



## Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 12:24 PM JST

PDB ID : 9IMN / pdb\_00009imn  
EMDB ID : EMD-60694  
Title : Cryo-EM structure of a TEF30-associated intermediate PSII core dimer complex, type I, from *Chlamydomonas reinhardtii*  
Authors : Wang, Y.; Wang, C.; Li, A.; Liu, Z.  
Deposited on : 2024-07-03  
Resolution : 2.97 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

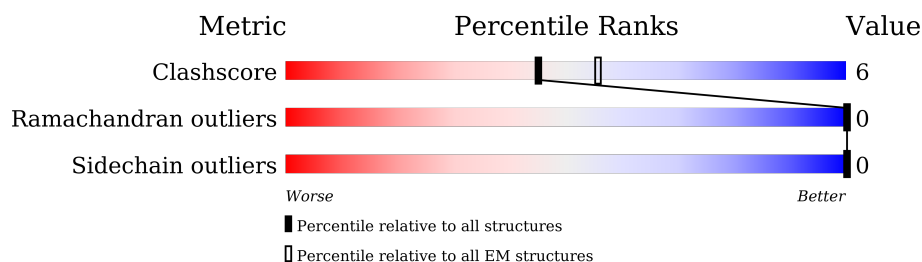
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	327	 82%      12%      6%
1	a	327	 82%      12%      6%
2	B	480	 87%      13%
2	b	480	 90%      10%
3	C	450	 85%      13%      .
3	c	450	 89%      9%      .
4	D	351	 85%      11%      .
4	d	351	 87%      9%      .

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Mol	Chain	Length	Quality of chain
5	E	75	
5	e	75	
6	F	31	
6	f	31	
7	G	240	
7	g	240	
8	H	69	
8	h	69	
9	I	34	
9	i	34	
10	K	37	
10	k	37	
11	L	38	
11	l	38	
12	M	27	
12	m	27	
13	T	31	
13	t	31	
14	V	31	
14	v	31	
15	W	19	
15	w	19	
16	X	32	
16	x	32	
17	Z	61	

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Mol	Chain	Length	Quality of chain
17	z	61	<div> <div>62%</div> <div>92%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	A	404	X	-	-	-
19	CLA	A	406	X	-	-	-
19	CLA	B	501	X	-	-	-
19	CLA	B	502	X	-	-	-
19	CLA	B	503	X	-	-	-
19	CLA	B	504	X	-	-	-
19	CLA	B	506	X	-	-	-
19	CLA	B	507	X	-	-	-
19	CLA	B	508	X	-	-	-
19	CLA	B	509	X	-	-	-
19	CLA	B	510	X	-	-	-
19	CLA	B	511	X	-	-	-
19	CLA	B	512	X	-	-	-
19	CLA	B	513	X	-	-	-
19	CLA	B	514	X	-	-	-
19	CLA	B	515	X	-	-	-
19	CLA	B	516	X	-	-	-
19	CLA	C	502	X	-	-	-
19	CLA	C	503	X	-	-	-
19	CLA	C	504	X	-	-	-
19	CLA	C	505	X	-	-	-
19	CLA	C	506	X	-	-	-
19	CLA	C	507	X	-	-	-
19	CLA	C	508	X	-	-	-
19	CLA	C	509	X	-	-	-
19	CLA	C	510	X	-	-	-
19	CLA	C	511	X	-	-	-
19	CLA	C	512	X	-	-	-
19	CLA	C	513	X	-	-	-
19	CLA	C	514	X	-	-	-
19	CLA	D	403	X	-	-	-
19	CLA	D	404	X	-	-	-
19	CLA	a	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	403	X	-	-	-
19	CLA	a	404	X	-	-	-
19	CLA	a	406	X	-	-	-
19	CLA	b	501	X	-	-	-
19	CLA	b	502	X	-	-	-
19	CLA	b	503	X	-	-	-
19	CLA	b	504	X	-	-	-
19	CLA	b	505	X	-	-	-
19	CLA	b	506	X	-	-	-
19	CLA	b	507	X	-	-	-
19	CLA	b	508	X	-	-	-
19	CLA	b	509	X	-	-	-
19	CLA	b	510	X	-	-	-
19	CLA	b	511	X	-	-	-
19	CLA	b	512	X	-	-	-
19	CLA	b	513	X	-	-	-
19	CLA	b	514	X	-	-	-
19	CLA	b	515	X	-	-	-
19	CLA	b	516	X	-	-	-
19	CLA	c	503	X	-	-	-
19	CLA	c	504	X	-	-	-
19	CLA	c	505	X	-	-	-
19	CLA	c	506	X	-	-	-
19	CLA	c	507	X	-	-	-
19	CLA	c	508	X	-	-	-
19	CLA	c	509	X	-	-	-
19	CLA	c	510	X	-	-	-
19	CLA	c	511	X	-	-	-
19	CLA	c	512	X	-	-	-
19	CLA	c	513	X	-	-	-
19	CLA	c	514	X	-	-	-
19	CLA	c	515	X	-	-	-
19	CLA	d	403	X	-	-	-
19	CLA	d	404	X	-	-	-

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 42392 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2388	1568	395	410	15		
1	a	306	Total	C	N	O	S	0	0
			2388	1568	395	410	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		
2	b	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	441	Total	C	N	O	S	0	0
			3444	2256	574	597	17		
3	c	441	Total	C	N	O	S	0	0
			3444	2256	574	597	17		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	337	Total	C	N	O	S	0	0
			2686	1777	439	458	12		
4	d	337	Total	C	N	O	S	0	0
			2686	1777	439	458	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total	C	N	O	0	0
			610	399	101	110		
5	e	75	Total	C	N	O	0	0
			610	399	101	110		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	31	Total	C	N	O	S	0	0
			251	171	42	37	1		
6	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

- Molecule 7 is a protein called PDZ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	182	Total	C	N	O	S	0	0
			1464	913	266	278	7		
7	g	182	Total	C	N	O	S	0	0
			1464	913	266	278	7		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	69	Total	C	N	O	S	0	0
			530	355	78	95	2		
8	h	69	Total	C	N	O	S	0	0
			530	355	78	95	2		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		
9	i	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			297	209	43	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			297	209	43	45		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	38	Total	C	N	O	S	0	0
			314	210	51	52	1		
11	l	38	Total	C	N	O	S	0	0
			314	210	51	52	1		

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	27	Total	C	N	O	0	0
			210	146	29	35		
12	m	27	Total	C	N	O	0	0
			210	146	29	35		

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	31	Total	C	N	O	S	0	0
			256	177	38	39	2		
13	t	31	Total	C	N	O	S	0	0
			256	177	38	39	2		

- Molecule 14 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	31	Total	C	N	O	0	0
			216	143	35	38		
14	v	31	Total	C	N	O	0	0
			216	143	35	38		

- Molecule 15 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	19	Total	C	N	O	S	0	0
			156	113	22	20	1		
15	w	19	Total	C	N	O	S	0	0
			156	113	22	20	1		



- Molecule 16 is a protein called Chloroplast photosystem II subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	32	Total	C	N	O	0	0
			214	140	35	39		
16	x	32	Total	C	N	O	0	0
			214	140	35	39		

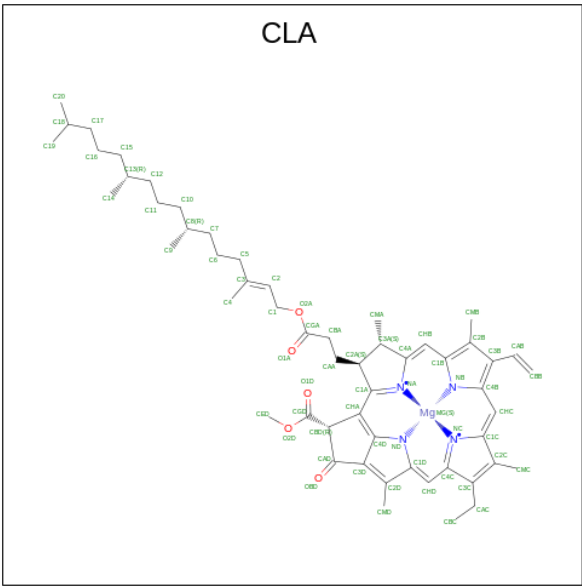
- Molecule 17 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
17	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 18 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Fe	0
			1	1	
18	a	1	Total	Fe	0
			1	1	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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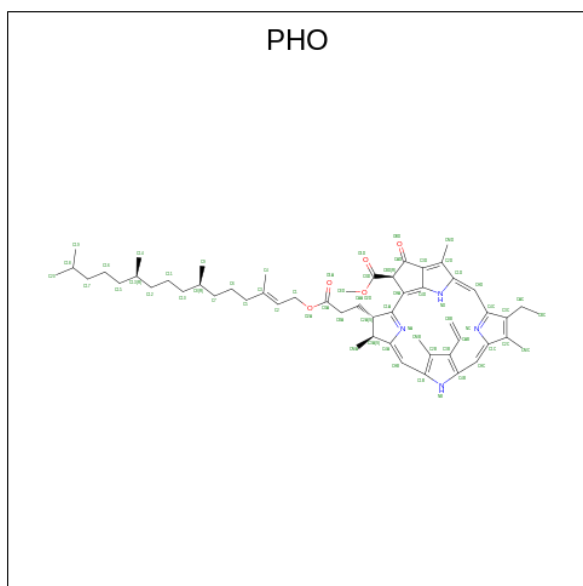
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

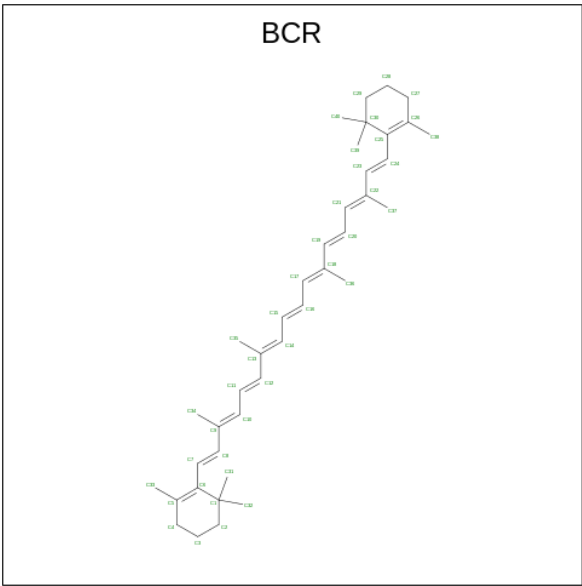
- Molecule 20 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	N	O	0
			64	55	4	5	
20	D	1	Total	C	N	O	0
			64	55	4	5	
20	a	1	Total	C	N	O	0
			64	55	4	5	
20	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand

of Interest" by depositor).



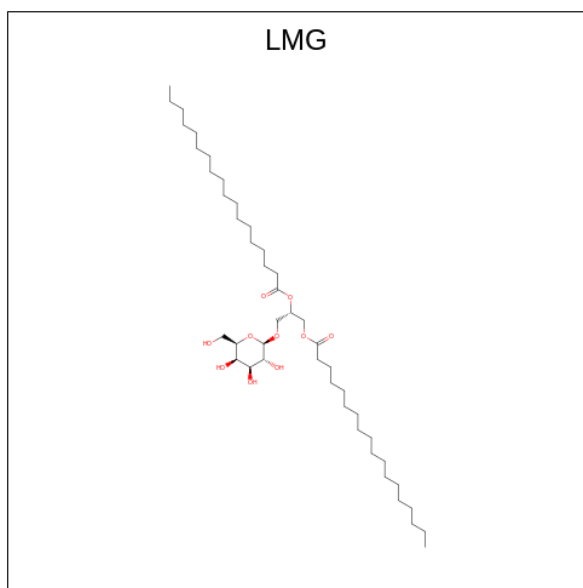
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	C	1	Total	C	0
			40	40	
21	C	1	Total	C	0
			40	40	
21	C	1	Total	C	0
			40	40	
21	D	1	Total	C	0
			40	40	
21	H	1	Total	C	0
			40	40	
21	V	1	Total	C	0
			40	40	
21	W	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	
21	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
21	c	1	Total C 40 40	0
21	c	1	Total C 40 40	0
21	c	1	Total C 40 40	0
21	d	1	Total C 40 40	0
21	h	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	w	1	Total C 40 40	0

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



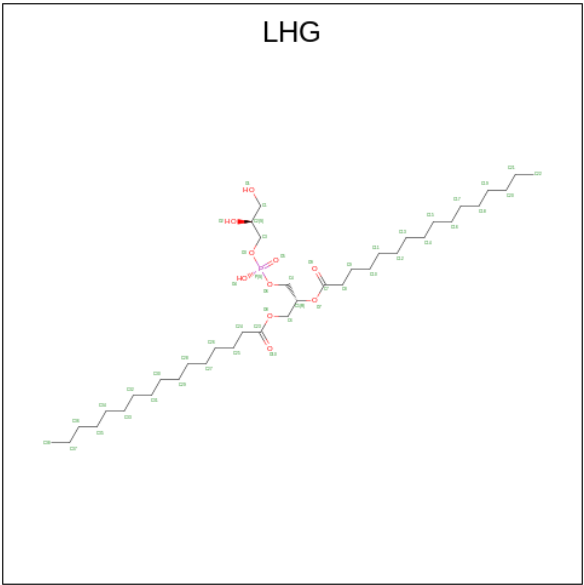
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C O 46 36 10	0
22	B	1	Total C O 42 32 10	0
22	C	1	Total C O 51 41 10	0
22	F	1	Total C O 46 36 10	0

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Mol	Chain	Residues	Atoms			AltConf
22	H	1	Total	C	O	0
			48	38	10	
22	b	1	Total	C	O	0
			42	32	10	
22	c	1	Total	C	O	0
			46	36	10	
22	c	1	Total	C	O	0
			51	41	10	
22	f	1	Total	C	O	0
			46	36	10	
22	h	1	Total	C	O	0
			48	38	10	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			43	32	10	1	
23	A	1	Total	C	O	P	0
			44	33	10	1	
23	B	1	Total	C	O	P	0
			44	33	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	D	1	Total	C	O	P	0
			49	38	10	1	

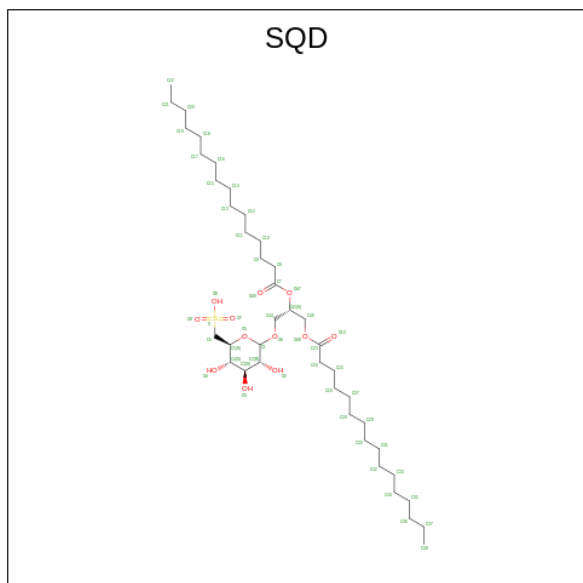
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Mol	Chain	Residues	Atoms				AltConf
23	L	1	Total	C	O	P	0
			49	38	10	1	
23	X	1	Total	C	O	P	0
			49	38	10	1	
23	a	1	Total	C	O	P	0
			43	32	10	1	
23	a	1	Total	C	O	P	0
			44	33	10	1	
23	b	1	Total	C	O	P	0
			49	38	10	1	
23	d	1	Total	C	O	P	0
			44	33	10	1	
23	d	1	Total	C	O	P	0
			49	38	10	1	
23	l	1	Total	C	O	P	0
			49	38	10	1	
23	x	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



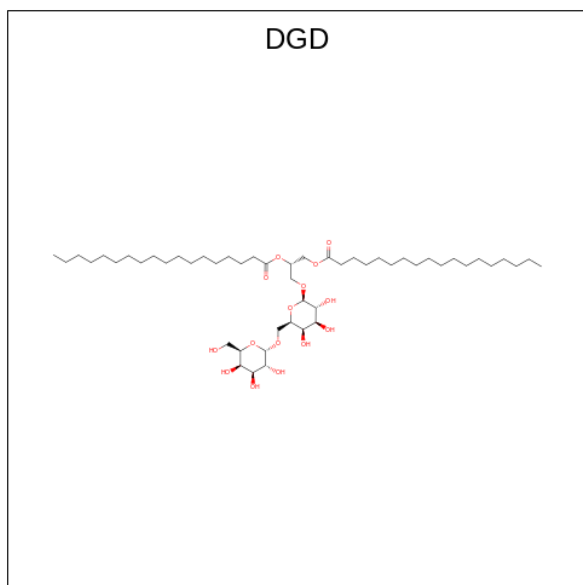
Mol	Chain	Residues	Atoms				AltConf
24	C	1	Total	C	O	S	0
			51	38	12	1	

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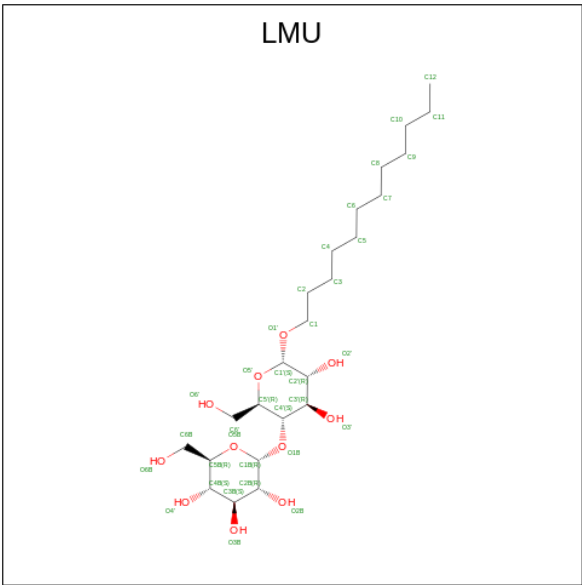
Mol	Chain	Residues	Atoms				AltConf
24	c	1	Total	C	O	S	0
			51	38	12	1	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



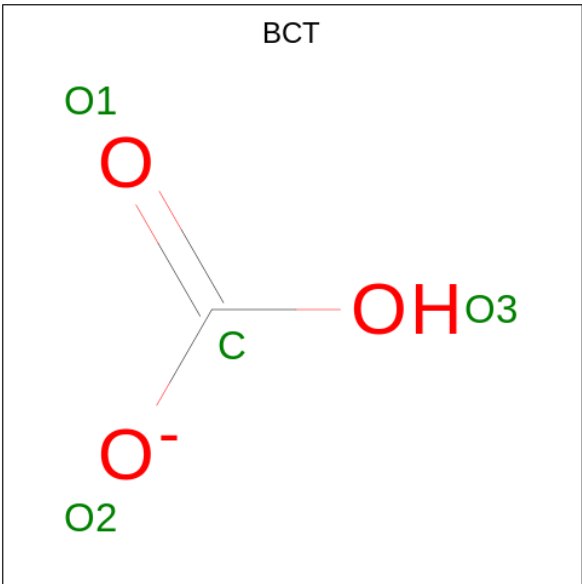
Mol	Chain	Residues	Atoms				AltConf
25	C	1	Total	C	O		0
			53	38	15		
25	C	1	Total	C	O		0
			49	34	15		
25	C	1	Total	C	O		0
			59	44	15		
25	c	1	Total	C	O		0
			53	38	15		
25	c	1	Total	C	O		0
			49	34	15		
25	c	1	Total	C	O		0
			59	44	15		

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula:  $C_{24}H_{46}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	C	1	Total	C	O	0
			35	24	11	
26	c	1	Total	C	O	0
			35	24	11	

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



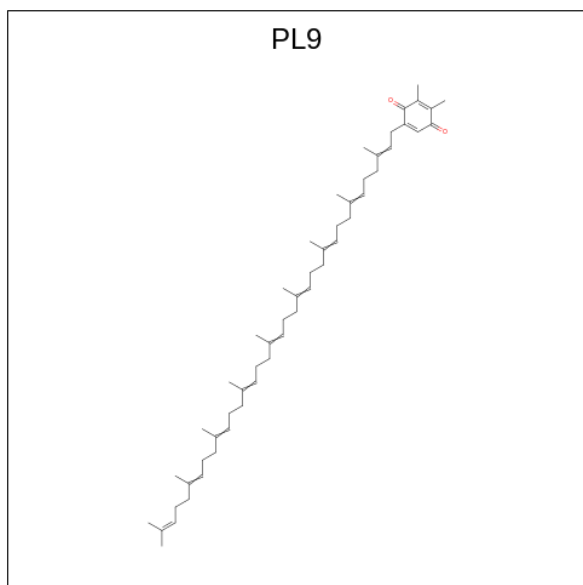
Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total	C	O	0
			4	1	3	

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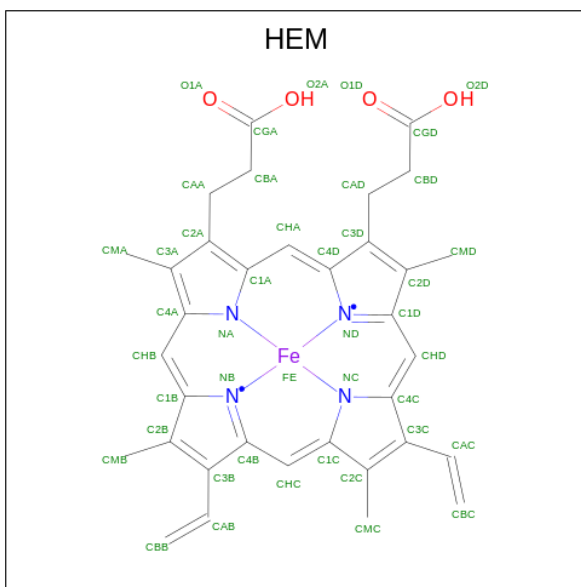
Mol	Chain	Residues	Atoms			AltConf
27	d	1	Total	C	O	0
			4	1	3	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	D	1	Total	C	O	0
			55	53	2	
28	d	1	Total	C	O	0
			55	53	2	

- Molecule 29 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).

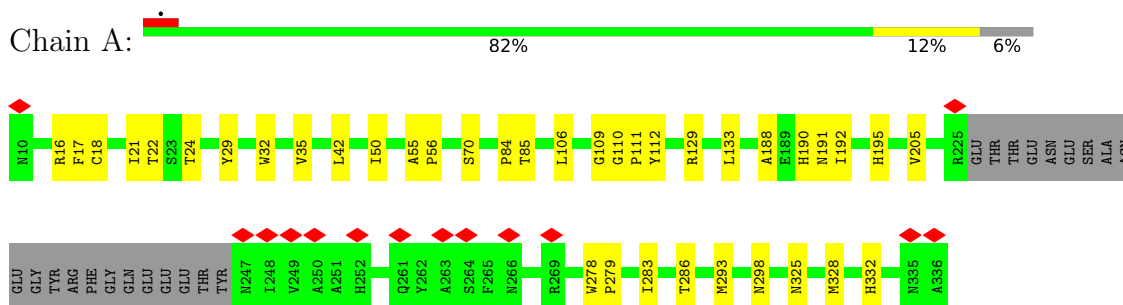


Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
29	e	1	Total 43	C 34	Fe 1	N 4	O 4	0

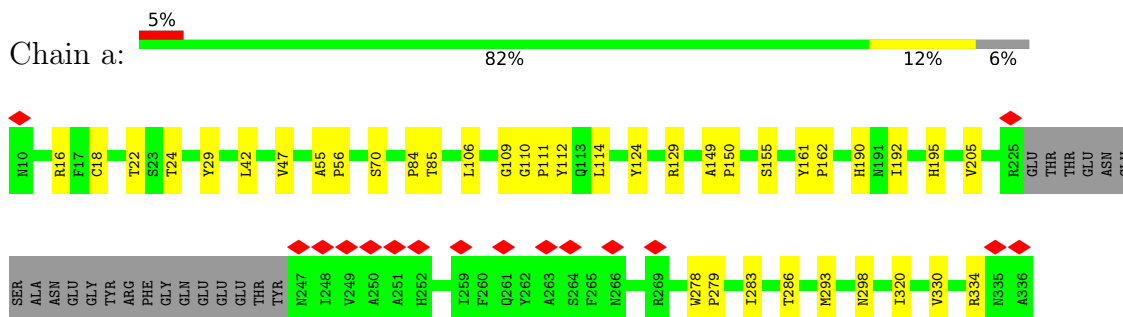
### 3 Residue-property plots [i](#)

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.

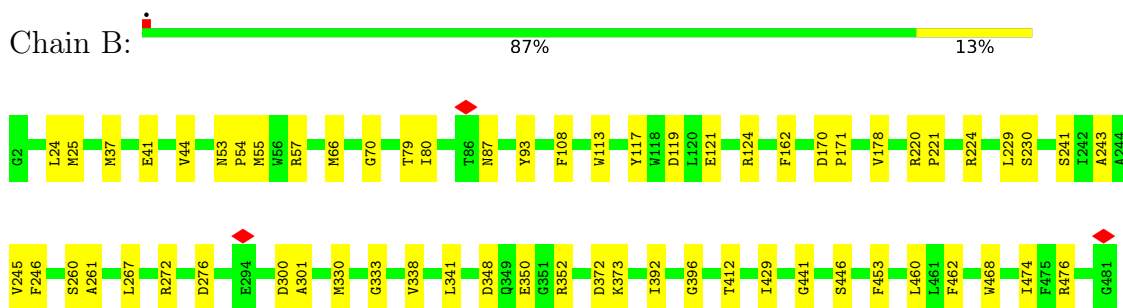
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

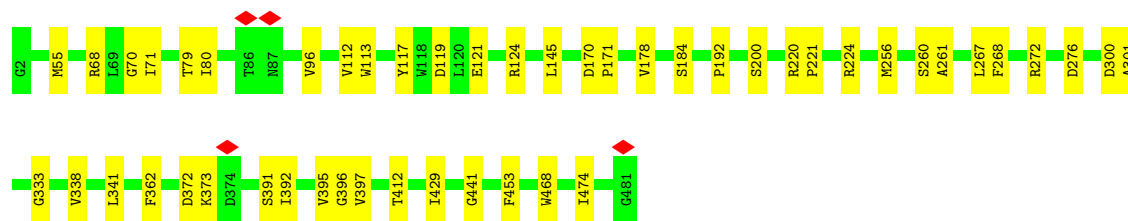


- Molecule 2: Photosystem II CP47 reaction center protein

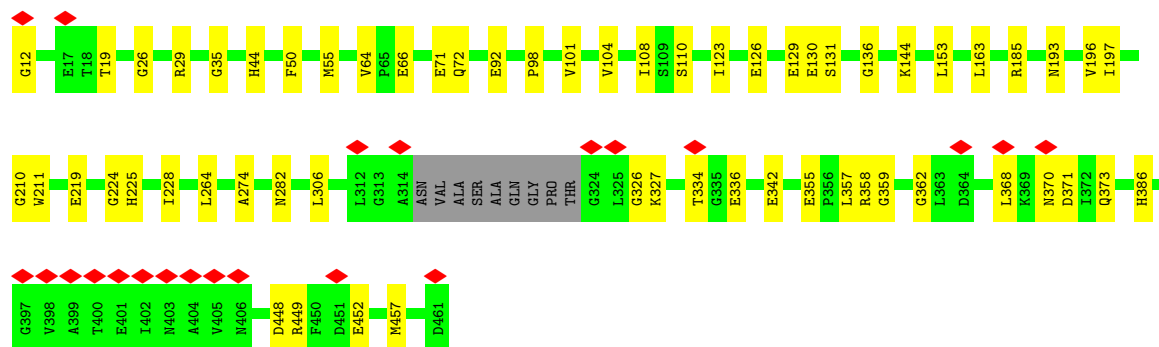
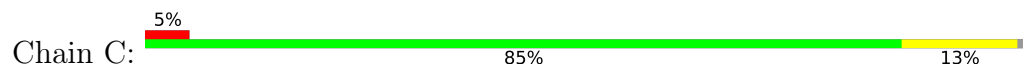


- Molecule 2: Photosystem II CP47 reaction center protein

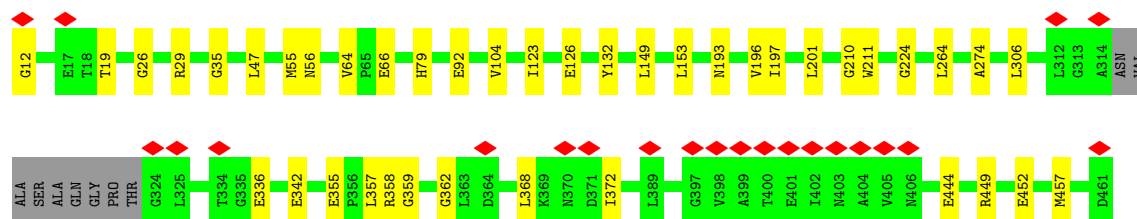
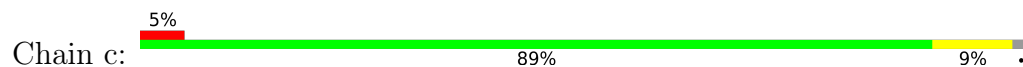




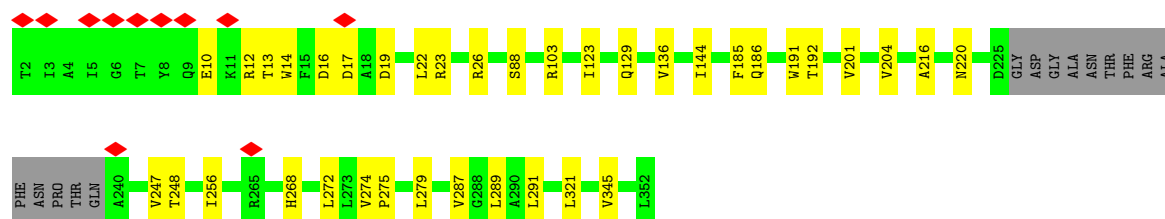
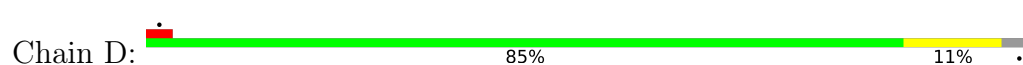
• Molecule 3: Photosystem II CP43 reaction center protein



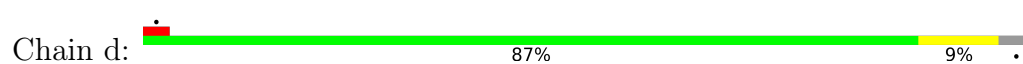
• Molecule 3: Photosystem II CP43 reaction center protein

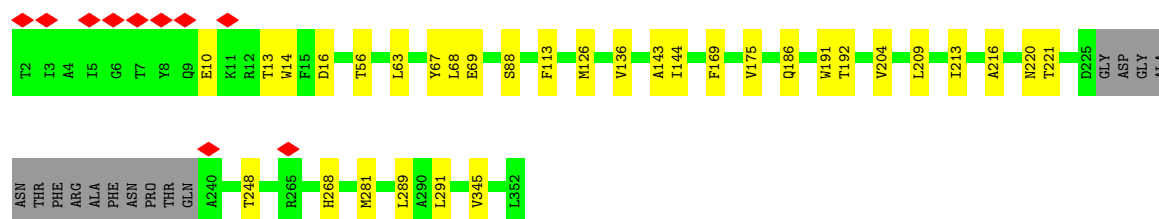


• Molecule 4: Photosystem II D2 protein

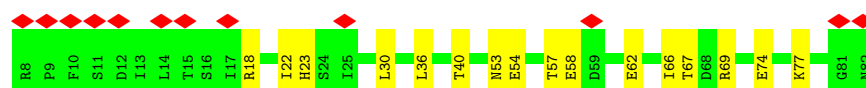
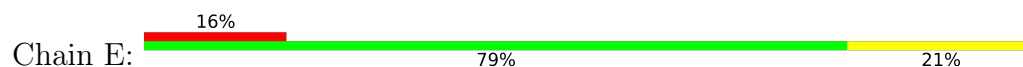


• Molecule 4: Photosystem II D2 protein

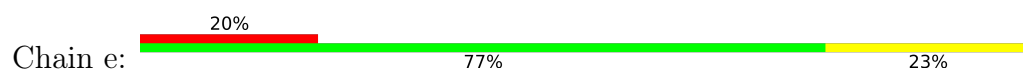




• Molecule 5: Cytochrome b559 subunit alpha



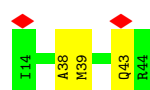
• Molecule 5: Cytochrome b559 subunit alpha



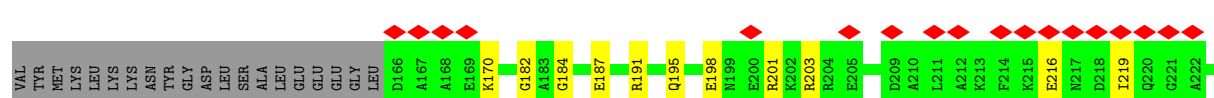
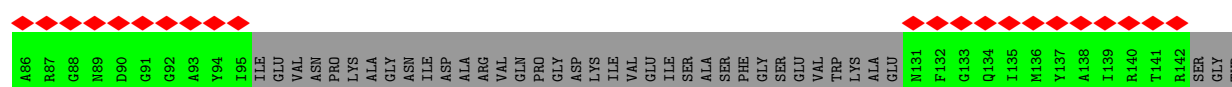
• Molecule 6: Cytochrome b559 subunit beta



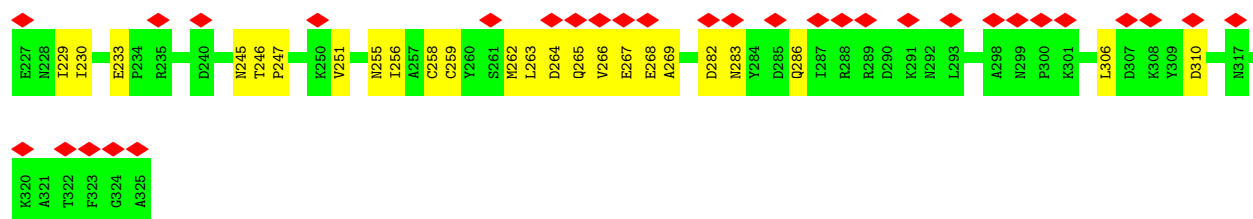
• Molecule 6: Cytochrome b559 subunit beta



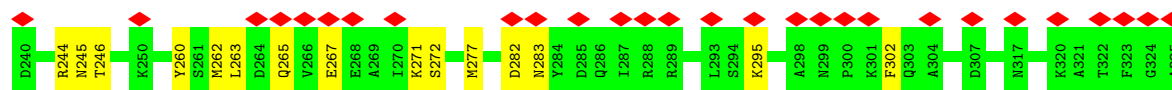
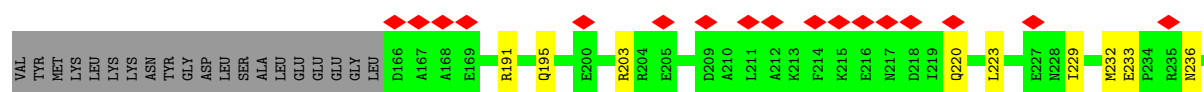
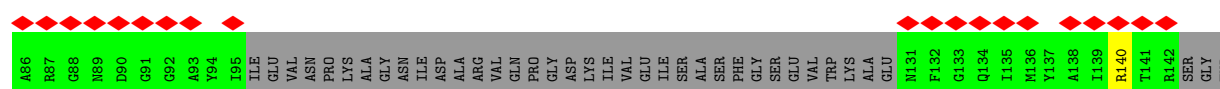
• Molecule 7: PDZ domain-containing protein



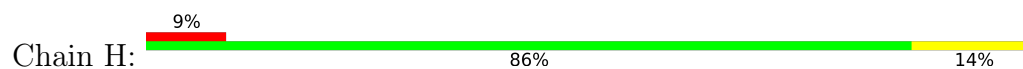




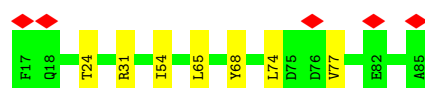
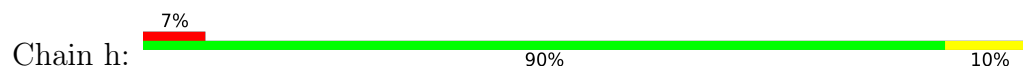
• Molecule 7: PDZ domain-containing protein



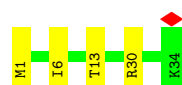
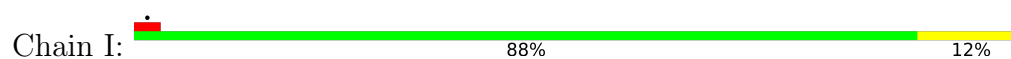
• Molecule 8: Photosystem II reaction center protein H



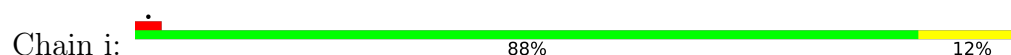
• Molecule 8: Photosystem II reaction center protein H



• Molecule 9: Photosystem II reaction center protein I

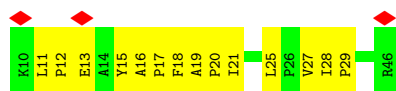


• Molecule 9: Photosystem II reaction center protein I

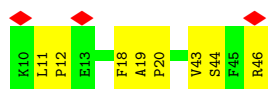
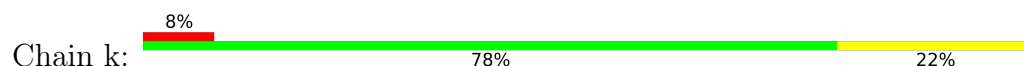




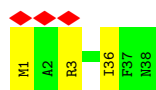
- Molecule 10: Photosystem II reaction center protein K



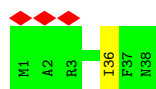
- Molecule 10: Photosystem II reaction center protein K



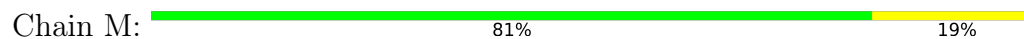
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



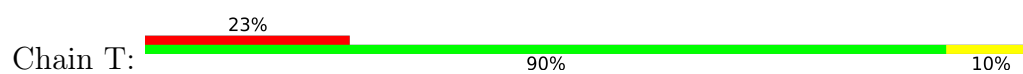
- Molecule 12: Photosystem II reaction center protein M



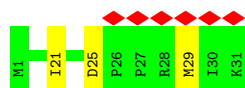
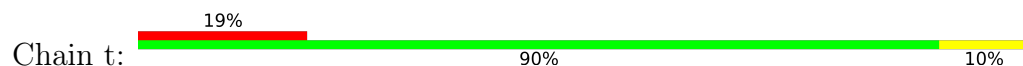
- Molecule 12: Photosystem II reaction center protein M



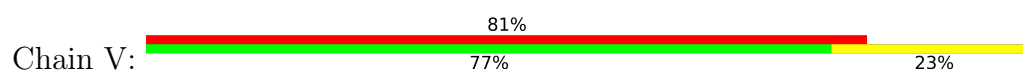
- Molecule 13: Photosystem II reaction center protein T



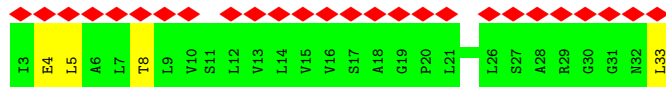
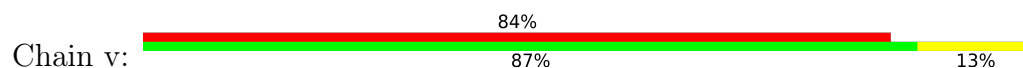
- Molecule 13: Photosystem II reaction center protein T



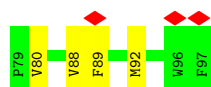
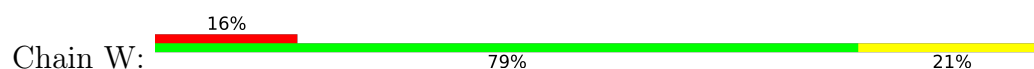
- Molecule 14: Photosystem II reaction center protein Psb30



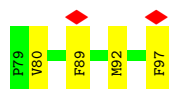
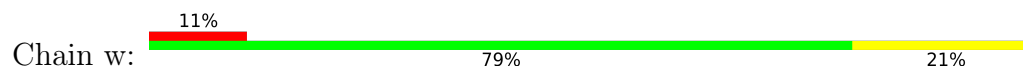
- Molecule 14: Photosystem II reaction center protein Psb30



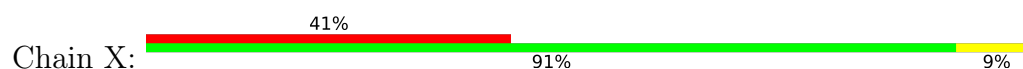
- Molecule 15: Photosystem II reaction center W protein, chloroplastic



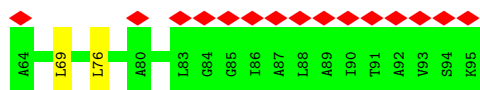
- Molecule 15: Photosystem II reaction center W protein, chloroplastic



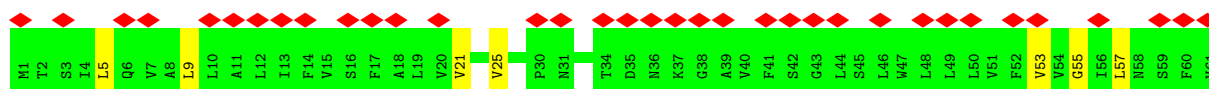
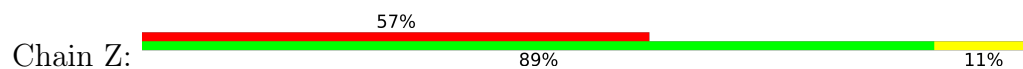
- Molecule 16: Chloroplast photosystem II subunit X



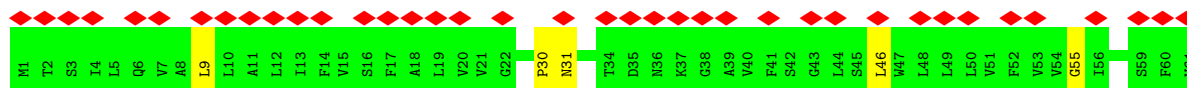
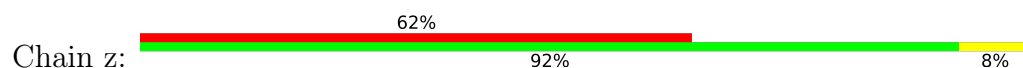
- Molecule 16: Chloroplast photosystem II subunit X



- Molecule 17: Photosystem II reaction center protein Z



- Molecule 17: Photosystem II reaction center protein Z



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61267	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.008	Depositor
Minimum map value	-0.544	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.16	Depositor
Map size ( $\text{\AA}$ )	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, SQD, LMU, FE2, DGD, BCT, HEM, PHO, LMG, BCR, PL9, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.19	0/2463	0.30	0/3358
1	a	0.18	0/2463	0.26	0/3358
2	B	0.17	0/3883	0.29	0/5286
2	b	0.16	0/3883	0.24	0/5286
3	C	0.15	0/3563	0.28	0/4851
3	c	0.14	0/3563	0.25	0/4851
4	D	0.18	0/2777	0.28	0/3787
4	d	0.18	0/2777	0.26	0/3787
5	E	0.15	0/628	0.31	0/857
5	e	0.12	0/628	0.27	0/857
6	F	0.16	0/258	0.36	0/349
6	f	0.17	0/258	0.47	0/349
7	G	0.12	0/1487	0.32	0/1993
7	g	0.10	0/1487	0.26	0/1993
8	H	0.13	0/542	0.27	0/742
8	h	0.14	0/542	0.28	0/742
9	I	0.18	0/283	0.27	0/383
9	i	0.18	0/283	0.22	0/383
10	K	0.13	0/309	0.33	0/425
10	k	0.12	0/309	0.31	0/425
11	L	0.21	0/322	0.28	0/437
11	l	0.19	0/322	0.26	0/437
12	M	0.14	0/214	0.36	0/293
12	m	0.15	0/214	0.25	0/293
13	T	0.18	0/263	0.26	0/354
13	t	0.17	0/263	0.24	0/354
14	V	0.12	0/216	0.28	0/296
14	v	0.09	0/216	0.24	0/296
15	W	0.79	0/164	1.14	0/225
15	w	0.80	0/164	1.15	0/225
16	X	0.11	0/215	0.23	0/292
16	x	0.09	0/215	0.21	0/292

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Z	0.14	0/469	0.27	0/644
17	z	0.12	0/469	0.24	0/644
All	All	0.17	0/36112	0.29	0/49144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2327	27	0
1	a	2388	0	2327	28	0
2	B	3755	0	3642	46	0
2	b	3755	0	3642	38	0
3	C	3444	0	3319	47	0
3	c	3444	0	3319	39	0
4	D	2686	0	2585	31	0
4	d	2686	0	2585	30	0
5	E	610	0	599	12	0
5	e	610	0	599	14	0
6	F	251	0	263	4	0
6	f	251	0	263	7	0
7	G	1464	0	1422	26	0
7	g	1464	0	1422	18	0
8	H	530	0	553	10	0
8	h	530	0	553	7	0
9	I	275	0	287	11	0
9	i	275	0	287	10	0
10	K	297	0	308	11	0
10	k	297	0	308	7	0
11	L	314	0	327	2	0
11	l	314	0	327	1	0
12	M	210	0	231	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	m	210	0	231	2	0
13	T	256	0	273	3	0
13	t	256	0	273	3	0
14	V	216	0	250	10	0
14	v	216	0	250	3	0
15	W	156	0	156	10	0
15	w	156	0	156	9	0
16	X	214	0	240	3	0
16	x	214	0	240	3	0
17	Z	458	0	490	11	0
17	z	458	0	490	8	0
18	A	1	0	0	0	0
18	a	1	0	0	0	0
19	A	239	0	242	0	0
19	B	1020	0	1113	17	0
19	C	845	0	936	14	0
19	D	130	0	144	6	0
19	a	239	0	242	4	0
19	b	1020	0	1113	11	0
19	c	845	0	936	14	0
19	d	130	0	144	5	0
20	A	64	0	74	1	0
20	D	64	0	74	2	0
20	a	64	0	74	0	0
20	d	64	0	74	1	0
21	A	40	0	56	9	0
21	B	80	0	112	7	0
21	C	120	0	168	21	0
21	D	40	0	56	1	0
21	H	40	0	56	7	0
21	V	40	0	56	4	0
21	W	40	0	56	8	0
21	a	40	0	56	5	0
21	b	80	0	112	10	0
21	c	120	0	168	18	0
21	d	40	0	56	1	0
21	h	40	0	56	6	0
21	k	40	0	56	2	0
21	w	40	0	56	7	0
22	A	46	0	62	0	0
22	B	42	0	54	0	0
22	C	51	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	46	0	62	0	0
22	H	48	0	66	2	0
22	b	42	0	54	0	0
22	c	97	0	134	0	0
22	f	46	0	62	0	0
22	h	48	0	66	1	0
23	A	87	0	117	1	0
23	B	93	0	135	1	0
23	D	49	0	74	1	0
23	L	49	0	74	0	0
23	X	49	0	74	0	0
23	a	87	0	117	0	0
23	b	49	0	74	1	0
23	d	93	0	135	1	0
23	l	49	0	74	0	0
23	x	49	0	74	0	0
24	C	51	0	69	0	0
24	c	51	0	69	0	0
25	C	161	0	196	1	0
25	c	161	0	196	0	0
26	C	35	0	46	0	0
26	c	35	0	46	0	0
27	D	4	0	0	1	0
27	d	4	0	0	1	0
28	D	55	0	80	0	0
28	d	55	0	80	1	0
29	F	43	0	30	6	0
29	e	43	0	30	5	0
All	All	42392	0	43252	518	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:6:ILE:CD1	15:W:80:VAL:HG13	1.85	1.07
9:i:6:ILE:HD11	15:w:80:VAL:HG13	1.30	1.05
9:i:6:ILE:CD1	15:w:80:VAL:HG13	1.85	1.05
9:I:6:ILE:CD1	15:W:80:VAL:CG1	2.33	1.05
9:i:6:ILE:CD1	15:w:80:VAL:CG1	2.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:6:ILE:HD11	15:W:80:VAL:HG13	1.39	0.99
9:i:6:ILE:HD11	15:w:80:VAL:CG1	1.96	0.92
9:I:6:ILE:HD13	15:W:80:VAL:CG1	1.99	0.92
9:i:6:ILE:HD13	15:w:80:VAL:CG1	2.01	0.89
9:I:6:ILE:HD11	15:W:80:VAL:CG1	2.01	0.89
1:a:192:ILE:HD12	1:a:293:MET:HE1	1.58	0.86
2:B:350:GLU:OE2	2:B:352:ARG:NH1	2.09	0.86
21:W:101:BCR:H403	2:b:113:TRP:CD1	2.13	0.83
3:C:452:GLU:OE2	4:D:248:THR:OG1	1.95	0.83
29:e:101:HEM:HHC	29:e:101:HEM:HBB2	1.64	0.79
2:B:272:ARG:NH1	2:B:276:ASP:OD2	2.16	0.79
3:C:12:GLY:N	14:V:33:LEU:O	2.17	0.78
29:F:102:HEM:HHC	29:F:102:HEM:HBB2	1.65	0.78
3:C:66:GLU:N	3:C:66:GLU:OE1	2.18	0.77
5:e:62:GLU:OE2	5:e:62:GLU:N	2.18	0.76
4:D:186:GLN:HB2	19:D:403:CLA:HBC1	1.68	0.76
3:C:71:GLU:OE2	3:C:386:HIS:NE2	2.19	0.76
21:C:517:BCR:C31	17:Z:9:LEU:HD21	2.16	0.76
10:K:13:GLU:N	10:K:13:GLU:OE1	2.19	0.76
2:B:119:ASP:OD1	2:B:124:ARG:NH2	2.19	0.75
5:E:62:GLU:OE2	5:E:62:GLU:N	2.18	0.75
9:I:6:ILE:CD1	15:W:80:VAL:HG11	2.17	0.74
9:I:6:ILE:HD13	15:W:80:VAL:HG11	1.67	0.74
3:c:66:GLU:N	3:c:66:GLU:OE1	2.19	0.74
2:b:272:ARG:NH1	2:b:276:ASP:OD2	2.21	0.74
3:c:12:GLY:N	14:v:33:LEU:O	2.20	0.74
1:A:29:TYR:O	1:A:129:ARG:NH1	2.20	0.74
5:E:74:GLU:N	5:E:74:GLU:OE2	2.21	0.74
2:b:119:ASP:OD1	2:b:124:ARG:NH2	2.20	0.73
21:A:407:BCR:H382	21:A:407:BCR:H23C	1.70	0.73
2:B:113:TRP:CD1	21:w:101:BCR:H403	2.23	0.73
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.25	0.72
19:B:506:CLA:H62	21:w:101:BCR:HC7	1.72	0.72
21:c:518:BCR:H383	21:c:518:BCR:H23C	1.70	0.72
2:b:372:ASP:OD1	2:b:373:LYS:N	2.23	0.72
21:a:407:BCR:H382	21:a:407:BCR:H23C	1.72	0.71
2:B:372:ASP:OD1	2:B:373:LYS:N	2.23	0.71
21:C:517:BCR:H383	21:C:517:BCR:H23C	1.71	0.71
9:i:6:ILE:CD1	15:w:80:VAL:HG11	2.21	0.70
21:W:101:BCR:H401	2:b:117:TYR:HE2	1.55	0.70
4:d:186:GLN:HB2	19:d:403:CLA:HBC1	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:101:BCR:H23C	21:V:101:BCR:H402	1.73	0.70
1:a:42:LEU:HB3	21:a:407:BCR:H353	1.74	0.70
7:g:203:ARG:NH1	7:g:229:ILE:O	2.25	0.69
7:G:203:ARG:NH2	7:G:233:GLU:OE1	2.25	0.69
4:D:192:THR:HG23	19:D:403:CLA:HBC2	1.73	0.69
9:i:6:ILE:HD13	15:w:80:VAL:HG11	1.73	0.69
3:C:92:GLU:OE1	3:C:92:GLU:N	2.25	0.69
21:C:516:BCR:H23C	21:C:516:BCR:H382	1.74	0.69
19:D:404:CLA:H43	16:X:76:LEU:HD23	1.72	0.69
2:b:224:ARG:NE	4:d:10:GLU:OE2	2.26	0.69
7:g:220:GLN:OE1	7:g:220:GLN:N	2.22	0.69
3:c:92:GLU:N	3:c:92:GLU:OE1	2.25	0.69
3:c:357:LEU:HD21	3:c:372:ILE:HG22	1.73	0.69
2:B:117:TYR:HE2	21:w:101:BCR:H401	1.57	0.68
2:B:113:TRP:HB2	21:w:101:BCR:H23C	1.76	0.68
21:W:101:BCR:H23C	2:b:113:TRP:HB2	1.75	0.68
2:b:145:LEU:HD21	19:b:515:CLA:HMB2	1.74	0.68
21:c:516:BCR:H321	21:c:516:BCR:HC8	1.76	0.67
5:e:35:TRP:CD2	6:f:38:ALA:HB2	2.29	0.67
2:b:224:ARG:NH2	4:d:16:ASP:OD2	2.26	0.67
3:C:136:GLY:O	3:C:144:LYS:NZ	2.25	0.66
3:c:224:GLY:HA3	21:c:517:BCR:H402	1.76	0.66
1:A:42:LEU:HB3	21:A:407:BCR:H353	1.77	0.66
21:C:515:BCR:HC8	21:C:515:BCR:H321	1.77	0.66
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.31	0.66
1:a:286:THR:OG1	19:a:402:CLA:O1D	2.13	0.66
1:A:85:THR:HG22	1:A:109:GLY:O	1.96	0.65
2:B:241:SER:O	2:B:245:VAL:HG23	1.96	0.65
4:d:221:THR:HG22	4:d:221:THR:O	1.96	0.64
3:C:224:GLY:HA3	21:C:516:BCR:H402	1.79	0.64
2:B:230:SER:OG	2:B:476:ARG:NH2	2.30	0.64
14:v:5:LEU:O	14:v:8:THR:OG1	2.14	0.64
14:V:4:GLU:N	14:V:4:GLU:OE2	2.31	0.63
2:B:341:LEU:HD12	2:B:429:ILE:HG22	1.80	0.63
3:C:163:LEU:HD23	3:C:225:HIS:CD2	2.34	0.63
2:b:341:LEU:HD12	2:b:429:ILE:HG22	1.81	0.63
14:V:5:LEU:O	14:V:8:THR:OG1	2.16	0.63
7:g:267:GLU:N	7:g:267:GLU:OE1	2.32	0.63
21:b:518:BCR:H383	21:b:518:BCR:H23C	1.81	0.63
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.80	0.62
29:F:102:HEM:HMC1	29:F:102:HEM:HBC2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:18:PHE:CZ	17:z:9:LEU:HD23	2.34	0.62
21:c:516:BCR:H323	17:z:55:GLY:CA	2.30	0.62
7:g:282:ASP:OD1	7:g:283:ASN:N	2.33	0.62
21:B:518:BCR:H383	21:B:518:BCR:H23C	1.80	0.62
21:c:517:BCR:H382	21:c:517:BCR:H23C	1.81	0.62
1:a:24:THR:HG21	3:c:457:MET:HE2	1.81	0.62
7:g:223:LEU:HD11	7:g:260:TYR:CE1	2.35	0.62
7:G:263:LEU:HD23	7:G:265:GLN:H	1.65	0.62
21:k:101:BCR:H321	21:k:101:BCR:HC8	1.81	0.62
4:D:216:ALA:O	4:D:220:ASN:ND2	2.31	0.61
23:d:408:LHG:H322	13:t:21:ILE:HD11	1.82	0.61
21:H:101:BCR:H383	21:H:101:BCR:H23C	1.82	0.61
2:b:55:MET:CE	2:b:267:LEU:HD12	2.31	0.61
19:d:404:CLA:H43	16:x:76:LEU:HD23	1.82	0.61
7:g:233:GLU:OE2	7:g:246:THR:HG22	2.01	0.60
7:G:203:ARG:NH1	7:G:229:ILE:O	2.32	0.60
29:e:101:HEM:HBC2	29:e:101:HEM:HMC2	1.82	0.60
2:B:224:ARG:NH2	4:D:16:ASP:OD2	2.34	0.60
21:C:517:BCR:H312	17:Z:9:LEU:HD21	1.83	0.60
1:a:55:ALA:O	1:a:70:SER:OG	2.16	0.60
19:c:513:CLA:H93	21:c:518:BCR:C27	2.32	0.60
7:G:198:GLU:OE2	7:G:201:ARG:NH2	2.35	0.60
10:K:18:PHE:CE1	17:Z:9:LEU:HD22	2.37	0.60
11:L:1:MET:SD	11:L:3:ARG:N	2.75	0.59
14:v:4:GLU:N	14:v:4:GLU:OE2	2.32	0.59
19:b:516:CLA:OBD	8:h:24:THR:HG21	2.02	0.59
3:C:334:THR:OG1	3:C:336:GLU:OE1	2.19	0.59
5:E:22:ILE:HG23	5:E:23:HIS:HD1	1.67	0.59
3:C:355:GLU:OE2	3:C:358:ARG:NH1	2.35	0.58
21:b:517:BCR:H382	21:b:517:BCR:H23C	1.83	0.58
1:a:124:TYR:HH	1:a:155:SER:HG	1.51	0.58
21:B:517:BCR:H23C	21:B:517:BCR:H382	1.86	0.58
5:e:58:GLU:O	5:e:61:GLN:NE2	2.36	0.58
21:h:101:BCR:H383	21:h:101:BCR:H23C	1.84	0.58
19:C:512:CLA:H93	21:C:517:BCR:C27	2.33	0.58
19:B:502:CLA:H43	8:H:65:LEU:HA	1.86	0.58
3:C:197:ILE:HG23	21:C:516:BCR:H403	1.86	0.58
14:V:4:GLU:O	14:V:8:THR:HG23	2.04	0.58
21:C:515:BCR:H323	17:Z:55:GLY:CA	2.33	0.58
5:e:36:LEU:O	5:e:40:THR:HG22	2.04	0.58
3:C:274:ALA:HB2	19:C:503:CLA:HMD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:71:ILE:HD13	2:b:96:VAL:HG21	1.85	0.58
23:D:407:LHG:H322	13:T:21:ILE:HD11	1.85	0.57
4:d:192:THR:HG23	19:d:403:CLA:HBC2	1.85	0.57
2:B:117:TYR:CE2	21:w:101:BCR:H401	2.40	0.57
19:a:404:CLA:HED1	4:d:175:VAL:CG1	2.35	0.57
19:a:404:CLA:HED1	4:d:175:VAL:HG13	1.86	0.57
3:c:452:GLU:OE2	4:d:248:THR:OG1	2.23	0.56
8:H:54:ILE:HG12	21:H:101:BCR:H333	1.87	0.56
7:g:191:ARG:NH1	7:g:195:GLN:OE1	2.38	0.56
8:h:54:ILE:HG13	21:h:101:BCR:H333	1.86	0.56
5:e:22:ILE:HG23	5:e:23:HIS:HD1	1.71	0.56
2:B:55:MET:CE	2:B:267:LEU:HD23	2.36	0.55
7:g:223:LEU:HD11	7:g:260:TYR:HE1	1.69	0.55
4:d:68:LEU:HA	6:f:39:MET:HE3	1.88	0.55
19:B:502:CLA:H42	22:H:102:LMG:H112	1.88	0.55
3:C:342:GLU:N	3:C:342:GLU:OE1	2.40	0.55
4:d:68:LEU:CA	6:f:39:MET:HE3	2.37	0.55
7:G:306:LEU:O	7:G:310:ASP:N	2.35	0.55
2:B:66:MET:SD	19:B:505:CLA:HED3	2.46	0.55
12:M:12:ALA:O	12:M:16:ILE:HG12	2.07	0.55
1:a:205:VAL:HG12	4:d:204:VAL:HG12	1.89	0.55
3:c:342:GLU:N	3:c:342:GLU:OE1	2.39	0.54
3:C:19:THR:HG21	3:C:29:ARG:HG2	1.89	0.54
3:C:44:HIS:CE1	19:C:510:CLA:HMA3	2.42	0.54
7:G:265:GLN:OE1	7:G:266:VAL:N	2.40	0.54
1:a:85:THR:HG22	1:a:109:GLY:O	2.07	0.54
19:B:506:CLA:C6	21:w:101:BCR:HC7	2.37	0.54
9:I:13:THR:CG2	15:W:88:VAL:HG21	2.38	0.54
19:b:502:CLA:H42	22:h:102:LMG:H112	1.90	0.54
3:c:444:GLU:OE1	3:c:444:GLU:N	2.33	0.54
4:d:281:MET:HE2	4:d:281:MET:HA	1.89	0.54
7:g:203:ARG:HG2	7:g:232:MET:HE3	1.89	0.54
3:c:26:GLY:HA3	19:c:513:CLA:HMD2	1.90	0.54
3:c:123:ILE:HG23	3:c:123:ILE:O	2.08	0.53
7:G:282:ASP:OD1	7:G:283:ASN:N	2.41	0.53
1:a:195:HIS:CD2	1:a:293:MET:HE2	2.43	0.53
3:C:26:GLY:HA3	19:C:512:CLA:HMD2	1.90	0.53
14:V:5:LEU:HD23	14:V:9:LEU:HD23	1.89	0.53
2:b:392:ILE:O	2:b:396:GLY:N	2.41	0.53
3:c:355:GLU:OE2	3:c:358:ARG:NH1	2.41	0.53
21:b:517:BCR:HC8	21:b:517:BCR:H331	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:O	1:A:70:SER:OG	2.17	0.53
4:d:216:ALA:O	4:d:220:ASN:ND2	2.38	0.53
3:C:264:LEU:HD21	19:C:509:CLA:HAB	1.91	0.53
7:g:277:MET:HE2	7:g:277:MET:HA	1.91	0.53
10:k:43:VAL:HG12	10:k:43:VAL:O	2.09	0.53
2:B:121:GLU:OE2	8:H:21:GLY:N	2.39	0.53
23:A:409:LHG:O3	23:A:409:LHG:O1	2.18	0.52
2:B:300:ASP:OD1	2:B:301:ALA:N	2.42	0.52
3:c:201:LEU:HD11	21:c:517:BCR:H20C	1.90	0.52
3:C:163:LEU:HD22	19:C:502:CLA:C2D	2.40	0.52
19:b:504:CLA:HAA2	19:b:512:CLA:H141	1.90	0.52
4:d:136:VAL:HG12	4:d:136:VAL:O	2.09	0.52
1:a:190:HIS:ND1	1:a:298:ASN:OD1	2.34	0.52
4:d:88:SER:OG	5:e:69:ARG:NH2	2.42	0.52
2:B:162:PHE:O	19:B:506:CLA:HMD3	2.10	0.52
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.44	0.52
7:g:267:GLU:O	7:g:271:LYS:NZ	2.40	0.52
19:b:502:CLA:H43	8:h:65:LEU:HA	1.92	0.52
8:H:75:ASP:OD2	16:X:64:ALA:N	2.43	0.52
7:G:265:GLN:OE1	7:G:267:GLU:N	2.42	0.52
8:H:54:ILE:CG1	21:H:101:BCR:H333	2.39	0.52
2:b:333:GLY:O	2:b:441:GLY:N	2.41	0.52
3:c:264:LEU:HD21	19:c:510:CLA:HAB	1.92	0.52
21:c:516:BCR:H382	21:c:516:BCR:H23C	1.91	0.52
7:G:191:ARG:NH1	7:G:195:GLN:OE1	2.40	0.52
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.52
3:c:357:LEU:HD23	3:c:368:LEU:HD23	1.92	0.51
2:B:24:LEU:HD21	19:B:516:CLA:HAB	1.91	0.51
17:z:30:PRO:O	17:z:31:ASN:OD1	2.28	0.51
3:c:19:THR:HG21	3:c:29:ARG:HG2	1.93	0.51
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.45	0.51
7:G:258:CYS:SG	7:G:262:MET:HE1	2.51	0.51
2:B:224:ARG:NE	4:D:10:GLU:OE2	2.44	0.51
2:B:330:MET:HE1	2:B:446:SER:HB3	1.92	0.51
21:V:101:BCR:H321	21:V:101:BCR:HC8	1.92	0.51
29:e:101:HEM:HBC2	29:e:101:HEM:CMC	2.41	0.51
19:B:504:CLA:HAA2	19:B:512:CLA:H141	1.92	0.51
21:H:101:BCR:HC8	21:H:101:BCR:H331	1.93	0.51
7:g:203:ARG:NH2	7:g:246:THR:HG21	2.25	0.50
29:F:102:HEM:HBC2	29:F:102:HEM:CMC	2.40	0.50
1:a:29:TYR:O	1:a:129:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLY:N	1:A:111:PRO:HD2	2.27	0.50
3:C:123:ILE:HG23	3:C:123:ILE:O	2.11	0.50
1:A:16:ARG:HD3	1:A:16:ARG:C	2.37	0.50
19:B:507:CLA:H203	11:L:36:ILE:HG13	1.92	0.50
19:B:509:CLA:CGA	8:H:50:MET:HE3	2.41	0.50
4:D:136:VAL:O	4:D:136:VAL:HG12	2.11	0.50
6:F:27:VAL:HB	6:F:28:PRO:HD3	1.93	0.50
4:d:113:PHE:CZ	21:d:405:BCR:H323	2.47	0.50
2:B:260:SER:OG	2:B:261:ALA:N	2.45	0.50
19:C:512:CLA:H93	21:C:517:BCR:H271	1.94	0.50
2:b:260:SER:OG	2:b:261:ALA:N	2.45	0.50
21:B:517:BCR:HC8	21:B:517:BCR:H331	1.93	0.49
19:b:502:CLA:H41	19:b:502:CLA:C7	2.42	0.49
3:C:370:ASN:OD1	3:C:371:ASP:N	2.44	0.49
3:c:35:GLY:N	3:c:126:GLU:O	2.45	0.49
21:c:518:BCR:H312	17:z:9:LEU:HD11	1.93	0.49
1:A:24:THR:HG21	3:C:457:MET:HE2	1.94	0.49
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.94	0.49
1:a:283:ILE:HA	1:a:286:THR:HG22	1.94	0.49
3:c:104:VAL:HG11	21:c:516:BCR:HC42	1.94	0.49
10:k:44:SER:O	10:k:44:SER:OG	2.30	0.49
4:D:19:ASP:OD1	4:D:23:ARG:NH1	2.46	0.49
19:B:502:CLA:H41	19:B:502:CLA:C7	2.42	0.49
21:W:101:BCR:H312	19:b:506:CLA:H62	1.94	0.49
21:c:516:BCR:H323	17:z:55:GLY:HA3	1.95	0.49
1:A:283:ILE:HG13	20:A:405:PHO:HBC3	1.95	0.49
2:B:333:GLY:O	2:B:441:GLY:N	2.42	0.49
10:K:21:ILE:O	10:K:25:LEU:HG	2.13	0.49
17:Z:53:VAL:O	17:Z:57:LEU:HD13	2.13	0.49
3:c:64:VAL:HG23	3:c:64:VAL:O	2.13	0.49
21:W:101:BCR:H401	2:b:117:TYR:CE2	2.41	0.49
10:k:18:PHE:CE1	17:z:9:LEU:HD23	2.48	0.48
1:A:325:ASN:HA	1:A:328:MET:HE3	1.95	0.48
2:B:392:ILE:O	2:B:396:GLY:N	2.42	0.48
3:C:64:VAL:O	3:C:64:VAL:HG23	2.12	0.48
21:C:515:BCR:H382	21:C:515:BCR:H23C	1.94	0.48
4:D:22:LEU:O	4:D:26:ARG:NH2	2.47	0.48
1:A:18:CYS:O	1:A:22:THR:HG22	2.13	0.48
5:E:57:THR:HG22	5:E:58:GLU:N	2.28	0.48
21:h:101:BCR:HC8	21:h:101:BCR:H331	1.95	0.48
10:K:27:VAL:HG22	10:K:27:VAL:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:517:BCR:H331	21:B:517:BCR:C8	2.44	0.48
1:A:190:HIS:ND1	1:A:298:ASN:OD1	2.35	0.48
2:B:170:ASP:OD1	2:B:171:PRO:HD2	2.14	0.48
3:C:224:GLY:CA	21:C:516:BCR:H402	2.43	0.48
4:D:12:ARG:NH1	4:D:17:ASP:OD1	2.46	0.48
4:D:185:PHE:CD2	19:D:403:CLA:HMD1	2.49	0.48
2:b:170:ASP:OD1	2:b:171:PRO:HD2	2.13	0.48
3:c:132:TYR:OH	19:c:515:CLA:O1D	2.31	0.48
5:e:18:ARG:O	5:e:22:ILE:HG22	2.12	0.48
7:g:263:LEU:HD22	7:g:265:GLN:HG3	1.95	0.48
5:E:18:ARG:O	5:E:22:ILE:HG22	2.14	0.48
21:C:515:BCR:H323	17:Z:55:GLY:HA3	1.94	0.47
2:b:184:SER:N	2:b:200:SER:OG	2.46	0.47
10:k:43:VAL:HG12	10:k:46:ARG:HG2	1.96	0.47
7:G:245:ASN:OD1	9:I:30:ARG:NH1	2.47	0.47
1:a:330:VAL:HG12	1:a:330:VAL:O	2.14	0.47
3:c:193:ASN:HB3	3:c:196:VAL:HG12	1.96	0.47
1:A:42:LEU:HD12	21:A:407:BCR:H341	1.97	0.47
19:B:513:CLA:HMB3	19:B:513:CLA:HBB1	1.96	0.47
7:g:140:ARG:NH2	7:g:272:SER:OG	2.47	0.47
1:A:205:VAL:HG12	4:D:204:VAL:HG12	1.95	0.47
19:c:503:CLA:H143	21:c:517:BCR:C35	2.44	0.47
21:h:101:BCR:H382	16:x:69:LEU:HD21	1.95	0.47
9:I:1:MET:SD	9:I:1:MET:N	2.80	0.47
2:b:395:VAL:HG23	2:b:397:VAL:HG13	1.97	0.47
2:B:87:ASN:OD1	2:B:87:ASN:O	2.32	0.47
4:D:88:SER:OG	5:E:69:ARG:NH2	2.47	0.47
9:I:13:THR:HG21	15:W:88:VAL:HG21	1.95	0.47
1:a:42:LEU:HD12	21:a:407:BCR:H341	1.96	0.47
3:c:197:ILE:HG23	21:c:517:BCR:H403	1.96	0.47
15:w:89:PHE:HA	15:w:92:MET:HE2	1.96	0.47
21:b:517:BCR:H331	21:b:517:BCR:C8	2.43	0.47
1:a:56:PRO:CD	1:a:106:LEU:HD13	2.45	0.47
1:a:110:GLY:N	1:a:111:PRO:HD2	2.30	0.46
19:b:507:CLA:H203	11:l:36:ILE:HG13	1.97	0.46
10:K:20:PRO:HB3	14:V:8:THR:HG22	1.98	0.46
4:d:67:TYR:HB2	6:f:39:MET:HE2	1.97	0.46
17:z:46:LEU:C	17:z:46:LEU:HD23	2.40	0.46
7:G:286:GLN:OE1	7:G:286:GLN:N	2.41	0.46
19:a:403:CLA:H203	28:d:406:PL9:H502	1.97	0.46
19:c:513:CLA:H93	21:c:518:BCR:H272	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:236:ASN:OD1	7:g:244:ARG:NH2	2.49	0.46
4:D:13:THR:HG22	4:D:14:TRP:N	2.31	0.46
7:G:216:GLU:HG2	7:G:216:GLU:O	2.16	0.46
4:d:13:THR:HG22	4:d:14:TRP:N	2.30	0.46
21:V:101:BCR:H23C	21:V:101:BCR:C40	2.42	0.46
3:c:153:LEU:HD21	19:c:508:CLA:HAB	1.97	0.46
21:c:518:BCR:H383	21:c:518:BCR:C23	2.44	0.46
3:C:50:PHE:HB2	3:C:110:SER:OG	2.15	0.46
21:C:517:BCR:H383	21:C:517:BCR:C23	2.43	0.46
4:D:279:LEU:HD22	20:D:401:PHO:HBC3	1.96	0.46
19:D:403:CLA:HBC3	19:D:403:CLA:HHD	1.98	0.46
10:K:11:LEU:HD23	10:K:12:PRO:O	2.16	0.46
2:B:341:LEU:HD12	2:B:429:ILE:CG2	2.45	0.46
1:A:56:PRO:CD	1:A:106:LEU:HD13	2.46	0.46
19:b:504:CLA:HBB1	19:b:513:CLA:HBC2	1.98	0.46
19:B:504:CLA:HBB1	19:B:513:CLA:HBC2	1.98	0.46
19:B:513:CLA:H142	21:B:518:BCR:H313	1.98	0.46
3:C:55:MET:HE1	19:C:505:CLA:ND	2.31	0.46
21:c:516:BCR:H323	17:z:55:GLY:HA2	1.98	0.46
2:B:468:TRP:CE3	4:D:144:ILE:HD13	2.51	0.46
3:C:371:ASP:O	3:C:373:GLN:NE2	2.47	0.46
14:V:15:VAL:CG2	21:V:101:BCR:H322	2.46	0.46
2:B:412:THR:HG22	2:B:412:THR:O	2.17	0.45
3:C:35:GLY:N	3:C:126:GLU:O	2.43	0.45
19:C:502:CLA:H143	21:C:516:BCR:C35	2.46	0.45
8:H:22:LEU:HD12	8:H:22:LEU:H	1.82	0.45
1:a:192:ILE:CD1	1:a:293:MET:HE1	2.37	0.45
10:k:11:LEU:HD12	10:k:12:PRO:HD2	1.97	0.45
19:C:512:CLA:H41	14:V:26:LEU:HD12	1.98	0.45
7:G:263:LEU:HD23	7:G:264:ASP:N	2.31	0.45
12:M:17:ILE:HB	12:M:18:PRO:HD3	1.98	0.45
17:Z:5:LEU:HD21	17:Z:57:LEU:CB	2.46	0.45
2:b:184:SER:C	2:b:200:SER:HG	2.24	0.45
3:c:336:GLU:N	3:c:336:GLU:OE1	2.49	0.45
3:C:130:GLU:OE1	3:C:131:SER:OG	2.28	0.45
8:h:74:LEU:HB2	8:h:77:VAL:HG22	1.98	0.45
3:C:359:GLY:N	3:C:362:GLY:O	2.48	0.45
8:H:48:VAL:HG23	8:H:49:LEU:HD22	1.99	0.45
12:M:5:ILE:HD12	12:M:5:ILE:H	1.81	0.45
21:W:101:BCR:H15C	21:W:101:BCR:H351	1.81	0.45
1:A:191:ASN:OD1	1:A:325:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:74:LEU:HB2	8:H:77:VAL:HG22	1.98	0.45
1:a:47:VAL:HG21	1:a:114:LEU:HD22	1.99	0.45
21:a:407:BCR:H15C	21:a:407:BCR:H351	1.84	0.45
3:c:224:GLY:CA	21:c:517:BCR:H402	2.44	0.45
4:d:67:TYR:CB	6:f:39:MET:HE2	2.47	0.45
4:d:209:LEU:HD23	4:d:213:ILE:HD12	1.99	0.45
7:G:182:GLY:N	13:T:31:LYS:O	2.50	0.45
3:c:149:LEU:HD23	3:c:149:LEU:C	2.41	0.45
7:g:262:MET:O	7:g:295:LYS:NZ	2.47	0.45
17:Z:21:VAL:O	17:Z:25:VAL:HG23	2.17	0.45
2:b:121:GLU:OE2	8:h:31:ARG:NH1	2.49	0.45
2:b:412:THR:O	2:b:412:THR:HG22	2.17	0.45
3:c:372:ILE:HG13	3:c:372:ILE:O	2.16	0.45
9:i:1:MET:SD	9:i:1:MET:N	2.84	0.45
1:A:283:ILE:HA	1:A:286:THR:HG22	1.97	0.44
21:B:517:BCR:HC8	21:B:517:BCR:C33	2.47	0.44
3:C:306:LEU:HD23	3:C:306:LEU:C	2.42	0.44
19:b:513:CLA:H142	21:b:518:BCR:H313	1.99	0.44
4:D:103:ARG:HE	5:E:77:LYS:HE2	1.82	0.44
29:F:102:HEM:HBD1	29:F:102:HEM:HHA	1.99	0.44
15:W:89:PHE:HA	15:W:92:MET:HE2	1.99	0.44
1:a:18:CYS:O	1:a:22:THR:HG22	2.17	0.44
5:e:23:HIS:CD2	29:e:101:HEM:NC	2.85	0.44
1:A:133:LEU:HD23	4:D:256:ILE:HG12	2.00	0.44
5:E:23:HIS:CD2	29:F:102:HEM:NC	2.85	0.44
21:b:517:BCR:HC8	21:b:517:BCR:C33	2.47	0.44
5:e:35:TRP:CG	6:f:38:ALA:HB2	2.52	0.44
4:D:129:GLN:NE2	20:D:401:PHO:OBD	2.49	0.44
5:E:30:LEU:HD11	6:F:27:VAL:HG13	1.98	0.44
3:c:274:ALA:HB2	19:c:504:CLA:HMD2	1.99	0.44
3:c:359:GLY:N	3:c:362:GLY:O	2.50	0.44
21:A:407:BCR:H15C	21:A:407:BCR:H351	1.86	0.44
21:H:101:BCR:H331	21:H:101:BCR:C8	2.48	0.44
2:b:68:ARG:HB2	2:b:267:LEU:HD21	1.99	0.44
3:C:225:HIS:HA	3:C:228:ILE:HG22	2.00	0.44
3:C:326:GLY:O	3:C:327:LYS:HG2	2.18	0.44
2:b:55:MET:HE1	2:b:267:LEU:HD12	1.99	0.44
4:d:268:HIS:CE1	27:d:402:BCT:O3	2.70	0.44
3:C:193:ASN:HB3	3:C:196:VAL:HG12	2.00	0.44
7:G:246:THR:HG23	7:G:247:PRO:HD2	2.00	0.44
2:b:192:PRO:HG3	8:h:68:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:66:ILE:O	5:e:75:GLN:NE2	2.51	0.44
4:D:201:VAL:HG22	19:D:403:CLA:C1B	2.48	0.44
1:a:16:ARG:HD3	1:a:16:ARG:C	2.42	0.44
3:C:104:VAL:HG11	21:C:515:BCR:HC42	1.98	0.44
3:C:357:LEU:HD23	3:C:368:LEU:HD23	2.00	0.44
6:F:23:HIS:NE2	29:F:102:HEM:C1B	2.85	0.44
3:c:449:ARG:O	3:c:449:ARG:HG2	2.18	0.44
3:C:104:VAL:O	3:C:108:ILE:HG12	2.18	0.43
1:A:42:LEU:CB	21:A:407:BCR:H353	2.46	0.43
21:H:101:BCR:H382	16:X:69:LEU:HD21	1.99	0.43
3:C:185:ARG:NH2	3:C:219:GLU:OE2	2.48	0.43
10:K:11:LEU:HD21	10:K:15:TYR:HB2	1.99	0.43
17:Z:5:LEU:HD21	17:Z:57:LEU:HB3	2.00	0.43
3:c:29:ARG:HB3	19:c:513:CLA:HED1	1.99	0.43
3:C:153:LEU:HD21	19:C:507:CLA:HAB	2.00	0.43
21:b:518:BCR:H383	21:b:518:BCR:C23	2.47	0.43
13:t:29:MET:SD	13:t:29:MET:N	2.91	0.43
4:D:274:VAL:HB	4:D:275:PRO:HD3	2.01	0.43
12:m:17:ILE:HB	12:m:18:PRO:HD3	2.00	0.43
5:E:36:LEU:O	5:E:40:THR:HG22	2.19	0.43
7:G:170:LYS:HD2	7:G:170:LYS:O	2.18	0.43
8:h:54:ILE:CG1	21:h:101:BCR:H333	2.49	0.43
2:B:468:TRP:HE3	4:D:144:ILE:HD13	1.83	0.43
19:c:503:CLA:H143	21:c:517:BCR:H351	1.99	0.43
12:m:5:ILE:HD12	12:m:5:ILE:H	1.84	0.43
15:w:97:PHE:O	21:w:101:BCR:H393	2.19	0.43
2:B:453:PHE:HB2	4:D:291:LEU:HD12	2.00	0.43
21:b:517:BCR:H15C	21:b:517:BCR:H351	1.92	0.43
2:B:53:ASN:N	2:B:54:PRO:HD3	2.34	0.43
2:B:79:THR:HG22	2:B:80:ILE:N	2.34	0.43
21:a:407:BCR:H382	21:a:407:BCR:C23	2.46	0.43
2:b:474:ILE:HD12	23:b:520:LHG:HC5	2.01	0.43
5:e:40:THR:HG23	5:e:42:LEU:H	1.84	0.43
2:B:462:PHE:CE2	19:B:513:CLA:HMB2	2.54	0.42
19:C:502:CLA:H143	21:C:516:BCR:H351	2.01	0.42
1:a:24:THR:CG2	3:c:457:MET:HE2	2.48	0.42
19:d:403:CLA:HBC3	19:d:403:CLA:HHD	2.01	0.42
13:T:25:ASP:OD1	13:T:25:ASP:C	2.62	0.42
1:a:205:VAL:CG1	4:d:204:VAL:HG12	2.48	0.42
21:k:101:BCR:HC7	21:k:101:BCR:H331	1.71	0.42
2:B:220:ARG:HE	2:B:221:PRO:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:84:PRO:HA	1:a:112:TYR:CG	2.54	0.42
2:b:341:LEU:HD12	2:b:429:ILE:CG2	2.48	0.42
7:g:245:ASN:OD1	9:i:30:ARG:NH1	2.53	0.42
21:h:101:BCR:H331	21:h:101:BCR:C8	2.49	0.42
10:k:19:ALA:N	10:k:20:PRO:HD2	2.34	0.42
21:A:407:BCR:H382	21:A:407:BCR:C23	2.46	0.42
19:B:501:CLA:HHC	19:B:501:CLA:CBB	2.49	0.42
3:C:29:ARG:HB3	19:C:512:CLA:HED1	2.01	0.42
1:A:50:ILE:HG22	21:A:407:BCR:H271	2.01	0.42
2:B:57:ARG:NH1	2:B:330:MET:HG2	2.34	0.42
3:C:282:ASN:OD1	25:C:518:DGD:O5E	2.32	0.42
3:c:79:HIS:NE2	19:c:504:CLA:O1D	2.52	0.42
4:d:56:THR:OG1	4:d:69:GLU:OE2	2.35	0.42
2:B:44:VAL:HG12	2:B:44:VAL:O	2.20	0.42
10:K:16:ALA:N	10:K:17:PRO:HD2	2.35	0.42
1:a:320:ILE:HD11	4:d:63:LEU:HD21	2.00	0.42
1:a:334:ARG:HB2	1:a:334:ARG:CZ	2.49	0.42
3:c:55:MET:HE1	19:c:506:CLA:ND	2.35	0.42
19:d:404:CLA:C4	16:x:76:LEU:HD23	2.47	0.42
1:A:84:PRO:HA	1:A:112:TYR:CG	2.54	0.42
2:B:348:ASP:OD2	2:B:352:ARG:NH2	2.53	0.42
4:D:247:VAL:HG23	4:D:248:THR:N	2.35	0.42
10:K:20:PRO:CB	14:V:8:THR:HG22	2.49	0.42
2:b:300:ASP:OD1	2:b:301:ALA:N	2.52	0.42
2:b:468:TRP:CE3	4:d:144:ILE:HD13	2.54	0.42
3:c:210:GLY:O	3:c:211:TRP:C	2.63	0.42
7:g:302:PHE:CD1	7:g:302:PHE:C	2.97	0.42
2:B:66:MET:HE3	2:B:93:TYR:HD1	1.84	0.42
3:C:129:GLU:OE1	3:C:129:GLU:N	2.52	0.42
7:G:259:CYS:HA	7:G:262:MET:HE2	2.02	0.42
10:K:19:ALA:N	10:K:20:PRO:HD2	2.34	0.42
2:b:79:THR:HG22	2:b:80:ILE:N	2.35	0.42
4:d:345:VAL:O	4:d:345:VAL:HG22	2.20	0.42
2:B:338:VAL:HG13	2:B:338:VAL:O	2.19	0.42
4:D:272:LEU:C	4:D:272:LEU:HD23	2.45	0.42
21:C:517:BCR:H312	17:Z:9:LEU:HD11	2.02	0.41
4:D:268:HIS:CE1	27:D:402:BCT:O3	2.73	0.41
7:G:251:VAL:O	7:G:255:ASN:ND2	2.53	0.41
21:W:101:BCR:H272	2:b:112:VAL:HG12	2.00	0.41
2:b:338:VAL:O	2:b:338:VAL:HG13	2.19	0.41
9:i:27:ASP:OD1	9:i:27:ASP:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ILE:HA	1:A:293:MET:HE1	2.02	0.41
3:C:210:GLY:O	3:C:211:TRP:C	2.63	0.41
21:D:405:BCR:H352	6:F:28:PRO:HB2	2.01	0.41
7:G:266:VAL:O	7:G:269:ALA:HB3	2.20	0.41
3:c:306:LEU:HD23	3:c:306:LEU:C	2.45	0.41
21:B:518:BCR:H383	21:B:518:BCR:C23	2.47	0.41
5:E:53:ASN:OD1	5:E:54:GLU:N	2.53	0.41
2:b:453:PHE:HB2	4:d:291:LEU:HD12	2.03	0.41
5:e:71:ASN:OD1	5:e:71:ASN:O	2.38	0.41
4:D:123:ILE:HD11	22:H:102:LMG:H401	2.02	0.41
7:G:266:VAL:O	7:G:269:ALA:N	2.53	0.41
8:H:75:ASP:OD1	8:H:75:ASP:N	2.51	0.41
2:B:37:MET:O	2:B:41:GLU:HG3	2.20	0.41
2:b:391:SER:O	2:b:395:VAL:HG22	2.20	0.41
6:f:43:GLN:OE1	6:f:43:GLN:HA	2.19	0.41
21:C:516:BCR:H351	21:C:516:BCR:H15C	1.97	0.41
5:E:66:ILE:O	5:E:67:THR:HG22	2.20	0.41
7:G:184:GLY:O	7:G:187:GLU:HG2	2.21	0.41
19:C:514:CLA:H62	19:C:514:CLA:H41	1.94	0.41
21:H:101:BCR:H383	21:H:101:BCR:C23	2.50	0.41
20:d:401:PHO:O1A	20:d:401:PHO:C2	2.69	0.41
1:A:32:TRP:O	1:A:35:VAL:HG22	2.21	0.41
1:A:188:ALA:HB2	1:A:328:MET:HB3	2.02	0.41
1:A:195:HIS:CD2	1:A:293:MET:HE3	2.56	0.41
2:B:229:LEU:HD21	19:B:509:CLA:O2A	2.21	0.41
21:C:516:BCR:H11C	21:C:516:BCR:H341	1.89	0.41
7:G:266:VAL:HG13	7:G:267:GLU:N	2.35	0.41
1:a:161:TYR:HB3	1:a:162:PRO:HD3	2.03	0.41
4:d:126:MET:HE3	4:d:143:ALA:O	2.20	0.41
3:C:104:VAL:HG11	21:C:515:BCR:H333	2.03	0.41
7:G:219:ILE:HD12	7:G:219:ILE:H	1.84	0.41
10:K:28:ILE:N	10:K:29:PRO:HD2	2.36	0.41
14:V:26:LEU:HD21	17:Z:25:VAL:HA	2.02	0.41
21:W:101:BCR:H11C	21:W:101:BCR:H341	1.79	0.41
2:b:220:ARG:HE	2:b:221:PRO:HD2	1.84	0.41
3:c:149:LEU:HD11	19:c:508:CLA:CMB	2.51	0.41
29:e:101:HEM:HBD1	29:e:101:HEM:HHA	2.03	0.41
4:D:345:VAL:HG22	4:D:345:VAL:O	2.20	0.41
21:b:517:BCR:HC7	21:b:517:BCR:H311	1.94	0.41
13:t:25:ASP:OD1	13:t:25:ASP:C	2.63	0.41
21:A:407:BCR:C33	21:A:407:BCR:HC8	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:278:TRP:HB3	1:a:279:PRO:HD3	2.02	0.40
21:A:407:BCR:H24C	21:A:407:BCR:H371	1.92	0.40
5:e:27:VAL:N	5:e:28:PRO:HD2	2.36	0.40
7:G:230:ILE:HD12	7:G:256:ILE:CD1	2.51	0.40
2:b:256:MET:HE1	2:b:268:PHE:CD1	2.56	0.40
19:b:501:CLA:CBB	19:b:501:CLA:HHC	2.51	0.40
3:c:56:ASN:O	3:c:56:ASN:ND2	2.53	0.40
5:e:66:ILE:O	5:e:67:THR:HG22	2.21	0.40
3:C:98:PRO:O	3:C:101:VAL:HG12	2.21	0.40
3:C:448:ASP:O	3:C:449:ARG:HB3	2.22	0.40
3:C:449:ARG:O	3:C:449:ARG:HG2	2.22	0.40
1:a:149:ALA:HB3	1:a:150:PRO:CD	2.51	0.40
21:b:518:BCR:H15C	21:b:518:BCR:H351	1.99	0.40
3:c:47:LEU:HD13	19:c:512:CLA:HMD1	2.03	0.40
1:A:17:PHE:CZ	1:A:21:ILE:HD11	2.56	0.40
1:A:332:HIS:HB3	4:D:321:LEU:HD21	2.02	0.40
2:B:460:LEU:CD1	4:D:287:VAL:HG21	2.52	0.40
2:B:474:ILE:HD12	23:B:521:LHG:HC5	2.04	0.40
3:C:64:VAL:HG22	3:C:72:GLN:OE1	2.22	0.40
7:G:268:GLU:OE1	7:G:268:GLU:HA	2.21	0.40
2:b:362:PHE:HE2	4:d:169:PHE:CZ	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/327 (92%)	296 (98%)	6 (2%)	0	100	100
1	a	302/327 (92%)	295 (98%)	7 (2%)	0	100	100
2	B	478/480 (100%)	464 (97%)	14 (3%)	0	100	100
2	b	478/480 (100%)	465 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	437/450 (97%)	426 (98%)	11 (2%)	0	100	100
3	c	437/450 (97%)	424 (97%)	13 (3%)	0	100	100
4	D	333/351 (95%)	327 (98%)	6 (2%)	0	100	100
4	d	333/351 (95%)	325 (98%)	8 (2%)	0	100	100
5	E	73/75 (97%)	73 (100%)	0	0	100	100
5	e	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	F	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	f	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	G	176/240 (73%)	172 (98%)	4 (2%)	0	100	100
7	g	176/240 (73%)	174 (99%)	2 (1%)	0	100	100
8	H	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
8	h	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	36 (100%)	0	0	100	100
12	M	25/27 (93%)	25 (100%)	0	0	100	100
12	m	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
13	T	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	t	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
14	V	29/31 (94%)	29 (100%)	0	0	100	100
14	v	29/31 (94%)	29 (100%)	0	0	100	100
15	W	17/19 (90%)	17 (100%)	0	0	100	100
15	w	17/19 (90%)	17 (100%)	0	0	100	100
16	X	30/32 (94%)	30 (100%)	0	0	100	100
16	x	30/32 (94%)	30 (100%)	0	0	100	100
17	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
17	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
All	All	4374/4666 (94%)	4275 (98%)	99 (2%)	0	100	100



