



Full wwPDB EM Validation Report ⓘ

Dec 2, 2025 – 12:07 AM JST

PDB ID : 8ZOG / pdb_00008zog
EMDB ID : EMD-60292
Title : Structure of the astaxanthin mutant PSI-9VCPI supercomplex in Nan-
nochloropsis oceanica
Authors : Shen, L.L.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 3.16 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

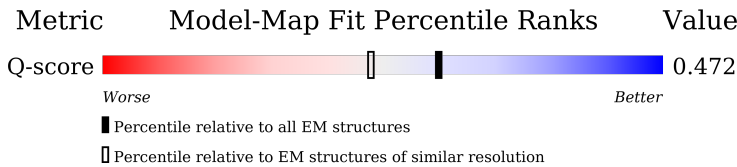
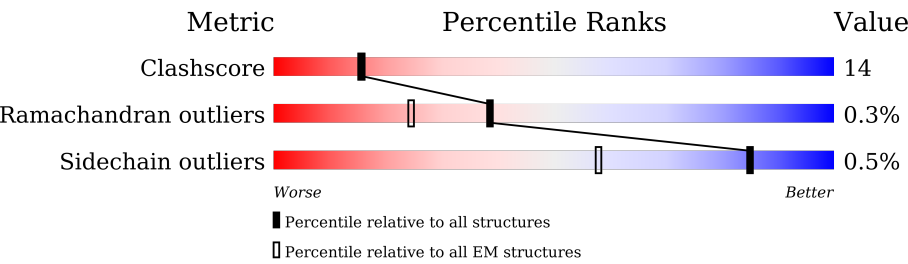
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14474 (2.66 - 3.66)

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

Mol	Chain	Length	Quality of chain
1	5	244	<div><div>11%</div><div>52%</div><div>17%</div><div>31%</div></div>
2	9	232	<div><div>21%</div><div>65%</div><div>21%</div><div>13%</div></div>
3	8	200	<div><div>12%</div><div>62%</div><div>18%</div><div>18%</div></div>
4	4	202	<div><div>11%</div><div>71%</div><div>12%</div><div>17%</div></div>

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Mol	Chain	Length	Quality of chain
4	7	202	
5	3	220	
6	6	259	
7	2	223	
8	1	208	
9	a	745	
10	b	737	
11	d	136	
12	e	67	
13	f	185	
14	h	128	
15	i	45	
16	j	41	
17	l	172	
18	m	30	
19	g	55	
20	c	81	

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
23	CLA	1	305	X	-	-	-
23	CLA	1	306	X	-	-	-
23	CLA	1	307	X	-	-	-
23	CLA	1	308	X	-	-	-
23	CLA	1	309	X	-	-	-
23	CLA	1	310	X	-	-	-
23	CLA	1	311	X	-	-	-
23	CLA	1	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	1	313	X	-	-	-
23	CLA	1	314	X	-	-	-
23	CLA	2	306	X	-	-	-
23	CLA	2	307	X	-	-	-
23	CLA	2	308	X	-	-	-
23	CLA	2	309	X	-	-	-
23	CLA	2	310	X	-	-	-
23	CLA	2	311	X	-	-	-
23	CLA	2	312	X	-	-	-
23	CLA	2	313	X	-	-	-
23	CLA	2	314	X	-	-	-
23	CLA	2	315	X	-	-	-
23	CLA	2	316	X	-	-	-
23	CLA	3	307	X	-	-	-
23	CLA	3	308	X	-	-	-
23	CLA	3	309	X	-	-	-
23	CLA	3	310	X	-	-	-
23	CLA	3	311	X	-	-	-
23	CLA	3	312	X	-	-	-
23	CLA	3	313	X	-	-	-
23	CLA	3	314	X	-	-	-
23	CLA	3	315	X	-	-	-
23	CLA	4	305	X	-	-	-
23	CLA	4	306	X	-	-	-
23	CLA	4	307	X	-	-	-
23	CLA	4	308	X	-	-	-
23	CLA	4	309	X	-	-	-
23	CLA	4	310	X	-	-	-
23	CLA	4	311	X	-	-	-
23	CLA	4	312	X	-	-	-
23	CLA	4	313	X	-	-	-
23	CLA	4	314	X	-	-	-
23	CLA	4	315	X	-	-	-
23	CLA	4	316	X	-	-	-
23	CLA	5	306	X	-	-	-
23	CLA	5	307	X	-	-	-
23	CLA	5	308	X	-	-	-
23	CLA	5	309	X	-	-	-
23	CLA	5	310	X	-	-	-
23	CLA	5	311	X	-	-	-
23	CLA	5	312	X	-	-	-
23	CLA	5	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	5	314	X	-	-	-
23	CLA	5	315	X	-	-	-
23	CLA	5	316	X	-	-	-
23	CLA	6	307	X	-	-	-
23	CLA	6	308	X	-	-	-
23	CLA	6	309	X	-	-	-
23	CLA	6	310	X	-	-	-
23	CLA	6	311	X	-	-	-
23	CLA	6	312	X	-	-	-
23	CLA	6	313	X	-	-	-
23	CLA	6	314	X	-	-	-
23	CLA	6	315	X	-	-	-
23	CLA	6	316	X	-	-	-
23	CLA	7	306	X	-	-	-
23	CLA	7	307	X	-	-	-
23	CLA	7	308	X	-	-	-
23	CLA	7	309	X	-	-	-
23	CLA	7	310	X	-	-	-
23	CLA	7	311	X	-	-	-
23	CLA	7	312	X	-	-	-
23	CLA	7	313	X	-	-	-
23	CLA	7	314	X	-	-	-
23	CLA	7	315	X	-	-	-
23	CLA	7	316	X	-	-	-
23	CLA	7	317	X	-	-	-
23	CLA	8	305	X	-	-	-
23	CLA	8	306	X	-	-	-
23	CLA	8	307	X	-	-	-
23	CLA	8	308	X	-	-	-
23	CLA	8	309	X	-	-	-
23	CLA	8	310	X	-	-	-
23	CLA	8	311	X	-	-	-
23	CLA	8	312	X	-	-	-
23	CLA	8	313	X	-	-	-
23	CLA	8	314	X	-	-	-
23	CLA	9	308	X	-	-	-
23	CLA	9	309	X	-	-	-
23	CLA	9	310	X	-	-	-
23	CLA	9	311	X	-	-	-
23	CLA	9	312	X	-	-	-
23	CLA	9	313	X	-	-	-
23	CLA	9	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	9	315	X	-	-	-
23	CLA	9	316	X	-	-	-
23	CLA	a	801	X	-	-	-
23	CLA	a	802	X	-	-	-
23	CLA	a	803	X	-	-	-
23	CLA	a	804	X	-	-	-
23	CLA	a	805	X	-	-	-
23	CLA	a	806	X	-	-	-
23	CLA	a	807	X	-	-	-
23	CLA	a	808	X	-	-	-
23	CLA	a	809	X	-	-	-
23	CLA	a	810	X	-	-	-
23	CLA	a	811	X	-	-	-
23	CLA	a	812	X	-	-	-
23	CLA	a	813	X	-	-	-
23	CLA	a	814	X	-	-	-
23	CLA	a	815	X	-	-	-
23	CLA	a	816	X	-	-	-
23	CLA	a	817	X	-	-	-
23	CLA	a	818	X	-	-	-
23	CLA	a	819	X	-	-	-
23	CLA	a	820	X	-	-	-
23	CLA	a	821	X	-	-	-
23	CLA	a	822	X	-	-	-
23	CLA	a	823	X	-	-	-
23	CLA	a	824	X	-	-	-
23	CLA	a	825	X	-	-	-
23	CLA	a	826	X	-	-	-
23	CLA	a	827	X	-	-	-
23	CLA	a	828	X	-	-	-
23	CLA	a	829	X	-	-	-
23	CLA	a	830	X	-	-	-
23	CLA	a	831	X	-	-	-
23	CLA	a	832	X	-	-	-
23	CLA	a	833	X	-	-	-
23	CLA	a	834	X	-	-	-
23	CLA	a	835	X	-	-	-
23	CLA	a	836	X	-	-	-
23	CLA	a	837	X	-	-	-
23	CLA	a	838	X	-	-	-
23	CLA	a	839	X	-	-	-
23	CLA	a	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	a	841	X	-	-	-
23	CLA	a	842	X	-	-	-
23	CLA	a	844	X	-	-	-
23	CLA	a	852	X	-	-	-
23	CLA	a	856	X	-	X	-
23	CLA	b	801	X	-	-	-
23	CLA	b	802	X	-	-	-
23	CLA	b	803	X	-	-	-
23	CLA	b	804	X	-	-	-
23	CLA	b	805	X	-	-	-
23	CLA	b	806	X	-	-	-
23	CLA	b	807	X	-	-	-
23	CLA	b	808	X	-	-	-
23	CLA	b	809	X	-	-	-
23	CLA	b	810	X	-	X	-
23	CLA	b	811	X	-	-	-
23	CLA	b	812	X	-	-	-
23	CLA	b	813	X	-	-	-
23	CLA	b	814	X	-	-	-
23	CLA	b	815	X	-	-	-
23	CLA	b	816	X	-	-	-
23	CLA	b	817	X	-	-	-
23	CLA	b	818	X	-	-	-
23	CLA	b	819	X	-	-	-
23	CLA	b	820	X	-	-	-
23	CLA	b	821	X	-	-	-
23	CLA	b	822	X	-	-	-
23	CLA	b	823	X	-	-	-
23	CLA	b	824	X	-	-	-
23	CLA	b	825	X	-	-	-
23	CLA	b	826	X	-	-	-
23	CLA	b	827	X	-	-	-
23	CLA	b	828	X	-	-	-
23	CLA	b	829	X	-	-	-
23	CLA	b	830	X	-	-	-
23	CLA	b	831	X	-	-	-
23	CLA	b	832	X	-	-	-
23	CLA	b	833	X	-	-	-
23	CLA	b	834	X	-	-	-
23	CLA	b	835	X	-	-	-
23	CLA	b	836	X	-	-	-
23	CLA	b	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	b	838	X	-	-	-
23	CLA	b	839	X	-	-	-
23	CLA	b	840	X	-	-	-
23	CLA	b	841	X	-	-	-
23	CLA	f	802	X	-	-	-
23	CLA	f	803	X	-	-	-
23	CLA	h	201	X	-	-	-
23	CLA	h	203	X	-	-	-
23	CLA	j	101	X	-	-	-
23	CLA	l	201	X	-	-	-
23	CLA	l	202	X	-	-	-
23	CLA	l	203	X	-	-	-
30	BCR	f	801	-	-	X	-
31	SF4	c	102	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 43749 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 VCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	169	Total	C	N	O	S	0	0
			1317	867	222	222	6		

- Molecule 2 is a protein called VCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	201	Total	C	N	O	S	0	0
			1466	936	256	269	5		

- Molecule 3 is a protein called VCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	164	Total	C	N	O	S	0	0
			1258	822	203	227	6		

- Molecule 4 is a protein called VCPI-4/7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	168	Total	C	N	O	S	0	0
			1268	822	211	229	6		
4	7	166	Total	C	N	O	S	0	0
			1220	791	202	222	5		

- Molecule 5 is a protein called VCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	177	Total	C	N	O	S	0	0
			1324	846	225	245	8		

- Molecule 6 is a protein called VCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	180	Total	C	N	O	S	0	0
			1352	880	223	244	5		

- Molecule 7 is a protein called VCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	185	Total	C	N	O	S	0	0
			1372	892	224	249	7		

- Molecule 8 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	739	Total	C	N	O	S	0	0
			5827	3828	982	1000	17		

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	735	Total	C	N	O	S	0	0
			5865	3874	985	989	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	130	Total	C	N	O	S	0	0
			1014	652	175	184	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	61	Total	C	N	O	0	0
			494	314	86	94		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	f	160	Total	C	N	O	S	0	0
			1266	815	213	235	3		

- Molecule 14 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	85	Total	C	N	O	S	0	0
			646	427	100	117	2		

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	i	34	Total	C	N	O	S	0	0
			271	189	36	45	1		

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	41	Total	C	N	O	S	0	0
			339	233	48	57	1		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	l	171	Total	C	N	O		0	0
			1283	848	203	232			

- Molecule 18 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	m	30	Total	C	N	O		0	0
			210	137	35	38			

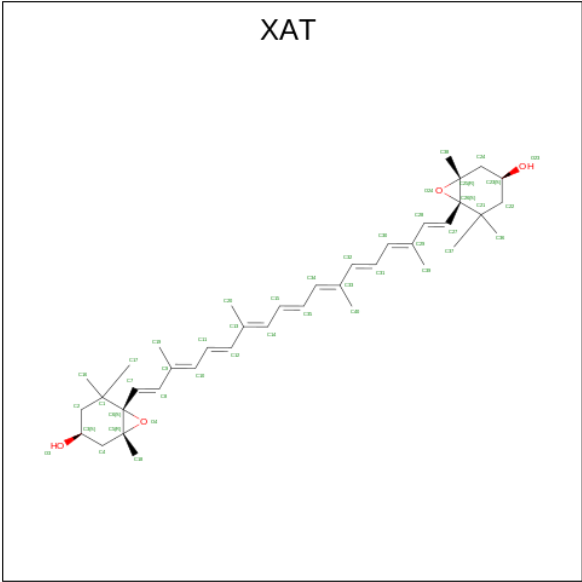
- Molecule 19 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	50	Total	C	N	O		0	0
			250	150	50	50			

- Molecule 20 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	80	Total	C	N	O	S	0	0
			596	366	103	117	10		

- Molecule 21 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	5	1	Total	C	O	0
			44	40	4	
21	5	1	Total	C	O	0
			44	40	4	
21	5	1	Total	C	O	0
			44	40	4	
21	5	1	Total	C	O	0
			44	40	4	
21	9	1	Total	C	O	0
			44	40	4	
21	9	1	Total	C	O	0
			44	40	4	
21	9	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	
21	8	1	Total	C	O	0
			44	40	4	

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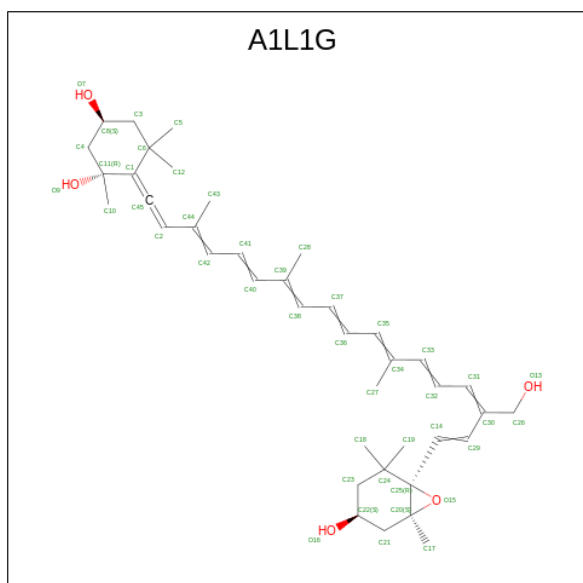
Mol	Chain	Residues	Atoms			AltConf
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	2	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	
21	7	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	1	1	Total	C	O	0
			44	40	4	
21	a	1	Total	C	O	0
			44	40	4	
21	a	1	Total	C	O	0
			44	40	4	

- Molecule 22 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxa bicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



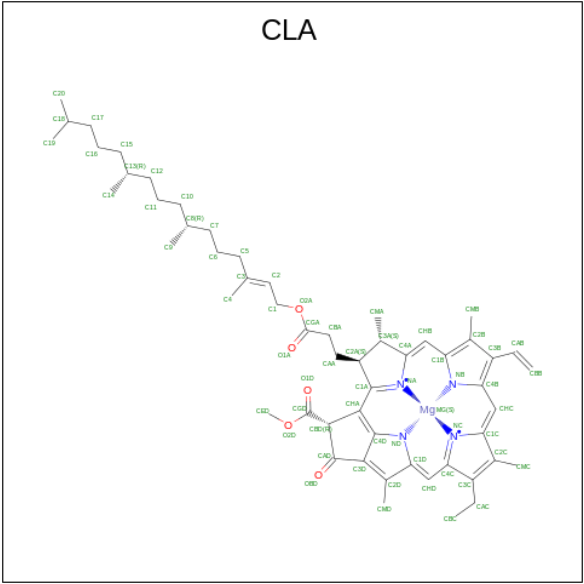
Mol	Chain	Residues	Atoms			AltConf
22	5	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	

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Mol	Chain	Residues	Atoms			AltConf
22	7	1	Total	C	O	0
			45	40	5	
22	1	1	Total	C	O	0
			45	40	5	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	9	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
23	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	4	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
23	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	b	1	Total 59	C 49	Mg 1	N 4	O 5	0

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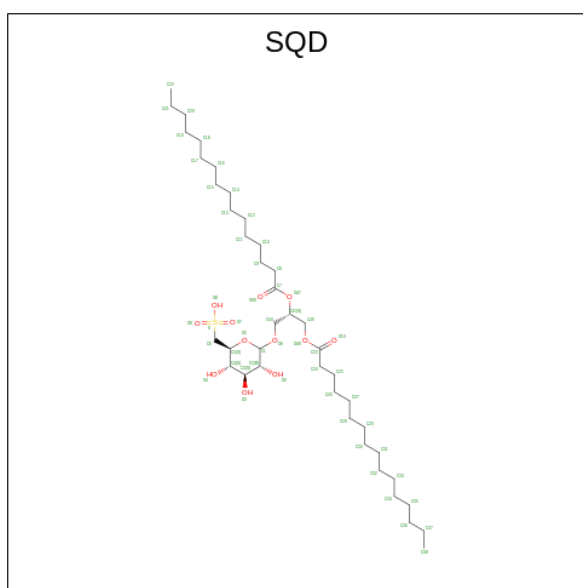
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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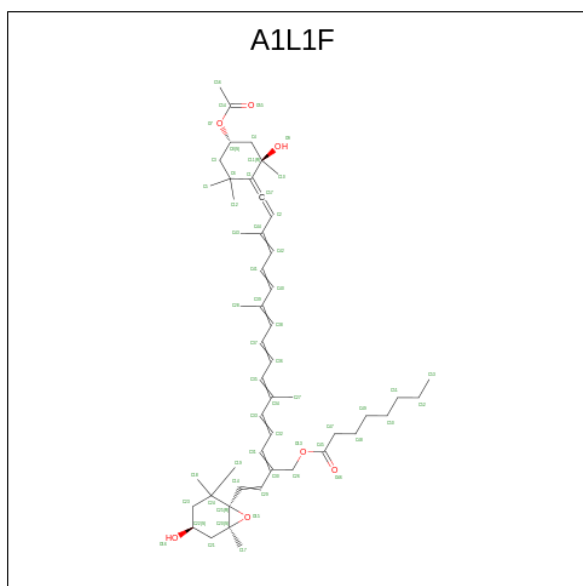
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- 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).



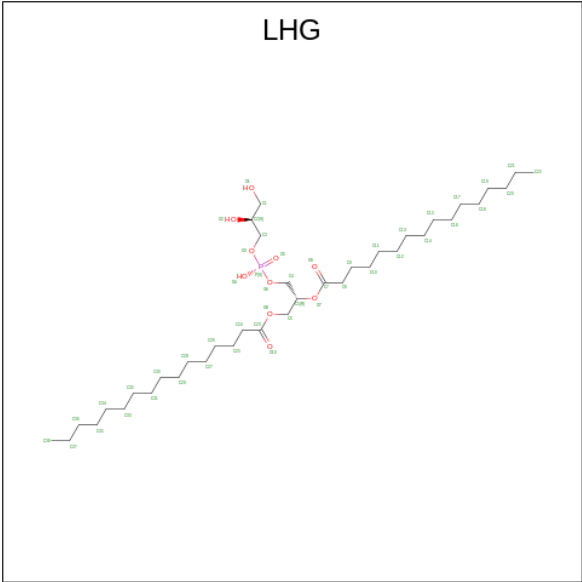
Mol	Chain	Residues	Atoms				AltConf
24	5	1	Total	C	O	S	0
			35	22	12	1	
24	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 25 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: C₅₀H₇₂O₇) (labeled as "Ligand of Interest" by depositor).



