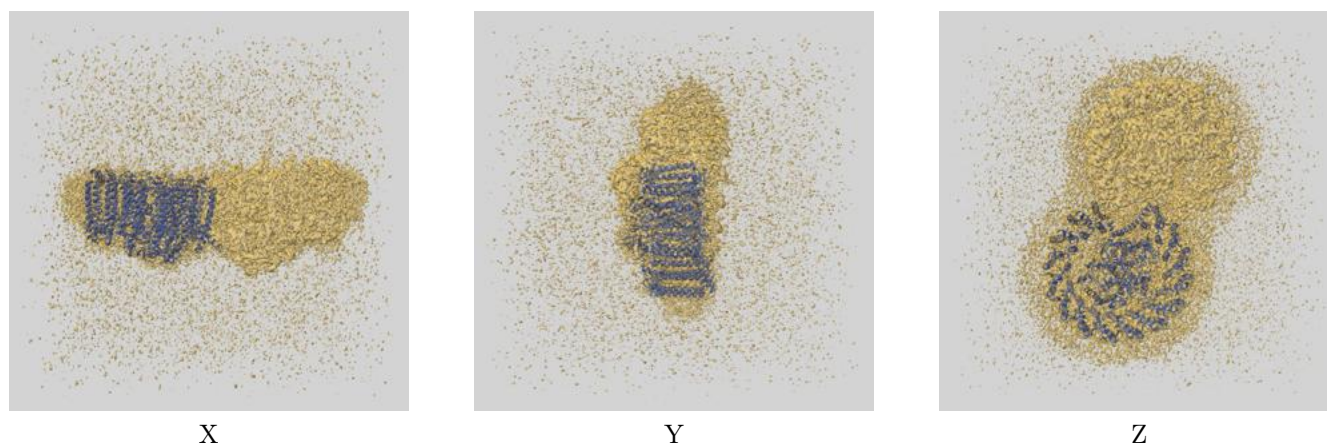
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.81 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

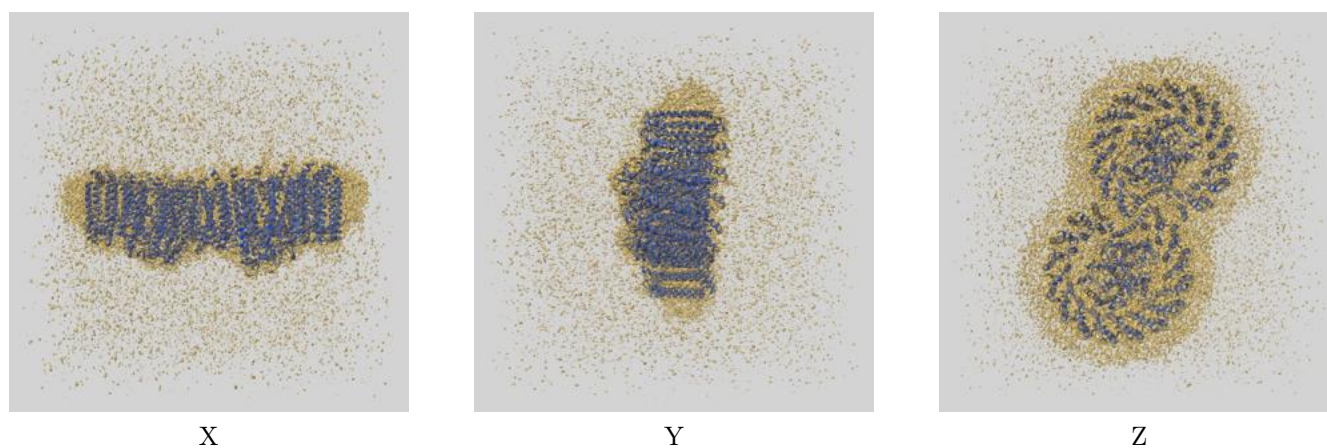
This section contains information regarding the fit between EMDB map EMD-39244 and PDB model 8YGD. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