There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/266 (93%)	248 (100%)	0	100	100
1	a	248/266 (93%)	248 (100%)	0	100	100
2	B	382/382 (100%)	382 (100%)	0	100	100
2	b	382/382 (100%)	382 (100%)	0	100	100
3	C	346/352 (98%)	346 (100%)	0	100	100
3	c	346/352 (98%)	346 (100%)	0	100	100
4	D	270/280 (96%)	270 (100%)	0	100	100
4	d	270/280 (96%)	270 (100%)	0	100	100
5	E	66/66 (100%)	66 (100%)	0	100	100
5	e	66/66 (100%)	66 (100%)	0	100	100
6	F	25/25 (100%)	25 (100%)	0	100	100
6	f	25/25 (100%)	25 (100%)	0	100	100
7	G	148/195 (76%)	148 (100%)	0	100	100
7	g	148/195 (76%)	148 (100%)	0	100	100
8	H	59/59 (100%)	59 (100%)	0	100	100
8	h	59/59 (100%)	59 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	K	31/31 (100%)	31 (100%)	0	100	100
10	k	31/31 (100%)	31 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	23/23 (100%)	23 (100%)	0	100	100
12	m	23/23 (100%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	T	28/28 (100%)	28 (100%)	0	100	100
13	t	28/28 (100%)	28 (100%)	0	100	100
14	V	25/25 (100%)	25 (100%)	0	100	100
14	v	25/25 (100%)	25 (100%)	0	100	100
15	W	15/15 (100%)	15 (100%)	0	100	100
15	w	15/15 (100%)	15 (100%)	0	100	100
16	X	22/22 (100%)	22 (100%)	0	100	100
16	x	22/22 (100%)	22 (100%)	0	100	100
17	Z	51/51 (100%)	51 (100%)	0	100	100
17	z	51/51 (100%)	51 (100%)	0	100	100
All	All	3610/3772 (96%)	3610 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	ASN
1	A	322	ASN
1	A	335	ASN
2	B	53	ASN
2	B	100	HIS
3	C	16	GLN
4	D	9	GLN
4	D	164	GLN
4	D	186	GLN
7	G	220	GLN
1	a	322	ASN
2	b	331	ASN
3	c	56	ASN
11	l	5	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 2 are monoatomic - leaving 134 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$
19	CLA	c	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.27	9 (11%)
19	CLA	c	508	-	65,73,73	1.52	7 (10%)	76,113,113	1.20	7 (9%)
21	BCR	a	407	-	41,41,41	0.76	0	56,56,56	1.93	19 (33%)
19	CLA	B	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.23	8 (10%)
19	CLA	c	511	-	65,73,73	1.49	9 (13%)	76,113,113	1.24	7 (9%)
19	CLA	C	509	-	65,73,73	1.50	8 (12%)	76,113,113	1.19	7 (9%)
19	CLA	c	514	-	65,73,73	1.50	7 (10%)	76,113,113	1.28	7 (9%)
25	DGD	C	520	-	60,60,67	0.88	2 (3%)	74,74,81	0.87	2 (2%)
19	CLA	C	502	-	65,73,73	1.51	7 (10%)	76,113,113	1.17	9 (11%)
19	CLA	b	509	-	65,73,73	1.51	7 (10%)	76,113,113	1.21	9 (11%)
19	CLA	b	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.23	9 (11%)
19	CLA	b	513	-	65,73,73	1.49	8 (12%)	76,113,113	1.25	8 (10%)
19	CLA	c	515	-	65,73,73	1.50	6 (9%)	76,113,113	1.22	7 (9%)
22	LMG	H	102	-	48,48,55	0.95	2 (4%)	56,56,63	0.95	2 (3%)
28	PL9	d	406	-	55,55,55	1.32	5 (9%)	68,69,69	1.50	12 (17%)
19	CLA	B	510	-	65,73,73	1.47	7 (10%)	76,113,113	1.29	9 (11%)
19	CLA	d	404	-	65,73,73	1.49	7 (10%)	76,113,113	1.25	9 (11%)
21	BCR	V	101	-	41,41,41	0.66	0	56,56,56	2.19	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	b	514	-	45,53,73	1.77	6 (13%)	52,89,113	1.46	7 (13%)
23	LHG	a	408	-	42,42,48	0.98	2 (4%)	45,48,54	1.02	2 (4%)
19	CLA	B	516	-	65,73,73	1.50	8 (12%)	76,113,113	1.22	8 (10%)
19	CLA	C	505	-	65,73,73	1.51	7 (10%)	76,113,113	1.23	7 (9%)
27	BCT	D	402	18	2,3,3	1.28	0	2,3,3	4.12	2 (100%)
26	LMU	c	523	-	36,36,36	1.18	2 (5%)	47,47,47	0.89	1 (2%)
19	CLA	A	402	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	8 (10%)
19	CLA	B	512	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	8 (10%)
19	CLA	a	402	-	65,73,73	1.48	8 (12%)	76,113,113	1.27	9 (11%)
25	DGD	C	519	-	50,50,67	0.97	2 (4%)	64,64,81	0.92	2 (3%)
24	SQD	C	501	-	50,51,54	1.21	4 (8%)	59,62,65	1.09	5 (8%)
20	PHO	a	405	-	51,69,69	1.03	5 (9%)	47,99,99	1.21	6 (12%)
19	CLA	a	404	-	49,57,73	1.72	8 (16%)	55,93,113	1.39	8 (14%)
23	LHG	B	521	-	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
21	BCR	C	516	-	41,41,41	0.79	0	56,56,56	1.83	17 (30%)
22	LMG	C	521	-	51,51,55	0.93	2 (3%)	59,59,63	0.88	2 (3%)
19	CLA	B	506	-	65,73,73	1.50	7 (10%)	76,113,113	1.20	8 (10%)
21	BCR	h	101	-	41,41,41	0.70	0	56,56,56	2.09	23 (41%)
23	LHG	x	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	3 (5%)
21	BCR	A	407	-	41,41,41	0.76	0	56,56,56	1.88	17 (30%)
29	HEM	F	102	5,6	41,50,50	1.49	4 (9%)	45,82,82	1.39	5 (11%)
25	DGD	c	520	-	50,50,67	0.97	2 (4%)	64,64,81	0.92	2 (3%)
19	CLA	C	506	-	65,73,73	1.48	7 (10%)	76,113,113	1.16	7 (9%)
23	LHG	D	407	-	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
19	CLA	c	507	-	65,73,73	1.49	7 (10%)	76,113,113	1.19	8 (10%)
19	CLA	b	503	-	65,73,73	1.50	8 (12%)	76,113,113	1.26	8 (10%)
19	CLA	b	516	-	65,73,73	1.48	8 (12%)	76,113,113	1.27	7 (9%)
19	CLA	a	406	-	60,68,73	1.54	7 (11%)	70,107,113	1.29	8 (11%)
21	BCR	b	518	-	41,41,41	0.74	0	56,56,56	1.91	19 (33%)
19	CLA	b	501	-	65,73,73	1.52	7 (10%)	76,113,113	1.20	7 (9%)
24	SQD	c	501	-	50,51,54	1.21	4 (8%)	59,62,65	1.09	5 (8%)
23	LHG	b	520	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
21	BCR	B	518	-	41,41,41	0.74	0	56,56,56	1.92	20 (35%)
21	BCR	b	517	-	41,41,41	0.76	1 (2%)	56,56,56	2.04	20 (35%)
19	CLA	b	502	-	65,73,73	1.49	6 (9%)	76,113,113	1.22	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	PL9	D	406	-	55,55,55	1.34	5 (9%)	68,69,69	1.50	12 (17%)
26	LMU	C	522	-	36,36,36	1.17	2 (5%)	47,47,47	0.89	1 (2%)
19	CLA	B	509	-	65,73,73	1.51	7 (10%)	76,113,113	1.19	9 (11%)
19	CLA	b	510	-	65,73,73	1.47	6 (9%)	76,113,113	1.31	9 (11%)
19	CLA	C	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.24	7 (9%)
19	CLA	B	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.27	8 (10%)
19	CLA	B	508	-	65,73,73	1.49	7 (10%)	76,113,113	1.22	9 (11%)
19	CLA	B	501	-	65,73,73	1.52	6 (9%)	76,113,113	1.19	7 (9%)
19	CLA	b	515	-	65,73,73	1.51	7 (10%)	76,113,113	1.22	9 (11%)
19	CLA	a	403	-	65,73,73	1.53	8 (12%)	76,113,113	1.28	9 (11%)
23	LHG	B	520	-	43,43,48	0.99	2 (4%)	46,49,54	0.93	2 (4%)
25	DGD	c	519	-	54,54,67	0.93	2 (3%)	68,68,81	0.98	3 (4%)
19	CLA	C	512	3	65,73,73	1.53	6 (9%)	76,113,113	1.19	8 (10%)
19	CLA	B	502	-	65,73,73	1.50	6 (9%)	76,113,113	1.25	8 (10%)
19	CLA	c	510	-	65,73,73	1.50	8 (12%)	76,113,113	1.19	7 (9%)
19	CLA	B	514	-	45,53,73	1.76	6 (13%)	52,89,113	1.46	7 (13%)
21	BCR	d	405	-	41,41,41	0.76	0	56,56,56	1.98	17 (30%)
19	CLA	d	403	-	65,73,73	1.50	8 (12%)	76,113,113	1.22	7 (9%)
29	HEM	e	101	5,6	41,50,50	1.49	3 (7%)	45,82,82	1.38	5 (11%)
21	BCR	c	516	-	41,41,41	0.79	1 (2%)	56,56,56	1.93	19 (33%)
22	LMG	f	101	-	46,46,55	0.97	2 (4%)	54,54,63	0.94	2 (3%)
19	CLA	b	512	-	65,73,73	1.47	7 (10%)	76,113,113	1.30	8 (10%)
19	CLA	B	515	-	65,73,73	1.50	8 (12%)	76,113,113	1.23	9 (11%)
19	CLA	c	505	-	65,73,73	1.51	7 (10%)	76,113,113	1.23	9 (11%)
23	LHG	d	407	-	43,43,48	0.99	2 (4%)	46,49,54	0.93	2 (4%)
19	CLA	B	505	-	65,73,73	1.53	8 (12%)	76,113,113	1.15	6 (7%)
21	BCR	W	101	-	41,41,41	0.84	2 (4%)	56,56,56	2.30	20 (35%)
25	DGD	c	521	-	60,60,67	0.89	2 (3%)	74,74,81	0.87	2 (2%)
22	LMG	A	408	-	46,46,55	0.99	3 (6%)	54,54,63	1.03	3 (5%)
22	LMG	b	519	-	42,42,55	0.99	2 (4%)	50,50,63	1.03	3 (6%)
21	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	2.04	19 (33%)
19	CLA	b	506	-	65,73,73	1.50	7 (10%)	76,113,113	1.19	8 (10%)
20	PHO	A	405	-	51,69,69	1.03	5 (9%)	47,99,99	1.21	6 (12%)
21	BCR	D	405	-	41,41,41	0.77	0	56,56,56	1.98	17 (30%)
19	CLA	D	404	-	65,73,73	1.50	7 (10%)	76,113,113	1.24	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	c	503	-	65,73,73	1.51	7 (10%)	76,113,113	1.19	8 (10%)
21	BCR	C	517	-	41,41,41	0.75	1 (2%)	56,56,56	1.93	17 (30%)
22	LMG	c	502	-	46,46,55	0.99	2 (4%)	54,54,63	1.02	3 (5%)
21	BCR	H	101	-	41,41,41	0.69	0	56,56,56	2.10	23 (41%)
21	BCR	c	517	-	41,41,41	0.81	1 (2%)	56,56,56	1.84	16 (28%)
19	CLA	A	404	-	49,57,73	1.72	8 (16%)	55,93,113	1.41	9 (16%)
22	LMG	c	522	-	51,51,55	0.93	2 (3%)	59,59,63	0.88	2 (3%)
19	CLA	c	509	-	65,73,73	1.47	7 (10%)	76,113,113	1.25	8 (10%)
19	CLA	c	513	3	65,73,73	1.52	6 (9%)	76,113,113	1.19	7 (9%)
27	BCT	d	402	18	2,3,3	1.27	0	2,3,3	4.13	2 (100%)
21	BCR	c	518	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
19	CLA	C	508	-	65,73,73	1.47	7 (10%)	76,113,113	1.25	8 (10%)
19	CLA	B	513	-	65,73,73	1.48	8 (12%)	76,113,113	1.25	8 (10%)
19	CLA	b	505	-	65,73,73	1.50	8 (12%)	76,113,113	1.17	8 (10%)
21	BCR	k	101	-	41,41,41	0.70	0	56,56,56	1.91	20 (35%)
20	PHO	D	401	-	51,69,69	1.03	5 (9%)	47,99,99	1.09	4 (8%)
19	CLA	b	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.28	8 (10%)
19	CLA	b	507	-	65,73,73	1.52	7 (10%)	76,113,113	1.26	8 (10%)
19	CLA	b	508	-	65,73,73	1.50	7 (10%)	76,113,113	1.22	8 (10%)
23	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.98	2 (3%)
23	LHG	A	409	-	42,42,48	0.98	2 (4%)	45,48,54	1.02	2 (4%)
22	LMG	F	101	-	46,46,55	0.97	2 (4%)	54,54,63	0.96	2 (3%)
19	CLA	D	403	-	65,73,73	1.49	8 (12%)	76,113,113	1.23	6 (7%)
22	LMG	h	102	-	48,48,55	0.96	2 (4%)	56,56,63	1.04	2 (3%)
19	CLA	B	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.22	9 (11%)
19	CLA	c	512	-	65,73,73	1.51	9 (13%)	76,113,113	1.23	7 (9%)
23	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	0.89	2 (3%)
23	LHG	X	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.02	3 (5%)
19	CLA	A	406	-	60,68,73	1.55	7 (11%)	70,107,113	1.28	9 (12%)
23	LHG	A	410	-	43,43,48	1.00	2 (4%)	46,49,54	0.93	2 (4%)
21	BCR	w	101	-	41,41,41	0.84	1 (2%)	56,56,56	2.24	18 (32%)
19	CLA	B	507	-	65,73,73	1.51	7 (10%)	76,113,113	1.26	8 (10%)
23	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	0.89	2 (3%)
19	CLA	c	506	-	65,73,73	1.49	7 (10%)	76,113,113	1.23	7 (9%)
22	LMG	B	519	-	42,42,55	0.99	2 (4%)	50,50,63	1.03	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	LHG	a	409	-	43,43,48	1.00	2 (4%)	46,49,54	0.93	2 (4%)
19	CLA	C	504	-	65,73,73	1.51	7 (10%)	76,113,113	1.22	9 (11%)
19	CLA	C	513	-	65,73,73	1.50	7 (10%)	76,113,113	1.28	7 (9%)
21	BCR	B	517	-	41,41,41	0.76	1 (2%)	56,56,56	2.05	20 (35%)
19	CLA	C	503	-	65,73,73	1.48	9 (13%)	76,113,113	1.29	9 (11%)
19	CLA	C	507	-	65,73,73	1.51	6 (9%)	76,113,113	1.23	7 (9%)
19	CLA	C	510	-	65,73,73	1.49	7 (10%)	76,113,113	1.26	7 (9%)
20	PHO	d	401	-	51,69,69	1.03	5 (9%)	47,99,99	1.10	4 (8%)
19	CLA	C	514	-	65,73,73	1.50	5 (7%)	76,113,113	1.21	7 (9%)
25	DGD	C	518	-	54,54,67	0.93	2 (3%)	68,68,81	0.97	3 (4%)
19	CLA	A	403	-	65,73,73	1.53	8 (12%)	76,113,113	1.29	9 (11%)

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
19	CLA	c	504	-	1/1/15/20	19/37/115/115	-
19	CLA	c	508	-	1/1/15/20	17/37/115/115	-
21	BCR	a	407	-	-	4/29/63/63	0/2/2/2
19	CLA	B	503	-	1/1/15/20	14/37/115/115	-
19	CLA	c	511	-	1/1/15/20	15/37/115/115	-
19	CLA	C	509	-	1/1/15/20	12/37/115/115	-
19	CLA	c	514	-	1/1/15/20	14/37/115/115	-
25	DGD	C	520	-	-	10/48/88/95	0/2/2/2
19	CLA	C	502	-	1/1/15/20	11/37/115/115	-
19	CLA	b	509	-	1/1/15/20	18/37/115/115	-
19	CLA	b	511	-	1/1/15/20	21/37/115/115	-
19	CLA	b	513	-	1/1/15/20	14/37/115/115	-
19	CLA	c	515	-	1/1/15/20	15/37/115/115	-
22	LMG	H	102	-	-	12/43/63/70	0/1/1/1
28	PL9	d	406	-	-	7/53/73/73	0/1/1/1
19	CLA	B	510	-	1/1/15/20	9/37/115/115	-
19	CLA	d	404	-	1/1/15/20	20/37/115/115	-
21	BCR	V	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	514	-	1/1/11/20	7/13/91/115	-
23	LHG	a	408	-	-	11/47/47/53	-
19	CLA	B	516	-	1/1/15/20	10/37/115/115	-
19	CLA	C	505	-	1/1/15/20	12/37/115/115	-
26	LMU	c	523	-	-	8/21/61/61	0/2/2/2
19	CLA	A	402	-	1/1/15/20	8/37/115/115	-
19	CLA	B	512	-	1/1/15/20	12/37/115/115	-
19	CLA	a	402	-	1/1/15/20	10/37/115/115	-
25	DGD	C	519	-	-	7/38/78/95	0/2/2/2
24	SQD	C	501	-	-	9/46/66/69	0/1/1/1
20	PHO	a	405	-	-	12/37/103/103	0/5/6/6
19	CLA	a	404	-	1/1/11/20	9/18/96/115	-
23	LHG	B	521	-	-	10/53/53/53	-
21	BCR	C	516	-	-	5/29/63/63	0/2/2/2
22	LMG	C	521	-	-	5/46/66/70	0/1/1/1
19	CLA	B	506	-	1/1/15/20	8/37/115/115	-
21	BCR	h	101	-	-	5/29/63/63	0/2/2/2
23	LHG	x	101	-	-	11/53/53/53	-
21	BCR	A	407	-	-	4/29/63/63	0/2/2/2
29	HEM	F	102	5,6	-	4/12/54/54	-
25	DGD	c	520	-	-	7/38/78/95	0/2/2/2
19	CLA	C	506	-	1/1/15/20	15/37/115/115	-
23	LHG	D	407	-	-	12/53/53/53	-
19	CLA	c	507	-	1/1/15/20	16/37/115/115	-
19	CLA	b	503	-	1/1/15/20	13/37/115/115	-
19	CLA	b	516	-	1/1/15/20	11/37/115/115	-
19	CLA	a	406	-	1/1/14/20	9/31/109/115	-
21	BCR	b	518	-	-	4/29/63/63	0/2/2/2
19	CLA	b	501	-	1/1/15/20	15/37/115/115	-
24	SQD	c	501	-	-	9/46/66/69	0/1/1/1
23	LHG	b	520	-	-	10/53/53/53	-
21	BCR	B	518	-	-	4/29/63/63	0/2/2/2
21	BCR	b	517	-	-	4/29/63/63	0/2/2/2
19	CLA	b	502	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	D	406	-	-	8/53/73/73	0/1/1/1
26	LMU	C	522	-	-	9/21/61/61	0/2/2/2
19	CLA	B	509	-	1/1/15/20	18/37/115/115	-
19	CLA	b	510	-	1/1/15/20	10/37/115/115	-
19	CLA	C	511	-	1/1/15/20	14/37/115/115	-
19	CLA	B	504	-	1/1/15/20	15/37/115/115	-
19	CLA	B	508	-	1/1/15/20	9/37/115/115	-
19	CLA	B	501	-	1/1/15/20	16/37/115/115	-
19	CLA	b	515	-	1/1/15/20	5/37/115/115	-
19	CLA	a	403	-	1/1/15/20	10/37/115/115	-
23	LHG	B	520	-	-	11/48/48/53	-
25	DGD	c	519	-	-	5/42/82/95	0/2/2/2
19	CLA	C	512	3	1/1/15/20	17/37/115/115	-
19	CLA	B	502	-	1/1/15/20	10/37/115/115	-
19	CLA	c	510	-	1/1/15/20	12/37/115/115	-
19	CLA	B	514	-	1/1/11/20	7/13/91/115	-
21	BCR	d	405	-	-	4/29/63/63	0/2/2/2
19	CLA	d	403	-	1/1/15/20	7/37/115/115	-
29	HEM	e	101	5,6	-	3/12/54/54	-
21	BCR	c	516	-	-	4/29/63/63	0/2/2/2
22	LMG	f	101	-	-	5/41/61/70	0/1/1/1
19	CLA	b	512	-	1/1/15/20	12/37/115/115	-
19	CLA	B	515	-	1/1/15/20	4/37/115/115	-
19	CLA	c	505	-	1/1/15/20	16/37/115/115	-
23	LHG	d	407	-	-	11/48/48/53	-
19	CLA	B	505	-	-	19/37/115/115	-
21	BCR	W	101	-	-	2/29/63/63	0/2/2/2
25	DGD	c	521	-	-	9/48/88/95	0/2/2/2
22	LMG	A	408	-	-	7/41/61/70	0/1/1/1
22	LMG	b	519	-	-	4/37/57/70	0/1/1/1
21	BCR	C	515	-	-	4/29/63/63	0/2/2/2
19	CLA	b	506	-	1/1/15/20	11/37/115/115	-
20	PHO	A	405	-	-	12/37/103/103	0/5/6/6
21	BCR	D	405	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	D	404	-	1/1/15/20	20/37/115/115	-
19	CLA	c	503	-	1/1/15/20	12/37/115/115	-
21	BCR	C	517	-	-	4/29/63/63	0/2/2/2
22	LMG	c	502	-	-	7/41/61/70	0/1/1/1
21	BCR	H	101	-	-	5/29/63/63	0/2/2/2
21	BCR	c	517	-	-	5/29/63/63	0/2/2/2
19	CLA	A	404	-	1/1/11/20	7/18/96/115	-
22	LMG	c	522	-	-	4/46/66/70	0/1/1/1
19	CLA	c	509	-	1/1/15/20	7/37/115/115	-
19	CLA	c	513	3	1/1/15/20	11/37/115/115	-
21	BCR	c	518	-	-	4/29/63/63	0/2/2/2
19	CLA	C	508	-	1/1/15/20	7/37/115/115	-
19	CLA	B	513	-	1/1/15/20	14/37/115/115	-
19	CLA	b	505	-	1/1/15/20	19/37/115/115	-
21	BCR	k	101	-	-	2/29/63/63	0/2/2/2
20	PHO	D	401	-	-	9/37/103/103	0/5/6/6
19	CLA	b	504	-	1/1/15/20	15/37/115/115	-
19	CLA	b	507	-	1/1/15/20	15/37/115/115	-
19	CLA	b	508	-	1/1/15/20	8/37/115/115	-
23	LHG	d	408	-	-	9/53/53/53	-
23	LHG	A	409	-	-	6/47/47/53	-
22	LMG	F	101	-	-	5/41/61/70	0/1/1/1
19	CLA	D	403	-	1/1/15/20	8/37/115/115	-
22	LMG	h	102	-	-	10/43/63/70	0/1/1/1
19	CLA	B	511	-	1/1/15/20	21/37/115/115	-
19	CLA	c	512	-	1/1/15/20	14/37/115/115	-
23	LHG	L	101	-	-	9/53/53/53	-
23	LHG	X	101	-	-	9/53/53/53	-
19	CLA	A	406	-	1/1/14/20	9/31/109/115	-
23	LHG	A	410	-	-	13/48/48/53	-
21	BCR	w	101	-	-	10/29/63/63	0/2/2/2
19	CLA	B	507	-	1/1/15/20	14/37/115/115	-
23	LHG	l	101	-	-	8/53/53/53	-
19	CLA	c	506	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMG	B	519	-	-	4/37/57/70	0/1/1/1
23	LHG	a	409	-	-	14/48/48/53	-
19	CLA	C	504	-	1/1/15/20	18/37/115/115	-
19	CLA	C	513	-	1/1/15/20	14/37/115/115	-
21	BCR	B	517	-	-	4/29/63/63	0/2/2/2
19	CLA	C	503	-	1/1/15/20	18/37/115/115	-
19	CLA	C	507	-	1/1/15/20	16/37/115/115	-
19	CLA	C	510	-	1/1/15/20	15/37/115/115	-
20	PHO	d	401	-	-	9/37/103/103	0/5/6/6
19	CLA	C	514	-	1/1/15/20	14/37/115/115	-
25	DGD	C	518	-	-	3/42/82/95	0/2/2/2
19	CLA	A	403	-	1/1/15/20	13/37/115/115	-

All (626) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	403	CLA	C4B-NB	7.68	1.42	1.35
19	B	501	CLA	C4B-NB	7.68	1.42	1.35
19	A	403	CLA	C4B-NB	7.66	1.42	1.35
19	b	501	CLA	C4B-NB	7.66	1.42	1.35
19	C	512	CLA	C4B-NB	7.65	1.42	1.35
19	c	508	CLA	C4B-NB	7.64	1.42	1.35
19	b	507	CLA	C4B-NB	7.63	1.42	1.35
19	b	515	CLA	C4B-NB	7.59	1.42	1.35
19	B	505	CLA	C4B-NB	7.59	1.42	1.35
19	B	511	CLA	C4B-NB	7.58	1.42	1.35
19	B	507	CLA	C4B-NB	7.57	1.42	1.35
19	B	515	CLA	C4B-NB	7.56	1.42	1.35
19	b	511	CLA	C4B-NB	7.55	1.41	1.35
19	C	514	CLA	C4B-NB	7.55	1.41	1.35
19	C	507	CLA	C4B-NB	7.53	1.41	1.35
19	C	505	CLA	C4B-NB	7.52	1.41	1.35
19	c	513	CLA	C4B-NB	7.52	1.41	1.35
19	c	515	CLA	C4B-NB	7.51	1.41	1.35
19	B	509	CLA	C4B-NB	7.51	1.41	1.35
19	C	511	CLA	C4B-NB	7.50	1.41	1.35
19	b	509	CLA	C4B-NB	7.50	1.41	1.35
19	C	504	CLA	C4B-NB	7.49	1.41	1.35
19	C	513	CLA	C4B-NB	7.49	1.41	1.35
19	c	505	CLA	C4B-NB	7.48	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	514	CLA	C4B-NB	7.47	1.41	1.35
19	d	404	CLA	C4B-NB	7.47	1.41	1.35
19	D	404	CLA	C4B-NB	7.47	1.41	1.35
19	B	502	CLA	C4B-NB	7.46	1.41	1.35
19	b	506	CLA	C4B-NB	7.46	1.41	1.35
19	c	503	CLA	C4B-NB	7.46	1.41	1.35
19	b	503	CLA	C4B-NB	7.46	1.41	1.35
19	C	502	CLA	C4B-NB	7.45	1.41	1.35
19	c	510	CLA	C4B-NB	7.45	1.41	1.35
19	B	513	CLA	C4B-NB	7.44	1.41	1.35
19	C	509	CLA	C4B-NB	7.44	1.41	1.35
19	b	513	CLA	C4B-NB	7.44	1.41	1.35
19	c	512	CLA	C4B-NB	7.44	1.41	1.35
19	d	403	CLA	C4B-NB	7.44	1.41	1.35
19	B	504	CLA	C4B-NB	7.43	1.41	1.35
19	B	506	CLA	C4B-NB	7.43	1.41	1.35
19	b	504	CLA	C4B-NB	7.43	1.41	1.35
19	A	404	CLA	C4B-NB	7.43	1.41	1.35
19	C	506	CLA	C4B-NB	7.42	1.41	1.35
19	c	507	CLA	C4B-NB	7.42	1.41	1.35
19	b	508	CLA	C4B-NB	7.42	1.41	1.35
19	B	503	CLA	C4B-NB	7.41	1.41	1.35
19	C	510	CLA	C4B-NB	7.41	1.41	1.35
19	A	406	CLA	C4B-NB	7.40	1.41	1.35
19	b	505	CLA	C4B-NB	7.39	1.41	1.35
19	A	402	CLA	C4B-NB	7.39	1.41	1.35
19	b	502	CLA	C4B-NB	7.39	1.41	1.35
19	c	511	CLA	C4B-NB	7.39	1.41	1.35
19	B	508	CLA	C4B-NB	7.39	1.41	1.35
19	a	404	CLA	C4B-NB	7.37	1.41	1.35
19	B	516	CLA	C4B-NB	7.35	1.41	1.35
19	c	506	CLA	C4B-NB	7.33	1.41	1.35
19	B	514	CLA	C4B-NB	7.31	1.41	1.35
19	c	509	CLA	C4B-NB	7.31	1.41	1.35
19	B	512	CLA	C4B-NB	7.30	1.41	1.35
19	a	406	CLA	C4B-NB	7.30	1.41	1.35
19	C	503	CLA	C4B-NB	7.27	1.41	1.35
19	c	504	CLA	C4B-NB	7.26	1.41	1.35
19	D	403	CLA	C4B-NB	7.25	1.41	1.35
19	b	514	CLA	C4B-NB	7.24	1.41	1.35
19	C	508	CLA	C4B-NB	7.24	1.41	1.35
19	B	510	CLA	C4B-NB	7.21	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	402	CLA	C4B-NB	7.19	1.41	1.35
19	b	510	CLA	C4B-NB	7.18	1.41	1.35
19	b	512	CLA	C4B-NB	7.13	1.41	1.35
19	b	516	CLA	C4B-NB	7.02	1.41	1.35
24	c	501	SQD	O8-S	4.61	1.63	1.47
24	C	501	SQD	O8-S	4.60	1.63	1.47
28	D	406	PL9	C7-C3	-4.50	1.46	1.51
28	d	406	PL9	C7-C3	-4.37	1.46	1.51
22	C	521	LMG	O8-C28	4.28	1.45	1.33
23	A	410	LHG	O8-C23	4.28	1.45	1.33
23	a	409	LHG	O8-C23	4.28	1.45	1.33
25	c	520	DGD	O1G-C1A	4.27	1.45	1.33
29	F	102	HEM	C3C-C2C	-4.27	1.34	1.40
24	C	501	SQD	O48-C23	4.27	1.45	1.33
22	c	522	LMG	O8-C28	4.27	1.45	1.33
24	c	501	SQD	O48-C23	4.27	1.45	1.33
22	h	102	LMG	O8-C28	4.27	1.45	1.33
25	C	519	DGD	O1G-C1A	4.27	1.45	1.33
29	e	101	HEM	C3C-C2C	-4.26	1.34	1.40
23	x	101	LHG	O8-C23	4.25	1.45	1.33
22	H	102	LMG	O8-C28	4.22	1.45	1.33
28	D	406	PL9	C3-C4	-4.22	1.42	1.49
22	A	408	LMG	O8-C28	4.22	1.45	1.33
23	X	101	LHG	O8-C23	4.21	1.45	1.33
23	d	407	LHG	O8-C23	4.20	1.45	1.33
22	F	101	LMG	O8-C28	4.20	1.45	1.33
25	c	519	DGD	O1G-C1A	4.20	1.45	1.33
22	c	502	LMG	O8-C28	4.20	1.45	1.33
25	C	518	DGD	O1G-C1A	4.19	1.45	1.33
23	a	408	LHG	O8-C23	4.19	1.45	1.33
23	B	520	LHG	O8-C23	4.18	1.45	1.33
22	f	101	LMG	O8-C28	4.17	1.45	1.33
23	l	101	LHG	O8-C23	4.17	1.45	1.33
23	A	409	LHG	O8-C23	4.17	1.45	1.33
23	A	410	LHG	O7-C7	4.17	1.46	1.34
23	L	101	LHG	O8-C23	4.17	1.45	1.33
25	c	521	DGD	O1G-C1A	4.16	1.45	1.33
22	h	102	LMG	O7-C10	4.15	1.46	1.34
25	C	520	DGD	O1G-C1A	4.15	1.45	1.33
23	a	409	LHG	O7-C7	4.15	1.46	1.34
28	d	406	PL9	C3-C4	-4.15	1.42	1.49
23	b	520	LHG	O7-C7	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	520	LHG	O7-C7	4.14	1.46	1.34
22	f	101	LMG	O7-C10	4.14	1.46	1.34
22	b	519	LMG	O8-C28	4.13	1.45	1.33
22	F	101	LMG	O7-C10	4.13	1.45	1.34
23	d	407	LHG	O7-C7	4.12	1.45	1.34
22	c	522	LMG	O7-C10	4.12	1.45	1.34
22	A	408	LMG	O7-C10	4.12	1.45	1.34
22	c	502	LMG	O7-C10	4.12	1.45	1.34
22	B	519	LMG	O8-C28	4.11	1.45	1.33
25	C	518	DGD	O2G-C1B	4.11	1.45	1.34
23	B	521	LHG	O7-C7	4.11	1.45	1.34
22	C	521	LMG	O7-C10	4.10	1.45	1.34
25	c	521	DGD	O2G-C1B	4.10	1.45	1.34
23	x	101	LHG	O7-C7	4.10	1.45	1.34
25	c	519	DGD	O2G-C1B	4.10	1.45	1.34
23	b	520	LHG	O8-C23	4.09	1.45	1.33
23	B	521	LHG	O8-C23	4.09	1.45	1.33
23	D	407	LHG	O7-C7	4.08	1.45	1.34
25	C	520	DGD	O2G-C1B	4.08	1.45	1.34
22	H	102	LMG	O7-C10	4.08	1.45	1.34
23	X	101	LHG	O7-C7	4.08	1.45	1.34
23	d	408	LHG	O8-C23	4.08	1.45	1.33
23	D	407	LHG	O8-C23	4.07	1.45	1.33
23	d	408	LHG	O7-C7	4.07	1.45	1.34
24	c	501	SQD	O47-C7	4.03	1.45	1.34
24	C	501	SQD	O47-C7	4.02	1.45	1.34
25	C	519	DGD	O2G-C1B	4.01	1.45	1.34
25	c	520	DGD	O2G-C1B	4.01	1.45	1.34
23	A	409	LHG	O7-C7	4.00	1.45	1.34
23	a	408	LHG	O7-C7	4.00	1.45	1.34
23	l	101	LHG	O7-C7	3.98	1.45	1.34
23	L	101	LHG	O7-C7	3.95	1.45	1.34
22	B	519	LMG	O7-C10	3.93	1.45	1.34
22	b	519	LMG	O7-C10	3.92	1.45	1.34
19	B	501	CLA	C1D-ND	3.83	1.42	1.37
19	C	512	CLA	C1D-ND	3.82	1.42	1.37
19	c	513	CLA	C1D-ND	3.80	1.42	1.37
19	b	515	CLA	C1D-ND	3.77	1.42	1.37
19	b	516	CLA	C1D-ND	3.77	1.42	1.37
19	B	505	CLA	C1D-ND	3.76	1.42	1.37
19	C	504	CLA	C1D-ND	3.76	1.42	1.37
19	D	404	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	506	CLA	C1D-ND	3.75	1.42	1.37
19	b	501	CLA	C1D-ND	3.74	1.42	1.37
19	c	515	CLA	C1D-ND	3.73	1.42	1.37
19	C	514	CLA	C1D-ND	3.73	1.42	1.37
19	C	505	CLA	C1D-ND	3.73	1.42	1.37
19	C	507	CLA	C1D-ND	3.72	1.42	1.37
19	B	509	CLA	C1D-ND	3.72	1.42	1.37
19	c	511	CLA	C1D-ND	3.72	1.42	1.37
19	c	505	CLA	C1D-ND	3.72	1.42	1.37
19	c	512	CLA	C1D-ND	3.72	1.42	1.37
19	B	507	CLA	C1D-ND	3.71	1.42	1.37
19	B	516	CLA	C1D-ND	3.71	1.42	1.37
19	b	507	CLA	C1D-ND	3.70	1.42	1.37
19	b	514	CLA	C1D-ND	3.70	1.42	1.37
19	A	406	CLA	C1D-ND	3.69	1.42	1.37
19	C	511	CLA	C1D-ND	3.68	1.42	1.37
19	c	508	CLA	C1D-ND	3.68	1.42	1.37
19	b	511	CLA	C1D-ND	3.68	1.42	1.37
19	b	509	CLA	C1D-ND	3.67	1.42	1.37
19	C	510	CLA	C1D-ND	3.67	1.42	1.37
19	B	515	CLA	C1D-ND	3.66	1.42	1.37
19	b	502	CLA	C1D-ND	3.66	1.42	1.37
19	b	513	CLA	C1D-ND	3.65	1.42	1.37
19	d	404	CLA	C1D-ND	3.65	1.42	1.37
19	B	503	CLA	C1D-ND	3.65	1.42	1.37
19	c	503	CLA	C1D-ND	3.65	1.42	1.37
19	B	502	CLA	C1D-ND	3.64	1.42	1.37
19	A	404	CLA	C1D-ND	3.64	1.42	1.37
19	c	504	CLA	C1D-ND	3.63	1.42	1.37
19	B	506	CLA	C1D-ND	3.63	1.42	1.37
19	a	404	CLA	C1D-ND	3.63	1.42	1.37
19	b	505	CLA	C1D-ND	3.62	1.42	1.37
19	C	502	CLA	C1D-ND	3.62	1.42	1.37
19	C	509	CLA	C1D-ND	3.62	1.42	1.37
19	B	513	CLA	C1D-ND	3.62	1.42	1.37
19	B	514	CLA	C1D-ND	3.62	1.42	1.37
19	a	406	CLA	C1D-ND	3.61	1.42	1.37
19	c	510	CLA	C1D-ND	3.61	1.42	1.37
19	a	402	CLA	C1D-ND	3.60	1.42	1.37
19	b	504	CLA	C1D-ND	3.60	1.42	1.37
19	B	511	CLA	C1D-ND	3.59	1.42	1.37
19	b	506	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	402	CLA	C1D-ND	3.59	1.42	1.37
29	F	102	HEM	C3C-CAC	3.59	1.55	1.47
29	e	101	HEM	C3C-CAC	3.58	1.55	1.47
19	B	504	CLA	C1D-ND	3.58	1.42	1.37
19	C	508	CLA	C1D-ND	3.57	1.42	1.37
19	b	510	CLA	C1D-ND	3.56	1.42	1.37
19	B	508	CLA	C1D-ND	3.55	1.42	1.37
19	B	512	CLA	C1D-ND	3.55	1.42	1.37
19	C	503	CLA	C1D-ND	3.55	1.42	1.37
19	c	509	CLA	C1D-ND	3.55	1.42	1.37
19	A	403	CLA	C1D-ND	3.54	1.42	1.37
19	C	513	CLA	C1D-ND	3.54	1.42	1.37
19	b	508	CLA	C1D-ND	3.54	1.42	1.37
19	D	403	CLA	C1D-ND	3.54	1.42	1.37
19	a	403	CLA	C1D-ND	3.54	1.42	1.37
19	C	506	CLA	C1D-ND	3.53	1.42	1.37
19	b	503	CLA	C1D-ND	3.53	1.42	1.37
19	d	403	CLA	C1D-ND	3.52	1.42	1.37
19	c	514	CLA	C1D-ND	3.51	1.42	1.37
19	c	507	CLA	C1D-ND	3.51	1.42	1.37
19	B	510	CLA	C1D-ND	3.50	1.42	1.37
26	c	523	LMU	O5B-C1B	3.50	1.50	1.41
26	C	522	LMU	O5B-C1B	3.48	1.50	1.41
19	b	512	CLA	C1D-ND	3.46	1.42	1.37
19	A	404	CLA	C4D-ND	-3.35	1.33	1.37
26	C	522	LMU	O5'-C1'	3.34	1.50	1.41
19	a	403	CLA	C4D-ND	-3.34	1.33	1.37
19	A	403	CLA	C4D-ND	-3.33	1.33	1.37
19	B	505	CLA	C4D-ND	-3.31	1.33	1.37
26	c	523	LMU	O5'-C1'	3.30	1.50	1.41
19	a	404	CLA	C4D-ND	-3.25	1.33	1.37
19	b	505	CLA	C4D-ND	-3.22	1.33	1.37
28	d	406	PL9	C6-C1	-3.21	1.42	1.48
19	b	507	CLA	C4D-ND	-3.18	1.33	1.37
19	a	406	CLA	C4D-ND	-3.18	1.33	1.37
19	A	406	CLA	C4D-ND	-3.18	1.33	1.37
19	B	502	CLA	C4D-ND	-3.18	1.33	1.37
19	c	513	CLA	C4D-ND	-3.17	1.33	1.37
28	D	406	PL9	C6-C1	-3.17	1.42	1.48
19	B	504	CLA	C4D-ND	-3.16	1.33	1.37
19	B	507	CLA	C4D-ND	-3.16	1.33	1.37
19	c	503	CLA	C4D-ND	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	512	CLA	C4D-ND	-3.15	1.33	1.37
19	C	504	CLA	C4D-ND	-3.15	1.33	1.37
19	B	509	CLA	C4D-ND	-3.15	1.33	1.37
19	B	510	CLA	C4D-ND	-3.15	1.33	1.37
19	B	506	CLA	C4D-ND	-3.14	1.33	1.37
19	b	508	CLA	C4D-ND	-3.14	1.33	1.37
19	c	505	CLA	C4D-ND	-3.13	1.33	1.37
19	C	509	CLA	C4D-ND	-3.13	1.33	1.37
19	c	506	CLA	C4D-ND	-3.13	1.33	1.37
19	B	508	CLA	C4D-ND	-3.13	1.33	1.37
19	b	516	CLA	C4D-ND	-3.12	1.33	1.37
19	c	512	CLA	C4D-ND	-3.11	1.33	1.37
19	c	515	CLA	C4D-ND	-3.11	1.33	1.37
19	b	509	CLA	C4D-ND	-3.11	1.33	1.37
19	b	510	CLA	C4D-ND	-3.11	1.33	1.37
19	b	511	CLA	C4D-ND	-3.11	1.33	1.37
19	C	505	CLA	C4D-ND	-3.10	1.33	1.37
19	D	404	CLA	C4D-ND	-3.10	1.33	1.37
19	c	504	CLA	C4D-ND	-3.09	1.33	1.37
19	B	512	CLA	C4D-ND	-3.09	1.33	1.37
19	b	506	CLA	C4D-ND	-3.09	1.33	1.37
19	C	503	CLA	C4D-ND	-3.09	1.33	1.37
19	C	508	CLA	C4D-ND	-3.09	1.33	1.37
19	d	403	CLA	C4D-ND	-3.08	1.33	1.37
19	C	502	CLA	C4D-ND	-3.08	1.33	1.37
19	b	504	CLA	C4D-ND	-3.08	1.33	1.37
19	D	403	CLA	C4D-ND	-3.08	1.33	1.37
19	d	404	CLA	C4D-ND	-3.08	1.33	1.37
19	B	503	CLA	C4D-ND	-3.07	1.33	1.37
19	c	510	CLA	C4D-ND	-3.07	1.33	1.37
19	b	502	CLA	C4D-ND	-3.06	1.33	1.37
19	b	503	CLA	C4D-ND	-3.06	1.33	1.37
19	A	402	CLA	C4D-ND	-3.05	1.33	1.37
19	B	511	CLA	C4D-ND	-3.05	1.33	1.37
19	C	514	CLA	C4D-ND	-3.05	1.33	1.37
19	C	511	CLA	C4D-ND	-3.04	1.33	1.37
19	C	513	CLA	C4D-ND	-3.04	1.33	1.37
19	b	512	CLA	C4D-ND	-3.03	1.33	1.37
19	C	507	CLA	CHC-C1C	3.03	1.42	1.35
19	b	501	CLA	C4D-ND	-3.02	1.33	1.37
19	c	509	CLA	C4D-ND	-3.02	1.33	1.37
19	c	508	CLA	CHC-C1C	3.02	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	507	CLA	C4D-ND	-3.02	1.33	1.37
19	B	516	CLA	C4D-ND	-3.02	1.33	1.37
19	c	508	CLA	C4D-ND	-3.02	1.33	1.37
19	B	501	CLA	C4D-ND	-3.01	1.33	1.37
19	B	516	CLA	CHC-C1C	3.01	1.42	1.35
19	a	402	CLA	C4D-ND	-3.00	1.33	1.37
19	b	513	CLA	CHC-C1C	3.00	1.42	1.35
19	b	515	CLA	C4D-ND	-3.00	1.33	1.37
19	C	512	CLA	CHC-C1C	2.99	1.42	1.35
19	b	502	CLA	CHC-C1C	2.99	1.42	1.35
19	B	514	CLA	CHC-C1C	2.99	1.42	1.35
19	b	514	CLA	CHC-C1C	2.99	1.42	1.35
19	b	514	CLA	C4D-ND	-2.99	1.33	1.37
19	b	507	CLA	CHC-C1C	2.98	1.42	1.35
19	C	504	CLA	CHC-C1C	2.98	1.42	1.35
19	C	514	CLA	CHC-C1C	2.98	1.42	1.35
19	B	508	CLA	CHC-C1C	2.97	1.42	1.35
19	c	507	CLA	C4D-ND	-2.97	1.33	1.37
19	c	506	CLA	CHC-C1C	2.97	1.42	1.35
19	b	508	CLA	CHC-C1C	2.97	1.42	1.35
19	c	505	CLA	CHC-C1C	2.97	1.42	1.35
19	B	514	CLA	C4D-ND	-2.97	1.33	1.37
19	A	403	CLA	CHC-C1C	2.96	1.42	1.35
19	B	513	CLA	C4D-ND	-2.96	1.33	1.37
19	c	515	CLA	CHC-C1C	2.96	1.42	1.35
19	b	513	CLA	C4D-ND	-2.95	1.33	1.37
19	C	505	CLA	CHC-C1C	2.94	1.42	1.35
19	b	503	CLA	CHC-C1C	2.94	1.42	1.35
19	B	513	CLA	CHC-C1C	2.94	1.42	1.35
19	B	507	CLA	CHC-C1C	2.94	1.42	1.35
19	B	506	CLA	CHC-C1C	2.93	1.42	1.35
19	d	404	CLA	CHC-C1C	2.93	1.42	1.35
19	a	403	CLA	CHC-C1C	2.93	1.42	1.35
19	B	503	CLA	CHC-C1C	2.93	1.42	1.35
19	b	506	CLA	CHC-C1C	2.93	1.42	1.35
19	B	515	CLA	C4D-ND	-2.93	1.33	1.37
19	c	504	CLA	CHC-C1C	2.93	1.42	1.35
19	b	510	CLA	CHC-C1C	2.92	1.42	1.35
19	c	512	CLA	CHC-C1C	2.92	1.42	1.35
19	c	513	CLA	CHC-C1C	2.92	1.42	1.35
19	c	509	CLA	CHC-C1C	2.92	1.42	1.35
19	C	502	CLA	CHC-C1C	2.92	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	508	CLA	CHC-C1C	2.92	1.42	1.35
19	C	506	CLA	CHC-C1C	2.91	1.42	1.35
19	C	509	CLA	CHC-C1C	2.91	1.42	1.35
19	c	514	CLA	C4D-ND	-2.91	1.33	1.37
19	C	510	CLA	C4D-ND	-2.91	1.33	1.37
19	d	403	CLA	CHC-C1C	2.91	1.42	1.35
19	c	503	CLA	CHC-C1C	2.90	1.42	1.35
19	b	512	CLA	CHC-C1C	2.90	1.42	1.35
19	a	402	CLA	CHC-C1C	2.90	1.42	1.35
19	B	502	CLA	CHC-C1C	2.90	1.42	1.35
19	C	511	CLA	CHC-C1C	2.90	1.42	1.35
19	c	511	CLA	C4D-ND	-2.89	1.33	1.37
19	B	510	CLA	CHC-C1C	2.89	1.42	1.35
19	c	510	CLA	CHC-C1C	2.89	1.42	1.35
19	C	506	CLA	C4D-ND	-2.89	1.33	1.37
24	C	501	SQD	C6-S	-2.89	1.66	1.77
19	D	403	CLA	CHC-C1C	2.89	1.42	1.35
19	B	512	CLA	CHC-C1C	2.89	1.42	1.35
19	A	402	CLA	CHC-C1C	2.88	1.42	1.35
19	C	510	CLA	CHC-C1C	2.88	1.42	1.35
19	c	507	CLA	CHC-C1C	2.88	1.42	1.35
29	e	101	HEM	CAB-C3B	2.88	1.55	1.47
19	b	509	CLA	CHC-C1C	2.88	1.42	1.35
19	B	511	CLA	CHC-C1C	2.88	1.42	1.35
19	A	404	CLA	CHC-C1C	2.88	1.42	1.35
19	c	511	CLA	CHC-C1C	2.87	1.42	1.35
19	C	503	CLA	CHC-C1C	2.87	1.42	1.35
19	a	406	CLA	CHC-C1C	2.87	1.42	1.35
19	a	404	CLA	CHC-C1C	2.86	1.42	1.35
24	c	501	SQD	C6-S	-2.86	1.66	1.77
19	c	514	CLA	CHC-C1C	2.86	1.42	1.35
19	b	516	CLA	CHC-C1C	2.86	1.42	1.35
19	B	509	CLA	CHC-C1C	2.85	1.42	1.35
19	b	511	CLA	CHC-C1C	2.85	1.42	1.35
20	a	405	PHO	CAC-C3C	-2.85	1.47	1.52
19	C	513	CLA	CHC-C1C	2.85	1.42	1.35
19	b	501	CLA	CHC-C1C	2.84	1.42	1.35
19	B	501	CLA	CHC-C1C	2.83	1.42	1.35
29	F	102	HEM	CAB-C3B	2.83	1.55	1.47
19	A	406	CLA	CHC-C1C	2.83	1.42	1.35
19	b	515	CLA	CHC-C1C	2.82	1.42	1.35
19	b	505	CLA	CHC-C1C	2.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	515	CLA	CHC-C1C	2.81	1.42	1.35
19	B	505	CLA	CHC-C1C	2.81	1.42	1.35
19	D	404	CLA	CHC-C1C	2.81	1.42	1.35
20	A	405	PHO	CAC-C3C	-2.80	1.47	1.52
19	a	403	CLA	CMB-C2B	-2.76	1.45	1.51
19	B	504	CLA	CHC-C1C	2.75	1.42	1.35
19	b	504	CLA	CHC-C1C	2.75	1.42	1.35
19	b	512	CLA	CMB-C2B	-2.72	1.46	1.51
19	A	403	CLA	CMB-C2B	-2.72	1.46	1.51
19	B	512	CLA	CMB-C2B	-2.69	1.46	1.51
20	d	401	PHO	CAC-C3C	-2.66	1.47	1.52
19	a	404	CLA	CMB-C2B	-2.66	1.46	1.51
20	D	401	PHO	CAC-C3C	-2.65	1.47	1.52
19	A	404	CLA	CMB-C2B	-2.64	1.46	1.51
19	b	511	CLA	CMB-C2B	-2.63	1.46	1.51
19	B	508	CLA	CMB-C2B	-2.59	1.46	1.51
19	B	511	CLA	CMB-C2B	-2.59	1.46	1.51
19	b	508	CLA	CMB-C2B	-2.58	1.46	1.51
19	b	503	CLA	CMB-C2B	-2.56	1.46	1.51
19	C	509	CLA	CMB-C2B	-2.56	1.46	1.51
19	B	503	CLA	CMB-C2B	-2.56	1.46	1.51
19	D	403	CLA	CMB-C2B	-2.55	1.46	1.51
19	C	507	CLA	CMB-C2B	-2.55	1.46	1.51
19	c	513	CLA	CMB-C2B	-2.55	1.46	1.51
19	c	507	CLA	CMB-C2B	-2.54	1.46	1.51
19	b	507	CLA	CMB-C2B	-2.54	1.46	1.51
19	C	511	CLA	CMB-C2B	-2.53	1.46	1.51
19	d	403	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	514	CLA	CMB-C2B	-2.53	1.46	1.51
19	c	508	CLA	CMB-C2B	-2.52	1.46	1.51
19	C	505	CLA	CMB-C2B	-2.52	1.46	1.51
19	B	516	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	505	CLA	CMB-C2B	-2.52	1.46	1.51
19	c	510	CLA	CMB-C2B	-2.52	1.46	1.51
19	B	506	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	504	CLA	CMB-C2B	-2.51	1.46	1.51
19	B	507	CLA	CMB-C2B	-2.51	1.46	1.51
19	B	505	CLA	CMB-C2B	-2.51	1.46	1.51
19	B	504	CLA	CMB-C2B	-2.51	1.46	1.51
19	A	402	CLA	CMB-C2B	-2.51	1.46	1.51
19	b	510	CLA	CMB-C2B	-2.51	1.46	1.51
19	c	512	CLA	CMB-C2B	-2.50	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	402	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	506	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	501	CLA	CMB-C2B	-2.50	1.46	1.51
19	c	511	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	406	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	509	CLA	CMB-C2B	-2.49	1.46	1.51
19	C	503	CLA	CMB-C2B	-2.49	1.46	1.51
19	c	506	CLA	CMB-C2B	-2.49	1.46	1.51
19	c	503	CLA	CMB-C2B	-2.49	1.46	1.51
19	C	502	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	510	CLA	CMB-C2B	-2.49	1.46	1.51
19	C	506	CLA	CMB-C2B	-2.49	1.46	1.51
19	C	510	CLA	CMB-C2B	-2.49	1.46	1.51
19	b	516	CLA	CMB-C2B	-2.49	1.46	1.51
19	c	514	CLA	CMB-C2B	-2.48	1.46	1.51
19	c	504	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	514	CLA	CMB-C2B	-2.48	1.46	1.51
19	C	513	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	509	CLA	CMB-C2B	-2.48	1.46	1.51
21	w	101	BCR	C30-C25	-2.47	1.50	1.53
19	d	404	CLA	CMB-C2B	-2.47	1.46	1.51
19	B	502	CLA	CMB-C2B	-2.47	1.46	1.51
19	B	513	CLA	CMB-C2B	-2.46	1.46	1.51
19	b	513	CLA	CMB-C2B	-2.46	1.46	1.51
19	C	512	CLA	CMB-C2B	-2.46	1.46	1.51
19	c	505	CLA	CMB-C2B	-2.45	1.46	1.51
19	A	406	CLA	CMB-C2B	-2.45	1.46	1.51
19	C	504	CLA	CMB-C2B	-2.44	1.46	1.51
19	B	501	CLA	CMB-C2B	-2.44	1.46	1.51
19	D	404	CLA	CMB-C2B	-2.43	1.46	1.51
19	b	502	CLA	CMB-C2B	-2.43	1.46	1.51
19	A	403	CLA	C3B-C2B	-2.42	1.37	1.40
19	c	509	CLA	CMB-C2B	-2.42	1.46	1.51
28	d	406	PL9	C53-C6	-2.42	1.45	1.50
19	C	508	CLA	CMB-C2B	-2.41	1.46	1.51
19	b	515	CLA	CMB-C2B	-2.41	1.46	1.51
19	c	515	CLA	CMB-C2B	-2.41	1.46	1.51
19	B	515	CLA	CMB-C2B	-2.41	1.46	1.51
28	D	406	PL9	C53-C6	-2.39	1.45	1.50
21	W	101	BCR	C30-C25	-2.38	1.50	1.53
19	D	403	CLA	CMD-C2D	-2.38	1.45	1.50
19	C	514	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	403	CLA	C3B-C2B	-2.37	1.37	1.40
19	B	505	CLA	C3B-C2B	-2.36	1.37	1.40
19	d	403	CLA	CMD-C2D	-2.34	1.45	1.50
19	c	503	CLA	C3B-C2B	-2.34	1.37	1.40
19	C	502	CLA	C3B-C2B	-2.34	1.37	1.40
28	D	406	PL9	C52-C5	-2.31	1.45	1.50
28	d	406	PL9	C52-C5	-2.30	1.45	1.50
19	c	512	CLA	C3B-C2B	-2.28	1.37	1.40
19	B	503	CLA	C3B-C2B	-2.27	1.37	1.40
19	B	512	CLA	C3B-C2B	-2.25	1.37	1.40
19	c	514	CLA	CMD-C2D	-2.24	1.46	1.50
19	C	513	CLA	CMD-C2D	-2.23	1.46	1.50
20	d	401	PHO	C3B-C2B	-2.23	1.37	1.40
19	c	507	CLA	CMD-C2D	-2.23	1.46	1.50
19	b	505	CLA	C3B-C2B	-2.22	1.37	1.40
20	A	405	PHO	CMC-C2C	-2.22	1.46	1.51
19	C	506	CLA	CMD-C2D	-2.22	1.46	1.50
19	A	402	CLA	CMD-C2D	-2.22	1.46	1.50
19	b	509	CLA	C3B-C2B	-2.21	1.37	1.40
21	B	517	BCR	C30-C25	-2.21	1.50	1.53
19	a	402	CLA	CMD-C2D	-2.21	1.46	1.50
19	b	503	CLA	C3B-C2B	-2.21	1.37	1.40
19	C	511	CLA	C3B-C2B	-2.21	1.37	1.40
19	C	503	CLA	C3B-C2B	-2.21	1.37	1.40
19	b	515	CLA	C3B-C2B	-2.20	1.37	1.40
19	B	509	CLA	C3B-C2B	-2.20	1.37	1.40
19	a	404	CLA	C3B-C2B	-2.19	1.37	1.40
19	b	513	CLA	CMD-C2D	-2.19	1.46	1.50
20	a	405	PHO	CMC-C2C	-2.19	1.46	1.51
19	B	503	CLA	CMD-C2D	-2.18	1.46	1.50
19	A	404	CLA	CMD-C2D	-2.18	1.46	1.50
21	c	516	BCR	C30-C25	-2.18	1.50	1.53
20	D	401	PHO	C3B-C2B	-2.18	1.37	1.40
19	b	511	CLA	C3B-C2B	-2.18	1.37	1.40
19	B	508	CLA	CMD-C2D	-2.17	1.46	1.50
19	b	512	CLA	CMD-C2D	-2.17	1.46	1.50
20	A	405	PHO	C3B-C2B	-2.17	1.37	1.40
19	C	502	CLA	CMD-C2D	-2.17	1.46	1.50
19	C	503	CLA	CMD-C2D	-2.17	1.46	1.50
19	b	505	CLA	CMC-C2C	-2.17	1.46	1.50
19	c	509	CLA	CMD-C2D	-2.17	1.46	1.50
19	c	514	CLA	C3B-C2B	-2.17	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	508	CLA	CMD-C2D	-2.17	1.46	1.50
19	B	511	CLA	C3B-C2B	-2.17	1.37	1.40
19	C	513	CLA	C3B-C2B	-2.17	1.37	1.40
19	b	508	CLA	CMD-C2D	-2.16	1.46	1.50
19	a	403	CLA	CMD-C2D	-2.16	1.46	1.50
19	A	403	CLA	CMD-C2D	-2.16	1.46	1.50
19	B	516	CLA	C3B-C2B	-2.15	1.37	1.40
19	a	404	CLA	CMD-C2D	-2.15	1.46	1.50
20	d	401	PHO	CMD-C2D	-2.15	1.46	1.51
20	D	401	PHO	CMC-C2C	-2.15	1.46	1.51
19	B	506	CLA	CMD-C2D	-2.15	1.46	1.50
19	b	507	CLA	CMD-C2D	-2.15	1.46	1.50
19	B	513	CLA	CMD-C2D	-2.15	1.46	1.50
19	C	506	CLA	C3B-C2B	-2.14	1.37	1.40
21	b	517	BCR	C30-C25	-2.14	1.50	1.53
19	b	513	CLA	C3B-C2B	-2.14	1.37	1.40
19	b	512	CLA	C3B-C2B	-2.14	1.37	1.40
19	B	515	CLA	C3B-C2B	-2.14	1.37	1.40
19	C	505	CLA	C3B-C2B	-2.14	1.37	1.40
19	b	501	CLA	C3B-C2B	-2.14	1.37	1.40
21	C	515	BCR	C30-C25	-2.14	1.50	1.53
19	b	503	CLA	CMD-C2D	-2.14	1.46	1.50
19	c	504	CLA	CMD-C2D	-2.14	1.46	1.50
20	D	401	PHO	CMD-C2D	-2.14	1.46	1.51
19	C	509	CLA	CMD-C2D	-2.13	1.46	1.50
19	B	507	CLA	C3B-C2B	-2.13	1.37	1.40
19	B	512	CLA	CMD-C2D	-2.13	1.46	1.50
21	W	101	BCR	C1-C6	-2.13	1.50	1.53
19	C	512	CLA	C3B-C2B	-2.13	1.37	1.40
20	A	405	PHO	CMD-C2D	-2.13	1.46	1.51
19	B	509	CLA	CMD-C2D	-2.13	1.46	1.50
20	d	401	PHO	CMC-C2C	-2.13	1.46	1.51
19	C	510	CLA	C3B-C2B	-2.13	1.37	1.40
19	b	509	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	506	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	511	CLA	CMC-C2C	-2.12	1.46	1.50
19	A	402	CLA	C3B-C2B	-2.12	1.37	1.40
19	c	504	CLA	C3B-C2B	-2.12	1.37	1.40
20	a	405	PHO	CMD-C2D	-2.12	1.46	1.51
19	b	515	CLA	CMD-C2D	-2.12	1.46	1.50
19	c	510	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	504	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	505	CLA	CMD-C2D	-2.12	1.46	1.50
19	c	513	CLA	C3B-C2B	-2.12	1.37	1.40
19	b	510	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	402	CLA	C3B-C2B	-2.11	1.37	1.40
19	b	516	CLA	CMD-C2D	-2.11	1.46	1.50
19	B	507	CLA	CMD-C2D	-2.11	1.46	1.50
19	B	515	CLA	CMD-C2D	-2.11	1.46	1.50
19	A	404	CLA	C3B-C2B	-2.11	1.37	1.40
19	b	504	CLA	CMD-C2D	-2.11	1.46	1.50
19	c	503	CLA	CMD-C2D	-2.11	1.46	1.50
19	c	508	CLA	CMD-C2D	-2.11	1.46	1.50
19	c	510	CLA	C3B-C2B	-2.11	1.37	1.40
19	a	406	CLA	CMD-C2D	-2.11	1.46	1.50
19	b	504	CLA	CMC-C2C	-2.10	1.46	1.50
20	a	405	PHO	C3B-C2B	-2.10	1.37	1.40
19	c	507	CLA	C3B-C2B	-2.10	1.37	1.40
19	b	516	CLA	C3B-CAB	-2.10	1.43	1.47
19	C	504	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	505	CLA	CMD-C2D	-2.10	1.46	1.50
19	B	510	CLA	CMD-C2D	-2.10	1.46	1.50
20	d	401	PHO	CMB-C2B	-2.10	1.46	1.51
19	b	511	CLA	CMD-C2D	-2.10	1.46	1.50
19	B	516	CLA	CMD-C2D	-2.10	1.46	1.50
20	D	401	PHO	CMB-C2B	-2.10	1.46	1.51
19	b	514	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	405	PHO	CMB-C2B	-2.10	1.46	1.51
19	C	511	CLA	C3B-CAB	-2.09	1.43	1.47
19	C	511	CLA	CMD-C2D	-2.09	1.46	1.50
19	B	501	CLA	C3B-C2B	-2.09	1.37	1.40
19	B	516	CLA	C3B-CAB	-2.08	1.43	1.47
19	B	511	CLA	CMD-C2D	-2.08	1.46	1.50
20	a	405	PHO	CMB-C2B	-2.08	1.46	1.51
19	C	510	CLA	CMD-C2D	-2.08	1.46	1.50
19	c	505	CLA	CMD-C2D	-2.08	1.46	1.50
19	d	403	CLA	CMC-C2C	-2.08	1.46	1.50
19	b	506	CLA	C3B-C2B	-2.08	1.37	1.40
19	B	504	CLA	CMC-C2C	-2.07	1.46	1.50
19	B	514	CLA	CMD-C2D	-2.07	1.46	1.50
19	C	507	CLA	CMD-C2D	-2.07	1.46	1.50
19	B	504	CLA	C3B-C2B	-2.07	1.37	1.40
19	B	502	CLA	CMD-C2D	-2.07	1.46	1.50
19	D	403	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	506	CLA	CMD-C2D	-2.07	1.46	1.50
19	B	508	CLA	C3B-C2B	-2.07	1.37	1.40
19	D	404	CLA	CMD-C2D	-2.06	1.46	1.50
19	c	510	CLA	CMC-C2C	-2.06	1.46	1.50
19	c	511	CLA	C3B-C2B	-2.06	1.37	1.40
19	c	506	CLA	C3B-C2B	-2.06	1.37	1.40
19	c	512	CLA	CMD-C2D	-2.05	1.46	1.50
19	b	507	CLA	C3B-C2B	-2.05	1.37	1.40
19	b	502	CLA	CMD-C2D	-2.05	1.46	1.50
19	c	511	CLA	CMD-C2D	-2.05	1.46	1.50
19	A	406	CLA	C3B-C2B	-2.05	1.37	1.40
19	C	505	CLA	CMD-C2D	-2.05	1.46	1.50
19	b	516	CLA	C3B-C2B	-2.05	1.37	1.40
19	B	513	CLA	CMC-C2C	-2.05	1.46	1.50
19	d	404	CLA	CMD-C2D	-2.05	1.46	1.50
19	B	511	CLA	CMC-C2C	-2.04	1.46	1.50
19	b	508	CLA	C3B-C2B	-2.04	1.37	1.40
19	C	509	CLA	CMC-C2C	-2.04	1.46	1.50
19	c	511	CLA	CMC-C2C	-2.04	1.46	1.50
21	c	517	BCR	C30-C25	-2.04	1.51	1.53
22	A	408	LMG	O1-C1	2.04	1.43	1.40
29	F	102	HEM	FE-ND	2.04	2.06	1.96
19	c	512	CLA	C3B-CAB	-2.03	1.43	1.47
19	C	509	CLA	C3B-C2B	-2.03	1.37	1.40
19	c	508	CLA	C3B-C2B	-2.03	1.37	1.40
19	d	403	CLA	C3B-C2B	-2.03	1.37	1.40
19	d	404	CLA	C3B-C2B	-2.03	1.37	1.40
19	a	402	CLA	CMC-C2C	-2.03	1.46	1.50
19	A	404	CLA	CMC-C2C	-2.02	1.46	1.50
19	a	403	CLA	CMC-C2C	-2.02	1.46	1.50
19	c	504	CLA	CMC-C2C	-2.02	1.46	1.50
19	b	513	CLA	CMC-C2C	-2.02	1.46	1.50
19	D	404	CLA	C3B-C2B	-2.02	1.37	1.40
19	a	404	CLA	CMC-C2C	-2.02	1.46	1.50
19	b	501	CLA	CMD-C2D	-2.02	1.46	1.50
19	a	406	CLA	C3B-C2B	-2.02	1.37	1.40
19	c	509	CLA	CMC-C2C	-2.02	1.46	1.50
19	c	515	CLA	CMD-C2D	-2.02	1.46	1.50
19	c	505	CLA	C3B-C2B	-2.02	1.37	1.40
19	A	403	CLA	CMC-C2C	-2.02	1.46	1.50
19	B	505	CLA	CMC-C2C	-2.01	1.46	1.50
19	c	512	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	513	CLA	C3B-C2B	-2.01	1.37	1.40
19	C	504	CLA	C3B-C2B	-2.01	1.37	1.40
19	A	406	CLA	CMD-C2D	-2.01	1.46	1.50
19	c	511	CLA	C3B-CAB	-2.01	1.43	1.47
19	B	515	CLA	CMC-C2C	-2.01	1.46	1.50
19	B	506	CLA	C3B-C2B	-2.01	1.37	1.40
19	b	504	CLA	C3B-C2B	-2.01	1.37	1.40
21	C	517	BCR	C1-C6	-2.01	1.51	1.53
19	D	403	CLA	C3B-C2B	-2.01	1.37	1.40
19	C	508	CLA	CMC-C2C	-2.00	1.46	1.50
19	B	510	CLA	CMC-C2C	-2.00	1.46	1.50
19	C	503	CLA	C3B-CAB	-2.00	1.43	1.47
19	C	503	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	503	CLA	CMC-C2C	-2.00	1.46	1.50