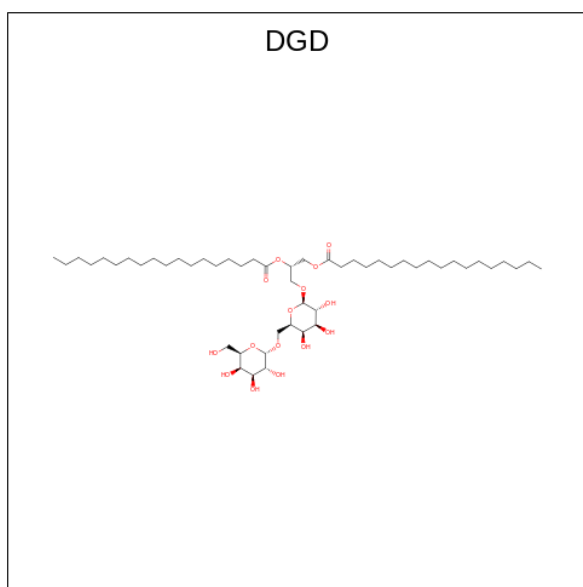
Mol	Chain	Residues	Atoms				AltConf
25	9	1	Total	C	O		0
			57	50	7		
25	8	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			53	46	7		
25	1	1	Total	C	O		0
			57	50	7		
25	h	1	Total	C	O		0
			57	50	7		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



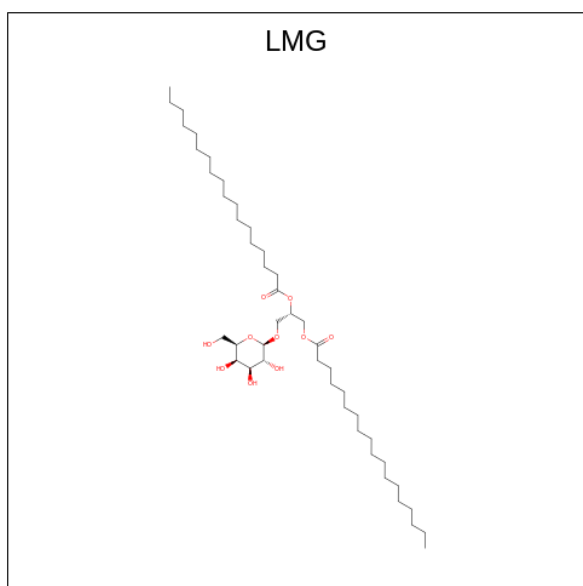
Mol	Chain	Residues	Atoms				AltConf
26	9	1	Total	C	O	P	0
			36	25	10	1	
26	a	1	Total	C	O	P	0
			48	37	10	1	
26	a	1	Total	C	O	P	0
			27	16	10	1	
26	b	1	Total	C	O	P	0
			31	20	10	1	
26	m	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



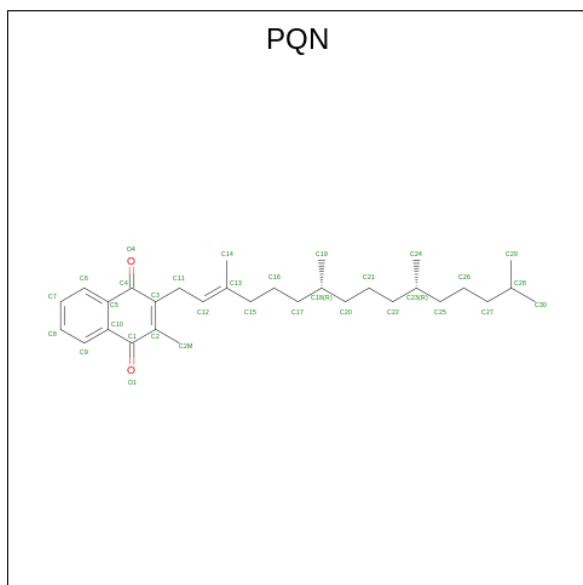
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	8	1	40	25	15	0
27	4	1	40	25	15	0
27	b	1	57	42	15	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



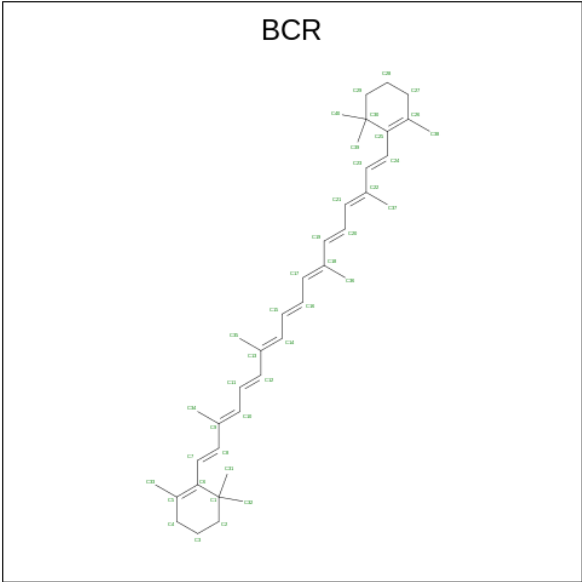
Mol	Chain	Residues	Atoms			AltConf
28	2	1	Total	C	O	0
			35	25	10	
28	a	1	Total	C	O	0
			34	24	10	
28	j	1	Total	C	O	0
			32	22	10	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	a	1	Total	C	O	0
			33	31	2	
29	b	1	Total	C	O	0
			33	31	2	

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



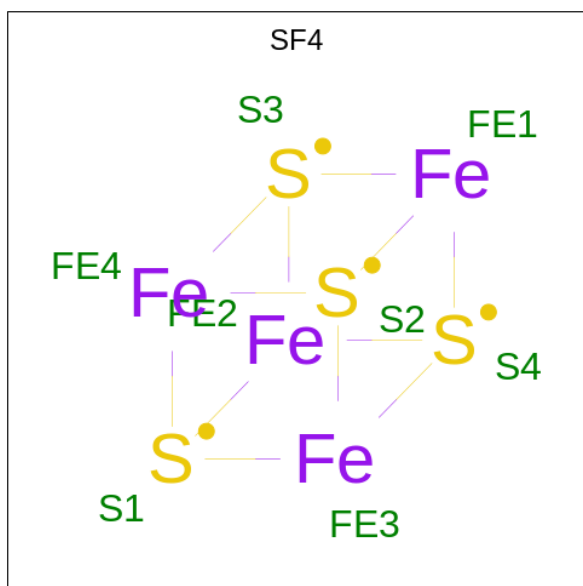
Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	f	1	Total C 40 40	0

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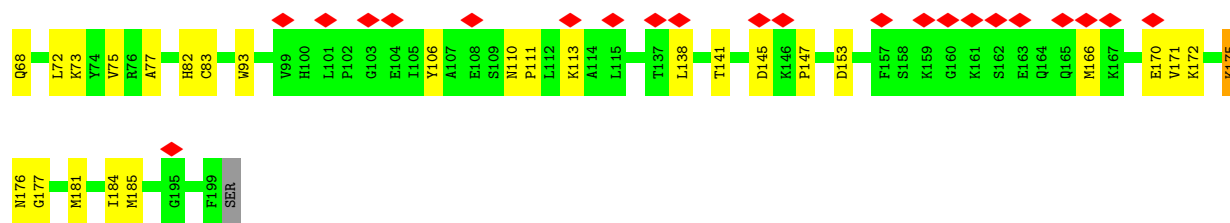
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
30	f	1	Total C 40 40	0
30	i	1	Total C 40 40	0
30	i	1	Total C 40 40	0
30	j	1	Total C 40 40	0
30	m	1	Total C 40 40	0

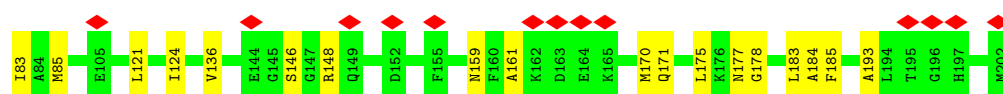
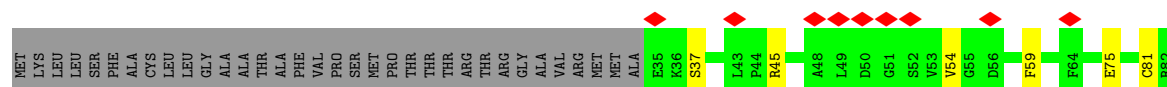
- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



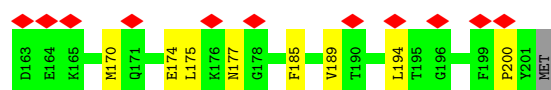
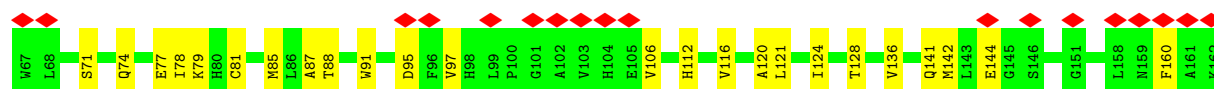
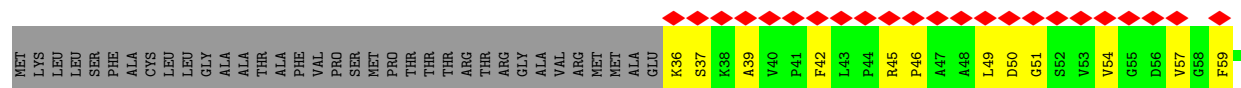
Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total Fe S 8 4 4	0
31	c	1	Total Fe S 8 4 4	0
31	c	1	Total Fe S 8 4 4	0



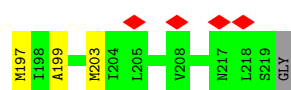
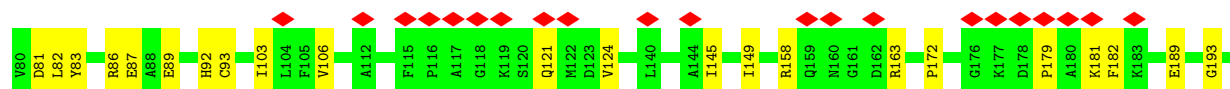
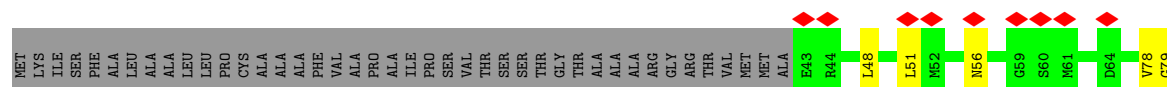
• Molecule 4: VCPI-4/7



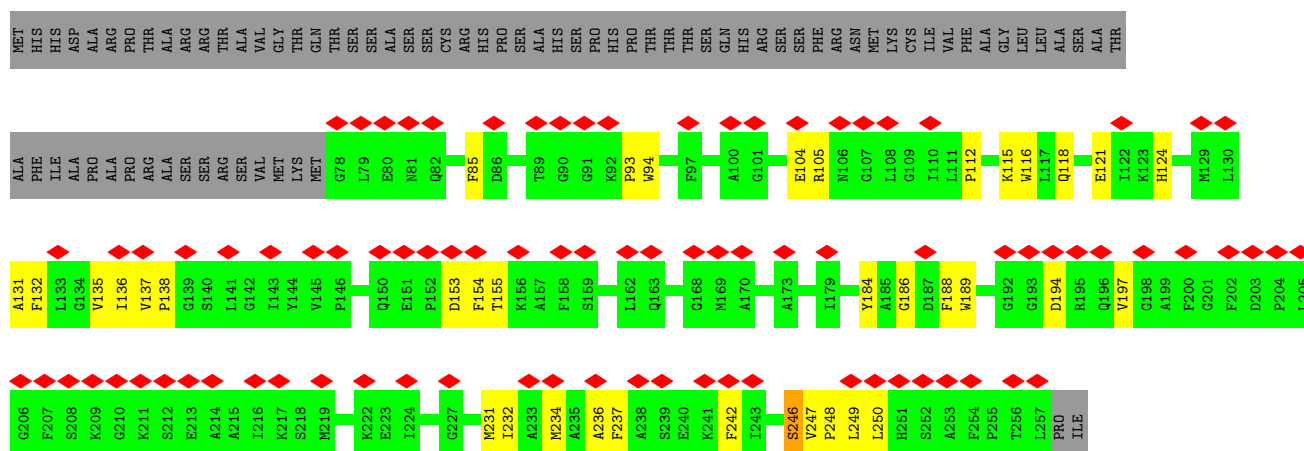
• Molecule 4: VCPI-4/7



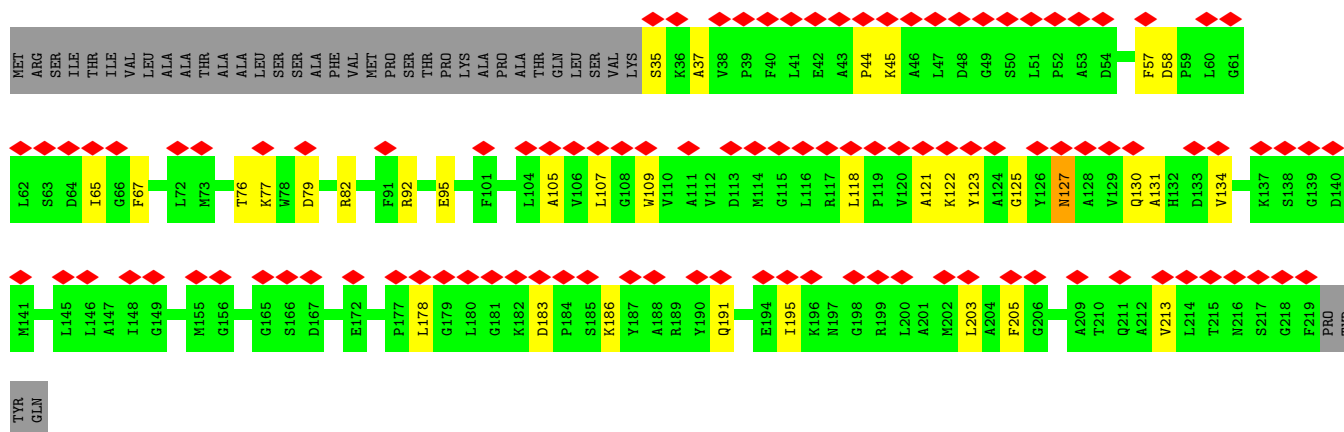
• Molecule 5: VCPI-3



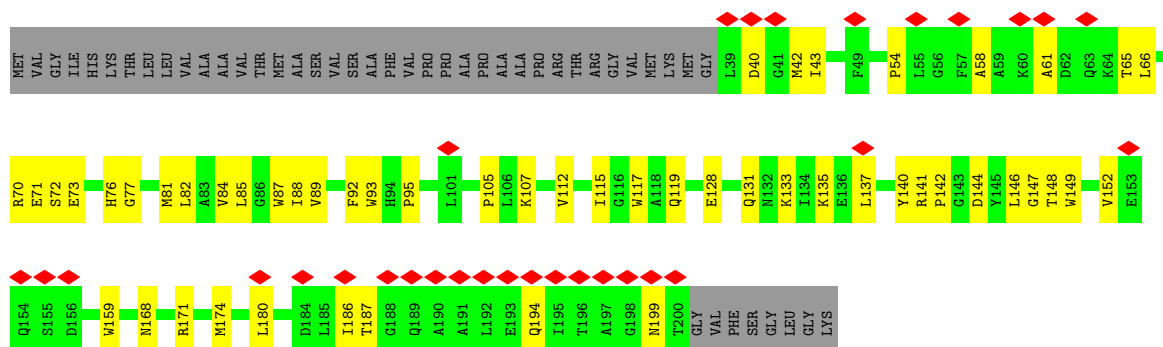
• Molecule 6: VCPI-6



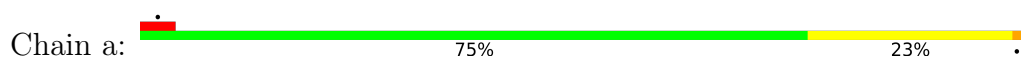
• Molecule 7: VCPI-2

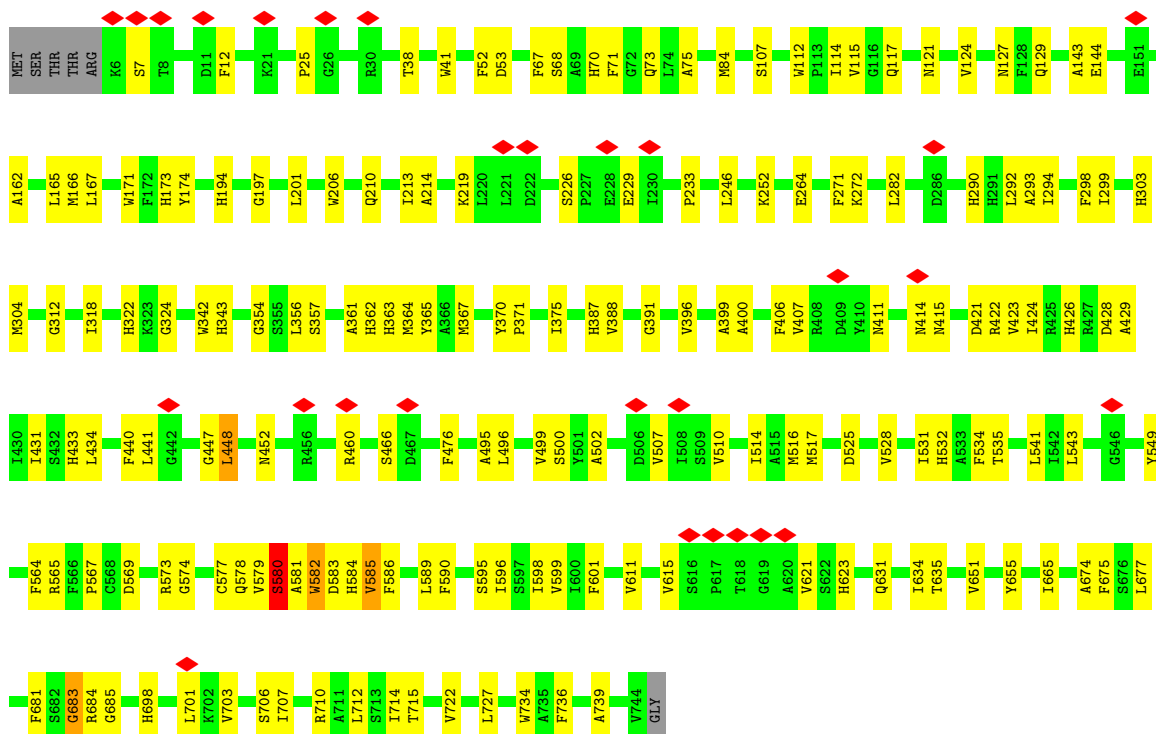


• Molecule 8: VCPI-1



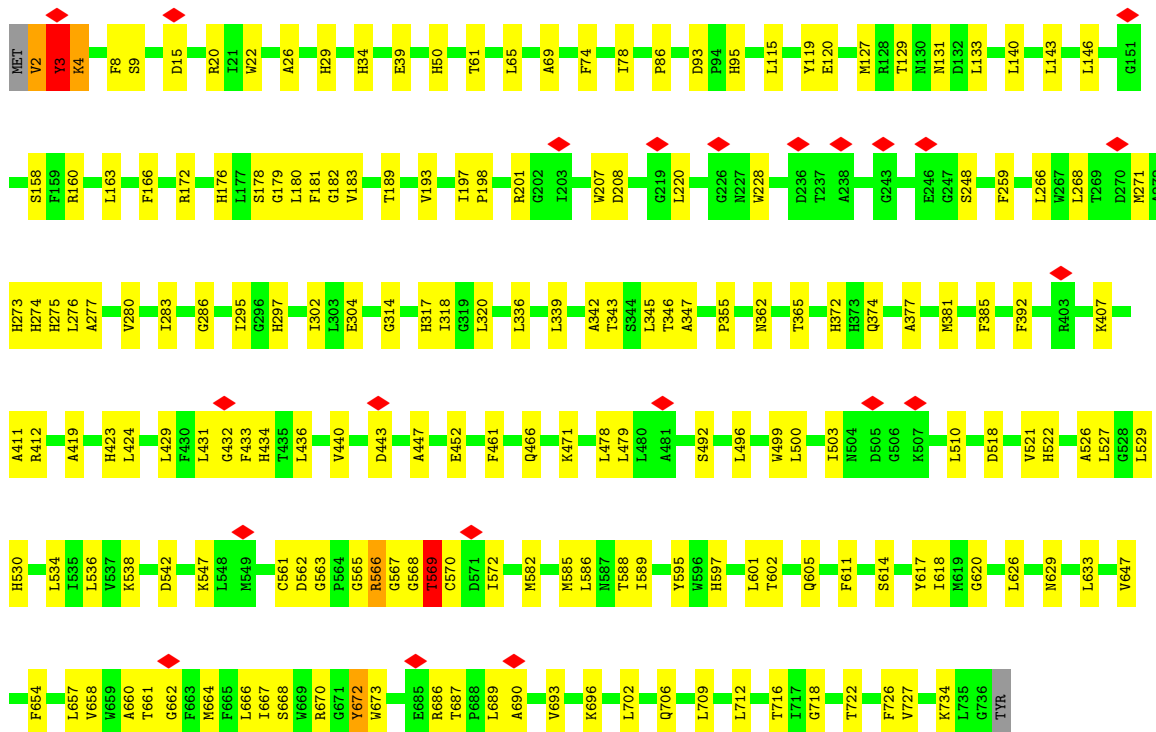
• Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1



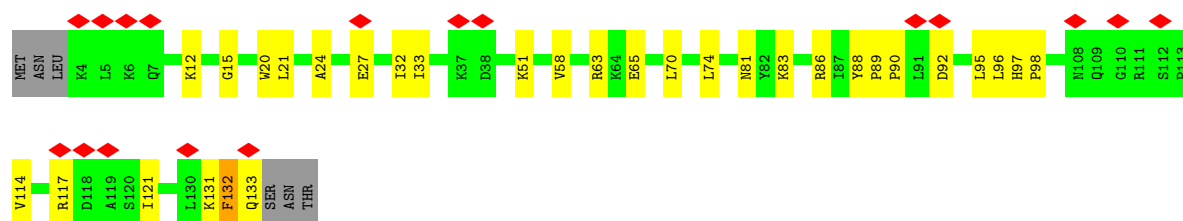
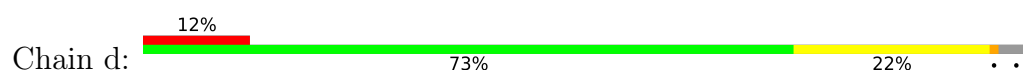


• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A2

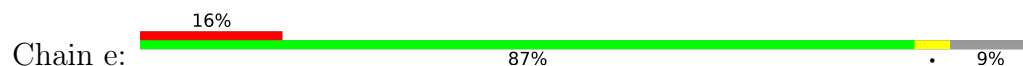
Chain b: 74% 24%



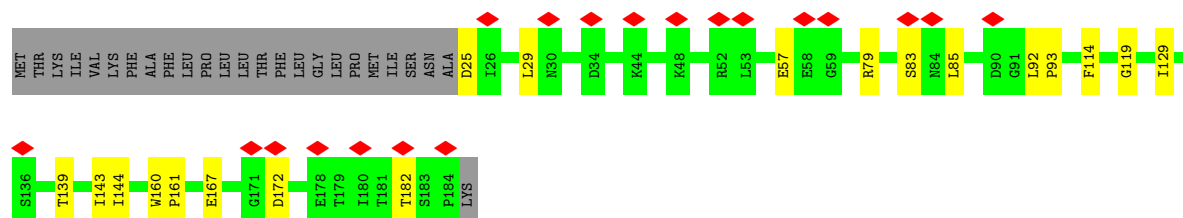
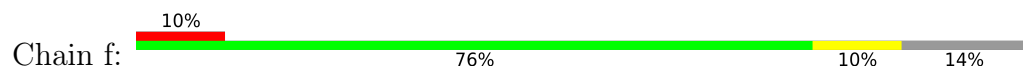
• Molecule 11: Photosystem I reaction center subunit II



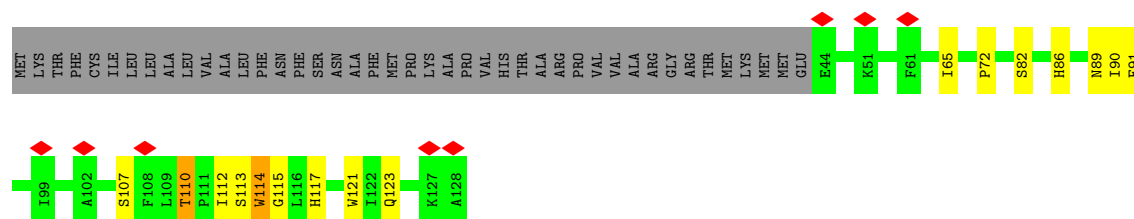
• Molecule 12: Photosystem I reaction center subunit IV



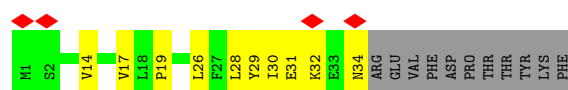
• Molecule 13: Photosystem I reaction center subunit III