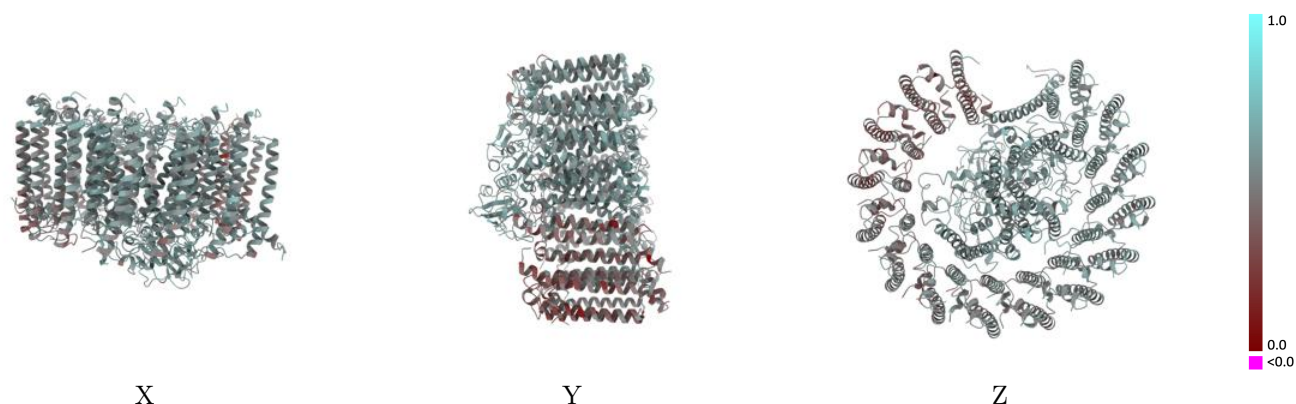


9.1.2 Map-model assembly overlay [i](#)



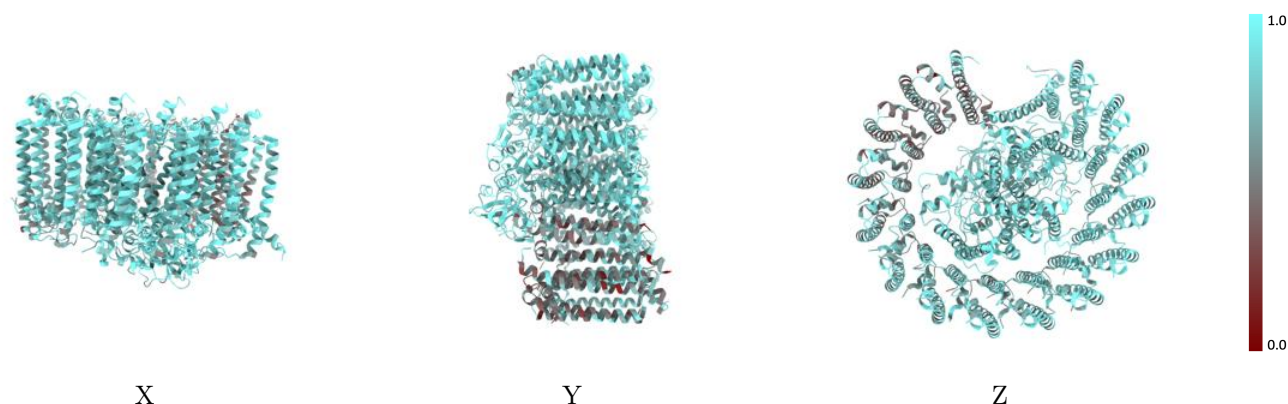
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