All (1074) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	w	101	BCR	C7-C8-C9	-5.78	117.49	126.23
19	B	512	CLA	C4A-NA-C1A	5.78	109.30	106.71
21	W	101	BCR	C38-C26-C25	-5.69	118.13	124.53
19	b	512	CLA	C4A-NA-C1A	5.63	109.24	106.71
19	C	503	CLA	C4A-NA-C1A	5.48	109.17	106.71
27	d	402	BCT	O2-C-O1	5.48	133.76	119.55
27	D	402	BCT	O2-C-O1	5.45	133.69	119.55
21	b	517	BCR	C3-C4-C5	-5.39	104.46	114.08
21	B	517	BCR	C3-C4-C5	-5.36	104.51	114.08
21	w	101	BCR	C16-C17-C18	-5.36	119.67	127.31
19	b	513	CLA	C4A-NA-C1A	5.34	109.11	106.71
19	B	513	CLA	C4A-NA-C1A	5.33	109.10	106.71
21	H	101	BCR	C7-C8-C9	-5.24	118.31	126.23
19	D	403	CLA	C4A-NA-C1A	5.19	109.04	106.71
19	C	511	CLA	C4A-NA-C1A	5.17	109.03	106.71
21	w	101	BCR	C38-C26-C25	-5.16	118.74	124.53
19	C	508	CLA	C4A-NA-C1A	5.15	109.02	106.71
19	c	509	CLA	C4A-NA-C1A	5.15	109.02	106.71
19	d	403	CLA	C4A-NA-C1A	5.13	109.01	106.71
21	H	101	BCR	C28-C27-C26	-5.12	104.93	114.08
19	c	504	CLA	C4A-NA-C1A	5.08	108.99	106.71
19	b	510	CLA	C4A-NA-C1A	5.08	108.99	106.71
21	W	101	BCR	C16-C17-C18	-5.06	120.09	127.31
21	h	101	BCR	C7-C8-C9	-5.04	118.62	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	406	PL9	C7-C3-C4	5.02	120.96	116.88
19	C	507	CLA	C4A-NA-C1A	5.01	108.96	106.71
19	C	513	CLA	C4A-NA-C1A	5.00	108.95	106.71
19	c	514	CLA	C4A-NA-C1A	4.98	108.94	106.71
21	h	101	BCR	C28-C27-C26	-4.95	105.23	114.08
21	V	101	BCR	C30-C25-C26	-4.92	115.68	122.61
19	B	510	CLA	C4A-NA-C1A	4.92	108.92	106.71
19	B	516	CLA	C4A-NA-C1A	4.92	108.92	106.71
28	D	406	PL9	C7-C3-C4	4.91	120.87	116.88
19	B	502	CLA	C4A-NA-C1A	4.91	108.91	106.71
19	c	508	CLA	C4A-NA-C1A	4.83	108.88	106.71
19	b	505	CLA	C4A-NA-C1A	4.83	108.88	106.71
21	C	515	BCR	C33-C5-C6	-4.82	119.11	124.53
19	c	512	CLA	C4A-NA-C1A	4.80	108.87	106.71
22	h	102	LMG	O7-C10-C11	4.77	121.79	111.50
19	b	516	CLA	C4A-NA-C1A	4.77	108.85	106.71
19	D	404	CLA	C4A-NA-C1A	4.76	108.84	106.71
19	b	515	CLA	C4A-NA-C1A	4.73	108.83	106.71
21	C	517	BCR	C28-C27-C26	-4.72	105.64	114.08
21	c	518	BCR	C28-C27-C26	-4.72	105.64	114.08
19	C	512	CLA	C4A-NA-C1A	4.72	108.83	106.71
19	C	510	CLA	C4A-NA-C1A	4.71	108.82	106.71
19	B	501	CLA	C4A-NA-C1A	4.64	108.79	106.71
19	c	510	CLA	C4A-NA-C1A	4.64	108.79	106.71
21	b	518	BCR	C28-C27-C26	-4.60	105.86	114.08
19	b	502	CLA	C4A-NA-C1A	4.60	108.78	106.71
19	b	511	CLA	C4A-NA-C1A	4.60	108.77	106.71
21	B	518	BCR	C28-C27-C26	-4.58	105.90	114.08
19	B	515	CLA	C4A-NA-C1A	4.56	108.76	106.71
19	c	511	CLA	C4A-NA-C1A	4.55	108.75	106.71
21	D	405	BCR	C30-C25-C26	-4.55	116.21	122.61
19	d	404	CLA	C4A-NA-C1A	4.54	108.75	106.71
19	a	406	CLA	C4A-NA-C1A	4.51	108.73	106.71
21	d	405	BCR	C30-C25-C26	-4.50	116.27	122.61
19	b	504	CLA	C4A-NA-C1A	4.50	108.73	106.71
19	c	513	CLA	C4A-NA-C1A	4.49	108.73	106.71
19	C	509	CLA	C4A-NA-C1A	4.49	108.72	106.71
21	c	517	BCR	C24-C23-C22	-4.48	119.46	126.23
19	A	403	CLA	C4A-NA-C1A	4.48	108.72	106.71
19	b	501	CLA	C4A-NA-C1A	4.48	108.72	106.71
21	w	101	BCR	C15-C14-C13	-4.47	120.93	127.31
19	B	505	CLA	C4A-NA-C1A	4.46	108.71	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	101	BCR	C20-C21-C22	-4.45	120.96	127.31
19	c	515	CLA	C4A-NA-C1A	4.44	108.70	106.71
19	C	514	CLA	C4A-NA-C1A	4.43	108.70	106.71
21	w	101	BCR	C11-C10-C9	-4.43	120.99	127.31
19	b	508	CLA	C4A-NA-C1A	4.43	108.70	106.71
19	B	504	CLA	C4A-NA-C1A	4.42	108.69	106.71
19	B	514	CLA	C4A-NA-C1A	4.42	108.69	106.71
19	a	403	CLA	C4A-NA-C1A	4.40	108.69	106.71
19	C	505	CLA	C4A-NA-C1A	4.40	108.68	106.71
21	W	101	BCR	C15-C14-C13	-4.40	121.03	127.31
21	a	407	BCR	C3-C4-C5	-4.38	106.26	114.08
19	b	514	CLA	C4A-NA-C1A	4.36	108.66	106.71
19	B	511	CLA	C4A-NA-C1A	4.33	108.65	106.71
21	c	516	BCR	C33-C5-C6	-4.32	119.67	124.53
21	A	407	BCR	C3-C4-C5	-4.32	106.36	114.08
19	A	406	CLA	C4A-NA-C1A	4.32	108.65	106.71
21	C	516	BCR	C20-C21-C22	-4.26	121.23	127.31
19	A	402	CLA	C4A-NA-C1A	4.25	108.62	106.71
19	B	507	CLA	C4A-NA-C1A	4.25	108.61	106.71
19	c	506	CLA	C4A-NA-C1A	4.24	108.61	106.71
21	V	101	BCR	C40-C30-C25	4.24	117.18	110.30
21	c	517	BCR	C20-C21-C22	-4.23	121.27	127.31
19	b	507	CLA	C4A-NA-C1A	4.22	108.60	106.71
21	C	515	BCR	C11-C10-C9	-4.20	121.32	127.31
21	W	101	BCR	C24-C23-C22	-4.19	119.91	126.23
21	W	101	BCR	C11-C10-C9	-4.14	121.40	127.31
19	a	402	CLA	C4A-NA-C1A	4.14	108.57	106.71
21	h	101	BCR	C20-C21-C22	-4.13	121.42	127.31
22	b	519	LMG	O7-C10-C11	4.13	120.39	111.50
21	C	516	BCR	C24-C23-C22	-4.13	120.00	126.23
21	C	515	BCR	C30-C25-C26	-4.12	116.81	122.61
21	k	101	BCR	C38-C26-C25	-4.11	119.91	124.53
19	b	503	CLA	C4A-NA-C1A	4.11	108.55	106.71
22	B	519	LMG	O7-C10-C11	4.09	120.31	111.50
19	B	508	CLA	C4A-NA-C1A	4.07	108.54	106.71
19	a	404	CLA	C4A-NA-C1A	4.07	108.53	106.71
21	H	101	BCR	C20-C21-C22	-4.07	121.50	127.31
21	V	101	BCR	C30-C25-C24	4.07	127.28	115.78
21	W	101	BCR	C3-C4-C5	-4.05	106.85	114.08
21	w	101	BCR	C3-C4-C5	-4.04	106.87	114.08
19	B	503	CLA	C4A-NA-C1A	4.04	108.52	106.71
19	C	502	CLA	C4A-NA-C1A	4.02	108.51	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	520	DGD	O2G-C1B-C2B	4.01	120.13	111.50
19	c	503	CLA	C4A-NA-C1A	4.00	108.50	106.71
25	C	518	DGD	O2G-C1B-C2B	3.99	120.10	111.50
25	c	519	DGD	O2G-C1B-C2B	3.99	120.10	111.50
21	c	518	BCR	C33-C5-C6	-3.98	120.06	124.53
25	c	521	DGD	O2G-C1B-C2B	3.98	120.08	111.50
21	c	516	BCR	C30-C25-C26	-3.98	117.01	122.61
22	A	408	LMG	O7-C10-C11	3.98	120.07	111.50
21	C	517	BCR	C33-C5-C6	-3.98	120.06	124.53
21	B	517	BCR	C20-C21-C22	-3.96	121.66	127.31
21	b	517	BCR	C20-C21-C22	-3.94	121.68	127.31
21	b	517	BCR	C36-C18-C19	3.94	124.28	118.08
19	B	514	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
21	B	517	BCR	C36-C18-C19	3.92	124.25	118.08
19	b	514	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
21	h	101	BCR	C3-C4-C5	-3.92	107.09	114.08
22	c	502	LMG	O7-C10-C11	3.91	119.93	111.50
19	A	404	CLA	C4A-NA-C1A	3.91	108.46	106.71
21	a	407	BCR	C7-C8-C9	-3.86	120.40	126.23
23	A	409	LHG	O7-C7-C8	3.85	119.80	111.50
22	C	521	LMG	O7-C10-C11	3.82	119.74	111.50
21	H	101	BCR	C11-C10-C9	-3.82	121.86	127.31
23	a	408	LHG	O7-C7-C8	3.82	119.72	111.50
21	A	407	BCR	C20-C21-C22	-3.82	121.86	127.31
21	a	407	BCR	C16-C17-C18	-3.81	121.88	127.31
21	C	517	BCR	C7-C8-C9	-3.81	120.48	126.23
19	B	508	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
21	V	101	BCR	C37-C22-C23	3.79	124.04	118.08
19	A	404	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
22	c	522	LMG	O7-C10-C11	3.78	119.65	111.50
19	c	515	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
21	A	407	BCR	C7-C8-C9	-3.77	120.54	126.23
19	a	404	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
22	H	102	LMG	O7-C10-C11	3.76	119.60	111.50
23	x	101	LHG	O7-C7-C8	3.75	119.58	111.50
21	W	101	BCR	C33-C5-C4	3.75	120.81	113.62
19	c	505	CLA	C4A-NA-C1A	3.73	108.38	106.71
21	w	101	BCR	C20-C21-C22	-3.72	121.99	127.31
23	X	101	LHG	O7-C7-C8	3.72	119.51	111.50
19	B	510	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
21	a	407	BCR	C20-C21-C22	-3.70	122.02	127.31
19	b	509	CLA	C4A-NA-C1A	3.70	108.37	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	509	CLA	C4A-NA-C1A	3.69	108.37	106.71
21	h	101	BCR	C16-C17-C18	-3.69	122.04	127.31
19	b	510	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
19	C	510	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
19	b	508	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
21	H	101	BCR	C3-C4-C5	-3.69	107.50	114.08
23	A	410	LHG	O7-C7-C8	3.69	119.44	111.50
21	W	101	BCR	C7-C8-C9	-3.67	120.68	126.23
21	H	101	BCR	C16-C17-C18	-3.67	122.08	127.31
24	C	501	SQD	O47-C7-C8	3.67	119.40	111.50
21	c	517	BCR	C38-C26-C25	-3.66	120.42	124.53
21	B	518	BCR	C33-C5-C6	-3.66	120.42	124.53
24	c	501	SQD	O47-C7-C8	3.66	119.38	111.50
21	D	405	BCR	C1-C6-C5	-3.65	117.47	122.61
23	D	407	LHG	O7-C7-C8	3.65	119.36	111.50
21	b	518	BCR	C33-C5-C6	-3.65	120.43	124.53
23	a	409	LHG	O7-C7-C8	3.65	119.36	111.50
21	c	517	BCR	C7-C8-C9	-3.64	120.73	126.23
23	d	408	LHG	O7-C7-C8	3.64	119.34	111.50
25	c	520	DGD	O2G-C1B-C2B	3.63	119.32	111.50
21	h	101	BCR	C11-C10-C9	-3.63	122.14	127.31
21	b	517	BCR	C37-C22-C21	-3.62	117.85	122.92
19	c	511	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
19	C	504	CLA	C4A-NA-C1A	3.62	108.33	106.71
23	B	521	LHG	O7-C7-C8	3.62	119.30	111.50
19	A	406	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
21	c	518	BCR	C20-C21-C22	-3.62	122.15	127.31
21	d	405	BCR	C20-C21-C22	-3.61	122.15	127.31
25	C	519	DGD	O2G-C1B-C2B	3.61	119.28	111.50
21	d	405	BCR	C1-C6-C5	-3.61	117.53	122.61
19	B	506	CLA	C4A-NA-C1A	3.60	108.32	106.71
19	b	506	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
21	C	516	BCR	C38-C26-C25	-3.59	120.50	124.53
23	b	520	LHG	O7-C7-C8	3.58	119.22	111.50
19	a	406	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
19	B	506	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
21	D	405	BCR	C20-C21-C22	-3.56	122.23	127.31
19	b	506	CLA	C4A-NA-C1A	3.56	108.31	106.71
21	V	101	BCR	C33-C5-C6	-3.55	120.54	124.53
21	C	516	BCR	C33-C5-C6	-3.55	120.54	124.53
21	c	516	BCR	C11-C10-C9	-3.54	122.26	127.31
21	B	517	BCR	C37-C22-C21	-3.53	117.97	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	514	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
21	B	517	BCR	C15-C16-C17	-3.52	116.27	123.47
21	b	517	BCR	C15-C16-C17	-3.51	116.28	123.47
22	f	101	LMG	O7-C10-C11	3.51	119.07	111.50
21	d	405	BCR	C28-C27-C26	-3.50	107.82	114.08
21	W	101	BCR	C4-C5-C6	-3.49	117.66	122.73
21	C	516	BCR	C7-C8-C9	-3.49	120.96	126.23
21	C	517	BCR	C20-C21-C22	-3.49	122.33	127.31
19	b	503	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
19	c	506	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
21	c	517	BCR	C11-C10-C9	-3.49	122.34	127.31
21	B	518	BCR	C37-C22-C23	3.48	123.56	118.08
22	F	101	LMG	O7-C10-C11	3.48	119.01	111.50
19	b	504	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
21	A	407	BCR	C16-C17-C18	-3.48	122.35	127.31
21	D	405	BCR	C28-C27-C26	-3.48	107.87	114.08
21	k	101	BCR	C16-C17-C18	-3.47	122.35	127.31
23	B	520	LHG	O7-C7-C8	3.47	118.99	111.50
21	d	405	BCR	C37-C22-C23	3.47	123.54	118.08
23	d	407	LHG	O7-C7-C8	3.47	118.97	111.50
19	B	512	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
21	c	518	BCR	C7-C8-C9	-3.46	121.01	126.23
21	D	405	BCR	C37-C22-C23	3.45	123.52	118.08
21	b	518	BCR	C37-C22-C23	3.45	123.52	118.08
19	B	504	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
21	B	518	BCR	C36-C18-C19	3.44	123.49	118.08
21	A	407	BCR	C24-C23-C22	-3.42	121.07	126.23
21	d	405	BCR	C16-C17-C18	-3.41	122.44	127.31
19	b	516	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
21	c	517	BCR	C33-C5-C6	-3.41	120.70	124.53
21	b	518	BCR	C20-C21-C22	-3.41	122.45	127.31
19	b	512	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
21	B	518	BCR	C20-C21-C22	-3.39	122.47	127.31
21	d	405	BCR	C38-C26-C27	3.39	120.13	113.62
21	a	407	BCR	C24-C23-C22	-3.39	121.11	126.23
19	c	507	CLA	C4A-NA-C1A	3.39	108.23	106.71
19	c	514	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
19	C	510	CLA	CMB-C2B-C3B	3.39	131.01	124.68
19	B	515	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
19	C	505	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
21	C	516	BCR	C11-C10-C9	-3.38	122.49	127.31
21	V	101	BCR	C16-C17-C18	-3.38	122.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	517	BCR	C37-C22-C23	3.37	123.39	118.08
19	c	515	CLA	CMB-C2B-C3B	3.37	130.99	124.68
21	b	518	BCR	C36-C18-C19	3.37	123.38	118.08
19	C	513	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
21	b	517	BCR	C37-C22-C23	3.36	123.37	118.08
21	k	101	BCR	C7-C8-C9	-3.36	121.16	126.23
21	h	101	BCR	C36-C18-C19	3.35	123.36	118.08
21	D	405	BCR	C38-C26-C27	3.35	120.05	113.62
19	A	404	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
21	a	407	BCR	C11-C10-C9	-3.35	122.53	127.31
21	H	101	BCR	C36-C18-C19	3.34	123.34	118.08
21	b	517	BCR	C2-C1-C6	3.33	115.61	110.48
21	A	407	BCR	C11-C10-C9	-3.32	122.57	127.31
21	C	515	BCR	C36-C18-C19	3.32	123.30	118.08
21	b	517	BCR	C7-C8-C9	-3.31	121.23	126.23
19	c	511	CLA	CMB-C2B-C3B	3.31	130.87	124.68
21	D	405	BCR	C33-C5-C6	-3.31	120.81	124.53
21	A	407	BCR	C36-C18-C19	3.31	123.28	118.08
21	k	101	BCR	C20-C21-C22	-3.30	122.60	127.31
19	B	514	CLA	CMB-C2B-C3B	3.30	130.85	124.68
19	B	511	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
21	B	517	BCR	C7-C8-C9	-3.29	121.26	126.23
19	b	515	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
19	b	514	CLA	CMB-C2B-C3B	3.28	130.82	124.68
21	k	101	BCR	C37-C22-C23	3.28	123.25	118.08
21	B	517	BCR	C2-C1-C6	3.28	115.53	110.48
19	B	511	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
21	D	405	BCR	C16-C17-C18	-3.28	122.63	127.31
19	A	403	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
19	b	511	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
25	C	519	DGD	O1G-C1A-C2A	3.25	119.92	111.38
28	D	406	PL9	C7-C3-C2	-3.25	119.02	123.30
19	a	403	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
28	d	406	PL9	C7-C3-C2	-3.25	119.03	123.30
21	a	407	BCR	C38-C26-C25	-3.25	120.88	124.53
25	c	520	DGD	O1G-C1A-C2A	3.23	119.86	111.38
21	c	518	BCR	C16-C17-C18	-3.23	122.70	127.31
19	C	507	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
21	W	101	BCR	C29-C30-C25	-3.23	105.51	110.48
21	c	517	BCR	C36-C18-C19	3.23	123.16	118.08
19	a	403	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
19	D	404	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	517	BCR	C15-C14-C13	-3.22	122.71	127.31
21	w	101	BCR	C33-C5-C6	-3.22	120.92	124.53
19	c	507	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
21	k	101	BCR	C36-C18-C19	3.21	123.13	118.08
19	d	404	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
19	A	404	CLA	CMB-C2B-C3B	3.20	130.67	124.68
21	C	515	BCR	C16-C17-C18	-3.20	122.74	127.31
19	b	511	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
19	A	403	CLA	CMB-C2B-C1B	-3.19	123.55	128.46
21	D	405	BCR	C27-C26-C25	-3.19	118.09	122.73
21	c	516	BCR	C38-C26-C25	-3.19	120.94	124.53
21	w	101	BCR	C29-C30-C25	-3.19	105.57	110.48
19	C	506	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
21	C	516	BCR	C36-C18-C19	3.19	123.10	118.08
21	d	405	BCR	C33-C5-C6	-3.19	120.95	124.53
19	a	402	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
19	B	508	CLA	CMB-C2B-C3B	3.18	130.63	124.68
19	a	404	CLA	CMB-C2B-C3B	3.18	130.63	124.68
21	W	101	BCR	C38-C26-C27	3.18	119.73	113.62
19	A	402	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	C	509	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
21	b	517	BCR	C15-C14-C13	-3.17	122.79	127.31
19	B	502	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
21	a	407	BCR	C36-C18-C19	3.16	123.06	118.08
19	B	516	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
19	b	502	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
19	c	510	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
19	C	514	CLA	CMB-C2B-C3B	3.14	130.56	124.68
19	c	505	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	b	502	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	B	502	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
19	b	501	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	b	510	CLA	CMB-C2B-C3B	3.13	130.53	124.68
21	b	518	BCR	C7-C8-C9	-3.13	121.51	126.23
21	V	101	BCR	C8-C9-C10	-3.12	114.15	118.94
19	b	508	CLA	CMB-C2B-C3B	3.12	130.52	124.68
19	B	507	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
21	c	516	BCR	C37-C22-C23	3.12	122.99	118.08
21	c	518	BCR	C29-C30-C25	3.12	115.28	110.48
19	B	510	CLA	CMB-C2B-C3B	3.12	130.51	124.68
19	B	514	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
19	b	506	CLA	CMB-C2B-C3B	3.11	130.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	405	PHO	C1-C2-C3	-3.10	120.67	126.04
21	H	101	BCR	C37-C22-C23	3.10	122.97	118.08
19	C	504	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
19	b	516	CLA	CMB-C2B-C3B	3.10	130.48	124.68
19	b	514	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
21	h	101	BCR	C37-C22-C23	3.10	122.96	118.08
19	B	506	CLA	CMB-C2B-C3B	3.10	130.48	124.68
19	b	507	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
21	V	101	BCR	C27-C26-C25	-3.09	118.24	122.73
21	c	516	BCR	C36-C18-C19	3.09	122.95	118.08
19	c	513	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
21	C	515	BCR	C20-C21-C22	-3.09	122.90	127.31
21	d	405	BCR	C27-C26-C25	-3.08	118.25	122.73
19	b	510	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	c	508	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
19	B	503	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
19	B	510	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	c	506	CLA	CMB-C2B-C3B	3.07	130.43	124.68
19	b	503	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
21	B	518	BCR	C7-C8-C9	-3.07	121.60	126.23
19	C	504	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
21	c	518	BCR	C37-C22-C23	3.06	122.90	118.08
21	C	517	BCR	C29-C30-C25	3.05	115.18	110.48
19	a	404	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
19	c	505	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
21	C	515	BCR	C37-C22-C23	3.05	122.89	118.08
21	w	101	BCR	C33-C5-C4	3.05	119.48	113.62
19	d	403	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
19	c	509	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
19	D	403	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
19	B	506	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
19	d	404	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
20	a	405	PHO	C1-C2-C3	-3.03	120.80	126.04
21	C	515	BCR	C38-C26-C27	3.03	119.44	113.62
19	c	514	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	D	405	BCR	C33-C5-C4	3.03	119.44	113.62
19	C	506	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
19	B	506	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
19	C	508	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
19	B	503	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
19	b	509	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
19	B	508	CLA	C1B-CHB-C4A	-3.02	124.13	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	c	507	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	A	406	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
24	c	501	SQD	O7-S-C6	3.01	110.52	106.94
19	b	504	CLA	CMB-C2B-C3B	3.01	130.31	124.68
19	D	403	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	a	406	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
19	b	506	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
21	C	515	BCR	C38-C26-C25	-3.00	121.16	124.53
19	B	504	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	B	504	CLA	CMB-C2B-C3B	3.00	130.29	124.68
21	B	517	BCR	C30-C25-C26	-3.00	118.39	122.61
21	k	101	BCR	C3-C4-C5	-3.00	108.72	114.08
20	a	405	PHO	O1D-CGD-CBD	3.00	129.73	124.74
24	C	501	SQD	O7-S-C6	3.00	110.50	106.94
19	b	512	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
19	B	509	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	b	506	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	B	513	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
19	A	404	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
19	B	513	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
19	b	513	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
19	b	509	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	B	512	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	c	512	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
21	C	517	BCR	C16-C17-C18	-2.97	123.08	127.31
19	d	403	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
19	b	504	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
21	C	515	BCR	C8-C9-C10	2.96	123.49	118.94
19	a	404	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
19	B	507	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
19	c	513	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
19	b	507	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
20	A	405	PHO	O1D-CGD-CBD	2.96	129.67	124.74
19	B	504	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
19	b	508	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
19	C	511	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
21	c	516	BCR	C15-C14-C13	-2.95	123.10	127.31
21	b	517	BCR	C4-C5-C6	-2.95	118.44	122.73
21	B	518	BCR	C1-C6-C5	-2.95	118.46	122.61
19	C	508	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	C	513	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
21	c	516	BCR	C20-C21-C22	-2.94	123.11	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	509	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
19	C	512	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
19	c	509	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
19	b	503	CLA	CMB-C2B-C3B	2.94	130.18	124.68
21	B	518	BCR	C16-C17-C18	-2.94	123.12	127.31
21	C	517	BCR	C37-C22-C23	2.93	122.70	118.08
21	c	518	BCR	C36-C18-C19	2.93	122.70	118.08
21	d	405	BCR	C33-C5-C4	2.93	119.25	113.62
19	C	506	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
21	c	517	BCR	C15-C16-C17	-2.93	117.48	123.47
21	C	517	BCR	C36-C18-C19	2.93	122.69	118.08
19	C	505	CLA	CMB-C2B-C3B	2.92	130.15	124.68
23	l	101	LHG	O7-C7-C8	2.92	117.80	111.50
21	h	101	BCR	C30-C25-C26	-2.92	118.50	122.61
21	C	515	BCR	C1-C6-C7	2.92	124.03	115.78
19	C	512	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
21	C	515	BCR	C15-C14-C13	-2.91	123.15	127.31
19	c	503	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
21	c	518	BCR	C1-C6-C5	-2.91	118.52	122.61
19	D	404	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
19	c	514	CLA	CMB-C2B-C3B	2.91	130.11	124.68
19	C	513	CLA	CMB-C2B-C3B	2.90	130.11	124.68
21	b	518	BCR	C16-C17-C18	-2.90	123.17	127.31
19	B	515	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
19	C	511	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
23	L	101	LHG	O7-C7-C8	2.90	117.75	111.50
19	C	509	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	b	504	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
19	B	511	CLA	CMB-C2B-C3B	2.90	130.10	124.68
19	b	503	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
19	c	507	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
19	c	508	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
19	C	510	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
19	A	402	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
19	c	506	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
19	b	508	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
19	a	402	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
19	C	510	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
21	B	517	BCR	C4-C5-C6	-2.88	118.54	122.73
19	c	512	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
19	c	510	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	d	403	CLA	C1B-CHB-C4A	-2.88	124.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	507	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
19	c	511	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
19	C	505	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	D	401	PHO	O1D-CGD-CBD	2.87	129.52	124.74
22	c	502	LMG	O8-C28-C29	2.87	120.92	111.91
19	D	403	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
19	c	511	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
21	V	101	BCR	C38-C26-C27	2.87	119.13	113.62
19	A	406	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
21	k	101	BCR	C38-C26-C27	2.87	119.12	113.62
21	b	517	BCR	C38-C26-C25	-2.86	121.31	124.53
21	b	518	BCR	C1-C6-C5	-2.86	118.58	122.61
19	C	505	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
19	b	513	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
19	B	503	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
21	a	407	BCR	C15-C14-C13	-2.86	123.23	127.31
21	V	101	BCR	C28-C27-C26	-2.85	108.98	114.08
23	L	101	LHG	O8-C23-C24	2.85	120.86	111.91
21	B	517	BCR	C38-C26-C25	-2.85	121.32	124.53
21	B	517	BCR	C11-C10-C9	-2.85	123.24	127.31
20	d	401	PHO	O1D-CGD-CBD	2.85	129.49	124.74
19	c	506	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
28	D	406	PL9	C40-C39-C41	2.85	120.06	115.27
19	C	503	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
21	C	516	BCR	C15-C16-C17	-2.85	117.64	123.47
21	c	518	BCR	C33-C5-C4	2.85	119.08	113.62
19	c	515	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
19	B	508	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
21	c	516	BCR	C38-C26-C27	2.84	119.08	113.62
29	e	101	HEM	C1B-NB-C4B	2.84	108.01	105.07
19	d	404	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
20	d	401	PHO	O2D-CGD-O1D	-2.84	118.28	123.84
19	b	512	CLA	CMB-C2B-C3B	2.84	129.99	124.68
19	B	501	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	b	501	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
19	B	511	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
19	B	514	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
20	a	405	PHO	O2D-CGD-O1D	-2.84	118.29	123.84
19	A	403	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
23	l	101	LHG	O8-C23-C24	2.83	120.80	111.91
19	c	503	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
19	B	512	CLA	CMB-C2B-C3B	2.83	129.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	511	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
22	A	408	LMG	O8-C28-C29	2.83	120.79	111.91
21	w	101	BCR	C38-C26-C27	2.83	119.05	113.62
19	a	406	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
19	D	404	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
19	C	514	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
21	c	516	BCR	C16-C17-C18	-2.83	123.28	127.31
19	b	514	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
29	F	102	HEM	C1B-NB-C4B	2.82	107.99	105.07
19	b	501	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	C	502	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
19	B	501	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
28	d	406	PL9	C40-C39-C41	2.80	119.99	115.27
19	c	510	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
19	B	501	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
21	B	518	BCR	C33-C5-C4	2.80	119.00	113.62
21	A	407	BCR	C37-C22-C23	2.80	122.49	118.08
20	D	401	PHO	O2D-CGD-O1D	-2.80	118.37	123.84
19	a	403	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
21	A	407	BCR	C38-C26-C25	-2.79	121.39	124.53
19	c	503	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
19	C	509	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
21	c	516	BCR	C8-C9-C10	2.79	123.22	118.94
21	C	515	BCR	C1-C6-C5	-2.79	118.69	122.61
21	b	518	BCR	C33-C5-C4	2.79	118.97	113.62
19	B	516	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
21	H	101	BCR	C37-C22-C21	-2.79	119.02	122.92
21	V	101	BCR	C36-C18-C19	2.78	122.46	118.08
21	w	101	BCR	C23-C24-C25	-2.78	119.39	127.20
21	C	517	BCR	C1-C6-C5	-2.78	118.69	122.61
19	a	402	CLA	CMB-C2B-C3B	2.78	129.88	124.68
19	b	511	CLA	CMB-C2B-C3B	2.78	129.88	124.68
19	B	505	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
19	c	514	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
20	A	405	PHO	O2D-CGD-O1D	-2.78	118.41	123.84
21	c	518	BCR	C24-C23-C22	-2.78	122.04	126.23
21	W	101	BCR	C1-C6-C5	-2.77	118.71	122.61
19	b	507	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
21	H	101	BCR	C30-C25-C26	-2.77	118.71	122.61
21	b	517	BCR	C11-C10-C9	-2.77	123.35	127.31
21	k	101	BCR	C30-C25-C26	-2.77	118.71	122.61
19	B	502	CLA	C1B-CHB-C4A	-2.77	124.63	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	517	BCR	C30-C25-C26	-2.77	118.71	122.61
19	C	513	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
21	A	407	BCR	C15-C14-C13	-2.77	123.36	127.31
19	B	515	CLA	CHB-C4A-NA	2.77	128.34	124.51
21	a	407	BCR	C37-C22-C23	2.77	122.44	118.08
21	h	101	BCR	C37-C22-C21	-2.76	119.05	122.92
21	V	101	BCR	C1-C6-C7	2.76	123.59	115.78
19	c	507	CLA	CMB-C2B-C3B	2.76	129.84	124.68
19	c	504	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
19	C	506	CLA	CMB-C2B-C3B	2.76	129.84	124.68
19	A	402	CLA	CMB-C2B-C3B	2.76	129.84	124.68
19	B	507	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
19	c	505	CLA	CMB-C2B-C3B	2.75	129.83	124.68
21	B	518	BCR	C30-C25-C26	-2.75	118.74	122.61
19	C	507	CLA	CMB-C2B-C3B	2.75	129.81	124.68
19	B	509	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
21	B	518	BCR	C37-C22-C21	-2.74	119.08	122.92
21	b	518	BCR	C30-C25-C26	-2.74	118.75	122.61
19	b	509	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
21	C	516	BCR	C16-C17-C18	-2.74	123.40	127.31
19	b	510	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
19	C	504	CLA	CMB-C2B-C3B	2.74	129.80	124.68
21	c	516	BCR	C1-C6-C7	2.73	123.51	115.78
19	B	515	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
21	a	407	BCR	C36-C18-C17	-2.73	119.10	122.92
19	b	502	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
19	A	402	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	b	505	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
21	V	101	BCR	C20-C21-C22	-2.72	123.42	127.31
21	C	517	BCR	C24-C23-C22	-2.72	122.12	126.23
23	B	520	LHG	O8-C23-C24	2.72	120.45	111.91
19	c	508	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
21	d	405	BCR	C38-C26-C25	-2.72	121.47	124.53
19	C	507	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
21	b	517	BCR	C24-C23-C22	-2.72	122.12	126.23
21	C	517	BCR	C8-C7-C6	-2.71	119.58	127.20
21	B	517	BCR	C38-C26-C27	2.71	118.83	113.62
19	B	502	CLA	CMB-C2B-C3B	2.71	129.75	124.68
19	c	504	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	c	510	CLA	CMB-C2B-C3B	2.71	129.75	124.68
19	b	501	CLA	CMB-C2B-C3B	2.71	129.75	124.68
21	h	101	BCR	C36-C18-C17	-2.71	119.13	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	516	CLA	CMB-C2B-C3B	2.71	129.75	124.68
19	C	508	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
19	B	505	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	C	509	CLA	CMB-C2B-C3B	2.71	129.75	124.68
19	B	510	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
22	C	521	LMG	O8-C28-C29	2.70	120.39	111.91
21	V	101	BCR	C3-C4-C5	-2.70	109.26	114.08
19	a	402	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	b	516	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
21	w	101	BCR	C24-C23-C22	-2.69	122.17	126.23
19	C	504	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
22	c	522	LMG	O8-C28-C29	2.69	120.35	111.91
21	k	101	BCR	C28-C27-C26	-2.69	109.28	114.08
23	d	407	LHG	O8-C23-C24	2.69	120.35	111.91
21	b	518	BCR	C37-C22-C21	-2.69	119.16	122.92
19	c	509	CLA	CMB-C2B-C3B	2.69	129.71	124.68
19	C	514	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
21	B	517	BCR	C24-C23-C22	-2.69	122.18	126.23
19	b	515	CLA	CHB-C4A-NA	2.69	128.22	124.51
21	C	516	BCR	C37-C22-C21	-2.68	119.16	122.92
19	C	502	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
21	W	101	BCR	C33-C5-C6	-2.68	121.52	124.53
19	c	509	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
19	C	508	CLA	CMB-C2B-C3B	2.68	129.69	124.68
21	D	405	BCR	C3-C4-C5	-2.68	109.30	114.08
21	c	516	BCR	C15-C16-C17	-2.67	118.00	123.47
19	C	502	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
21	h	101	BCR	C1-C6-C5	-2.67	118.85	122.61
19	C	503	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
19	d	404	CLA	CMB-C2B-C3B	2.67	129.68	124.68
19	C	512	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
19	c	512	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
21	A	407	BCR	C36-C18-C17	-2.66	119.19	122.92
19	b	507	CLA	CMB-C2B-C3B	2.66	129.66	124.68
21	H	101	BCR	C36-C18-C17	-2.66	119.19	122.92
19	c	515	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
19	A	406	CLA	CMB-C2B-C3B	2.66	129.65	124.68
29	e	101	HEM	C3B-C2B-C1B	2.66	108.46	106.49
19	B	512	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
19	b	502	CLA	CMB-C2B-C3B	2.66	129.65	124.68
28	d	406	PL9	C22-C23-C24	-2.66	121.27	127.66
21	c	517	BCR	C16-C17-C18	-2.65	123.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	507	CLA	CMB-C2B-C3B	2.65	129.64	124.68
19	C	511	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
21	d	405	BCR	C16-C15-C14	-2.65	118.05	123.47
19	a	406	CLA	CMB-C2B-C3B	2.65	129.63	124.68
21	b	518	BCR	C15-C16-C17	-2.64	118.06	123.47
19	c	513	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
19	d	403	CLA	CMB-C2B-C3B	2.64	129.62	124.68
19	b	512	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
21	a	407	BCR	C35-C13-C12	2.64	122.24	118.08
21	B	518	BCR	C15-C16-C17	-2.64	118.06	123.47
21	h	101	BCR	C38-C26-C27	2.64	118.68	113.62
19	c	514	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	d	405	BCR	C3-C4-C5	-2.63	109.38	114.08
23	X	101	LHG	O8-C23-C24	2.63	120.16	111.91
23	X	101	LHG	C5-O7-C7	-2.63	111.32	117.79
29	F	102	HEM	C4D-ND-C1D	2.63	107.79	105.07
19	c	505	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	D	403	CLA	CMB-C2B-C3B	2.62	129.58	124.68
21	c	517	BCR	C15-C14-C13	-2.62	123.57	127.31
19	a	403	CLA	CMB-C2B-C3B	2.61	129.57	124.68
19	B	503	CLA	CMB-C2B-C3B	2.61	129.56	124.68
21	B	518	BCR	C38-C26-C25	-2.61	121.60	124.53
28	D	406	PL9	C22-C23-C24	-2.61	121.38	127.66
19	b	515	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
21	b	518	BCR	C38-C26-C25	-2.60	121.61	124.53
24	C	501	SQD	O48-C23-C24	2.60	120.06	111.91
23	a	408	LHG	O8-C23-C24	2.60	120.06	111.91
19	b	516	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
24	c	501	SQD	O48-C23-C24	2.60	120.05	111.91
19	c	513	CLA	CMB-C2B-C3B	2.59	129.52	124.68
19	b	505	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
23	D	407	LHG	O8-C23-C24	2.59	120.03	111.91
19	c	508	CLA	CMB-C2B-C3B	2.59	129.52	124.68
21	H	101	BCR	C38-C26-C27	2.58	118.58	113.62
19	C	513	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	c	517	BCR	C1-C6-C5	-2.58	118.98	122.61
21	W	101	BCR	C8-C7-C6	-2.58	119.97	127.20
19	C	512	CLA	CHD-C1D-ND	-2.57	122.09	124.45
22	A	408	LMG	C8-O7-C10	-2.57	111.46	117.79
22	b	519	LMG	O8-C28-C29	2.57	119.97	111.91
19	A	406	CLA	O2D-CGD-CBD	2.57	115.83	111.27
19	C	506	CLA	C4A-NA-C1A	2.57	107.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	516	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
21	C	517	BCR	C33-C5-C4	2.56	118.54	113.62
21	C	516	BCR	C37-C22-C23	2.56	122.11	118.08
21	d	405	BCR	C36-C18-C19	2.56	122.11	118.08
21	k	101	BCR	C24-C23-C22	-2.56	122.37	126.23
23	x	101	LHG	C5-O7-C7	-2.56	111.49	117.79
21	D	405	BCR	C16-C15-C14	-2.56	118.24	123.47
21	h	101	BCR	C4-C5-C6	-2.55	119.02	122.73
25	c	519	DGD	O1G-C1A-C2A	2.55	119.92	111.91
19	b	504	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
23	d	408	LHG	O8-C23-C24	2.55	119.92	111.91
21	b	517	BCR	C32-C1-C6	-2.55	106.16	110.30
21	h	101	BCR	C38-C26-C25	-2.55	121.67	124.53
22	B	519	LMG	O8-C28-C29	2.55	119.90	111.91
21	b	517	BCR	C38-C26-C27	2.55	118.51	113.62
19	b	509	CLA	CMB-C2B-C3B	2.55	129.44	124.68
19	B	513	CLA	CMB-C2B-C3B	2.55	129.44	124.68
19	C	511	CLA	CMB-C2B-C3B	2.54	129.44	124.68
19	B	515	CLA	CMB-C2B-C3B	2.54	129.44	124.68
19	A	403	CLA	CMB-C2B-C3B	2.54	129.43	124.68
25	C	518	DGD	O1G-C1A-C2A	2.54	119.87	111.91
19	D	404	CLA	CMB-C2B-C3B	2.54	129.42	124.68
23	A	409	LHG	O8-C23-C24	2.54	119.86	111.91
19	B	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	d	405	BCR	C37-C22-C21	-2.53	119.38	122.92
19	b	507	CLA	C4-C3-C5	2.53	119.52	115.27
19	b	513	CLA	CHB-C4A-NA	2.53	128.00	124.51
19	B	509	CLA	CMB-C2B-C3B	2.53	129.40	124.68
21	c	517	BCR	C30-C25-C26	-2.53	119.06	122.61
29	e	101	HEM	C4D-ND-C1D	2.52	107.68	105.07
19	a	406	CLA	O2D-CGD-CBD	2.52	115.75	111.27
21	B	518	BCR	C11-C10-C9	-2.52	123.71	127.31
19	c	513	CLA	CHD-C1D-ND	-2.52	122.14	124.45
29	F	102	HEM	C4B-CHC-C1C	2.52	125.89	122.56
19	B	507	CLA	C4-C3-C5	2.52	119.51	115.27
19	B	504	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
19	c	504	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
19	c	512	CLA	CMB-C2B-C3B	2.52	129.39	124.68
21	C	516	BCR	C15-C14-C13	-2.52	123.72	127.31
19	C	508	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	C	503	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
21	W	101	BCR	C30-C25-C26	-2.51	119.08	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	405	BCR	C38-C26-C25	-2.51	121.71	124.53
19	b	513	CLA	CMB-C2B-C3B	2.51	129.37	124.68
21	V	101	BCR	C10-C11-C12	-2.51	115.39	123.22
21	b	518	BCR	C11-C10-C9	-2.51	123.73	127.31
23	x	101	LHG	O8-C23-C24	2.51	119.78	111.91
19	C	512	CLA	CMB-C2B-C3B	2.51	129.37	124.68
19	b	505	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
20	d	401	PHO	CMB-C2B-C3B	2.50	129.36	124.68
19	b	515	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
19	B	501	CLA	CMB-C2B-C3B	2.50	129.36	124.68
29	F	102	HEM	C3B-C2B-C1B	2.50	108.34	106.49
21	V	101	BCR	C39-C30-C25	-2.50	106.25	110.30
19	b	504	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	c	504	CLA	C1-C2-C3	-2.49	121.73	126.04
19	B	513	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	B	505	CLA	CHD-C1D-ND	-2.49	122.17	124.45
20	D	401	PHO	CMC-C2C-C3C	2.49	129.63	124.94
19	c	503	CLA	CMB-C2B-C3B	2.49	129.33	124.68
21	H	101	BCR	C1-C6-C5	-2.49	119.11	122.61
21	A	407	BCR	C35-C13-C12	2.48	121.99	118.08
21	D	405	BCR	C37-C22-C21	-2.48	119.44	122.92
19	c	509	CLA	CHB-C4A-NA	2.48	127.95	124.51
20	A	405	PHO	CMC-C2C-C3C	2.48	129.62	124.94
19	A	402	CLA	C7-C6-C5	-2.48	106.62	113.36
21	D	405	BCR	C7-C8-C9	-2.48	122.49	126.23
22	F	101	LMG	O8-C28-C29	2.48	119.68	111.91
19	C	503	CLA	C1-C2-C3	-2.48	121.76	126.04
21	D	405	BCR	C36-C18-C19	2.47	121.97	118.08
19	A	403	CLA	CHD-C1D-ND	-2.47	122.18	124.45
21	c	516	BCR	C1-C6-C5	-2.47	119.13	122.61
21	h	101	BCR	C24-C23-C22	-2.47	122.50	126.23
19	c	512	CLA	CHB-C4A-NA	2.47	127.92	124.51
20	D	401	PHO	CMB-C2B-C3B	2.47	129.29	124.68
21	C	515	BCR	C15-C16-C17	-2.47	118.42	123.47
21	a	407	BCR	C4-C5-C6	-2.47	119.15	122.73
21	H	101	BCR	C24-C23-C22	-2.46	122.51	126.23
19	C	511	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	c	506	CLA	CHD-C1D-ND	-2.46	122.19	124.45
21	d	405	BCR	C7-C8-C9	-2.46	122.52	126.23
20	a	405	PHO	CMC-C2C-C3C	2.46	129.58	124.94
22	f	101	LMG	O8-C28-C29	2.45	119.60	111.91
21	H	101	BCR	C4-C5-C6	-2.45	119.17	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	c	505	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	H	102	LMG	O8-C28-C29	2.45	119.59	111.91
19	b	505	CLA	CHD-C1D-ND	-2.45	122.21	124.45
23	b	520	LHG	O8-C23-C24	2.44	119.57	111.91
21	H	101	BCR	C29-C30-C25	2.44	114.24	110.48
19	B	505	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
21	V	101	BCR	C34-C9-C8	2.43	121.91	118.08
21	B	517	BCR	C32-C1-C6	-2.43	106.36	110.30
19	a	402	CLA	C7-C6-C5	-2.43	106.76	113.36
21	H	101	BCR	C15-C14-C13	-2.43	123.84	127.31
22	h	102	LMG	O8-C28-C29	2.43	119.52	111.91
28	d	406	PL9	C7-C8-C9	-2.42	122.75	126.79
21	C	516	BCR	C1-C6-C5	-2.42	119.20	122.61
21	C	515	BCR	C27-C26-C25	-2.42	119.21	122.73
19	C	505	CLA	CHD-C1D-ND	-2.42	122.23	124.45
23	B	521	LHG	O8-C23-C24	2.42	119.50	111.91
19	C	514	CLA	CHD-C1D-ND	-2.42	122.23	124.45
20	d	401	PHO	CMC-C2C-C3C	2.41	129.50	124.94
19	c	505	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	a	403	CLA	CHD-C1D-ND	-2.41	122.24	124.45
21	B	517	BCR	C16-C17-C18	-2.41	123.87	127.31
21	H	101	BCR	C38-C26-C25	-2.41	121.82	124.53
21	c	518	BCR	C15-C14-C13	-2.41	123.88	127.31
21	b	517	BCR	C16-C17-C18	-2.40	123.88	127.31
21	h	101	BCR	C15-C14-C13	-2.40	123.88	127.31
21	B	518	BCR	C15-C14-C13	-2.40	123.89	127.31
19	C	507	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	C	504	CLA	CHB-C4A-NA	2.40	127.82	124.51
19	b	514	CLA	CHB-C4A-NA	2.40	127.82	124.51
19	C	504	CLA	CHD-C1D-ND	-2.40	122.25	124.45
19	B	514	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	B	511	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
19	C	503	CLA	CMB-C2B-C3B	2.39	129.15	124.68
19	b	511	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
19	c	504	CLA	CMB-C2B-C3B	2.39	129.15	124.68
21	C	517	BCR	C15-C14-C13	-2.38	123.91	127.31
19	B	502	CLA	CHD-C1D-ND	-2.38	122.26	124.45
21	a	407	BCR	C33-C5-C4	2.38	118.19	113.62
19	B	512	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	c	502	LMG	C8-O7-C10	-2.38	111.93	117.79
19	b	502	CLA	CHD-C1D-ND	-2.38	122.27	124.45
21	c	517	BCR	C36-C18-C17	-2.38	119.59	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	517	BCR	C19-C18-C17	-2.38	115.29	118.94
28	D	406	PL9	C7-C8-C9	-2.38	122.84	126.79
19	b	509	CLA	CHB-C4A-NA	2.37	127.80	124.51
21	C	516	BCR	C30-C25-C26	-2.37	119.27	122.61
29	e	101	HEM	C4B-CHC-C1C	2.37	125.69	122.56
21	k	101	BCR	C15-C14-C13	-2.37	123.93	127.31
19	b	514	CLA	CHD-C1D-ND	-2.37	122.28	124.45
19	B	502	CLA	CHB-C4A-NA	2.37	127.79	124.51
21	C	515	BCR	C33-C5-C4	2.37	118.17	113.62
19	C	502	CLA	CMB-C2B-C3B	2.37	129.11	124.68
21	h	101	BCR	C2-C1-C6	2.37	114.12	110.48
19	d	404	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	a	406	CLA	CHB-C4A-NA	2.36	127.78	124.51
21	c	518	BCR	C8-C7-C6	-2.36	120.56	127.20
19	C	503	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
19	A	406	CLA	CHB-C4A-NA	2.36	127.78	124.51
21	b	518	BCR	C15-C14-C13	-2.36	123.94	127.31
20	A	405	PHO	CMB-C2B-C3B	2.36	129.09	124.68
19	C	507	CLA	CHD-C1D-ND	-2.36	122.28	124.45
19	c	515	CLA	CHD-C1D-ND	-2.36	122.28	124.45
19	C	510	CLA	CHB-C4A-NA	2.36	127.78	124.51
29	e	101	HEM	C4C-CHD-C1D	2.36	125.67	122.56
19	b	513	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	V	101	BCR	C15-C16-C17	-2.36	118.65	123.47
19	D	404	CLA	CHB-C4A-NA	2.35	127.77	124.51
21	k	101	BCR	C1-C6-C7	2.35	122.43	115.78
23	a	409	LHG	O8-C23-C24	2.35	119.29	111.91
19	c	504	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
19	B	509	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
21	c	517	BCR	C38-C26-C27	2.35	118.13	113.62
25	c	521	DGD	O1G-C1A-C2A	2.35	119.27	111.91
21	B	518	BCR	C38-C26-C27	2.35	118.12	113.62
19	C	502	CLA	CHD-C1D-ND	-2.34	122.30	124.45
21	c	518	BCR	C27-C26-C25	-2.34	119.33	122.73
21	B	517	BCR	C28-C27-C26	-2.34	109.89	114.08
21	c	516	BCR	C34-C9-C8	-2.34	114.39	118.08
19	B	503	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A	402	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A	403	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
19	B	513	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	c	503	CLA	CHD-C1D-ND	-2.34	122.31	124.45
19	a	403	CLA	O2D-CGD-CBD	2.33	115.42	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	503	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	C	508	CLA	C1-C2-C3	-2.33	122.01	126.04
21	C	515	BCR	C36-C18-C17	-2.33	119.66	122.92
19	b	507	CLA	CHB-C4A-NA	2.33	127.73	124.51
20	a	405	PHO	CMB-C2B-C3B	2.33	129.03	124.68
21	k	101	BCR	C16-C15-C14	-2.33	118.71	123.47
21	B	517	BCR	C19-C18-C17	-2.33	115.37	118.94
21	C	515	BCR	C3-C4-C5	-2.33	109.92	114.08
23	A	410	LHG	O8-C23-C24	2.33	119.20	111.91
25	C	520	DGD	O1G-C1A-C2A	2.32	119.20	111.91
20	A	405	PHO	O2A-CGA-O1A	-2.32	117.73	123.59
19	c	508	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	b	510	CLA	C1-C2-C3	-2.32	122.03	126.04
21	H	101	BCR	C27-C26-C25	-2.32	119.37	122.73
21	b	518	BCR	C38-C26-C27	2.32	118.07	113.62
26	c	523	LMU	O5B-C5B-C4B	2.32	113.90	109.69
19	a	403	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
26	C	522	LMU	O5B-C5B-C4B	2.31	113.89	109.69
20	a	405	PHO	O2A-CGA-O1A	-2.31	117.77	123.59
19	c	510	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	c	518	BCR	C15-C16-C17	-2.30	118.75	123.47
21	C	516	BCR	C33-C5-C4	2.30	118.04	113.62
21	a	407	BCR	C1-C6-C5	-2.30	119.37	122.61
19	b	508	CLA	CHB-C4A-NA	2.30	127.69	124.51
21	H	101	BCR	C2-C1-C6	2.30	114.02	110.48
19	B	508	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	b	502	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	c	511	CLA	CHB-C4A-NA	2.29	127.68	124.51
21	c	517	BCR	C33-C5-C4	2.29	118.02	113.62
19	B	507	CLA	CHB-C4A-NA	2.29	127.68	124.51
21	C	517	BCR	C37-C22-C21	-2.29	119.71	122.92
21	b	518	BCR	C3-C4-C5	-2.29	109.99	114.08
22	b	519	LMG	C8-O7-C10	-2.29	112.15	117.79
28	d	406	PL9	C27-C28-C29	-2.29	122.15	127.66
28	D	406	PL9	C27-C28-C29	-2.29	122.15	127.66
21	B	518	BCR	C36-C18-C17	-2.29	119.72	122.92
19	C	503	CLA	CHB-C4A-NA	2.28	127.67	124.51
19	a	402	CLA	CHB-C4A-NA	2.28	127.67	124.51
19	b	512	CLA	CHB-C4A-NA	2.28	127.67	124.51
19	b	511	CLA	CHB-C4A-NA	2.28	127.67	124.51
21	h	101	BCR	C27-C26-C25	-2.28	119.42	122.73
19	a	404	CLA	CHD-C1D-ND	-2.28	122.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	102	HEM	C4C-CHD-C1D	2.28	125.57	122.56
19	c	510	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
19	B	509	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	b	509	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
19	A	406	CLA	C1-C2-C3	-2.28	122.11	126.04
19	C	509	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	c	514	CLA	C1-C2-C3	-2.28	122.11	126.04
19	c	504	CLA	CHB-C4A-NA	2.28	127.66	124.51
21	B	518	BCR	C3-C4-C5	-2.28	110.01	114.08
21	C	515	BCR	C28-C27-C26	-2.28	110.01	114.08
21	C	517	BCR	C15-C16-C17	-2.27	118.82	123.47
19	C	514	CLA	CHB-C4A-NA	2.27	127.65	124.51
28	D	406	PL9	C20-C19-C21	2.27	119.09	115.27
21	V	101	BCR	C40-C30-C39	-2.27	101.56	108.53
19	a	406	CLA	C1-C2-C3	-2.27	122.12	126.04
19	C	513	CLA	C1-C2-C3	-2.27	122.12	126.04
19	C	510	CLA	CHD-C1D-ND	-2.27	122.37	124.45
19	c	504	CLA	CHD-C1D-ND	-2.27	122.37	124.45
19	A	404	CLA	CHD-C1D-ND	-2.26	122.37	124.45
19	b	503	CLA	CHD-C1D-ND	-2.26	122.37	124.45
19	B	511	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	B	519	LMG	C8-O7-C10	-2.26	112.22	117.79
19	B	514	CLA	CHD-C1D-ND	-2.26	122.38	124.45
21	b	517	BCR	C28-C27-C26	-2.26	110.04	114.08
19	B	503	CLA	CHD-C1D-ND	-2.26	122.38	124.45
21	w	101	BCR	C16-C15-C14	-2.26	118.84	123.47
21	V	101	BCR	C23-C22-C21	-2.26	115.47	118.94
21	a	407	BCR	C37-C22-C21	-2.26	119.76	122.92
19	C	509	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
21	k	101	BCR	C8-C9-C10	-2.25	115.48	118.94
19	c	511	CLA	CHD-C1D-ND	-2.25	122.39	124.45
19	b	506	CLA	CHB-C4A-NA	2.25	127.62	124.51
19	c	515	CLA	CHB-C4A-NA	2.25	127.62	124.51
21	A	407	BCR	C1-C6-C5	-2.25	119.44	122.61
19	b	510	CLA	CHB-C4A-NA	2.25	127.62	124.51
19	d	404	CLA	C1-C2-C3	-2.25	122.16	126.04
19	C	512	CLA	CHB-C4A-NA	2.24	127.62	124.51
19	C	506	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
19	b	511	CLA	CHD-C1D-ND	-2.24	122.40	124.45
21	w	101	BCR	C30-C25-C26	-2.24	119.46	122.61
19	c	508	CLA	CHD-C1D-ND	-2.24	122.40	124.45
21	c	516	BCR	C3-C4-C5	-2.23	110.09	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	502	CLA	CHB-C4A-NA	2.23	127.60	124.51
21	k	101	BCR	C2-C3-C4	-2.23	106.39	111.38
19	b	508	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
19	B	511	CLA	CHD-C1D-ND	-2.23	122.41	124.45
19	B	508	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
21	A	407	BCR	C37-C22-C21	-2.22	119.81	122.92
19	c	507	CLA	CHD-C1D-ND	-2.22	122.41	124.45
19	c	512	CLA	CHD-C1D-ND	-2.22	122.41	124.45
19	B	513	CLA	C1-C2-C3	-2.22	122.20	126.04
21	c	517	BCR	C11-C12-C13	-2.22	120.18	126.42
19	B	510	CLA	C1-C2-C3	-2.22	122.21	126.04
19	B	506	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	C	504	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
19	b	516	CLA	CHB-C4A-NA	2.21	127.56	124.51
19	b	510	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	B	501	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	b	501	CLA	CHD-C1D-ND	-2.20	122.43	124.45
21	W	101	BCR	C16-C15-C14	-2.20	118.97	123.47
19	B	510	CLA	CHB-C4A-NA	2.19	127.55	124.51
21	V	101	BCR	C12-C13-C14	-2.19	115.58	118.94
21	C	516	BCR	C36-C18-C17	-2.19	119.86	122.92
21	H	101	BCR	C11-C12-C13	-2.19	120.27	126.42
21	h	101	BCR	C16-C15-C14	-2.19	118.99	123.47
19	b	513	CLA	C1-C2-C3	-2.19	122.26	126.04
19	c	505	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
19	B	516	CLA	CHB-C4A-NA	2.19	127.53	124.51
21	c	518	BCR	C37-C22-C21	-2.18	119.87	122.92
21	A	407	BCR	C4-C5-C6	-2.18	119.57	122.73
19	B	509	CLA	C1-C2-C3	-2.18	122.28	126.04
21	A	407	BCR	C33-C5-C4	2.18	117.80	113.62
19	b	512	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
19	A	403	CLA	CHB-C4A-NA	2.18	127.52	124.51
19	c	503	CLA	CHB-C4A-NA	2.17	127.52	124.51
19	b	509	CLA	C1-C2-C3	-2.17	122.29	126.04
21	k	101	BCR	C15-C16-C17	-2.17	119.03	123.47
19	C	503	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	b	505	CLA	CHB-C4A-NA	2.17	127.51	124.51
19	d	404	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	C	517	BCR	C27-C26-C25	-2.16	119.59	122.73
19	c	513	CLA	CHB-C4A-NA	2.16	127.50	124.51
21	C	516	BCR	C11-C12-C13	-2.16	120.34	126.42
28	d	406	PL9	O1-C4-C3	-2.16	118.34	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	513	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	B	501	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	c	518	BCR	C32-C1-C6	-2.16	106.80	110.30
21	H	101	BCR	C16-C15-C14	-2.15	119.06	123.47
21	w	101	BCR	C4-C5-C6	-2.15	119.61	122.73
19	b	501	CLA	CHB-C4A-NA	2.15	127.49	124.51
28	d	406	PL9	C20-C19-C21	2.15	118.89	115.27
19	b	504	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	b	515	CLA	O2D-CGD-CBD	2.15	115.09	111.27
19	B	509	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	a	407	BCR	C2-C1-C6	2.14	113.78	110.48
19	a	403	CLA	CHB-C4A-NA	2.14	127.48	124.51
28	D	406	PL9	O1-C4-C3	-2.14	118.36	120.72
19	c	507	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
21	h	101	BCR	C11-C12-C13	-2.14	120.40	126.42
19	b	515	CLA	CHD-C1D-ND	-2.14	122.49	124.45
19	B	507	CLA	CHD-C1D-ND	-2.14	122.49	124.45
19	B	510	CLA	CHD-C1D-ND	-2.14	122.49	124.45
19	B	512	CLA	CHD-C1D-ND	-2.14	122.49	124.45
19	D	404	CLA	CHD-C1D-ND	-2.14	122.49	124.45
19	b	515	CLA	CMB-C2B-C3B	2.14	128.68	124.68
19	B	515	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	b	508	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	b	505	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	B	512	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
19	B	508	CLA	CHD-C1D-ND	-2.13	122.50	124.45
28	d	406	PL9	O2-C1-C6	2.12	124.27	120.59
19	b	512	CLA	CHD-C1D-ND	-2.12	122.50	124.45
19	c	507	CLA	CHB-C4A-NA	2.12	127.44	124.51
28	D	406	PL9	C31-C32-C33	-2.12	104.92	111.88
19	b	503	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
19	C	511	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	c	501	SQD	O9-S-C6	2.11	109.45	106.94
19	a	404	CLA	CHB-C4A-NA	2.11	127.44	124.51
19	A	403	CLA	O2D-CGD-CBD	2.11	115.02	111.27
21	b	517	BCR	C1-C6-C5	-2.11	119.64	122.61
19	A	404	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
21	V	101	BCR	C7-C6-C5	-2.11	116.35	121.46
19	D	403	CLA	CHB-C4A-NA	2.11	127.43	124.51
21	V	101	BCR	C16-C15-C14	-2.11	119.15	123.47
21	B	518	BCR	C24-C23-C22	-2.11	123.05	126.23
19	B	503	CLA	O2A-CGA-O1A	-2.11	118.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	509	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	B	515	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	B	506	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
21	D	405	BCR	C4-C5-C6	-2.10	119.68	122.73
19	B	508	CLA	C1-C2-C3	-2.10	122.42	126.04
21	k	101	BCR	C2-C1-C6	2.10	113.71	110.48
28	D	406	PL9	O2-C1-C6	2.09	124.22	120.59
21	W	101	BCR	C30-C25-C24	2.09	121.70	115.78
19	c	506	CLA	CHB-C4A-NA	2.09	127.41	124.51
19	C	505	CLA	CHB-C4A-NA	2.09	127.40	124.51
19	B	505	CLA	CHB-C4A-NA	2.09	127.40	124.51
21	b	518	BCR	C36-C18-C17	-2.09	120.00	122.92
19	b	515	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
19	b	506	CLA	CHD-C1D-ND	-2.09	122.54	124.45
28	d	406	PL9	C32-C33-C34	-2.09	122.64	127.66
19	b	505	CLA	CMB-C2B-C3B	2.09	128.58	124.68
19	B	506	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	C	517	BCR	C32-C1-C6	-2.08	106.92	110.30
21	k	101	BCR	C11-C10-C9	-2.08	124.34	127.31
21	c	516	BCR	C28-C27-C26	-2.08	110.36	114.08
24	C	501	SQD	O9-S-C6	2.08	109.41	106.94
19	d	403	CLA	CHB-C4A-NA	2.08	127.39	124.51
19	A	402	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
21	k	101	BCR	C23-C24-C25	-2.08	121.37	127.20
21	b	518	BCR	C24-C23-C22	-2.08	123.10	126.23
19	B	513	CLA	CHD-C1D-ND	-2.08	122.55	124.45
19	C	506	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	A	404	CLA	O2D-CGD-CBD	2.07	114.95	111.27
19	B	504	CLA	CHD-C1D-ND	-2.07	122.55	124.45
24	C	501	SQD	O8-S-C6	2.07	109.04	105.74
19	a	402	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
19	a	404	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
21	d	405	BCR	C4-C5-C6	-2.06	119.74	122.73
19	B	516	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
21	B	517	BCR	C27-C26-C25	-2.06	119.74	122.73
19	A	404	CLA	CHB-C4A-NA	2.06	127.36	124.51
28	D	406	PL9	O2-C1-C2	-2.06	117.06	121.78
27	D	402	BCT	O3-C-O1	-2.06	114.20	119.55
19	c	509	CLA	C1-C2-C3	-2.06	122.48	126.04
24	c	501	SQD	O8-S-C6	2.06	109.02	105.74
19	b	510	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
21	w	101	BCR	C20-C19-C18	-2.06	120.64	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	406	PL9	C31-C32-C33	-2.05	105.13	111.88
19	C	502	CLA	C1-C2-C3	-2.05	122.49	126.04
28	d	406	PL9	O2-C1-C2	-2.05	117.08	121.78
19	B	510	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
19	C	504	CLA	C1-C2-C3	-2.05	122.51	126.04
19	d	404	CLA	C4-C3-C5	2.04	118.71	115.27
19	C	502	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
19	c	509	CLA	O2D-CGD-CBD	2.04	114.90	111.27
21	h	101	BCR	C31-C1-C6	-2.04	106.99	110.30
28	D	406	PL9	C32-C33-C34	-2.04	122.75	127.66
21	W	101	BCR	C23-C24-C25	-2.04	121.47	127.20
19	B	511	CLA	O1D-CGD-CBD	2.04	128.66	124.48
21	c	518	BCR	C11-C10-C9	-2.04	124.40	127.31
25	c	519	DGD	C2G-O2G-C1B	-2.04	112.78	117.79
19	B	515	CLA	O2D-CGD-CBD	2.04	114.89	111.27
19	A	406	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	B	516	CLA	CHD-C1D-ND	-2.03	122.58	124.45
21	c	516	BCR	C27-C26-C25	-2.03	119.78	122.73
19	d	403	CLA	CHD-C1D-ND	-2.03	122.58	124.45
21	h	101	BCR	C29-C30-C25	2.03	113.61	110.48
21	a	407	BCR	C16-C15-C14	-2.03	119.31	123.47
21	c	516	BCR	C37-C22-C21	-2.03	120.08	122.92
19	c	505	CLA	C1-C2-C3	-2.03	122.54	126.04
19	B	502	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
19	b	516	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
19	b	506	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
21	A	407	BCR	C2-C1-C6	2.02	113.59	110.48
27	d	402	BCT	O3-C-O1	-2.02	114.31	119.55
21	H	101	BCR	C31-C1-C6	-2.02	107.03	110.30
25	C	518	DGD	C2G-O2G-C1B	-2.02	112.83	117.79
19	b	511	CLA	O1D-CGD-CBD	2.02	128.61	124.48
21	B	518	BCR	C29-C30-C25	2.01	113.58	110.48
19	b	502	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
21	a	407	BCR	C35-C13-C14	-2.01	120.11	122.92
19	c	503	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	a	402	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	W	101	BCR	C36-C18-C17	-2.01	120.11	122.92
19	C	508	CLA	O2D-CGD-CBD	2.01	114.83	111.27
19	b	507	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	C	512	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
21	w	101	BCR	C15-C16-C17	-2.00	119.38	123.47
21	V	101	BCR	C21-C20-C19	-2.00	116.97	123.22

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	402	CLA	ND
19	A	403	CLA	ND
19	A	404	CLA	ND
19	A	406	CLA	ND
19	B	501	CLA	ND
19	B	502	CLA	ND
19	B	503	CLA	ND
19	B	504	CLA	ND
19	B	506	CLA	ND
19	B	507	CLA	ND
19	B	508	CLA	ND
19	B	509	CLA	ND
19	B	510	CLA	ND
19	B	511	CLA	ND
19	B	512	CLA	ND
19	B	513	CLA	ND
19	B	514	CLA	ND
19	B	515	CLA	ND
19	B	516	CLA	ND
19	C	502	CLA	ND
19	C	503	CLA	ND
19	C	504	CLA	ND
19	C	505	CLA	ND
19	C	506	CLA	ND
19	C	507	CLA	ND
19	C	508	CLA	ND
19	C	509	CLA	ND
19	C	510	CLA	ND
19	C	511	CLA	ND
19	C	512	CLA	ND
19	C	513	CLA	ND
19	C	514	CLA	ND
19	D	403	CLA	ND
19	D	404	CLA	ND
19	a	402	CLA	ND
19	a	403	CLA	ND
19	a	404	CLA	ND
19	a	406	CLA	ND
19	b	501	CLA	ND
19	b	502	CLA	ND
19	b	503	CLA	ND
19	b	504	CLA	ND

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Mol	Chain	Res	Type	Atom
19	b	505	CLA	ND
19	b	506	CLA	ND
19	b	507	CLA	ND
19	b	508	CLA	ND
19	b	509	CLA	ND
19	b	510	CLA	ND
19	b	511	CLA	ND
19	b	512	CLA	ND
19	b	513	CLA	ND
19	b	514	CLA	ND
19	b	515	CLA	ND
19	b	516	CLA	ND
19	c	503	CLA	ND
19	c	504	CLA	ND
19	c	505	CLA	ND
19	c	506	CLA	ND
19	c	507	CLA	ND
19	c	508	CLA	ND
19	c	509	CLA	ND
19	c	510	CLA	ND
19	c	511	CLA	ND
19	c	512	CLA	ND
19	c	513	CLA	ND
19	c	514	CLA	ND
19	c	515	CLA	ND
19	d	403	CLA	ND
19	d	404	CLA	ND