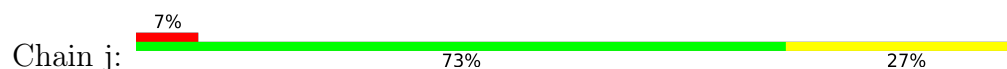
• Molecule 14: PsarR

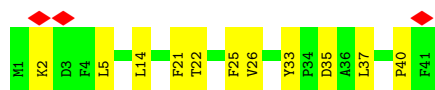


• Molecule 15: Photosystem I reaction center subunit VIII

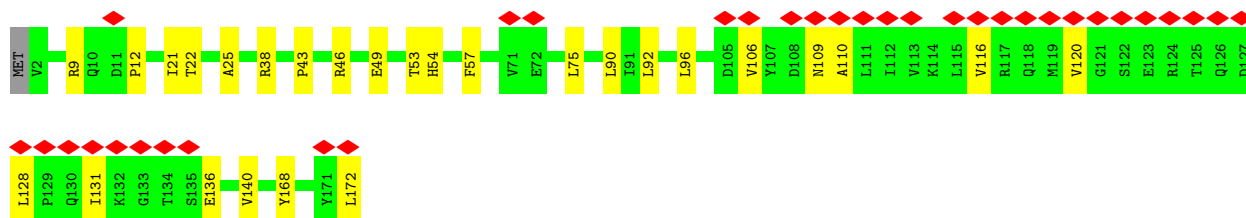
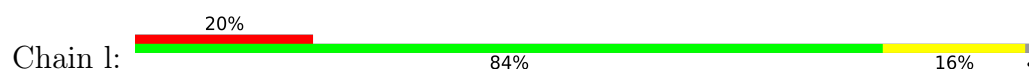


• Molecule 16: Photosystem I reaction center subunit IX





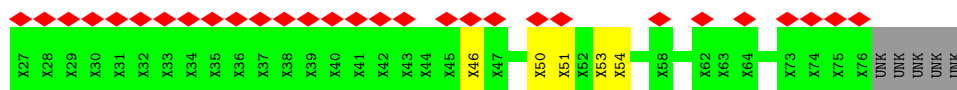
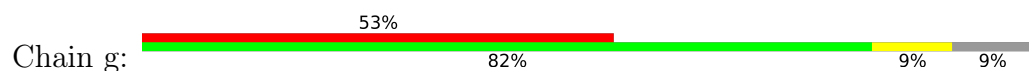
• Molecule 17: PSI subunit V