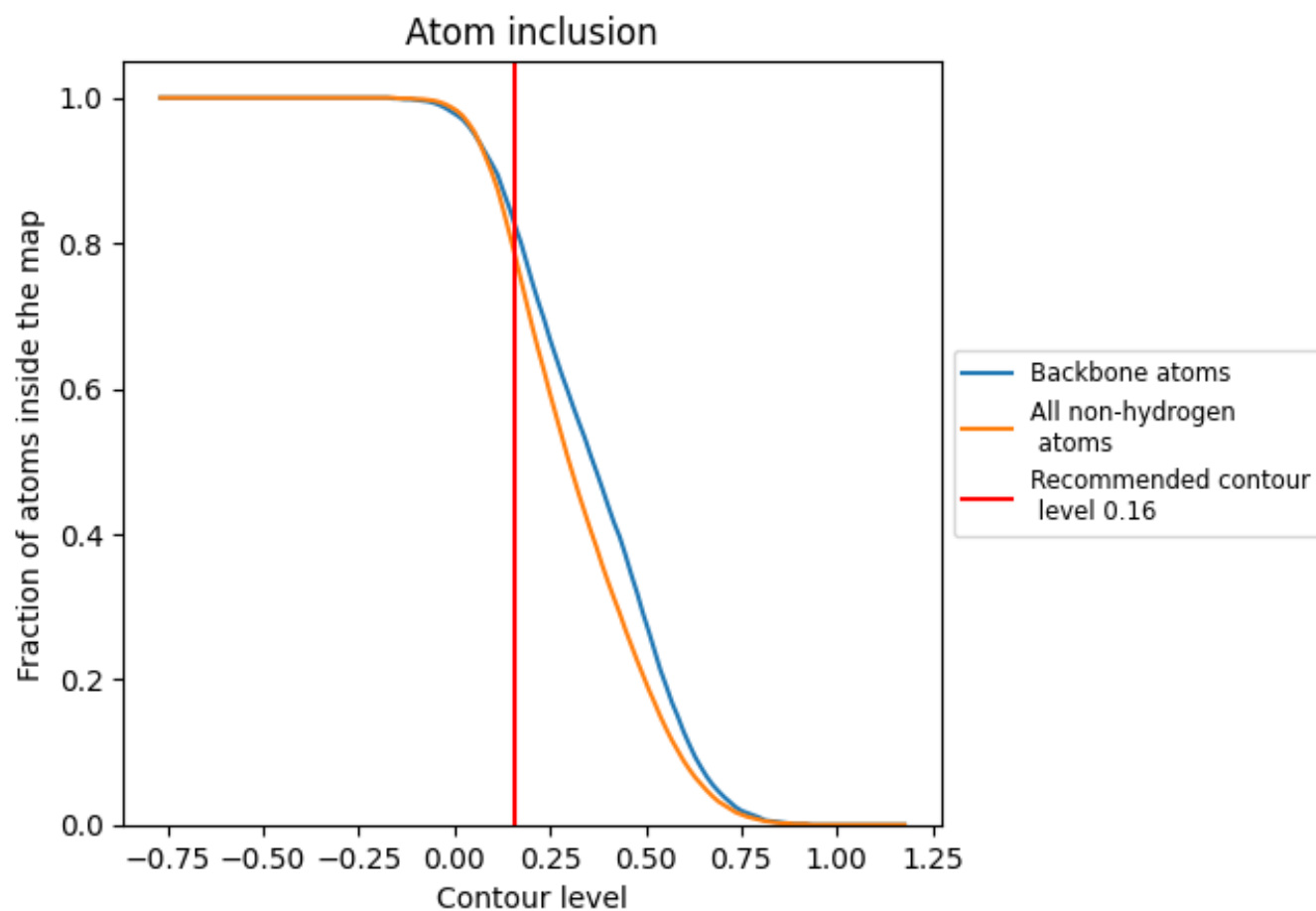
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.5170
0	 0.8460	 0.5400
1	 0.5350	 0.3930
2	 0.4540	 0.3430
3	 0.5160	 0.4100
7	 0.9210	 0.5730
8	 0.8390	 0.5570
9	 0.8780	 0.5730
A	 0.8660	 0.5660
B	 0.8350	 0.5370
C	 0.5550	 0.3730
D	 0.9040	 0.5680
E	 0.8150	 0.5290
F	 0.8280	 0.5400
G	 0.8440	 0.5220
H	 0.8740	 0.5680
I	 0.8130	 0.5190
J	 0.8060	 0.5160
K	 0.7980	 0.5050
L	 0.8700	 0.5770
M	 0.8580	 0.5640
N	 0.7330	 0.4690
O	 0.7700	 0.5130
P	 0.7480	 0.4960
Q	 0.8080	 0.5140
R	 0.7010	 0.4760
S	 0.7440	 0.4890
T	 0.7060	 0.4610
U	 0.6980	 0.4760
V	 0.6810	 0.4420
W	 0.6350	 0.4590
X	 0.7870	 0.5370
Z	 0.4910	 0.3700
a	 0.5070	 0.3920
b	 0.6090	 0.4210