All (1327) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	403	CLA	C3A-C2A-CAA-CBA
19	A	406	CLA	C1A-C2A-CAA-CBA
19	A	406	CLA	C3A-C2A-CAA-CBA
19	B	501	CLA	C1A-C2A-CAA-CBA
19	B	501	CLA	CBD-CGD-O2D-CED
19	B	503	CLA	C1A-C2A-CAA-CBA
19	B	503	CLA	C3A-C2A-CAA-CBA
19	B	504	CLA	CAD-CBD-CGD-O1D
19	B	504	CLA	CAD-CBD-CGD-O2D
19	B	506	CLA	C1A-C2A-CAA-CBA
19	B	506	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	506	CLA	CHA-CBD-CGD-O1D
19	B	506	CLA	CHA-CBD-CGD-O2D
19	B	507	CLA	C1A-C2A-CAA-CBA
19	B	507	CLA	C3A-C2A-CAA-CBA
19	B	509	CLA	C3A-C2A-CAA-CBA
19	B	509	CLA	CHA-CBD-CGD-O1D
19	B	509	CLA	CHA-CBD-CGD-O2D
19	B	509	CLA	CAD-CBD-CGD-O1D
19	B	509	CLA	CBD-CGD-O2D-CED
19	B	511	CLA	CHA-CBD-CGD-O1D
19	B	511	CLA	CHA-CBD-CGD-O2D
19	B	511	CLA	CAD-CBD-CGD-O1D
19	B	511	CLA	CAD-CBD-CGD-O2D
19	B	511	CLA	CBD-CGD-O2D-CED
19	B	514	CLA	CHA-CBD-CGD-O1D
19	B	514	CLA	CHA-CBD-CGD-O2D
19	B	514	CLA	CAD-CBD-CGD-O1D
19	B	514	CLA	CAD-CBD-CGD-O2D
19	B	516	CLA	CHA-CBD-CGD-O1D
19	B	516	CLA	CHA-CBD-CGD-O2D
19	B	516	CLA	CAD-CBD-CGD-O1D
19	C	502	CLA	C3A-C2A-CAA-CBA
19	C	502	CLA	CHA-CBD-CGD-O1D
19	C	502	CLA	CHA-CBD-CGD-O2D
19	C	502	CLA	CAD-CBD-CGD-O1D
19	C	502	CLA	CAD-CBD-CGD-O2D
19	C	503	CLA	CHA-CBD-CGD-O1D
19	C	503	CLA	CHA-CBD-CGD-O2D
19	C	503	CLA	CAD-CBD-CGD-O1D
19	C	503	CLA	CBD-CGD-O2D-CED
19	C	504	CLA	C1A-C2A-CAA-CBA
19	C	506	CLA	CHA-CBD-CGD-O1D
19	C	506	CLA	CHA-CBD-CGD-O2D
19	C	507	CLA	C1A-C2A-CAA-CBA
19	C	507	CLA	C3A-C2A-CAA-CBA
19	C	508	CLA	CHA-CBD-CGD-O2D
19	C	512	CLA	CHA-CBD-CGD-O1D
19	C	512	CLA	CHA-CBD-CGD-O2D
19	C	512	CLA	CAD-CBD-CGD-O1D
19	C	512	CLA	CAD-CBD-CGD-O2D
19	C	513	CLA	CHA-CBD-CGD-O1D
19	C	513	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	C	514	CLA	CBD-CGD-O2D-CED
19	D	404	CLA	CHA-CBD-CGD-O1D
19	D	404	CLA	CHA-CBD-CGD-O2D
19	D	404	CLA	CAD-CBD-CGD-O1D
19	D	404	CLA	C2-C3-C5-C6
19	D	404	CLA	C4-C3-C5-C6
19	a	402	CLA	CBD-CGD-O2D-CED
19	a	403	CLA	C3A-C2A-CAA-CBA
19	a	403	CLA	O1A-CGA-O2A-C1
19	a	406	CLA	C1A-C2A-CAA-CBA
19	a	406	CLA	C3A-C2A-CAA-CBA
19	b	501	CLA	C1A-C2A-CAA-CBA
19	b	501	CLA	CBD-CGD-O2D-CED
19	b	503	CLA	C1A-C2A-CAA-CBA
19	b	503	CLA	C3A-C2A-CAA-CBA
19	b	504	CLA	CAD-CBD-CGD-O1D
19	b	504	CLA	CAD-CBD-CGD-O2D
19	b	505	CLA	C1A-C2A-CAA-CBA
19	b	506	CLA	C1A-C2A-CAA-CBA
19	b	506	CLA	C3A-C2A-CAA-CBA
19	b	506	CLA	CHA-CBD-CGD-O1D
19	b	506	CLA	CHA-CBD-CGD-O2D
19	b	506	CLA	CAD-CBD-CGD-O1D
19	b	507	CLA	C1A-C2A-CAA-CBA
19	b	507	CLA	C3A-C2A-CAA-CBA
19	b	509	CLA	C1A-C2A-CAA-CBA
19	b	509	CLA	C3A-C2A-CAA-CBA
19	b	509	CLA	CHA-CBD-CGD-O1D
19	b	509	CLA	CHA-CBD-CGD-O2D
19	b	509	CLA	CAD-CBD-CGD-O1D
19	b	509	CLA	CBD-CGD-O2D-CED
19	b	511	CLA	CHA-CBD-CGD-O1D
19	b	511	CLA	CHA-CBD-CGD-O2D
19	b	511	CLA	CAD-CBD-CGD-O1D
19	b	511	CLA	CAD-CBD-CGD-O2D
19	b	514	CLA	CHA-CBD-CGD-O1D
19	b	514	CLA	CHA-CBD-CGD-O2D
19	b	514	CLA	CAD-CBD-CGD-O1D
19	b	514	CLA	CAD-CBD-CGD-O2D
19	b	515	CLA	O2A-C1-C2-C3
19	b	516	CLA	CHA-CBD-CGD-O1D
19	b	516	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	b	516	CLA	CAD-CBD-CGD-O1D
19	b	516	CLA	CAD-CBD-CGD-O2D
19	c	503	CLA	C3A-C2A-CAA-CBA
19	c	503	CLA	CHA-CBD-CGD-O1D
19	c	503	CLA	CHA-CBD-CGD-O2D
19	c	503	CLA	CAD-CBD-CGD-O1D
19	c	503	CLA	CBD-CGD-O2D-CED
19	c	504	CLA	CHA-CBD-CGD-O1D
19	c	504	CLA	CHA-CBD-CGD-O2D
19	c	504	CLA	CAD-CBD-CGD-O1D
19	c	504	CLA	CBD-CGD-O2D-CED
19	c	505	CLA	C1A-C2A-CAA-CBA
19	c	507	CLA	C1A-C2A-CAA-CBA
19	c	507	CLA	CHA-CBD-CGD-O1D
19	c	507	CLA	CHA-CBD-CGD-O2D
19	c	508	CLA	C1A-C2A-CAA-CBA
19	c	509	CLA	CHA-CBD-CGD-O2D
19	c	513	CLA	CHA-CBD-CGD-O1D
19	c	513	CLA	CHA-CBD-CGD-O2D
19	c	513	CLA	CAD-CBD-CGD-O1D
19	c	513	CLA	CAD-CBD-CGD-O2D
19	c	514	CLA	CHA-CBD-CGD-O1D
19	c	514	CLA	CHA-CBD-CGD-O2D
19	d	404	CLA	CHA-CBD-CGD-O1D
19	d	404	CLA	CHA-CBD-CGD-O2D
19	d	404	CLA	CAD-CBD-CGD-O1D
21	A	407	BCR	C5-C6-C7-C8
21	A	407	BCR	C23-C24-C25-C26
21	B	517	BCR	C23-C24-C25-C26
21	B	517	BCR	C23-C24-C25-C30
21	B	518	BCR	C5-C6-C7-C8
21	C	515	BCR	C23-C24-C25-C26
21	C	516	BCR	C5-C6-C7-C8
21	C	516	BCR	C23-C24-C25-C26
21	D	405	BCR	C1-C6-C7-C8
21	D	405	BCR	C5-C6-C7-C8
21	D	405	BCR	C23-C24-C25-C26
21	D	405	BCR	C23-C24-C25-C30
21	H	101	BCR	C1-C6-C7-C8
21	H	101	BCR	C5-C6-C7-C8
21	H	101	BCR	C23-C24-C25-C26
21	a	407	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	a	407	BCR	C23-C24-C25-C26
21	b	517	BCR	C23-C24-C25-C26
21	b	517	BCR	C23-C24-C25-C30
21	b	518	BCR	C5-C6-C7-C8
21	c	516	BCR	C23-C24-C25-C26
21	c	517	BCR	C5-C6-C7-C8
21	c	517	BCR	C23-C24-C25-C26
21	d	405	BCR	C1-C6-C7-C8
21	d	405	BCR	C5-C6-C7-C8
21	d	405	BCR	C23-C24-C25-C26
21	d	405	BCR	C23-C24-C25-C30
21	h	101	BCR	C1-C6-C7-C8
21	h	101	BCR	C5-C6-C7-C8
21	h	101	BCR	C23-C24-C25-C26
21	w	101	BCR	C17-C18-C19-C20
21	w	101	BCR	C36-C18-C19-C20
22	A	408	LMG	O6-C1-O1-C7
22	c	502	LMG	O6-C1-O1-C7
23	A	410	LHG	C3-O3-P-O4
23	A	410	LHG	C3-O3-P-O5
23	A	410	LHG	C4-O6-P-O5
23	B	520	LHG	C3-O3-P-O4
23	B	520	LHG	C4-O6-P-O3
23	B	520	LHG	C4-O6-P-O4
23	B	520	LHG	C4-O6-P-O5
23	D	407	LHG	C3-O3-P-O5
23	D	407	LHG	C4-O6-P-O3
23	L	101	LHG	C3-O3-P-O6
23	X	101	LHG	C4-O6-P-O4
23	a	409	LHG	C3-O3-P-O4
23	a	409	LHG	C4-O6-P-O5
23	d	407	LHG	C3-O3-P-O4
23	d	407	LHG	C4-O6-P-O3
23	d	407	LHG	C4-O6-P-O4
23	d	407	LHG	C4-O6-P-O5
23	d	408	LHG	C3-O3-P-O5
23	d	408	LHG	C3-O3-P-O6
23	d	408	LHG	C4-O6-P-O3
23	l	101	LHG	C3-O3-P-O4
23	x	101	LHG	C4-O6-P-O4
24	C	501	SQD	C5-C6-S-O7
24	c	501	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
25	C	519	DGD	C4D-C5D-C6D-O5D
25	c	520	DGD	C4D-C5D-C6D-O5D
26	C	522	LMU	O5B-C1B-O1B-C4'
26	c	523	LMU	O5B-C1B-O1B-C4'
28	D	406	PL9	C42-C43-C44-C46
28	D	406	PL9	C47-C48-C49-C51
19	b	509	CLA	O1D-CGD-O2D-CED
19	B	509	CLA	O1D-CGD-O2D-CED
19	A	402	CLA	CBD-CGD-O2D-CED
19	B	505	CLA	CBD-CGD-O2D-CED
19	B	507	CLA	CBD-CGD-O2D-CED
19	C	504	CLA	CBD-CGD-O2D-CED
19	C	507	CLA	CBD-CGD-O2D-CED
19	b	505	CLA	CBD-CGD-O2D-CED
19	b	506	CLA	CBD-CGD-O2D-CED
19	b	507	CLA	CBD-CGD-O2D-CED
19	b	511	CLA	CBD-CGD-O2D-CED
19	c	508	CLA	CBD-CGD-O2D-CED
19	c	515	CLA	CBD-CGD-O2D-CED
19	B	505	CLA	O1D-CGD-O2D-CED
19	C	507	CLA	O1D-CGD-O2D-CED
19	c	508	CLA	O1D-CGD-O2D-CED
19	c	515	CLA	O1D-CGD-O2D-CED
19	A	402	CLA	O1D-CGD-O2D-CED
19	B	511	CLA	O1D-CGD-O2D-CED
19	C	514	CLA	O1D-CGD-O2D-CED
19	a	402	CLA	O1D-CGD-O2D-CED
19	b	501	CLA	O1D-CGD-O2D-CED
19	c	503	CLA	O1D-CGD-O2D-CED
19	c	504	CLA	O1D-CGD-O2D-CED
19	a	403	CLA	CBA-CGA-O2A-C1
28	d	406	PL9	C47-C48-C49-C51
19	C	512	CLA	CBD-CGD-O2D-CED
19	c	513	CLA	CBD-CGD-O2D-CED
20	D	401	PHO	CBD-CGD-O2D-CED
20	d	401	PHO	CBD-CGD-O2D-CED
19	A	403	CLA	O1A-CGA-O2A-C1
19	B	505	CLA	O1A-CGA-O2A-C1
19	B	508	CLA	O1A-CGA-O2A-C1
19	C	507	CLA	O1A-CGA-O2A-C1
19	b	505	CLA	O1A-CGA-O2A-C1
19	b	508	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	c	508	CLA	O1A-CGA-O2A-C1
20	A	405	PHO	O1A-CGA-O2A-C1
20	a	405	PHO	O1A-CGA-O2A-C1
19	B	501	CLA	O1D-CGD-O2D-CED
19	C	503	CLA	O1D-CGD-O2D-CED
25	C	520	DGD	O6D-C5D-C6D-O5D
19	A	406	CLA	C3-C5-C6-C7
19	B	503	CLA	C3-C5-C6-C7
19	C	513	CLA	C3-C5-C6-C7
19	a	406	CLA	C3-C5-C6-C7
19	b	503	CLA	C3-C5-C6-C7
19	c	514	CLA	C3-C5-C6-C7
20	d	401	PHO	C3-C5-C6-C7
19	A	403	CLA	CBA-CGA-O2A-C1
19	A	406	CLA	CBA-CGA-O2A-C1
19	B	507	CLA	CBA-CGA-O2A-C1
19	b	506	CLA	CBA-CGA-O2A-C1
19	b	507	CLA	CBA-CGA-O2A-C1
20	A	405	PHO	CBA-CGA-O2A-C1
20	a	405	PHO	CBA-CGA-O2A-C1
19	c	510	CLA	CBD-CGD-O2D-CED
25	C	519	DGD	O6D-C5D-C6D-O5D
25	c	520	DGD	O6D-C5D-C6D-O5D
25	C	520	DGD	C4D-C5D-C6D-O5D
19	B	511	CLA	C2A-CAA-CBA-CGA
19	C	503	CLA	C2A-CAA-CBA-CGA
19	b	511	CLA	C2A-CAA-CBA-CGA
19	c	504	CLA	C2A-CAA-CBA-CGA
19	B	511	CLA	O1A-CGA-O2A-C1
19	C	507	CLA	C3-C5-C6-C7
19	B	502	CLA	CBA-CGA-O2A-C1
19	B	505	CLA	CBA-CGA-O2A-C1
19	B	506	CLA	CBA-CGA-O2A-C1
19	B	508	CLA	CBA-CGA-O2A-C1
19	C	507	CLA	CBA-CGA-O2A-C1
19	C	509	CLA	CBA-CGA-O2A-C1
19	a	406	CLA	CBA-CGA-O2A-C1
19	b	502	CLA	CBA-CGA-O2A-C1
19	b	505	CLA	CBA-CGA-O2A-C1
19	b	508	CLA	CBA-CGA-O2A-C1
19	c	508	CLA	CBA-CGA-O2A-C1
19	c	510	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	c	521	DGD	O6D-C5D-C6D-O5D
19	B	507	CLA	O1D-CGD-O2D-CED
19	b	507	CLA	O1D-CGD-O2D-CED
28	d	406	PL9	C47-C48-C49-C50
19	C	504	CLA	O1D-CGD-O2D-CED
19	b	505	CLA	O1D-CGD-O2D-CED
19	B	502	CLA	O1A-CGA-O2A-C1
19	C	509	CLA	O1A-CGA-O2A-C1
19	b	502	CLA	O1A-CGA-O2A-C1
19	b	506	CLA	O1A-CGA-O2A-C1
19	b	511	CLA	O1A-CGA-O2A-C1
19	c	510	CLA	O1A-CGA-O2A-C1
21	w	101	BCR	C13-C14-C15-C16
19	C	509	CLA	CBD-CGD-O2D-CED
19	b	503	CLA	CBD-CGD-O2D-CED
19	b	511	CLA	O1D-CGD-O2D-CED
19	B	508	CLA	C3-C5-C6-C7
19	b	508	CLA	C3-C5-C6-C7
19	c	508	CLA	C3-C5-C6-C7
19	d	404	CLA	C3-C5-C6-C7
20	D	401	PHO	C3-C5-C6-C7
25	c	521	DGD	C4D-C5D-C6D-O5D
19	C	506	CLA	CBA-CGA-O2A-C1
19	A	406	CLA	O1A-CGA-O2A-C1
19	B	507	CLA	O1A-CGA-O2A-C1
19	a	406	CLA	O1A-CGA-O2A-C1
19	b	507	CLA	O1A-CGA-O2A-C1
28	D	406	PL9	C47-C48-C49-C50
19	a	404	CLA	CBD-CGD-O2D-CED
19	c	505	CLA	CBD-CGD-O2D-CED
19	B	511	CLA	CBA-CGA-O2A-C1
19	b	511	CLA	CBA-CGA-O2A-C1
19	B	506	CLA	O1A-CGA-O2A-C1
19	C	506	CLA	O1A-CGA-O2A-C1
19	C	505	CLA	CBA-CGA-O2A-C1
19	c	506	CLA	CBA-CGA-O2A-C1
19	c	507	CLA	CBA-CGA-O2A-C1
19	b	506	CLA	O1D-CGD-O2D-CED
20	d	401	PHO	O1D-CGD-O2D-CED
19	C	512	CLA	O1D-CGD-O2D-CED
19	c	507	CLA	O1A-CGA-O2A-C1
19	A	402	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	509	CLA	CBA-CGA-O2A-C1
19	B	510	CLA	CBA-CGA-O2A-C1
19	C	514	CLA	CBA-CGA-O2A-C1
19	a	402	CLA	CBA-CGA-O2A-C1
19	b	509	CLA	CBA-CGA-O2A-C1
19	b	510	CLA	CBA-CGA-O2A-C1
19	c	515	CLA	CBA-CGA-O2A-C1
23	A	409	LHG	O6-C4-C5-O7
22	h	102	LMG	O7-C8-C9-O8
19	B	509	CLA	O1A-CGA-O2A-C1
19	B	507	CLA	C4-C3-C5-C6
19	b	507	CLA	C4-C3-C5-C6
19	B	509	CLA	C6-C7-C8-C9
19	B	511	CLA	C11-C12-C13-C14
19	C	505	CLA	C11-C12-C13-C14
19	C	514	CLA	C11-C10-C8-C9
19	D	404	CLA	C6-C7-C8-C9
19	b	509	CLA	C6-C7-C8-C9
19	b	511	CLA	C11-C12-C13-C14
19	c	506	CLA	C6-C7-C8-C9
19	c	506	CLA	C11-C12-C13-C14
19	c	515	CLA	C11-C10-C8-C9
19	d	404	CLA	C6-C7-C8-C9
20	D	401	PHO	O1D-CGD-O2D-CED
21	C	515	BCR	C7-C8-C9-C34
21	c	516	BCR	C7-C8-C9-C34
21	w	101	BCR	C7-C8-C9-C34
21	w	101	BCR	C11-C12-C13-C35
21	C	515	BCR	C7-C8-C9-C10
21	c	516	BCR	C7-C8-C9-C10
21	w	101	BCR	C7-C8-C9-C10
19	b	509	CLA	O1A-CGA-O2A-C1
19	C	508	CLA	C8-C10-C11-C12
19	c	513	CLA	O1D-CGD-O2D-CED
19	B	512	CLA	CBA-CGA-O2A-C1
19	B	504	CLA	C10-C11-C12-C13
19	c	503	CLA	C13-C15-C16-C17
19	C	502	CLA	C13-C15-C16-C17
19	c	509	CLA	C8-C10-C11-C12
19	D	404	CLA	CBD-CGD-O2D-CED
19	b	516	CLA	C10-C11-C12-C13
19	B	507	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	b	512	CLA	CBA-CGA-O2A-C1
22	f	101	LMG	O6-C5-C6-O5
25	C	518	DGD	O6E-C5E-C6E-O5E
25	c	519	DGD	O6E-C5E-C6E-O5E
19	A	403	CLA	C2-C1-O2A-CGA
19	C	509	CLA	C2-C1-O2A-CGA
19	a	403	CLA	C2-C1-O2A-CGA
19	c	510	CLA	C2-C1-O2A-CGA
19	b	504	CLA	C10-C11-C12-C13
19	b	510	CLA	C15-C16-C17-C18
19	b	502	CLA	C5-C6-C7-C8
19	B	508	CLA	C11-C12-C13-C15
19	B	511	CLA	C11-C12-C13-C15
19	C	503	CLA	C12-C13-C15-C16
19	c	514	CLA	C11-C12-C13-C15
19	b	507	CLA	C3-C5-C6-C7
19	b	510	CLA	O1A-CGA-O2A-C1
19	B	502	CLA	C5-C6-C7-C8
19	C	509	CLA	C5-C6-C7-C8
19	A	402	CLA	O1A-CGA-O2A-C1
19	B	510	CLA	O1A-CGA-O2A-C1
19	B	503	CLA	CBD-CGD-O2D-CED
19	c	506	CLA	CBD-CGD-O2D-CED
22	F	101	LMG	C10-C11-C12-C13
19	D	404	CLA	C3-C5-C6-C7
19	B	511	CLA	C13-C15-C16-C17
19	c	510	CLA	C5-C6-C7-C8
20	d	401	PHO	CBA-CGA-O2A-C1
19	C	505	CLA	O1A-CGA-O2A-C1
19	C	514	CLA	O1A-CGA-O2A-C1
19	a	402	CLA	O1A-CGA-O2A-C1
19	c	506	CLA	O1A-CGA-O2A-C1
19	c	515	CLA	O1A-CGA-O2A-C1
19	A	402	CLA	C15-C16-C17-C18
19	B	515	CLA	C8-C10-C11-C12
19	C	513	CLA	C8-C10-C11-C12
19	a	402	CLA	C15-C16-C17-C18
19	b	515	CLA	C8-C10-C11-C12
19	c	514	CLA	C8-C10-C11-C12
19	B	512	CLA	O1A-CGA-O2A-C1
23	A	410	LHG	C3-O3-P-O6
23	A	410	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
23	B	520	LHG	C3-O3-P-O6
23	B	521	LHG	C4-O6-P-O3
23	X	101	LHG	C4-O6-P-O3
23	a	409	LHG	C3-O3-P-O6
23	a	409	LHG	C4-O6-P-O3
23	b	520	LHG	C4-O6-P-O3
23	d	407	LHG	C3-O3-P-O6
23	l	101	LHG	C3-O3-P-O6
23	x	101	LHG	C3-O3-P-O6
23	x	101	LHG	C4-O6-P-O3
23	d	407	LHG	C23-C24-C25-C26
19	B	513	CLA	CBA-CGA-O2A-C1
19	a	404	CLA	CBA-CGA-O2A-C1
19	c	510	CLA	O1D-CGD-O2D-CED
19	d	404	CLA	C4-C3-C5-C6
19	b	507	CLA	C2-C3-C5-C6
19	C	514	CLA	C2A-CAA-CBA-CGA
22	F	101	LMG	O6-C5-C6-O5
19	A	404	CLA	CBA-CGA-O2A-C1
19	D	404	CLA	CBA-CGA-O2A-C1
19	b	513	CLA	CBA-CGA-O2A-C1
19	d	404	CLA	CBA-CGA-O2A-C1
20	D	401	PHO	CBA-CGA-O2A-C1
22	f	101	LMG	C10-C11-C12-C13
23	X	101	LHG	C8-C7-O7-C5
23	A	410	LHG	C29-C30-C31-C32
19	c	515	CLA	C16-C17-C18-C20
23	A	410	LHG	C31-C32-C33-C34
23	a	409	LHG	C31-C32-C33-C34
23	x	101	LHG	C26-C27-C28-C29
22	C	521	LMG	C37-C38-C39-C40
22	c	522	LMG	C37-C38-C39-C40
23	a	409	LHG	C29-C30-C31-C32
22	F	101	LMG	C28-C29-C30-C31
19	C	510	CLA	CBA-CGA-O2A-C1
23	X	101	LHG	C26-C27-C28-C29
19	a	404	CLA	O1A-CGA-O2A-C1
19	b	512	CLA	O1A-CGA-O2A-C1
19	b	513	CLA	O1A-CGA-O2A-C1
20	D	401	PHO	O1A-CGA-O2A-C1
19	C	514	CLA	C16-C17-C18-C20
28	d	406	PL9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
19	B	507	CLA	C2-C3-C5-C6
19	B	502	CLA	C6-C7-C8-C9
19	B	510	CLA	C11-C10-C8-C9
19	B	511	CLA	C6-C7-C8-C9
19	C	503	CLA	C6-C7-C8-C9
19	C	510	CLA	C14-C13-C15-C16
19	C	513	CLA	C11-C12-C13-C14
19	a	403	CLA	C11-C12-C13-C14
19	b	510	CLA	C11-C10-C8-C9
19	b	511	CLA	C6-C7-C8-C9
19	c	504	CLA	C6-C7-C8-C9
19	c	511	CLA	C11-C12-C13-C14
19	c	511	CLA	C14-C13-C15-C16
22	f	101	LMG	C28-C29-C30-C31
19	B	513	CLA	O1A-CGA-O2A-C1
23	X	101	LHG	O9-C7-O7-C5
19	C	509	CLA	O1D-CGD-O2D-CED
19	b	503	CLA	O1D-CGD-O2D-CED
19	D	404	CLA	O1A-CGA-O2A-C1
19	d	404	CLA	O1A-CGA-O2A-C1
19	B	501	CLA	C3A-C2A-CAA-CBA
19	B	504	CLA	C3A-C2A-CAA-CBA
19	C	508	CLA	C3A-C2A-CAA-CBA
19	D	403	CLA	C3A-C2A-CAA-CBA
19	b	501	CLA	C3A-C2A-CAA-CBA
19	b	504	CLA	C3A-C2A-CAA-CBA
19	c	509	CLA	C3A-C2A-CAA-CBA
19	d	403	CLA	C3A-C2A-CAA-CBA
19	b	504	CLA	C8-C10-C11-C12
19	A	404	CLA	O1A-CGA-O2A-C1
20	d	401	PHO	O1A-CGA-O2A-C1
19	C	514	CLA	C16-C17-C18-C19
23	a	409	LHG	C12-C13-C14-C15
22	A	408	LMG	O1-C7-C8-C9
23	b	520	LHG	C4-C5-C6-O8
23	x	101	LHG	C4-C5-C6-O8
23	A	410	LHG	C12-C13-C14-C15
23	A	410	LHG	C7-C8-C9-C10
23	a	409	LHG	C7-C8-C9-C10
20	A	405	PHO	C4-C3-C5-C6
20	a	405	PHO	C4-C3-C5-C6
19	c	511	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	405	PHO	C2-C3-C5-C6
20	a	405	PHO	C2-C3-C5-C6
23	x	101	LHG	C8-C7-O7-C5
19	B	501	CLA	C2C-C3C-CAC-CBC
25	C	518	DGD	C4B-C5B-C6B-C7B
23	B	520	LHG	C23-C24-C25-C26
23	x	101	LHG	O9-C7-O7-C5
19	C	506	CLA	C2-C1-O2A-CGA
19	C	510	CLA	O1A-CGA-O2A-C1
21	A	407	BCR	C1-C6-C7-C8
21	A	407	BCR	C23-C24-C25-C30
21	B	517	BCR	C1-C6-C7-C8
21	B	517	BCR	C5-C6-C7-C8
21	B	518	BCR	C1-C6-C7-C8
21	B	518	BCR	C23-C24-C25-C26
21	B	518	BCR	C23-C24-C25-C30
21	C	515	BCR	C23-C24-C25-C30
21	C	516	BCR	C1-C6-C7-C8
21	C	516	BCR	C23-C24-C25-C30
21	C	517	BCR	C5-C6-C7-C8
21	C	517	BCR	C23-C24-C25-C26
21	H	101	BCR	C23-C24-C25-C30
21	a	407	BCR	C1-C6-C7-C8
21	a	407	BCR	C23-C24-C25-C30
21	b	517	BCR	C1-C6-C7-C8
21	b	517	BCR	C5-C6-C7-C8
21	b	518	BCR	C1-C6-C7-C8
21	b	518	BCR	C23-C24-C25-C26
21	b	518	BCR	C23-C24-C25-C30
21	c	516	BCR	C23-C24-C25-C30
21	c	517	BCR	C1-C6-C7-C8
21	c	517	BCR	C23-C24-C25-C30
21	c	518	BCR	C5-C6-C7-C8
21	c	518	BCR	C23-C24-C25-C26
21	c	518	BCR	C23-C24-C25-C30
21	h	101	BCR	C23-C24-C25-C30
21	k	101	BCR	C23-C24-C25-C26
21	k	101	BCR	C23-C24-C25-C30
21	w	101	BCR	C1-C6-C7-C8
21	w	101	BCR	C5-C6-C7-C8
19	B	510	CLA	C15-C16-C17-C18
19	B	516	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	b	511	CLA	C13-C15-C16-C17
19	d	404	CLA	CBD-CGD-O2D-CED
19	B	502	CLA	C6-C7-C8-C10
19	B	510	CLA	C11-C10-C8-C7
19	B	511	CLA	C6-C7-C8-C10
19	C	504	CLA	C6-C7-C8-C10
19	C	509	CLA	C6-C7-C8-C10
19	C	510	CLA	C12-C13-C15-C16
19	C	513	CLA	C11-C10-C8-C7
19	C	513	CLA	C11-C12-C13-C15
19	a	403	CLA	C11-C12-C13-C15
19	b	508	CLA	C11-C12-C13-C15
19	b	510	CLA	C11-C10-C8-C7
19	b	511	CLA	C6-C7-C8-C10
19	b	511	CLA	C11-C12-C13-C15
19	c	504	CLA	C6-C7-C8-C10
19	c	511	CLA	C12-C13-C15-C16
19	c	514	CLA	C11-C10-C8-C7
28	d	406	PL9	C43-C44-C46-C47
19	c	511	CLA	O1A-CGA-O2A-C1
20	A	405	PHO	C8-C10-C11-C12
19	c	515	CLA	C16-C17-C18-C19
22	A	408	LMG	O9-C10-O7-C8
19	C	509	CLA	C2A-CAA-CBA-CGA
19	b	505	CLA	C2A-CAA-CBA-CGA
19	c	515	CLA	C2A-CAA-CBA-CGA
19	c	505	CLA	O1D-CGD-O2D-CED
19	a	404	CLA	O1D-CGD-O2D-CED
19	b	501	CLA	C2C-C3C-CAC-CBC
22	f	101	LMG	C29-C30-C31-C32
22	A	408	LMG	C11-C10-O7-C8
22	c	502	LMG	C11-C10-O7-C8
23	L	101	LHG	C8-C7-O7-C5
23	l	101	LHG	C8-C7-O7-C5
23	a	408	LHG	O6-C4-C5-O7
20	a	405	PHO	C8-C10-C11-C12
23	L	101	LHG	O9-C7-O7-C5
22	A	408	LMG	O1-C7-C8-O7
22	H	102	LMG	O7-C8-C9-O8
22	c	502	LMG	O1-C7-C8-O7
23	x	101	LHG	O7-C5-C6-O8
26	C	522	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
22	F	101	LMG	C29-C30-C31-C32
26	c	523	LMU	O5B-C5B-C6B-O6B
19	b	503	CLA	C8-C10-C11-C12
28	D	406	PL9	C30-C29-C31-C32
28	D	406	PL9	C45-C44-C46-C47
19	d	404	CLA	C2-C3-C5-C6
19	A	403	CLA	C11-C12-C13-C14
19	B	508	CLA	C11-C12-C13-C14
19	C	503	CLA	C14-C13-C15-C16
19	C	504	CLA	C6-C7-C8-C9
19	C	509	CLA	C6-C7-C8-C9
19	b	508	CLA	C11-C12-C13-C14
19	b	513	CLA	C14-C13-C15-C16
19	c	505	CLA	C6-C7-C8-C9
19	c	510	CLA	C6-C7-C8-C9
19	c	514	CLA	C11-C12-C13-C14
25	c	519	DGD	C4B-C5B-C6B-C7B
19	b	502	CLA	C3-C5-C6-C7
19	c	510	CLA	C2A-CAA-CBA-CGA
19	A	403	CLA	C1A-C2A-CAA-CBA
19	B	504	CLA	C1A-C2A-CAA-CBA
19	B	505	CLA	C1A-C2A-CAA-CBA
19	B	509	CLA	C1A-C2A-CAA-CBA
19	B	514	CLA	C1A-C2A-CAA-CBA
19	C	502	CLA	C1A-C2A-CAA-CBA
19	C	506	CLA	C1A-C2A-CAA-CBA
19	C	508	CLA	C1A-C2A-CAA-CBA
19	C	512	CLA	C1A-C2A-CAA-CBA
19	D	403	CLA	C1A-C2A-CAA-CBA
19	a	403	CLA	C1A-C2A-CAA-CBA
19	b	504	CLA	C1A-C2A-CAA-CBA
19	b	514	CLA	C1A-C2A-CAA-CBA
19	c	503	CLA	C1A-C2A-CAA-CBA
19	c	509	CLA	C1A-C2A-CAA-CBA
19	d	403	CLA	C1A-C2A-CAA-CBA
19	d	404	CLA	C1A-C2A-CAA-CBA
19	C	511	CLA	C16-C17-C18-C20
22	c	502	LMG	O9-C10-O7-C8
23	l	101	LHG	O9-C7-O7-C5
23	B	521	LHG	C8-C7-O7-C5
23	D	407	LHG	C3-O3-P-O6
19	B	502	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	C	519	DGD	O6E-C5E-C6E-O5E
19	c	512	CLA	C16-C17-C18-C20
22	B	519	LMG	O6-C5-C6-O5
22	C	521	LMG	O6-C5-C6-O5
22	b	519	LMG	O6-C5-C6-O5
22	c	522	LMG	O6-C5-C6-O5
23	B	520	LHG	C28-C29-C30-C31
22	B	519	LMG	C11-C10-O7-C8
19	C	506	CLA	C16-C17-C18-C20
19	c	507	CLA	C16-C17-C18-C20
25	c	520	DGD	O6E-C5E-C6E-O5E
19	B	502	CLA	C3-C5-C6-C7
22	H	102	LMG	C7-C8-C9-O8
22	h	102	LMG	C7-C8-C9-O8
23	B	521	LHG	C4-C5-C6-O8
25	C	520	DGD	C5D-C6D-O5D-C1E
23	D	407	LHG	C23-C24-C25-C26
19	b	516	CLA	C13-C15-C16-C17
22	h	102	LMG	O6-C5-C6-O5
26	C	522	LMU	C4'-C5'-C6'-O6'
19	B	503	CLA	C8-C10-C11-C12
22	H	102	LMG	O6-C5-C6-O5
19	c	508	CLA	C2-C3-C5-C6
23	d	408	LHG	C23-C24-C25-C26
19	b	505	CLA	C16-C17-C18-C19
19	B	501	CLA	CBA-CGA-O2A-C1
19	C	503	CLA	CBA-CGA-O2A-C1
19	c	504	CLA	CBA-CGA-O2A-C1
19	B	504	CLA	C8-C10-C11-C12
19	b	502	CLA	C10-C11-C12-C13
19	c	508	CLA	C8-C10-C11-C12
22	h	102	LMG	C15-C16-C17-C18
22	A	408	LMG	O6-C5-C6-O5
19	B	505	CLA	C2A-CAA-CBA-CGA
19	B	509	CLA	C2-C1-O2A-CGA
22	c	502	LMG	O6-C5-C6-O5
19	B	503	CLA	O1D-CGD-O2D-CED
19	c	506	CLA	C13-C15-C16-C17
19	C	506	CLA	C16-C17-C18-C19
19	c	507	CLA	C16-C17-C18-C19
19	c	511	CLA	C15-C16-C17-C18
23	B	521	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
19	c	506	CLA	O1D-CGD-O2D-CED
26	C	522	LMU	C4-C5-C6-C7
19	B	503	CLA	C4-C3-C5-C6
19	C	512	CLA	C4-C3-C5-C6
19	b	503	CLA	C4-C3-C5-C6
19	c	508	CLA	C4-C3-C5-C6
19	A	403	CLA	C11-C12-C13-C15
19	B	513	CLA	C12-C13-C15-C16
19	B	515	CLA	C12-C13-C15-C16
19	C	503	CLA	C6-C7-C8-C10
19	C	504	CLA	C11-C10-C8-C7
19	C	506	CLA	C12-C13-C15-C16
19	C	507	CLA	C12-C13-C15-C16
19	C	512	CLA	C12-C13-C15-C16
19	b	512	CLA	C11-C10-C8-C7
19	b	513	CLA	C12-C13-C15-C16
19	c	504	CLA	C12-C13-C15-C16
19	c	505	CLA	C6-C7-C8-C10
19	c	505	CLA	C11-C10-C8-C7
19	c	506	CLA	C6-C7-C8-C10
19	c	506	CLA	C11-C12-C13-C15
19	c	508	CLA	C12-C13-C15-C16
19	c	510	CLA	C6-C7-C8-C10
19	d	404	CLA	C6-C7-C8-C10
19	d	404	CLA	C12-C13-C15-C16
19	B	513	CLA	C3-C5-C6-C7
19	b	513	CLA	C3-C5-C6-C7
19	B	505	CLA	C11-C12-C13-C14
19	B	512	CLA	C11-C10-C8-C9
19	B	513	CLA	C14-C13-C15-C16
19	C	505	CLA	C6-C7-C8-C9
19	C	507	CLA	C14-C13-C15-C16
19	C	510	CLA	C11-C12-C13-C14
19	C	512	CLA	C14-C13-C15-C16
19	C	513	CLA	C11-C10-C8-C9
19	D	404	CLA	C14-C13-C15-C16
19	b	505	CLA	C11-C12-C13-C14
19	b	512	CLA	C11-C10-C8-C9
19	c	504	CLA	C14-C13-C15-C16
19	c	507	CLA	C14-C13-C15-C16
19	c	508	CLA	C14-C13-C15-C16
19	c	513	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	c	514	CLA	C11-C10-C8-C9
19	d	404	CLA	C14-C13-C15-C16
19	D	404	CLA	O1D-CGD-O2D-CED
19	b	505	CLA	C16-C17-C18-C20
19	b	510	CLA	C8-C10-C11-C12
22	b	519	LMG	C11-C10-O7-C8
19	C	511	CLA	CBD-CGD-O2D-CED
23	A	409	LHG	O6-C4-C5-C6
23	a	408	LHG	O6-C4-C5-C6
19	C	505	CLA	CBD-CGD-O2D-CED
28	d	406	PL9	C45-C44-C46-C47
19	C	512	CLA	C2-C3-C5-C6
19	B	504	CLA	CBA-CGA-O2A-C1
19	C	511	CLA	CBA-CGA-O2A-C1
19	b	504	CLA	CBA-CGA-O2A-C1
19	C	506	CLA	C3A-C2A-CAA-CBA
19	D	404	CLA	C3A-C2A-CAA-CBA
19	b	505	CLA	C3A-C2A-CAA-CBA
19	c	507	CLA	C3A-C2A-CAA-CBA
19	c	508	CLA	C3A-C2A-CAA-CBA
19	d	404	CLA	C3A-C2A-CAA-CBA
19	b	513	CLA	C5-C6-C7-C8
21	w	101	BCR	C19-C20-C21-C22
26	C	522	LMU	C2-C1-O1'-C1'
26	c	523	LMU	C2-C1-O1'-C1'
24	C	501	SQD	C15-C16-C17-C18
19	B	501	CLA	C8-C10-C11-C12
25	c	521	DGD	C9B-CAB-CBB-CCB
22	c	502	LMG	O1-C7-C8-C9
25	c	521	DGD	C2A-C3A-C4A-C5A
19	c	504	CLA	O1A-CGA-O2A-C1
23	b	520	LHG	C25-C26-C27-C28
19	B	501	CLA	O1A-CGA-O2A-C1
19	C	507	CLA	C8-C10-C11-C12
23	d	407	LHG	C28-C29-C30-C31
19	C	503	CLA	O1A-CGA-O2A-C1
19	B	509	CLA	C16-C17-C18-C20
19	C	511	CLA	C16-C17-C18-C19
19	c	512	CLA	C16-C17-C18-C19
19	B	510	CLA	C8-C10-C11-C12
23	D	407	LHG	O2-C2-C3-O3
24	C	501	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
24	c	501	SQD	O6-C44-C45-O47
23	b	520	LHG	C31-C32-C33-C34
23	b	520	LHG	C8-C7-O7-C5
25	c	521	DGD	C2B-C1B-O2G-C2G
19	B	512	CLA	C16-C17-C18-C20
23	B	520	LHG	C11-C12-C13-C14
22	B	519	LMG	O9-C10-O7-C8
22	b	519	LMG	O9-C10-O7-C8
29	e	101	HEM	C4D-C3D-CAD-CBD
19	B	508	CLA	C14-C13-C15-C16
19	B	511	CLA	C11-C10-C8-C9
19	C	506	CLA	C14-C13-C15-C16
19	b	504	CLA	C11-C12-C13-C14
19	b	511	CLA	C11-C10-C8-C9
20	A	405	PHO	C14-C13-C15-C16
26	C	522	LMU	O5'-C5'-C6'-O6'
19	C	510	CLA	C2A-CAA-CBA-CGA
19	c	511	CLA	C2A-CAA-CBA-CGA
19	B	504	CLA	C16-C17-C18-C20
19	a	404	CLA	O2A-C1-C2-C3
21	C	517	BCR	C23-C24-C25-C30
21	c	518	BCR	C1-C6-C7-C8
19	B	513	CLA	C5-C6-C7-C8
19	B	507	CLA	C13-C15-C16-C17
19	B	516	CLA	C13-C15-C16-C17
19	b	501	CLA	C13-C15-C16-C17
23	b	520	LHG	O9-C7-O7-C5
22	h	102	LMG	C35-C36-C37-C38
25	C	520	DGD	C2A-C3A-C4A-C5A
22	H	102	LMG	C15-C16-C17-C18
25	C	519	DGD	C6B-C7B-C8B-C9B
19	b	507	CLA	C13-C15-C16-C17
25	c	520	DGD	C6B-C7B-C8B-C9B
19	B	505	CLA	C11-C12-C13-C15
19	B	509	CLA	C6-C7-C8-C10
19	B	511	CLA	C11-C10-C8-C7
19	B	512	CLA	C11-C10-C8-C7
19	C	502	CLA	C11-C12-C13-C15
19	C	505	CLA	C11-C12-C13-C15
19	C	510	CLA	C6-C7-C8-C10
19	C	511	CLA	C11-C10-C8-C7
19	C	512	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	D	404	CLA	C6-C7-C8-C10
19	D	404	CLA	C12-C13-C15-C16
19	b	504	CLA	C11-C12-C13-C15
19	b	505	CLA	C11-C12-C13-C15
19	b	509	CLA	C6-C7-C8-C10
19	b	511	CLA	C11-C10-C8-C7
19	b	515	CLA	C12-C13-C15-C16
19	c	503	CLA	C11-C12-C13-C15
19	c	507	CLA	C12-C13-C15-C16
19	c	511	CLA	C6-C7-C8-C10
19	c	512	CLA	C11-C10-C8-C7
19	c	513	CLA	C12-C13-C15-C16
20	D	401	PHO	C11-C10-C8-C7
20	a	405	PHO	C11-C12-C13-C15
28	D	406	PL9	C43-C44-C46-C47
19	b	501	CLA	C16-C17-C18-C19
19	b	509	CLA	C16-C17-C18-C20
25	C	520	DGD	C9B-CAB-CBB-CCB
19	B	501	CLA	C13-C15-C16-C17
22	H	102	LMG	C35-C36-C37-C38
25	C	520	DGD	C2B-C1B-O2G-C2G
24	c	501	SQD	C15-C16-C17-C18
19	B	509	CLA	C16-C17-C18-C19
19	b	501	CLA	C16-C17-C18-C20
19	b	509	CLA	C16-C17-C18-C19
19	b	510	CLA	C13-C15-C16-C17
19	A	404	CLA	CAD-CBD-CGD-O2D
19	B	516	CLA	CAD-CBD-CGD-O2D
19	C	509	CLA	CAD-CBD-CGD-O2D
19	D	403	CLA	CAD-CBD-CGD-O2D
19	D	404	CLA	CAD-CBD-CGD-O2D
19	a	404	CLA	CAD-CBD-CGD-O2D
19	b	501	CLA	CAD-CBD-CGD-O2D
19	b	510	CLA	CAD-CBD-CGD-O2D
19	b	512	CLA	CAD-CBD-CGD-O2D
19	b	515	CLA	CAD-CBD-CGD-O2D
19	c	504	CLA	CAD-CBD-CGD-O2D
19	c	508	CLA	CAD-CBD-CGD-O2D
19	c	510	CLA	CAD-CBD-CGD-O2D
19	d	404	CLA	CAD-CBD-CGD-O2D
23	d	408	LHG	C32-C33-C34-C35
23	B	521	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	B	519	LMG	O6-C1-O1-C7
22	b	519	LMG	O6-C1-O1-C7
22	H	102	LMG	C11-C10-O7-C8
23	X	101	LHG	O6-C4-C5-O7
19	B	505	CLA	C8-C10-C11-C12
20	a	405	PHO	C5-C6-C7-C8
20	a	405	PHO	C3-C5-C6-C7
23	x	101	LHG	C14-C15-C16-C17
29	F	102	HEM	C4B-C3B-CAB-CBB
29	e	101	HEM	C4B-C3B-CAB-CBB
19	B	504	CLA	C16-C17-C18-C19
19	B	507	CLA	C16-C17-C18-C20
19	B	512	CLA	C16-C17-C18-C19
19	d	404	CLA	O1D-CGD-O2D-CED
25	c	521	DGD	O1B-C1B-O2G-C2G
19	A	406	CLA	CHA-CBD-CGD-O1D
19	A	406	CLA	CHA-CBD-CGD-O2D
19	B	501	CLA	CHA-CBD-CGD-O1D
19	B	505	CLA	CHA-CBD-CGD-O1D
19	B	505	CLA	CHA-CBD-CGD-O2D
19	C	504	CLA	CHA-CBD-CGD-O1D
19	C	504	CLA	CHA-CBD-CGD-O2D
19	C	508	CLA	CHA-CBD-CGD-O1D
19	C	510	CLA	CHA-CBD-CGD-O1D
19	C	510	CLA	CHA-CBD-CGD-O2D
19	C	511	CLA	CHA-CBD-CGD-O1D
19	C	511	CLA	CHA-CBD-CGD-O2D
19	a	406	CLA	CHA-CBD-CGD-O1D
19	a	406	CLA	CHA-CBD-CGD-O2D
19	b	505	CLA	CHA-CBD-CGD-O1D
19	b	505	CLA	CHA-CBD-CGD-O2D
19	c	509	CLA	CHA-CBD-CGD-O1D
19	c	511	CLA	CHA-CBD-CGD-O1D
19	c	511	CLA	CHA-CBD-CGD-O2D
19	c	512	CLA	CHA-CBD-CGD-O1D
19	c	512	CLA	CHA-CBD-CGD-O2D
22	A	408	LMG	C2-C1-O1-C7
23	B	521	LHG	O7-C5-C6-O8
19	C	511	CLA	O1A-CGA-O2A-C1
19	b	504	CLA	O1A-CGA-O2A-C1
26	c	523	LMU	C4-C5-C6-C7
19	B	501	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	B	513	CLA	C16-C17-C18-C20
19	b	513	CLA	C16-C17-C18-C20
19	B	504	CLA	O1A-CGA-O2A-C1
25	C	520	DGD	O1B-C1B-O2G-C2G
19	B	513	CLA	C11-C10-C8-C9
19	c	512	CLA	C11-C12-C13-C14
20	D	401	PHO	C11-C10-C8-C9
20	a	405	PHO	C11-C12-C13-C14
22	H	102	LMG	C36-C37-C38-C39
19	C	504	CLA	C8-C10-C11-C12
24	C	501	SQD	C5-C6-S-O8
24	c	501	SQD	C5-C6-S-O8
19	B	505	CLA	C16-C17-C18-C19
19	c	513	CLA	C16-C17-C18-C19
19	c	512	CLA	CBD-CGD-O2D-CED
20	a	405	PHO	CBD-CGD-O2D-CED
29	F	102	HEM	C4D-C3D-CAD-CBD
29	e	101	HEM	C2D-C3D-CAD-CBD
21	w	101	BCR	C11-C12-C13-C14
19	D	404	CLA	C1A-C2A-CAA-CBA
19	D	404	CLA	C2-C1-O2A-CGA
19	b	509	CLA	C2-C1-O2A-CGA
19	d	404	CLA	C2-C1-O2A-CGA
19	B	506	CLA	C5-C6-C7-C8
23	X	101	LHG	C3-O3-P-O6
19	C	507	CLA	C4-C3-C5-C6
23	A	410	LHG	C4-O6-P-O4
23	B	521	LHG	C4-O6-P-O5
23	D	407	LHG	C4-O6-P-O4
23	L	101	LHG	C3-O3-P-O4
23	a	409	LHG	C4-O6-P-O4
23	b	520	LHG	C4-O6-P-O5
23	d	408	LHG	C4-O6-P-O4
23	x	101	LHG	C3-O3-P-O4
19	C	512	CLA	C16-C17-C18-C19
19	A	404	CLA	O2A-C1-C2-C3
23	X	101	LHG	O6-C4-C5-C6
22	h	102	LMG	C38-C39-C40-C41
19	b	501	CLA	C8-C10-C11-C12
22	H	102	LMG	O9-C10-O7-C8
23	B	521	LHG	C25-C26-C27-C28
23	d	407	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	C	505	CLA	O1D-CGD-O2D-CED
19	B	503	CLA	CAD-CBD-CGD-O1D
19	B	505	CLA	CAD-CBD-CGD-O1D
19	B	506	CLA	CAD-CBD-CGD-O1D
19	C	504	CLA	CAD-CBD-CGD-O1D
19	C	506	CLA	CAD-CBD-CGD-O1D
19	C	510	CLA	CAD-CBD-CGD-O1D
19	b	503	CLA	CAD-CBD-CGD-O1D
19	b	505	CLA	CAD-CBD-CGD-O1D
19	c	507	CLA	CAD-CBD-CGD-O1D
19	c	511	CLA	CAD-CBD-CGD-O1D
24	C	501	SQD	C5-C6-S-O9
24	c	501	SQD	C5-C6-S-O9
23	d	407	LHG	C11-C12-C13-C14
20	A	405	PHO	C5-C6-C7-C8
23	A	410	LHG	C14-C15-C16-C17
19	b	507	CLA	C16-C17-C18-C20
19	A	403	CLA	C12-C13-C15-C16
19	B	516	CLA	C6-C7-C8-C10
19	C	504	CLA	C3A-C2A-CAA-CBA
19	C	514	CLA	C11-C10-C8-C7
19	D	403	CLA	C6-C7-C8-C10
19	b	503	CLA	C2-C3-C5-C6
19	b	516	CLA	C6-C7-C8-C10
19	c	505	CLA	C3A-C2A-CAA-CBA
19	c	507	CLA	C11-C12-C13-C15
19	c	511	CLA	C11-C12-C13-C15
19	c	515	CLA	C11-C10-C8-C7
19	d	403	CLA	C6-C7-C8-C10
20	A	405	PHO	C11-C12-C13-C15
20	d	401	PHO	C11-C10-C8-C7
23	B	520	LHG	C32-C33-C34-C35
23	A	410	LHG	C26-C27-C28-C29
19	C	505	CLA	C10-C11-C12-C13
23	a	409	LHG	C14-C15-C16-C17
23	L	101	LHG	C14-C15-C16-C17
23	b	520	LHG	O7-C5-C6-O8
23	l	101	LHG	C14-C15-C16-C17
26	c	523	LMU	C4'-C5'-C6'-O6'
25	c	521	DGD	C5D-C6D-O5D-C1E
19	C	510	CLA	C15-C16-C17-C18
19	b	505	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	c	521	DGD	C7B-C8B-C9B-CAB
19	C	511	CLA	O1D-CGD-O2D-CED
19	C	508	CLA	O1A-CGA-O2A-C1
19	C	508	CLA	CBA-CGA-O2A-C1
23	d	407	LHG	C32-C33-C34-C35
19	B	503	CLA	C2-C3-C5-C6
19	B	515	CLA	C14-C13-C15-C16
19	C	502	CLA	C11-C12-C13-C14
19	C	504	CLA	C11-C10-C8-C9
19	C	510	CLA	C6-C7-C8-C9
19	C	511	CLA	C11-C10-C8-C9
19	b	502	CLA	C6-C7-C8-C9
19	b	515	CLA	C14-C13-C15-C16
19	c	512	CLA	C11-C10-C8-C9
20	A	405	PHO	C11-C12-C13-C14
20	d	401	PHO	C11-C10-C8-C9
19	B	501	CLA	C16-C17-C18-C20
19	B	513	CLA	C16-C17-C18-C19
19	b	513	CLA	C16-C17-C18-C19
19	c	513	CLA	C16-C17-C18-C20
25	C	519	DGD	C9B-CAB-CBB-CCB
19	B	505	CLA	C16-C17-C18-C20
19	b	503	CLA	C16-C17-C18-C20
19	c	509	CLA	O1A-CGA-O2A-C1
23	A	410	LHG	C25-C26-C27-C28
19	C	503	CLA	C4-C3-C5-C6
19	B	509	CLA	C5-C6-C7-C8
19	C	502	CLA	C15-C16-C17-C18
19	c	507	CLA	C2-C1-O2A-CGA
19	a	402	CLA	C4C-C3C-CAC-CBC
23	a	409	LHG	C26-C27-C28-C29
25	c	520	DGD	C9B-CAB-CBB-CCB
19	C	504	CLA	O1A-CGA-O2A-C1
23	X	101	LHG	C14-C15-C16-C17
19	C	507	CLA	C5-C6-C7-C8
19	C	504	CLA	CBA-CGA-O2A-C1
23	a	409	LHG	C25-C26-C27-C28
19	c	506	CLA	C10-C11-C12-C13
19	c	504	CLA	C4-C3-C5-C6
19	A	402	CLA	C4C-C3C-CAC-CBC
20	a	405	PHO	O1D-CGD-O2D-CED
21	V	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	W	101	BCR	C23-C24-C25-C26
19	C	507	CLA	C2-C3-C5-C6
19	c	509	CLA	CBA-CGA-O2A-C1
19	c	505	CLA	O1A-CGA-O2A-C1
19	B	501	CLA	C4C-C3C-CAC-CBC
19	C	513	CLA	C16-C17-C18-C20
22	c	502	LMG	C2-C1-O1-C7
23	A	409	LHG	C3-O3-P-O6
23	A	409	LHG	C4-O6-P-O3
23	B	521	LHG	C3-O3-P-O6
23	L	101	LHG	C4-O6-P-O3
23	a	408	LHG	C3-O3-P-O6
23	a	408	LHG	C4-O6-P-O3
23	b	520	LHG	C3-O3-P-O6
23	l	101	LHG	C4-O6-P-O3
24	C	501	SQD	C31-C32-C33-C34
25	C	520	DGD	C7B-C8B-C9B-CAB
26	c	523	LMU	O1'-C1-C2-C3
19	c	505	CLA	C8-C10-C11-C12
19	c	512	CLA	O1D-CGD-O2D-CED
19	B	513	CLA	C11-C10-C8-C7
19	C	505	CLA	C6-C7-C8-C10
19	C	510	CLA	C11-C12-C13-C15
19	A	403	CLA	C14-C13-C15-C16
19	B	516	CLA	C6-C7-C8-C9
19	C	514	CLA	C14-C13-C15-C16
19	b	516	CLA	C6-C7-C8-C9
19	c	503	CLA	C11-C12-C13-C14
19	c	505	CLA	C11-C10-C8-C9
19	c	511	CLA	C6-C7-C8-C9
19	d	403	CLA	C6-C7-C8-C9
19	c	514	CLA	C16-C17-C18-C20
19	c	505	CLA	CBA-CGA-O2A-C1
19	b	506	CLA	C5-C6-C7-C8
19	C	512	CLA	C16-C17-C18-C20
19	C	503	CLA	C13-C15-C16-C17
19	c	507	CLA	C10-C11-C12-C13
29	F	102	HEM	C2D-C3D-CAD-CBD
19	c	512	CLA	CBA-CGA-O2A-C1
19	B	514	CLA	CBD-CGD-O2D-CED
19	c	503	CLA	C15-C16-C17-C18
19	b	501	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	b	501	CLA	CBA-CGA-O2A-C1
19	B	504	CLA	C3-C5-C6-C7
23	B	520	LHG	C11-C10-C9-C8
19	c	512	CLA	O1A-CGA-O2A-C1
19	b	501	CLA	C4C-C3C-CAC-CBC
19	b	504	CLA	C16-C17-C18-C20
19	D	403	CLA	C15-C16-C17-C18
19	B	511	CLA	C8-C10-C11-C12
19	b	511	CLA	C8-C10-C11-C12
19	B	508	CLA	C2A-CAA-CBA-CGA
19	C	511	CLA	C2A-CAA-CBA-CGA
19	b	508	CLA	C2A-CAA-CBA-CGA
19	c	512	CLA	C2A-CAA-CBA-CGA
19	b	516	CLA	C4C-C3C-CAC-CBC
19	A	404	CLA	C3A-C2A-CAA-CBA
19	B	505	CLA	C3A-C2A-CAA-CBA
19	B	512	CLA	C3A-C2A-CAA-CBA
19	a	404	CLA	C3A-C2A-CAA-CBA
19	b	512	CLA	C3A-C2A-CAA-CBA
19	A	406	CLA	C11-C12-C13-C15
19	B	503	CLA	C16-C17-C18-C20
19	a	406	CLA	C11-C12-C13-C15
22	H	102	LMG	C38-C39-C40-C41
19	B	508	CLA	C6-C7-C8-C9
19	C	504	CLA	C11-C12-C13-C14
19	C	511	CLA	C11-C12-C13-C14
19	b	508	CLA	C6-C7-C8-C9
19	b	508	CLA	C14-C13-C15-C16
19	c	505	CLA	C11-C12-C13-C14
20	a	405	PHO	C14-C13-C15-C16
23	D	407	LHG	C1-C2-C3-O3
19	C	504	CLA	C2A-CAA-CBA-CGA
19	c	505	CLA	C2A-CAA-CBA-CGA
19	b	509	CLA	C5-C6-C7-C8
19	C	513	CLA	C16-C17-C18-C19
19	A	402	CLA	O2A-C1-C2-C3
19	C	506	CLA	O2A-C1-C2-C3
19	C	513	CLA	O2A-C1-C2-C3
19	a	402	CLA	O2A-C1-C2-C3
19	b	516	CLA	O2A-C1-C2-C3
19	c	514	CLA	O2A-C1-C2-C3
21	C	516	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	A	404	CLA	C1A-C2A-CAA-CBA
19	B	510	CLA	C12-C13-C15-C16
19	C	506	CLA	C11-C12-C13-C15
19	C	513	CLA	C12-C13-C15-C16
19	b	502	CLA	C6-C7-C8-C10
19	c	514	CLA	C12-C13-C15-C16
19	B	505	CLA	C13-C15-C16-C17
19	b	502	CLA	C2A-CAA-CBA-CGA
19	C	507	CLA	C10-C11-C12-C13
24	C	501	SQD	C25-C26-C27-C28
23	d	407	LHG	C11-C10-C9-C8
25	C	520	DGD	C8B-C9B-CAB-CBB
22	f	101	LMG	C31-C32-C33-C34
19	c	508	CLA	C10-C11-C12-C13
25	c	521	DGD	C8B-C9B-CAB-CBB
22	C	521	LMG	O7-C8-C9-O8
19	B	502	CLA	C2A-CAA-CBA-CGA
19	D	404	CLA	C16-C17-C18-C19
19	d	403	CLA	C15-C16-C17-C18
19	C	505	CLA	C13-C15-C16-C17
19	C	503	CLA	C2-C3-C5-C6
24	c	501	SQD	C25-C26-C27-C28
19	b	507	CLA	C6-C7-C8-C9
19	c	515	CLA	C14-C13-C15-C16
26	c	523	LMU	C1-C2-C3-C4
23	B	521	LHG	C27-C28-C29-C30
19	c	504	CLA	C16-C17-C18-C20
19	c	514	CLA	C16-C17-C18-C19
23	D	407	LHG	C30-C31-C32-C33
21	C	517	BCR	C1-C6-C7-C8
21	W	101	BCR	C23-C24-C25-C30
22	F	101	LMG	C31-C32-C33-C34
26	C	522	LMU	O1'-C1-C2-C3
19	c	504	CLA	C2-C3-C5-C6
22	h	102	LMG	O7-C10-C11-C12
19	a	402	CLA	C2C-C3C-CAC-CBC
23	b	520	LHG	C27-C28-C29-C30
19	b	504	CLA	C16-C17-C18-C19
20	A	405	PHO	C3-C5-C6-C7
19	B	514	CLA	O1D-CGD-O2D-CED
20	d	401	PHO	C2A-CAA-CBA-CGA
19	C	509	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	B	516	CLA	C5-C6-C7-C8
23	D	407	LHG	C32-C33-C34-C35
19	b	505	CLA	C13-C15-C16-C17
19	B	503	CLA	C12-C13-C15-C16
19	B	508	CLA	C12-C13-C15-C16
19	D	403	CLA	C12-C13-C15-C16
20	D	401	PHO	C11-C12-C13-C15
20	d	401	PHO	C11-C12-C13-C15
19	b	516	CLA	C5-C6-C7-C8
19	b	514	CLA	CBD-CGD-O2D-CED
19	a	403	CLA	C13-C15-C16-C17
19	B	509	CLA	CAA-CBA-CGA-O2A
23	D	407	LHG	C7-C8-C9-C10
19	A	403	CLA	C16-C17-C18-C20
22	H	102	LMG	C32-C33-C34-C35
19	C	512	CLA	CBA-CGA-O2A-C1
22	h	102	LMG	C32-C33-C34-C35
19	C	514	CLA	C4-C3-C5-C6
19	b	505	CLA	C4-C3-C5-C6
19	c	513	CLA	C4-C3-C5-C6
23	L	101	LHG	O8-C23-C24-C25
25	c	520	DGD	O2G-C1B-C2B-C3B
19	B	510	CLA	C14-C13-C15-C16
19	C	503	CLA	C11-C10-C8-C9
19	C	506	CLA	C11-C12-C13-C14
19	C	513	CLA	C14-C13-C15-C16
19	D	403	CLA	C6-C7-C8-C9
19	c	504	CLA	C11-C10-C8-C9
19	c	507	CLA	C11-C12-C13-C14
19	c	515	CLA	C11-C12-C13-C14
25	C	519	DGD	O2G-C1B-C2B-C3B
19	B	501	CLA	CAD-CBD-CGD-O2D
19	B	509	CLA	CAD-CBD-CGD-O2D
19	C	503	CLA	CAD-CBD-CGD-O2D
19	b	506	CLA	CAD-CBD-CGD-O2D
19	b	509	CLA	CAD-CBD-CGD-O2D
19	d	403	CLA	CAD-CBD-CGD-O2D
20	A	405	PHO	CAD-CBD-CGD-O2D
23	d	408	LHG	C7-C8-C9-C10
23	B	520	LHG	C30-C31-C32-C33
19	B	513	CLA	C2A-CAA-CBA-CGA
25	c	519	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
19	C	512	CLA	O1A-CGA-O2A-C1
28	d	406	PL9	C42-C43-C44-C46
19	c	512	CLA	CAA-CBA-CGA-O2A
23	l	101	LHG	O8-C23-C24-C25
19	B	505	CLA	C4-C3-C5-C6
19	c	515	CLA	C4-C3-C5-C6
22	h	102	LMG	C36-C37-C38-C39
19	B	510	CLA	C13-C15-C16-C17
19	B	505	CLA	CAA-CBA-CGA-O2A
19	B	511	CLA	CAA-CBA-CGA-O2A
19	b	501	CLA	CAA-CBA-CGA-O2A
19	b	505	CLA	CAA-CBA-CGA-O2A
19	b	511	CLA	CAA-CBA-CGA-O2A
19	b	512	CLA	CAA-CBA-CGA-O2A
21	H	101	BCR	C7-C8-C9-C10
21	h	101	BCR	C7-C8-C9-C10
24	C	501	SQD	O6-C44-C45-C46
24	c	501	SQD	O6-C44-C45-C46
19	B	501	CLA	CAA-CBA-CGA-O2A
19	C	511	CLA	CAA-CBA-CGA-O2A
19	A	402	CLA	C2C-C3C-CAC-CBC
26	C	522	LMU	C3-C4-C5-C6
19	B	515	CLA	O2A-C1-C2-C3
19	B	516	CLA	O2A-C1-C2-C3
19	D	403	CLA	O2A-C1-C2-C3
19	c	507	CLA	O2A-C1-C2-C3
19	d	403	CLA	O2A-C1-C2-C3
20	D	401	PHO	C2A-CAA-CBA-CGA
19	B	512	CLA	CAA-CBA-CGA-O2A
19	b	509	CLA	CAA-CBA-CGA-O2A
19	c	515	CLA	CAA-CBA-CGA-O2A
22	c	522	LMG	O8-C28-C29-C30
19	A	406	CLA	C11-C12-C13-C14
19	a	406	CLA	C11-C12-C13-C14
19	B	504	CLA	CHA-CBD-CGD-O1D
19	B	504	CLA	CHA-CBD-CGD-O2D
19	B	513	CLA	CHA-CBD-CGD-O1D
19	C	505	CLA	CHA-CBD-CGD-O1D
19	b	504	CLA	CHA-CBD-CGD-O1D
19	b	504	CLA	CHA-CBD-CGD-O2D
19	b	513	CLA	CHA-CBD-CGD-O1D
26	c	523	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
22	C	521	LMG	O8-C28-C29-C30
19	C	510	CLA	CAA-CBA-CGA-O2A
19	c	508	CLA	CAA-CBA-CGA-O2A
19	c	511	CLA	CAA-CBA-CGA-O2A
19	c	504	CLA	C13-C15-C16-C17
19	B	504	CLA	C2A-CAA-CBA-CGA
19	b	511	CLA	C16-C17-C18-C19
26	C	522	LMU	C1-C2-C3-C4
19	C	514	CLA	CAA-CBA-CGA-O2A
19	a	403	CLA	CAA-CBA-CGA-O2A
23	a	408	LHG	O8-C23-C24-C25
23	a	408	LHG	C24-C25-C26-C27
19	B	503	CLA	C11-C12-C13-C15
19	b	503	CLA	C11-C12-C13-C15
19	b	513	CLA	C6-C7-C8-C10
19	b	513	CLA	C11-C10-C8-C7
20	A	405	PHO	C12-C13-C15-C16
19	D	404	CLA	C16-C17-C18-C20
19	b	512	CLA	C16-C17-C18-C20
19	c	504	CLA	C16-C17-C18-C19
25	C	518	DGD	O1B-C1B-O2G-C2G
19	C	512	CLA	C6-C7-C8-C9
19	a	402	CLA	C14-C13-C15-C16
19	b	513	CLA	C6-C7-C8-C9
19	b	513	CLA	C11-C10-C8-C9
19	c	510	CLA	C13-C15-C16-C17
19	C	507	CLA	CAA-CBA-CGA-O2A
19	B	501	CLA	CAA-CBA-CGA-O1A
24	C	501	SQD	C4-C5-C6-S
24	c	501	SQD	C4-C5-C6-S
25	C	520	DGD	CCB-CDB-CEB-CFB
22	H	102	LMG	C34-C35-C36-C37
25	c	519	DGD	C2B-C1B-O2G-C2G
19	b	513	CLA	C2A-CAA-CBA-CGA
28	d	406	PL9	C21-C22-C23-C24
19	b	505	CLA	CAA-CBA-CGA-O1A
19	B	511	CLA	C16-C17-C18-C19
19	d	404	CLA	C16-C17-C18-C19
19	B	511	CLA	CAA-CBA-CGA-O1A
19	b	511	CLA	CAA-CBA-CGA-O1A
19	b	512	CLA	CAA-CBA-CGA-O1A
22	c	522	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
21	c	517	BCR	C21-C22-C23-C24
19	B	512	CLA	C1A-C2A-CAA-CBA
19	a	404	CLA	C1A-C2A-CAA-CBA
19	b	512	CLA	C1A-C2A-CAA-CBA
19	B	509	CLA	CAA-CBA-CGA-O1A
19	B	512	CLA	CAA-CBA-CGA-O1A
23	l	101	LHG	O10-C23-C24-C25
25	C	519	DGD	O1B-C1B-C2B-C3B
28	D	406	PL9	C21-C22-C23-C24
19	B	505	CLA	CAA-CBA-CGA-O1A
19	B	512	CLA	C13-C15-C16-C17
19	b	511	CLA	C16-C17-C18-C20
19	C	511	CLA	CAA-CBA-CGA-O1A
19	b	501	CLA	CAA-CBA-CGA-O1A
23	L	101	LHG	O10-C23-C24-C25
25	c	520	DGD	O1B-C1B-C2B-C3B
19	A	403	CLA	CAA-CBA-CGA-O2A
19	c	508	CLA	CAA-CBA-CGA-O1A
19	c	512	CLA	CAA-CBA-CGA-O1A
23	A	409	LHG	C4-O6-P-O5
23	L	101	LHG	C4-O6-P-O5
23	a	408	LHG	C4-O6-P-O5
23	a	409	LHG	C3-O3-P-O5
25	c	519	DGD	O6D-C5D-C6D-O5D
21	V	101	BCR	C23-C24-C25-C30
28	D	406	PL9	C34-C36-C37-C38
19	A	403	CLA	C13-C15-C16-C17
19	C	510	CLA	CAA-CBA-CGA-O1A
19	c	511	CLA	CAA-CBA-CGA-O1A
19	c	515	CLA	CAA-CBA-CGA-O1A
22	C	521	LMG	O10-C28-C29-C30
19	b	510	CLA	CAA-CBA-CGA-O2A
23	A	409	LHG	O8-C23-C24-C25
19	C	503	CLA	C16-C17-C18-C20
19	b	514	CLA	O1D-CGD-O2D-CED
24	c	501	SQD	C31-C32-C33-C34
19	b	509	CLA	CAA-CBA-CGA-O1A
23	x	101	LHG	C30-C31-C32-C33
19	C	505	CLA	CAD-CBD-CGD-O1D
19	C	514	CLA	CAD-CBD-CGD-O1D
19	c	505	CLA	CAD-CBD-CGD-O1D
19	c	506	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	c	515	CLA	CAD-CBD-CGD-O1D
23	a	408	LHG	O10-C23-C24-C25
23	D	407	LHG	O7-C7-C8-C9
23	d	408	LHG	O7-C7-C8-C9
19	B	503	CLA	C11-C12-C13-C14
19	B	503	CLA	C14-C13-C15-C16
19	B	504	CLA	C11-C12-C13-C14
19	B	507	CLA	C6-C7-C8-C9
19	B	513	CLA	C6-C7-C8-C9
19	C	502	CLA	C14-C13-C15-C16
19	b	503	CLA	C11-C12-C13-C14
19	c	503	CLA	C14-C13-C15-C16
19	c	514	CLA	C14-C13-C15-C16
19	B	502	CLA	CAA-CBA-CGA-O2A
19	C	504	CLA	CAA-CBA-CGA-O2A
19	c	508	CLA	C5-C6-C7-C8
19	b	502	CLA	CAA-CBA-CGA-O2A
19	C	507	CLA	CAA-CBA-CGA-O1A
19	C	514	CLA	CAA-CBA-CGA-O1A
23	a	408	LHG	O9-C7-O7-C5
19	B	513	CLA	C6-C7-C8-C10
19	C	504	CLA	C12-C13-C15-C16
19	a	402	CLA	C12-C13-C15-C16
19	b	503	CLA	C12-C13-C15-C16
19	b	507	CLA	C6-C7-C8-C10
19	B	507	CLA	CAA-CBA-CGA-O1A
19	a	403	CLA	CAA-CBA-CGA-O1A
23	d	408	LHG	O9-C7-C8-C9
19	A	404	CLA	CAA-CBA-CGA-O2A
19	B	507	CLA	CAA-CBA-CGA-O2A
19	b	507	CLA	CAA-CBA-CGA-O2A
19	c	510	CLA	CAA-CBA-CGA-O2A
22	h	102	LMG	C33-C34-C35-C36
19	b	502	CLA	CAA-CBA-CGA-O1A
19	B	511	CLA	C16-C17-C18-C20
23	a	408	LHG	C33-C34-C35-C36
19	A	403	CLA	CAA-CBA-CGA-O1A
19	B	502	CLA	CAA-CBA-CGA-O1A
19	b	512	CLA	C8-C10-C11-C12
19	d	404	CLA	C13-C15-C16-C17
19	C	509	CLA	CAA-CBA-CGA-O2A
19	C	513	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	a	404	CLA	CAA-CBA-CGA-O2A
19	c	505	CLA	CAA-CBA-CGA-O2A
19	c	514	CLA	CAA-CBA-CGA-O2A
19	b	507	CLA	CAA-CBA-CGA-O1A
19	b	510	CLA	CAA-CBA-CGA-O1A
19	B	512	CLA	C2A-CAA-CBA-CGA
19	b	504	CLA	C2A-CAA-CBA-CGA
19	b	512	CLA	C16-C17-C18-C19
22	H	102	LMG	C33-C34-C35-C36
23	a	408	LHG	C25-C26-C27-C28
19	c	505	CLA	CAA-CBA-CGA-O1A
23	D	407	LHG	O9-C7-C8-C9
23	a	409	LHG	C11-C10-C9-C8
29	F	102	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

78 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	c	504	CLA	2	0
19	c	508	CLA	2	0
21	a	407	BCR	5	0
19	C	509	CLA	1	0
19	C	502	CLA	3	0
19	b	513	CLA	2	0
19	c	515	CLA	1	0
22	H	102	LMG	2	0
28	d	406	PL9	1	0
19	d	404	CLA	2	0
21	V	101	BCR	4	0
19	B	516	CLA	1	0
19	C	505	CLA	1	0
27	D	402	BCT	1	0
19	B	512	CLA	1	0
19	a	402	CLA	1	0
19	a	404	CLA	2	0
23	B	521	LHG	1	0
21	C	516	BCR	8	0
19	B	506	CLA	3	0
21	h	101	BCR	6	0
21	A	407	BCR	9	0
29	F	102	HEM	6	0

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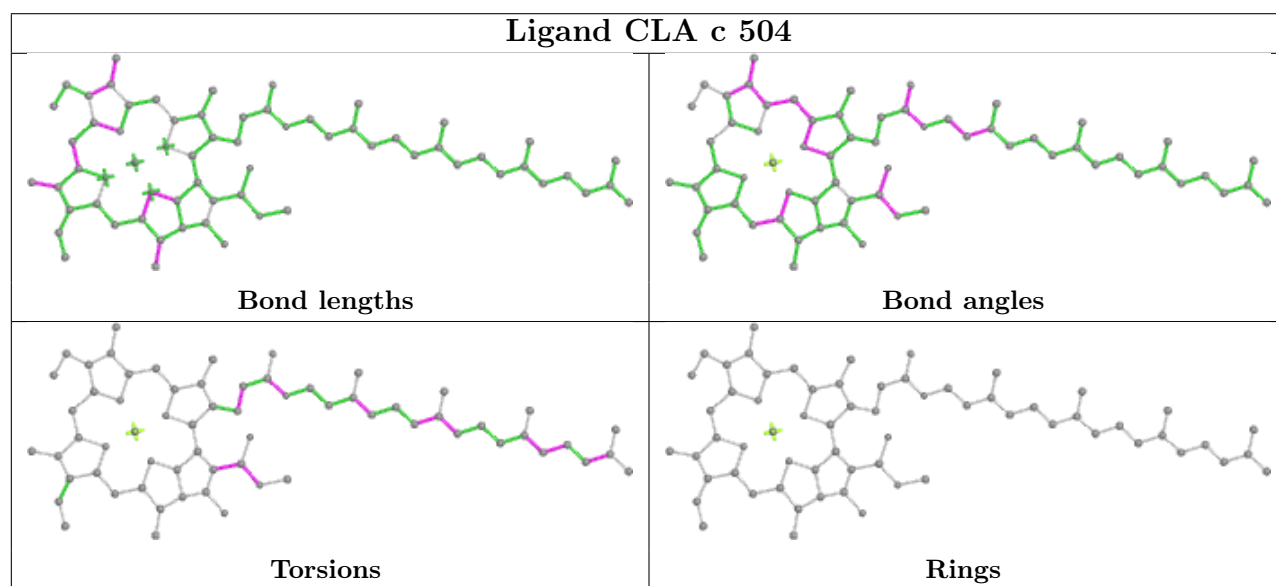
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	407	LHG	1	0
19	b	516	CLA	1	0
21	b	518	BCR	4	0
19	b	501	CLA	1	0
23	b	520	LHG	1	0
21	B	518	BCR	3	0
21	b	517	BCR	6	0
19	b	502	CLA	3	0
19	B	509	CLA	2	0
19	B	504	CLA	2	0
19	B	501	CLA	1	0
19	b	515	CLA	1	0
19	a	403	CLA	1	0
19	C	512	CLA	5	0
19	B	502	CLA	3	0
19	c	510	CLA	1	0
21	d	405	BCR	1	0
19	d	403	CLA	3	0
29	e	101	HEM	5	0
21	c	516	BCR	6	0
19	b	512	CLA	1	0
19	B	505	CLA	1	0
21	W	101	BCR	8	0
21	C	515	BCR	6	0
19	b	506	CLA	1	0
20	A	405	PHO	1	0
21	D	405	BCR	1	0
19	D	404	CLA	1	0
19	c	503	CLA	2	0
21	C	517	BCR	7	0
21	H	101	BCR	7	0
21	c	517	BCR	7	0
19	c	513	CLA	4	0
27	d	402	BCT	1	0
21	c	518	BCR	5	0
19	B	513	CLA	4	0
21	k	101	BCR	2	0
20	D	401	PHO	2	0
19	b	504	CLA	2	0
19	b	507	CLA	1	0
23	d	408	LHG	1	0
23	A	409	LHG	1	0

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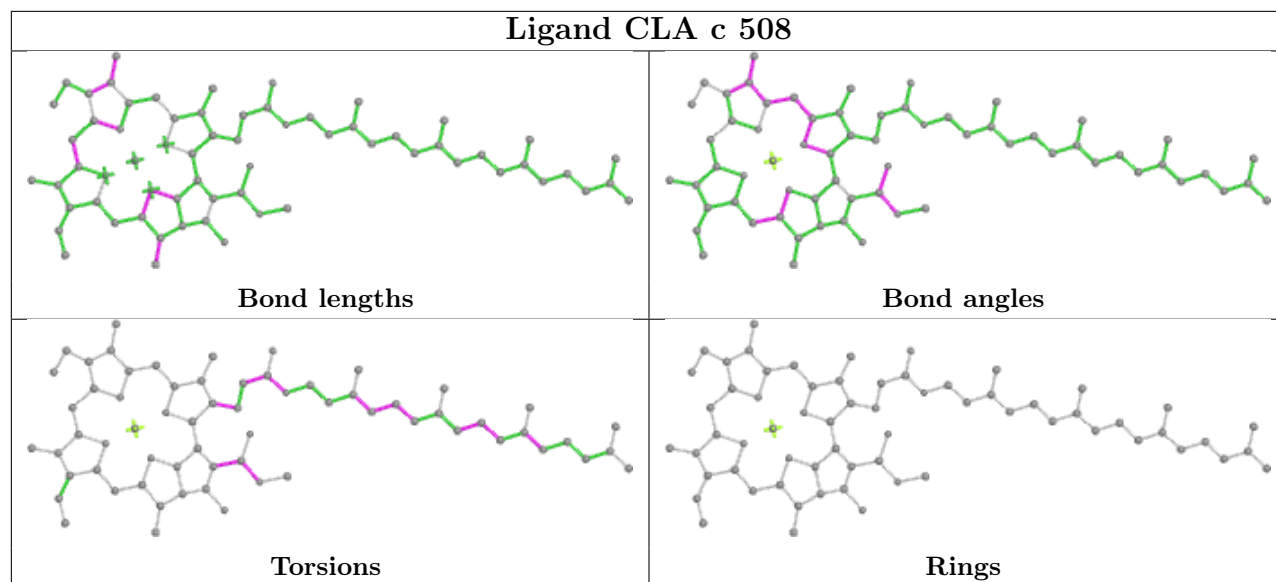
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	D	403	CLA	5	0
22	h	102	LMG	1	0
19	c	512	CLA	1	0
21	w	101	BCR	7	0
19	B	507	CLA	1	0
19	c	506	CLA	1	0
21	B	517	BCR	4	0
19	C	503	CLA	1	0
19	C	507	CLA	1	0
19	C	510	CLA	1	0
20	d	401	PHO	1	0
19	C	514	CLA	1	0
25	C	518	DGD	1	0

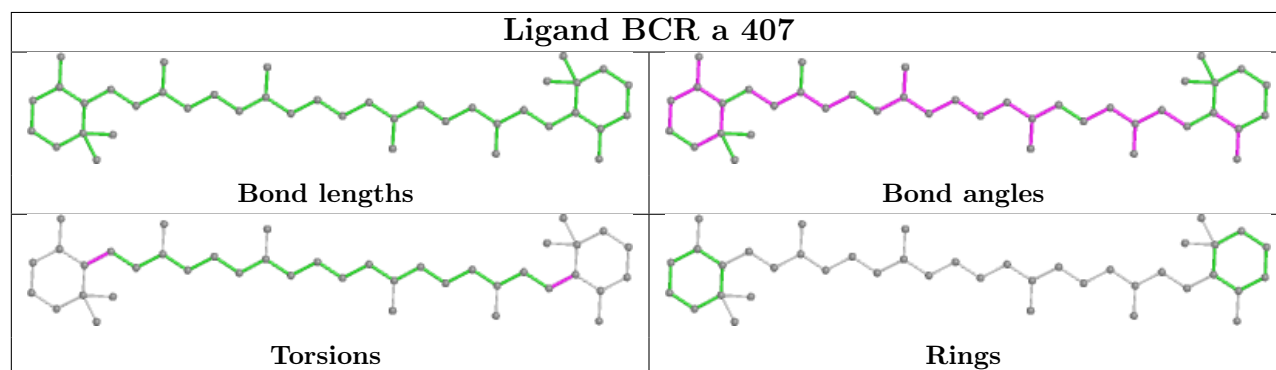
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



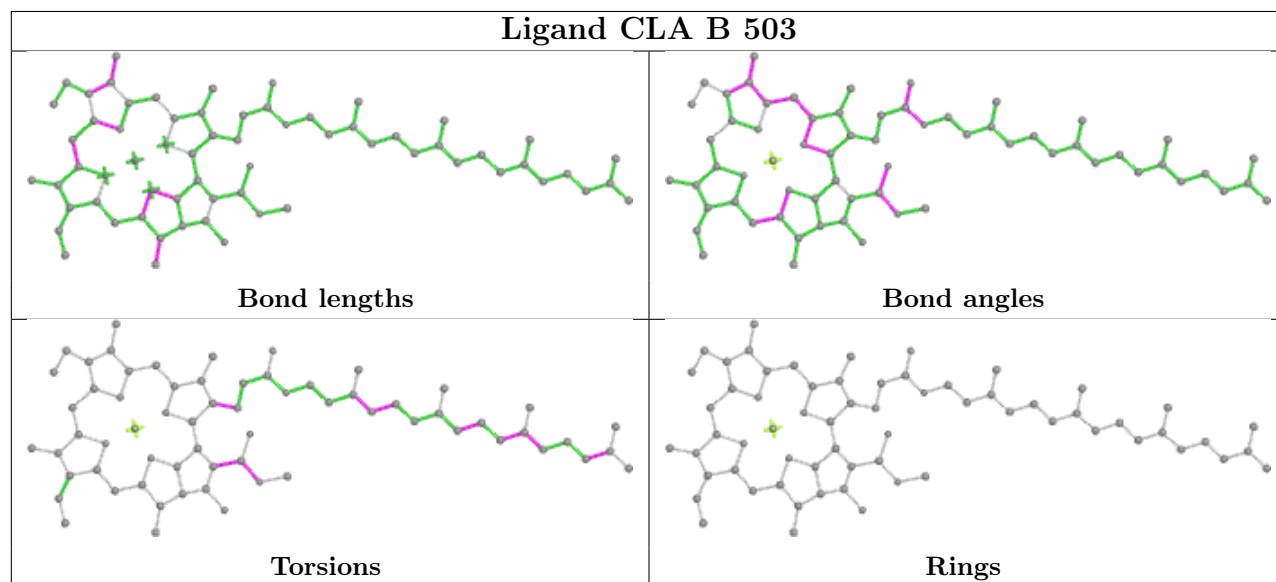
## Ligand CLA c 508



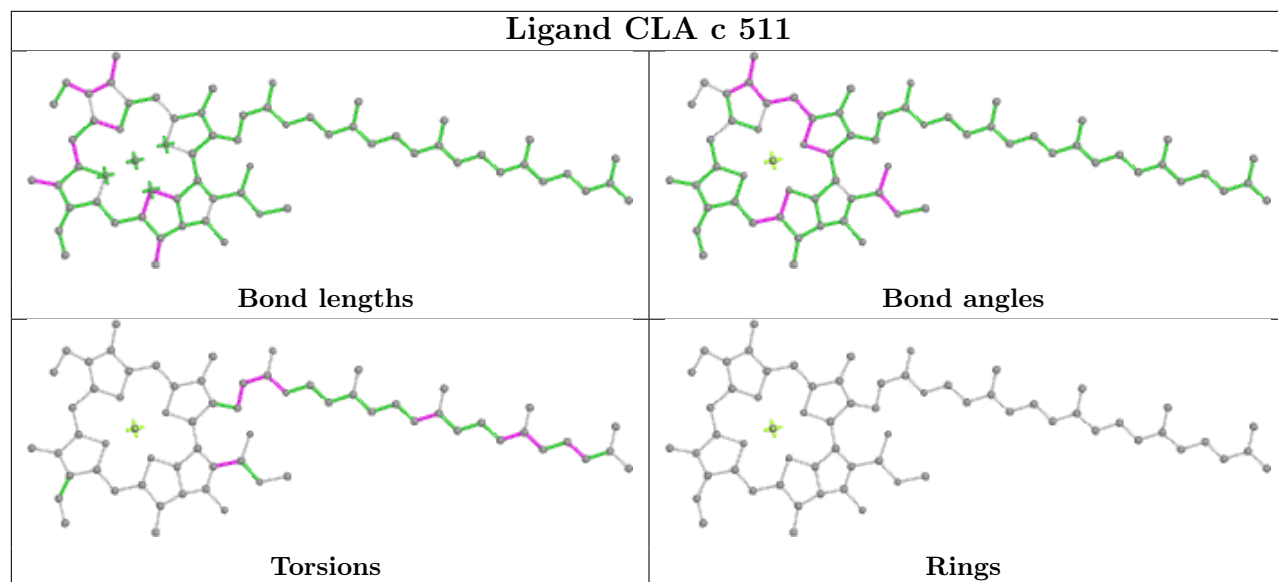
## Ligand BCR a 407



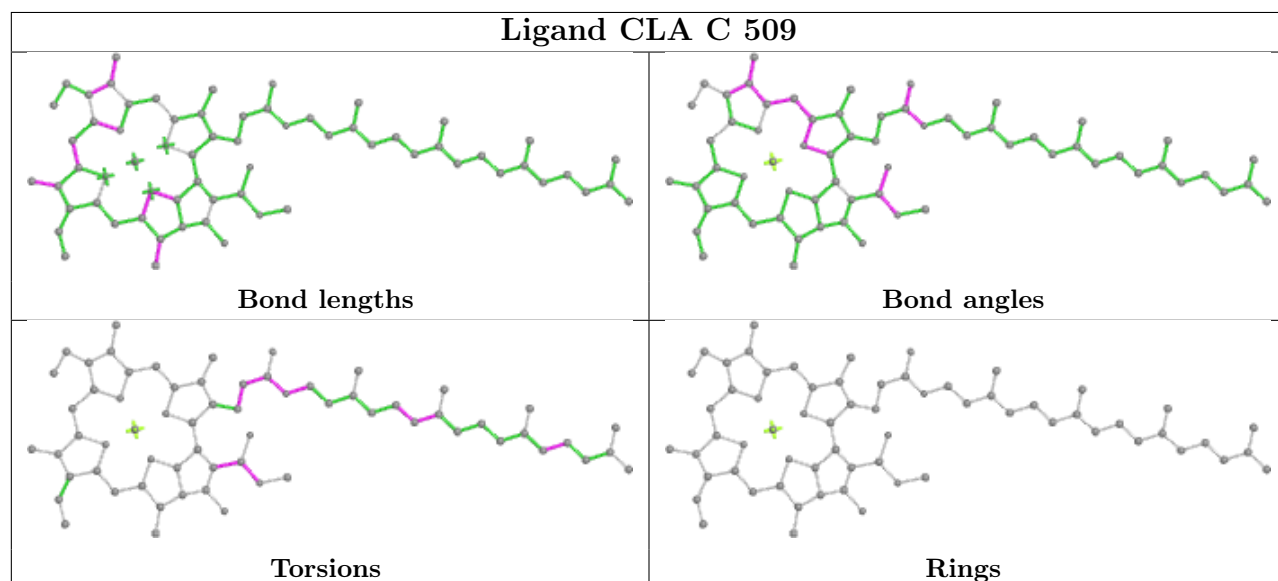
## Ligand CLA B 503



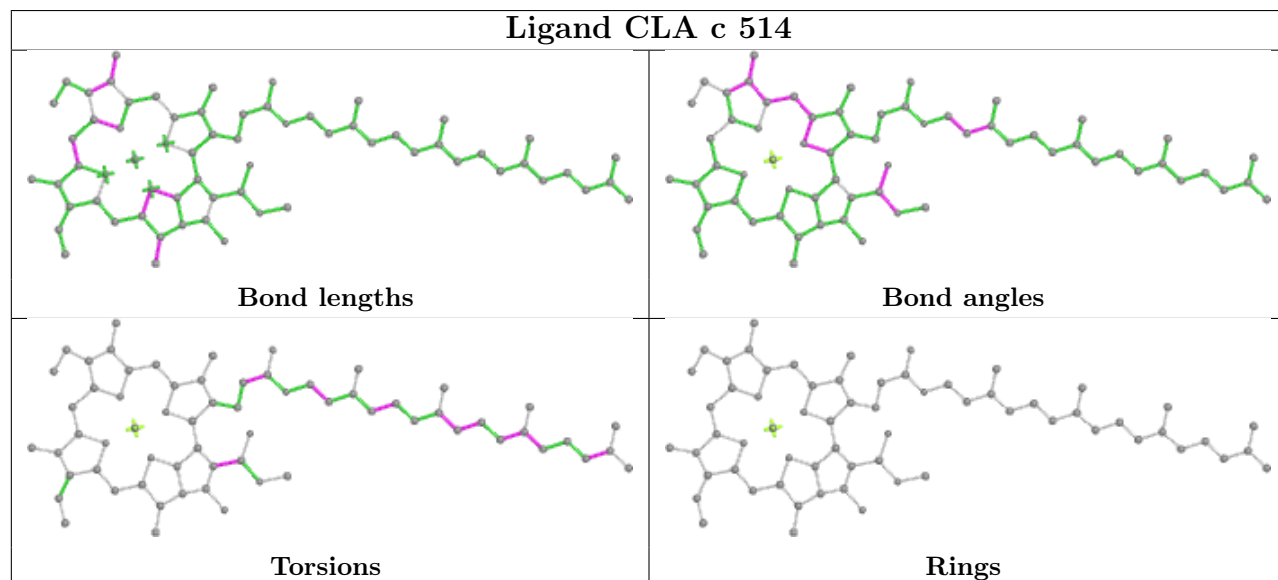
## Ligand CLA c 511



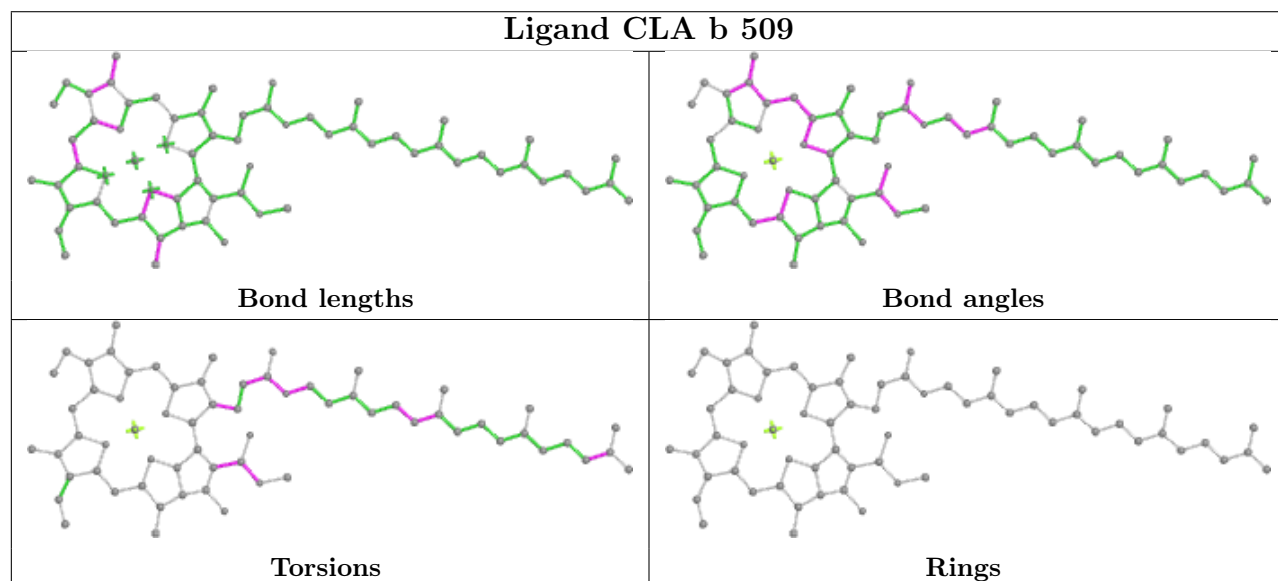
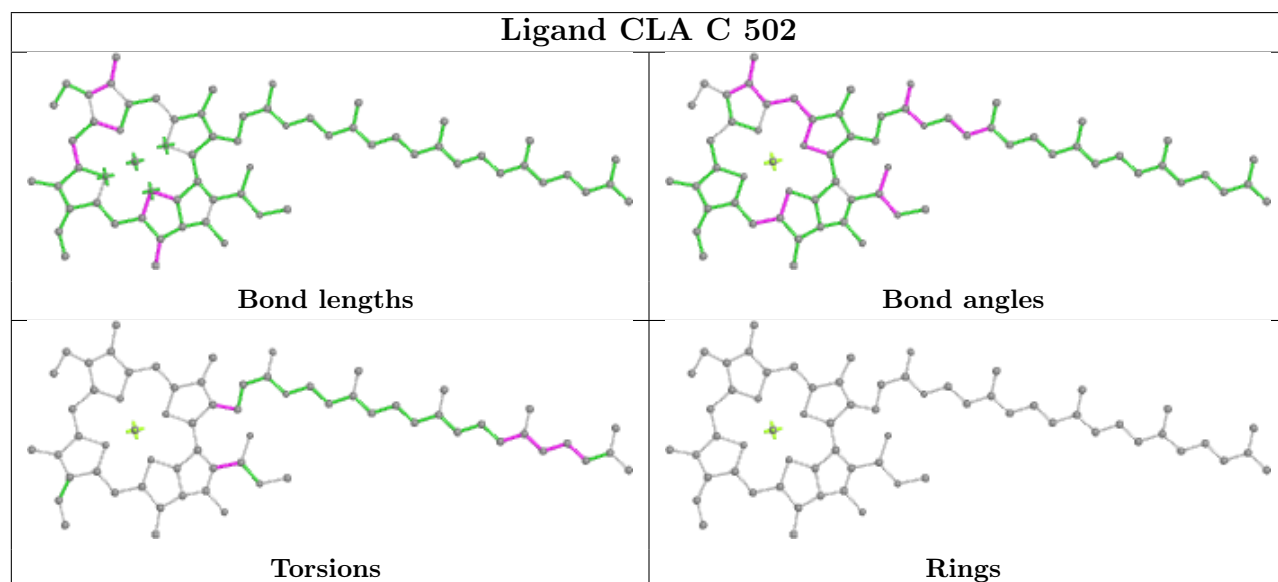
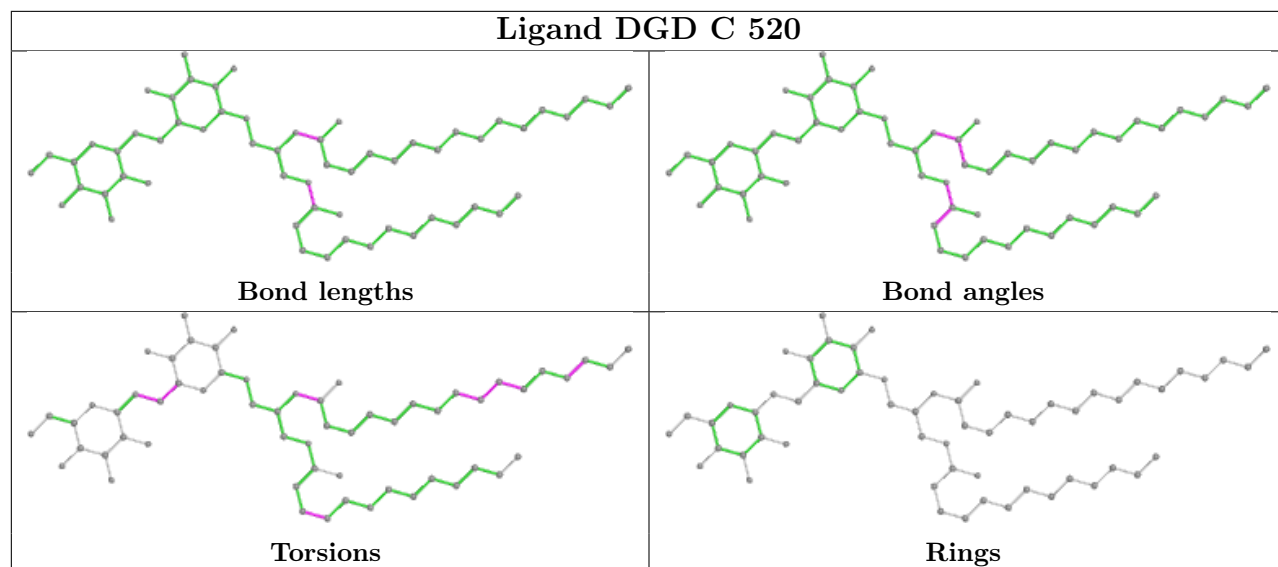
## Ligand CLA C 509