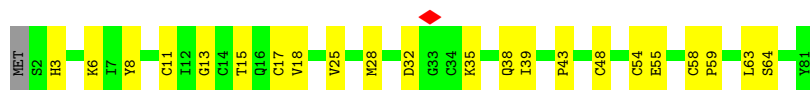
• Molecule 18: PsaM



• Molecule 19: PsaS



• Molecule 20: Photosystem I iron-sulfur center



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31137	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.682	Depositor
Minimum map value	-0.465	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.293	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: A1L1G, BCR, SQD, A1L1F, DGD, PQN, CLA, LMG, SF4, XAT, 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	5	0.14	0/1353	0.29	0/1823
2	9	0.35	0/1496	0.34	0/2032
3	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
4	4	0.17	0/1298	0.32	0/1761
4	7	0.19	0/1248	0.37	0/1700
5	3	0.12	0/1350	0.28	0/1821
6	6	0.17	0/1390	0.32	0/1883
7	2	0.14	0/1405	0.36	0/1904
8	1	0.14	0/1293	0.33	0/1759
9	a	0.30	3/6024 (0.0%)	0.35	5/8219 (0.1%)
10	b	0.26	0/6080	0.35	2/8302 (0.0%)
11	d	0.18	0/1040	0.36	0/1402
12	e	0.09	0/502	0.20	0/681
13	f	0.14	0/1297	0.31	0/1762
14	h	0.51	1/667 (0.1%)	0.52	0/915
15	i	0.15	0/278	0.33	0/378
16	j	0.16	0/351	0.35	0/478
17	l	0.14	0/1315	0.31	0/1796
18	m	0.09	0/210	0.28	0/288
20	c	0.13	0/606	0.34	0/822
All	All	0.25	5/30489 (0.0%)	0.35	10/41469 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	580	SER	CA-C	-7.00	1.43	1.52
3	8	44	LEU	C-O	-6.14	1.15	1.23
9	a	581	ALA	CA-C	-5.39	1.45	1.52
14	h	114	TRP	C-O	-5.33	1.18	1.24
9	a	582	TRP	CA-C	-5.06	1.45	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	581	ALA	N-CA-C	-8.65	102.47	113.72
9	a	683	GLY	O-C-N	-8.45	116.29	123.73
10	b	568	GLY	N-CA-C	-7.50	100.71	110.69
3	8	39	LYS	N-CA-C	-6.12	105.65	113.23
9	a	448	LEU	N-CA-C	-6.06	104.24	111.69
9	a	584	HIS	N-CA-C	-5.88	106.44	113.97
10	b	672	TYR	N-CA-C	-5.62	106.26	113.23
3	8	41	LEU	CA-C-N	5.07	124.78	119.82
3	8	41	LEU	C-N-CA	5.07	124.78	119.82
9	a	585	VAL	N-CA-C	-5.04	105.50	112.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1317	0	1318	36	0
2	9	1466	0	1470	56	0
3	8	1258	0	1280	32	0
4	4	1268	0	1288	24	0
4	7	1220	0	1209	40	0
5	3	1324	0	1340	20	0
6	6	1352	0	1334	30	0
7	2	1372	0	1347	23	0
8	1	1262	0	1237	37	0
9	a	5827	0	5697	156	0
10	b	5865	0	5711	202	0
11	d	1014	0	1015	29	0
12	e	494	0	495	3	0
13	f	1266	0	1262	29	0
14	h	646	0	649	11	0
15	i	271	0	292	19	0
16	j	339	0	342	15	0
17	l	1283	0	1278	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	m	210	0	226	2	0
19	g	250	0	57	4	0
20	c	596	0	583	23	0
21	1	88	0	112	7	0
21	2	220	0	280	24	0
21	3	176	0	224	14	0
21	4	176	0	224	24	0
21	5	176	0	224	24	0
21	6	176	0	224	18	0
21	7	176	0	224	28	0
21	8	132	0	168	15	0
21	9	132	0	168	16	0
21	a	88	0	112	7	0
22	1	45	0	0	1	0
22	3	90	0	0	0	0
22	5	45	0	0	1	0
22	7	45	0	0	2	0
22	9	90	0	0	3	0
23	1	547	0	508	15	0
23	2	544	0	452	10	0
23	3	458	0	378	8	0
23	4	613	0	522	30	0
23	5	563	0	472	26	0
23	6	499	0	413	12	0
23	7	576	0	444	24	0
23	8	507	0	429	22	0
23	9	454	0	380	35	0
23	a	2644	0	2634	215	0
23	b	2468	0	2519	173	0
23	f	117	0	115	2	0
23	h	120	0	121	7	0
23	j	42	0	31	2	0
23	l	148	0	123	10	0
24	1	45	0	54	3	0
24	5	35	0	34	1	0
25	1	57	0	0	11	0
25	6	110	0	0	5	0
25	8	57	0	0	2	0
25	9	57	0	0	1	0
25	h	57	0	0	4	0
26	9	36	0	45	1	0
26	a	75	0	93	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	b	31	0	32	2	0
26	m	46	0	65	2	0
27	4	40	0	38	11	0
27	8	40	0	38	2	0
27	b	57	0	72	6	0
28	2	35	0	40	3	0
28	a	34	0	38	10	0
28	j	32	0	34	6	0
29	a	33	0	46	4	0
29	b	33	0	46	6	0
30	a	160	0	224	13	0
30	b	360	0	504	57	0
30	f	80	0	112	31	0
30	i	80	0	112	17	0
30	j	40	0	56	14	0
30	m	40	0	56	0	0
31	a	8	0	0	0	0
31	c	16	0	0	3	0
All	All	43749	0	42670	1242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1242) 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:a:698:HIS:NE2	23:a:856:CLA:HAC1	1.52	1.25
23:a:834:CLA:H151	29:b:842:PQN:H202	1.21	1.21
23:a:803:CLA:H151	23:b:810:CLA:HBC3	1.24	1.15
25:1:304:A1L1F:C2	23:a:844:CLA:H42	1.80	1.11
23:a:802:CLA:HED3	30:f:801:BCR:C40	1.80	1.10
23:a:833:CLA:H61	23:l:202:CLA:H101	1.28	1.09
4:4:193:ALA:HB1	27:4:317:DGD:HE62	1.13	1.08
23:b:801:CLA:H142	23:b:839:CLA:H111	1.29	1.07
23:a:834:CLA:C14	30:b:848:BCR:H17C	1.85	1.06
4:4:193:ALA:HB1	27:4:317:DGD:C6E	1.85	1.06
23:a:802:CLA:HED3	30:f:801:BCR:H401	1.31	1.06
10:b:452:GLU:HA	13:f:92:LEU:HD22	1.32	1.06
23:a:834:CLA:H142	30:b:848:BCR:C17	1.86	1.05
10:b:686:ARG:NH2	11:d:21:LEU:HD23	1.72	1.03
2:9:37:VAL:HG21	10:b:158:SER:O	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:681:PHE:HE1	10:b:667:ILE:HG13	1.20	1.02
25:1:304:A1L1F:C2	23:a:844:CLA:H11	1.91	1.00
9:a:681:PHE:CE1	10:b:667:ILE:HG13	1.95	1.00
9:a:681:PHE:HE1	10:b:667:ILE:CG1	1.76	0.97
23:b:810:CLA:HED2	30:b:853:BCR:H393	1.44	0.96
23:b:801:CLA:C14	23:b:839:CLA:H111	1.94	0.96
9:a:706:SER:HB3	13:f:139:THR:HG22	1.47	0.94
23:b:810:CLA:H202	17:l:90:LEU:HD22	1.47	0.94
23:b:801:CLA:H143	23:b:839:CLA:H142	1.49	0.94
23:a:834:CLA:H142	30:b:848:BCR:H17C	0.95	0.93
23:a:810:CLA:H102	30:j:102:BCR:H332	1.51	0.93
10:b:687:THR:HG21	23:b:801:CLA:CMA	2.00	0.91
23:9:316:CLA:HAB	23:b:810:CLA:H112	1.53	0.91
21:5:303:XAT:H12	23:5:308:CLA:HAB	1.53	0.90
27:4:317:DGD:O5E	27:4:317:DGD:O4E	1.61	0.90
23:a:810:CLA:H11	30:j:102:BCR:C12	2.02	0.88
23:a:841:CLA:H203	23:a:856:CLA:H2	1.55	0.88
21:2:303:XAT:H32	23:2:308:CLA:HAB	1.52	0.88
2:9:41:GLU:CG	10:b:160:ARG:HH21	1.87	0.88
10:b:689:LEU:O	23:l:202:CLA:HBC2	1.72	0.88
10:b:3:TYR:HD1	15:i:34:ASN:HD22	1.20	0.88
23:a:833:CLA:H61	23:l:202:CLA:C10	2.05	0.86
9:a:698:HIS:CG	23:a:856:CLA:HBC1	2.11	0.85
23:b:810:CLA:HED2	30:b:853:BCR:C39	2.05	0.85
9:a:698:HIS:CE1	23:a:856:CLA:HAC1	2.12	0.85
25:1:304:A1L1F:C10	23:a:844:CLA:C3	2.54	0.85
10:b:3:TYR:CD1	15:i:34:ASN:HB2	2.12	0.84
23:a:833:CLA:C2	23:l:202:CLA:H93	2.06	0.84
23:b:840:CLA:H18	30:i:101:BCR:C21	2.07	0.84
23:a:803:CLA:H151	23:b:810:CLA:CBC	2.08	0.83
25:1:304:A1L1F:C2	23:a:844:CLA:C4	2.56	0.82
9:a:698:HIS:CD2	23:a:856:CLA:CBC	2.62	0.82
10:b:547:LYS:HD3	13:f:182:THR:HA	1.60	0.82
23:a:810:CLA:H11	30:j:102:BCR:H12C	1.60	0.81
23:b:839:CLA:H152	30:b:853:BCR:H17C	1.62	0.81
25:1:304:A1L1F:C57	23:a:844:CLA:H11	2.10	0.81
9:a:655:TYR:CE2	10:b:447:ALA:HB2	2.16	0.81
13:f:114:PHE:CD1	30:f:801:BCR:H343	2.17	0.80
23:a:834:CLA:C15	29:b:842:PQN:H202	2.08	0.80
4:4:193:ALA:CB	27:4:317:DGD:HE62	2.07	0.80
23:a:806:CLA:O1A	23:a:814:CLA:HBA1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:703:VAL:O	23:a:856:CLA:HMD2	1.82	0.80
10:b:689:LEU:O	23:l:202:CLA:CBC	2.30	0.79
29:b:842:PQN:H272	30:i:102:BCR:H343	1.65	0.79
2:9:120:TRP:CH2	23:9:316:CLA:H43	2.18	0.79
9:a:531:ILE:HD12	23:a:801:CLA:H172	1.63	0.79
23:a:802:CLA:CED	30:f:801:BCR:H401	2.10	0.78
10:b:3:TYR:HD1	15:i:34:ASN:ND2	1.80	0.78
9:a:698:HIS:NE2	23:a:856:CLA:CAC	2.41	0.78
9:a:681:PHE:CE1	10:b:667:ILE:CG1	2.62	0.78
23:b:825:CLA:HMA1	30:b:847:BCR:H17C	1.66	0.78
21:8:303:XAT:H12	23:8:312:CLA:HAB	1.67	0.77
23:a:810:CLA:H42	30:j:102:BCR:H10C	1.67	0.77
25:1:304:A1L1F:C10	23:a:844:CLA:C2	2.63	0.76
23:a:810:CLA:H42	30:j:102:BCR:C10	2.15	0.76
10:b:696:LYS:HD3	15:i:31:GLU:OE1	1.85	0.76
2:9:41:GLU:HG2	10:b:160:ARG:HH21	1.50	0.76
9:a:703:VAL:HG22	23:a:856:CLA:CMD	2.16	0.75
9:a:698:HIS:CG	23:a:856:CLA:CBC	2.70	0.75
23:a:810:CLA:C10	30:j:102:BCR:H332	2.16	0.75
1:5:164:PHE:HE1	23:f:802:CLA:H121	1.52	0.74
21:4:302:XAT:H12	23:4:307:CLA:HAB	1.67	0.74
9:a:698:HIS:CD2	23:a:856:CLA:HAC1	2.23	0.74
23:1:312:CLA:HHC	23:1:312:CLA:HBB1	1.69	0.74
21:2:303:XAT:H181	23:2:314:CLA:HBB1	1.70	0.73
15:i:26:LEU:HB3	30:i:102:BCR:H323	1.71	0.73
23:a:802:CLA:H12	10:b:433:PHE:CD1	2.23	0.73
23:b:839:CLA:H12	30:i:102:BCR:H351	1.69	0.73
23:a:841:CLA:H18	23:a:856:CLA:H52	1.70	0.73
10:b:547:LYS:HG2	13:f:182:THR:HG22	1.70	0.72
23:a:808:CLA:HMB2	30:j:102:BCR:HC8	1.71	0.72
23:b:832:CLA:H142	30:f:804:BCR:HC8	1.70	0.72
2:9:41:GLU:HG2	10:b:160:ARG:NH2	2.05	0.71
23:4:316:CLA:H2A	27:4:317:DGD:HE62	1.73	0.70
30:a:847:BCR:H362	30:a:848:BCR:H21C	1.73	0.70
9:a:706:SER:HB3	13:f:139:THR:CG2	2.20	0.70
23:b:806:CLA:H151	23:b:828:CLA:HBB2	1.74	0.70
9:a:574:GLY:C	10:b:670:ARG:NH1	2.49	0.70
23:a:802:CLA:H12	10:b:433:PHE:CE1	2.26	0.70
8:1:43:ILE:O	8:1:70:ARG:NH2	2.25	0.69
23:a:833:CLA:H11	17:l:21:ILE:HG22	1.72	0.69
23:a:802:CLA:HED3	30:f:801:BCR:H402	1.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:802:CLA:H41	10:b:436:LEU:HD22	1.75	0.69
10:b:686:ARG:HH21	11:d:21:LEU:HD23	1.55	0.69
9:a:363:HIS:ND1	23:a:819:CLA:OBD	2.26	0.69
10:b:273:HIS:HD1	23:b:817:CLA:HAB	1.58	0.69
29:b:842:PQN:H272	30:i:102:BCR:C34	2.23	0.69
23:b:834:CLA:H72	30:b:847:BCR:H391	1.72	0.68
13:f:167:GLU:HG3	13:f:172:ASP:HB3	1.73	0.68
16:j:22:THR:HA	16:j:25:PHE:CE1	2.28	0.68
10:b:2:VAL:N	15:i:32:LYS:O	2.26	0.68
9:a:698:HIS:CD2	23:a:856:CLA:HBC3	2.29	0.68
9:a:569:ASP:OD2	9:a:573:ARG:NH2	2.27	0.68
23:a:803:CLA:H192	23:b:810:CLA:HMC1	1.76	0.68
10:b:686:ARG:NH2	11:d:21:LEU:CD2	2.53	0.68
10:b:689:LEU:HD12	30:b:853:BCR:HC41	1.75	0.68
8:1:194:GLN:HG3	8:1:199:ASN:HB3	1.77	0.67
23:b:839:CLA:H12	30:i:102:BCR:H15C	1.73	0.67
21:4:301:XAT:H14	23:4:309:CLA:H12	1.76	0.67
10:b:295:ILE:HG13	23:b:820:CLA:HED1	1.77	0.67
23:a:803:CLA:H152	23:b:803:CLA:H202	1.76	0.67
25:1:304:A1L1F:C44	23:a:844:CLA:H42	2.23	0.67
2:9:41:GLU:CB	10:b:160:ARG:HH21	2.08	0.66
10:b:689:LEU:HB3	30:b:853:BCR:HC31	1.76	0.66
23:b:810:CLA:H92	30:b:853:BCR:H291	1.77	0.66
6:6:236:ALA:HB1	6:6:247:VAL:HG21	1.77	0.66
13:f:114:PHE:CE1	30:f:801:BCR:H343	2.30	0.66
21:6:303:XAT:H30	23:6:308:CLA:HAB	1.77	0.66
8:1:70:ARG:NH1	8:1:73:GLU:OE1	2.28	0.66
2:9:120:TRP:HH2	23:9:316:CLA:H43	1.60	0.66
23:6:309:CLA:H172	26:b:849:LHG:H281	1.78	0.66
23:a:833:CLA:H11	17:l:21:ILE:CG2	2.24	0.66
21:4:302:XAT:H193	23:4:307:CLA:H142	1.78	0.66
10:b:9:SER:HB2	27:b:851:DGD:HE62	1.78	0.66
1:5:113:ARG:NH1	1:5:116:GLU:OE1	2.29	0.65
9:a:112:TRP:HB3	21:a:853:XAT:H373	1.77	0.65
10:b:452:GLU:CA	13:f:92:LEU:HD22	2.18	0.65
4:7:120:ALA:HB1	23:7:311:CLA:HMD1	1.79	0.65
23:a:841:CLA:C5	30:f:801:BCR:H17C	2.27	0.65
10:b:547:LYS:CD	13:f:182:THR:HA	2.27	0.65
9:a:698:HIS:CD2	23:a:856:CLA:HHH	2.31	0.65
23:4:316:CLA:HAA2	27:4:317:DGD:HE5	1.77	0.65
9:a:698:HIS:CE1	23:a:856:CLA:CAC	2.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:336:LEU:HD21	23:b:829:CLA:HAB	1.78	0.65
15:i:29:TYR:HA	15:i:32:LYS:HE2	1.78	0.65
13:f:25:ASP:N	13:f:29:LEU:O	2.30	0.65
23:b:823:CLA:HBB1	23:b:838:CLA:H151	1.79	0.64
2:9:191:ALA:O	2:9:195:ASN:ND2	2.30	0.64
2:9:41:GLU:HB3	10:b:160:ARG:HH21	1.62	0.64
14:h:114:TRP:HA	14:h:117:HIS:NE2	2.11	0.64
9:a:197:GLY:O	9:a:201:LEU:HB2	1.97	0.64
16:j:21:PHE:HA	23:j:101:CLA:HBB2	1.80	0.64
23:b:810:CLA:C20	17:l:90:LEU:HD22	2.25	0.64
23:b:813:CLA:H121	23:b:818:CLA:H72	1.79	0.64
9:a:356:LEU:HD11	23:a:820:CLA:H71	1.79	0.64
9:a:703:VAL:HG22	23:a:856:CLA:HMD2	1.80	0.64
6:6:246:SER:HB2	23:6:315:CLA:CAA	2.28	0.63
4:7:136:VAL:HG22	23:7:312:CLA:HMA1	1.80	0.63
9:a:171:TRP:HB2	23:a:812:CLA:HMC2	1.80	0.63
9:a:362:HIS:HA	9:a:365:TYR:CE1	2.33	0.63
21:3:305:XAT:H32	23:3:313:CLA:HAB	1.79	0.63
10:b:304:GLU:HG2	10:b:318:ILE:HG13	1.78	0.63
16:j:26:VAL:HG11	30:j:102:BCR:H24C	1.81	0.63
9:a:298:PHE:HE1	23:a:822:CLA:HAB	1.64	0.63
1:5:120:GLY:O	1:5:124:MET:HG3	1.98	0.63
23:b:840:CLA:H13	30:i:101:BCR:H19C	1.81	0.63
9:a:114:ILE:HB	21:a:853:XAT:H372	1.81	0.63
23:a:810:CLA:H102	30:j:102:BCR:C33	2.28	0.63
21:4:304:XAT:H363	21:3:301:XAT:H10	1.80	0.63
9:a:589:LEU:HD21	23:a:831:CLA:HBC1	1.81	0.62
10:b:115:LEU:HA	10:b:365:THR:HG22	1.80	0.62
23:a:829:CLA:C17	30:j:102:BCR:HC7	2.28	0.62
23:a:833:CLA:C4	17:l:21:ILE:HG23	2.29	0.62
21:5:303:XAT:H162	23:5:308:CLA:H2	1.82	0.62
10:b:424:LEU:HD13	10:b:534:LEU:HA	1.81	0.62
11:d:86:ARG:HB2	11:d:96:LEU:HD11	1.82	0.62
11:d:117:ARG:NH2	20:c:6:LYS:HE2	2.13	0.62
25:1:304:A1L1F:C57	23:a:844:CLA:H42	2.25	0.62
1:5:130:PHE:CE1	21:5:303:XAT:O24	2.52	0.62
23:8:305:CLA:CGA	27:8:315:DGD:HE5	2.29	0.62
21:4:303:XAT:H32	23:4:312:CLA:HAB	1.80	0.62
9:a:298:PHE:CE1	23:a:822:CLA:HAB	2.35	0.62
10:b:129:THR:HG22	10:b:131:ASN:H	1.63	0.62
11:d:12:LYS:HB2	11:d:51:LYS:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:15:ASP:HB3	10:b:20:ARG:HB2	1.82	0.62
21:5:301:XAT:H373	24:5:317:SQD:H2	1.82	0.62
2:9:182:ALA:HB3	2:9:190:GLU:HG2	1.82	0.62
23:a:802:CLA:CED	30:f:801:BCR:C40	2.70	0.62
11:d:88:TYR:HB2	11:d:92:ASP:HB2	1.82	0.62
1:5:225:ILE:HG22	23:5:315:CLA:HAB	1.82	0.62
25:h:202:A1L1F:C4	25:h:202:A1L1F:C12	2.78	0.62
7:2:76:THR:O	7:2:82:ARG:NH1	2.33	0.61
9:a:429:ALA:O	9:a:433:HIS:ND1	2.31	0.61
23:a:841:CLA:H2	23:b:832:CLA:H42	1.82	0.61
23:a:841:CLA:H51	30:f:801:BCR:H17C	1.81	0.61
23:a:833:CLA:H42	17:l:21:ILE:HG23	1.82	0.61
23:b:832:CLA:H18	30:f:804:BCR:H17C	1.80	0.61
21:7:303:XAT:H362	23:7:308:CLA:H51	1.81	0.61
8:1:186:ILE:HG13	8:1:187:THR:HG23	1.83	0.61
4:7:50:ASP:OD1	4:7:51:GLY:N	2.32	0.61
10:b:660:ALA:HB3	23:b:803:CLA:HBB2	1.83	0.61
23:b:830:CLA:HAB	23:b:838:CLA:HBB2	1.82	0.61
3:8:185:MET:HE2	23:8:308:CLA:HBB2	1.83	0.61
9:a:162:ALA:O	9:a:166:MET:HG2	2.00	0.61
23:a:818:CLA:C3D	28:a:855:LMG:HC91	2.30	0.61
13:f:79:ARG:NH1	16:j:35:ASP:O	2.33	0.61
11:d:117:ARG:NE	20:c:6:LYS:HE2	2.16	0.61
5:3:199:ALA:O	5:3:203:MET:HG3	2.01	0.61
9:a:167:LEU:HD11	23:a:810:CLA:H193	1.83	0.61
9:a:698:HIS:CD2	23:a:856:CLA:CAC	2.83	0.60
1:5:190:ARG:NH1	1:5:191:GLU:O	2.34	0.60
23:4:316:CLA:H2A	27:4:317:DGD:C6E	2.30	0.60
7:2:44:PRO:HG3	7:2:58:ASP:HB3	1.83	0.60
11:d:131:LYS:O	11:d:132:PHE:C	2.44	0.60
23:a:833:CLA:HBC2	23:a:840:CLA:HMC2	1.83	0.60
10:b:689:LEU:CD1	30:b:853:BCR:HC41	2.31	0.60
5:3:92:HIS:HB3	5:3:197:MET:SD	2.42	0.60
23:b:837:CLA:HBC3	30:f:804:BCR:H401	1.83	0.60
9:a:121:ASN:HB3	9:a:129:GLN:HB3	1.83	0.60
17:l:38:ARG:O	17:l:46:ARG:NH2	2.35	0.60
22:1:301:A1L1G:C18	23:1:306:CLA:HAC2	2.32	0.60
23:a:841:CLA:C20	23:a:856:CLA:H2	2.30	0.60
10:b:412:ARG:NH2	23:b:830:CLA:O1D	2.35	0.60
23:a:802:CLA:HBA2	10:b:429:LEU:HD23	1.83	0.59
26:9:307:LHG:H301	23:b:810:CLA:H141	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:8:305:CLA:HAA2	27:8:315:DGD:HE5	1.82	0.59
23:a:820:CLA:H92	23:a:830:CLA:H91	1.84	0.59
23:b:804:CLA:H18	15:i:14:VAL:HG22	1.84	0.59
4:4:185:PHE:CZ	21:4:302:XAT:H30	2.37	0.59
30:b:846:BCR:H342	23:h:201:CLA:H172	1.84	0.59
5:3:83:TYR:OH	5:3:163:ARG:NH1	2.35	0.59
9:a:53:ASP:OD2	9:a:343:HIS:NE2	2.35	0.59
9:a:507:VAL:HG22	9:a:517:MET:HG3	1.85	0.58
2:9:120:TRP:CZ2	23:9:316:CLA:H43	2.38	0.58
23:a:803:CLA:H51	10:b:657:LEU:HD22	1.85	0.58
10:b:3:TYR:HD1	15:i:34:ASN:HB2	1.65	0.58
13:f:114:PHE:CE1	30:f:801:BCR:C34	2.87	0.58
2:9:185:PRO:HA	23:9:313:CLA:HBA2	1.85	0.58
4:4:170:MET:HE1	23:4:312:CLA:H43	1.84	0.58
9:a:734:TRP:NE1	23:a:829:CLA:O1A	2.36	0.58
10:b:74:PHE:O	10:b:78:ILE:HG12	2.04	0.58
23:a:826:CLA:HBA1	23:a:830:CLA:H193	1.86	0.58
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.58
21:8:302:XAT:H32	23:8:307:CLA:HAB	1.85	0.58
4:7:88:THR:HG21	21:7:304:XAT:H12	1.85	0.58
23:b:839:CLA:C15	30:b:853:BCR:H17C	2.30	0.58
14:h:121:TRP:CD1	23:h:201:CLA:HAA1	2.39	0.58
8:1:72:SER:O	8:1:76:HIS:ND1	2.28	0.58
9:a:70:HIS:ND1	23:a:814:CLA:OBD	2.31	0.58
9:a:706:SER:CB	13:f:139:THR:HG22	2.28	0.58
23:a:803:CLA:C19	23:b:810:CLA:HMC1	2.34	0.58
21:5:302:XAT:H14	23:5:310:CLA:H12	1.86	0.58
5:3:87:GLU:OE2	5:3:163:ARG:NH2	2.31	0.58
21:2:303:XAT:H363	23:2:308:CLA:H2	1.84	0.57
9:a:292:LEU:HD21	23:a:818:CLA:CAB	2.34	0.57
10:b:561:CYS:HB2	10:b:569:THR:O	2.04	0.57
9:a:517:MET:HE1	9:a:623:HIS:NE2	2.19	0.57
10:b:69:ALA:HB2	10:b:133:LEU:HB2	1.86	0.57
1:5:112:LEU:HD22	23:5:308:CLA:H12	1.86	0.57
2:9:222:ASP:HB2	2:9:230:LEU:HD13	1.86	0.57
23:a:818:CLA:C1D	28:a:855:LMG:H291	2.34	0.57
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.57
5:3:86:ARG:NH1	5:3:89:GLU:OE1	2.38	0.57
4:7:185:PHE:CD2	21:7:303:XAT:H12	2.39	0.57
9:a:114:ILE:HG13	9:a:115:VAL:HG13	1.86	0.57
23:b:803:CLA:CGA	23:b:803:CLA:H3A	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:802:CLA:CGA	23:a:802:CLA:H3A	2.35	0.57
10:b:178:SER:HB3	10:b:286:GLY:HA3	1.86	0.57
9:a:324:GLY:HA3	26:a:846:LHG:HC32	1.87	0.57
5:3:182:PHE:HZ	23:3:313:CLA:HED3	1.70	0.57
30:b:843:BCR:H23C	30:b:850:BCR:H323	1.86	0.57
9:a:107:SER:HB2	9:a:124:VAL:HG11	1.86	0.57
10:b:39:GLU:HB3	10:b:163:LEU:HD11	1.87	0.57
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.56
23:a:833:CLA:C6	23:l:202:CLA:H101	2.19	0.56
10:b:562:ASP:HB3	10:b:569:THR:HG21	1.86	0.56
11:d:117:ARG:HH21	20:c:6:LYS:HE2	1.70	0.56
1:5:155:VAL:HG21	23:5:310:CLA:HAA2	1.86	0.56
2:9:41:GLU:HB3	10:b:160:ARG:NH2	2.20	0.56
9:a:598:ILE:HG13	23:a:801:CLA:H192	1.86	0.56
28:a:855:LMG:H112	28:a:855:LMG:C9	2.35	0.56
10:b:29:HIS:ND1	23:b:806:CLA:O1A	2.28	0.56
11:d:97:HIS:HB3	11:d:98:PRO:HD3	1.86	0.56
23:a:818:CLA:CHD	28:a:855:LMG:H291	2.36	0.56
23:b:821:CLA:HHB	23:b:822:CLA:H2	1.88	0.56
23:b:833:CLA:H43	30:f:801:BCR:HC32	1.86	0.56
21:2:303:XAT:C36	23:2:308:CLA:H2	2.35	0.56
9:a:213:ILE:HG23	9:a:233:PRO:HB3	1.87	0.56
3:8:60:PHE:HE1	23:8:305:CLA:HBC3	1.70	0.56
11:d:117:ARG:HE	20:c:6:LYS:HE2	1.71	0.56
23:a:822:CLA:HBC3	23:a:828:CLA:H172	1.88	0.56
1:5:111:TRP:NE1	23:5:309:CLA:O1A	2.33	0.56
4:4:136:VAL:HG22	23:4:311:CLA:HMA1	1.87	0.56
6:6:248:PRO:HG2	23:6:315:CLA:HBC2	1.87	0.56
10:b:93:ASP:OD1	10:b:95:HIS:ND1	2.33	0.56
12:e:32:VAL:HG11	20:c:35:LYS:HD3	1.87	0.56
17:l:54:HIS:HA	17:l:57:PHE:CE2	2.41	0.56
23:a:825:CLA:H12	30:a:849:BCR:H14C	1.88	0.56
28:a:855:LMG:H112	28:a:855:LMG:O8	2.05	0.55
10:b:3:TYR:O	15:i:34:ASN:ND2	2.39	0.55
3:8:75:VAL:HG23	23:8:307:CLA:HMA2	1.89	0.55
6:6:248:PRO:HD2	25:6:304:A1L1F:C56	2.36	0.55
9:a:651:VAL:HG22	9:a:739:ALA:HB3	1.87	0.55
9:a:651:VAL:HG21	9:a:736:PHE:HA	1.88	0.55
2:9:93:ILE:HG13	21:9:304:XAT:H8	1.88	0.55
5:3:48:LEU:HD13	5:3:51:LEU:HD12	1.87	0.55
7:2:35:SER:OG	7:2:37:ALA:O	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:7:SER:H	9:a:12:PHE:HE2	1.53	0.55
30:b:852:BCR:H23C	16:j:33:TYR:CD2	2.42	0.55
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.55
2:9:162:LYS:NZ	23:9:312:CLA:O1A	2.39	0.55
23:b:805:CLA:HBA1	23:b:813:CLA:HBA1	1.87	0.55
8:1:88:ILE:HG22	8:1:92:PHE:HE1	1.71	0.55
30:i:102:BCR:H401	17:l:92:LEU:HB3	1.88	0.55
17:l:9:ARG:HH21	19:g:54:UNK:CB	2.19	0.55
20:c:15:THR:HG22	20:c:28:MET:HG3	1.89	0.55
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.55
2:9:149:ALA:O	2:9:153:PHE:HD1	1.90	0.55
10:b:687:THR:HG21	23:b:801:CLA:HMA1	1.84	0.55
2:9:85:GLY:O	2:9:89:MET:HG3	2.07	0.55
8:1:115:ILE:O	8:1:119:GLN:NE2	2.40	0.55
9:a:290:HIS:HB2	23:a:819:CLA:C1B	2.37	0.55
2:9:117:TRP:O	2:9:120:TRP:CD1	2.60	0.55
11:d:117:ARG:CZ	20:c:6:LYS:HE2	2.37	0.55
4:4:185:PHE:CE2	21:4:302:XAT:H30	2.42	0.55
9:a:441:LEU:HB3	9:a:534:PHE:HB2	1.88	0.55
25:1:304:A1L1F:C44	23:a:844:CLA:C4	2.83	0.54
10:b:561:CYS:SG	10:b:563:GLY:N	2.77	0.54
10:b:582:MET:HG3	10:b:712:LEU:HD21	1.87	0.54
10:b:633:LEU:HD22	10:b:726:PHE:HA	1.89	0.54
15:i:30:ILE:HG21	30:i:102:BCR:H322	1.88	0.54
16:j:14:LEU:HD21	28:j:103:LMG:H141	1.89	0.54
22:5:304:A1L1G:C41	23:5:313:CLA:HMC1	2.37	0.54
10:b:317:HIS:HB3	10:b:320:LEU:HD12	1.89	0.54
2:9:107:LEU:HD11	2:9:140:ILE:HD11	1.87	0.54
4:4:83:ILE:HD11	21:4:301:XAT:H362	1.90	0.54
10:b:521:VAL:HG21	10:b:595:TYR:HB2	1.89	0.54
10:b:565:GLY:O	10:b:567:GLY:N	2.40	0.54
11:d:63:ARG:NH2	11:d:65:GLU:OE1	2.41	0.54
23:b:823:CLA:HBB2	23:b:841:CLA:H52	1.90	0.54
23:9:312:CLA:HBA1	23:9:312:CLA:HBD	1.89	0.54
4:4:121:LEU:HD23	4:4:124:ILE:HD12	1.90	0.54
9:a:210:GLN:HA	9:a:214:ALA:HB3	1.89	0.54
23:9:316:CLA:CAB	23:b:810:CLA:H112	2.34	0.53
9:a:388:VAL:HG12	9:a:596:ILE:HG23	1.89	0.53
9:a:703:VAL:HG22	23:a:856:CLA:HMD3	1.89	0.53
4:7:46:PRO:HG2	4:7:49:LEU:HD12	1.90	0.53
6:6:154:PHE:HB2	21:6:303:XAT:H22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:200:PRO:O	21:7:304:XAT:O3	2.26	0.53
8:1:146:LEU:HD13	23:a:844:CLA:H91	1.90	0.53
23:a:820:CLA:HAB	23:a:820:CLA:H8	1.90	0.53
9:a:698:HIS:ND1	23:a:856:CLA:HBC1	2.22	0.53
23:a:825:CLA:HMA3	23:a:844:CLA:HAB	1.90	0.53
3:8:36:ALA:N	3:8:44:LEU:O	2.42	0.53
23:a:841:CLA:H203	23:a:856:CLA:C2	2.34	0.53
10:b:22:TRP:CG	10:b:706:GLN:HE22	2.26	0.53
10:b:355:PRO:HG3	23:b:818:CLA:HBA1	1.90	0.53
4:7:128:THR:HG23	22:7:302:A1L1G:C17	2.39	0.53
23:a:831:CLA:H42	26:a:845:LHG:H251	1.90	0.53
10:b:443:ASP:OD1	10:b:617:TYR:HB2	2.08	0.53
4:4:81:CYS:HB3	4:4:178:GLY:HA3	1.91	0.53
23:4:316:CLA:O2D	27:4:317:DGD:HE61	2.09	0.53
9:a:197:GLY:HA3	23:a:814:CLA:HBB1	1.89	0.53
9:a:219:LYS:HD3	9:a:246:LEU:HB3	1.90	0.53
10:b:661:THR:O	10:b:664:MET:HB3	2.09	0.53
8:1:61:ALA:HB1	8:1:65:THR:HB	1.90	0.53
23:a:835:CLA:O2D	23:a:835:CLA:H2A	2.09	0.53
23:b:801:CLA:H101	23:b:801:CLA:HBB1	1.91	0.53
6:6:232:ILE:HD13	25:6:301:A1L1F:C31	2.39	0.52
9:a:683:GLY:HA3	10:b:570:CYS:HB2	1.91	0.52
10:b:140:LEU:HG	30:b:845:BCR:H382	1.90	0.52
23:a:809:CLA:CHC	23:a:810:CLA:HMD2	2.39	0.52