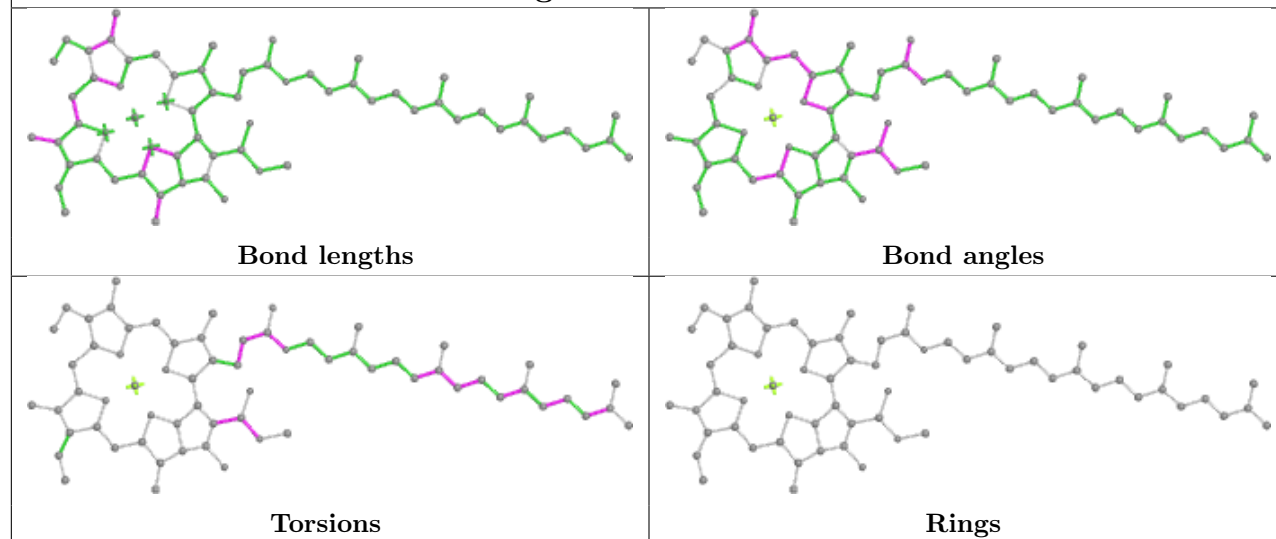
## Ligand CLA c 514



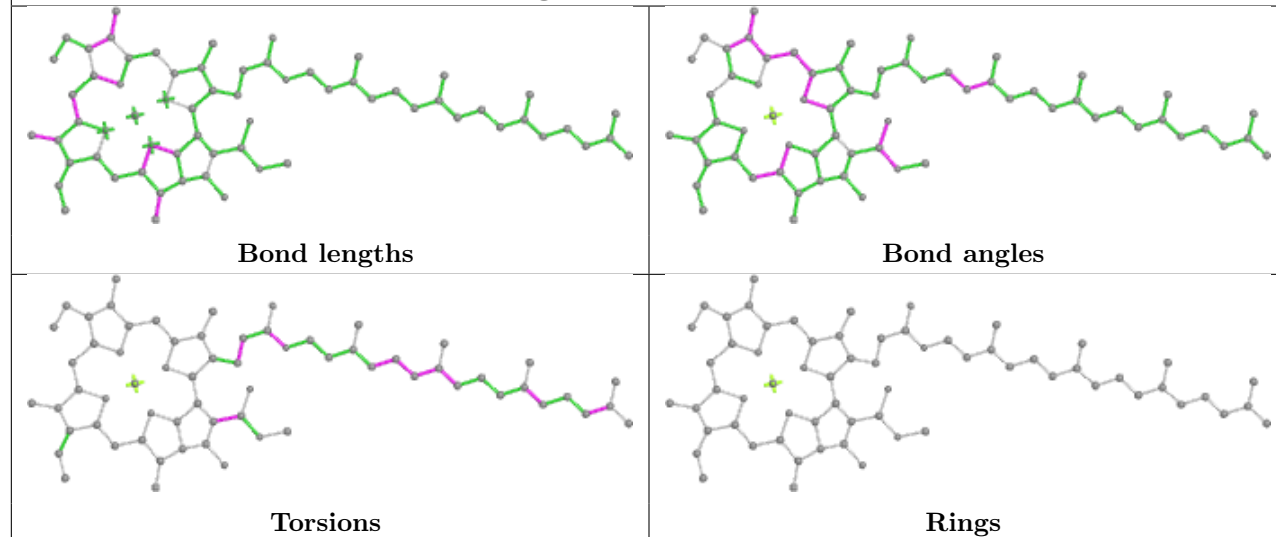




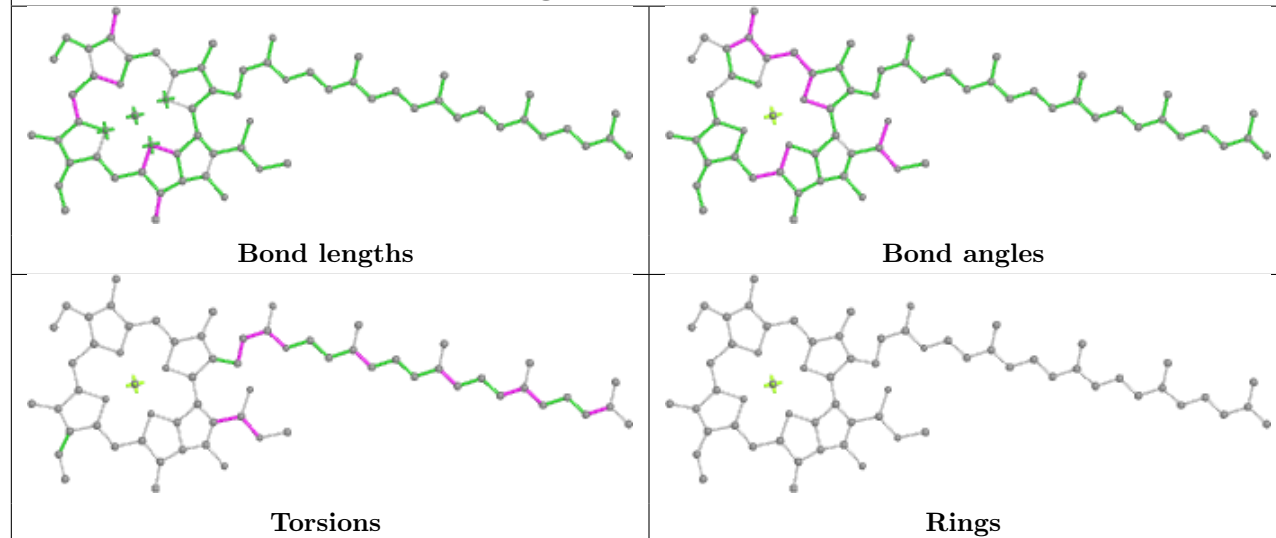
## Ligand CLA b 511

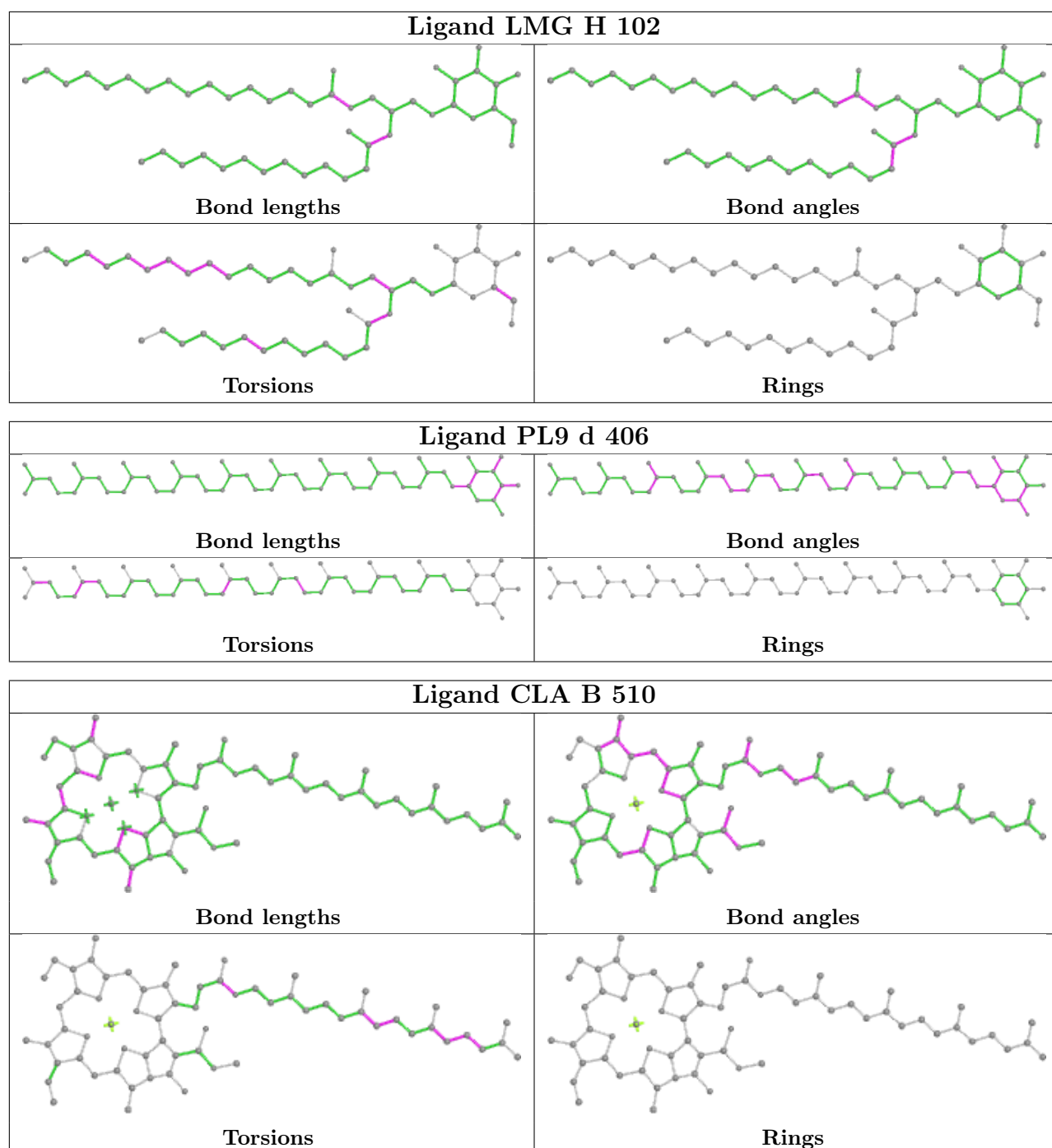


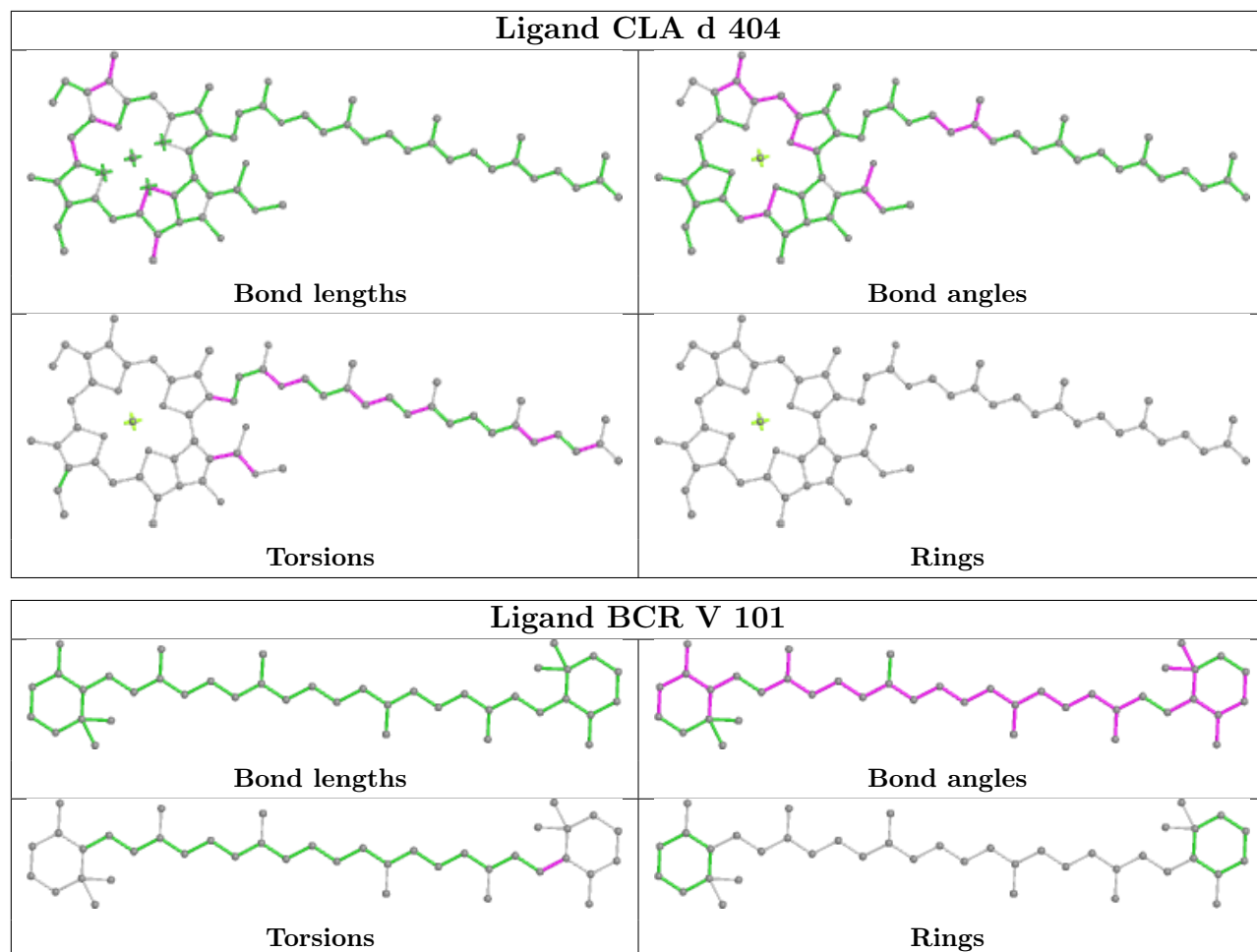
## Ligand CLA b 513



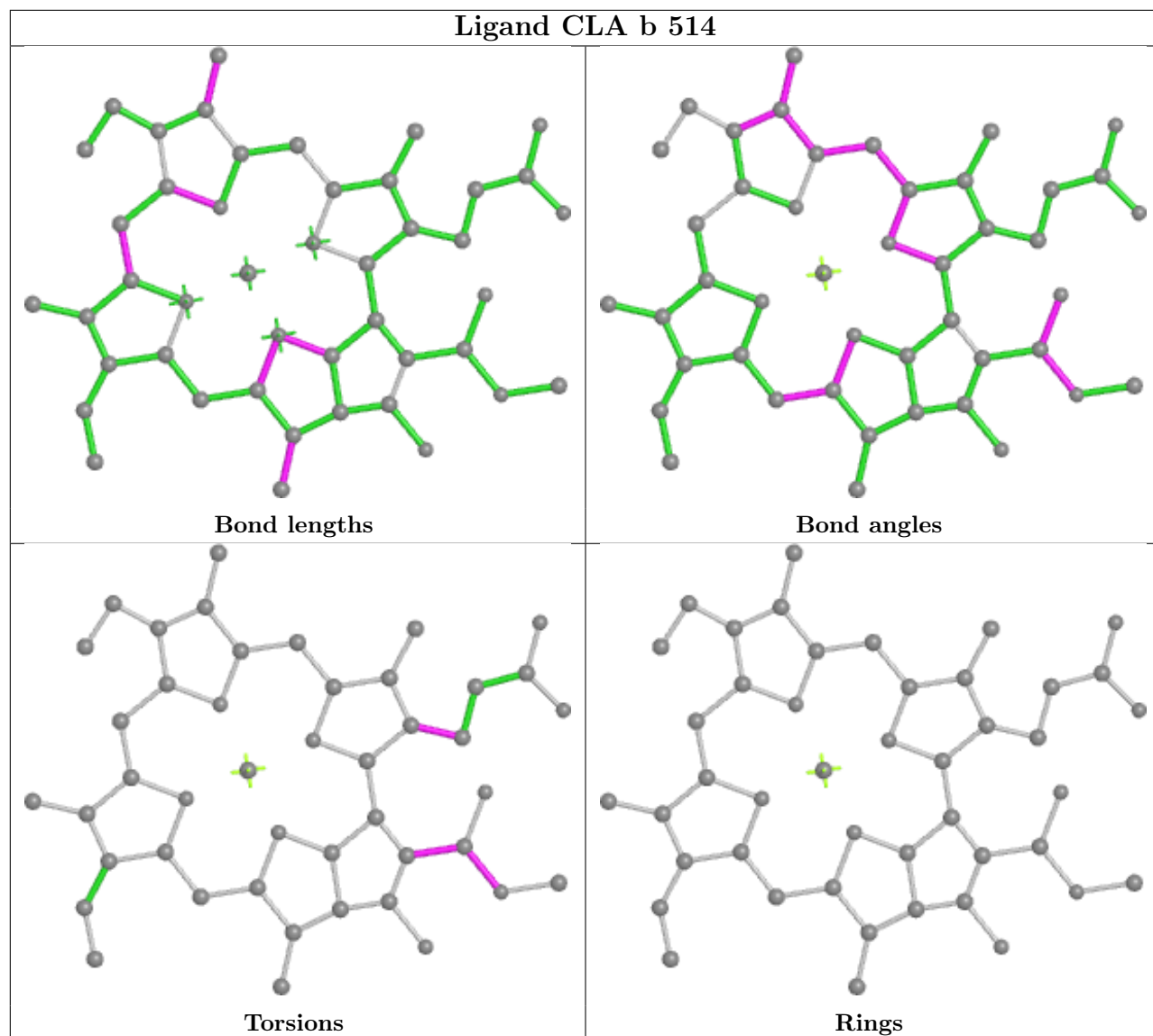
## Ligand CLA c 515

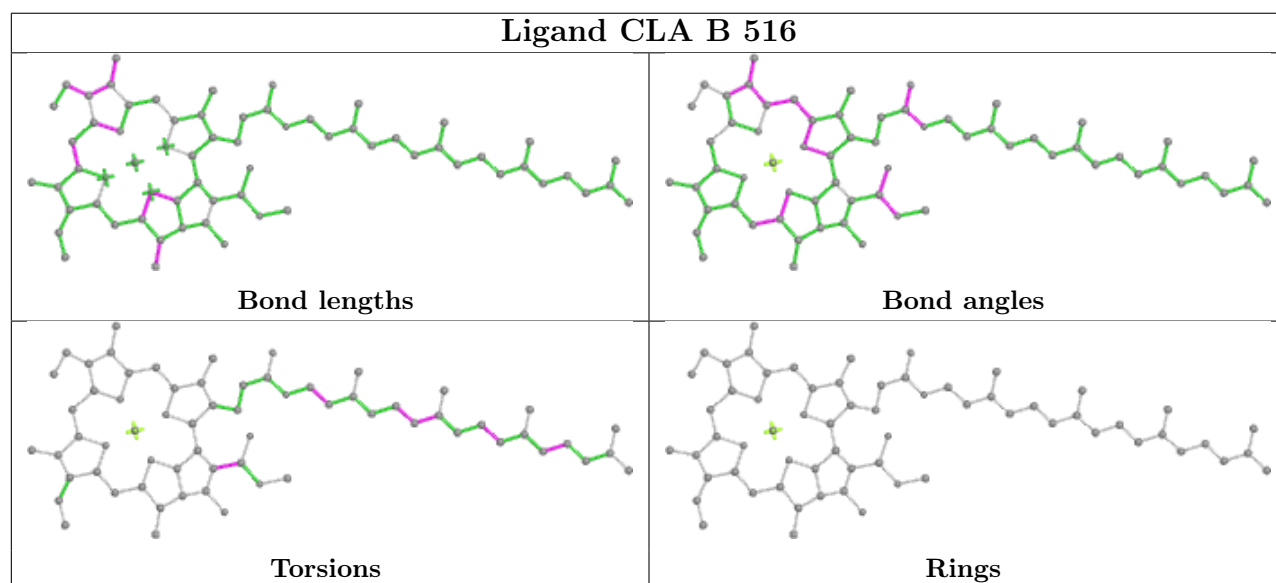
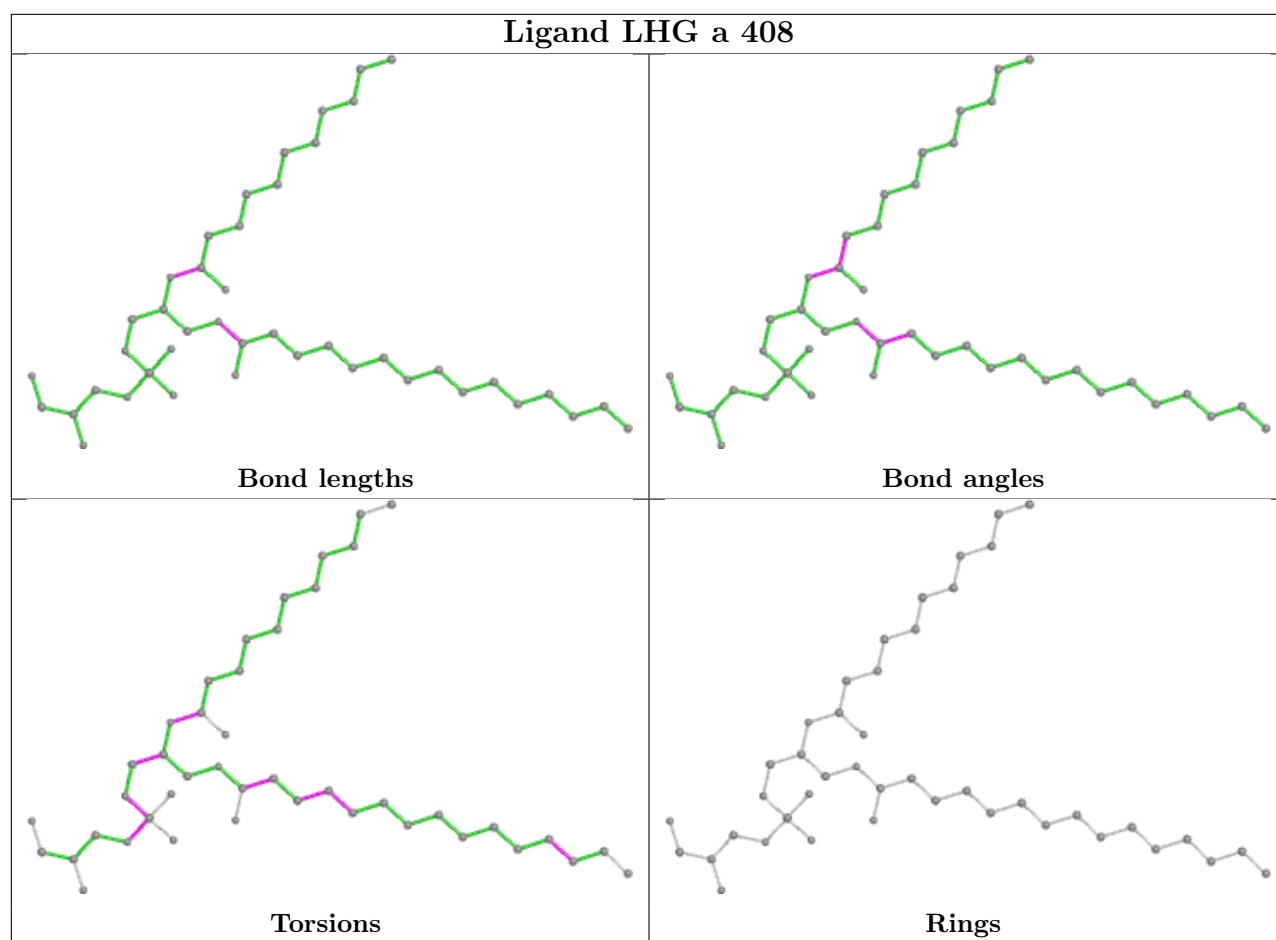


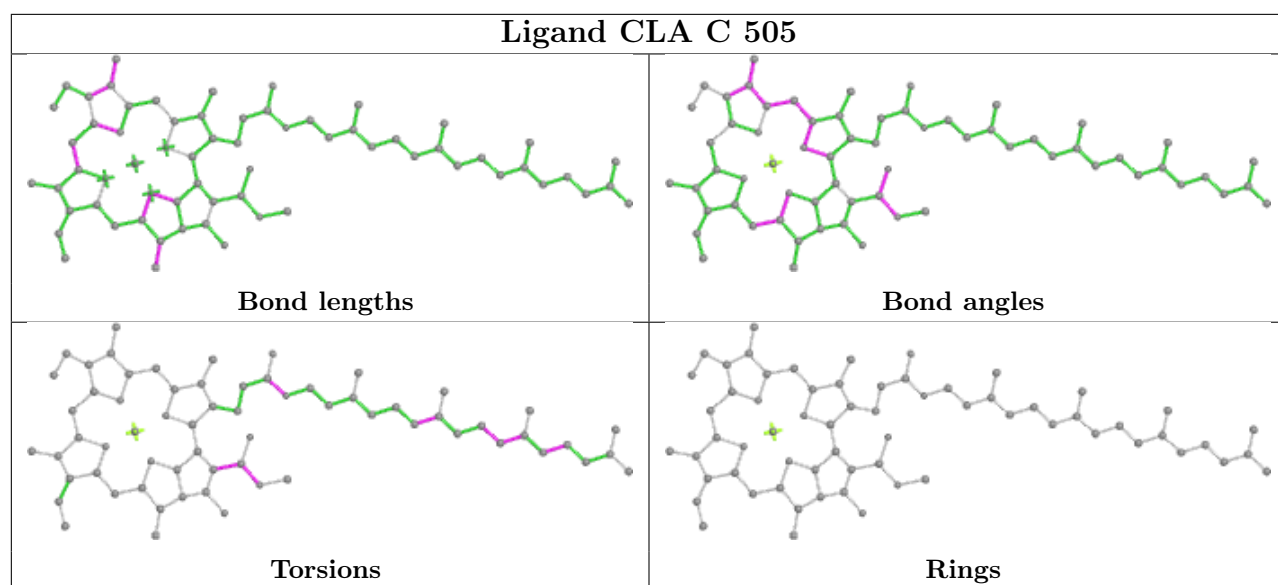


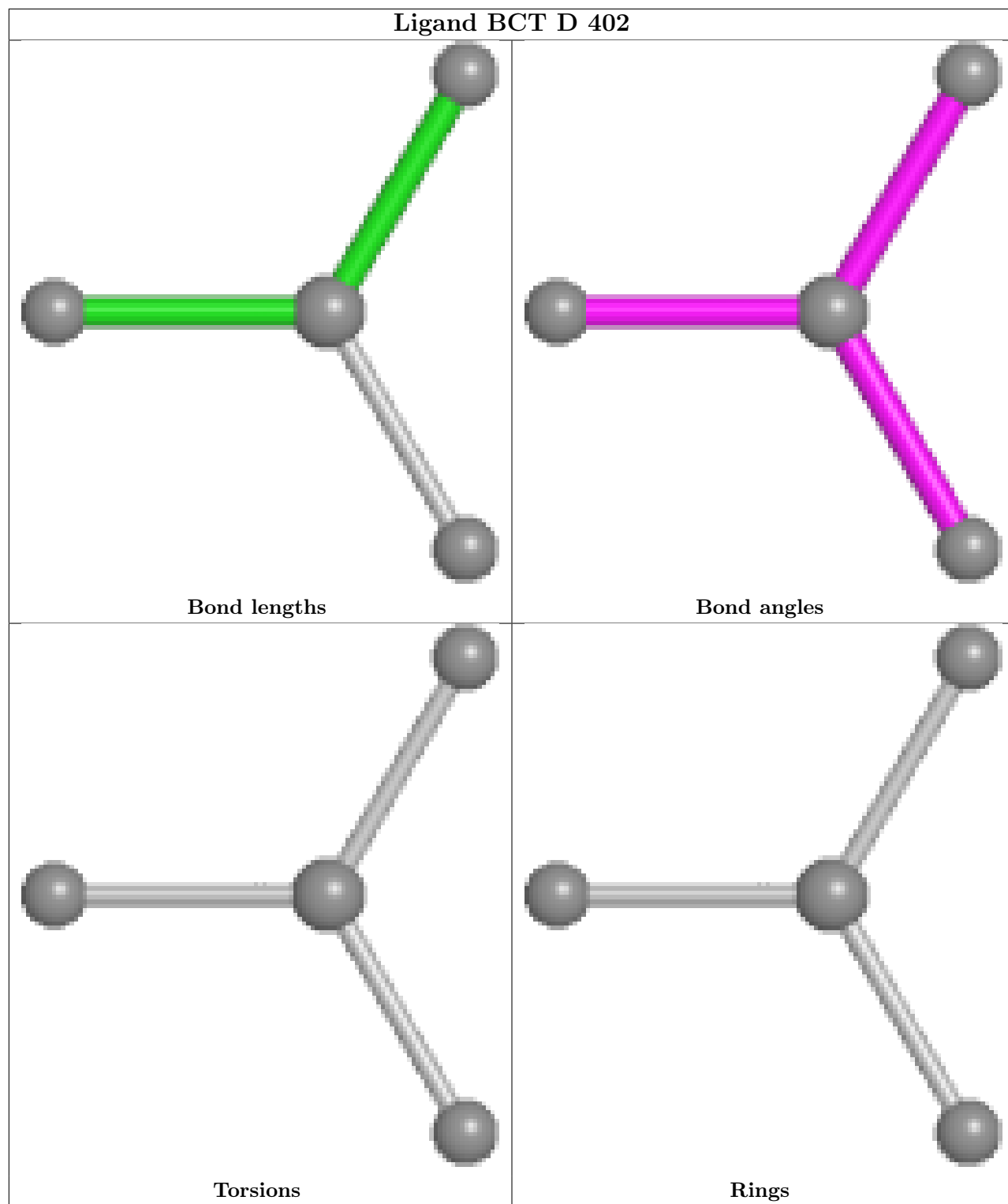


## Ligand CLA b 514

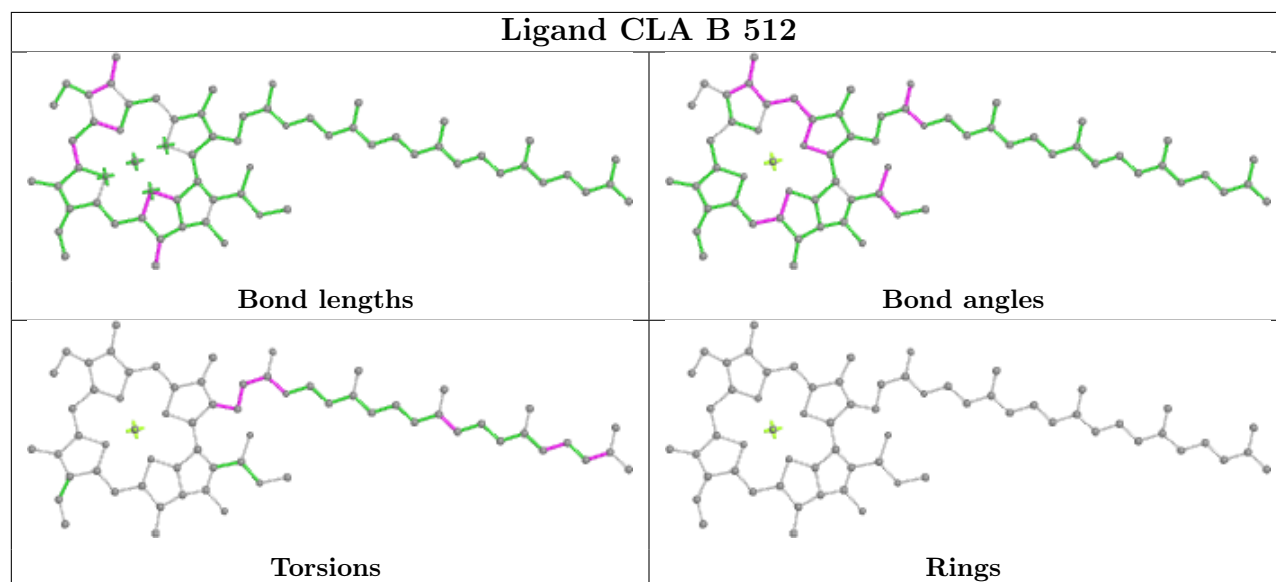
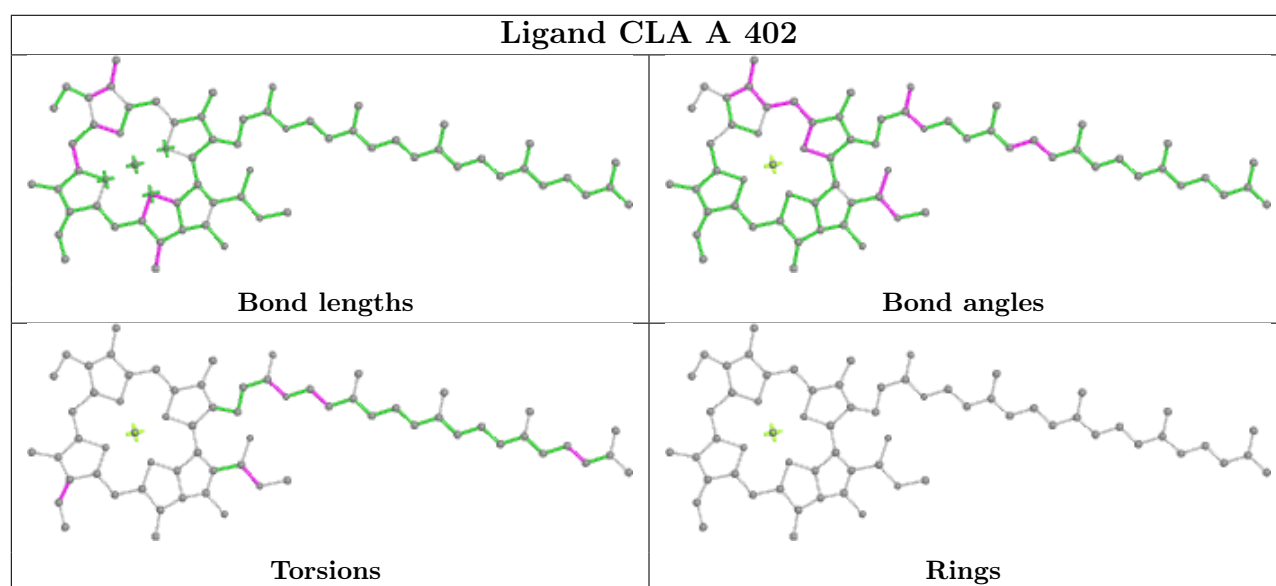
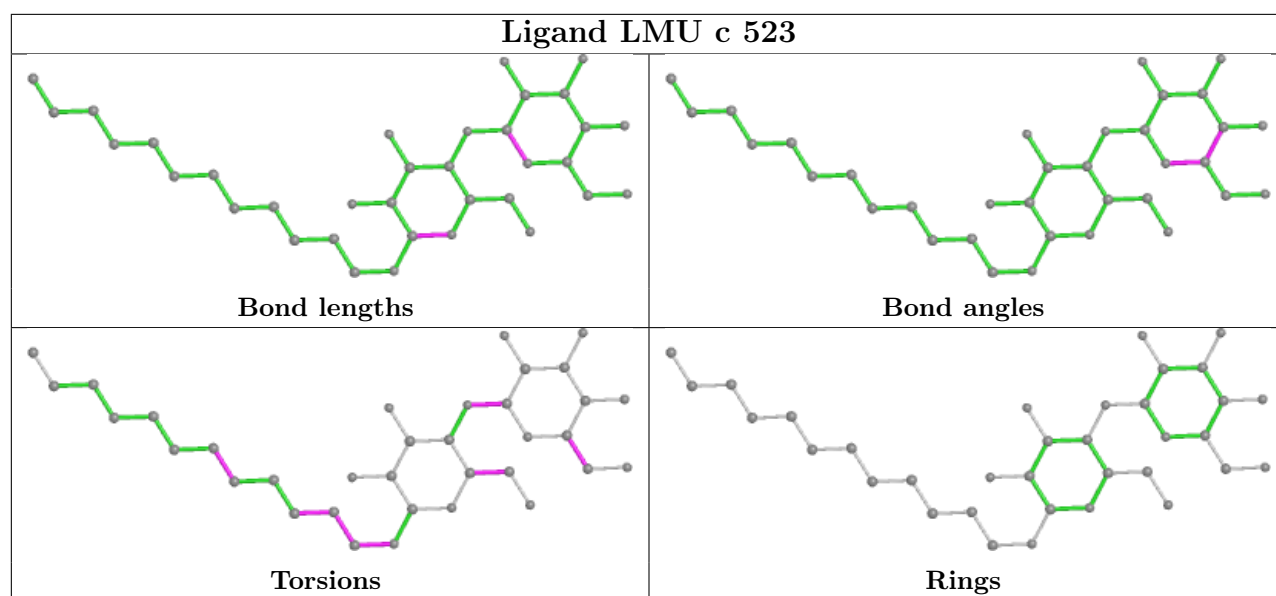


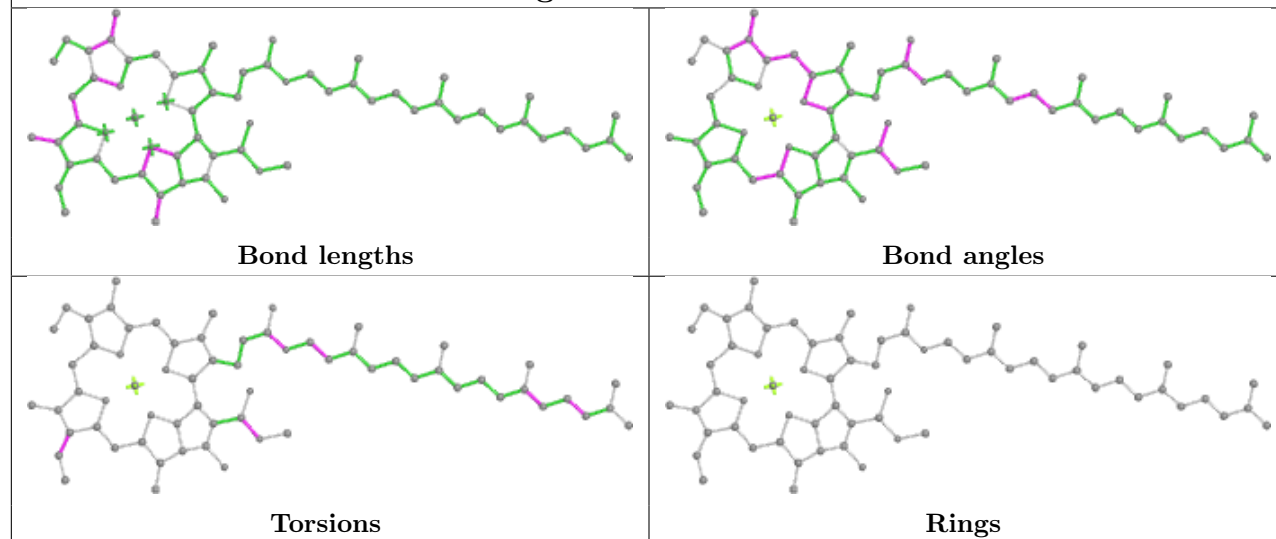
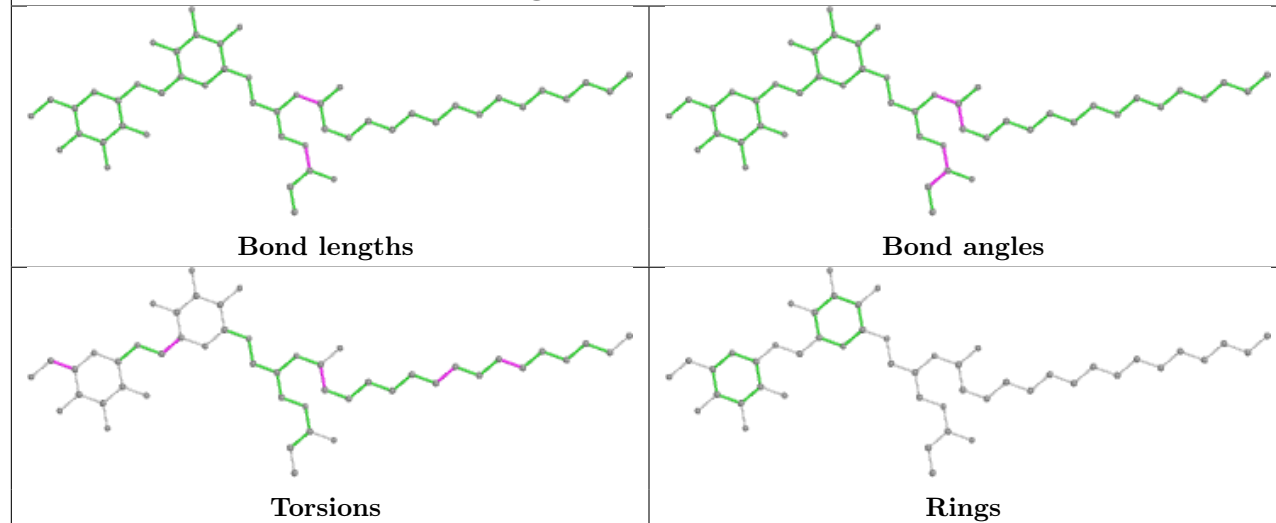


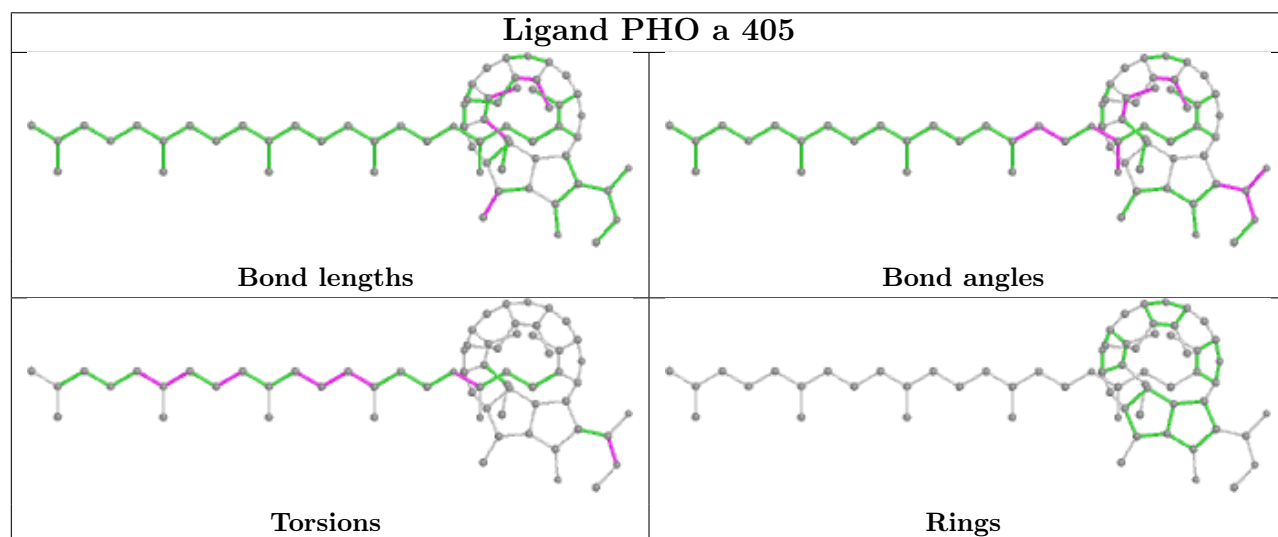
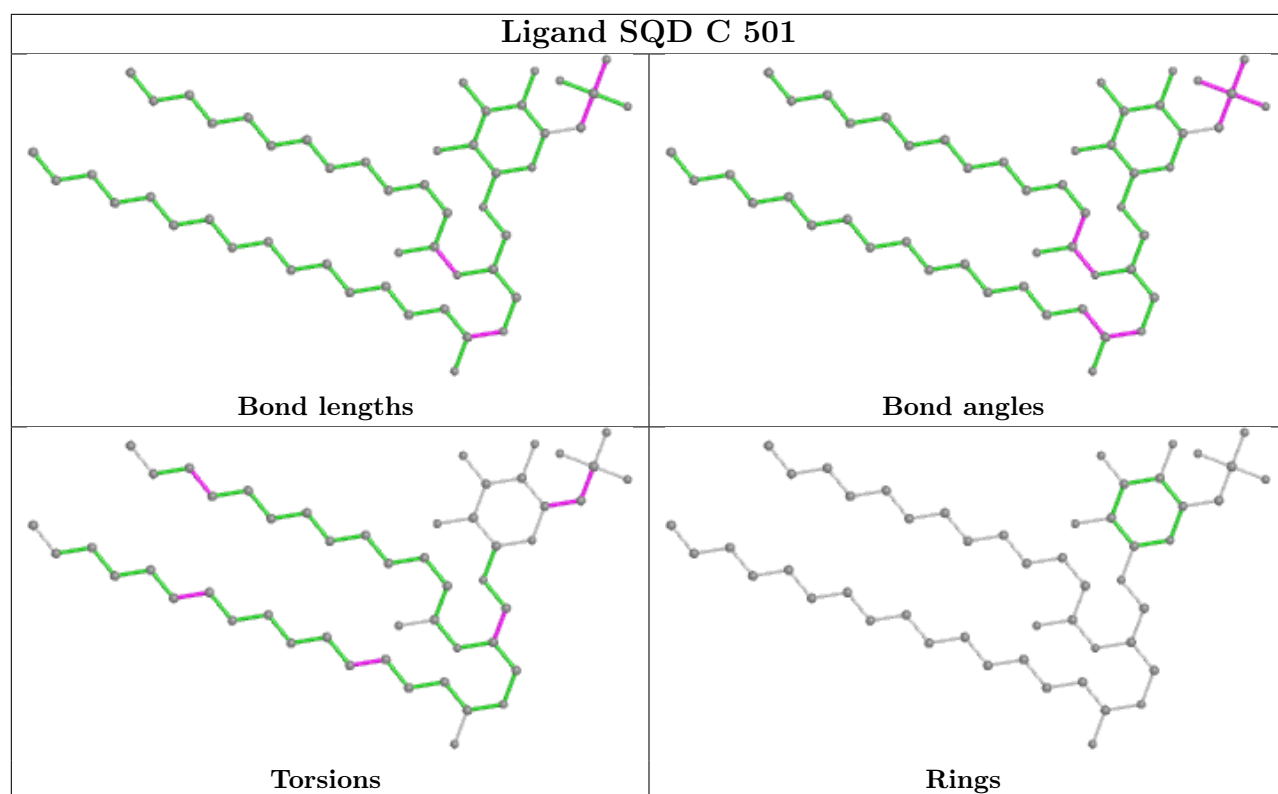


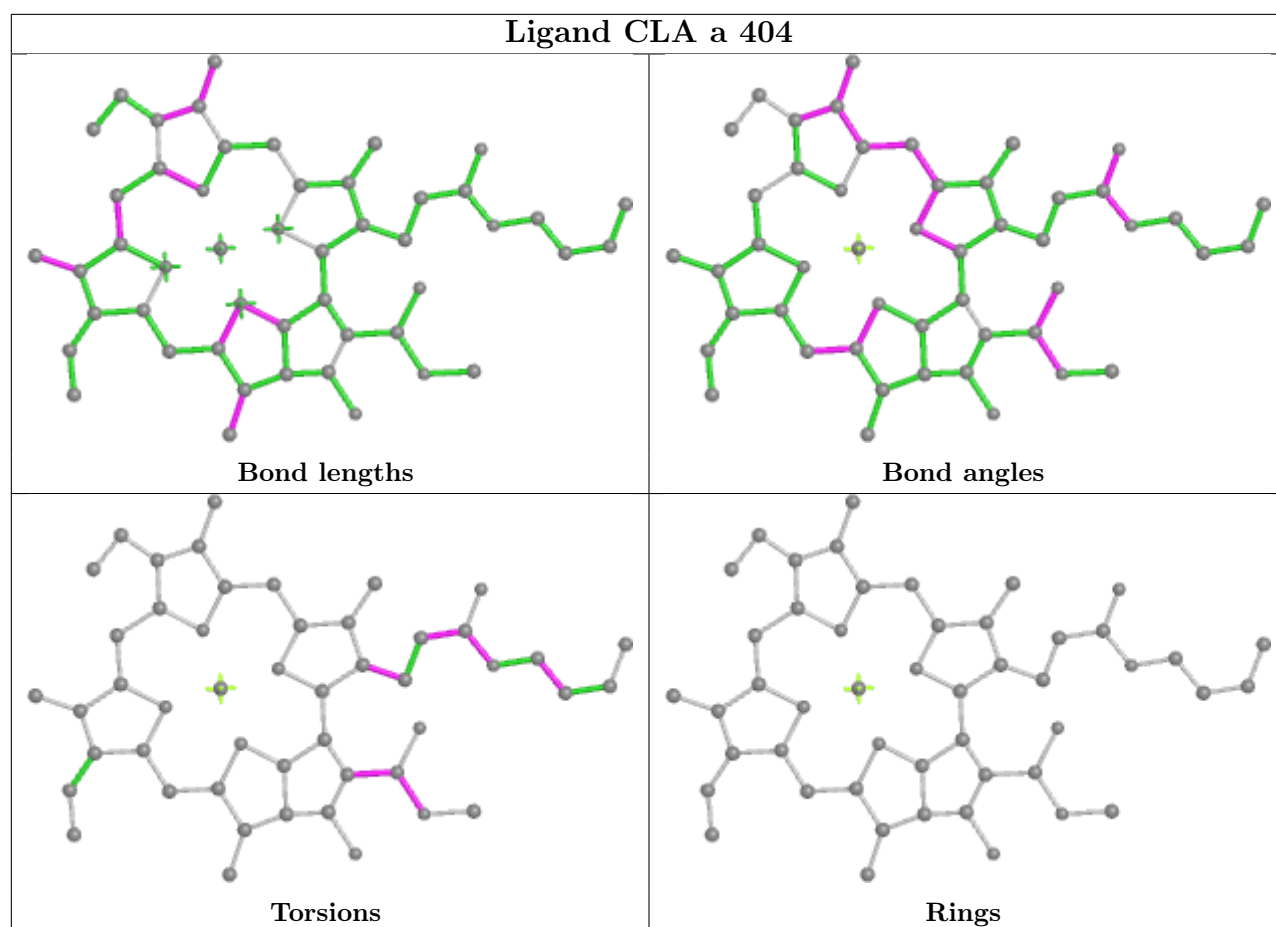


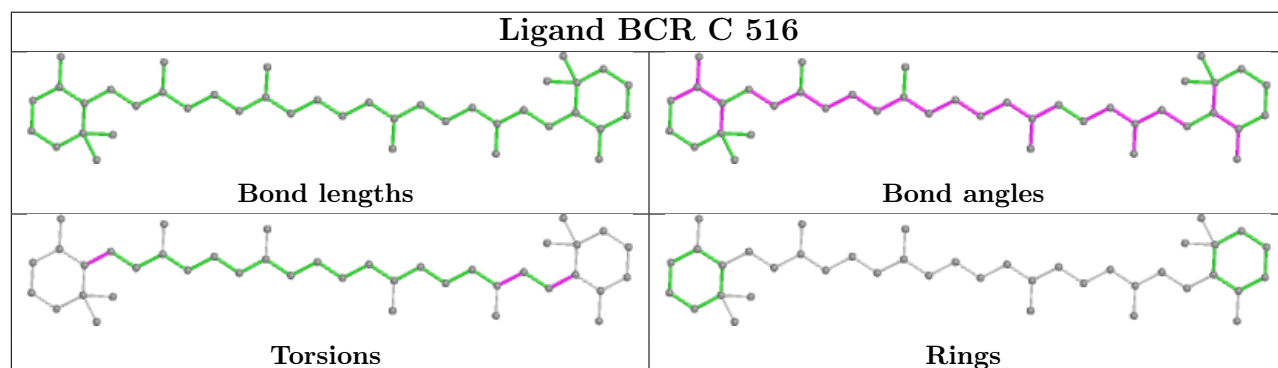
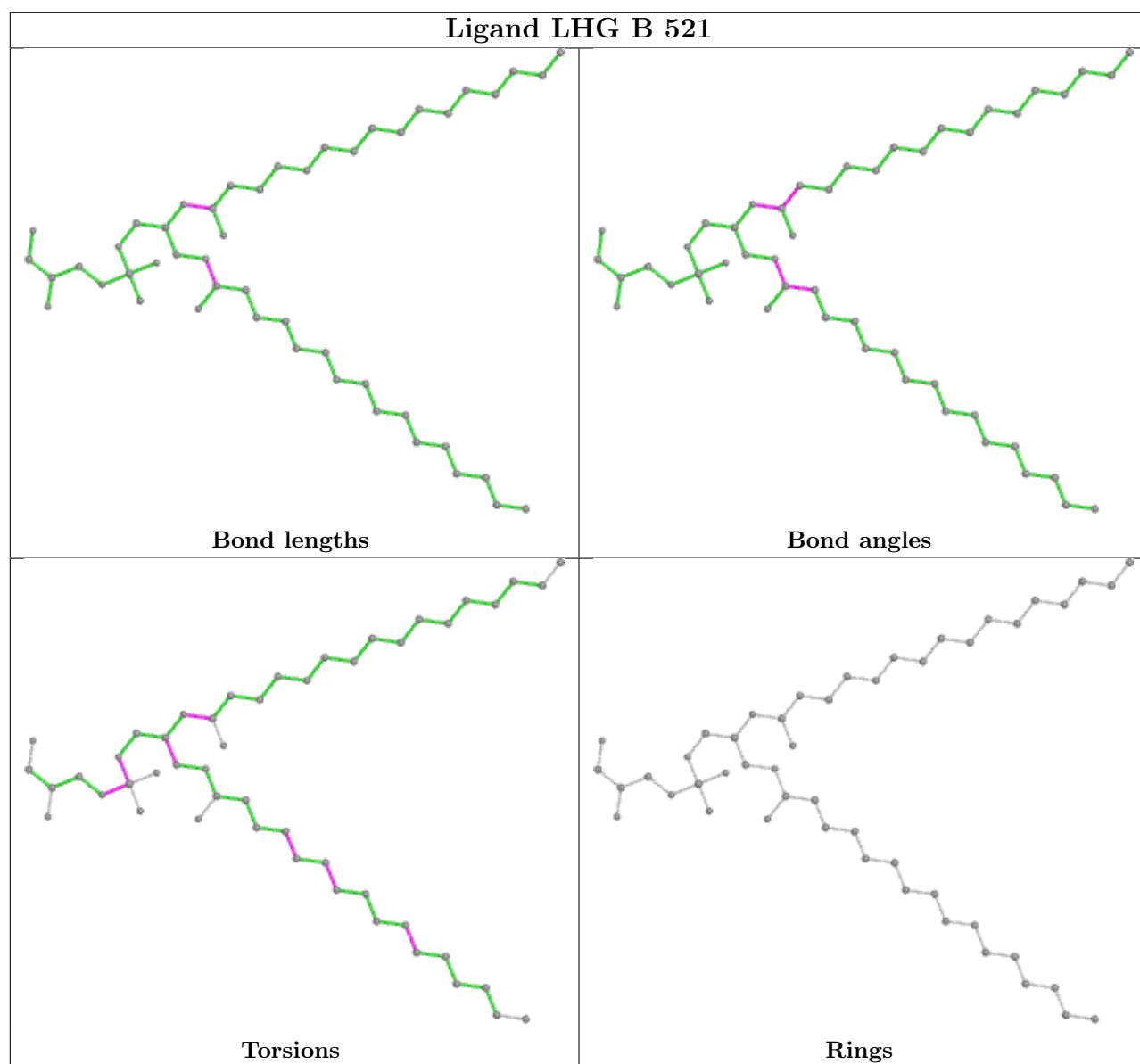


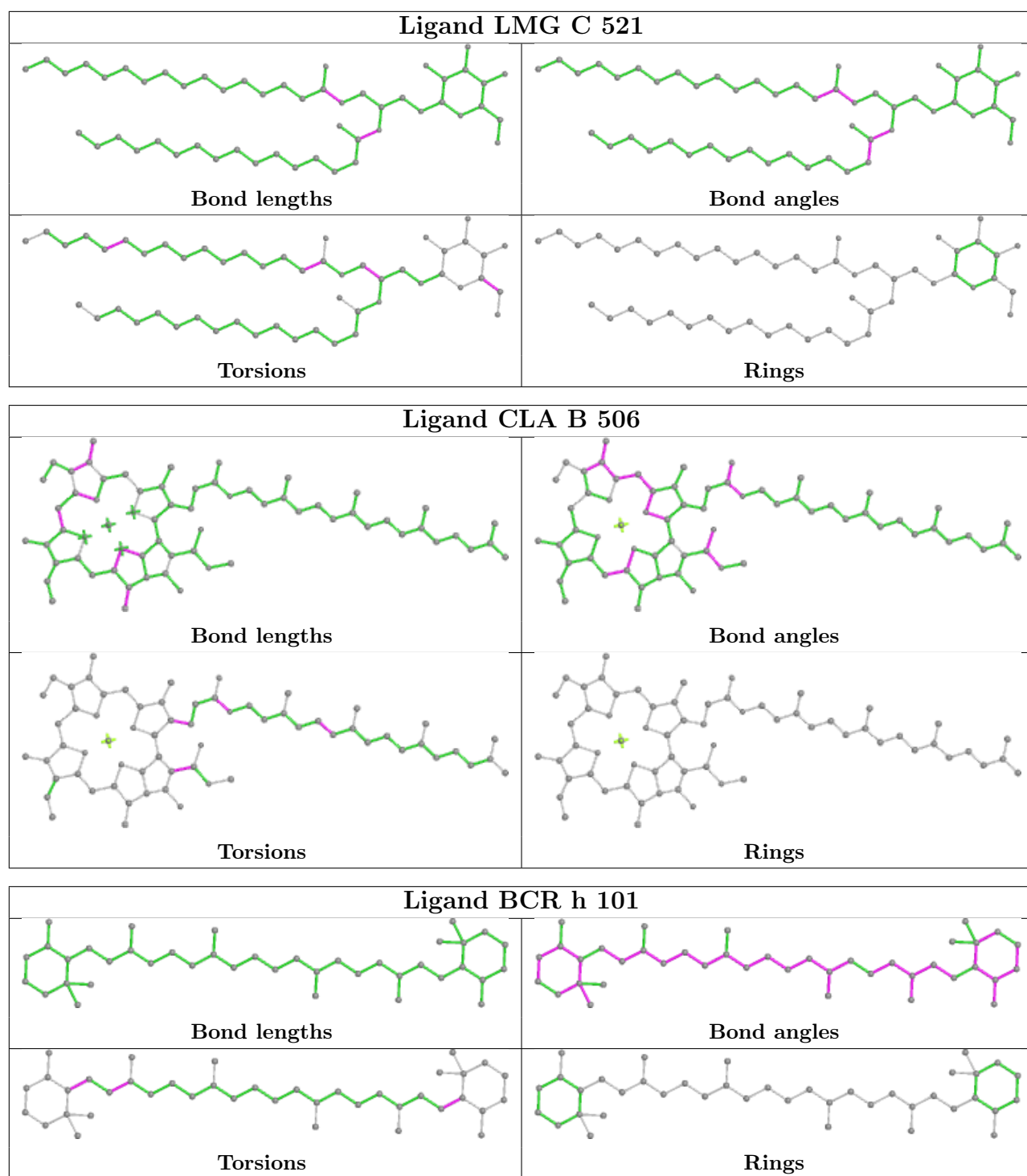


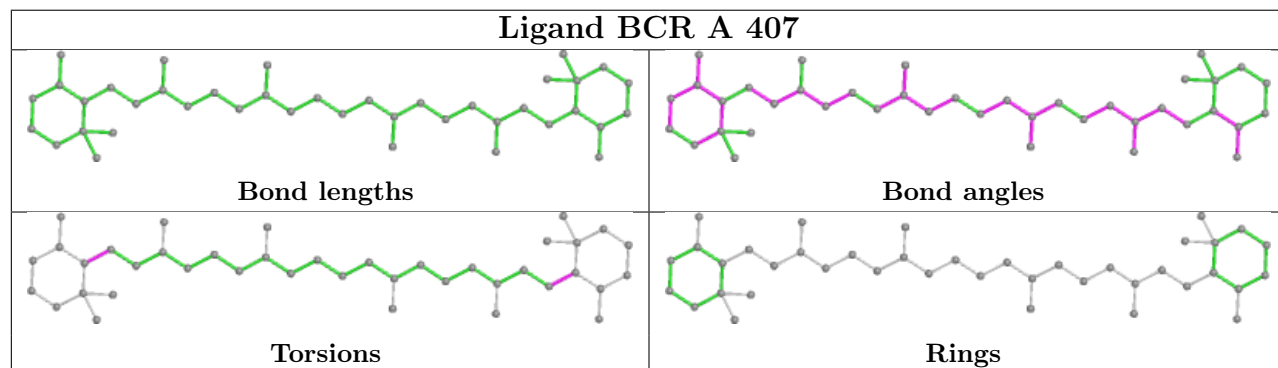
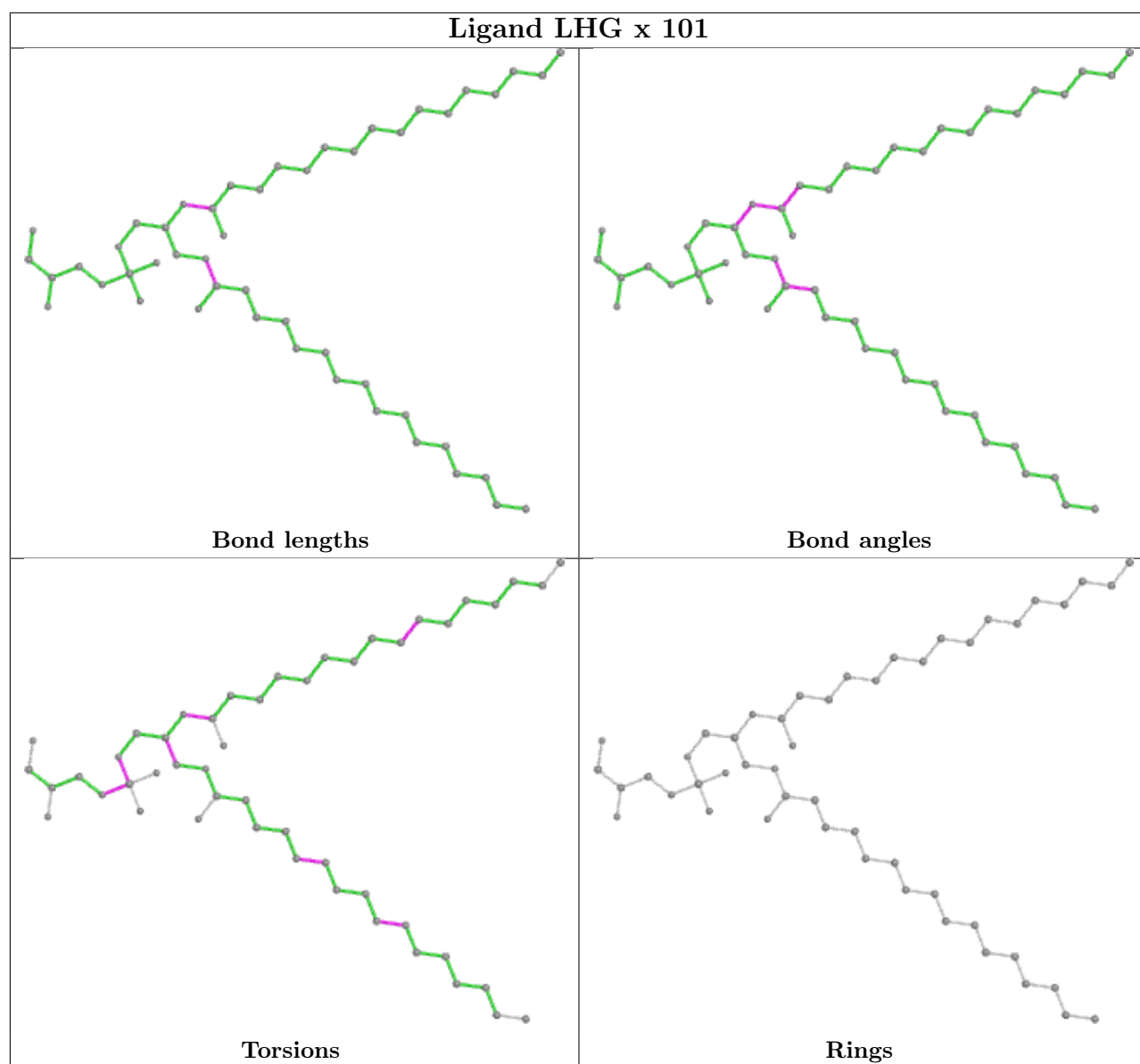
**Ligand CLA a 402****Ligand DGD C 519**

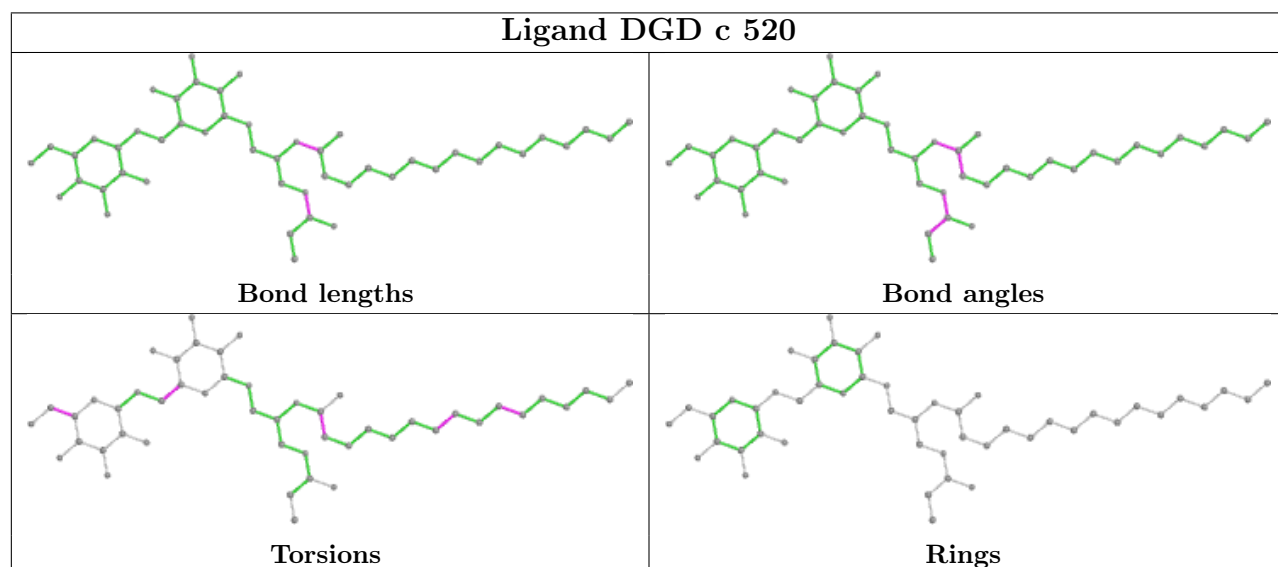
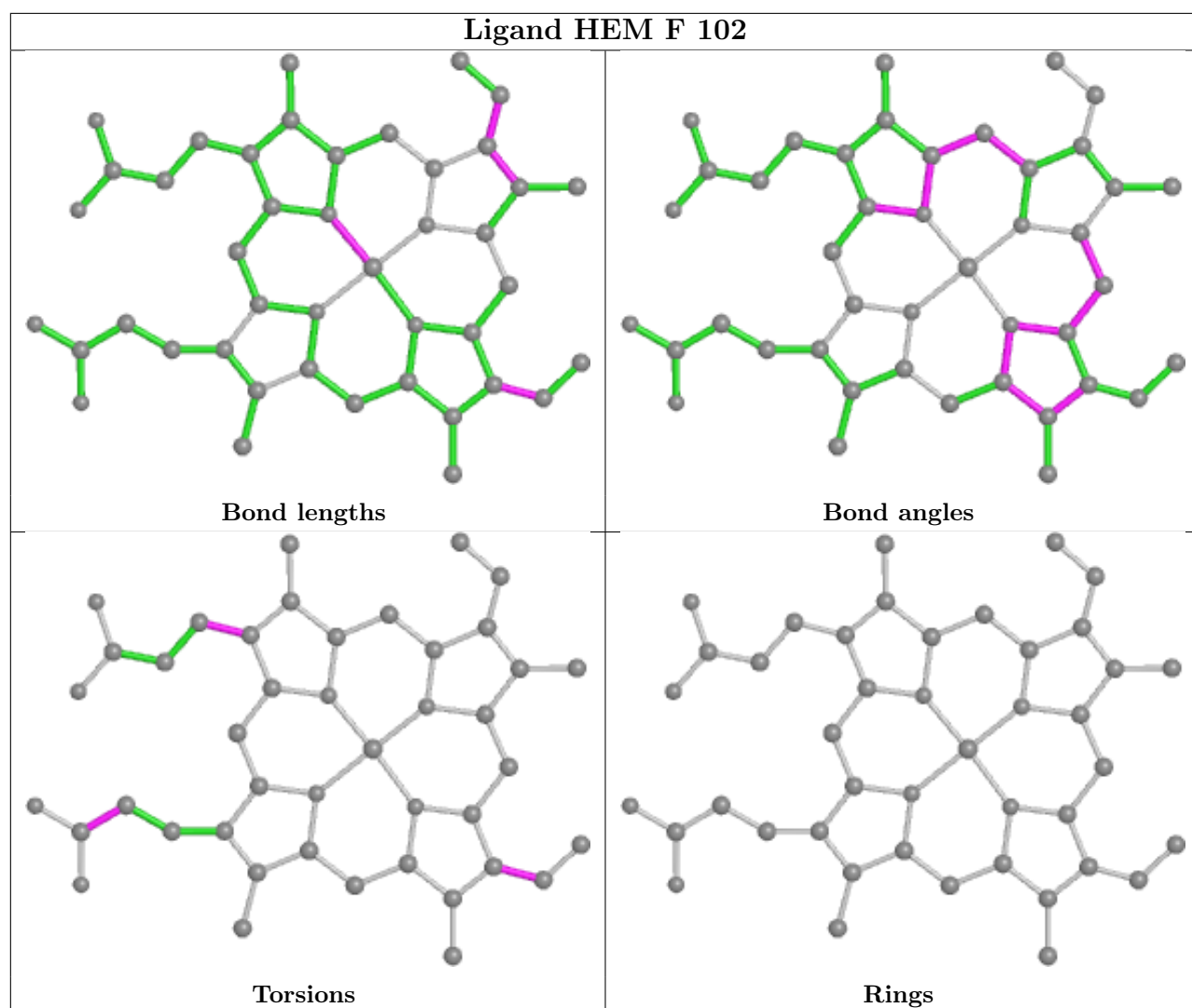




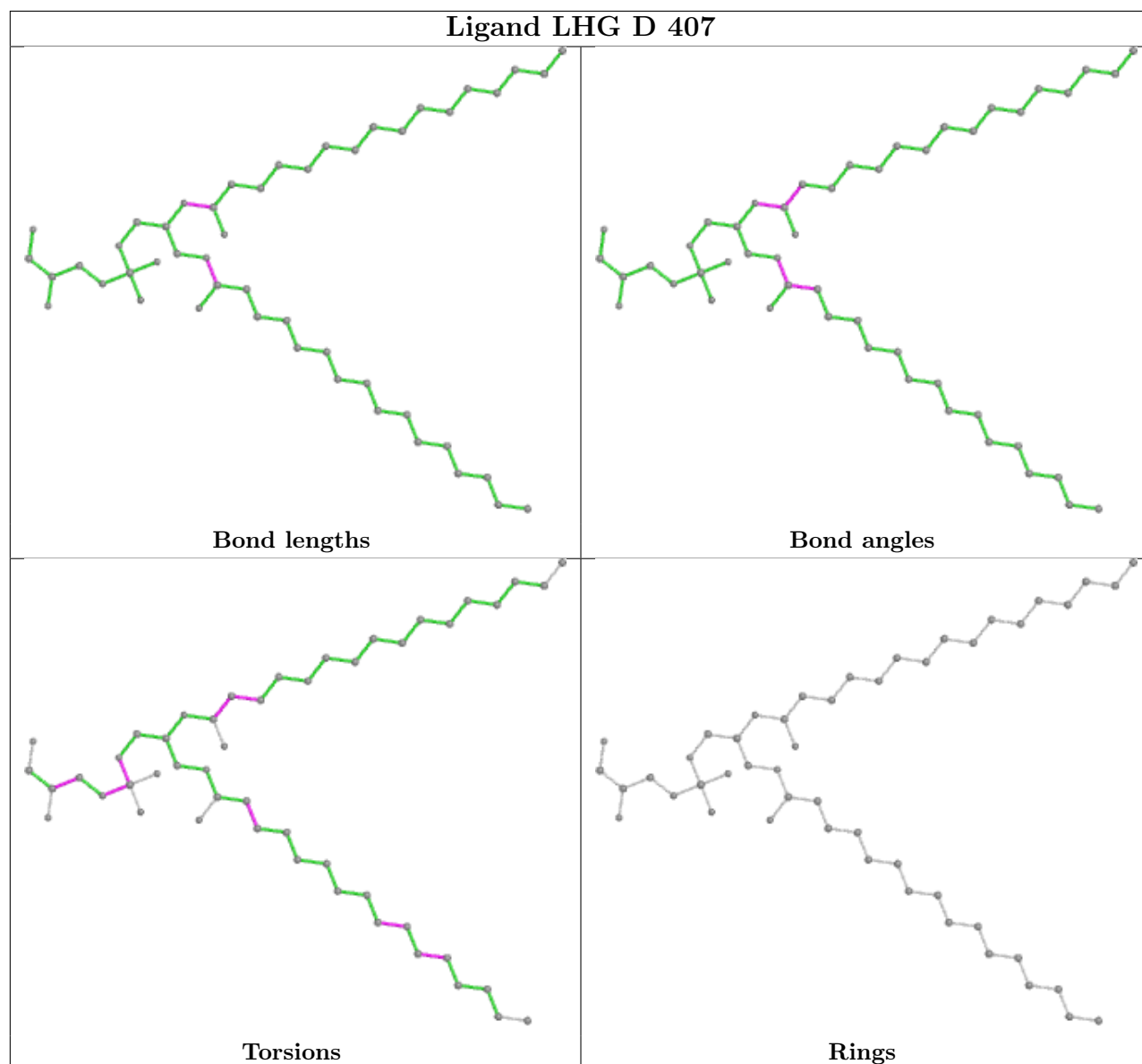
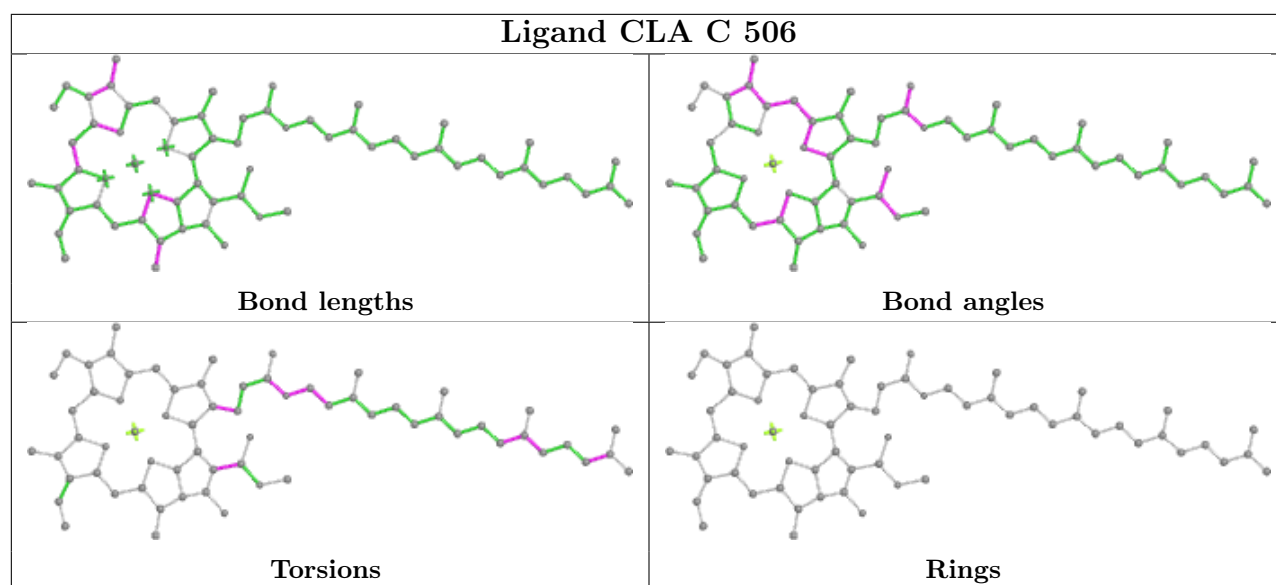




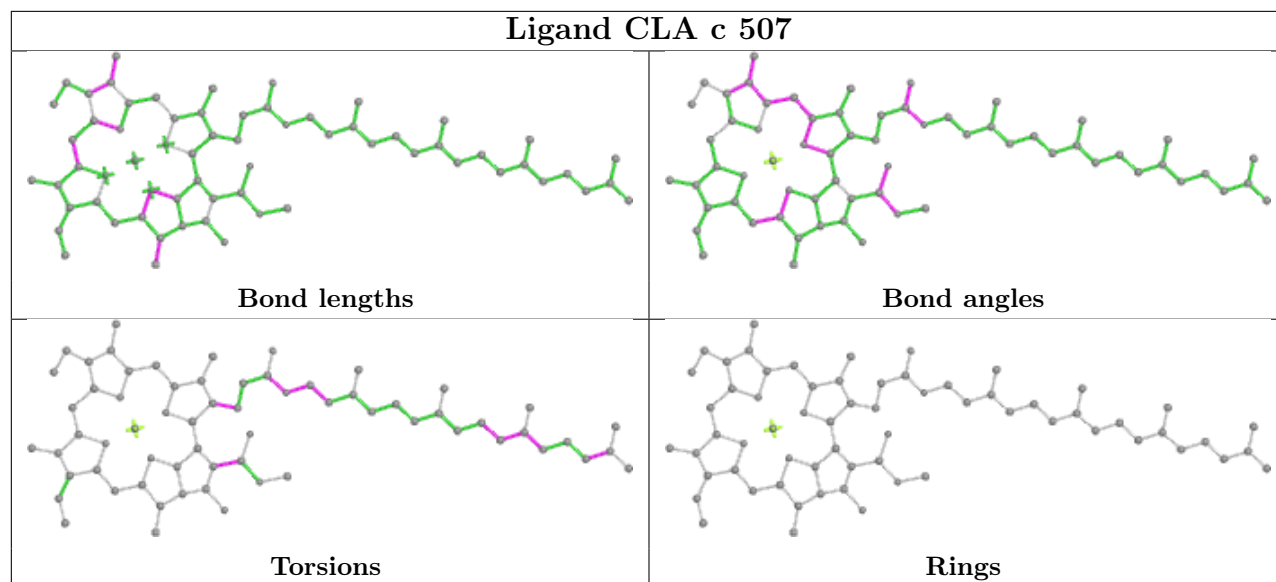




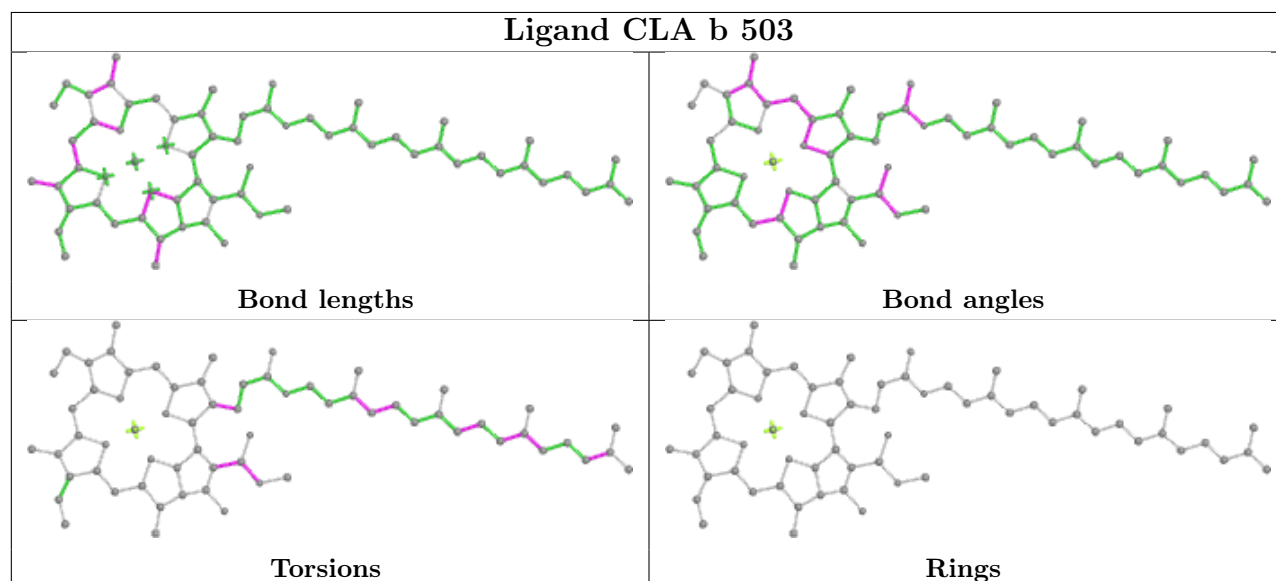




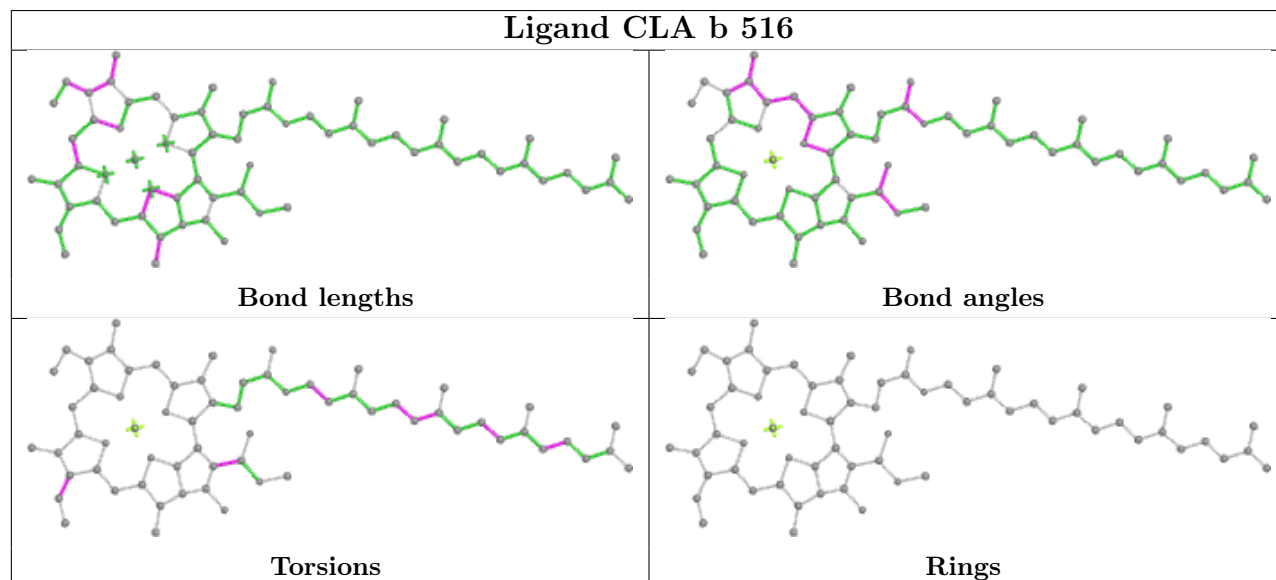
## Ligand CLA c 507

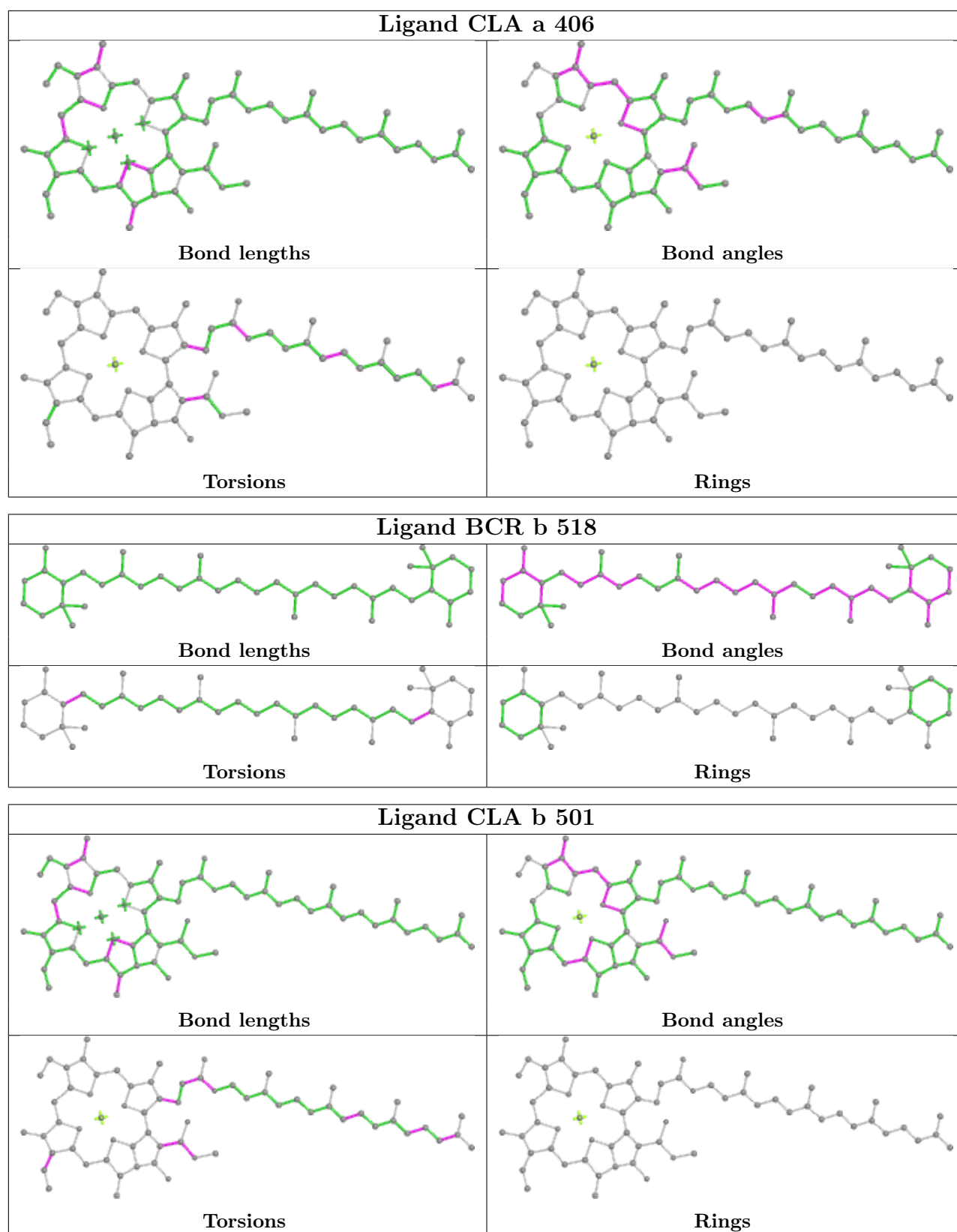


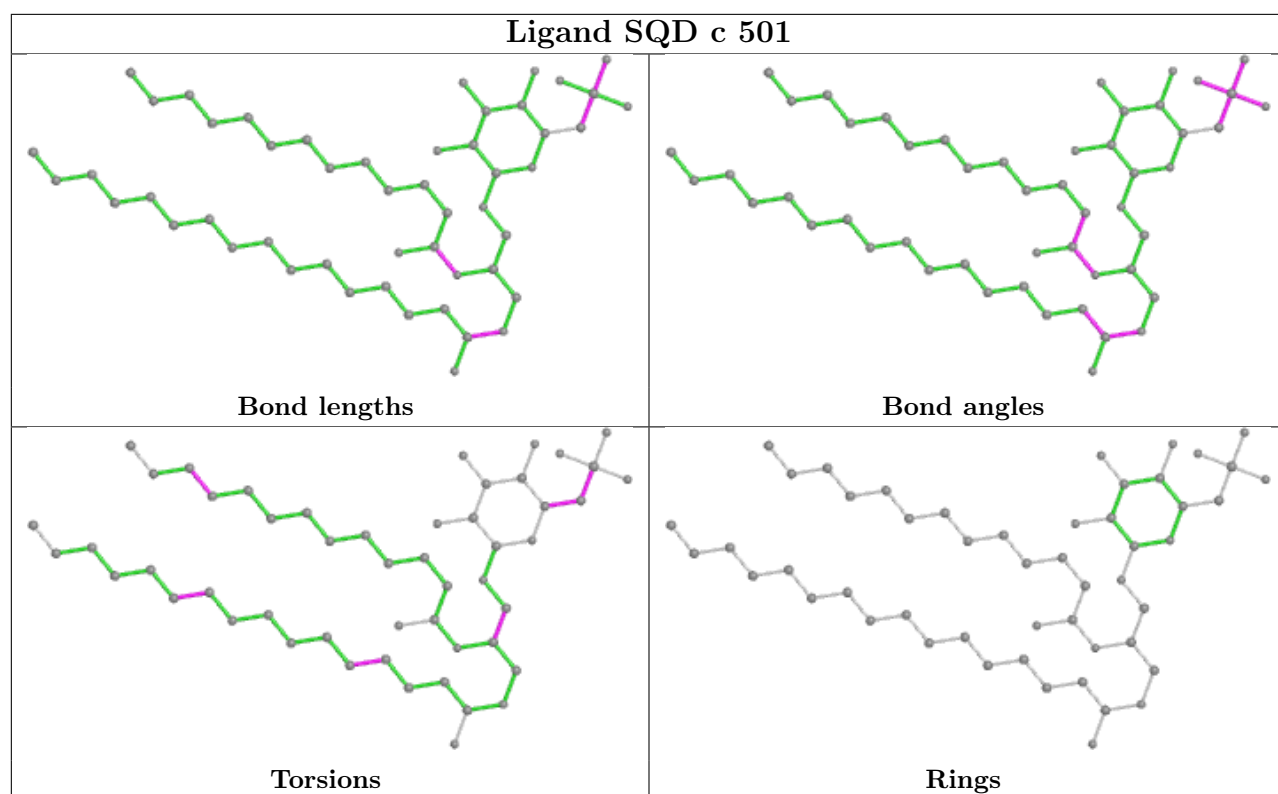
## Ligand CLA b 503



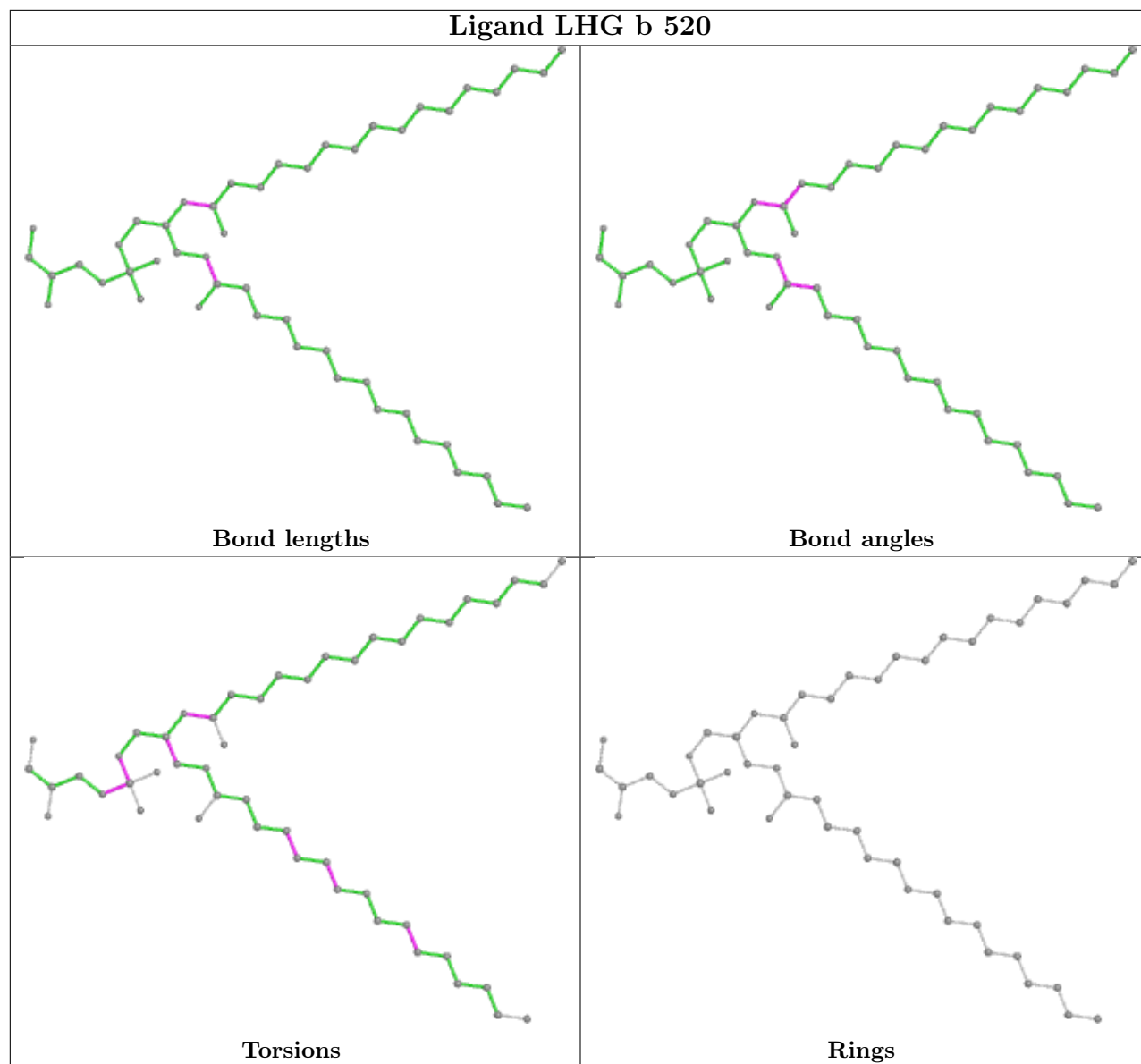
## Ligand CLA b 516



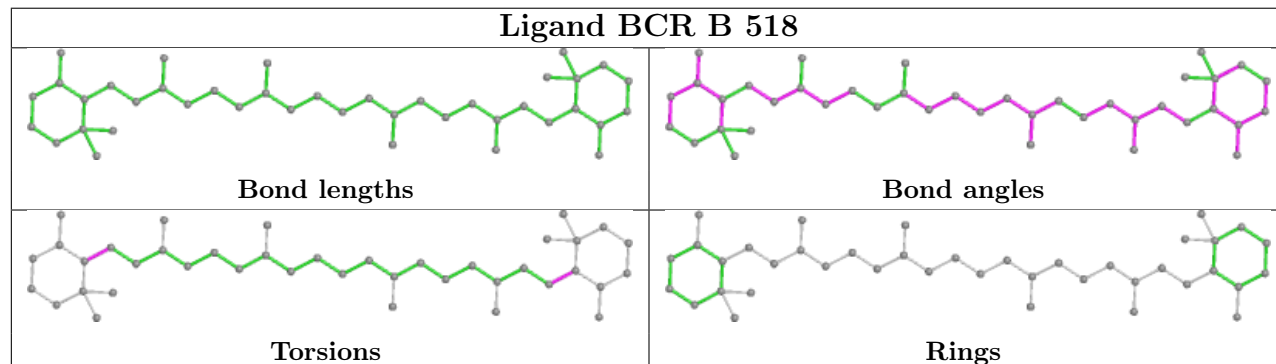


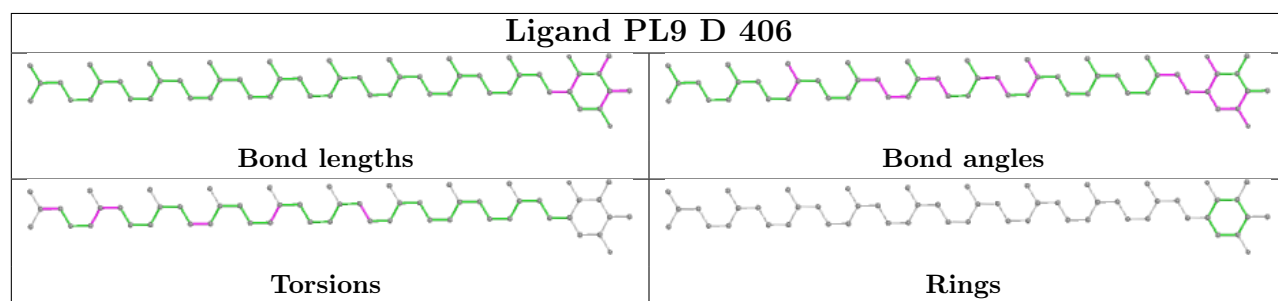
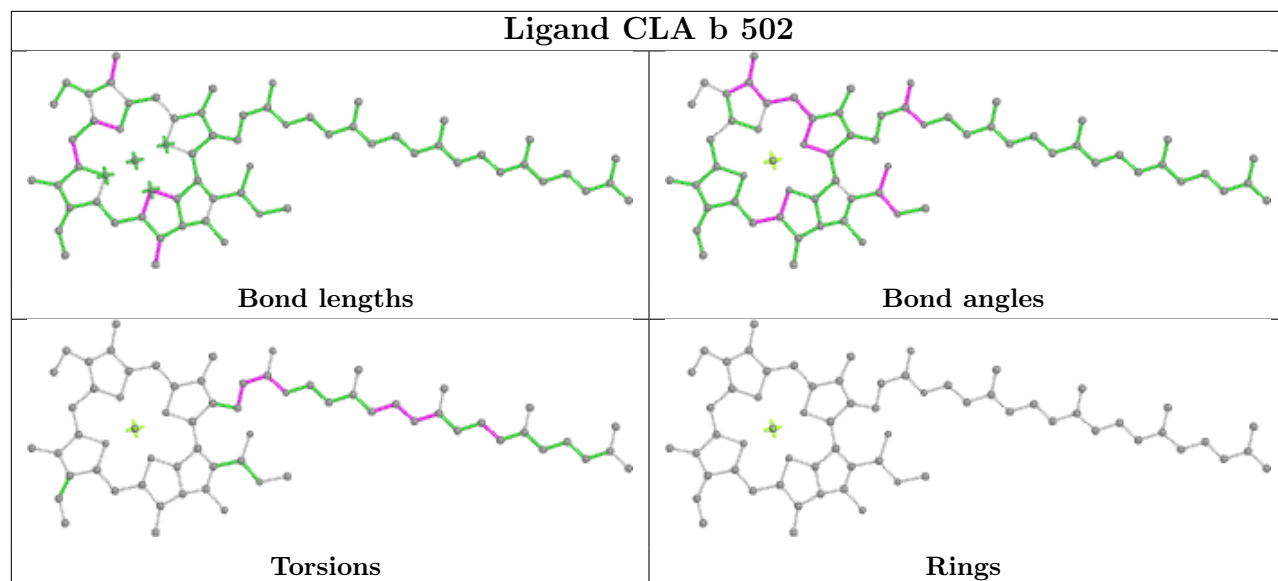
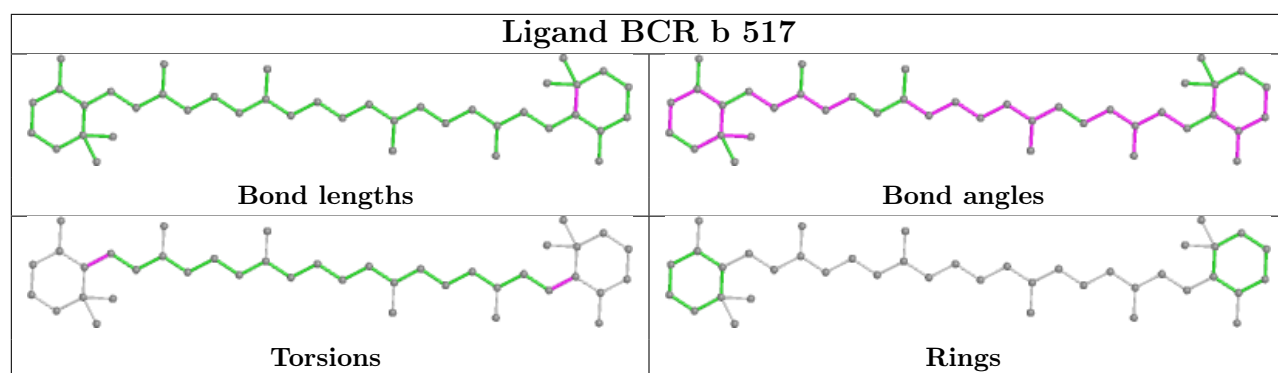


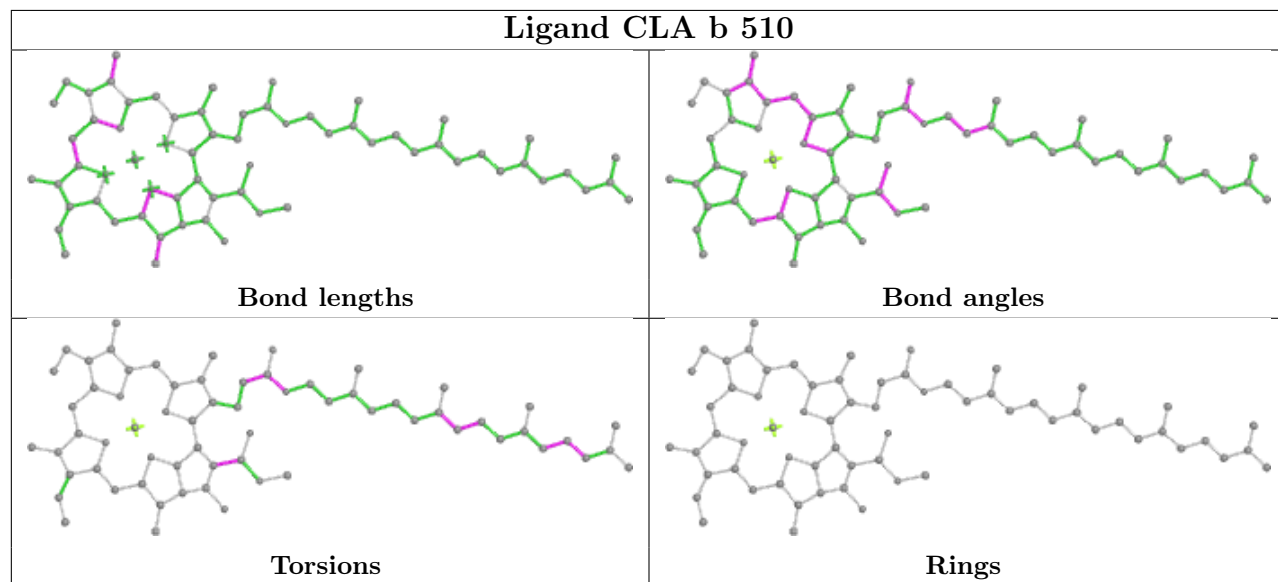
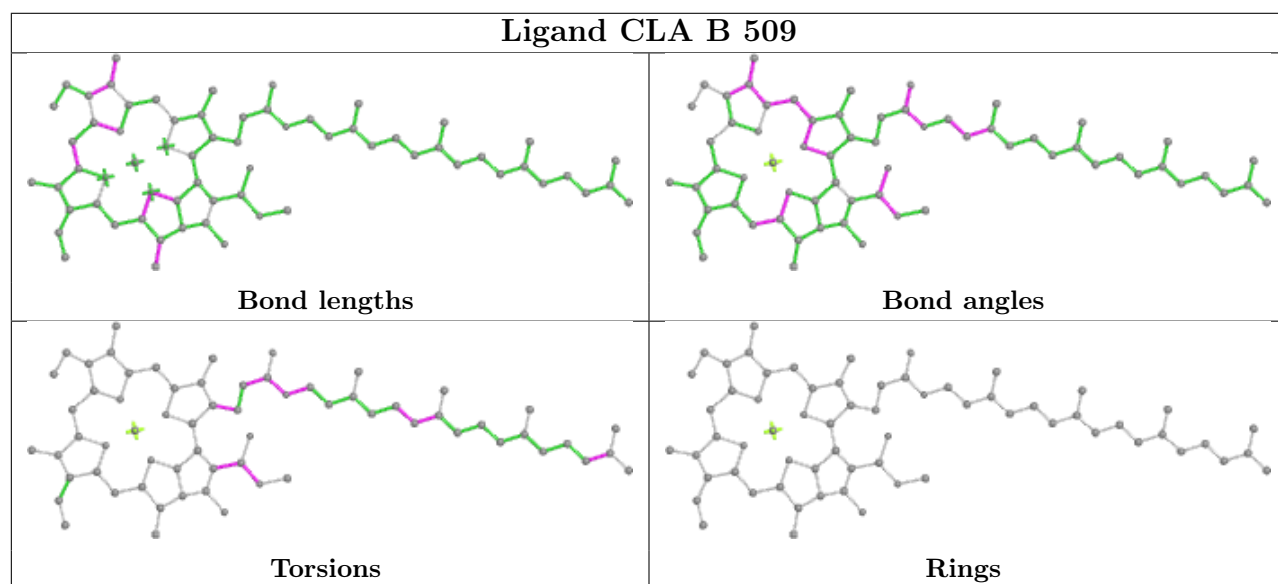
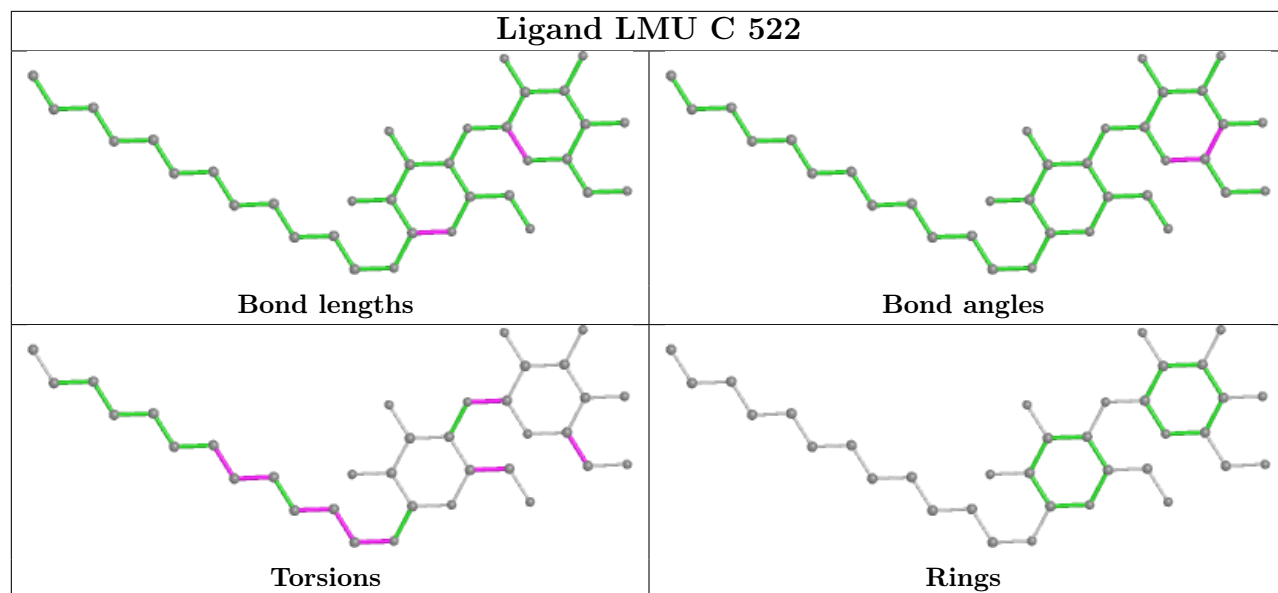
## Ligand LHG b 520



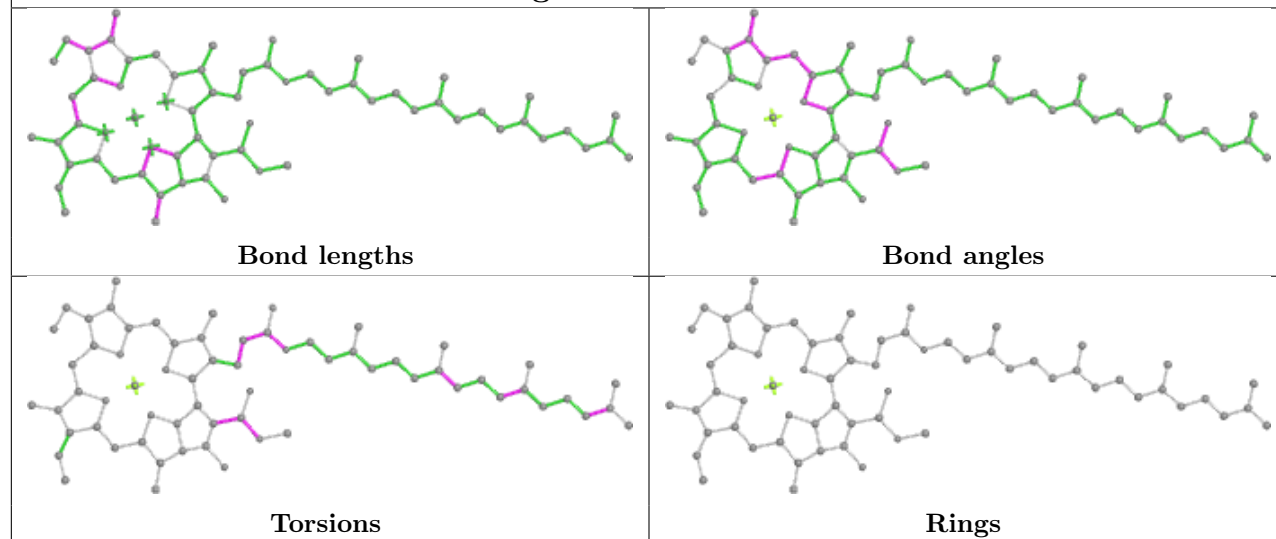
## Ligand BCR B 518



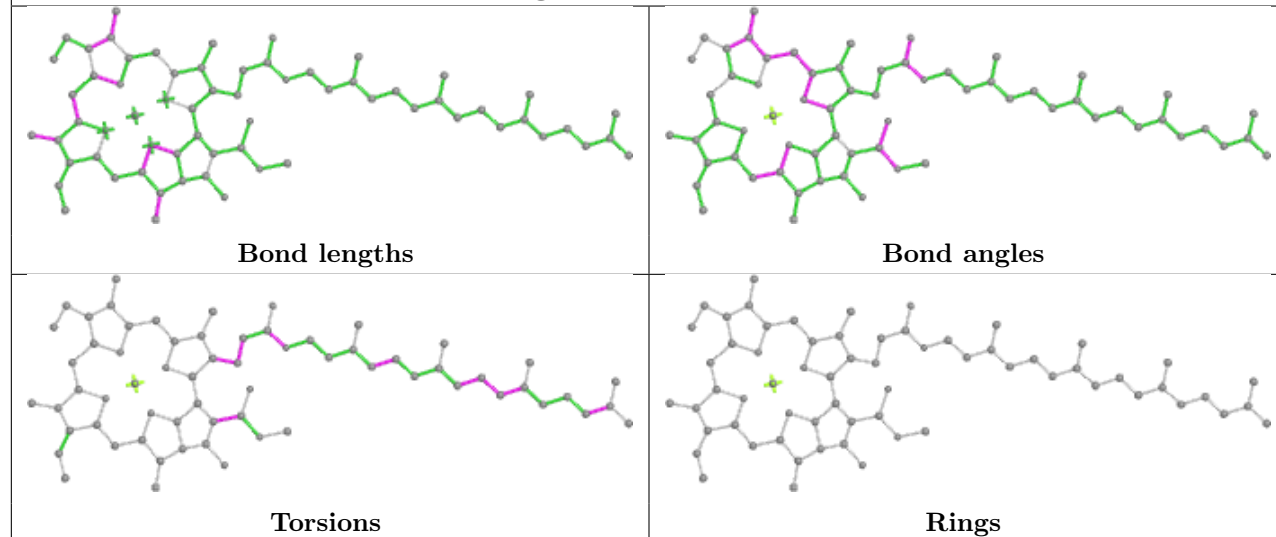




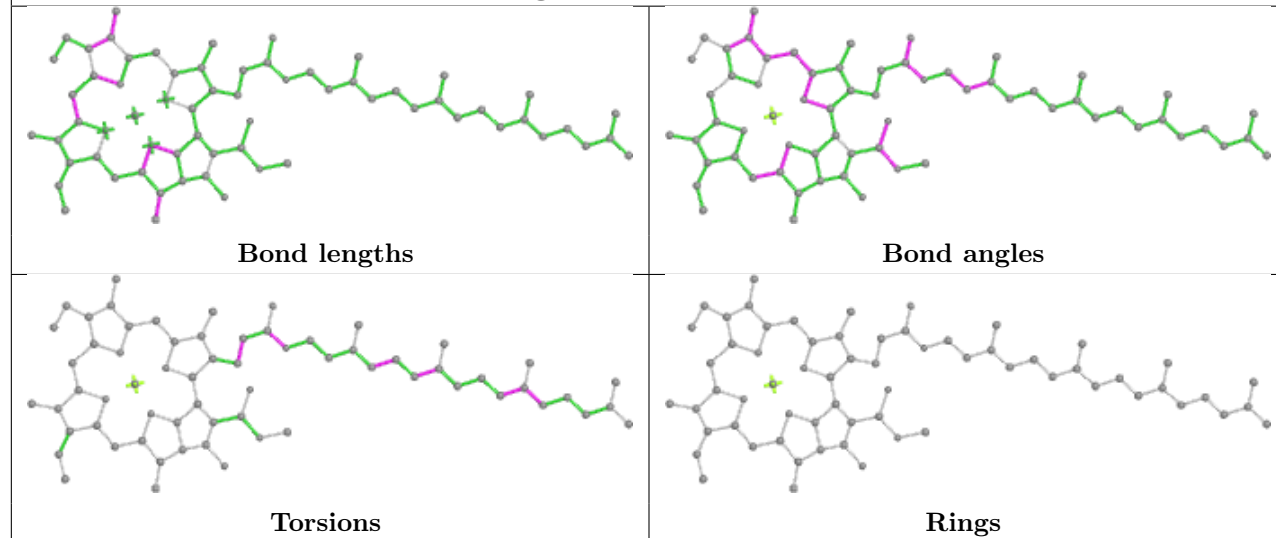
## Ligand CLA C 511



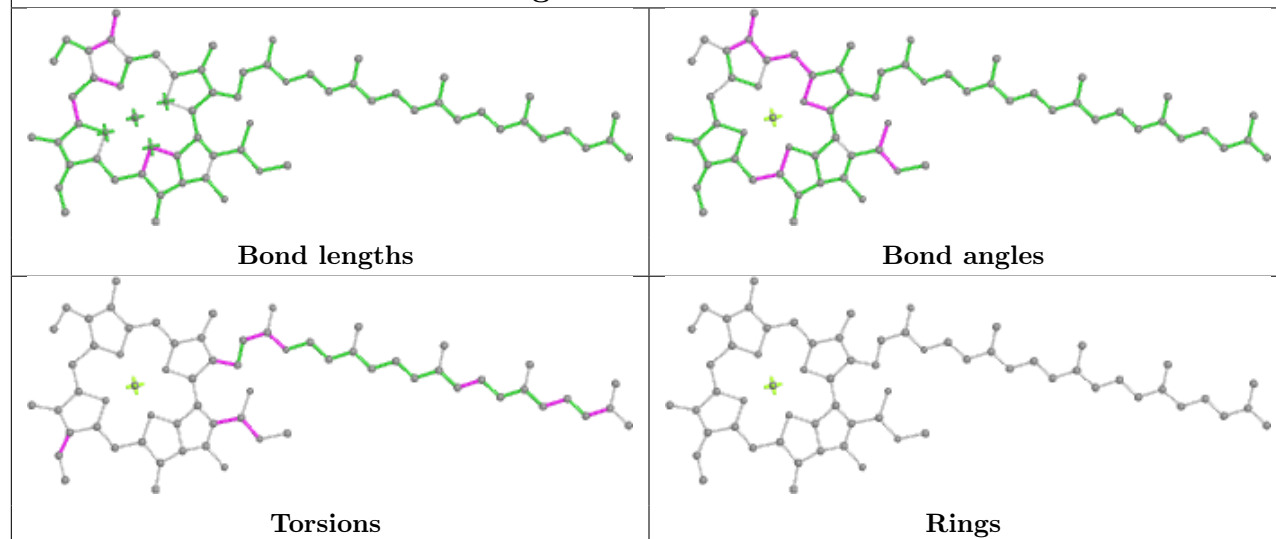
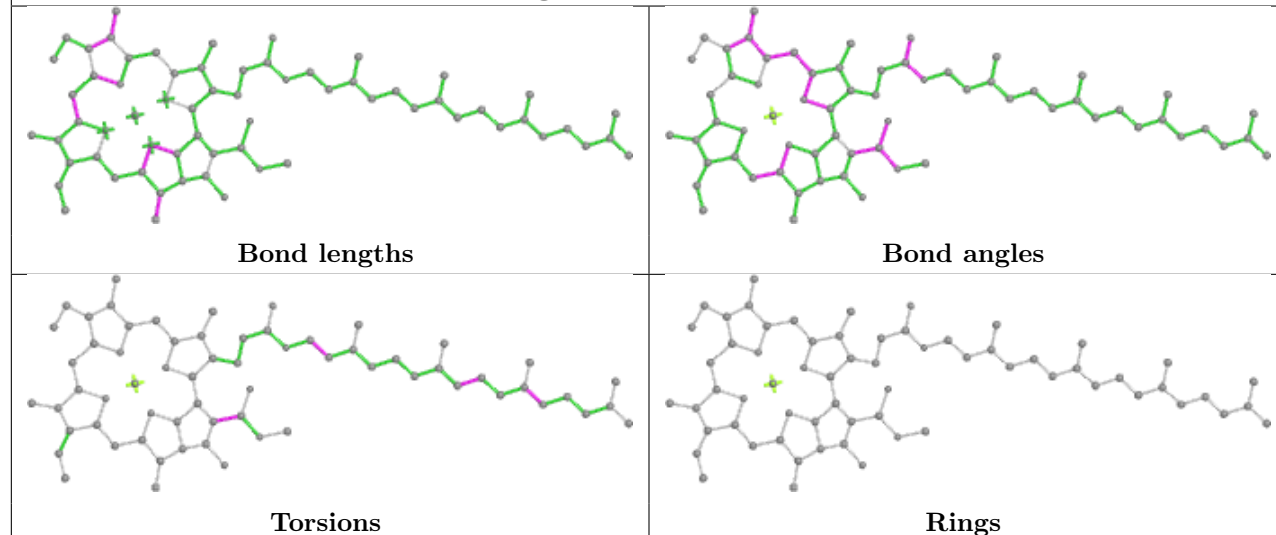
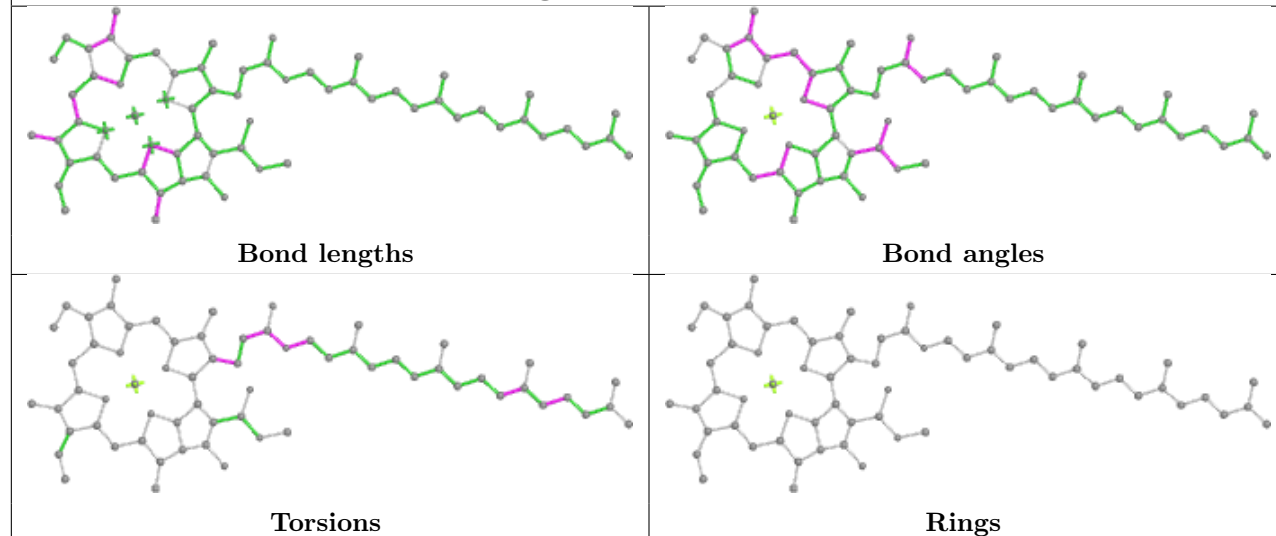
## Ligand CLA B 504



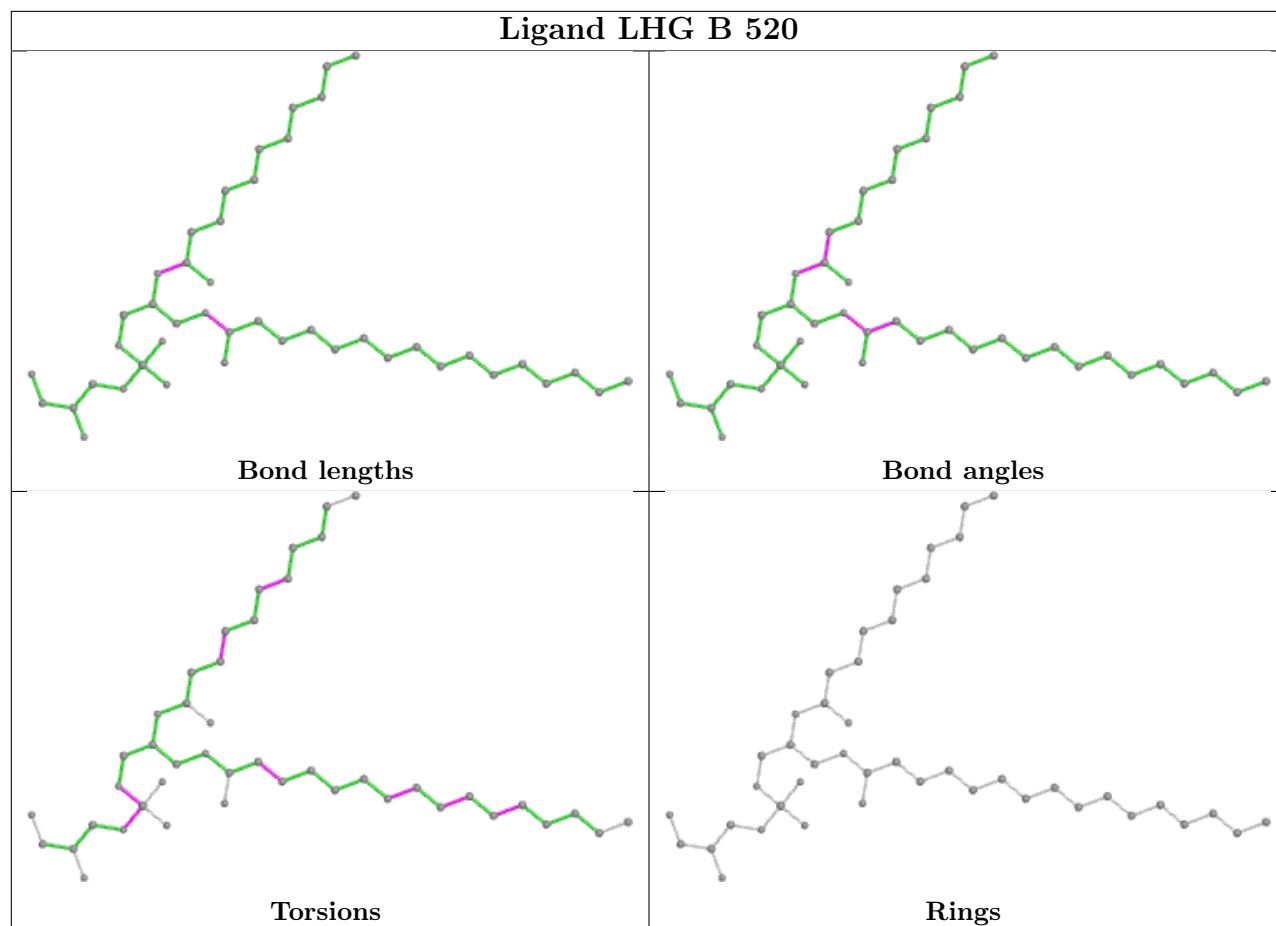
## Ligand CLA B 508



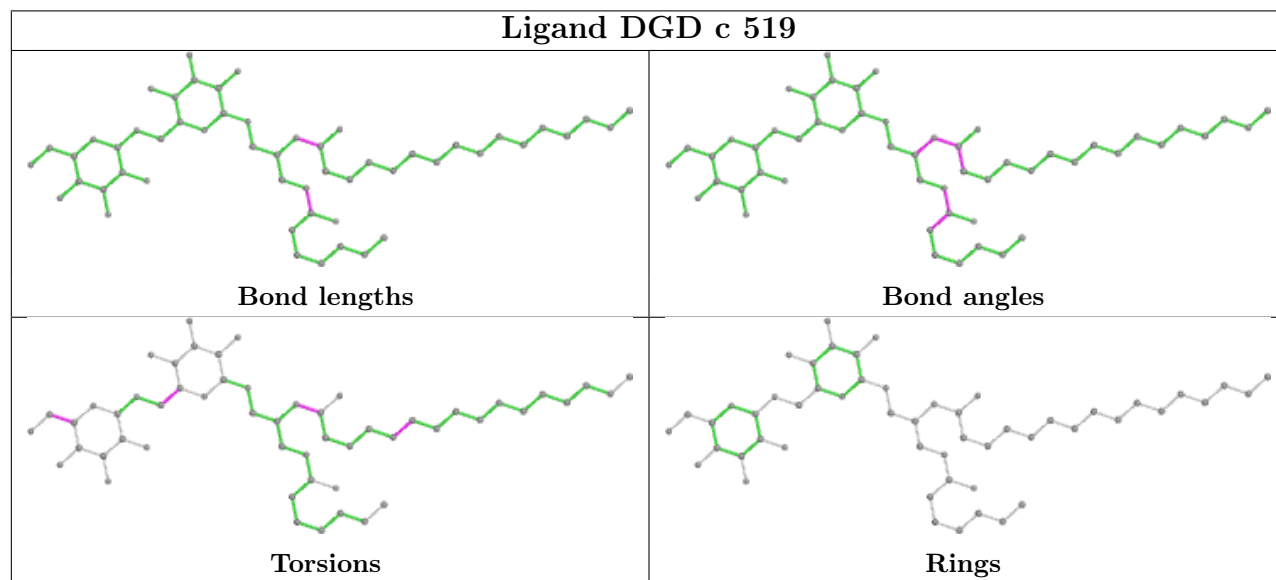


**Ligand CLA B 501****Ligand CLA b 515****Ligand CLA a 403**

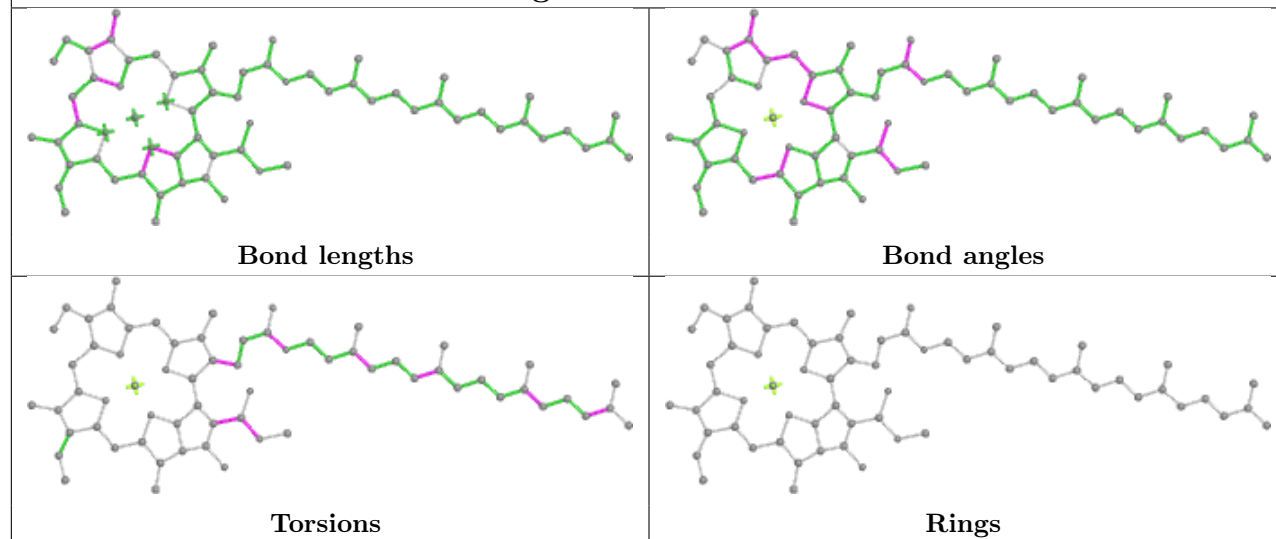
## Ligand LHG B 520



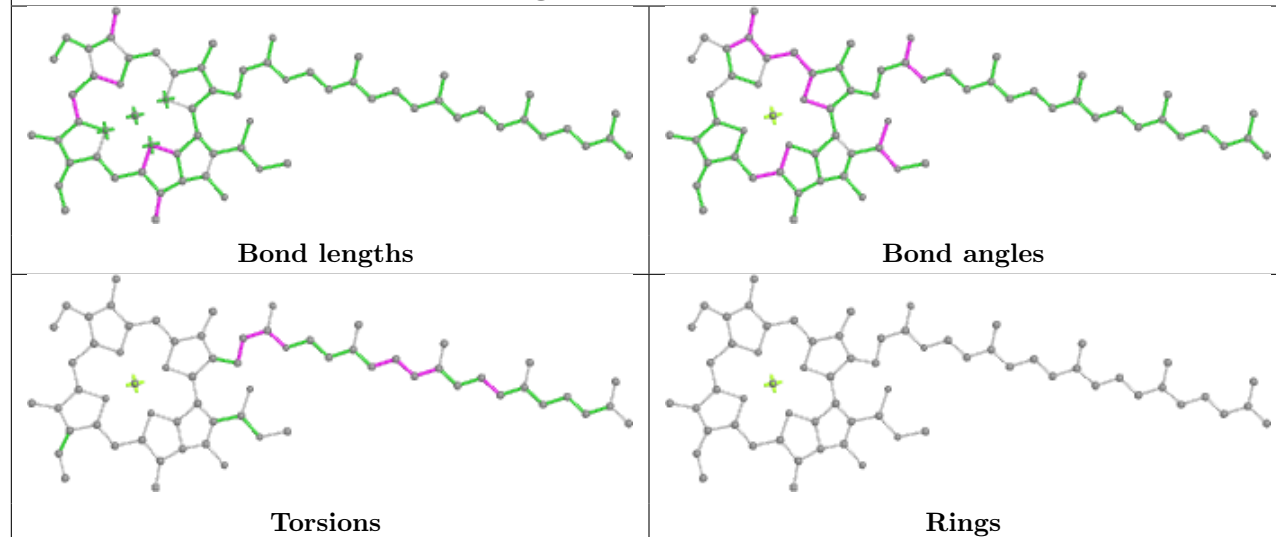
## Ligand DGD c 519



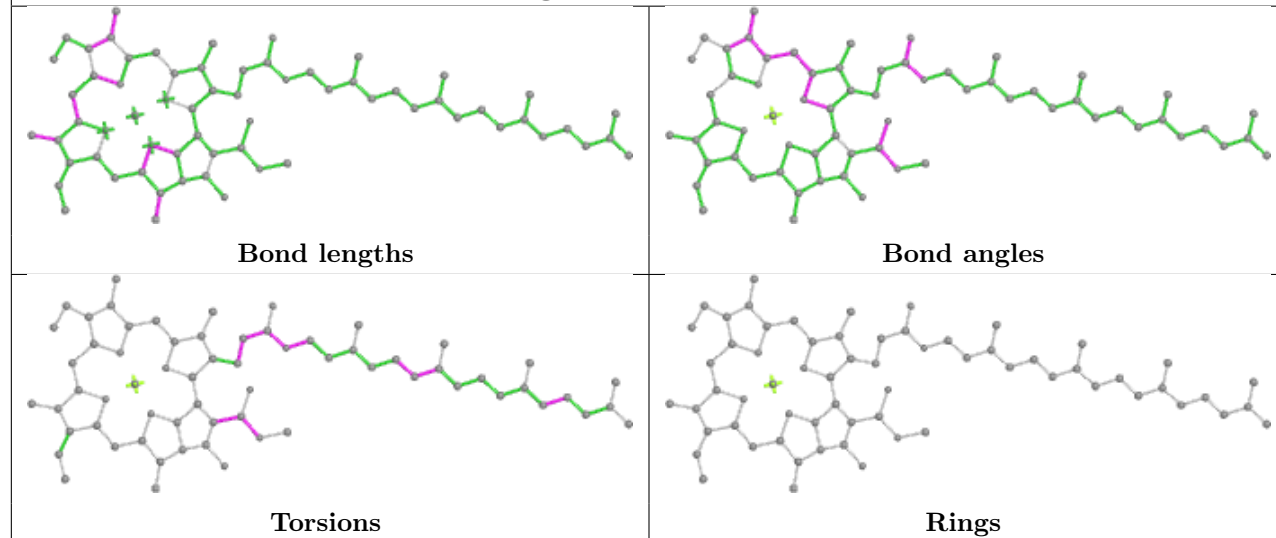
## Ligand CLA C 512



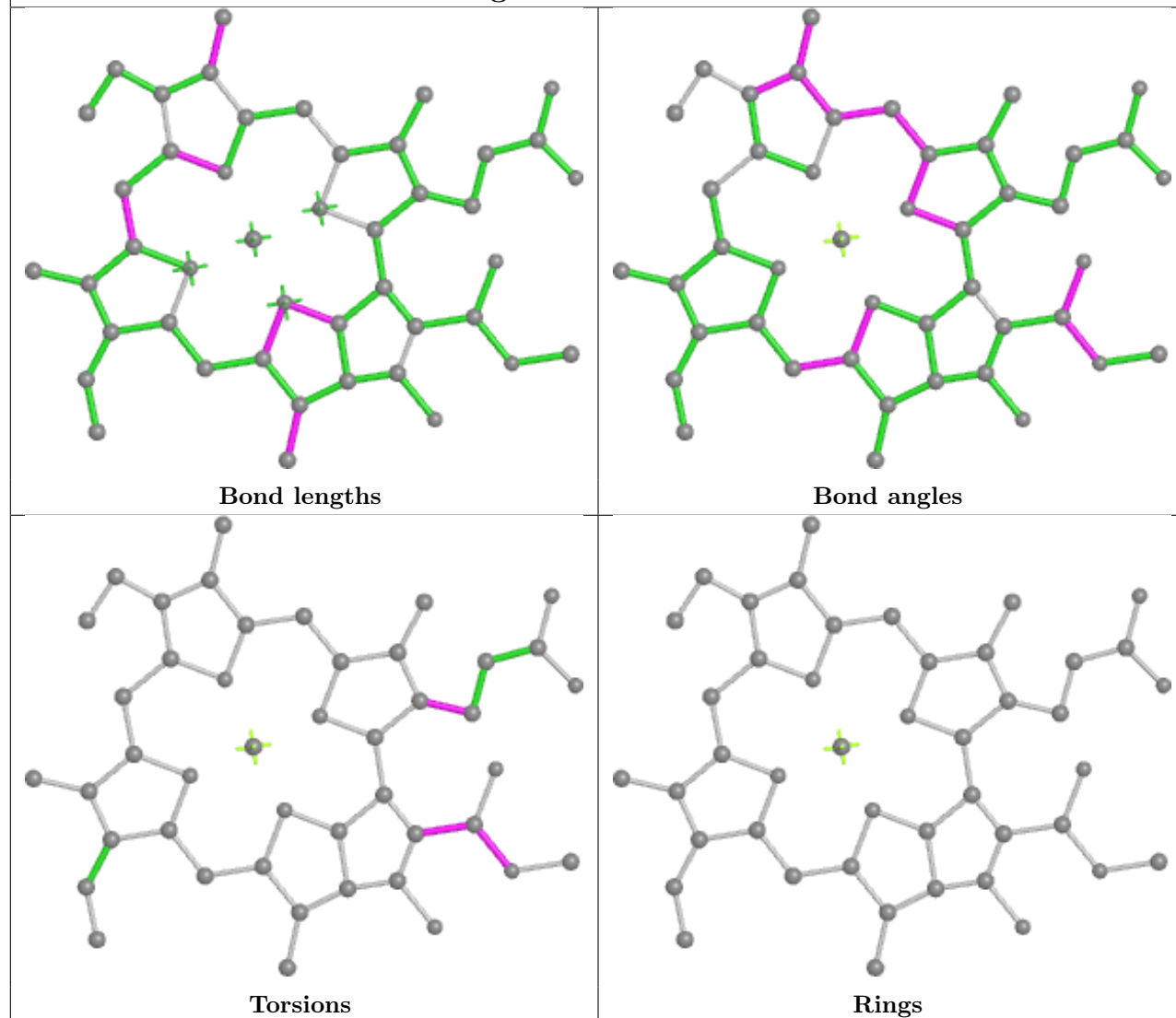
## Ligand CLA B 502



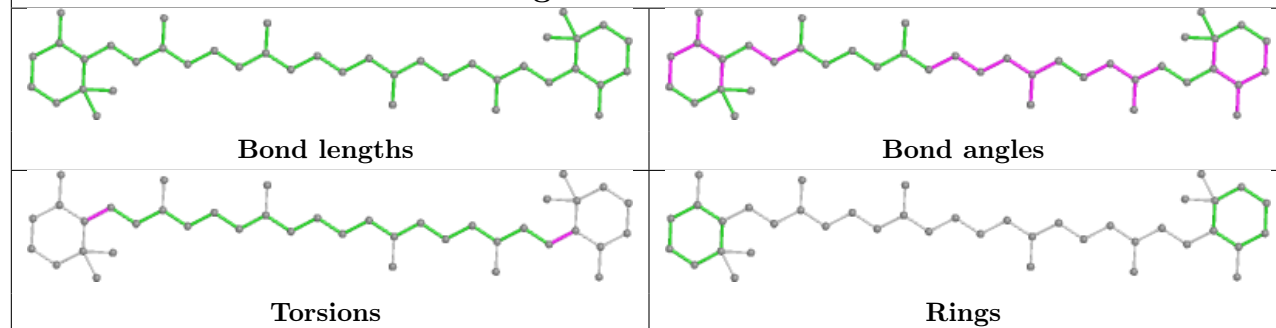
## Ligand CLA c 510



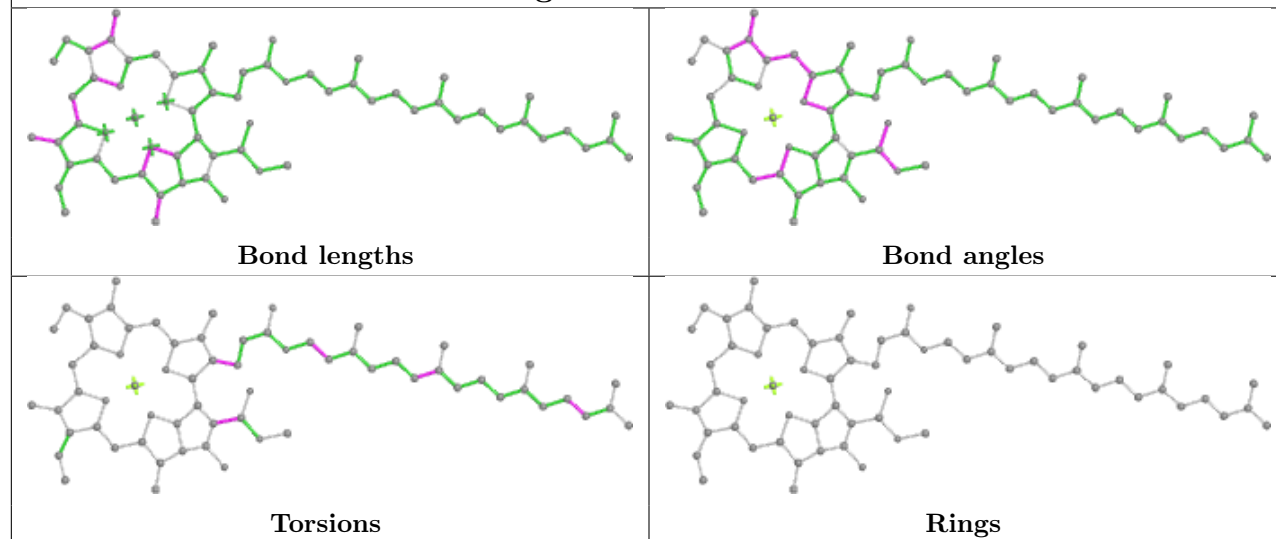
## Ligand CLA B 514



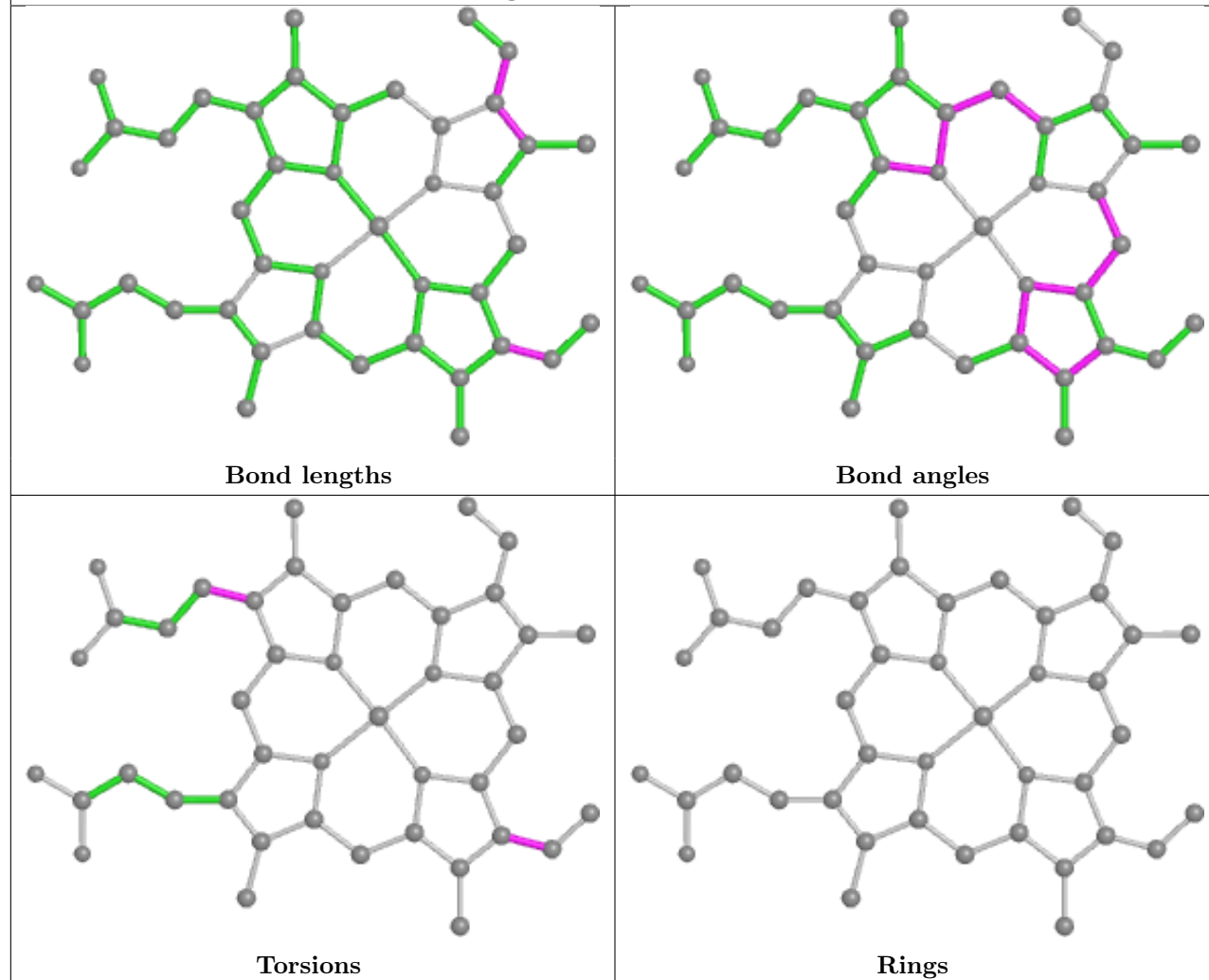
## Ligand BCR d 405

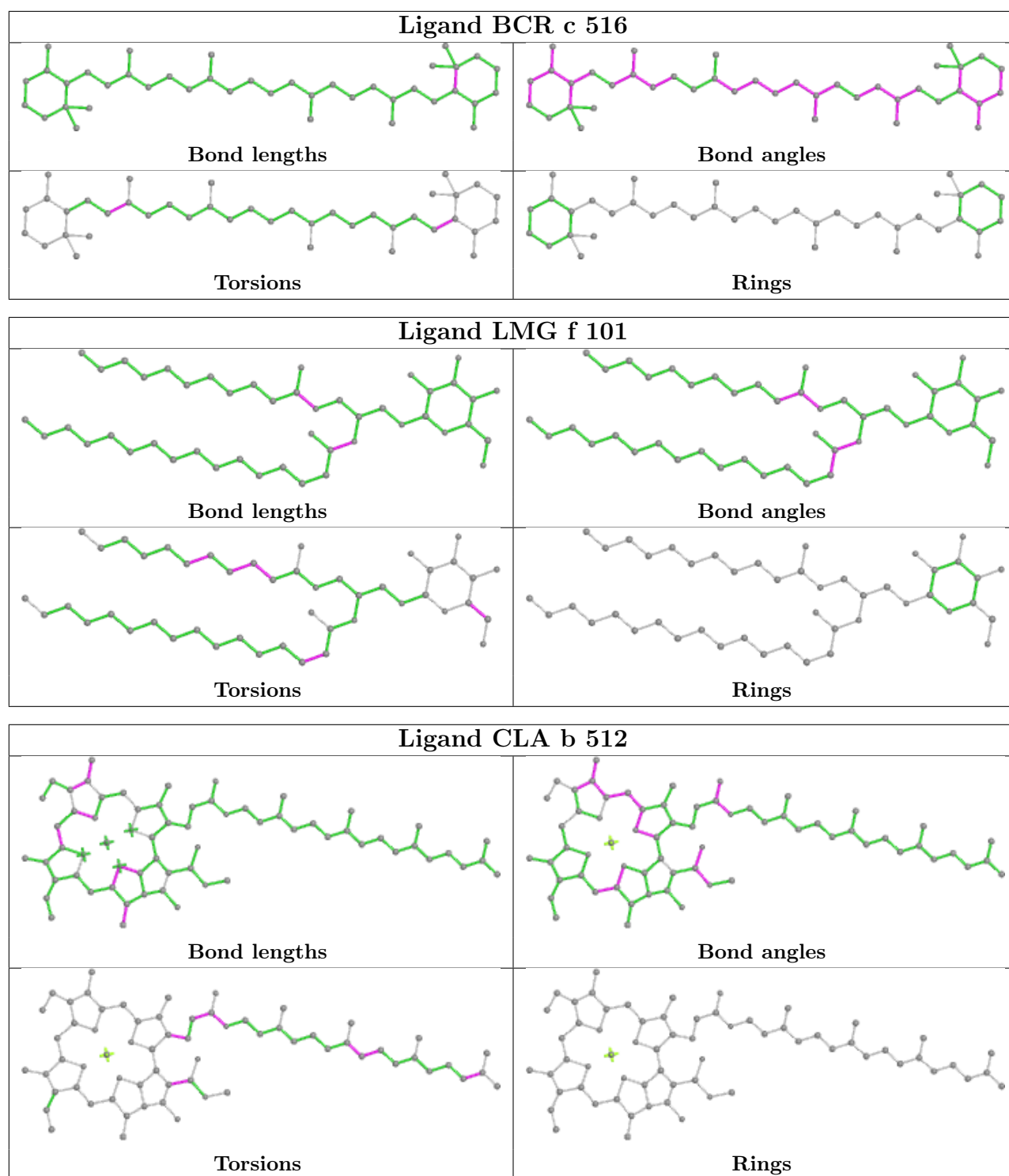


## Ligand CLA d 403

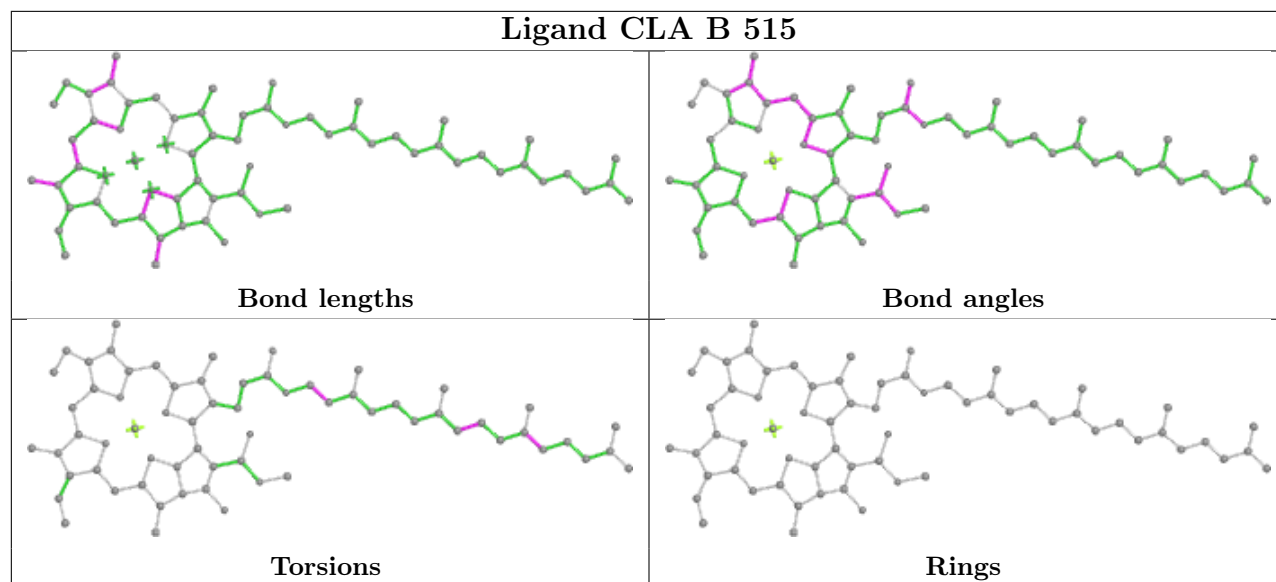


## Ligand HEM e 101

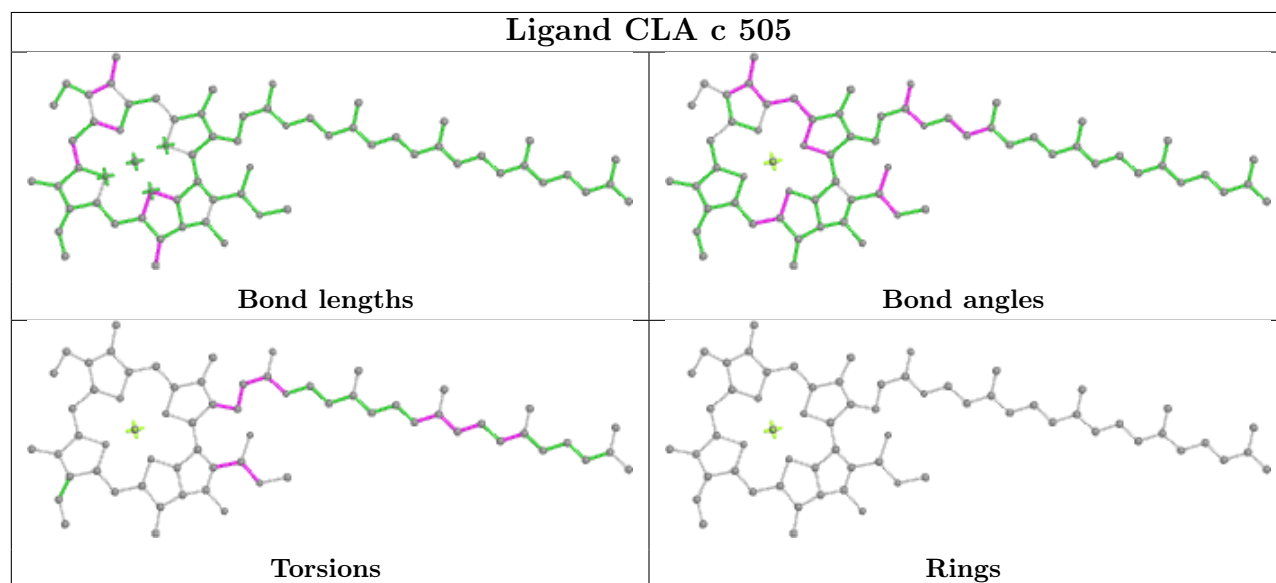




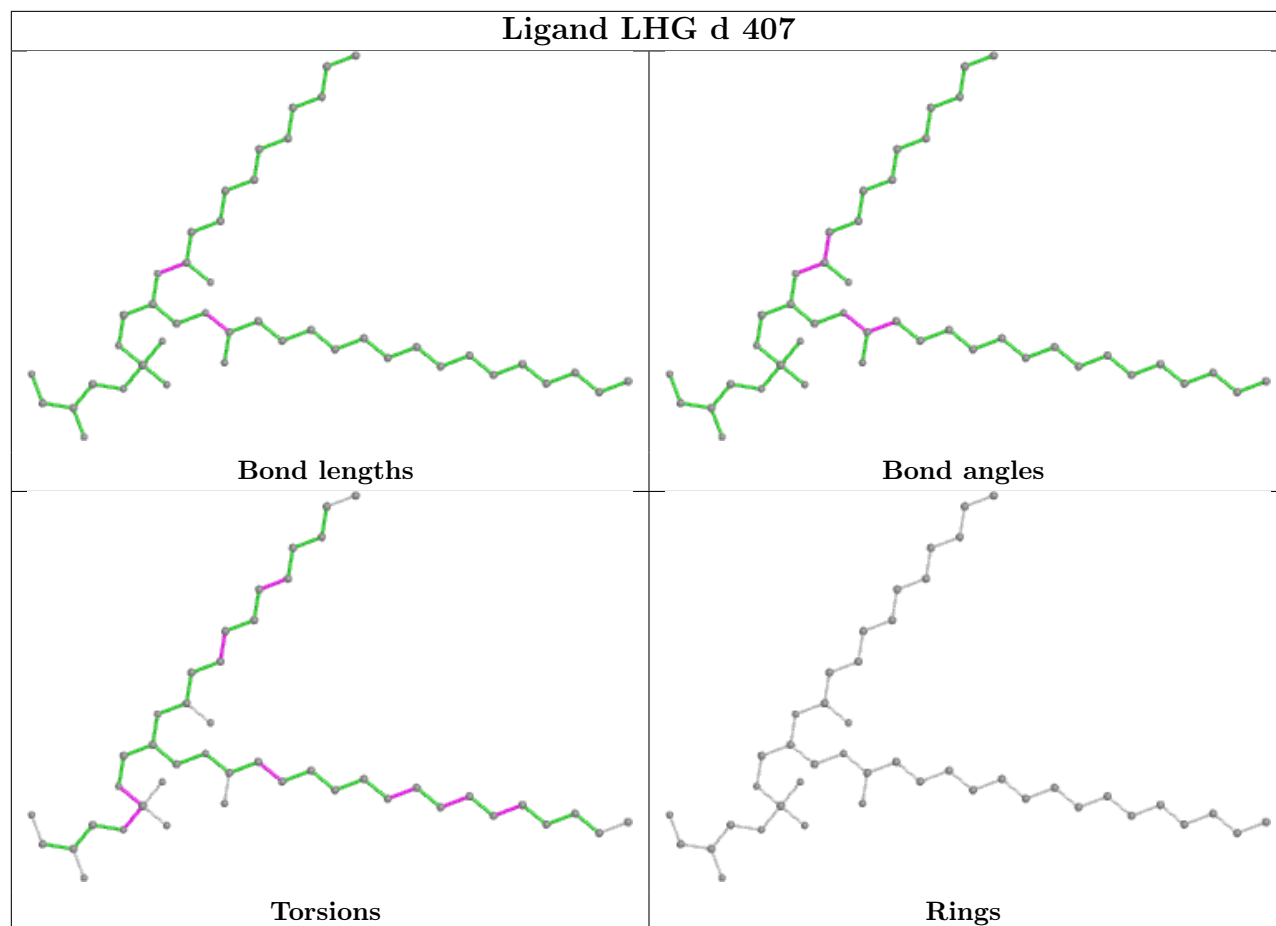
## Ligand CLA B 515



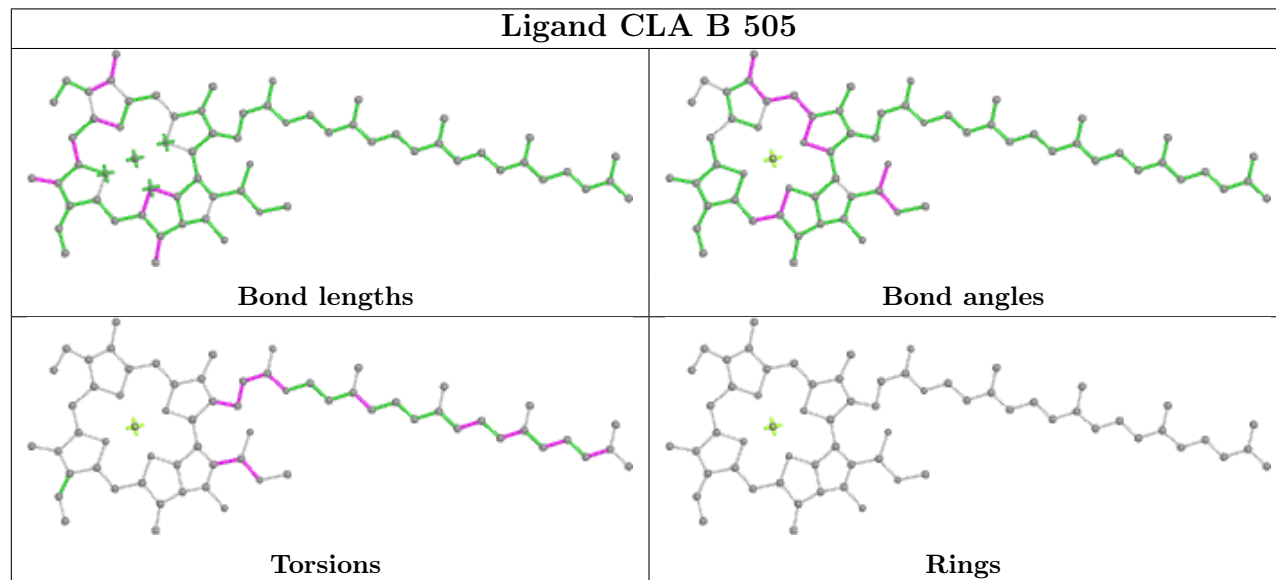
## Ligand CLA c 505



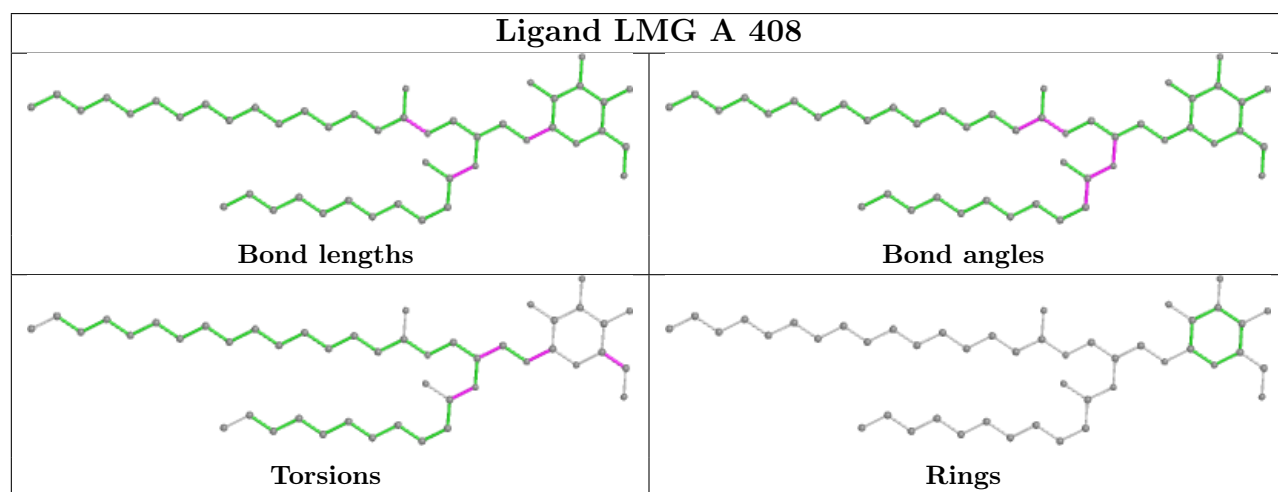
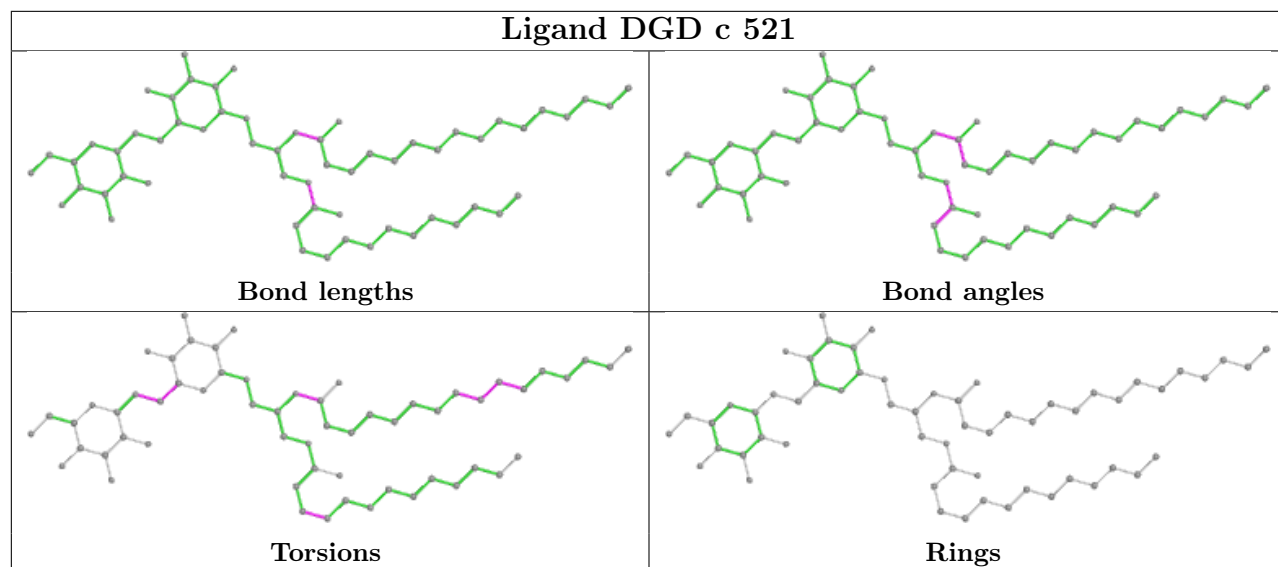
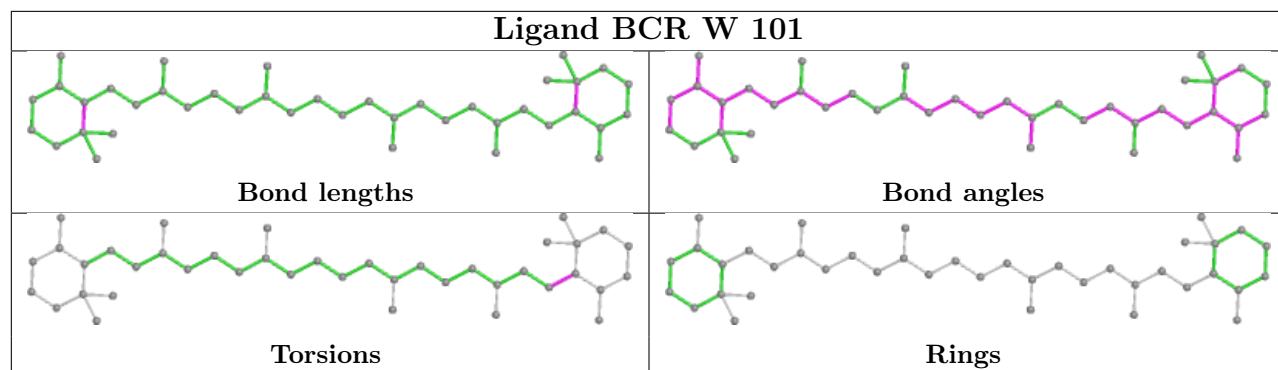
## Ligand LHG d 407