2:9:179:LEU:HD23	23:9:308:CLA:HMD3	1.90	0.52
2:9:192:GLU:HB2	23:9:312:CLA:C1B	2.40	0.52
5:3:79:GLY:O	5:3:158:ARG:NH1	2.43	0.52
6:6:184:TYR:CZ	6:6:186:GLY:HA3	2.44	0.52
8:1:77:GLY:O	8:1:81:MET:HG3	2.09	0.52
23:1:311:CLA:C3	23:a:844:CLA:H93	2.40	0.52
10:b:189:THR:HG21	10:b:276:LEU:HB2	1.91	0.52
23:b:833:CLA:CED	16:j:37:LEU:HD13	2.39	0.52
19:g:51:UNK:O	19:g:53:UNK:N	2.42	0.52
3:8:177:GLY:O	3:8:181:MET:HG3	2.09	0.52
4:4:193:ALA:O	27:4:317:DGD:O6E	2.28	0.52
10:b:709:LEU:HD11	27:b:851:DGD:HB41	1.90	0.52
23:9:316:CLA:HAB	23:b:810:CLA:C11	2.33	0.52
10:b:689:LEU:CB	30:b:853:BCR:HC31	2.39	0.52
20:c:11:CYS:SG	20:c:39:ILE:HG13	2.50	0.52
21:5:303:XAT:C16	23:5:308:CLA:H2	2.39	0.52
3:8:175:LYS:HB3	23:8:306:CLA:HMD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:718:GLY:O	10:b:722:THR:HG22	2.09	0.52
2:9:107:LEU:HG	2:9:136:ALA:HB1	1.91	0.52
2:9:218:LEU:HG	23:9:314:CLA:HMA2	1.92	0.52
9:a:396:VAL:HG11	9:a:589:LEU:HG	1.91	0.52
6:6:131:ALA:HB2	21:6:303:XAT:H10	1.92	0.52
23:b:810:CLA:CED	30:b:853:BCR:C39	2.84	0.52
23:b:829:CLA:H42	27:b:851:DGD:HB42	1.91	0.52
23:a:802:CLA:O1D	30:f:801:BCR:H401	2.09	0.51
6:6:249:LEU:HB2	25:6:304:A1L1F:O55	2.10	0.51
7:2:121:ALA:O	7:2:122:LYS:HG2	2.10	0.51
23:a:827:CLA:H93	23:a:840:CLA:H52	1.92	0.51
10:b:342:ALA:O	10:b:346:THR:HG23	2.11	0.51
10:b:693:VAL:HG11	23:b:801:CLA:HAB	1.92	0.51
25:h:202:A1L1F:O46	23:h:203:CLA:H52	2.11	0.51
4:7:121:LEU:HD13	23:7:316:CLA:HBC3	1.92	0.51
10:b:179:GLY:O	10:b:183:VAL:HB	2.10	0.51
23:b:832:CLA:CMC	30:b:852:BCR:H10C	2.40	0.51
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.92	0.51
7:2:77:LYS:O	7:2:79:ASP:N	2.43	0.51
9:a:431:ILE:HG13	9:a:549:TYR:HE1	1.74	0.51
9:a:574:GLY:O	10:b:670:ARG:HD3	2.11	0.51
23:a:818:CLA:HHC	23:a:818:CLA:HBB1	1.93	0.51
10:b:26:ALA:HA	23:b:829:CLA:H43	1.93	0.51
10:b:689:LEU:HD22	23:l:202:CLA:C2D	2.40	0.51
13:f:85:LEU:HD13	13:f:93:PRO:HB3	1.92	0.51
20:c:58:CYS:SG	20:c:63:LEU:HA	2.51	0.51
8:1:85:LEU:HB3	23:1:308:CLA:HMC2	1.92	0.51
9:a:681:PHE:HE1	10:b:667:ILE:CD1	2.22	0.51
10:b:274:HIS:HB2	23:b:817:CLA:C1B	2.41	0.51
10:b:662:GLY:O	10:b:666:LEU:HG	2.10	0.51
23:b:806:CLA:H52	27:b:851:DGD:HB72	1.93	0.51
13:f:143:ILE:HG13	13:f:144:ILE:HG13	1.92	0.51
3:8:50:LEU:HD11	3:8:61:ASP:HB2	1.93	0.51
4:7:45:ARG:NH1	4:7:49:LEU:O	2.42	0.51
9:a:422:ARG:O	9:a:426:HIS:ND1	2.41	0.51
10:b:602:THR:HG21	10:b:611:PHE:HB2	1.93	0.51
30:b:852:BCR:H23C	16:j:33:TYR:HD2	1.75	0.51
11:d:33:ILE:HG22	11:d:58:VAL:HG22	1.92	0.51
13:f:160:TRP:CD1	13:f:161:PRO:HD3	2.46	0.51
21:4:302:XAT:C16	23:4:307:CLA:H2	2.41	0.51
6:6:124:HIS:HB3	6:6:231:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.50
23:b:810:CLA:H202	17:l:90:LEU:CD2	2.32	0.50
9:a:655:TYR:CD2	10:b:447:ALA:HA	2.46	0.50
23:b:840:CLA:H18	30:i:101:BCR:C20	2.39	0.50
21:5:302:XAT:H193	23:5:311:CLA:HBA2	1.94	0.50
23:5:313:CLA:H3A	23:5:313:CLA:CGA	2.41	0.50
5:3:93:CYS:HB3	5:3:193:GLY:HA3	1.92	0.50
9:a:460:ARG:NH2	23:a:835:CLA:O1D	2.44	0.50
10:b:722:THR:HG23	23:b:802:CLA:O1D	2.11	0.50
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.50
2:9:31:GLY:O	3:8:68:GLN:OE1	2.29	0.50
2:9:191:ALA:HB1	23:9:313:CLA:HAA1	1.93	0.50
9:a:440:PHE:HE2	23:a:839:CLA:HAB	1.76	0.50
17:l:38:ARG:NH1	17:l:49:GLU:OE1	2.40	0.50
17:l:106:VAL:H	17:l:140:VAL:HG23	1.77	0.50
20:c:13:GLY:O	20:c:38:GLN:NE2	2.44	0.50
28:a:855:LMG:H131	28:a:855:LMG:H292	1.94	0.50
22:9:301:A1L1G:C44	23:9:315:CLA:HBC3	2.41	0.50
6:6:112:PRO:HB3	6:6:116:TRP:CD1	2.47	0.50
25:1:304:A1L1F:C2	23:a:844:CLA:C1	2.79	0.50
23:b:823:CLA:HAB	23:b:830:CLA:HMD1	1.93	0.50
3:8:172:LYS:O	3:8:176:ASN:ND2	2.39	0.49
6:6:104:GLU:OE2	6:6:105:ARG:NH1	2.45	0.49
9:a:565:ARG:HG2	9:a:715:THR:HG21	1.93	0.49
9:a:712:LEU:N	29:a:843:PQN:O4	2.45	0.49
23:a:818:CLA:O1A	28:a:855:LMG:O10	2.30	0.49
23:b:839:CLA:H203	17:l:92:LEU:HD11	1.93	0.49
9:a:674:ALA:HB3	23:a:802:CLA:HBB2	1.94	0.49
23:a:818:CLA:CHD	23:a:819:CLA:HBB2	2.43	0.49
10:b:3:TYR:CD1	15:i:34:ASN:ND2	2.68	0.49
23:b:832:CLA:HBB2	30:f:801:BCR:HC41	1.94	0.49
4:7:54:VAL:HG21	4:7:74:GLN:HE21	1.77	0.49
10:b:3:TYR:HD1	15:i:34:ASN:CB	2.24	0.49
23:b:811:CLA:H72	23:b:812:CLA:HBC3	1.93	0.49
20:c:17:CYS:SG	20:c:18:VAL:N	2.85	0.49
3:8:60:PHE:CE1	23:8:305:CLA:HBC3	2.47	0.49
21:7:301:XAT:H10	23:7:315:CLA:HMD1	1.93	0.49
23:a:803:CLA:OBD	23:b:802:CLA:HMB3	2.12	0.49
10:b:3:TYR:CD1	15:i:34:ASN:CB	2.93	0.49
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.49
8:1:112:VAL:HB	8:1:117:TRP:NE1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:802:CLA:H41	10:b:436:LEU:CD2	2.41	0.49
2:9:91:GLY:HA3	21:9:303:XAT:H173	1.94	0.49
23:4:308:CLA:HAC1	23:4:315:CLA:HAB	1.95	0.49
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.49
9:a:574:GLY:HA3	10:b:670:ARG:NH1	2.27	0.49
10:b:407:LYS:HB3	10:b:411:ALA:HB3	1.95	0.49
17:l:109:ASN:OD1	17:l:110:ALA:N	2.35	0.49
2:9:117:TRP:O	2:9:120:TRP:NE1	2.45	0.49
2:9:172:LYS:HB3	2:9:172:LYS:HE2	1.45	0.49
23:9:316:CLA:H142	23:9:316:CLA:H111	1.61	0.49
25:6:304:A1L1F:C33	23:6:313:CLA:HAB	2.43	0.49
10:b:478:LEU:HG	10:b:479:LEU:HG	1.93	0.49
19:g:46:UNK:O	19:g:50:UNK:N	2.45	0.49
5:3:145:ILE:O	5:3:149:ILE:HG12	2.13	0.49
4:7:91:TRP:CE3	21:7:303:XAT:H22	2.48	0.49
4:7:97:VAL:O	4:7:97:VAL:HG13	2.13	0.49
23:a:803:CLA:H51	10:b:657:LEU:CD2	2.41	0.49
23:b:832:CLA:C3C	30:b:852:BCR:C33	2.91	0.49
23:h:201:CLA:HBA1	23:h:201:CLA:HBD	1.93	0.49
23:3:308:CLA:HED2	23:3:308:CLA:H2A	1.94	0.49
9:a:252:LYS:NZ	9:a:264:GLU:OE1	2.41	0.49
10:b:597:HIS:CE1	10:b:601:LEU:HD11	2.48	0.49
23:b:801:CLA:H142	23:b:839:CLA:H71	1.93	0.49
17:l:43:PRO:HD3	17:l:136:GLU:CD	2.38	0.49
20:c:17:CYS:HB3	31:c:102:SF4:S4	2.52	0.49
4:4:184:ALA:HA	23:4:314:CLA:HBB1	1.95	0.48
4:7:124:ILE:HA	23:7:311:CLA:HBC3	1.95	0.48
4:7:185:PHE:O	4:7:189:VAL:HG22	2.13	0.48
10:b:166:PHE:O	10:b:172:ARG:NH2	2.46	0.48
23:b:837:CLA:HMC3	30:b:852:BCR:HC31	1.94	0.48
11:d:95:LEU:HD11	11:d:98:PRO:HD2	1.95	0.48
9:a:615:VAL:HG22	9:a:621:VAL:HG22	1.95	0.48
5:3:203:MET:HE2	21:3:305:XAT:O4	2.13	0.48
7:2:107:LEU:HB3	23:2:310:CLA:HMC2	1.94	0.48
23:1:306:CLA:H202	23:1:306:CLA:H162	1.69	0.48
9:a:114:ILE:HG23	9:a:115:VAL:HG22	1.95	0.48
23:a:818:CLA:HBA2	23:a:818:CLA:H3A	1.57	0.48
28:a:855:LMG:HC92	28:a:855:LMG:C11	2.41	0.48
10:b:65:LEU:HD11	30:b:845:BCR:H281	1.95	0.48
10:b:266:LEU:HD22	23:b:817:CLA:HBA1	1.95	0.48
10:b:412:ARG:HH21	23:b:830:CLA:CGD	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:72:PRO:HG3	25:h:202:A1L1F:C56	2.43	0.48
2:9:32:THR:H	2:9:33:PRO:HD2	1.77	0.48
6:6:118:GLN:HB3	6:6:197:VAL:HG11	1.96	0.48
10:b:419:ALA:O	10:b:423:HIS:ND1	2.40	0.48
10:b:443:ASP:OD1	10:b:618:ILE:N	2.46	0.48
1:5:171:GLU:HG3	23:5:312:CLA:NB	2.28	0.48
9:a:292:LEU:HD12	23:a:816:CLA:HMC3	1.95	0.48
10:b:526:ALA:O	10:b:530:HIS:ND1	2.37	0.48
25:8:304:A1L1F:C36	23:8:311:CLA:H51	2.43	0.48
7:2:118:LEU:N	23:2:310:CLA:OBD	2.47	0.48
4:7:81:CYS:O	4:7:85:MET:HG3	2.13	0.48
23:a:832:CLA:HAB	23:a:840:CLA:HBB2	1.96	0.48
23:b:831:CLA:O2A	30:f:804:BCR:H353	2.13	0.48
10:b:181:PHE:HE2	23:b:819:CLA:HAB	1.78	0.48
16:j:2:LYS:O	28:j:103:LMG:HC61	2.13	0.48
5:3:78:VAL:HG12	5:3:78:VAL:O	2.14	0.48
10:b:277:ALA:HA	23:b:816:CLA:HMC2	1.95	0.48
10:b:492:SER:HA	10:b:496:LEU:HD12	1.94	0.48
2:9:201:LEU:HD21	21:9:304:XAT:H371	1.96	0.48
3:8:58:PHE:HZ	3:8:175:LYS:HZ1	1.62	0.48
23:3:308:CLA:H2A	23:3:308:CLA:CED	2.44	0.48
9:a:423:VAL:HA	9:a:426:HIS:CE1	2.47	0.48
23:a:803:CLA:H192	23:b:810:CLA:CMC	2.42	0.48
10:b:8:PHE:HB2	10:b:34:HIS:CG	2.49	0.48
10:b:176:HIS:O	10:b:180:LEU:HB3	2.14	0.48
10:b:565:GLY:O	10:b:566:ARG:C	2.55	0.48
23:b:801:CLA:H141	23:b:801:CLA:H161	1.63	0.48
23:b:821:CLA:CHB	23:b:822:CLA:H2	2.44	0.48
14:h:114:TRP:HA	14:h:117:HIS:CD2	2.49	0.48
1:5:130:PHE:HE1	21:5:303:XAT:O24	1.94	0.48
21:5:305:XAT:C10	23:5:316:CLA:HBC3	2.43	0.48
2:9:187:LEU:HA	23:9:312:CLA:HMB1	1.96	0.48
23:9:316:CLA:H91	23:9:316:CLA:H112	1.69	0.48
9:a:411:ASN:ND2	9:a:414:ASN:OD1	2.37	0.48
23:a:825:CLA:H71	23:a:840:CLA:H62	1.96	0.48
10:b:670:ARG:C	10:b:672:TYR:H	2.22	0.48
23:b:839:CLA:HAB	29:b:842:PQN:H172	1.96	0.48
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.47
3:8:110:ASN:HB3	3:8:113:LYS:HB2	1.96	0.47
29:b:842:PQN:H303	30:i:102:BCR:HC7	1.95	0.47
30:b:845:BCR:H15C	30:b:845:BCR:H351	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:89:ASN:O	14:h:91:PHE:N	2.46	0.47
2:9:49:MET:HA	2:9:52:LYS:HD3	1.97	0.47
3:8:44:LEU:HD22	4:7:141:GLN:NE2	2.29	0.47
7:2:92:ARG:NH1	7:2:95:GLU:OE1	2.47	0.47
4:7:42:PHE:HE2	23:7:306:CLA:HAB	1.77	0.47
23:1:306:CLA:H93	23:1:306:CLA:H61	1.70	0.47
9:a:712:LEU:HD21	29:a:843:PQN:H151	1.95	0.47
23:b:806:CLA:H192	23:b:806:CLA:H161	1.72	0.47
9:a:655:TYR:CZ	10:b:447:ALA:HB2	2.48	0.47
10:b:297:HIS:HB3	10:b:302:ILE:HD11	1.97	0.47
10:b:466:GLN:NE2	23:b:836:CLA:OBD	2.34	0.47
23:b:824:CLA:H141	23:b:824:CLA:H193	1.95	0.47
6:6:131:ALA:CB	21:6:303:XAT:H10	2.44	0.47
23:2:316:CLA:C2C	28:2:317:LMG:H111	2.44	0.47
9:a:290:HIS:HB2	23:a:819:CLA:CHB	2.44	0.47
23:a:820:CLA:H203	23:a:828:CLA:H3A	1.96	0.47
10:b:687:THR:HG21	23:b:801:CLA:HMA2	1.88	0.47
23:b:830:CLA:HAB	23:b:838:CLA:CBB	2.44	0.47
30:b:845:BCR:H311	30:b:845:BCR:HC8	1.96	0.47
21:4:301:XAT:H35	21:4:301:XAT:H401	1.76	0.47
21:7:303:XAT:H32	23:7:308:CLA:HAB	1.97	0.47
8:1:84:VAL:O	8:1:88:ILE:HG12	2.14	0.47
10:b:432:GLY:HA2	10:b:527:LEU:HD22	1.96	0.47
2:9:88:ALA:HA	21:9:303:XAT:H8	1.95	0.47
3:8:36:ALA:HB3	3:8:45:LYS:HZ2	1.79	0.47
7:2:183:ASP:O	7:2:186:LYS:N	2.44	0.47
21:7:304:XAT:H11	21:7:304:XAT:H191	1.78	0.47
3:8:141:THR:HA	3:8:147:PRO:HB3	1.97	0.47
4:4:159:ASN:C	4:4:161:ALA:H	2.21	0.47
5:3:81:ASP:N	5:3:81:ASP:OD1	2.46	0.47
6:6:118:GLN:O	6:6:121:GLU:HB2	2.15	0.47
8:1:42:MET:HE1	8:1:66:LEU:HD22	1.96	0.47
8:1:88:ILE:HG22	8:1:92:PHE:CE1	2.49	0.47
9:a:38:THR:HB	9:a:710:ARG:HG3	1.97	0.47
9:a:476:PHE:HB3	23:a:838:CLA:H11	1.96	0.47
9:a:574:GLY:O	10:b:670:ARG:CD	2.62	0.47
10:b:127:MET:HE1	30:b:845:BCR:H282	1.97	0.47
10:b:143:LEU:HD23	10:b:146:LEU:HD12	1.97	0.47
10:b:271:MET:O	10:b:275:HIS:ND1	2.47	0.47
10:b:273:HIS:ND1	23:b:817:CLA:HAB	2.25	0.47
10:b:538:LYS:O	10:b:542:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:586:LEU:HD21	10:b:716:THR:HG23	1.96	0.47
10:b:595:TYR:CZ	23:b:836:CLA:HBC3	2.49	0.47
16:j:5:LEU:HB3	28:j:103:LMG:HC72	1.96	0.47
9:a:68:SER:OG	9:a:174:TYR:HB2	2.14	0.47
9:a:354:GLY:HA2	9:a:391:GLY:HA2	1.97	0.47
10:b:433:PHE:HZ	30:f:801:BCR:H372	1.79	0.47
23:b:810:CLA:H141	23:b:810:CLA:H162	1.75	0.47
30:b:844:BCR:H11C	30:b:844:BCR:H341	1.76	0.47
21:5:303:XAT:H11	21:5:303:XAT:H191	1.65	0.47
23:9:311:CLA:H2A	23:9:311:CLA:O2D	2.14	0.47
23:9:314:CLA:CED	23:9:314:CLA:H2A	2.45	0.47
7:2:191:GLN:O	7:2:195:ILE:HD12	2.15	0.47
9:a:502:ALA:HB2	9:a:516:MET:HE2	1.97	0.47
23:a:829:CLA:HBB1	23:a:829:CLA:HMB1	1.97	0.47
23:b:823:CLA:H2A	23:b:823:CLA:HED3	1.95	0.47
3:8:73:LYS:HD3	3:8:145:ASP:HA	1.95	0.47
3:8:83:CYS:HB3	3:8:177:GLY:HA3	1.97	0.47
21:2:301:XAT:H31	21:2:301:XAT:H391	1.72	0.47
23:a:841:CLA:H52	30:f:801:BCR:H17C	1.95	0.47
10:b:50:HIS:ND1	23:b:813:CLA:OBD	2.38	0.47
21:5:305:XAT:H15	21:5:305:XAT:H201	1.76	0.46
23:6:308:CLA:CGA	23:6:308:CLA:H3A	2.45	0.46
9:a:514:ILE:HD11	9:a:621:VAL:HG13	1.96	0.46
23:a:839:CLA:H62	23:a:839:CLA:H41	1.54	0.46
23:a:852:CLA:CMB	10:b:436:LEU:HD13	2.44	0.46
10:b:452:GLU:HA	13:f:92:LEU:CD2	2.22	0.46
23:b:801:CLA:HAC2	30:b:848:BCR:H381	1.95	0.46
8:1:73:GLU:HB2	23:1:306:CLA:C1B	2.45	0.46
10:b:687:THR:HG23	10:b:690:ALA:HB3	1.97	0.46
23:b:827:CLA:H143	23:b:827:CLA:H161	1.78	0.46
23:h:203:CLA:HED3	23:h:203:CLA:H2A	1.97	0.46
2:9:126:THR:OG1	2:9:129:GLU:OE2	2.34	0.46
21:3:303:XAT:H15	21:3:303:XAT:H201	1.79	0.46
21:7:303:XAT:H35	21:7:303:XAT:H401	1.76	0.46
23:b:832:CLA:HMC1	30:b:852:BCR:H10C	1.96	0.46
11:d:83:LYS:HG2	11:d:98:PRO:HG2	1.97	0.46
21:8:303:XAT:H34	23:8:313:CLA:HBB1	1.96	0.46
6:6:94:TRP:CZ3	21:6:303:XAT:H383	2.50	0.46
4:7:185:PHE:HE1	21:7:303:XAT:H162	1.79	0.46
9:a:144:GLU:HG2	9:a:206:TRP:HH2	1.80	0.46
23:b:812:CLA:H41	23:b:812:CLA:H62	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:96:VAL:HG12	23:5:308:CLA:OBD	2.15	0.46
4:4:185:PHE:CZ	21:4:302:XAT:H28	2.50	0.46
9:a:400:ALA:HB2	9:a:585:VAL:HG11	1.96	0.46
23:a:801:CLA:H61	23:a:803:CLA:O1D	2.15	0.46
10:b:372:HIS:HB2	23:b:827:CLA:C1B	2.45	0.46
23:b:801:CLA:H143	23:b:839:CLA:H111	1.91	0.46
23:b:811:CLA:H51	23:b:812:CLA:H43	1.97	0.46
23:b:838:CLA:H101	23:b:838:CLA:H13	1.78	0.46
4:7:160:PHE:HE2	21:7:304:XAT:H373	1.81	0.46
9:a:577:CYS:HB2	10:b:670:ARG:O	2.15	0.46
23:a:818:CLA:NC	28:a:855:LMG:H302	2.31	0.46
23:b:820:CLA:HBA2	23:b:820:CLA:H3A	1.33	0.46
23:8:311:CLA:HBB1	23:8:311:CLA:HMB3	1.97	0.46
7:2:105:ALA:HB1	21:2:303:XAT:H161	1.97	0.46
21:7:303:XAT:H31	21:7:303:XAT:H391	1.73	0.46
9:a:342:TRP:CD1	23:a:826:CLA:H192	2.51	0.46
23:a:803:CLA:C18	23:b:810:CLA:HMC1	2.44	0.46
10:b:392:PHE:CE2	30:b:847:BCR:HC42	2.51	0.46
23:b:801:CLA:H91	23:b:801:CLA:H111	1.70	0.46
3:8:166:MET:O	3:8:170:GLU:HG3	2.16	0.46
23:8:308:CLA:HBA1	23:8:308:CLA:H11	1.78	0.46
7:2:131:ALA:HA	7:2:134:VAL:HG12	1.98	0.46
23:2:316:CLA:C1C	28:2:317:LMG:H111	2.46	0.46
4:7:37:SER:HB2	4:7:45:ARG:HA	1.97	0.46
4:7:120:ALA:O	4:7:124:ILE:HG13	2.16	0.46
9:a:282:LEU:HD21	9:a:367:MET:HB3	1.98	0.46
23:a:826:CLA:H141	23:a:826:CLA:H161	1.81	0.46
14:h:112:ILE:O	14:h:115:GLY:N	2.49	0.46
28:j:103:LMG:H292	28:j:103:LMG:H111	1.98	0.46
22:9:306:A1L1G:C31	23:9:310:CLA:HBD	2.46	0.46
21:4:301:XAT:H30	23:4:309:CLA:H151	1.98	0.46
23:4:316:CLA:CGD	27:4:317:DGD:HE61	2.45	0.46
23:6:314:CLA:O1A	23:6:314:CLA:H2A	2.15	0.46
8:1:89:VAL:O	8:1:93:TRP:N	2.49	0.46
23:a:804:CLA:H41	23:a:841:CLA:HMC1	1.98	0.46
23:a:841:CLA:H18	23:a:856:CLA:C5	2.43	0.46
12:e:32:VAL:HG11	20:c:35:LYS:CD	2.46	0.46
13:f:119:GLY:HA3	13:f:160:TRP:CE2	2.51	0.46
14:h:65:ILE:O	14:h:123:GLN:NE2	2.49	0.46
17:l:168:TYR:O	17:l:172:LEU:HB2	2.15	0.46
26:m:101:LHG:H291	26:m:101:LHG:H321	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:82:HIS:HB3	3:8:181:MET:SD	2.56	0.46
28:2:317:LMG:H321	28:2:317:LMG:H292	1.35	0.46
21:7:304:XAT:H15	21:7:304:XAT:H201	1.73	0.46
9:a:665:ILE:HG23	23:a:809:CLA:H171	1.98	0.46
9:a:677:LEU:HB2	23:a:802:CLA:HMC2	1.97	0.46
23:a:841:CLA:HBA2	23:b:832:CLA:H51	1.97	0.46
10:b:385:PHE:HB3	10:b:536:LEU:HB3	1.97	0.46
22:9:301:A1L1G:O13	21:9:304:XAT:H28	2.16	0.45
21:7:301:XAT:H15	21:7:301:XAT:H201	1.82	0.45
10:b:50:HIS:HE1	23:b:805:CLA:H171	1.81	0.45
10:b:339:LEU:O	10:b:343:THR:HG22	2.16	0.45
23:b:822:CLA:HHC	23:b:841:CLA:HED1	1.98	0.45
30:b:843:BCR:H11C	30:b:843:BCR:H341	1.74	0.45
26:b:849:LHG:H101	23:h:201:CLA:H142	1.97	0.45
15:i:28:LEU:O	15:i:32:LYS:HG3	2.15	0.45
3:8:171:VAL:HG13	3:8:175:LYS:HE3	1.97	0.45
5:3:179:PRO:C	5:3:181:LYS:H	2.24	0.45
21:2:303:XAT:H35	21:2:303:XAT:H401	1.71	0.45
8:1:137:LEU:HD12	17:l:25:ALA:HB1	1.97	0.45
23:1:311:CLA:H62	23:a:844:CLA:H93	1.96	0.45
9:a:574:GLY:CA	10:b:670:ARG:NH1	2.79	0.45
10:b:268:LEU:HD23	10:b:271:MET:HE3	1.98	0.45
23:b:817:CLA:H41	23:b:834:CLA:HAA2	1.98	0.45
23:b:818:CLA:H3A	23:b:818:CLA:HBA2	1.37	0.45
23:b:823:CLA:HHB	23:b:841:CLA:O1D	2.16	0.45
20:c:3:HIS:HB2	20:c:48:CYS:SG	2.56	0.45
1:5:124:MET:HE3	23:5:313:CLA:HMC2	1.98	0.45
21:9:304:XAT:H35	21:9:304:XAT:H401	1.86	0.45
3:8:93:TRP:CE2	3:8:111:PRO:HG2	2.51	0.45
21:6:305:XAT:H11	21:6:305:XAT:H191	1.84	0.45
4:7:85:MET:HE3	4:7:177:ASN:HB3	1.98	0.45
9:a:114:ILE:O	9:a:117:GLN:HG2	2.15	0.45
9:a:312:GLY:HA2	23:a:823:CLA:HMD2	1.98	0.45
1:5:232:HIS:HE1	21:5:305:XAT:H14	1.81	0.45
23:5:310:CLA:H92	23:5:310:CLA:H61	1.77	0.45
21:3:304:XAT:H35	21:3:304:XAT:H401	1.68	0.45
6:6:153:ASP:OD1	6:6:155:THR:OG1	2.26	0.45
21:6:303:XAT:H15	21:6:303:XAT:H201	1.64	0.45
21:2:301:XAT:H35	21:2:301:XAT:H401	1.75	0.45
21:2:305:XAT:H31	21:2:305:XAT:H391	1.71	0.45
23:7:308:CLA:H91	23:7:308:CLA:H112	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:806:CLA:H162	23:a:806:CLA:H141	1.59	0.45
23:a:806:CLA:H62	23:a:806:CLA:H2	1.67	0.45
23:a:822:CLA:H12	23:a:825:CLA:HBA2	1.99	0.45
10:b:228:TRP:HZ3	30:b:850:BCR:H363	1.82	0.45
23:b:839:CLA:H62	23:b:839:CLA:H41	1.71	0.45
11:d:15:GLY:HA2	17:l:12:PRO:O	2.15	0.45
16:j:26:VAL:CG1	30:j:102:BCR:H403	2.47	0.45
4:4:37:SER:HB3	4:4:45:ARG:HA	1.98	0.45
21:4:303:XAT:H15	21:4:303:XAT:H201	1.87	0.45
21:7:304:XAT:H191	23:7:314:CLA:HAB	1.97	0.45
8:1:141:ARG:HD3	8:1:149:TRP:HB3	1.99	0.45
9:a:25:PRO:HB2	9:a:41:TRP:HH2	1.81	0.45
9:a:71:PHE:HD1	9:a:166:MET:HE3	1.82	0.45
9:a:447:GLY:HA3	23:a:835:CLA:HAB	1.99	0.45
23:b:825:CLA:HAA2	23:b:826:CLA:OBD	2.16	0.45
21:5:303:XAT:H15	21:5:303:XAT:H201	1.74	0.45
2:9:80:ALA:O	2:9:84:ASN:ND2	2.49	0.45
23:4:310:CLA:O2D	23:4:310:CLA:H2A	2.17	0.45
4:7:78:ILE:HG12	4:7:175:LEU:HD21	1.99	0.45
21:7:304:XAT:H171	23:7:315:CLA:HBB1	1.99	0.45
9:a:194:HIS:ND1	23:a:826:CLA:OBD	2.48	0.45
23:a:852:CLA:H122	23:a:852:CLA:H162	1.61	0.45
10:b:280:VAL:HG21	23:b:816:CLA:HAB	1.98	0.45
23:b:809:CLA:H142	23:b:809:CLA:H111	1.83	0.45
23:b:824:CLA:H92	23:b:824:CLA:H61	1.72	0.45
23:b:835:CLA:H62	23:b:835:CLA:H41	1.86	0.45
30:b:844:BCR:H15C	30:b:844:BCR:H351	1.78	0.45
5:3:121:GLN:HA	5:3:124:VAL:HG12	1.99	0.45
4:7:170:MET:HE2	23:7:313:CLA:H12	1.99	0.45
23:a:813:CLA:H62	23:a:813:CLA:H41	1.85	0.45
10:b:605:GLN:HE21	10:b:734:LYS:HB3	1.82	0.45
10:b:689:LEU:HD22	23:l:202:CLA:HMD2	1.98	0.45
23:b:812:CLA:H3A	23:b:812:CLA:HBA2	1.61	0.45
15:i:14:VAL:O	15:i:19:PRO:HD2	2.17	0.45
1:5:116:GLU:HB2	23:5:308:CLA:C1B	2.46	0.45
23:5:315:CLA:H11	23:4:310:CLA:CHB	2.47	0.45
9:a:375:ILE:HG21	9:a:510:VAL:HB	1.97	0.45
23:a:801:CLA:CED	23:a:801:CLA:HAA2	2.46	0.45
17:l:9:ARG:NH2	19:g:54:UNK:CB	2.79	0.45
7:2:65:ILE:HG22	7:2:67:PHE:H	1.80	0.45
21:1:303:XAT:H35	21:1:303:XAT:H401	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:407:VAL:HG11	9:a:564:PHE:N	2.32	0.45
23:a:806:CLA:H202	23:a:806:CLA:H161	1.70	0.45
23:a:834:CLA:H202	23:a:834:CLA:H162	1.79	0.45
23:a:840:CLA:H112	23:a:840:CLA:H152	1.80	0.45
2:9:120:TRP:HH2	23:9:316:CLA:C4	2.28	0.45
6:6:132:PHE:O	6:6:136:ILE:HG12	2.17	0.45
8:1:105:PRO:C	8:1:107:LYS:H	2.24	0.45
10:b:26:ALA:HB1	27:b:851:DGD:O1B	2.17	0.45
10:b:343:THR:HG23	10:b:377:ALA:HB2	1.99	0.45
23:b:808:CLA:H93	23:b:808:CLA:H62	1.80	0.45
23:b:813:CLA:H143	23:b:824:CLA:H51	1.99	0.45
14:h:107:SER:O	14:h:110:THR:OG1	2.32	0.45
16:j:14:LEU:HD23	16:j:14:LEU:HA	1.84	0.45
21:5:302:XAT:H15	21:5:302:XAT:H201	1.85	0.44
3:8:72:LEU:HD13	23:8:307:CLA:HED1	1.99	0.44
6:6:121:GLU:OE2	23:6:308:CLA:C1B	2.65	0.44
4:7:77:GLU:HB2	23:7:308:CLA:CHB	2.48	0.44
8:1:40:ASP:HB2	8:1:42:MET:HG3	1.97	0.44
8:1:95:PRO:HD2	23:1:308:CLA:HMD3	1.99	0.44
9:a:304:MET:HG3	23:a:823:CLA:C3C	2.47	0.44
23:a:803:CLA:H18	23:b:810:CLA:HMC1	1.99	0.44
11:d:20:TRP:HB2	11:d:24:ALA:HB3	1.99	0.44
13:f:114:PHE:HE1	30:f:801:BCR:C34	2.30	0.44
13:f:114:PHE:HD1	30:f:801:BCR:H343	1.76	0.44
30:j:102:BCR:H15C	30:j:102:BCR:H351	1.78	0.44
3:8:138:LEU:HB2	23:8:311:CLA:HMA1	1.99	0.44
21:2:303:XAT:H15	21:2:303:XAT:H201	1.79	0.44
8:1:144:ASP:OD2	8:1:148:THR:OG1	2.23	0.44
23:b:839:CLA:C1	30:i:102:BCR:H351	2.44	0.44
23:b:841:CLA:H141	23:b:841:CLA:H161	1.74	0.44
21:8:301:XAT:H382	23:8:312:CLA:HAC2	1.99	0.44
21:7:304:XAT:H32	23:7:313:CLA:HAB	1.98	0.44
23:a:806:CLA:H72	30:a:848:BCR:HC8	1.98	0.44
23:a:825:CLA:H62	23:a:825:CLA:H41	1.84	0.44
23:b:840:CLA:H3A	23:b:840:CLA:HBA1	1.59	0.44
13:f:114:PHE:HE1	30:f:801:BCR:C9	2.30	0.44
14:h:72:PRO:CG	25:h:202:A1L1F:C56	2.96	0.44
21:9:305:XAT:H11	21:9:305:XAT:H191	1.60	0.44
8:1:171:ARG:HA	8:1:174:MET:HE3	2.00	0.44
23:a:835:CLA:H141	23:a:835:CLA:H161	1.84	0.44
10:b:526:ALA:HB2	23:b:837:CLA:HMA1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:82:SER:O	14:h:86:HIS:ND1	2.27	0.44
4:4:170:MET:CE	23:4:312:CLA:H12	2.47	0.44
23:4:309:CLA:CGA	23:4:309:CLA:C1A	2.96	0.44
21:6:302:XAT:H11	21:6:302:XAT:H191	1.65	0.44
21:6:306:XAT:H31	21:6:306:XAT:H391	1.84	0.44
30:a:849:BCR:H371	30:a:849:BCR:H24C	1.86	0.44
23:b:836:CLA:H12	23:b:837:CLA:O1A	2.18	0.44
30:b:847:BCR:H20C	30:b:847:BCR:H361	1.86	0.44
13:f:160:TRP:CG	13:f:161:PRO:HD3	2.52	0.44
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.44
2:9:37:VAL:HG11	10:b:158:SER:HA	1.97	0.44
2:9:207:VAL:HG21	23:9:308:CLA:H191	1.99	0.44
6:6:85:PHE:HB3	6:6:93:PRO:HA	1.99	0.44
21:1:303:XAT:H183	23:1:308:CLA:C2B	2.47	0.44
9:a:415:ASN:O	9:a:421:ASP:HB2	2.18	0.44
23:a:828:CLA:H122	23:a:828:CLA:H162	1.66	0.44
23:b:823:CLA:HBA1	30:b:846:BCR:H16C	1.98	0.44
14:h:112:ILE:O	14:h:113:SER:C	2.60	0.44
20:c:59:PRO:HD2	31:c:102:SF4:S2	2.58	0.44
2:9:120:TRP:CH2	23:9:316:CLA:C4	2.97	0.44
4:4:175:LEU:HD23	4:4:175:LEU:HA	1.87	0.44
4:4:193:ALA:HB1	27:4:317:DGD:O5E	2.15	0.44
9:a:73:GLN:HG2	23:a:806:CLA:H3A	2.00	0.44
9:a:84:MET:SD	23:a:829:CLA:HED1	2.58	0.44