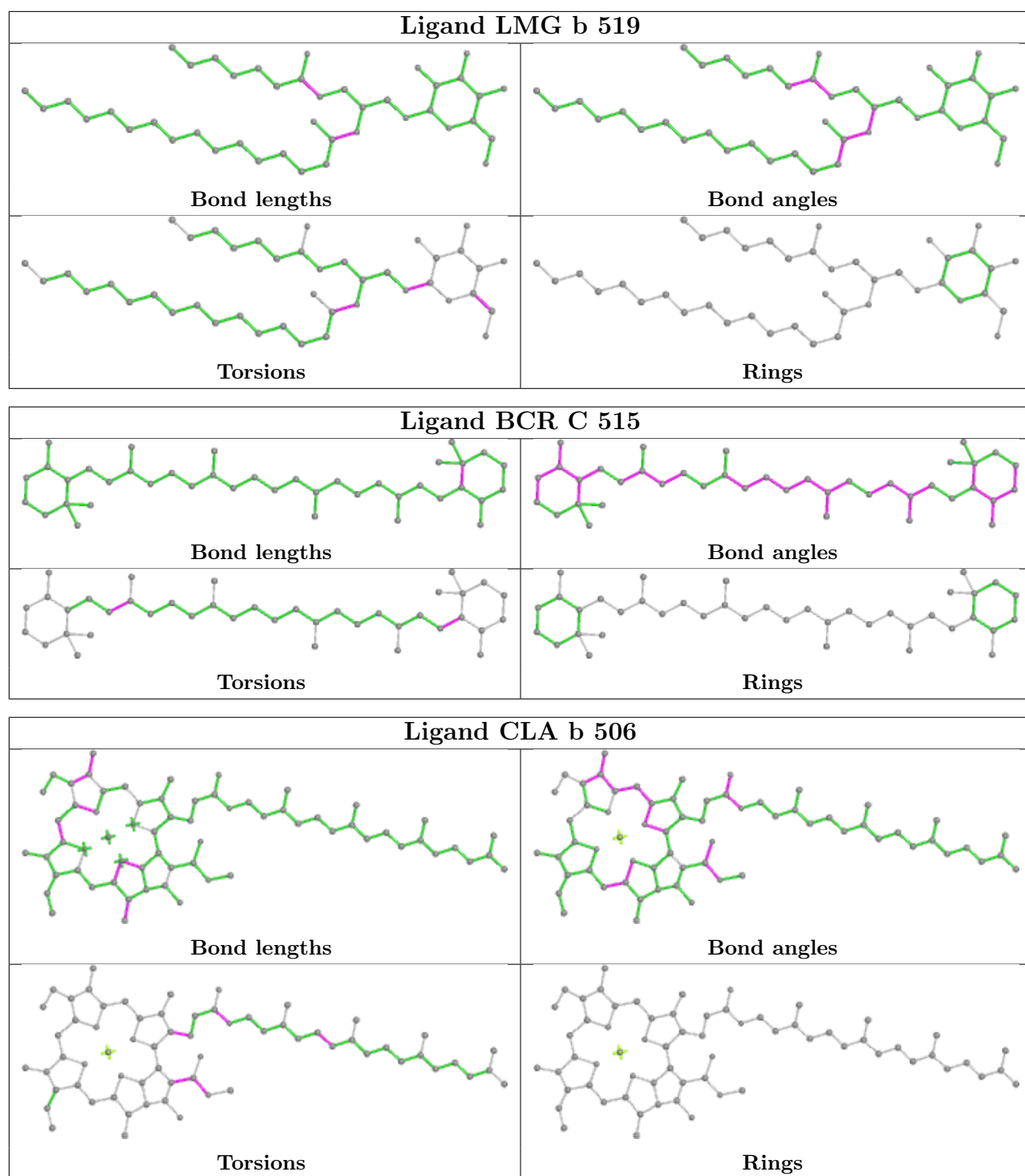


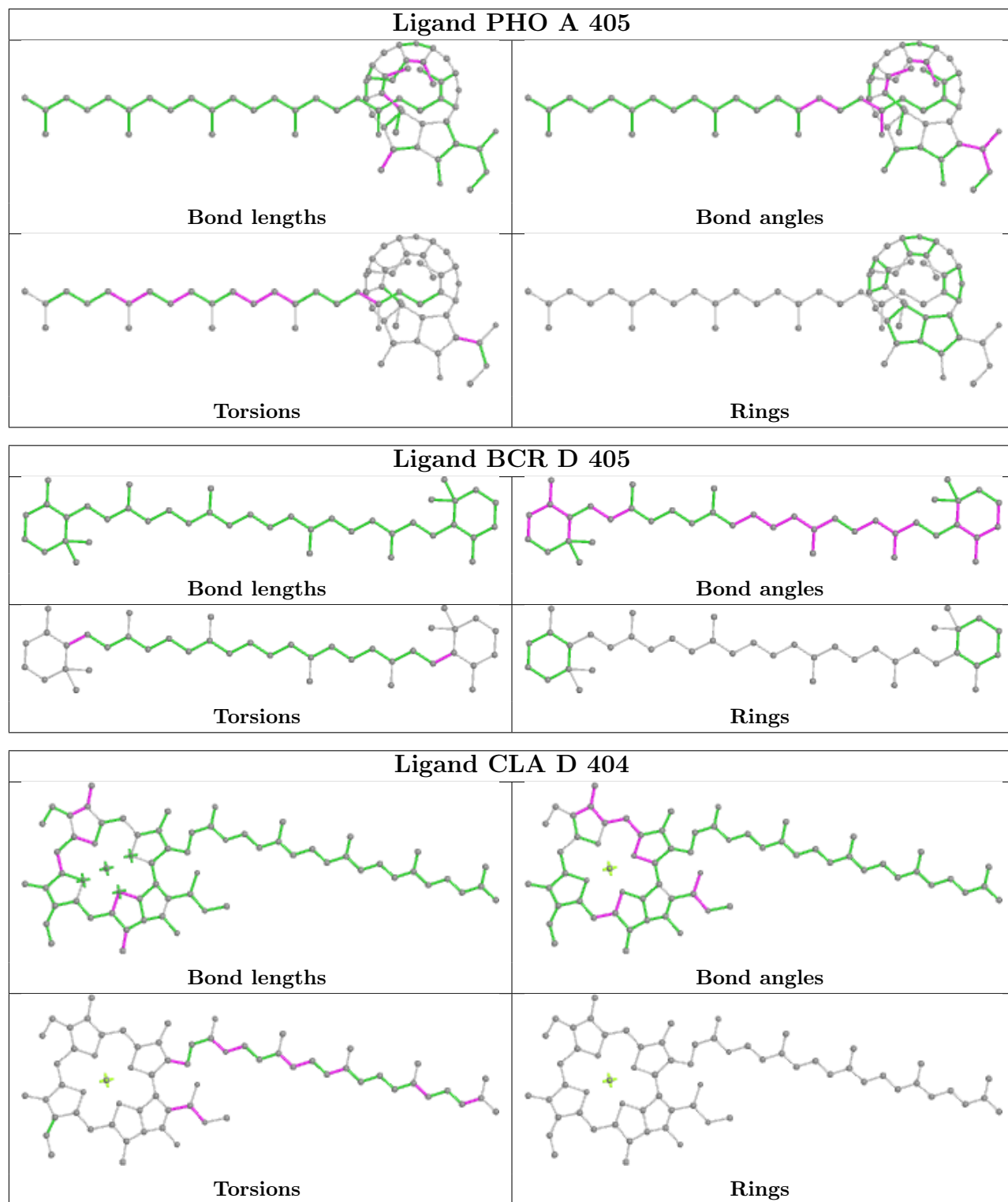
## Ligand CLA B 505

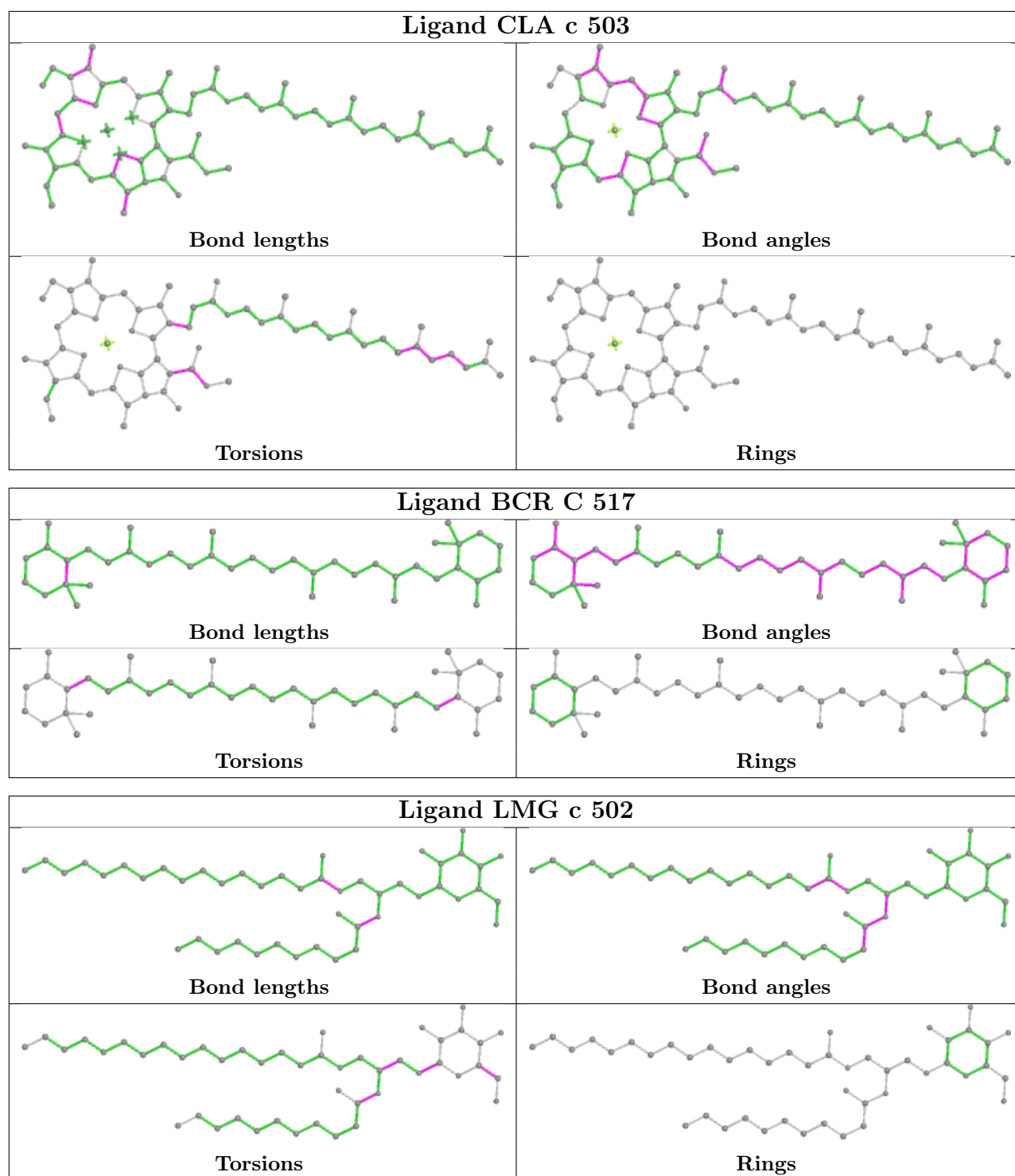


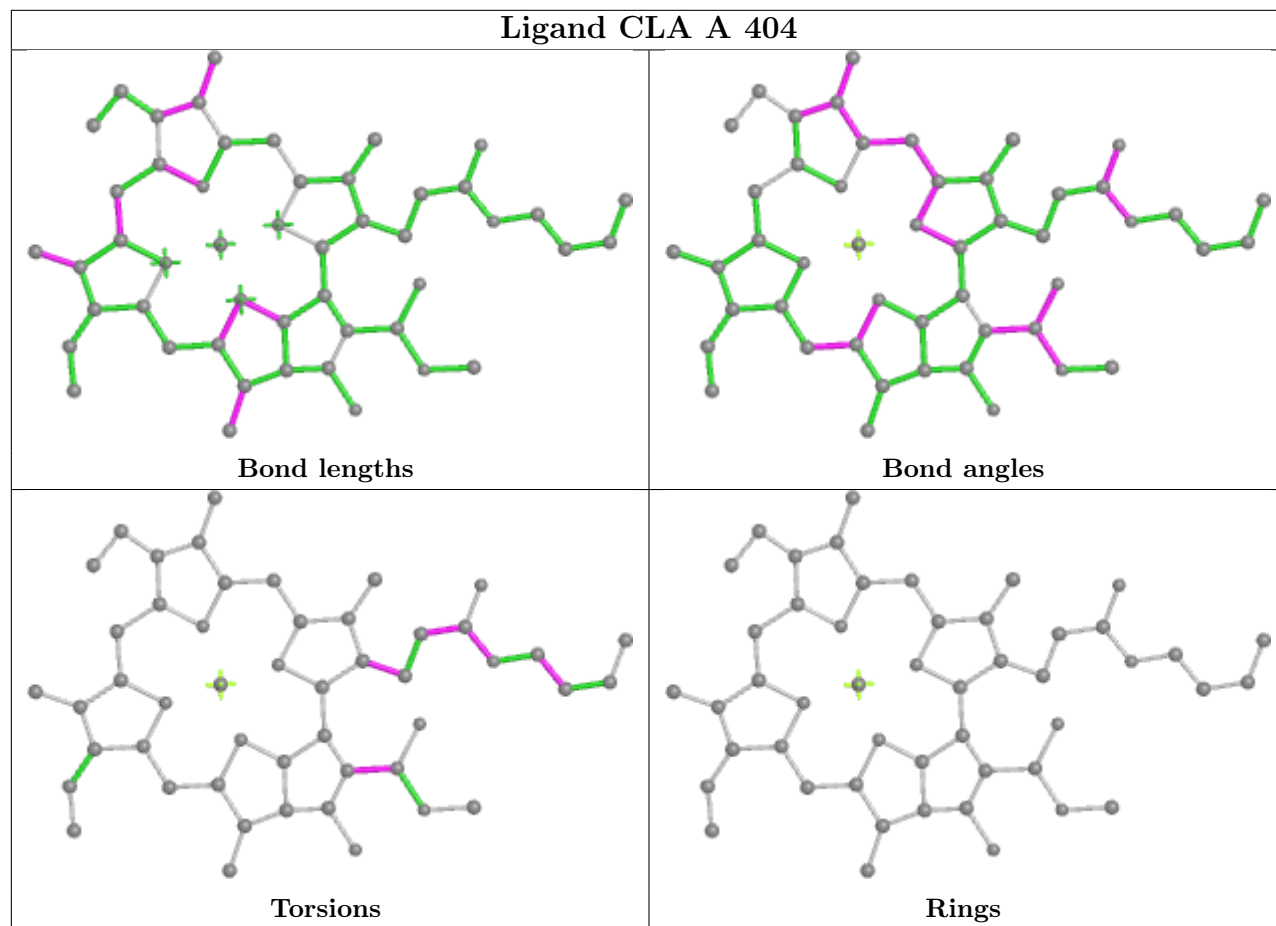
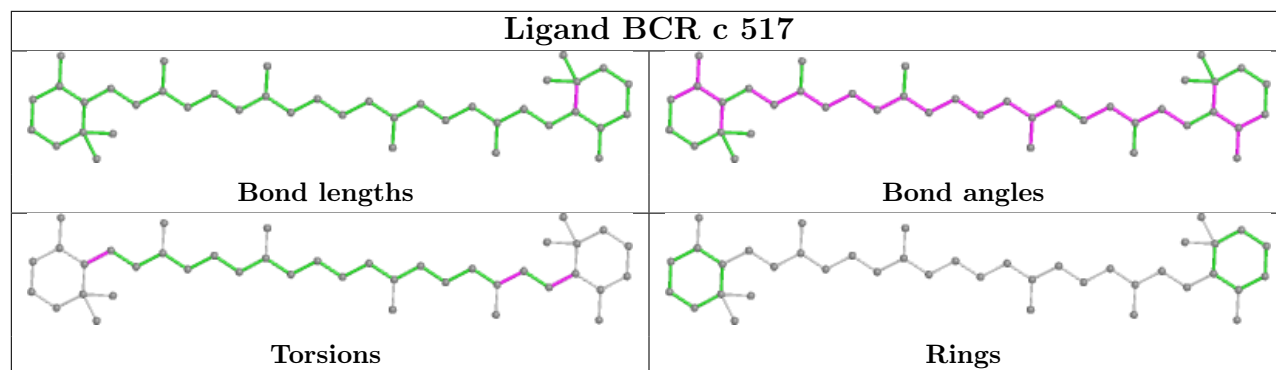
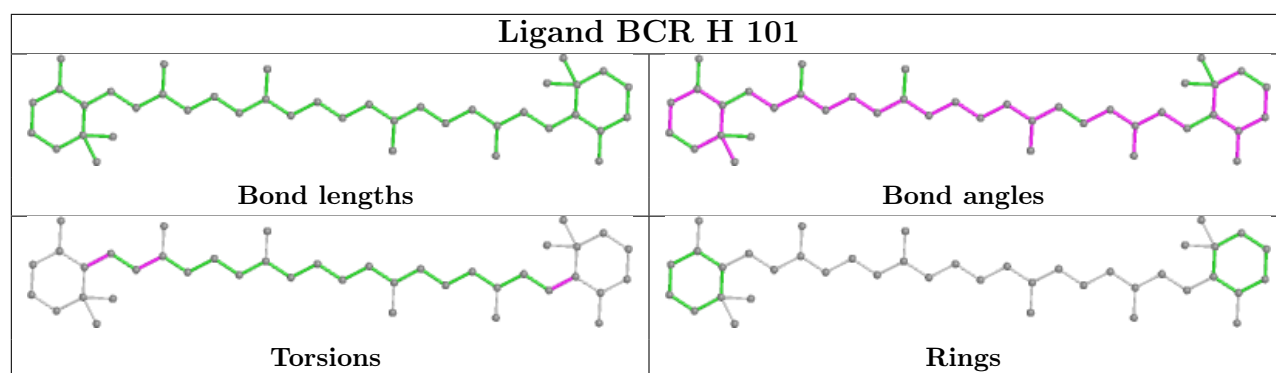


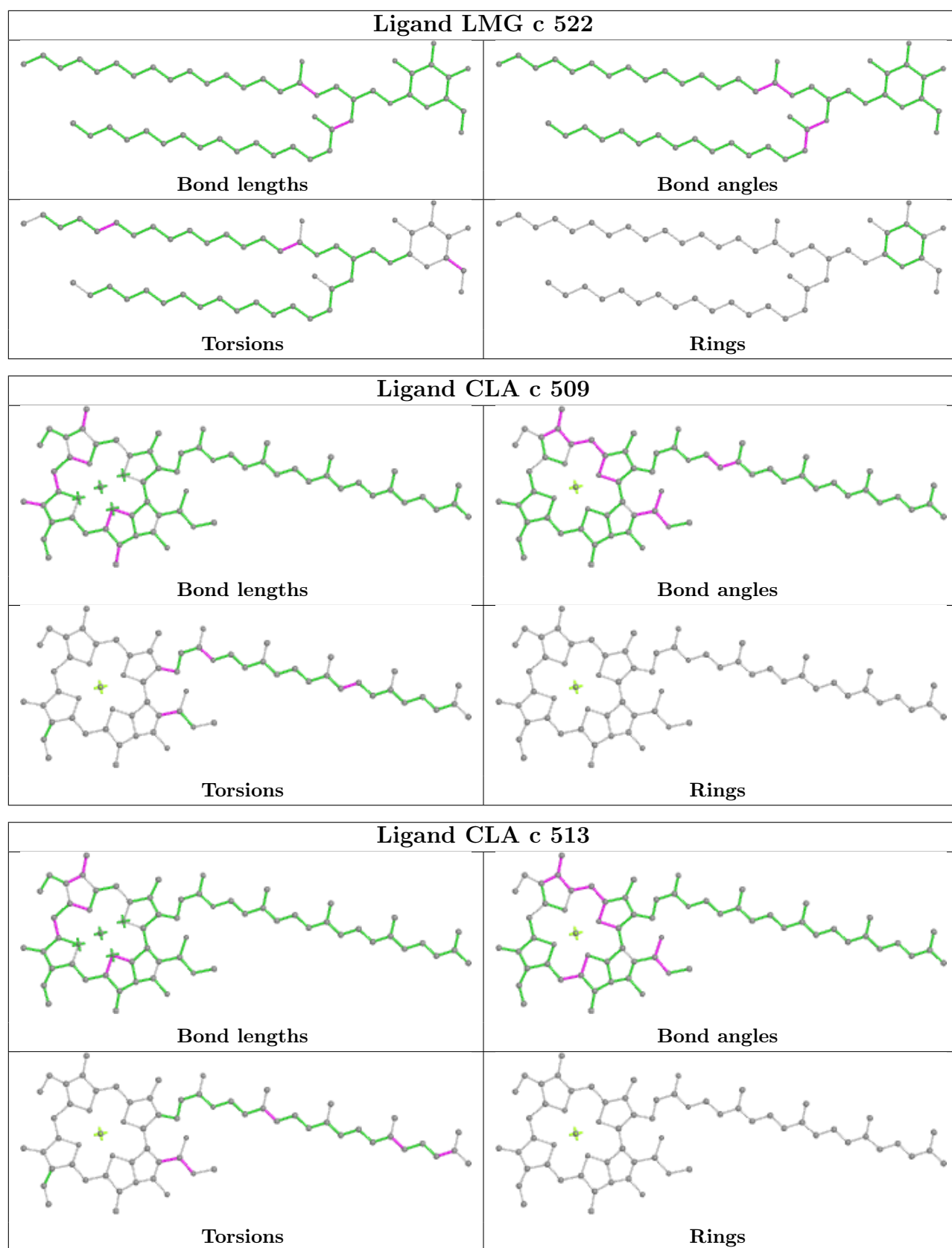


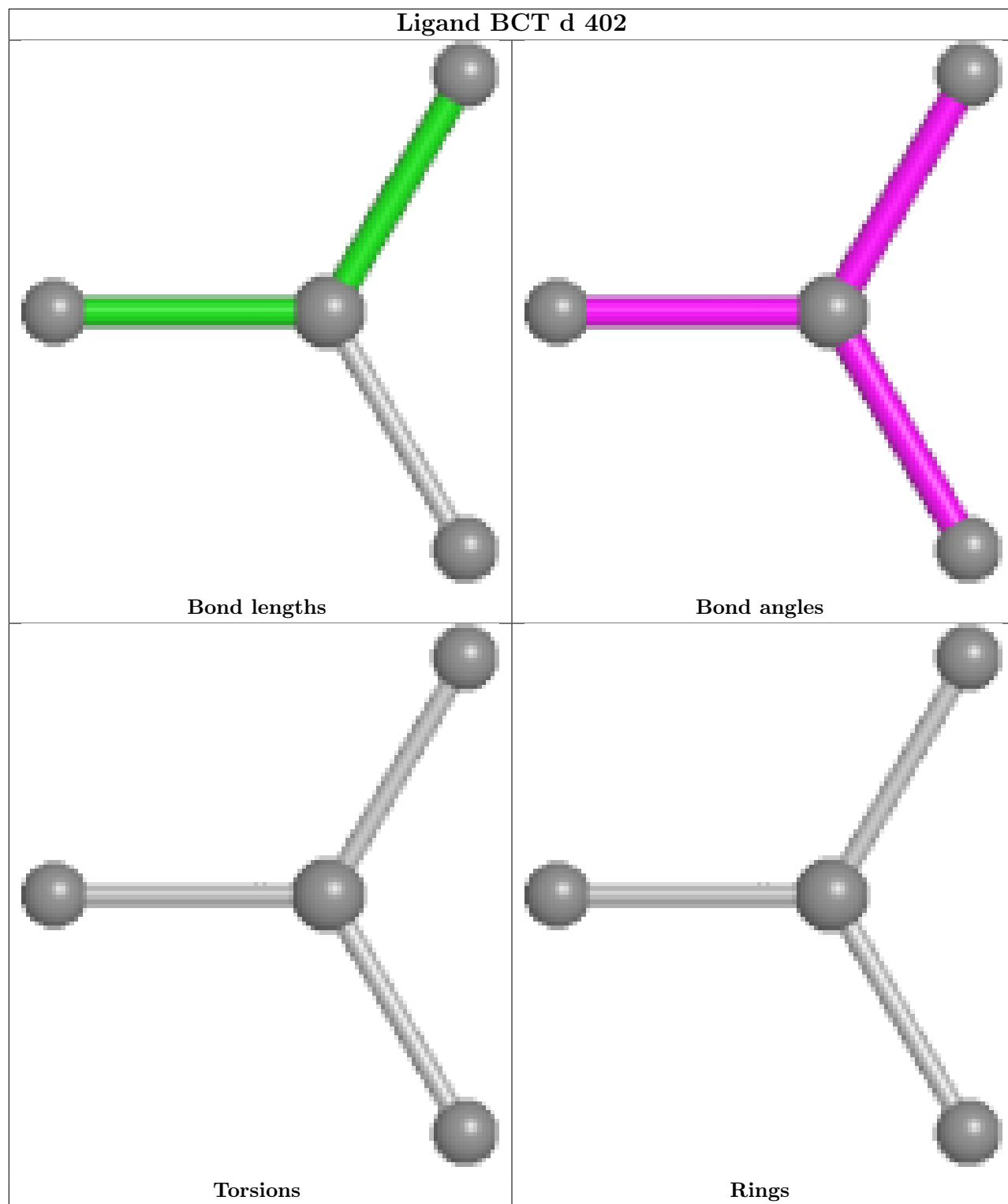


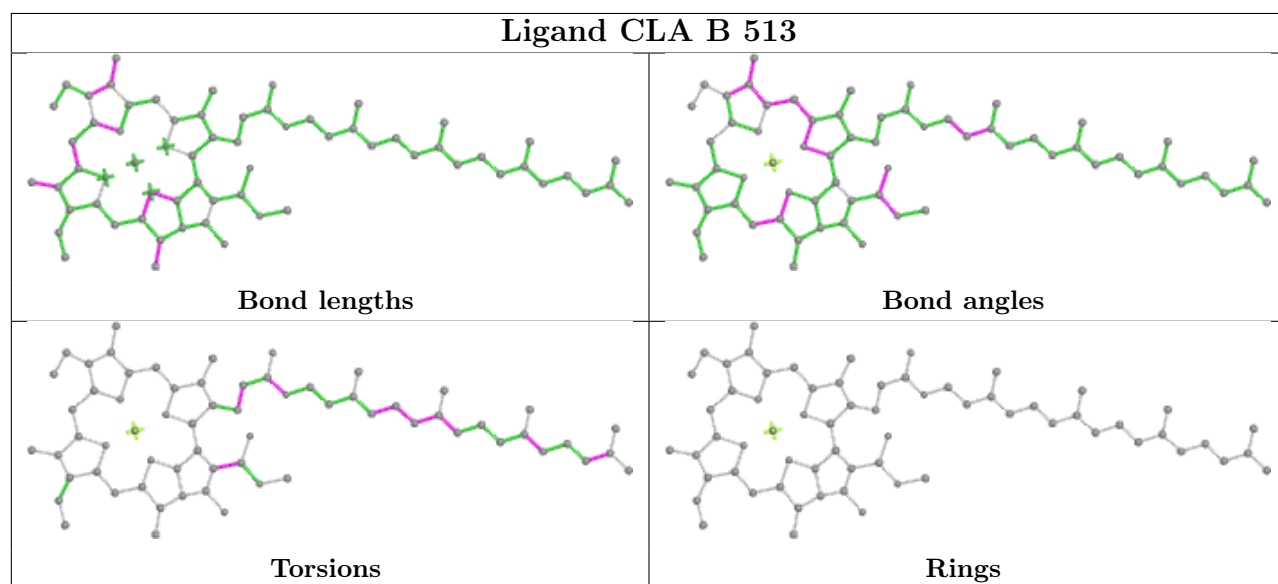
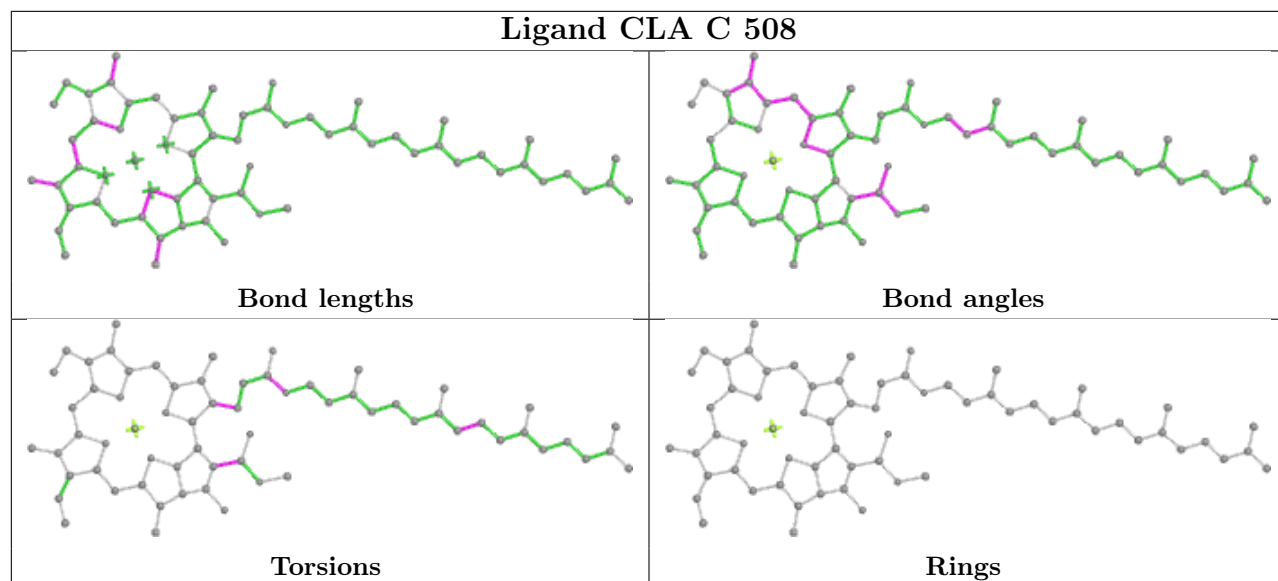
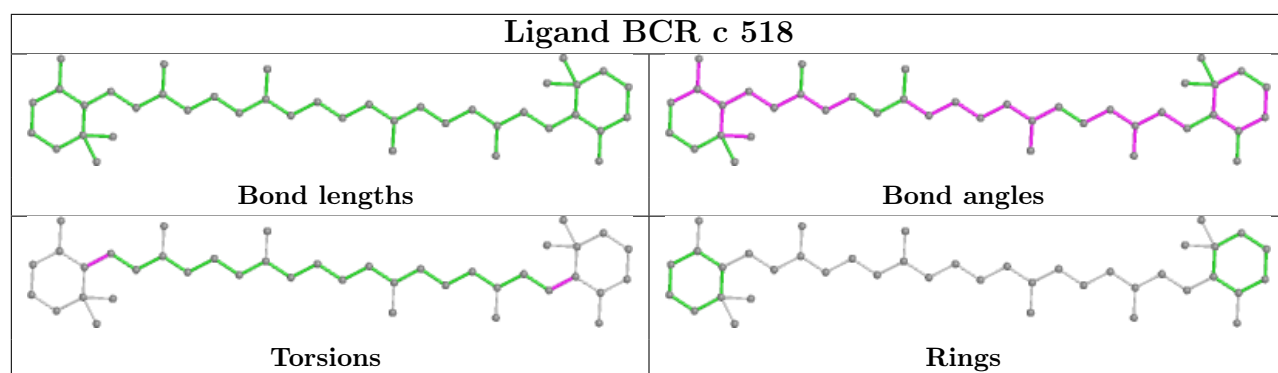




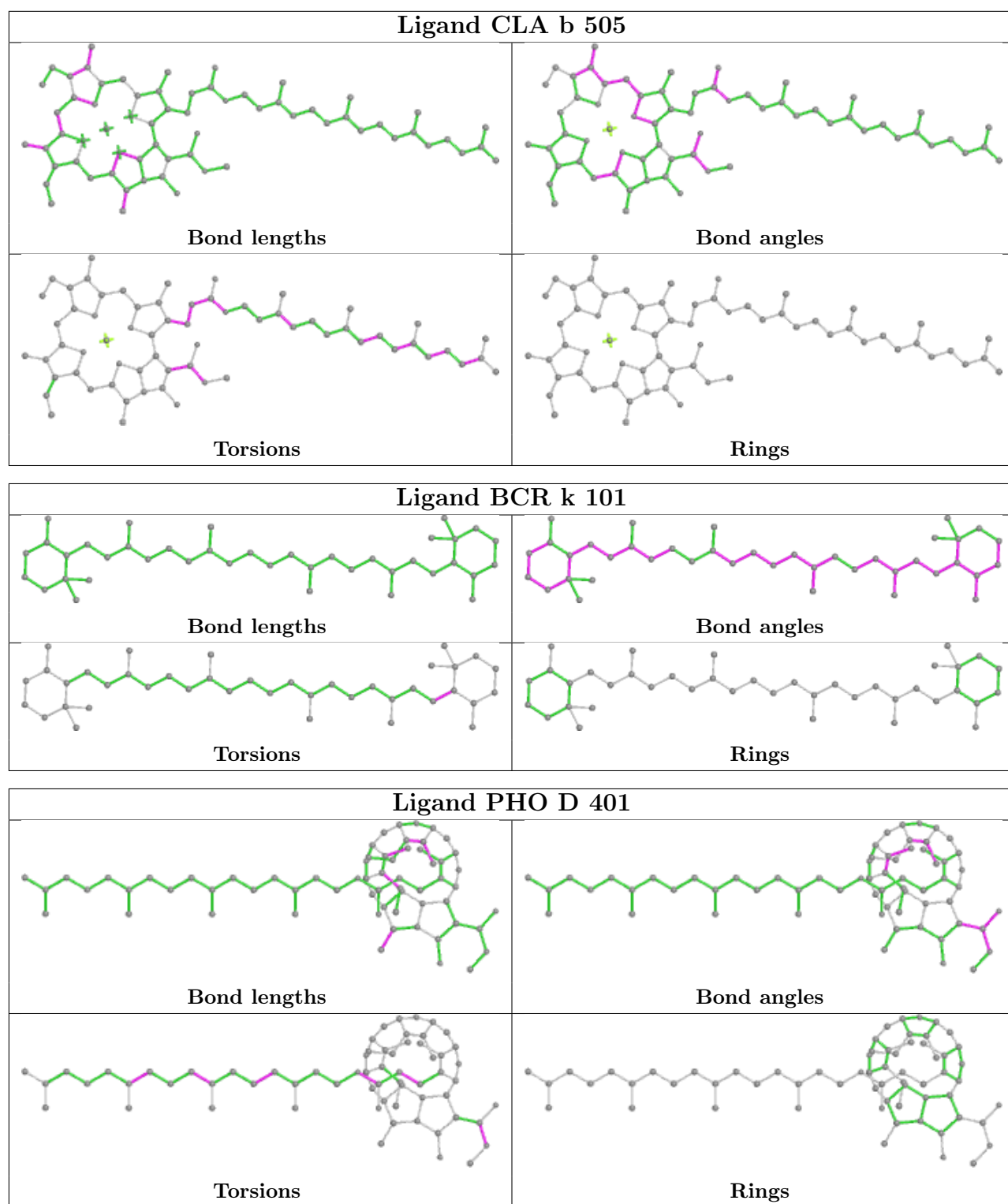




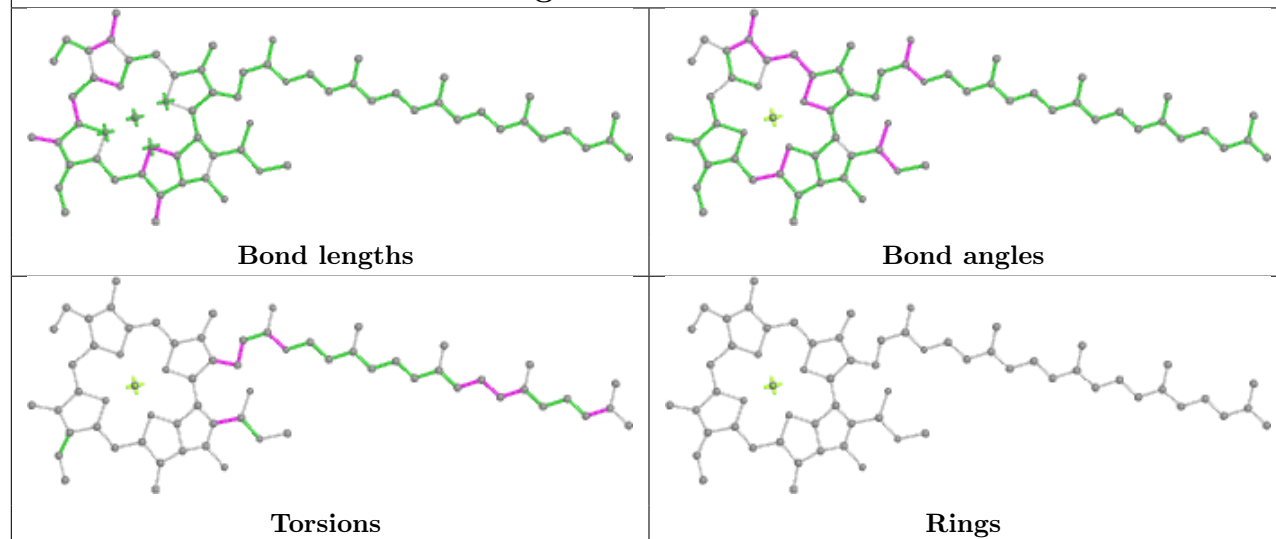




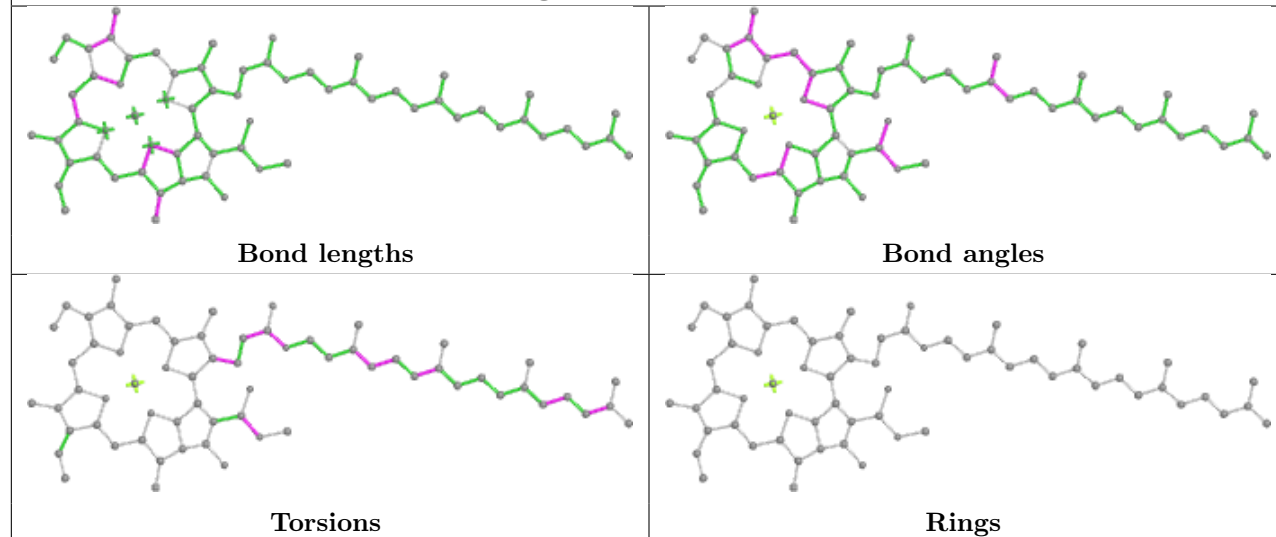




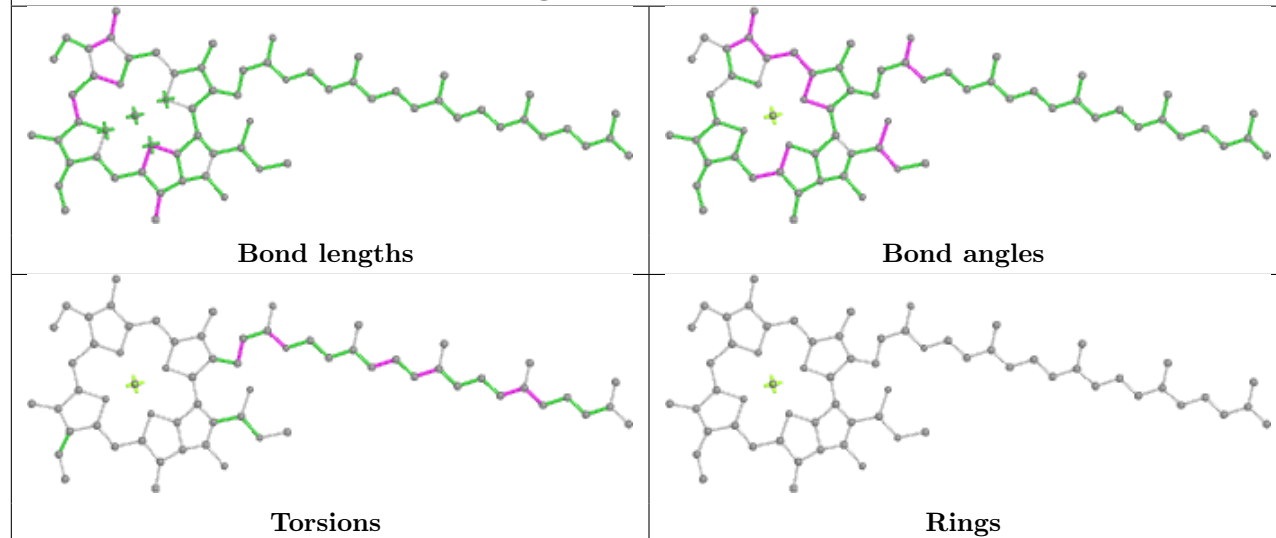
## Ligand CLA b 504

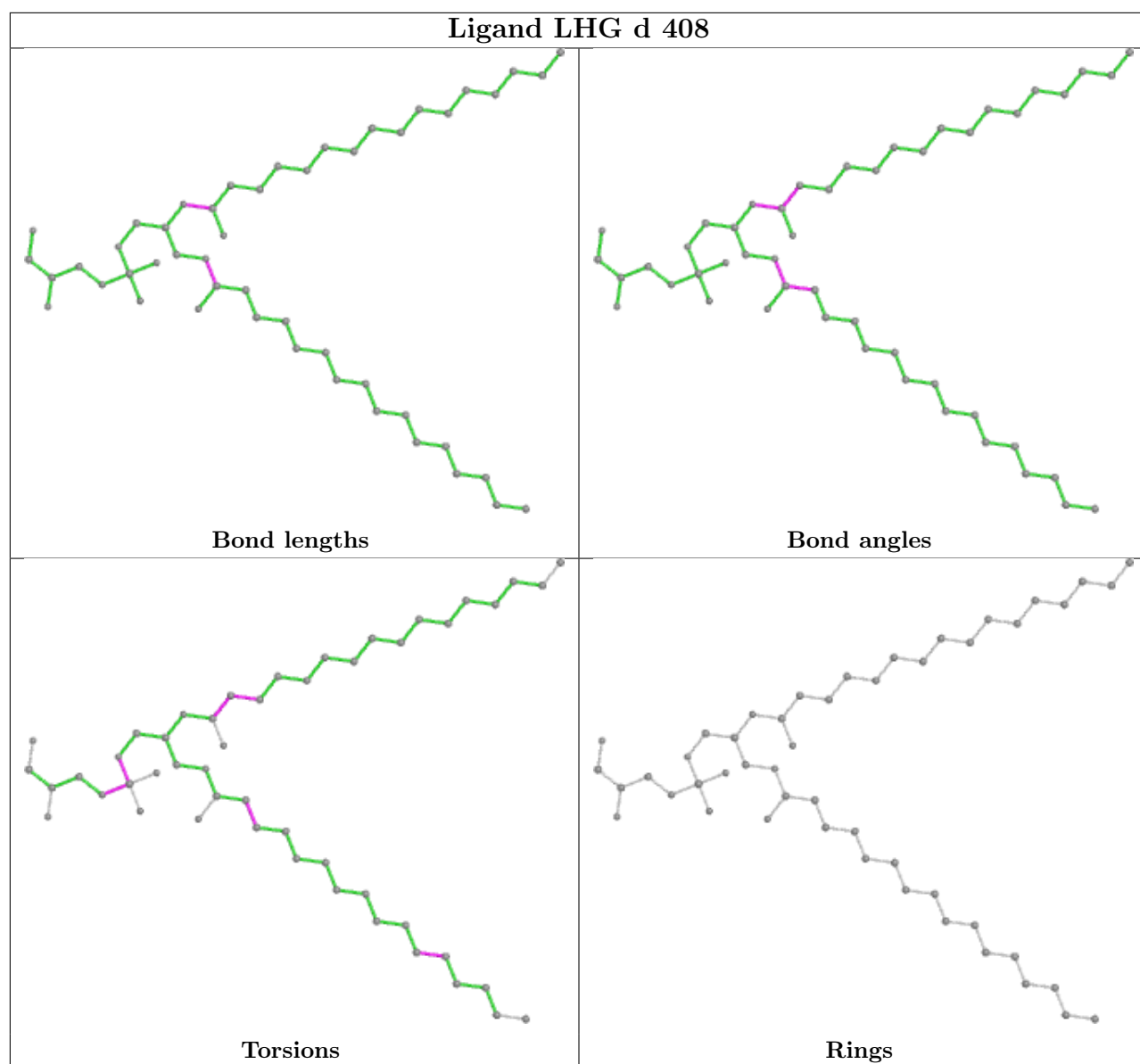


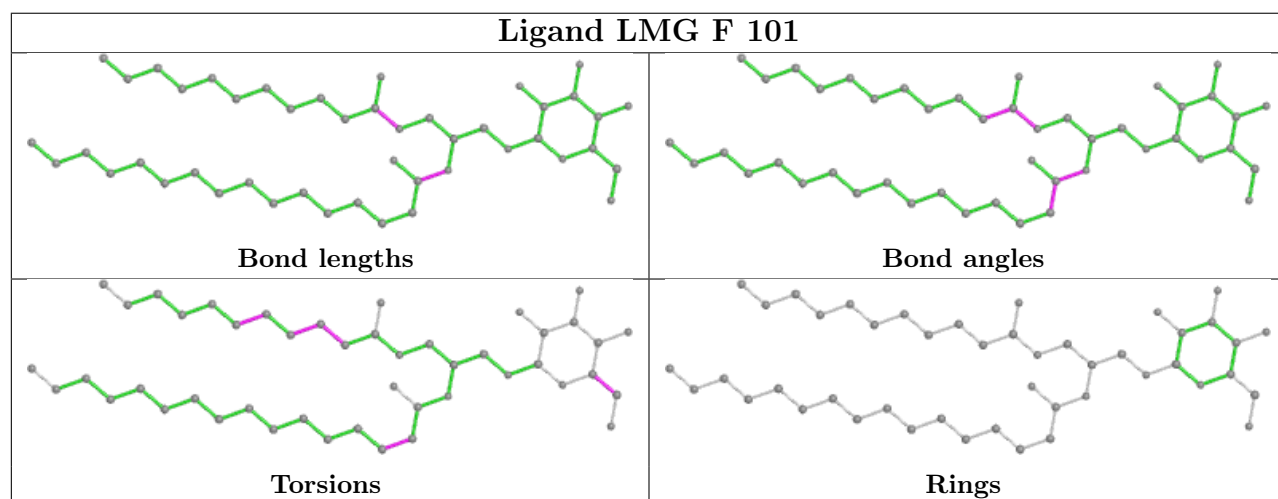
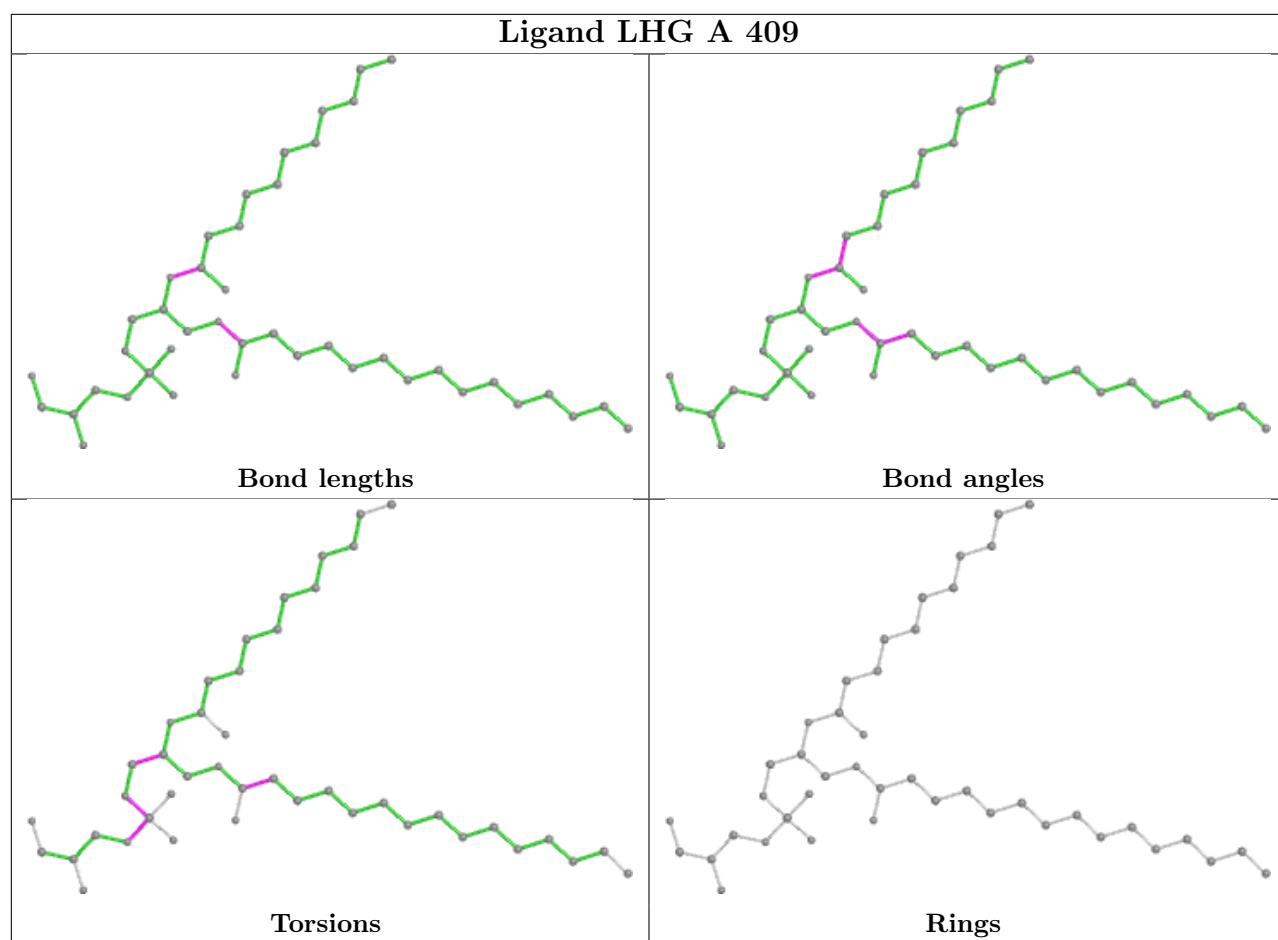
## Ligand CLA b 507

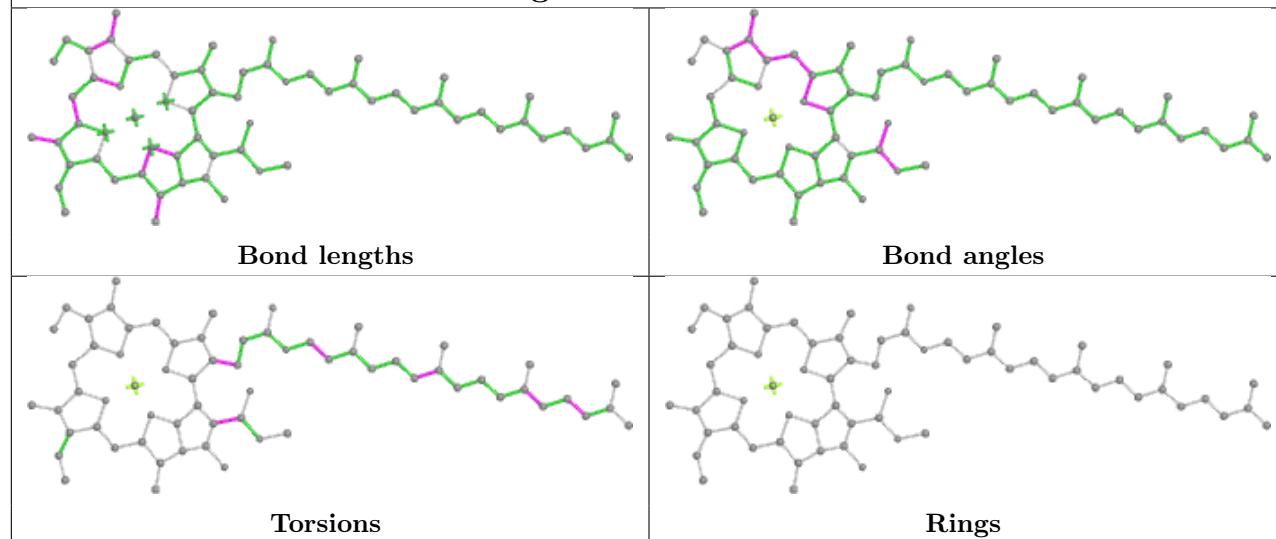
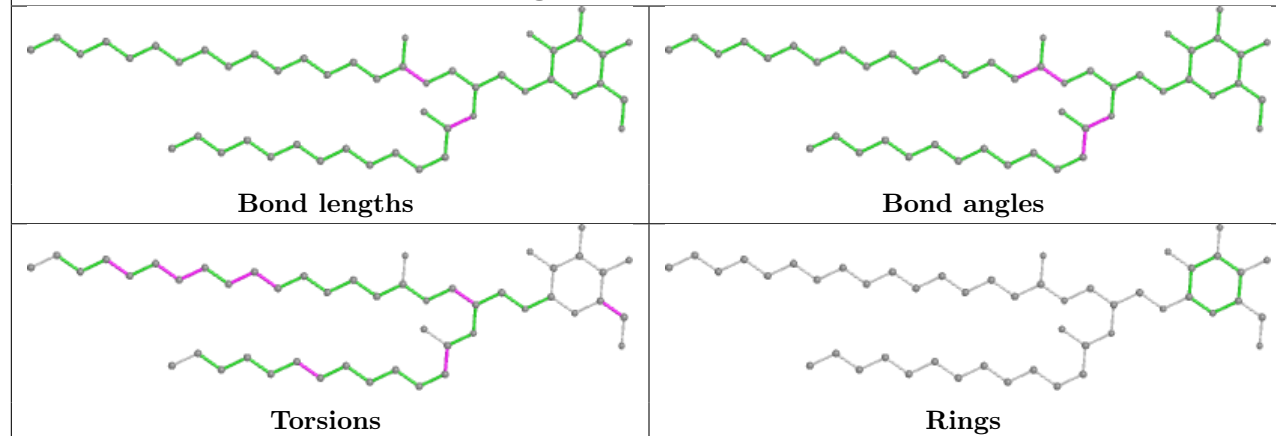
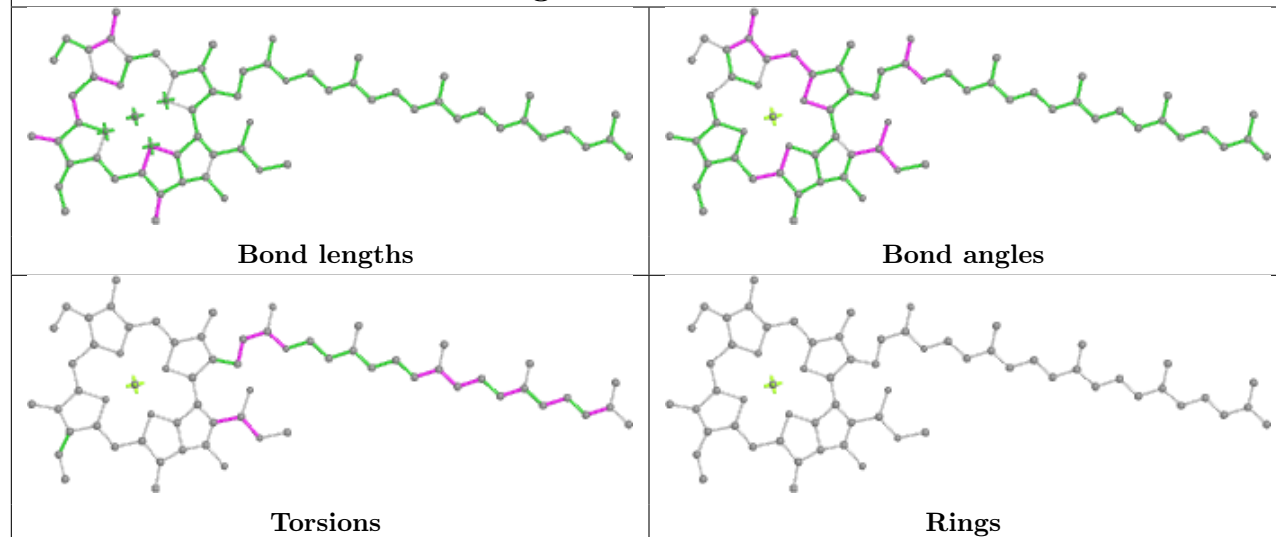


## Ligand CLA b 508

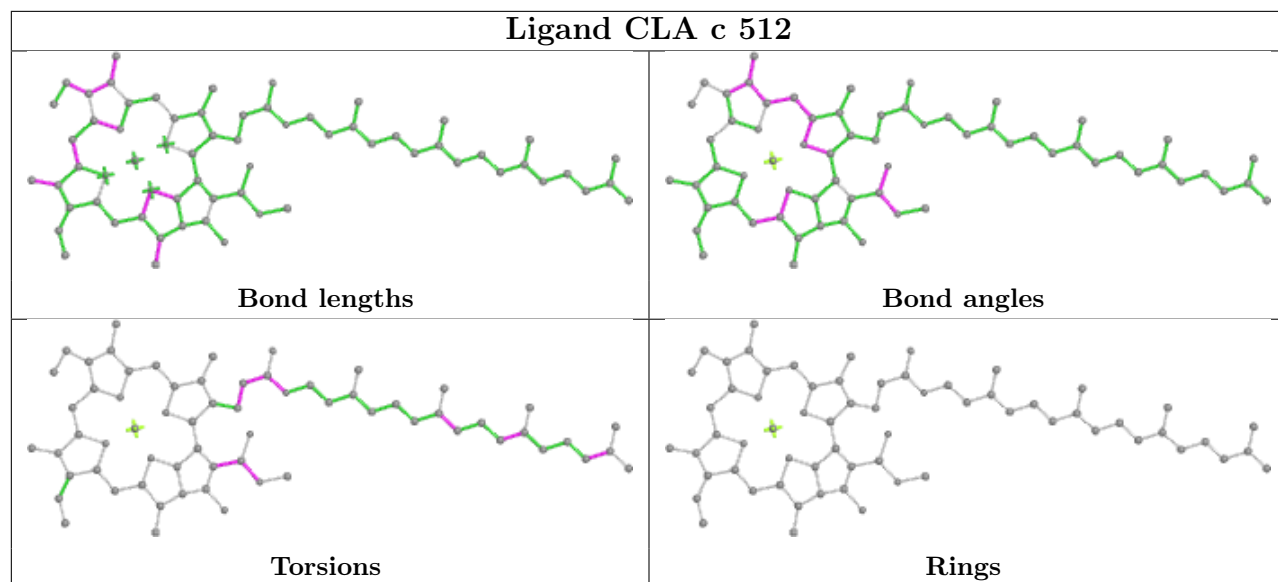




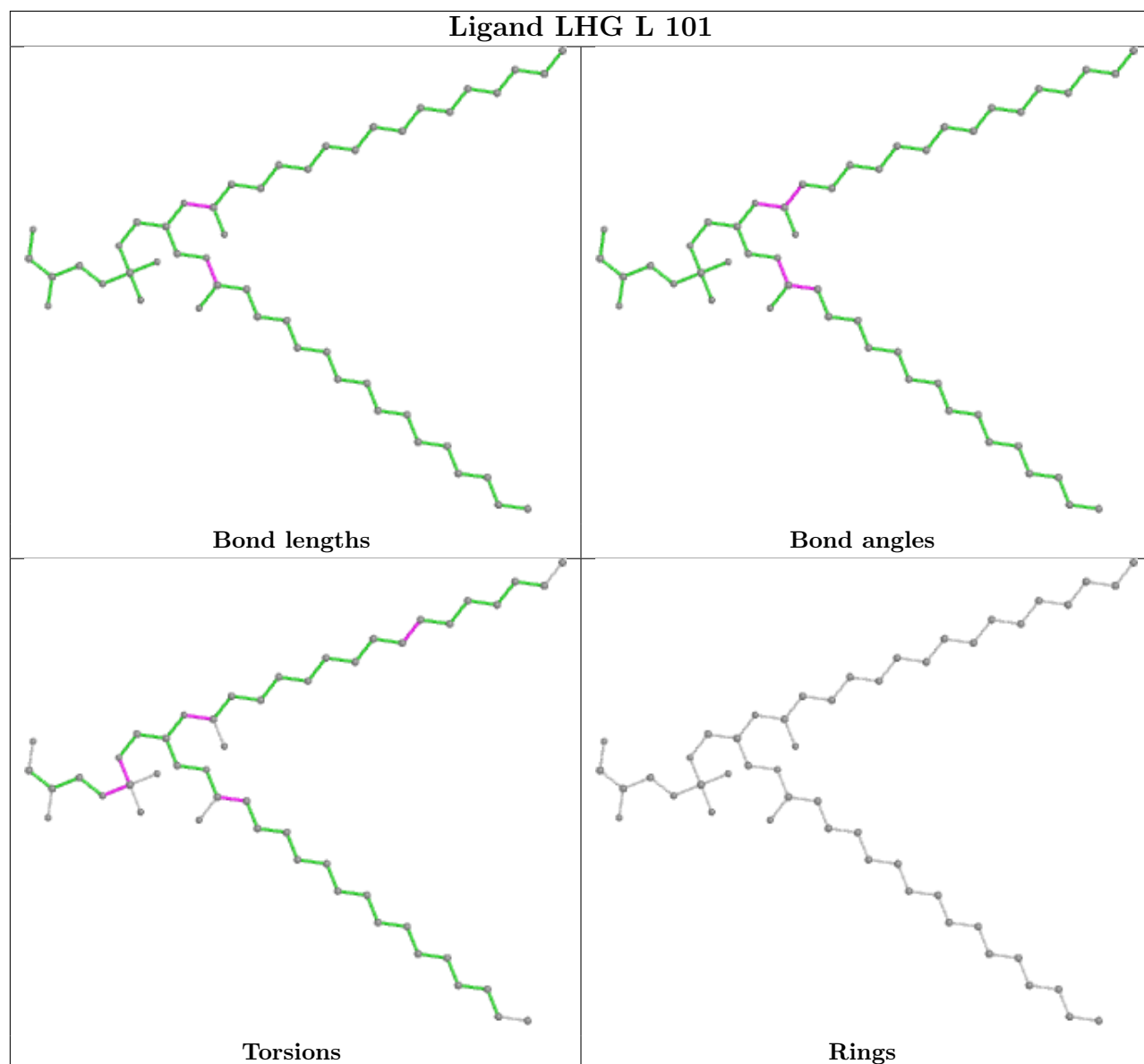


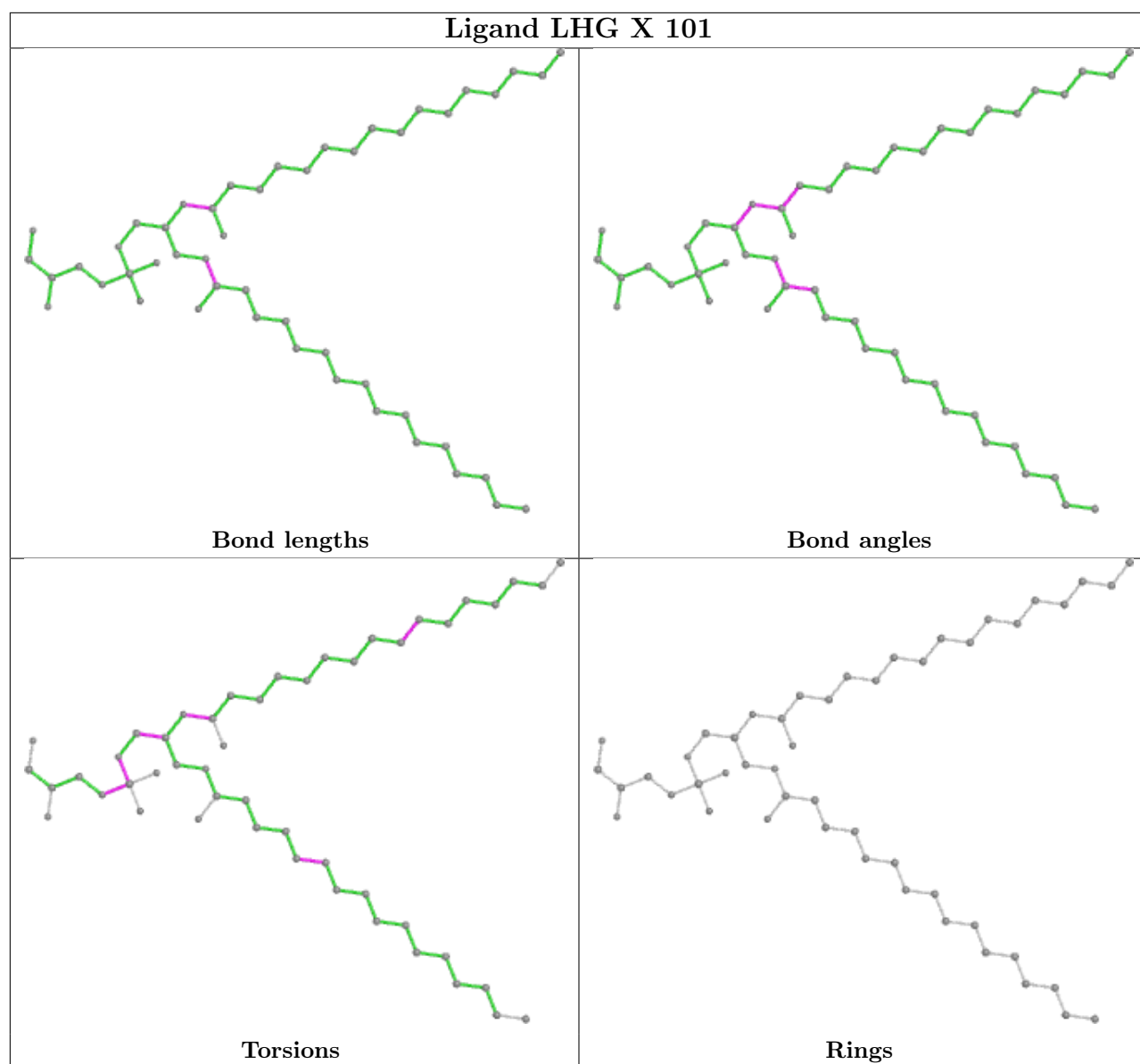
**Ligand CLA D 403****Ligand LMG h 102****Ligand CLA B 511**

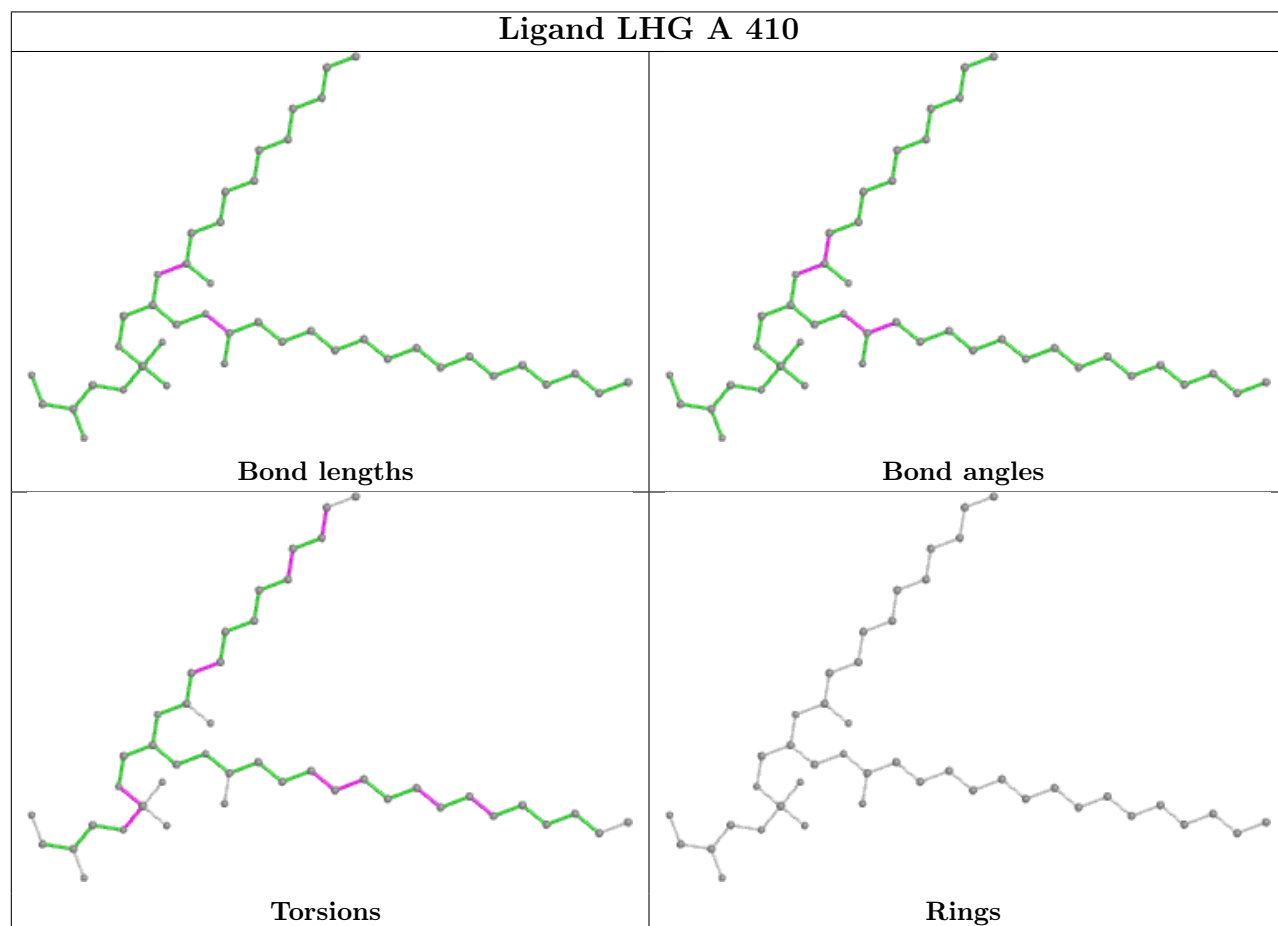
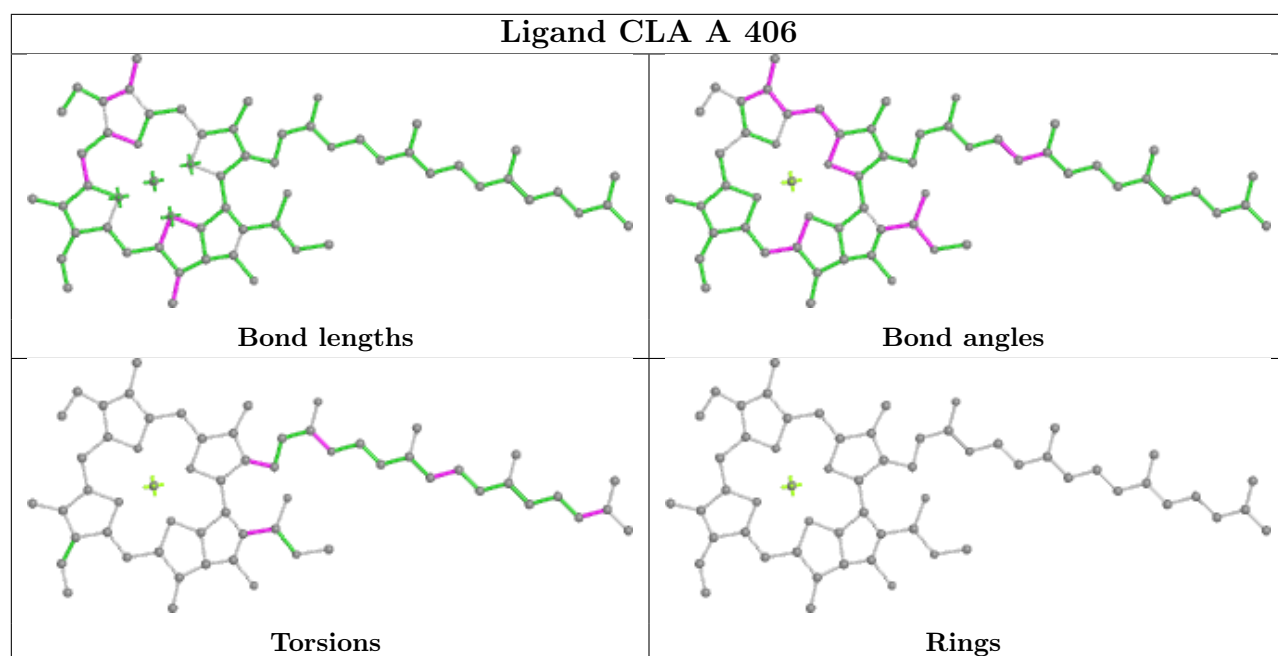
## Ligand CLA c 512