23:a:807:CLA:H43	26:a:845:LHG:H252	2.00	0.44
23:a:807:CLA:H92	23:a:807:CLA:H61	1.69	0.44
23:a:829:CLA:H91	23:a:831:CLA:H192	2.00	0.44
23:a:852:CLA:HMB1	10:b:436:LEU:HD13	2.00	0.44
10:b:201:ARG:HG2	10:b:248:SER:HB2	1.99	0.44
11:d:121:ILE:HD13	20:c:8:TYR:CZ	2.52	0.44
23:j:101:CLA:O1D	23:j:101:CLA:H2A	2.18	0.44
28:j:103:LMG:H122	28:j:103:LMG:H151	1.56	0.44
2:9:144:HIS:CD2	23:9:314:CLA:HBC3	2.53	0.44
6:6:124:HIS:CB	6:6:231:MET:HE2	2.47	0.44
21:6:303:XAT:H31	21:6:303:XAT:H391	1.87	0.44
23:2:310:CLA:H162	23:2:310:CLA:H192	1.71	0.44
9:a:127:ASN:ND2	13:f:57:GLU:OE2	2.51	0.44
9:a:532:HIS:CE1	9:a:599:VAL:HA	2.53	0.44
9:a:684:ARG:HH21	10:b:567:GLY:HA3	1.83	0.44
23:a:827:CLA:H13	23:a:827:CLA:H172	1.77	0.44
10:b:518:ASP:OD2	10:b:595:TYR:OH	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:654:PHE:O	10:b:658:VAL:HG23	2.17	0.44
23:b:817:CLA:H3A	23:b:817:CLA:HBA2	1.26	0.44
13:f:79:ARG:O	13:f:83:SER:HB2	2.17	0.44
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.44
21:5:303:XAT:H383	23:5:310:CLA:C2B	2.48	0.44
23:5:310:CLA:H93	23:5:310:CLA:H111	1.84	0.44
2:9:93:ILE:CG1	21:9:304:XAT:H8	2.47	0.44
25:9:302:A1L1F:C42	23:9:311:CLA:O1A	2.66	0.44
3:8:47:PRO:HG2	3:8:50:LEU:HG	2.00	0.44
25:8:304:A1L1F:C5	18:m:23:ARG:HD3	2.48	0.44
6:6:189:TRP:CZ3	21:6:305:XAT:H363	2.53	0.44
6:6:242:PHE:HZ	21:6:305:XAT:H183	1.83	0.44
7:2:118:LEU:HB2	7:2:123:TYR:HD2	1.83	0.44
21:7:305:XAT:H201	21:7:305:XAT:H15	1.69	0.44
9:a:517:MET:HE2	9:a:611:VAL:HA	2.00	0.44
10:b:172:ARG:HD2	23:b:824:CLA:OBD	2.18	0.44
10:b:585:MET:HE3	10:b:585:MET:HB3	1.83	0.44
23:b:828:CLA:H41	23:b:828:CLA:H61	1.75	0.44
21:9:304:XAT:H15	21:9:304:XAT:H201	1.76	0.43
23:4:307:CLA:H192	23:4:307:CLA:H161	1.76	0.43
5:3:189:GLU:HB2	23:3:313:CLA:C1B	2.47	0.43
21:7:303:XAT:H15	21:7:303:XAT:H201	1.78	0.43
24:1:315:SQD:H161	24:1:315:SQD:H132	1.72	0.43
9:a:52:PHE:CD2	23:a:806:CLA:HMC2	2.53	0.43
9:a:578:GLN:HA	9:a:583:ASP:OD2	2.18	0.43
23:a:805:CLA:H52	23:a:805:CLA:H12	1.77	0.43
23:a:826:CLA:HMB3	23:a:826:CLA:HBB1	1.99	0.43
30:a:848:BCR:H15C	30:a:848:BCR:H351	1.78	0.43
10:b:172:ARG:HB2	23:b:813:CLA:HBC2	2.00	0.43
21:5:302:XAT:H11	21:5:302:XAT:H191	1.86	0.43
23:9:314:CLA:H2A	23:9:314:CLA:O2D	2.17	0.43
4:4:59:PHE:HE1	23:4:305:CLA:HBC3	1.83	0.43
21:4:304:XAT:H35	21:4:304:XAT:H401	1.77	0.43
6:6:194:ASP:OD1	6:6:194:ASP:N	2.48	0.43
21:6:302:XAT:H15	21:6:302:XAT:H201	1.71	0.43
8:1:152:VAL:HG11	8:1:159:TRP:CD1	2.53	0.43
9:a:580:SER:HB2	9:a:582:TRP:H	1.82	0.43
23:b:824:CLA:H41	23:b:824:CLA:H62	1.78	0.43
25:6:301:A1L1F:C42	23:6:315:CLA:O1D	2.67	0.43
21:2:304:XAT:H31	21:2:304:XAT:H391	1.85	0.43
4:7:142:MET:C	4:7:144:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:58:ALA:HB1	8:1:66:LEU:HD21	2.01	0.43
9:a:364:MET:HE1	23:a:830:CLA:CAD	2.49	0.43
10:b:208:ASP:OD1	10:b:208:ASP:N	2.44	0.43
10:b:547:LYS:CG	13:f:182:THR:HG22	2.45	0.43
23:b:827:CLA:H61	23:b:827:CLA:H102	1.85	0.43
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.43
3:8:47:PRO:HG3	3:8:61:ASP:HB3	2.01	0.43
23:4:305:CLA:CHA	23:4:305:CLA:HBA1	2.48	0.43
23:4:308:CLA:HBA1	23:4:308:CLA:H3A	1.77	0.43
5:3:172:PRO:HD2	21:3:305:XAT:H242	2.00	0.43
9:a:367:MET:HG2	9:a:500:SER:HB2	1.99	0.43
10:b:259:PHE:CZ	10:b:510:LEU:HD12	2.52	0.43
10:b:689:LEU:HD13	30:b:853:BCR:HC31	2.00	0.43
30:b:843:BCR:H351	30:b:843:BCR:H15C	1.73	0.43
30:i:102:BCR:H24C	17:l:96:LEU:HG	2.01	0.43
17:l:75:LEU:HD23	17:l:75:LEU:HA	1.89	0.43
21:9:303:XAT:H15	21:9:303:XAT:H201	1.71	0.43
21:3:301:XAT:H35	21:3:301:XAT:H401	1.81	0.43
10:b:689:LEU:HB2	30:b:853:BCR:C2	2.48	0.43
23:b:804:CLA:H61	23:b:804:CLA:H2	1.62	0.43
30:b:853:BCR:H15C	30:b:853:BCR:H351	1.82	0.43
20:c:25:VAL:HG21	20:c:48:CYS:HA	1.99	0.43
2:9:83:TRP:O	2:9:87:HIS:ND1	2.51	0.43
23:9:316:CLA:HMC2	15:i:17:VAL:HG21	2.01	0.43
4:4:183:LEU:HD11	23:4:307:CLA:HAC1	2.00	0.43
8:1:128:GLU:HG3	21:1:302:XAT:H372	2.01	0.43
23:a:820:CLA:CAD	23:a:830:CLA:H41	2.48	0.43
23:a:822:CLA:OBD	23:a:824:CLA:HMD3	2.19	0.43
23:a:829:CLA:H101	30:j:102:BCR:H341	1.99	0.43
10:b:274:HIS:HB2	23:b:817:CLA:CHB	2.48	0.43
10:b:345:LEU:CD1	23:b:826:CLA:HAA1	2.49	0.43
10:b:424:LEU:HG	23:b:838:CLA:CBB	2.48	0.43
23:b:801:CLA:H143	23:b:839:CLA:C14	2.36	0.43
23:b:810:CLA:H2	23:b:810:CLA:H61	1.88	0.43
2:9:120:TRP:CD1	2:9:121:VAL:HG13	2.53	0.43
3:8:63:MET:HE2	23:b:812:CLA:H52	2.00	0.43
21:6:306:XAT:H35	21:6:306:XAT:H401	1.71	0.43
22:7:302:A1L1G:O9	23:7:311:CLA:O1A	2.37	0.43
8:1:82:LEU:HD11	23:1:311:CLA:HBC1	2.01	0.43
23:1:311:CLA:C3	23:a:844:CLA:C9	2.97	0.43
9:a:143:ALA:HB2	9:a:371:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:684:ARG:O	9:a:685:GLY:C	2.60	0.43
23:a:801:CLA:HBD	23:a:801:CLA:HED2	1.48	0.43
23:a:820:CLA:H3A	23:a:820:CLA:HBA2	1.48	0.43
10:b:440:VAL:HG12	23:b:833:CLA:HAC1	2.01	0.43
10:b:569:THR:HG22	10:b:572:ILE:HD12	2.01	0.43
11:d:81:ASN:H	11:d:81:ASN:ND2	2.16	0.43
20:c:54:CYS:SG	20:c:55:GLU:N	2.91	0.43
21:4:304:XAT:H15	21:4:304:XAT:H201	1.71	0.43
23:4:316:CLA:H92	23:4:316:CLA:H62	1.83	0.43
4:7:81:CYS:SG	4:7:175:LEU:HD23	2.59	0.43
4:7:112:HIS:O	4:7:116:VAL:HG13	2.18	0.43
9:a:567:PRO:HB3	9:a:714:ILE:HB	2.00	0.43
10:b:597:HIS:CE1	10:b:727:VAL:HG23	2.54	0.43
30:b:845:BCR:H24C	30:b:845:BCR:H371	1.70	0.43
30:f:804:BCR:H341	30:f:804:BCR:H11C	1.73	0.43
17:l:116:VAL:HG11	17:l:128:LEU:C	2.43	0.43
2:9:218:LEU:HD23	2:9:218:LEU:HA	1.84	0.43
4:4:85:MET:HE3	4:4:177:ASN:HB3	2.01	0.43
21:2:305:XAT:H35	21:2:305:XAT:H401	1.74	0.43
9:a:361:ALA:HB2	9:a:387:HIS:HB2	2.01	0.43
9:a:701:LEU:HD12	23:a:841:CLA:HMA2	2.00	0.43
9:a:727:LEU:HD22	23:a:842:CLA:HMA3	2.01	0.43
23:a:803:CLA:O1A	23:a:803:CLA:H3A	2.19	0.43
21:a:854:XAT:H173	21:a:854:XAT:H3	1.82	0.43
10:b:140:LEU:HD23	10:b:143:LEU:HD12	2.01	0.43
23:b:814:CLA:H2	23:b:814:CLA:H61	1.77	0.43
23:b:816:CLA:CHD	23:b:817:CLA:HBB2	2.49	0.43
12:e:16:TYR:CD2	12:e:44:ASN:HA	2.54	0.43
30:f:804:BCR:H20C	30:f:804:BCR:H361	1.88	0.43
21:9:303:XAT:H7	23:9:309:CLA:HAB	2.01	0.43
23:9:308:CLA:H93	23:9:308:CLA:H111	1.70	0.43
4:4:75:GLU:OE1	4:4:148:ARG:NH2	2.47	0.43
21:3:305:XAT:H15	21:3:305:XAT:H201	1.85	0.43
4:7:36:LYS:HB2	4:7:45:ARG:H	1.83	0.43
4:7:87:ALA:HB1	21:7:303:XAT:H161	2.01	0.43
21:7:304:XAT:H30	23:7:313:CLA:H71	2.01	0.43
23:a:844:CLA:C1C	26:a:846:LHG:HC31	2.48	0.43
30:a:847:BCR:H15C	30:a:847:BCR:H351	1.84	0.43
23:b:810:CLA:CED	30:b:853:BCR:H392	2.48	0.43
23:b:810:CLA:HMB3	23:b:810:CLA:HBB1	2.00	0.43
11:d:88:TYR:HB3	11:d:89:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:8:301:XAT:H15	21:8:301:XAT:H201	1.84	0.42
5:3:103:ILE:HD11	21:3:304:XAT:H363	2.01	0.42
7:2:205:PHE:CD2	21:2:303:XAT:H12	2.54	0.42
8:1:168:ASN:HA	8:1:171:ARG:HD2	2.01	0.42
21:1:302:XAT:H31	21:1:302:XAT:H391	1.88	0.42
9:a:165:LEU:HD23	9:a:165:LEU:HA	1.90	0.42
9:a:565:ARG:HD2	26:a:845:LHG:HC61	2.00	0.42
23:a:832:CLA:HBA1	23:a:832:CLA:H3A	1.81	0.42
23:a:833:CLA:O1A	17:l:22:THR:HG22	2.19	0.42
23:a:841:CLA:H51	30:f:801:BCR:C17	2.48	0.42
30:a:849:BCR:H11C	30:a:849:BCR:H341	1.84	0.42
30:a:850:BCR:H20C	30:a:850:BCR:H361	1.80	0.42
10:b:302:ILE:HD13	23:b:822:CLA:HMD2	1.99	0.42
10:b:461:PHE:CZ	23:f:803:CLA:HBB1	2.54	0.42
10:b:565:GLY:C	10:b:567:GLY:N	2.74	0.42
23:b:832:CLA:C3C	30:b:852:BCR:H332	2.49	0.42
23:h:201:CLA:H162	23:h:201:CLA:H141	1.78	0.42
17:l:53:THR:HG22	23:l:201:CLA:C1B	2.49	0.42
21:4:304:XAT:H363	21:3:301:XAT:C10	2.49	0.42
21:2:302:XAT:H15	21:2:302:XAT:H201	1.82	0.42
9:a:271:PHE:HE2	9:a:495:ALA:HB2	1.84	0.42
23:a:807:CLA:H102	23:a:807:CLA:H161	2.00	0.42
23:a:833:CLA:H43	17:l:21:ILE:HG23	2.00	0.42
30:a:847:BCR:H361	30:a:847:BCR:H20C	1.80	0.42
10:b:647:VAL:HG21	23:b:808:CLA:HAC1	2.00	0.42
30:b:852:BCR:H20C	30:b:852:BCR:H361	1.76	0.42
1:5:98:PHE:HE1	23:5:306:CLA:HBC3	1.84	0.42
21:6:303:XAT:H35	21:6:303:XAT:H401	1.83	0.42
21:2:304:XAT:H15	21:2:304:XAT:H201	1.91	0.42
21:7:303:XAT:H362	23:7:308:CLA:H2	2.01	0.42
21:7:303:XAT:C36	23:7:308:CLA:H2	2.49	0.42
21:7:305:XAT:H11	21:7:305:XAT:H191	1.84	0.42
24:1:315:SQD:H311	24:1:315:SQD:H282	1.84	0.42
9:a:357:SER:HB2	23:a:830:CLA:HMC2	2.01	0.42
28:a:855:LMG:H112	28:a:855:LMG:HC92	1.98	0.42
10:b:207:TRP:HE1	23:b:814:CLA:H11	1.84	0.42
10:b:500:LEU:HA	10:b:503:ILE:HG22	2.02	0.42
23:b:833:CLA:HED1	16:j:37:LEU:HD13	2.00	0.42
30:b:852:BCR:H11C	30:b:852:BCR:H341	1.73	0.42
4:7:71:SER:HB3	4:7:142:MET:CE	2.49	0.42
9:a:194:HIS:HE1	23:a:826:CLA:H72	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:831:CLA:H93	23:a:842:CLA:HED3	2.01	0.42
23:a:841:CLA:H141	23:a:856:CLA:O2A	2.20	0.42
23:b:801:CLA:CBC	30:b:848:BCR:C38	2.97	0.42
23:b:806:CLA:H161	23:b:806:CLA:H102	2.01	0.42
23:b:807:CLA:H93	23:b:807:CLA:H61	1.71	0.42
23:b:814:CLA:CHA	23:b:814:CLA:HBA1	2.49	0.42
11:d:32:ILE:HG21	11:d:70:LEU:HD23	2.00	0.42
13:f:114:PHE:CE1	30:f:801:BCR:C9	3.02	0.42
15:i:30:ILE:CG2	30:i:102:BCR:H322	2.48	0.42
30:i:102:BCR:H11C	30:i:102:BCR:H341	1.84	0.42
21:5:302:XAT:H31	21:5:302:XAT:H391	1.88	0.42
7:2:109:TRP:CE3	21:2:303:XAT:H22	2.54	0.42
21:2:304:XAT:H11	21:2:304:XAT:H191	1.89	0.42
23:a:812:CLA:H142	23:a:812:CLA:H112	1.85	0.42
23:a:823:CLA:CHD	21:a:854:XAT:H183	2.49	0.42
10:b:140:LEU:HD23	10:b:140:LEU:HA	1.86	0.42
10:b:220:LEU:HD23	10:b:220:LEU:HA	1.87	0.42
21:5:301:XAT:H383	23:5:308:CLA:HBC1	2.01	0.42
21:5:305:XAT:H31	21:5:305:XAT:H391	1.93	0.42
23:5:310:CLA:H202	23:5:310:CLA:H161	1.89	0.42
2:9:138:ALA:O	2:9:142:ILE:HG12	2.19	0.42
2:9:222:ASP:OD1	2:9:227:GLY:HA2	2.19	0.42
3:8:172:LYS:HD3	23:8:313:CLA:HAA2	2.01	0.42
21:4:301:XAT:H11	21:4:301:XAT:H191	1.89	0.42
9:a:75:ALA:HB2	9:a:166:MET:HB2	2.01	0.42
23:a:827:CLA:H3A	23:a:827:CLA:HBA2	1.79	0.42
10:b:120:GLU:OE2	10:b:362:ASN:ND2	2.39	0.42
10:b:626:LEU:HD22	23:b:802:CLA:HMD3	2.01	0.42
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.42
1:5:149:VAL:HG22	21:5:305:XAT:H182	2.02	0.42
2:9:91:GLY:HA3	21:9:303:XAT:O4	2.19	0.42
21:8:303:XAT:C34	23:8:313:CLA:HBB1	2.49	0.42
23:4:306:CLA:HBD	23:4:313:CLA:OBD	2.20	0.42
5:3:56:ASN:HB3	5:3:82:LEU:HD22	2.01	0.42
21:3:303:XAT:H35	21:3:303:XAT:H401	1.79	0.42
8:1:171:ARG:HA	8:1:174:MET:CE	2.49	0.42
9:a:525:ASP:HA	9:a:528:VAL:HG12	2.01	0.42
23:a:806:CLA:H72	30:a:848:BCR:C8	2.50	0.42
23:a:807:CLA:H161	23:a:807:CLA:H192	1.82	0.42
23:a:841:CLA:HED3	23:a:841:CLA:H2A	2.01	0.42
23:a:852:CLA:H93	23:a:852:CLA:H112	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:529:LEU:HD23	10:b:588:THR:HG21	2.00	0.42
23:b:832:CLA:H62	23:b:832:CLA:H2	1.80	0.42
21:4:302:XAT:H163	23:4:307:CLA:H2	2.02	0.42
21:3:304:XAT:H12	23:3:309:CLA:HAB	2.01	0.42
7:2:203:LEU:HD13	21:2:301:XAT:C10	2.50	0.42
21:2:303:XAT:H11	21:2:303:XAT:H191	1.66	0.42
9:a:67:PHE:HE2	9:a:173:HIS:CG	2.38	0.42
9:a:399:ALA:HB1	9:a:543:LEU:HB3	2.02	0.42
23:a:816:CLA:C4B	21:a:854:XAT:H242	2.50	0.42
23:a:840:CLA:H72	30:a:850:BCR:H373	2.01	0.42
23:a:841:CLA:HMD1	30:f:801:BCR:H383	2.01	0.42
21:a:853:XAT:H15	21:a:853:XAT:H201	1.82	0.42
10:b:471:LYS:HE2	10:b:471:LYS:HB2	1.89	0.42
23:b:827:CLA:H13	23:b:829:CLA:H141	2.02	0.42
21:5:301:XAT:H35	21:5:301:XAT:H401	1.66	0.42
2:9:198:VAL:HG12	21:9:304:XAT:H34	2.01	0.42
21:9:305:XAT:H15	21:9:305:XAT:H201	1.81	0.42
23:8:307:CLA:H203	23:8:307:CLA:H162	1.74	0.42
6:6:115:LYS:HE2	6:6:188:PHE:CE1	2.55	0.42
4:7:185:PHE:CE1	21:7:303:XAT:H162	2.53	0.42
8:1:54:PRO:HD2	21:1:303:XAT:H242	2.02	0.42
23:1:312:CLA:H42	24:1:315:SQD:H122	2.01	0.42
9:a:290:HIS:O	9:a:294:ILE:HG12	2.20	0.42
21:a:853:XAT:H35	21:a:853:XAT:H401	1.80	0.42
23:a:856:CLA:H142	23:a:856:CLA:H111	1.80	0.42
11:d:70:LEU:O	11:d:74:LEU:HG	2.19	0.42
21:5:302:XAT:H401	21:5:302:XAT:H35	1.77	0.42
21:9:305:XAT:H401	21:9:305:XAT:H35	1.74	0.42
8:1:140:TYR:OH	8:1:142:PRO:O	2.25	0.42
9:a:299:ILE:O	9:a:303:HIS:ND1	2.53	0.42
3:8:77:ALA:HB2	3:8:147:PRO:HB2	2.02	0.41
23:7:307:CLA:C3D	23:7:314:CLA:HMA3	2.50	0.41
8:1:71:GLU:HG2	8:1:142:PRO:O	2.20	0.41
23:a:826:CLA:H162	23:a:826:CLA:H202	1.79	0.41
23:a:831:CLA:H61	23:a:831:CLA:H92	1.70	0.41
10:b:220:LEU:HD21	30:b:843:BCR:H391	2.01	0.41
10:b:314:GLY:HA3	10:b:412:ARG:HD2	2.02	0.41
10:b:381:MET:HE1	30:b:847:BCR:H352	2.01	0.41
23:b:836:CLA:HBB1	23:b:836:CLA:HMB1	2.02	0.41
16:j:14:LEU:CD2	28:j:103:LMG:H141	2.49	0.41
2:9:204:VAL:HG22	23:9:308:CLA:H203	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:312:CLA:H11	23:3:312:CLA:H51	1.88	0.41
21:7:304:XAT:H31	21:7:304:XAT:H391	1.87	0.41
23:7:307:CLA:CAD	23:7:314:CLA:HMA3	2.51	0.41
23:b:804:CLA:HAA2	18:m:28:LEU:HB3	2.02	0.41
23:b:826:CLA:H141	23:b:826:CLA:H161	1.82	0.41
30:b:852:BCR:C21	16:j:40:PRO:HD3	2.50	0.41
20:c:32:ASP:OD1	20:c:32:ASP:N	2.53	0.41
1:5:143:TYR:OH	23:5:311:CLA:OBD	2.23	0.41
23:5:315:CLA:HBA1	23:5:315:CLA:H3A	1.96	0.41
21:8:302:XAT:H35	21:8:302:XAT:H401	1.76	0.41
21:4:304:XAT:H31	21:4:304:XAT:H391	1.62	0.41
21:2:302:XAT:H31	21:2:302:XAT:H391	1.83	0.41
4:7:174:GLU:HB2	23:7:313:CLA:C1B	2.50	0.41
9:a:293:ALA:HB1	23:a:818:CLA:HBC2	2.03	0.41
9:a:601:PHE:CZ	23:a:801:CLA:HED3	2.55	0.41
10:b:431:LEU:HD11	23:b:837:CLA:HMB1	2.03	0.41
23:b:808:CLA:C4A	23:b:808:CLA:HBA2	2.50	0.41
23:b:825:CLA:HBA2	23:b:825:CLA:H3A	1.72	0.41
2:9:217:ILE:HG21	23:9:314:CLA:HHB	2.01	0.41
6:6:121:GLU:OE2	23:6:308:CLA:C2B	2.68	0.41
7:2:178:LEU:HD23	7:2:178:LEU:HA	1.89	0.41
21:7:301:XAT:H35	21:7:301:XAT:H401	1.71	0.41
23:7:308:CLA:H142	23:7:308:CLA:H111	1.77	0.41
9:a:272:LYS:HG2	9:a:496:LEU:HD12	2.02	0.41
9:a:342:TRP:HB3	23:a:806:CLA:HAC1	2.02	0.41
9:a:356:LEU:HB2	23:a:828:CLA:H41	2.02	0.41
9:a:440:PHE:CE2	23:a:839:CLA:HAB	2.55	0.41
23:a:826:CLA:HMD2	23:a:826:CLA:H143	2.02	0.41
10:b:193:VAL:O	10:b:198:PRO:HD3	2.20	0.41
10:b:197:ILE:HB	10:b:198:PRO:HD3	2.02	0.41
10:b:668:SER:OG	10:b:673:TRP:NE1	2.52	0.41
10:b:689:LEU:CD1	30:b:853:BCR:C4	2.97	0.41
23:b:826:CLA:HED1	30:b:847:BCR:H21C	2.02	0.41
21:4:301:XAT:H15	21:4:301:XAT:H201	1.94	0.41
25:1:304:A1L1F:C10	23:a:844:CLA:C4	2.98	0.41
9:a:707:ILE:HD11	13:f:143:ILE:HG23	2.03	0.41
30:b:853:BCR:H352	23:l:202:CLA:HAB	2.01	0.41
23:9:314:CLA:H51	23:9:314:CLA:C1C	2.50	0.41
3:8:106:TYR:OH	23:8:310:CLA:OBD	2.28	0.41
21:8:301:XAT:H11	21:8:301:XAT:H191	1.84	0.41
6:6:137:VAL:HB	6:6:138:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:237:PHE:CE1	6:6:250:LEU:HD11	2.55	0.41
21:2:302:XAT:H35	21:2:302:XAT:H401	1.71	0.41
9:a:452:ASN:HD22	9:a:634:ILE:HB	1.85	0.41
23:a:818:CLA:OBD	23:a:837:CLA:HED2	2.21	0.41
10:b:342:ALA:HB2	23:b:824:CLA:H43	2.02	0.41
10:b:347:ALA:HB3	10:b:374:GLN:HE21	1.84	0.41
23:b:840:CLA:H18	30:i:101:BCR:C22	2.49	0.41
1:5:98:PHE:CD2	23:5:306:CLA:HMD2	2.56	0.41
23:4:316:CLA:HMB3	21:3:301:XAT:H392	2.03	0.41
21:3:304:XAT:H391	21:3:304:XAT:H31	1.78	0.41
7:2:57:PHE:CZ	21:2:305:XAT:H172	2.55	0.41
21:2:305:XAT:H11	21:2:305:XAT:H191	1.90	0.41
8:1:131:GLN:O	8:1:135:LYS:HG3	2.21	0.41
8:1:133:LYS:HD2	8:1:133:LYS:HA	1.82	0.41
10:b:4:LYS:HB3	10:b:4:LYS:HE2	1.48	0.41
10:b:702:LEU:HD22	10:b:706:GLN:NE2	2.35	0.41
23:b:832:CLA:H141	30:f:804:BCR:H10C	2.02	0.41
30:b:848:BCR:H15C	30:b:848:BCR:H351	1.85	0.41
11:d:114:VAL:HG21	20:c:43:PRO:HB3	2.03	0.41
30:i:102:BCR:H20C	30:i:102:BCR:H361	1.91	0.41
30:j:102:BCR:H20C	30:j:102:BCR:H361	1.91	0.41
3:8:153:ASP:OD1	21:8:303:XAT:O3	2.28	0.41
23:6:309:CLA:H152	23:6:309:CLA:H112	1.84	0.41
21:1:302:XAT:H15	21:1:302:XAT:H201	1.87	0.41
9:a:318:ILE:O	9:a:322:HIS:ND1	2.54	0.41
23:a:806:CLA:H52	30:a:848:BCR:HC8	2.03	0.41
10:b:585:MET:O	10:b:589:ILE:HG12	2.20	0.41
23:b:807:CLA:H122	23:b:807:CLA:H162	1.79	0.41
23:b:816:CLA:CBB	30:b:850:BCR:H14C	2.50	0.41
23:b:821:CLA:H12	23:b:822:CLA:H52	2.03	0.41
2:9:217:ILE:HB	23:9:314:CLA:H3A	2.02	0.41
3:8:184:ILE:HG21	21:8:302:XAT:H12	2.01	0.41
21:4:303:XAT:H35	21:4:303:XAT:H401	1.80	0.41
21:4:304:XAT:H11	21:4:304:XAT:H191	1.81	0.41
21:6:302:XAT:H31	21:6:302:XAT:H391	1.72	0.41
7:2:127:ASN:OD1	7:2:130:GLN:N	2.46	0.41
7:2:205:PHE:HE1	21:2:303:XAT:H162	1.84	0.41
4:7:160:PHE:CE2	21:7:304:XAT:H373	2.56	0.41
8:1:147:GLY:HA2	8:1:149:TRP:CZ3	2.55	0.41
9:a:370:TYR:OH	23:a:830:CLA:OBD	2.28	0.41
9:a:434:LEU:HG	9:a:541:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:466:SER:HG	9:a:631:GLN:HE22	1.64	0.41
9:a:499:VAL:HG12	23:a:819:CLA:H11	2.03	0.41
9:a:675:PHE:HZ	23:a:842:CLA:HBC2	1.86	0.41
10:b:433:PHE:CZ	30:f:801:BCR:H372	2.56	0.41
23:b:833:CLA:H41	23:b:833:CLA:H61	1.64	0.41
23:b:837:CLA:CMC	30:b:852:BCR:HC31	2.50	0.41
30:f:801:BCR:H11C	30:f:801:BCR:H341	1.95	0.41
2:9:72:LEU:HD23	2:9:72:LEU:HA	1.95	0.41
2:9:91:GLY:CA	21:9:303:XAT:H173	2.51	0.41
2:9:201:LEU:HD13	23:9:308:CLA:HBC1	2.03	0.41
21:8:302:XAT:H403	23:8:307:CLA:H202	2.02	0.41
23:4:308:CLA:HED2	23:4:308:CLA:HBD	1.83	0.41
4:7:59:PHE:HE1	23:7:306:CLA:HBC3	1.85	0.41
4:7:194:LEU:HD23	4:7:194:LEU:HA	1.89	0.41
23:1:306:CLA:H3A	23:1:306:CLA:O2A	2.20	0.41
10:b:86:PRO:HB3	10:b:119:TYR:CD2	2.56	0.41
10:b:182:GLY:HA3	10:b:283:ILE:HG13	2.03	0.41
3:8:55:ALA:HB1	3:8:171:VAL:HG23	2.03	0.40
21:8:303:XAT:H15	21:8:303:XAT:H201	1.72	0.40
6:6:135:VAL:HG13	21:6:303:XAT:H163	2.02	0.40
23:a:829:CLA:O1D	23:a:830:CLA:HMA1	2.21	0.40
23:a:842:CLA:H12	29:a:843:PQN:H301	2.02	0.40
30:a:849:BCR:H15C	30:a:849:BCR:H351	1.79	0.40
10:b:499:TRP:CD1	23:b:834:CLA:HED2	2.56	0.40
10:b:518:ASP:O	10:b:522:HIS:ND1	2.38	0.40
10:b:629:ASN:HA	10:b:734:LYS:HE2	2.02	0.40
11:d:121:ILE:CD1	20:c:8:TYR:CE1	3.04	0.40
26:m:101:LHG:H272	26:m:101:LHG:H302	1.86	0.40
1:5:117:LEU:HD23	1:5:117:LEU:HA	1.92	0.40
21:5:301:XAT:H31	21:5:301:XAT:H391	1.73	0.40
21:5:303:XAT:H35	21:5:303:XAT:H401	1.87	0.40
2:9:133:ILE:HD13	23:9:316:CLA:O1D	2.20	0.40
21:6:303:XAT:H28	23:6:308:CLA:H72	2.03	0.40
4:7:39:ALA:HB2	4:7:57:VAL:HG23	2.03	0.40
8:1:87:TRP:CG	8:1:180:LEU:HD13	2.56	0.40
9:a:226:SER:OG	9:a:229:GLU:HG2	2.21	0.40
23:b:801:CLA:C14	23:b:839:CLA:C11	2.84	0.40
23:b:826:CLA:HMB2	23:b:834:CLA:HBA1	2.03	0.40
11:d:89:PRO:HB2	11:d:90:PRO:HD3	2.03	0.40
20:c:64:SER:HB2	31:c:102:SF4:S3	2.62	0.40
21:8:303:XAT:H383	23:8:314:CLA:C3B	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:185:PHE:CD2	21:4:302:XAT:H32	2.57	0.40
21:4:302:XAT:H383	23:4:309:CLA:C2B	2.51	0.40
5:3:106:VAL:HG11	23:3:311:CLA:HED1	2.03	0.40
6:6:234:MET:HE3	6:6:234:MET:HB3	1.87	0.40
4:7:79:LYS:HB2	4:7:79:LYS:HE3	1.79	0.40
4:7:106:VAL:HG23	23:7:310:CLA:HED2	2.03	0.40
23:a:818:CLA:H62	23:a:818:CLA:H41	1.93	0.40
23:a:828:CLA:H61	23:a:828:CLA:H2	1.78	0.40
10:b:3:TYR:HD1	15:i:34:ASN:CG	2.29	0.40
10:b:346:THR:HG21	23:b:828:CLA:HHD	2.03	0.40
10:b:461:PHE:HB2	23:b:837:CLA:CAD	2.52	0.40
23:b:803:CLA:HHD	23:b:803:CLA:HBC2	2.03	0.40
21:8:302:XAT:H11	21:8:302:XAT:H191	1.71	0.40
21:8:302:XAT:H201	21:8:302:XAT:H15	1.73	0.40
4:4:54:VAL:HG11	4:4:171:GLN:HB3	2.04	0.40
9:a:452:ASN:HB3	9:a:635:THR:HG22	2.04	0.40
9:a:535:THR:HB	9:a:595:SER:HB2	2.04	0.40
9:a:586:PHE:CE1	9:a:722:VAL:HB	2.57	0.40
23:a:834:CLA:H143	23:a:834:CLA:H161	1.93	0.40
10:b:61:THR:HB	10:b:140:LEU:HD13	2.03	0.40
10:b:614:SER:O	10:b:620:GLY:HA3	2.21	0.40
10:b:709:LEU:CD1	27:b:851:DGD:HB41	2.51	0.40
11:d:121:ILE:HD13	20:c:8:TYR:CE1	2.56	0.40
13:f:129:ILE:HD13	13:f:129:ILE:HA	1.92	0.40
1:5:83:LEU:HD23	1:5:83:LEU:HA	1.94	0.40
7:2:92:ARG:NH2	23:2:308:CLA:HED3	2.36	0.40
7:2:125:GLY:O	7:2:127:ASN:N	2.44	0.40
21:1:303:XAT:H15	21:1:303:XAT:H201	1.85	0.40
23:1:308:CLA:H121	23:1:308:CLA:H8	1.97	0.40
9:a:406:PHE:HE2	9:a:424:ILE:HD11	1.86	0.40
9:a:586:PHE:CE1	9:a:590:PHE:HE2	2.39	0.40
23:a:804:CLA:H11	29:a:843:PQN:H201	2.04	0.40
23:a:841:CLA:C5	30:f:801:BCR:C17	2.97	0.40
10:b:434:HIS:CG	30:b:852:BCR:HC42	2.57	0.40
23:b:813:CLA:H161	23:b:813:CLA:H192	1.76	0.40
23:b:836:CLA:H11	23:b:836:CLA:H51	1.73	0.40
30:b:850:BCR:H20C	30:b:850:BCR:H361	1.88	0.40
11:d:27:GLU:O	11:d:89:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	25	57
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	22	54
4	7	164/202 (81%)	144 (88%)	20 (12%)	0	100	100
5	3	175/220 (80%)	166 (95%)	9 (5%)	0	100	100
6	6	178/259 (69%)	158 (89%)	20 (11%)	0	100	100
7	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	8	33
8	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
9	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	77
10	b	733/737 (100%)	697 (95%)	33 (4%)	3 (0%)	30	61
11	d	128/136 (94%)	112 (88%)	15 (12%)	1 (1%)	16	47
12	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
13	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
14	h	83/128 (65%)	77 (93%)	5 (6%)	1 (1%)	11	39
15	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
16	j	39/41 (95%)	39 (100%)	0	0	100	100
17	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	11	39
18	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
20	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3798/4357 (87%)	3546 (93%)	239 (6%)	13 (0%)	38	66

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	9	32	THR

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Mol	Chain	Res	Type
7	2	45	LYS
17	l	120	VAL
7	2	127	ASN
7	2	213	VAL
10	b	566	ARG
9	a	580	SER
10	b	569	THR
10	b	3	TYR
17	l	131	ILE
4	4	146	SER
11	d	132	PHE
14	h	90	ILE

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	5	133/182 (73%)	133 (100%)	0	100	100
2	9	141/167 (84%)	139 (99%)	2 (1%)	62	80
3	8	132/160 (82%)	131 (99%)	1 (1%)	79	89
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	122/159 (77%)	121 (99%)	1 (1%)	79	89
5	3	136/164 (83%)	136 (100%)	0	100	100
6	6	135/201 (67%)	134 (99%)	1 (1%)	81	90
7	2	134/172 (78%)	134 (100%)	0	100	100
8	1	128/165 (78%)	128 (100%)	0	100	100
9	a	607/613 (99%)	603 (99%)	4 (1%)	81	90
10	b	599/602 (100%)	595 (99%)	4 (1%)	81	90
11	d	107/113 (95%)	106 (99%)	1 (1%)	75	87
12	e	56/62 (90%)	56 (100%)	0	100	100
13	f	138/162 (85%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	h	71/107 (66%)	70 (99%)	1 (1%)	62	80
15	i	32/43 (74%)	32 (100%)	0	100	100
16	j	36/36 (100%)	36 (100%)	0	100	100
17	l	130/141 (92%)	130 (100%)	0	100	100
18	m	21/24 (88%)	21 (100%)	0	100	100
20	c	67/68 (98%)	67 (100%)	0	100	100
All	All	3058/3500 (87%)	3043 (100%)	15 (0%)	85	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	9	172	LYS
2	9	174	GLU
3	8	175	LYS
6	6	246	SER
4	7	95	ASP
9	a	428	ASP
9	a	448	LEU
9	a	579	VAL
9	a	580	SER
10	b	2	VAL
10	b	3	TYR
10	b	4	LYS
10	b	569	THR
11	d	133	GLN
14	h	110	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	133	GLN
2	9	104	HIS
3	8	156	ASN
4	4	123	GLN
5	3	211	HIS
8	1	63	GLN
8	1	119	GLN
8	1	132	ASN
8	1	194	GLN

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Mol	Chain	Res	Type
9	a	186	ASN
10	b	80	ASN
10	b	112	ASN
10	b	169	ASN
10	b	326	ASN
10	b	373	HIS
10	b	475	ASN
10	b	587	ASN
10	b	605	GLN
10	b	629	ASN
11	d	7	GLN
11	d	26	ASN
11	d	109	GLN
11	d	133	GLN
13	f	166	GLN
18	m	6	GLN
20	c	38	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

273 ligands are modelled in this entry.