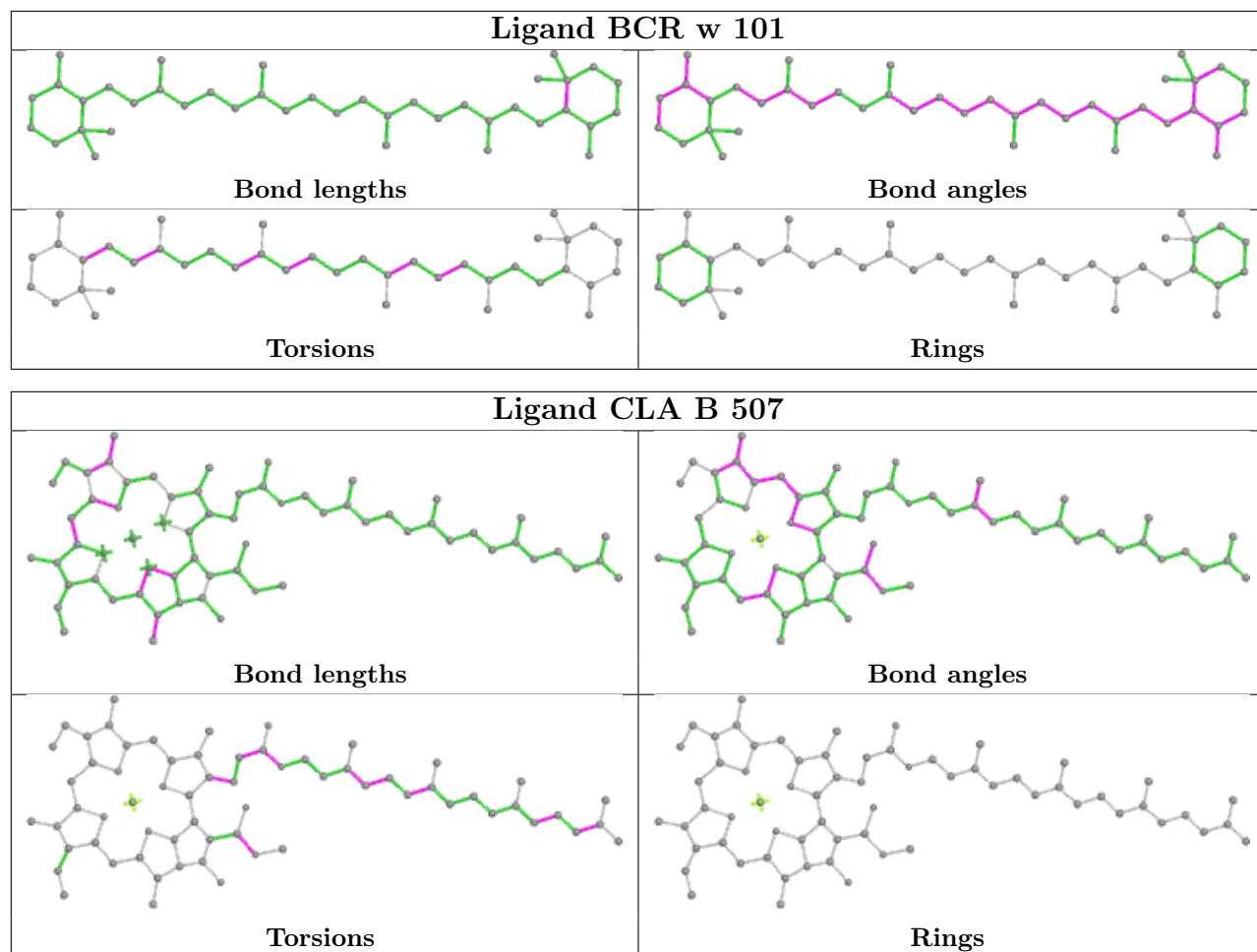
## Ligand LHG L 101

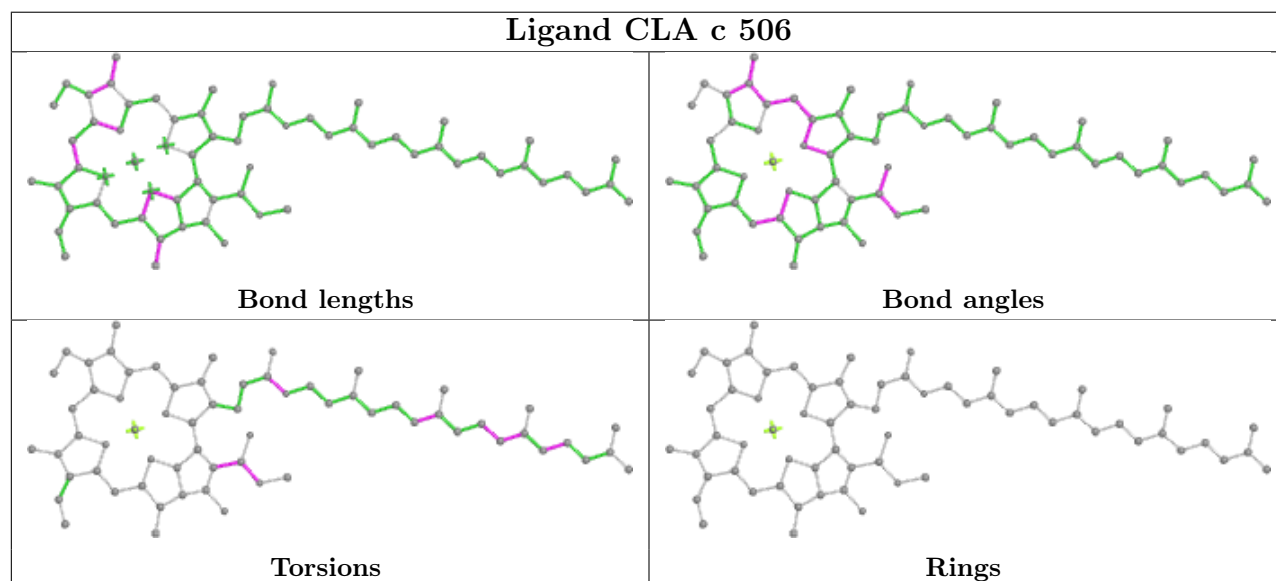
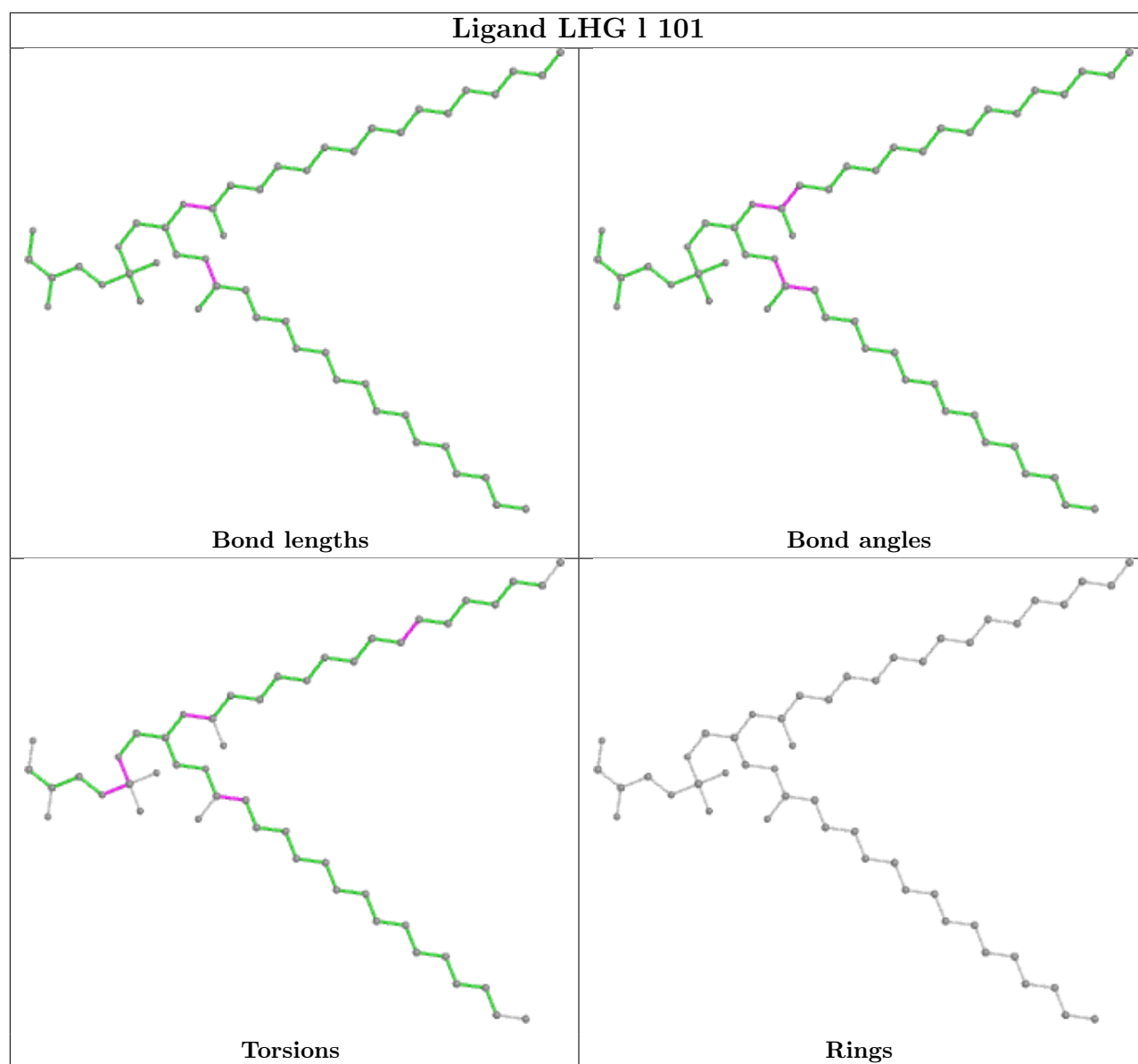


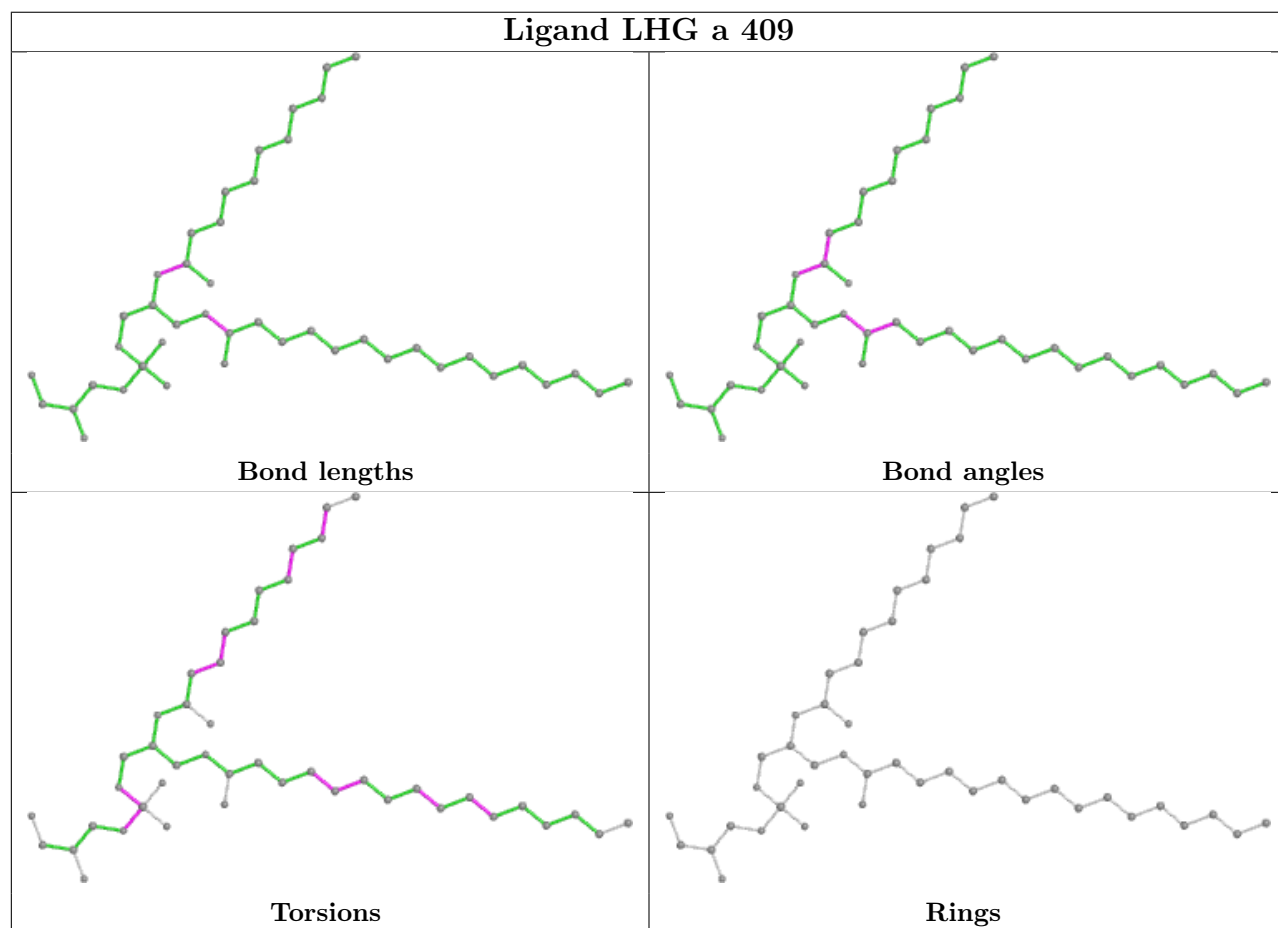
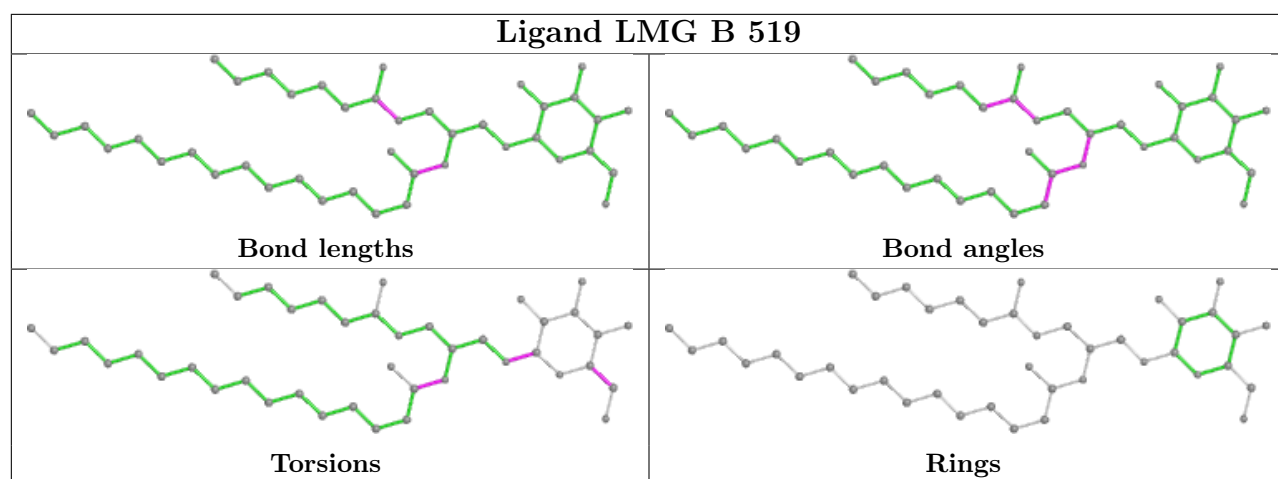


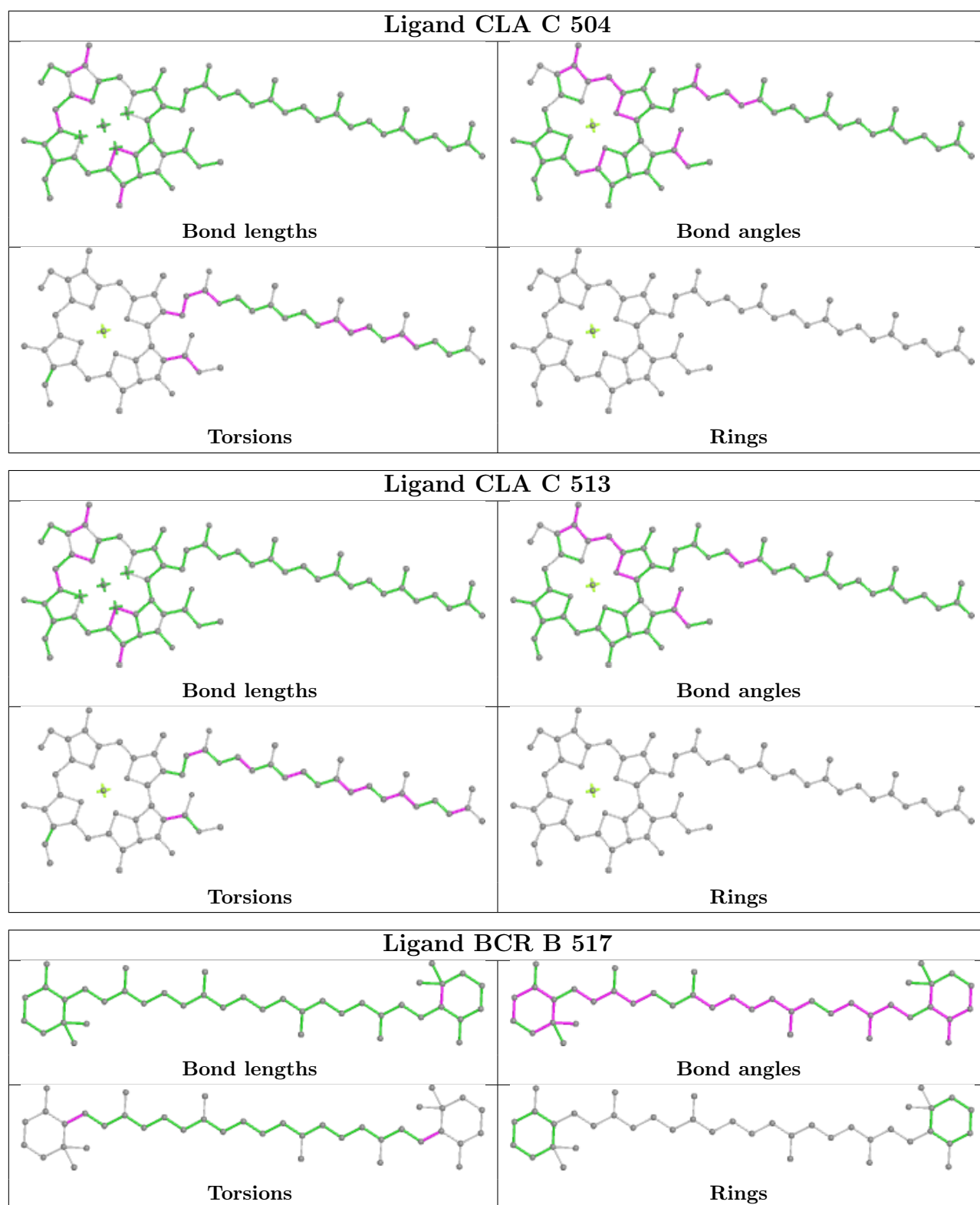




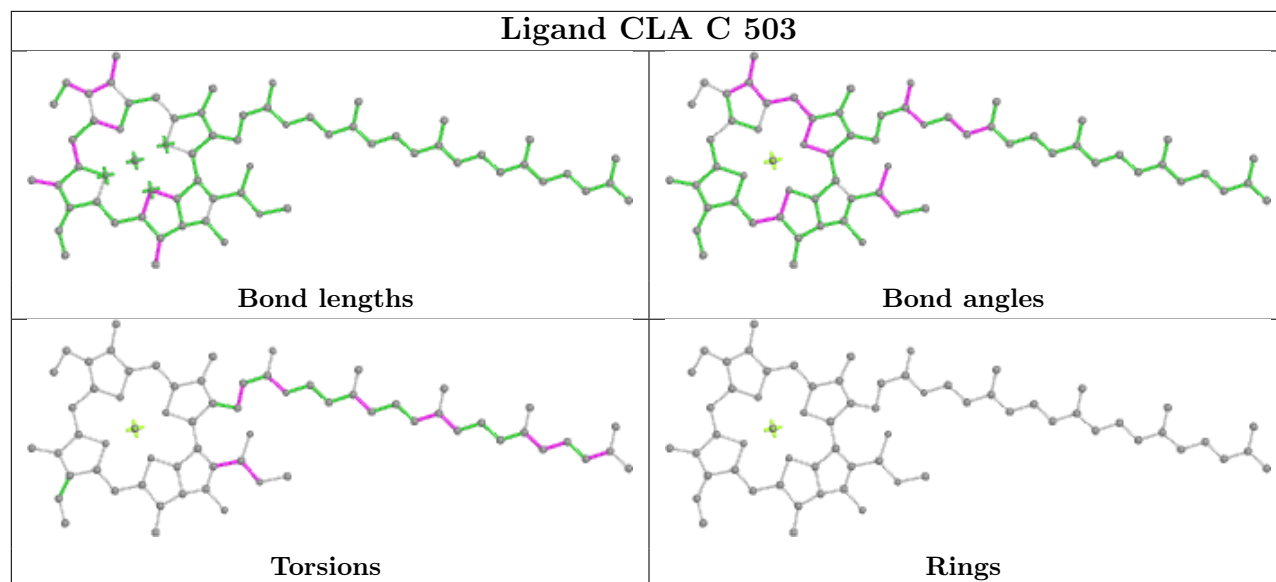




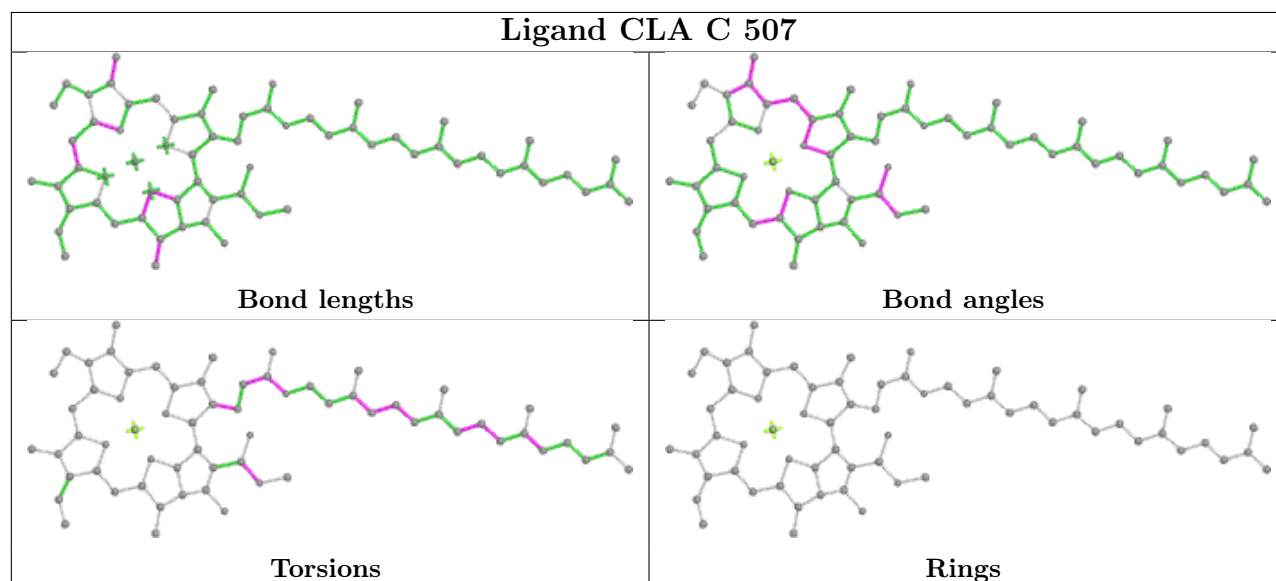




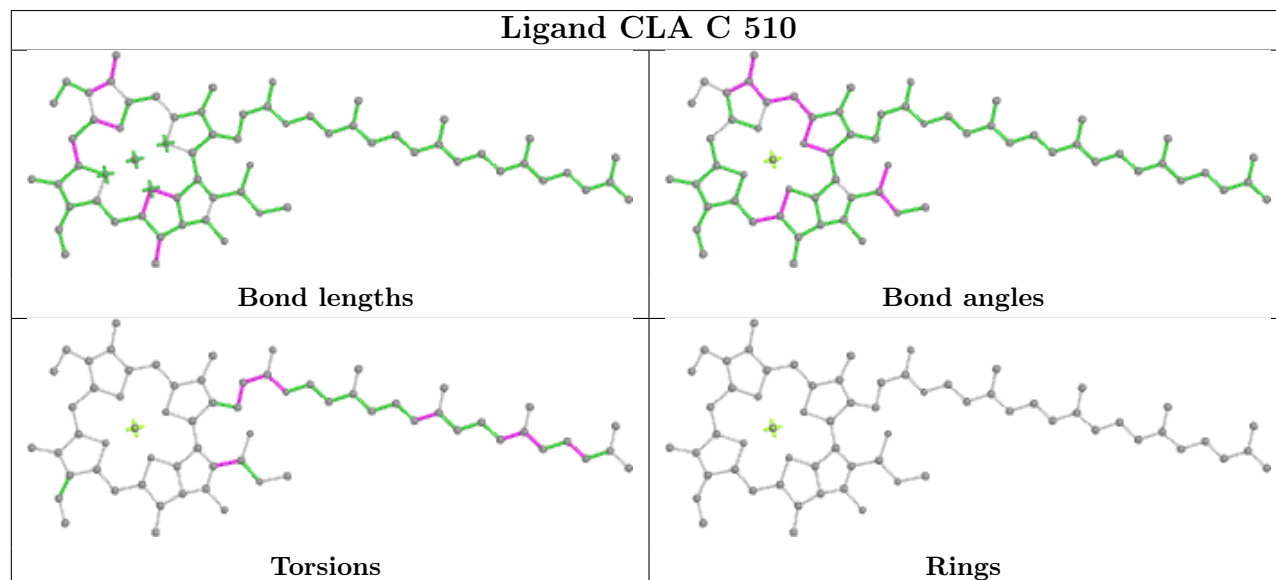
## Ligand CLA C 503

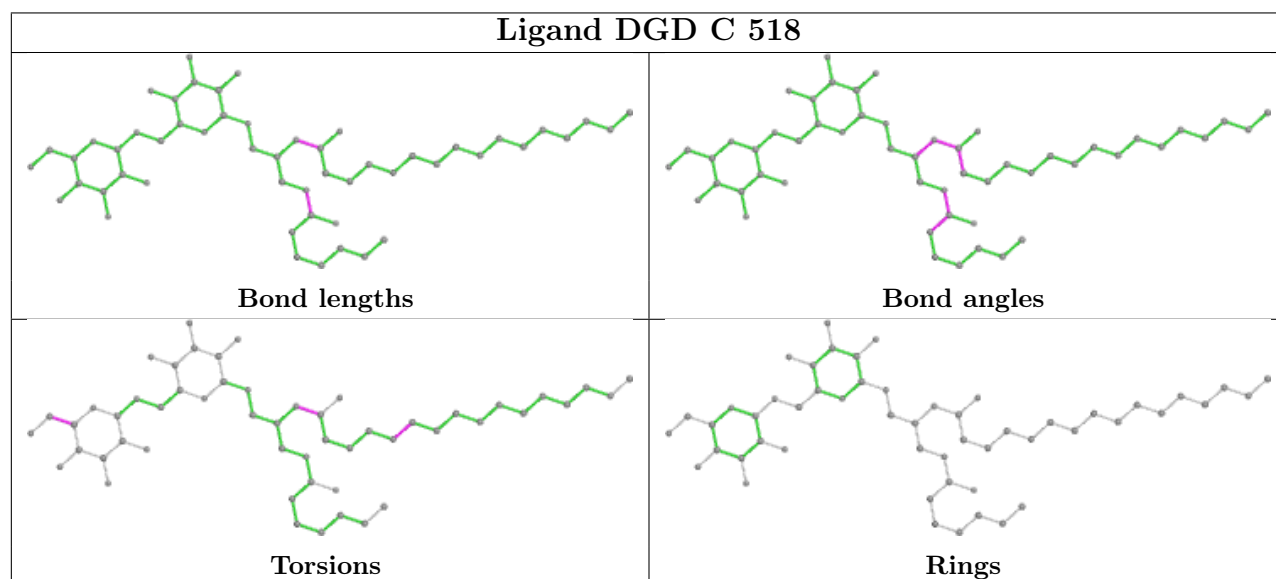
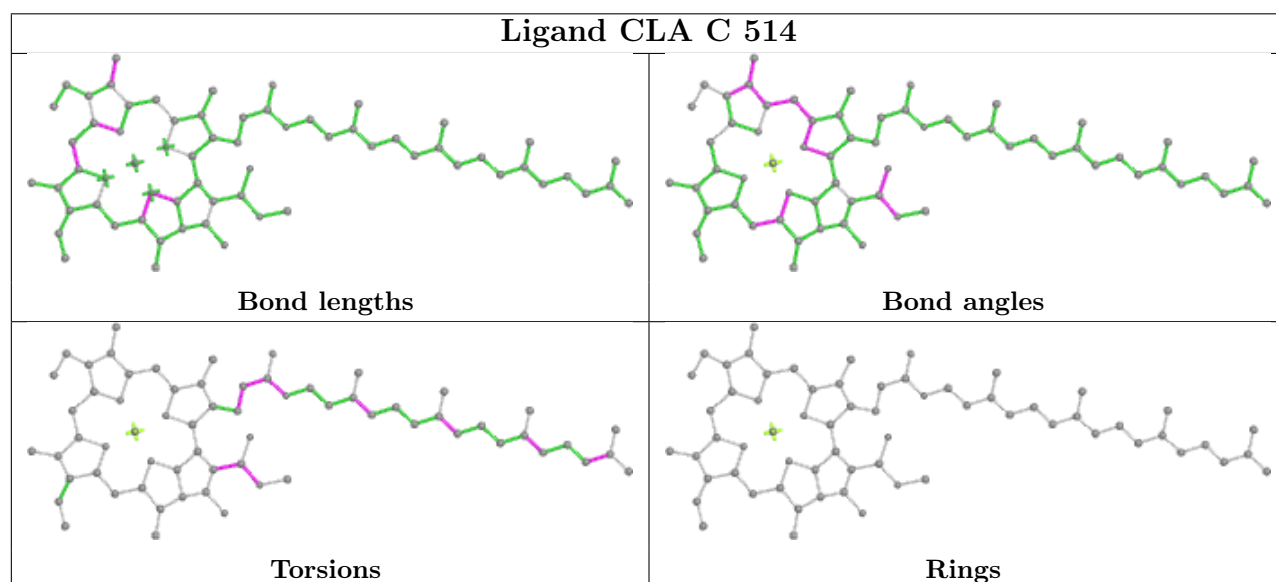
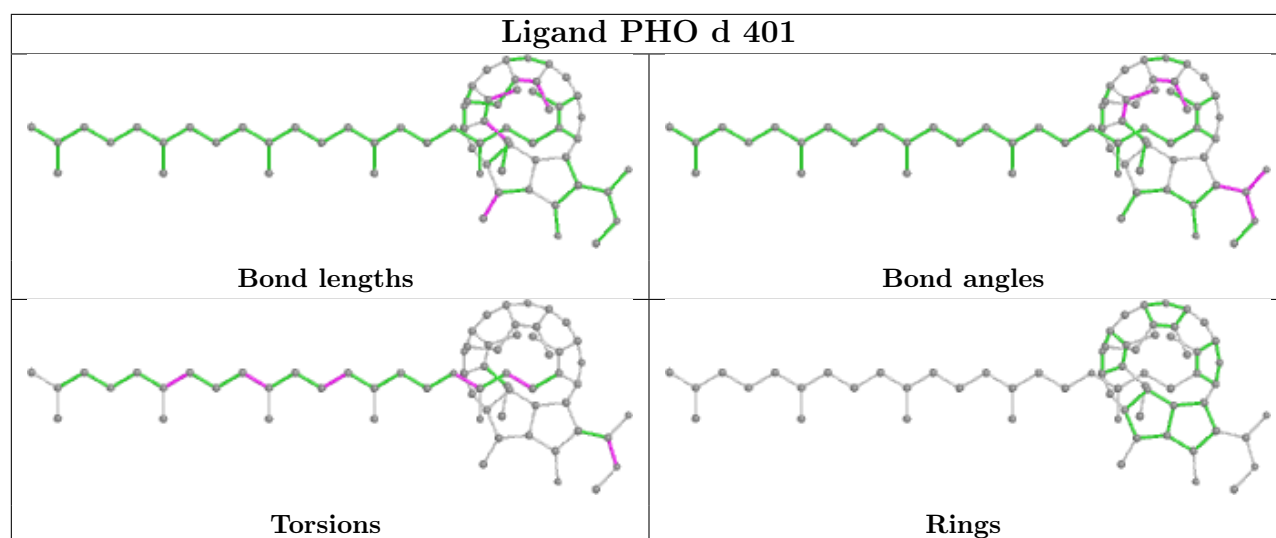


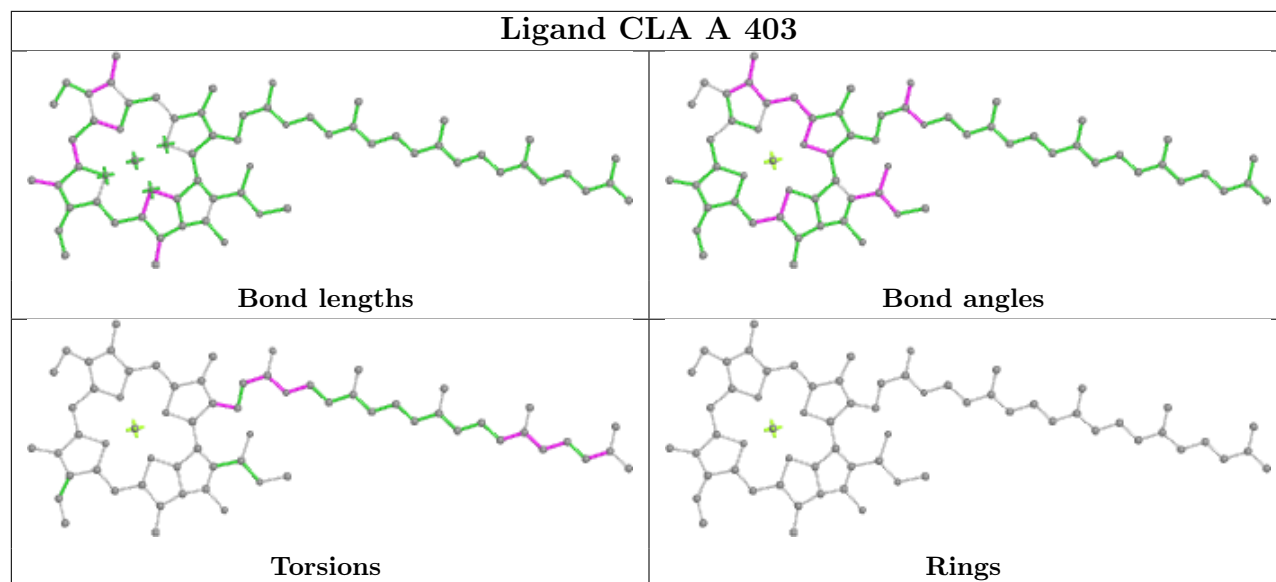
## Ligand CLA C 507



## Ligand CLA C 510







## 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.

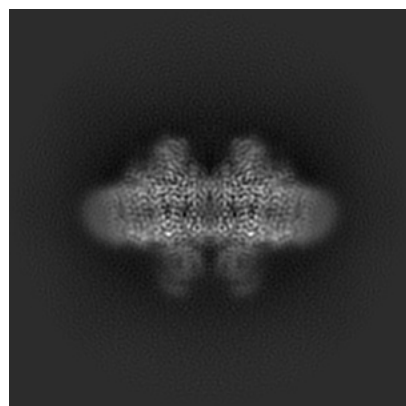
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60694. These allow visual inspection of the internal detail of the map and identification of artifacts.

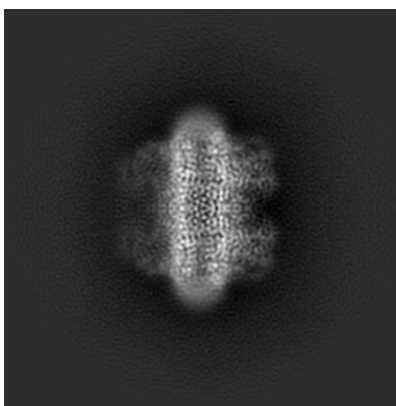
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

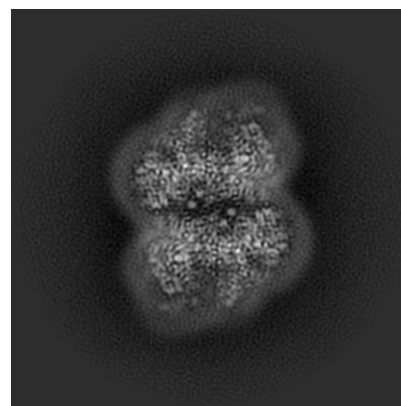
#### 6.1.1 Primary map



X

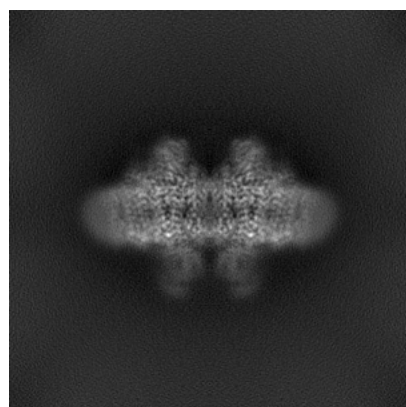


Y

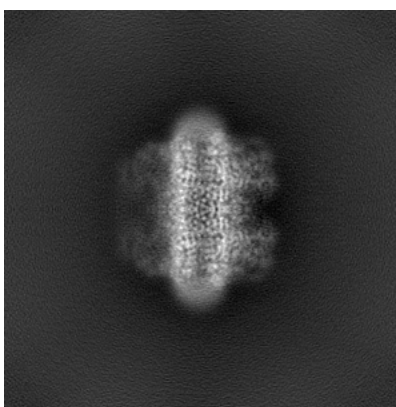


Z

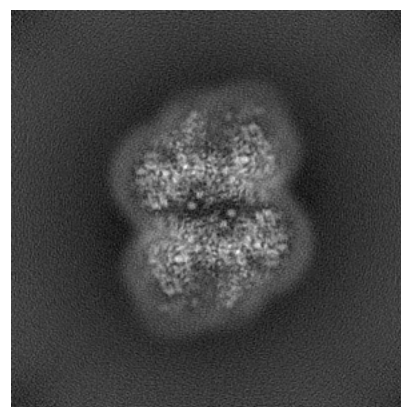
#### 6.1.2 Raw map



X



Y



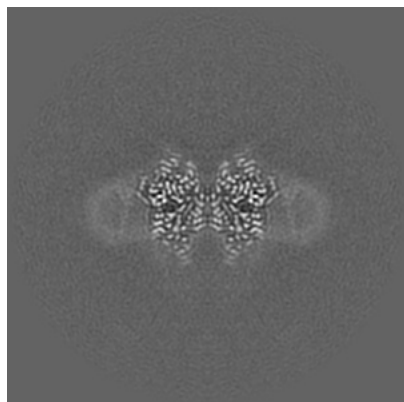
Z

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

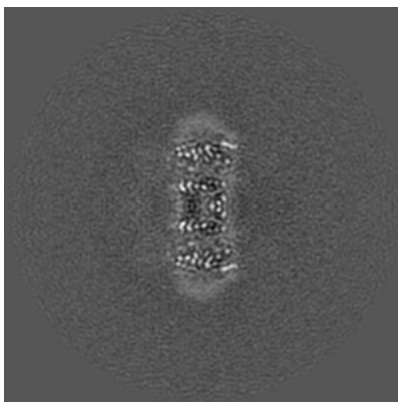


## 6.2 Central slices [i](#)

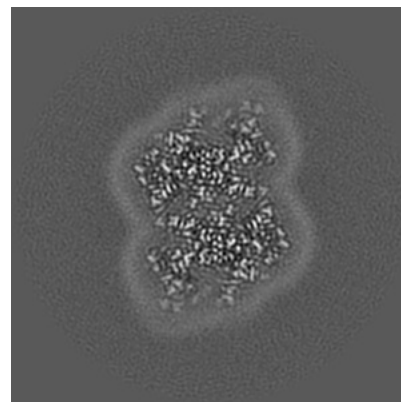
### 6.2.1 Primary map



X Index: 150

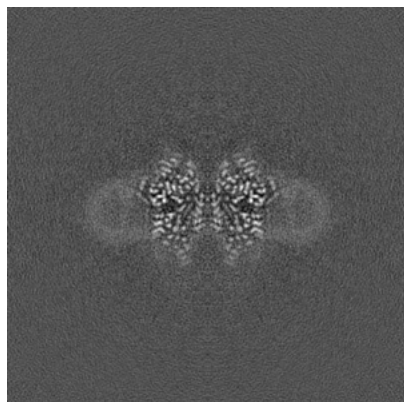


Y Index: 150

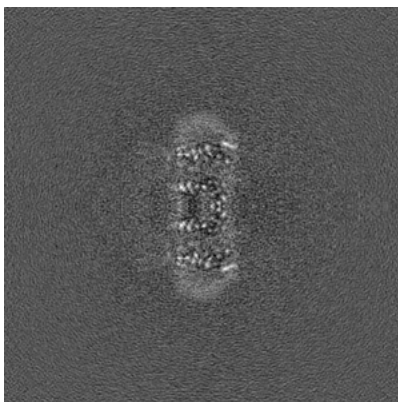


Z Index: 150

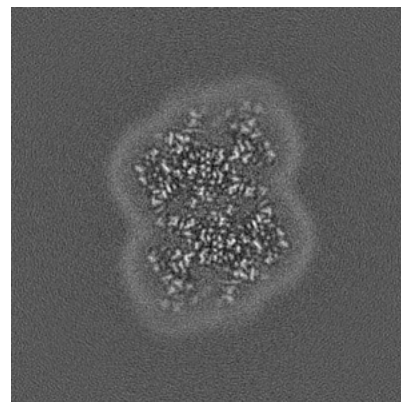
### 6.2.2 Raw map



X Index: 150



Y Index: 150

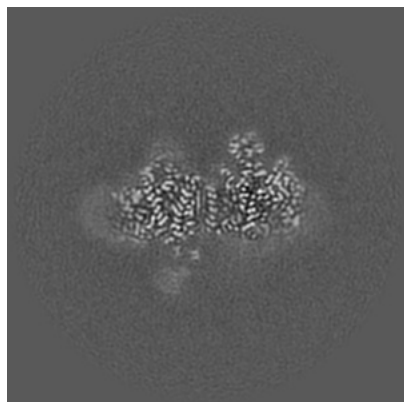


Z Index: 150

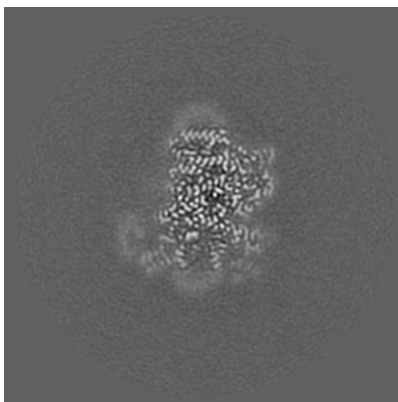
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

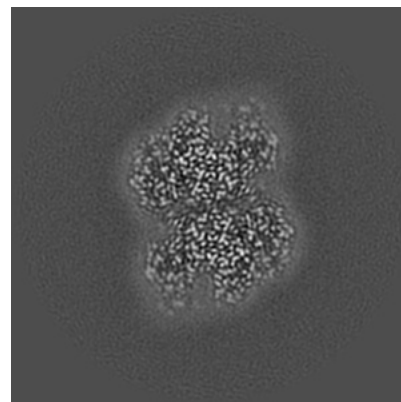
### 6.3.1 Primary map



X Index: 133

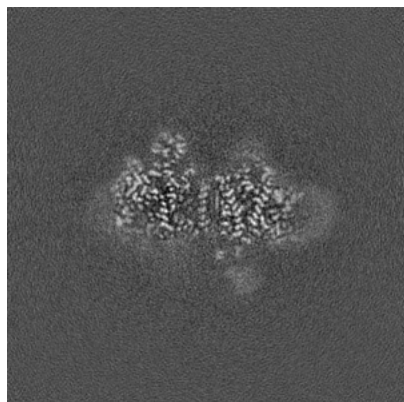


Y Index: 122

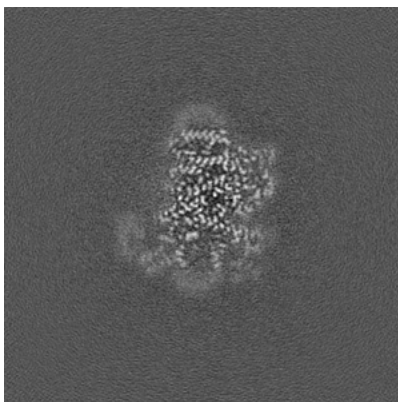


Z Index: 162

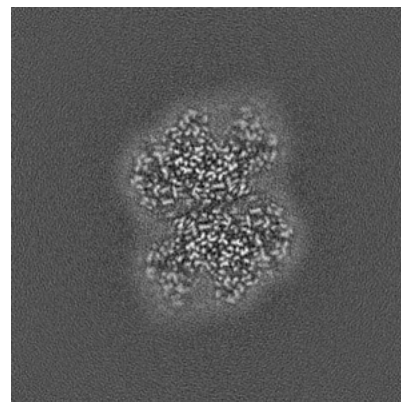
### 6.3.2 Raw map



X Index: 167



Y Index: 122

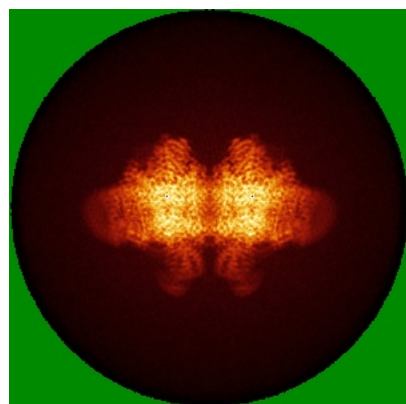


Z Index: 163

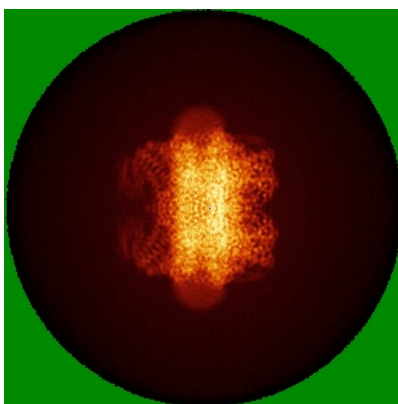
The images above show the largest variance slices of the map in three orthogonal directions.

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

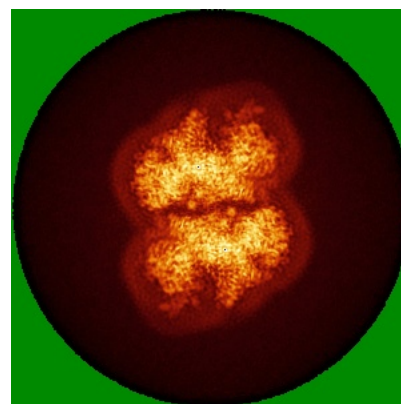
### 6.4.1 Primary map



X

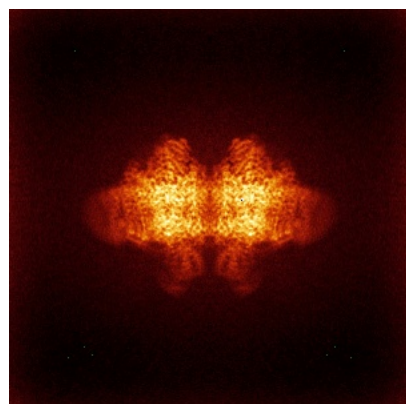


Y

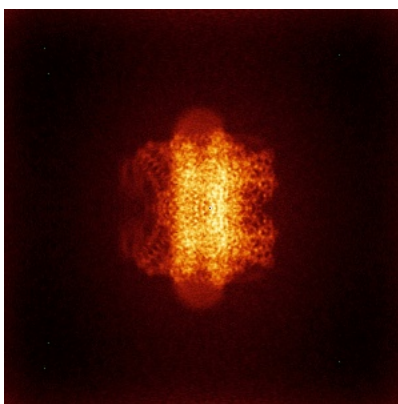


Z

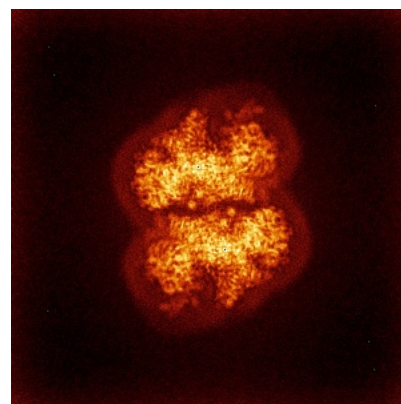
### 6.4.2 Raw map



X



Y

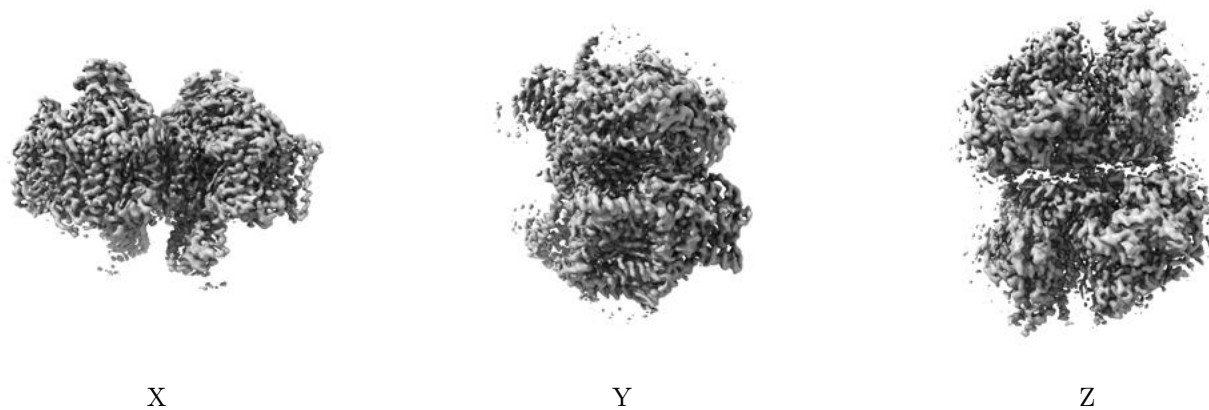


Z

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.

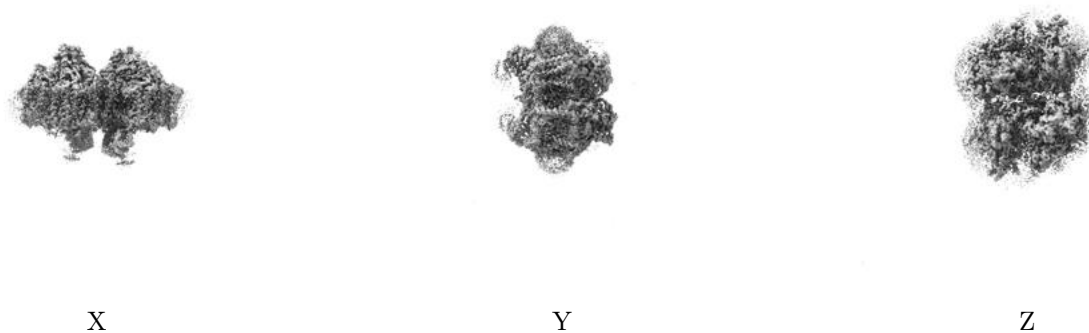
## 6.5 Orthogonal surface views [i](#)

### 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.

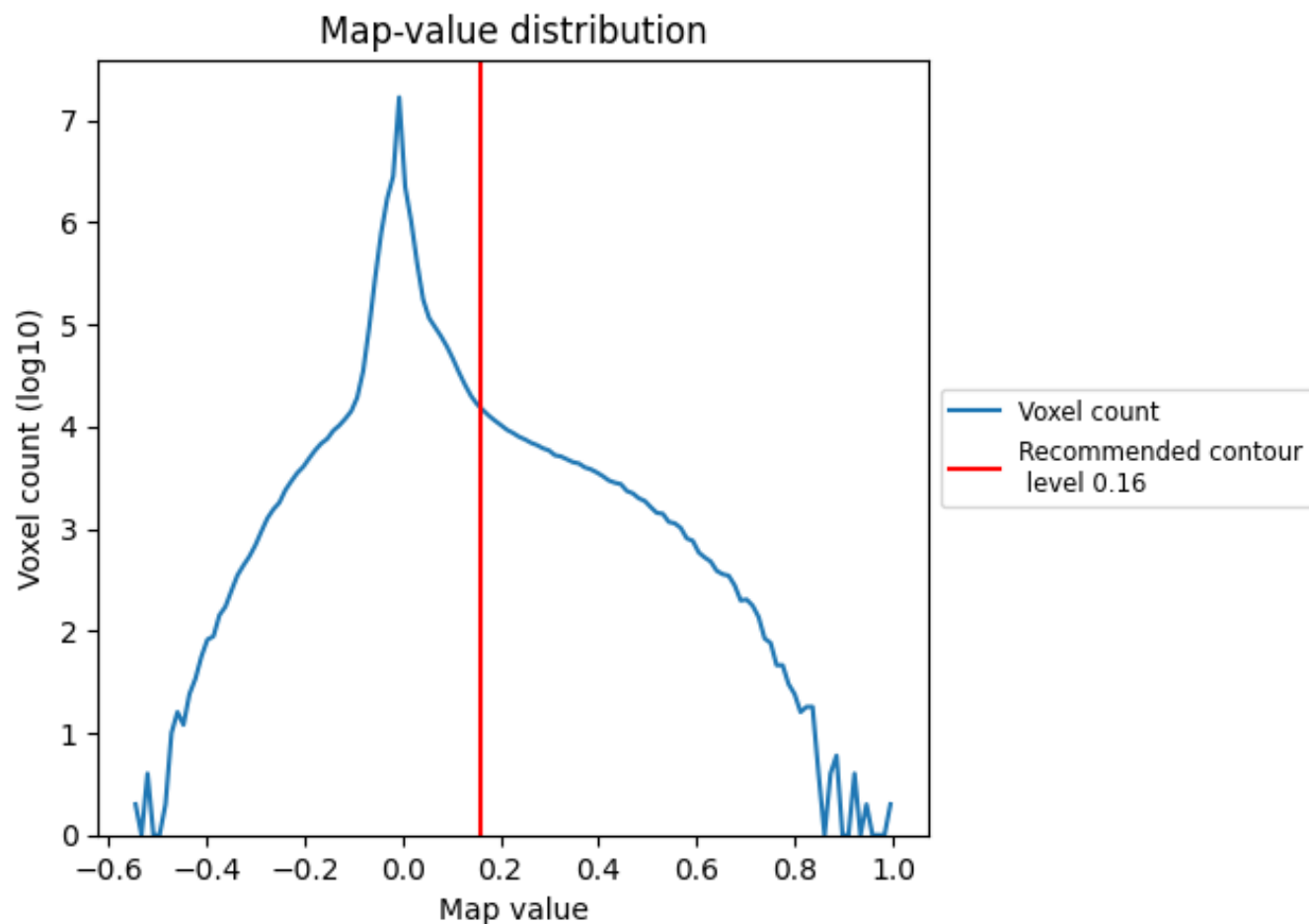
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

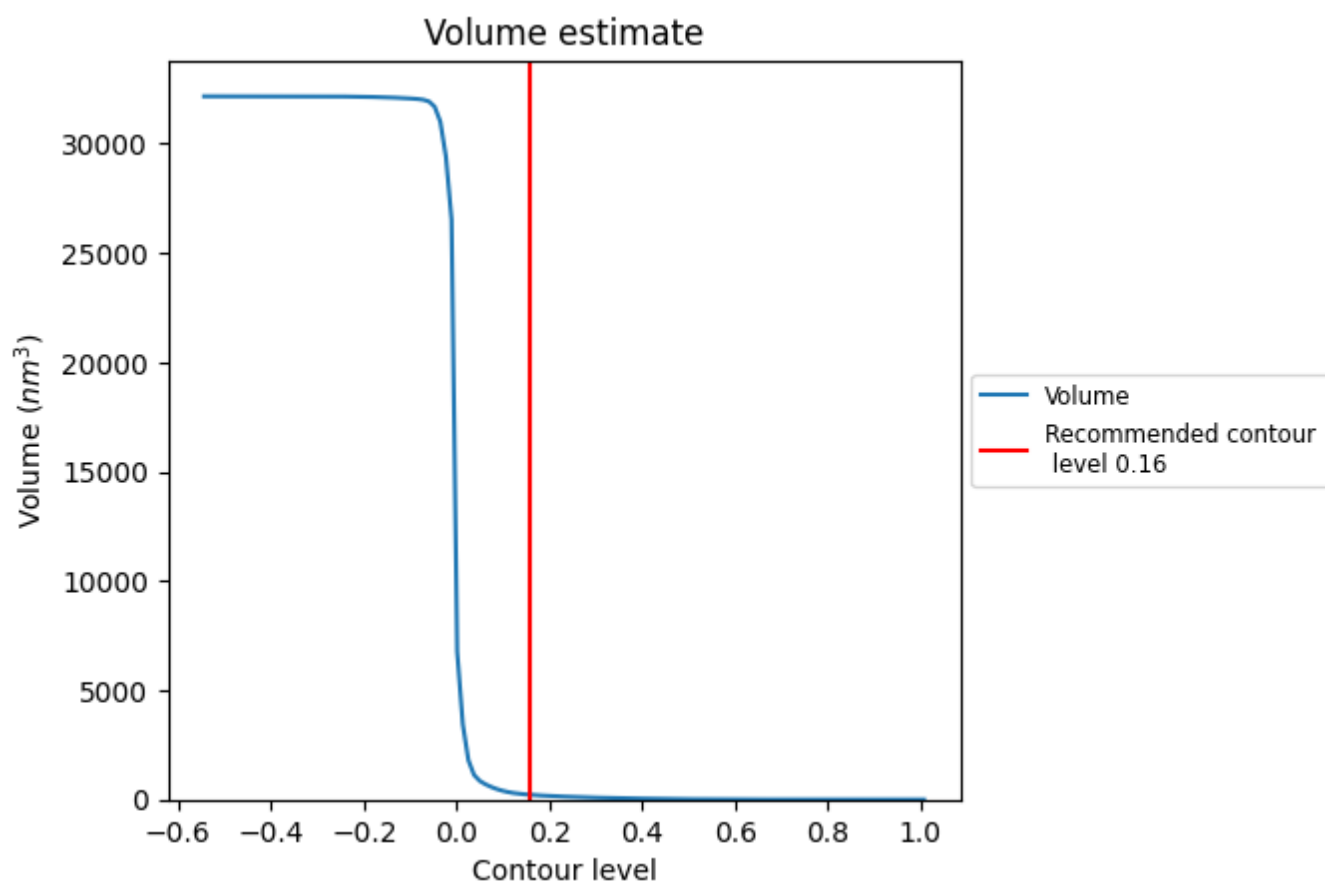
This section contains the results of statistical analysis of the map.

### 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](#)

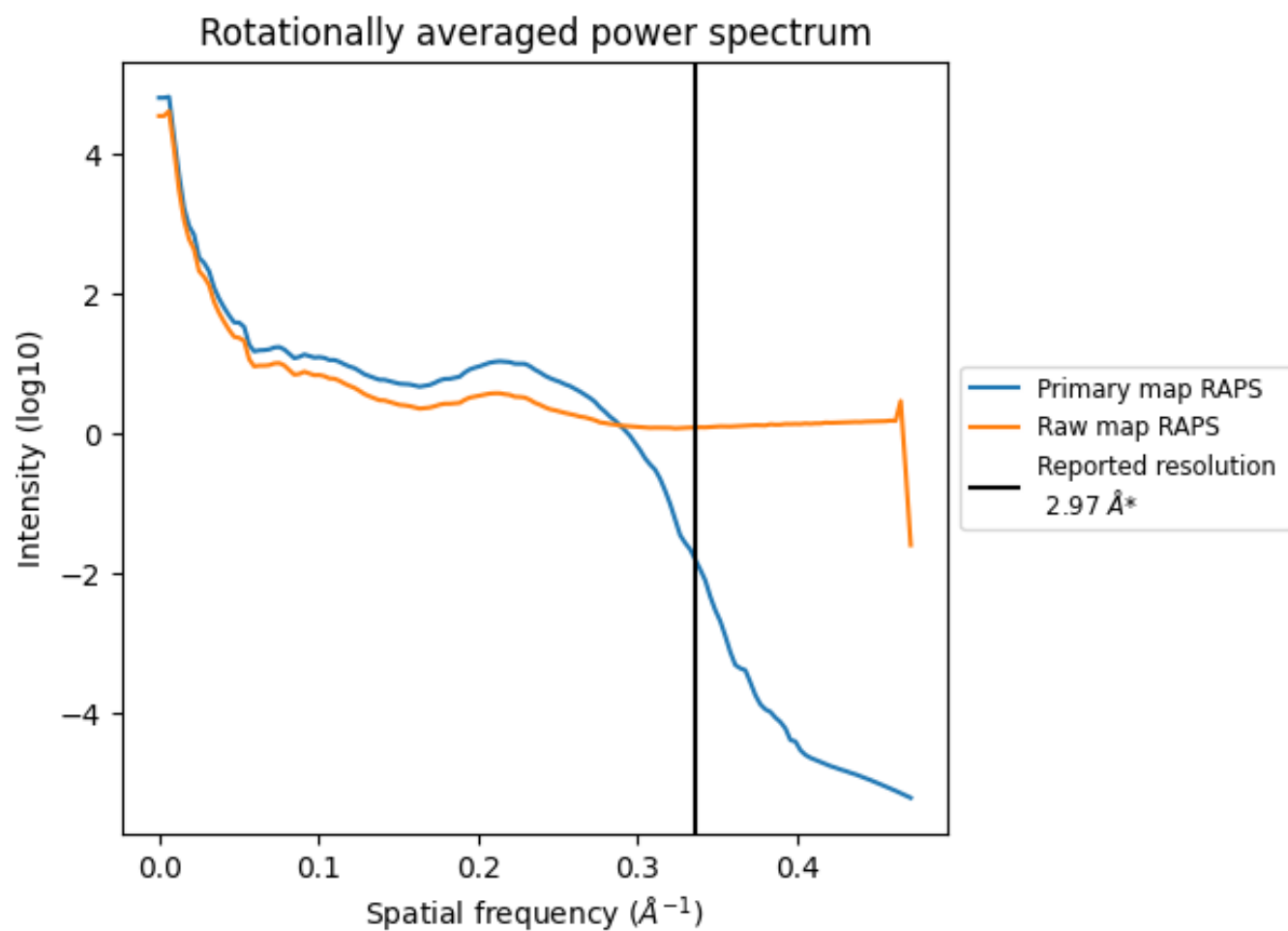


The volume at the recommended contour level is 217 nm<sup>3</sup>; this corresponds to an approximate mass of 196 kDa.

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 ⓘ

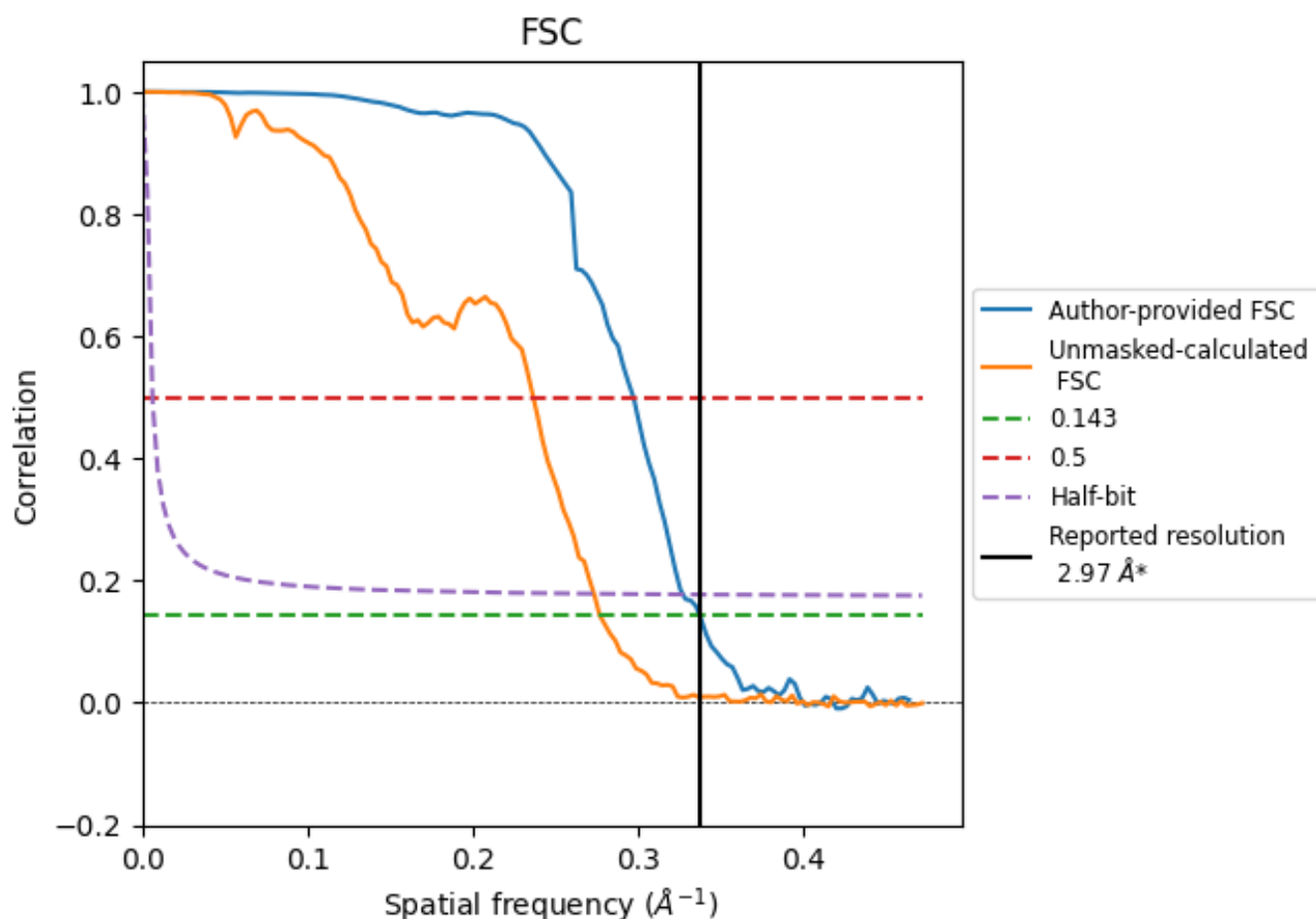


\*Reported resolution corresponds to spatial frequency of 0.337 Å<sup>-1</sup>

## 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 0.337 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

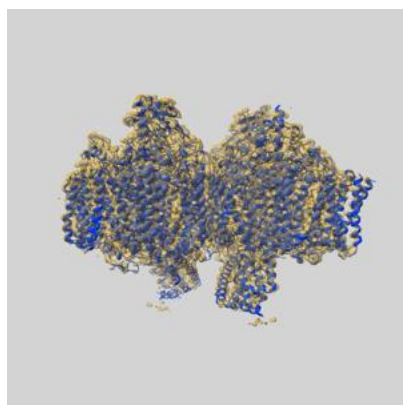
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.37	3.06
Unmasked-calculated*	3.61	4.23	3.66

\*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 3.61 differs from the reported value 2.97 by more than 10 %

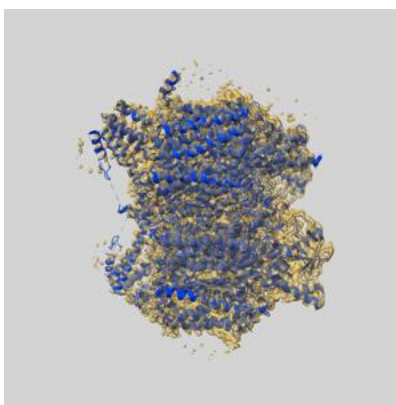
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60694 and PDB model 9IMN. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

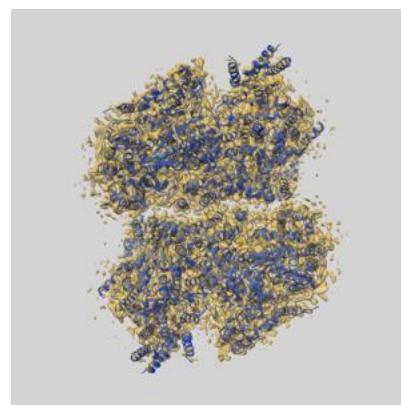
### 9.1 Map-model overlay [i](#)



X



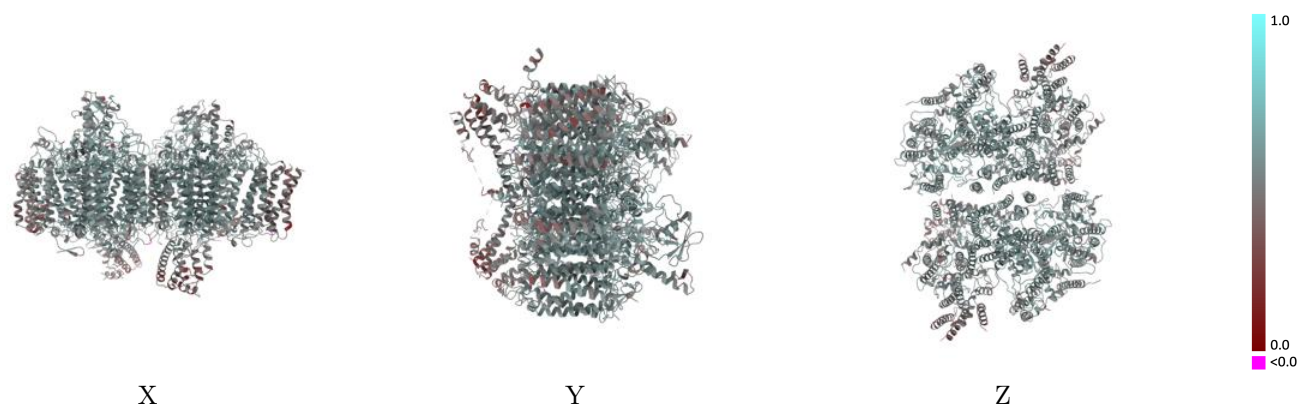
Y



Z

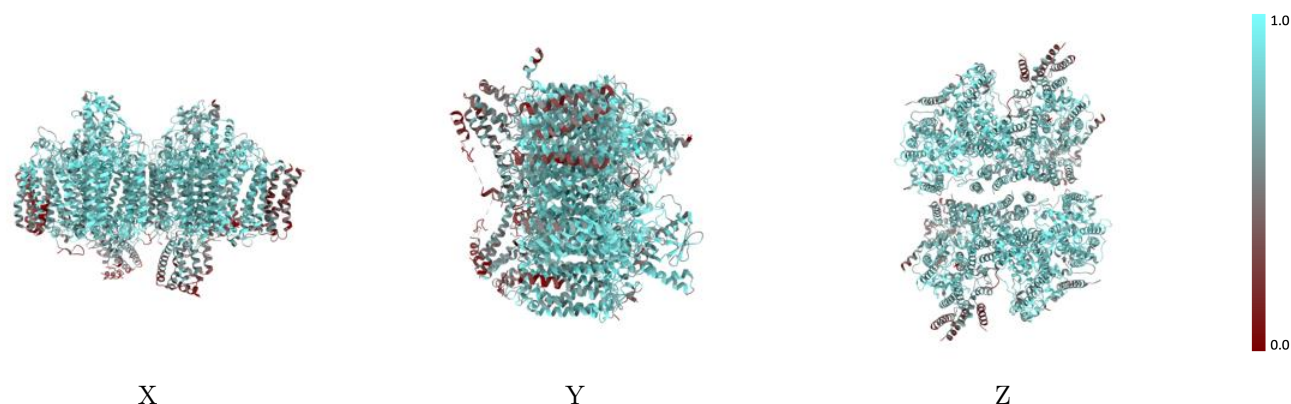
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



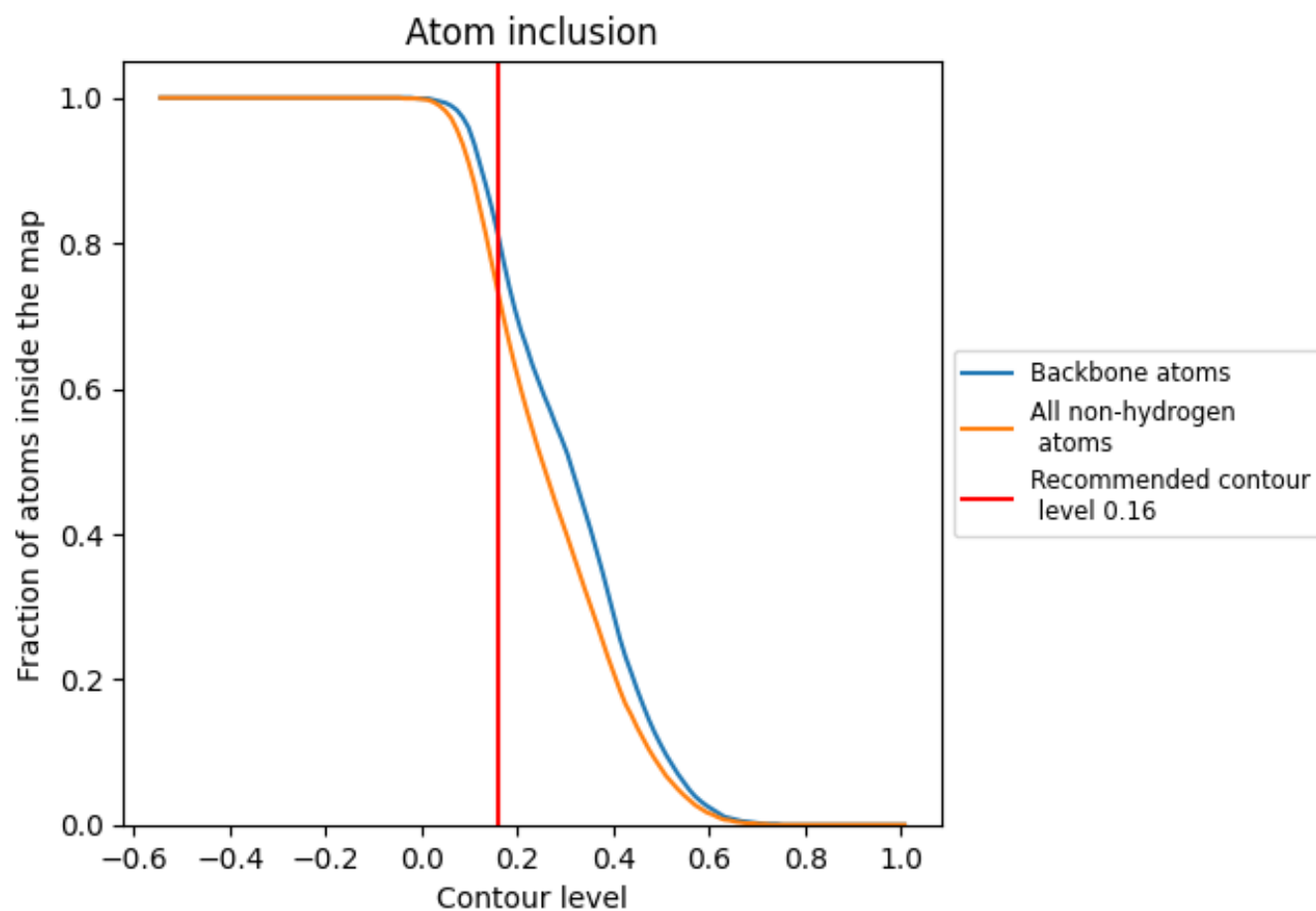
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 73% 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	 0.7320	 0.5340
A	 0.7970	 0.5650
B	 0.8200	 0.5560
C	 0.7180	 0.5270
D	 0.8410	 0.5710
E	 0.6720	 0.4780
F	 0.6710	 0.5120
G	 0.4790	 0.4310
H	 0.7150	 0.5290
I	 0.7430	 0.5360
K	 0.6310	 0.4870
L	 0.7500	 0.5430
M	 0.7600	 0.5420
T	 0.6330	 0.5230
V	 0.2830	 0.4370
W	 0.4710	 0.4890
X	 0.3760	 0.4700
Z	 0.3620	 0.4110
a	 0.8090	 0.5660
b	 0.8210	 0.5580
c	 0.7170	 0.5310
d	 0.8440	 0.5740
e	 0.6660	 0.4880
f	 0.6750	 0.5120
g	 0.4920	 0.4390
h	 0.7030	 0.5310
i	 0.7460	 0.5380
k	 0.6010	 0.4930
l	 0.7640	 0.5480
m	 0.7500	 0.5500
t	 0.6730	 0.5380
v	 0.2710	 0.4280
w	 0.4710	 0.4830
x	 0.3760	 0.4730
z	 0.3680	 0.4210