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
23	CLA	1	307	-	54,62,73	1.63	5 (9%)	62,99,113	1.52	7 (11%)
23	CLA	4	315	-	46,54,73	1.77	5 (10%)	53,90,113	1.57	7 (13%)
23	CLA	3	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.57	8 (14%)
23	CLA	a	856	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	8 (10%)
21	XAT	2	305	-	39,47,47	0.92	0	54,74,74	2.43	18 (33%)
23	CLA	5	310	1	65,73,73	1.49	5 (7%)	76,113,113	1.37	7 (9%)
23	CLA	b	840	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	6	308	-	58,66,73	1.61	6 (10%)	67,104,113	1.43	6 (8%)
21	XAT	2	301	-	39,47,47	0.91	0	54,74,74	2.71	19 (35%)
23	CLA	a	830	-	65,73,73	1.48	7 (10%)	76,113,113	1.40	8 (10%)
21	XAT	3	303	-	39,47,47	0.90	0	54,74,74	2.59	20 (37%)
25	A1L1F	6	301	-	50,59,59	1.30	5 (10%)	62,85,85	2.49	20 (32%)
26	LHG	b	849	23	30,30,48	1.34	6 (20%)	33,36,54	1.14	2 (6%)
23	CLA	a	813	-	54,62,73	1.65	6 (11%)	62,99,113	1.45	7 (11%)
23	CLA	b	836	-	58,66,73	1.56	6 (10%)	67,104,113	1.53	8 (11%)
23	CLA	4	308	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	8 (13%)
28	LMG	a	855	-	34,34,55	1.14	2 (5%)	42,42,63	1.15	3 (7%)
23	CLA	2	313	7	41,49,73	1.85	5 (12%)	47,84,113	1.70	8 (17%)
23	CLA	a	812	23	62,70,73	1.51	6 (9%)	72,109,113	1.45	8 (11%)
21	XAT	2	303	-	39,47,47	0.98	1 (2%)	54,74,74	2.63	20 (37%)
23	CLA	8	313	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	7 (13%)
23	CLA	1	312	8	52,60,73	1.71	5 (9%)	60,97,113	1.48	8 (13%)
21	XAT	9	305	-	39,47,47	0.96	1 (2%)	54,74,74	2.36	18 (33%)
23	CLA	b	833	-	58,66,73	1.58	6 (10%)	67,104,113	1.42	8 (11%)
23	CLA	b	837	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	8 (10%)
21	XAT	6	305	-	39,47,47	0.89	1 (2%)	54,74,74	2.73	19 (35%)
30	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
23	CLA	5	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
23	CLA	4	313	4	45,53,73	1.80	6 (13%)	52,89,113	1.56	7 (13%)
28	LMG	j	103	-	32,32,55	1.13	2 (6%)	40,40,63	1.14	3 (7%)
23	CLA	b	809	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	9 (11%)
21	XAT	5	301	-	39,47,47	0.95	2 (5%)	54,74,74	2.62	19 (35%)
25	A1L1F	8	304	-	50,59,59	1.30	4 (8%)	62,85,85	2.79	23 (37%)
30	BCR	f	801	-	41,41,41	0.69	0	56,56,56	2.14	15 (26%)
23	CLA	a	822	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	8	312	3	52,60,73	1.65	5 (9%)	60,97,113	1.53	8 (13%)
23	CLA	6	313	-	52,60,73	1.66	5 (9%)	60,97,113	1.51	7 (11%)
23	CLA	9	308	2	65,73,73	1.49	7 (10%)	76,113,113	1.42	9 (11%)
23	CLA	a	810	9	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)
21	XAT	8	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.66	20 (37%)
22	A1L1G	9	301	-	38,47,47	1.46	6 (15%)	49,71,71	1.57	10 (20%)
23	CLA	a	801	-	65,73,73	1.51	8 (12%)	76,113,113	1.38	7 (9%)
23	CLA	b	831	-	49,57,73	1.69	5 (10%)	55,93,113	1.55	8 (14%)
27	DGD	4	317	-	41,41,67	1.06	2 (4%)	55,55,81	1.81	5 (9%)
30	BCR	b	844	-	41,41,41	0.71	0	56,56,56	1.92	16 (28%)
31	SF4	a	851	-	0,12,12	-	-	-	-	-
23	CLA	1	306	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	9 (11%)
23	CLA	b	806	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	b	832	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
21	XAT	9	303	-	39,47,47	0.94	1 (2%)	54,74,74	2.61	19 (35%)
30	BCR	b	846	-	41,41,41	0.71	0	56,56,56	1.97	21 (37%)
23	CLA	2	312	-	47,55,73	1.75	6 (12%)	54,91,113	1.56	7 (12%)
23	CLA	5	308	1	60,68,73	1.55	5 (8%)	70,107,113	1.42	8 (11%)
23	CLA	a	811	-	56,64,73	1.59	6 (10%)	65,102,113	1.47	9 (13%)
23	CLA	3	314	5	47,55,73	1.74	5 (10%)	54,91,113	1.55	7 (12%)
23	CLA	a	808	-	51,59,73	1.70	5 (9%)	59,96,113	1.51	8 (13%)
30	BCR	b	845	-	41,41,41	0.68	0	56,56,56	2.10	16 (28%)
26	LHG	a	846	23	26,26,48	1.27	4 (15%)	29,32,54	1.20	2 (6%)
21	XAT	6	303	-	39,47,47	0.89	0	54,74,74	2.65	19 (35%)
23	CLA	5	313	-	52,60,73	1.65	5 (9%)	60,97,113	1.54	9 (15%)
23	CLA	6	314	-	46,54,73	1.73	5 (10%)	53,90,113	1.61	6 (11%)
23	CLA	b	816	-	55,63,73	1.63	5 (9%)	64,101,113	1.48	9 (14%)
23	CLA	2	307	-	47,55,73	1.74	5 (10%)	54,91,113	1.64	8 (14%)
23	CLA	1	313	-	41,49,73	1.84	6 (14%)	47,84,113	1.65	7 (14%)
23	CLA	b	819	-	55,63,73	1.62	6 (10%)	64,101,113	1.44	8 (12%)
21	XAT	8	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.53	19 (35%)
21	XAT	5	305	-	39,47,47	0.90	0	54,74,74	2.86	22 (40%)
23	CLA	2	310	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
23	CLA	b	820	-	50,58,73	1.69	6 (12%)	58,95,113	1.60	10 (17%)
23	CLA	2	316	7	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.13	14 (25%)
23	CLA	b	823	-	53,61,73	1.63	6 (11%)	61,98,113	1.46	8 (13%)
27	DGD	8	315	23	41,41,67	1.05	2 (4%)	55,55,81	1.11	4 (7%)
23	CLA	a	834	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	9 (11%)
23	CLA	b	828	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
23	CLA	6	316	6	46,54,73	1.75	5 (10%)	53,90,113	1.58	6 (11%)
23	CLA	3	307	5	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
23	CLA	2	309	-	46,54,73	1.76	5 (10%)	53,90,113	1.54	7 (13%)
23	CLA	j	101	16	42,50,73	1.81	5 (11%)	48,85,113	1.64	6 (12%)
23	CLA	4	316	-	55,63,73	1.63	6 (10%)	64,101,113	1.45	7 (10%)
23	CLA	3	310	-	56,64,73	1.60	5 (8%)	65,102,113	1.45	7 (10%)
23	CLA	4	309	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
24	SQD	5	317	23	34,35,54	1.47	4 (11%)	43,46,65	1.35	7 (16%)
23	CLA	7	317	-	45,53,73	1.80	5 (11%)	52,89,113	1.59	6 (11%)
23	CLA	a	806	-	65,73,73	1.50	11 (16%)	76,113,113	1.67	13 (17%)
23	CLA	7	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.58	7 (13%)
23	CLA	3	309	5	56,64,73	1.59	6 (10%)	65,102,113	1.45	7 (10%)
22	A1L1G	9	306	-	38,47,47	1.41	6 (15%)	49,71,71	1.54	8 (16%)
23	CLA	a	837	9	45,53,73	1.79	5 (11%)	52,89,113	1.58	7 (13%)
23	CLA	b	839	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
23	CLA	b	825	-	64,72,73	1.49	6 (9%)	74,111,113	1.44	7 (9%)
23	CLA	7	313	-	54,62,73	1.65	5 (9%)	62,99,113	1.49	9 (14%)
23	CLA	a	838	-	51,59,73	1.66	5 (9%)	59,96,113	1.55	8 (13%)
26	LHG	9	307	-	35,35,48	1.22	6 (17%)	38,41,54	0.97	2 (5%)
21	XAT	2	304	-	39,47,47	0.88	0	54,74,74	2.54	20 (37%)
23	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	9	316	-	62,70,73	1.55	6 (9%)	72,109,113	1.37	8 (11%)
23	CLA	a	817	-	45,53,73	1.79	5 (11%)	52,89,113	1.58	6 (11%)
23	CLA	b	808	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	8 (10%)
23	CLA	9	309	2	46,54,73	1.77	6 (13%)	53,90,113	1.55	7 (13%)
23	CLA	a	816	-	50,58,73	1.69	6 (12%)	58,95,113	1.57	9 (15%)
23	CLA	a	829	-	62,70,73	1.51	5 (8%)	72,109,113	1.39	8 (11%)
23	CLA	9	315	2	42,50,73	1.83	5 (11%)	48,85,113	1.61	7 (14%)
22	A1L1G	3	306	-	38,47,47	1.45	6 (15%)	49,71,71	1.49	9 (18%)
23	CLA	a	821	-	45,53,73	1.77	6 (13%)	52,89,113	1.61	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	815	-	45,53,73	1.76	6 (13%)	52,89,113	1.58	7 (13%)
23	CLA	8	305	3	43,51,73	1.79	5 (11%)	49,86,113	1.65	7 (14%)
23	CLA	h	201	-	65,73,73	1.51	6 (9%)	76,113,113	1.46	7 (9%)
30	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
23	CLA	4	307	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
23	CLA	7	308	-	60,68,73	1.53	5 (8%)	70,107,113	1.44	7 (10%)
23	CLA	b	817	-	59,67,73	1.56	5 (8%)	68,105,113	1.51	9 (13%)
30	BCR	b	850	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
31	SF4	c	101	-	0,12,12	-	-	-	-	-
23	CLA	5	309	-	55,63,73	1.63	6 (10%)	64,101,113	1.48	7 (10%)
23	CLA	b	813	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	8 (10%)
21	XAT	8	303	-	39,47,47	0.87	1 (2%)	54,74,74	2.64	18 (33%)
21	XAT	9	304	-	39,47,47	0.94	1 (2%)	54,74,74	2.42	19 (35%)
23	CLA	a	825	-	55,63,73	1.62	5 (9%)	64,101,113	1.46	8 (12%)
21	XAT	7	305	-	39,47,47	0.86	0	54,74,74	2.65	19 (35%)
23	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.54	8 (12%)
21	XAT	3	304	-	39,47,47	0.90	2 (5%)	54,74,74	2.62	19 (35%)
23	CLA	5	307	24	45,53,73	1.80	5 (11%)	52,89,113	1.56	6 (11%)
23	CLA	6	310	-	52,60,73	1.65	5 (9%)	60,97,113	1.53	7 (11%)
25	A1L1F	9	302	-	50,59,59	1.37	5 (10%)	62,85,85	2.71	19 (30%)
23	CLA	b	824	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	5	314	1	45,53,73	1.81	5 (11%)	52,89,113	1.58	6 (11%)
23	CLA	a	809	9	65,73,73	1.45	6 (9%)	76,113,113	1.44	9 (11%)
23	CLA	a	827	-	65,73,73	1.49	6 (9%)	76,113,113	1.45	9 (11%)
30	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.04	17 (30%)
30	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.79	16 (28%)
23	CLA	9	313	2	46,54,73	1.77	5 (10%)	53,90,113	1.62	7 (13%)
21	XAT	4	302	-	39,47,47	0.90	2 (5%)	54,74,74	2.57	17 (31%)
29	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.09	3 (7%)
23	CLA	7	310	-	46,54,73	1.77	5 (10%)	53,90,113	1.57	6 (11%)
21	XAT	7	303	-	39,47,47	0.96	1 (2%)	54,74,74	2.60	17 (31%)
21	XAT	a	854	-	39,47,47	0.94	2 (5%)	54,74,74	2.70	20 (37%)
23	CLA	1	305	-	61,69,73	1.55	6 (9%)	71,108,113	1.39	7 (9%)
21	XAT	a	853	-	39,47,47	0.88	1 (2%)	54,74,74	2.72	18 (33%)
23	CLA	a	804	-	55,63,73	1.63	6 (10%)	64,101,113	1.55	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	841	26	65,73,73	1.53	5 (7%)	76,113,113	1.36	8 (10%)
23	CLA	6	307	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
30	BCR	b	847	-	41,41,41	0.76	0	56,56,56	2.19	22 (39%)
23	CLA	7	312	-	48,56,73	1.71	5 (10%)	55,92,113	1.56	8 (14%)
23	CLA	a	818	-	56,64,73	1.62	6 (10%)	65,102,113	1.44	8 (12%)
23	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	7 (9%)
23	CLA	b	818	-	60,68,73	1.56	5 (8%)	70,107,113	1.40	7 (10%)
23	CLA	l	202	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	7 (10%)
26	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
26	LHG	m	101	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
23	CLA	3	312	5	59,67,73	1.57	5 (8%)	68,105,113	1.43	7 (10%)
23	CLA	a	852	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	7 (9%)
23	CLA	b	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
23	CLA	b	822	-	60,68,73	1.55	6 (10%)	70,107,113	1.37	7 (10%)
23	CLA	7	306	4	48,56,73	1.73	6 (12%)	55,92,113	1.53	6 (10%)
23	CLA	8	311	-	56,64,73	1.58	5 (8%)	65,102,113	1.50	8 (12%)
30	BCR	j	102	-	41,41,41	0.73	0	56,56,56	2.08	17 (30%)
24	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	4 (7%)
23	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	b	802	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	8 (10%)
30	BCR	b	852	-	41,41,41	0.72	0	56,56,56	2.06	15 (26%)
23	CLA	4	305	4	45,53,73	1.80	6 (13%)	52,89,113	1.57	7 (13%)
25	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
23	CLA	4	314	4	41,49,73	1.86	6 (14%)	47,84,113	1.64	7 (14%)
23	CLA	4	312	-	53,61,73	1.65	5 (9%)	61,98,113	1.48	8 (13%)
23	CLA	7	315	4	41,49,73	1.86	5 (12%)	47,84,113	1.65	8 (17%)
23	CLA	3	315	5	46,54,73	1.78	6 (13%)	53,90,113	1.53	7 (13%)
23	CLA	a	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.59	8 (15%)
23	CLA	1	308	8	65,73,73	1.48	5 (7%)	76,113,113	1.43	9 (11%)
23	CLA	8	308	-	55,63,73	1.61	6 (10%)	64,101,113	1.51	9 (14%)
23	CLA	a	831	-	65,73,73	1.51	5 (7%)	76,113,113	1.47	8 (10%)
23	CLA	7	307	-	45,53,73	1.81	5 (11%)	52,89,113	1.58	6 (11%)
31	SF4	c	102	-	0,12,12	-	-	-	-	-
23	CLA	5	315	-	52,60,73	1.66	5 (9%)	60,97,113	1.54	8 (13%)
23	CLA	6	311	6	42,50,73	1.84	5 (11%)	48,85,113	1.58	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	811	-	54,62,73	1.66	7 (12%)	67,100,113	1.50	9 (13%)
23	CLA	b	830	-	41,49,73	1.83	6 (14%)	47,84,113	1.64	9 (19%)
23	CLA	b	838	-	65,73,73	1.52	6 (9%)	76,113,113	1.34	8 (10%)
21	XAT	1	303	-	39,47,47	0.89	1 (2%)	54,74,74	2.52	20 (37%)
23	CLA	a	844	26	65,73,73	1.46	5 (7%)	76,113,113	1.39	9 (11%)
23	CLA	5	316	-	46,54,73	1.74	5 (10%)	53,90,113	1.57	7 (13%)
23	CLA	1	314	-	45,53,73	1.79	5 (11%)	52,89,113	1.56	6 (11%)
21	XAT	7	301	-	39,47,47	0.93	1 (2%)	54,74,74	2.62	19 (35%)
21	XAT	3	301	-	39,47,47	0.92	2 (5%)	54,74,74	2.54	19 (35%)
21	XAT	7	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.68	21 (38%)
23	CLA	b	804	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	b	812	-	53,61,73	1.65	5 (9%)	61,98,113	1.49	8 (13%)
23	CLA	l	201	-	42,50,73	1.82	6 (14%)	48,85,113	1.64	7 (14%)
30	BCR	b	843	-	41,41,41	0.70	0	56,56,56	2.29	21 (37%)
23	CLA	a	840	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	7 (9%)
23	CLA	9	312	-	46,54,73	1.75	6 (13%)	53,90,113	1.68	8 (15%)
23	CLA	b	803	-	65,73,73	1.45	6 (9%)	76,113,113	1.54	12 (15%)
23	CLA	6	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	6 (7%)
23	CLA	b	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
25	A1L1F	6	304	-	46,55,59	1.33	4 (8%)	58,81,85	2.55	20 (34%)
23	CLA	a	828	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
29	PQN	b	842	-	34,34,34	1.55	2 (5%)	42,45,45	1.21	4 (9%)
23	CLA	1	309	8	46,54,73	1.79	5 (10%)	53,90,113	1.51	7 (13%)
23	CLA	b	810	-	65,73,73	1.46	5 (7%)	76,113,113	1.45	8 (10%)
30	BCR	a	849	-	41,41,41	0.74	0	56,56,56	2.16	19 (33%)
23	CLA	a	823	-	49,57,73	1.69	6 (12%)	55,93,113	1.61	7 (12%)
23	CLA	8	314	-	41,49,73	1.85	5 (12%)	47,84,113	1.63	7 (14%)
23	CLA	5	312	-	51,59,73	1.65	5 (9%)	59,96,113	1.52	9 (15%)
23	CLA	h	203	-	55,63,73	1.62	6 (10%)	64,101,113	1.47	9 (14%)
23	CLA	b	821	-	51,59,73	1.66	6 (11%)	59,96,113	1.57	9 (15%)
23	CLA	3	311	-	50,58,73	1.71	5 (10%)	58,95,113	1.54	9 (15%)
27	DGD	b	851	-	58,58,67	1.15	7 (12%)	72,72,81	1.53	10 (13%)
23	CLA	8	306	27	46,54,73	1.75	5 (10%)	53,90,113	1.54	7 (13%)
30	BCR	b	853	-	41,41,41	0.71	0	56,56,56	1.97	18 (32%)
23	CLA	b	814	-	55,63,73	1.61	6 (10%)	64,101,113	1.56	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	XAT	6	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.81	20 (37%)
21	XAT	5	302	-	39,47,47	0.94	1 (2%)	54,74,74	2.57	19 (35%)
23	CLA	l	203	-	46,54,73	1.75	6 (13%)	53,90,113	1.57	7 (13%)
23	CLA	a	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
22	A1L1G	7	302	-	38,47,47	1.42	6 (15%)	49,71,71	1.51	9 (18%)
23	CLA	a	803	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	6 (7%)
23	CLA	a	832	-	50,58,73	1.68	6 (12%)	58,95,113	1.54	9 (15%)
23	CLA	a	824	-	46,54,73	1.77	6 (13%)	53,90,113	1.49	7 (13%)
23	CLA	b	829	-	65,73,73	1.52	6 (9%)	76,113,113	1.44	10 (13%)
23	CLA	a	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	6 (7%)
23	CLA	a	802	-	58,66,73	1.55	6 (10%)	67,104,113	1.50	8 (11%)
23	CLA	b	805	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	7 (9%)
21	XAT	4	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.75	19 (35%)
22	A1L1G	5	304	-	38,47,47	1.41	6 (15%)	49,71,71	1.44	7 (14%)
23	CLA	7	314	-	45,53,73	1.80	6 (13%)	52,89,113	1.64	7 (13%)
25	A1L1F	h	202	-	50,59,59	1.39	5 (10%)	62,85,85	2.60	22 (35%)
23	CLA	2	314	-	56,64,73	1.63	7 (12%)	65,102,113	1.45	7 (10%)
21	XAT	6	306	-	39,47,47	0.93	1 (2%)	54,74,74	2.61	19 (35%)
21	XAT	3	305	-	39,47,47	0.87	1 (2%)	54,74,74	2.57	17 (31%)
23	CLA	7	316	-	51,59,73	1.64	6 (11%)	59,96,113	1.58	8 (13%)
21	XAT	4	303	-	39,47,47	0.88	0	54,74,74	2.56	15 (27%)
23	CLA	b	826	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	6 (7%)
23	CLA	2	315	-	42,50,73	1.86	6 (14%)	48,85,113	1.55	7 (14%)
23	CLA	f	803	13	52,60,73	1.67	5 (9%)	60,97,113	1.49	8 (13%)
23	CLA	a	819	-	54,62,73	1.63	7 (12%)	62,99,113	1.46	7 (11%)
23	CLA	8	307	3	65,73,73	1.47	5 (7%)	76,113,113	1.39	8 (10%)
23	CLA	2	311	-	58,66,73	1.58	5 (8%)	67,104,113	1.41	7 (10%)
23	CLA	7	309	-	46,55,73	1.75	5 (10%)	52,91,113	1.52	7 (13%)
28	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.30	4 (9%)
22	A1L1G	3	302	-	38,47,47	1.46	6 (15%)	49,71,71	1.38	7 (14%)
30	BCR	i	102	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
23	CLA	8	309	-	57,65,73	1.60	5 (8%)	66,103,113	1.45	9 (13%)
23	CLA	1	310	8	65,73,73	1.50	5 (7%)	76,113,113	1.33	8 (10%)
23	CLA	a	842	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
23	CLA	b	835	-	53,61,73	1.67	5 (9%)	61,98,113	1.50	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	3	313	-	52,60,73	1.65	6 (11%)	60,97,113	1.52	9 (15%)
23	CLA	2	306	-	41,50,73	1.85	6 (14%)	46,85,113	1.57	6 (13%)
23	CLA	1	311	-	53,61,73	1.63	5 (9%)	61,98,113	1.50	9 (14%)
23	CLA	8	310	-	46,54,73	1.76	6 (13%)	53,90,113	1.54	7 (13%)
21	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.60	16 (29%)
23	CLA	6	315	6	41,49,73	1.87	6 (14%)	47,84,113	1.62	6 (12%)
23	CLA	a	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	a	841	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	9 (11%)
23	CLA	2	308	7	54,62,73	1.64	6 (11%)	62,99,113	1.46	8 (12%)
22	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.57	11 (22%)
21	XAT	5	303	-	39,47,47	0.93	1 (2%)	54,74,74	2.59	20 (37%)
23	CLA	4	310	-	46,54,73	1.78	6 (13%)	53,90,113	1.55	7 (13%)
23	CLA	a	814	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	6	312	6	51,59,73	1.67	6 (11%)	59,96,113	1.52	6 (10%)
23	CLA	a	820	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	9 (11%)
30	BCR	m	102	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	6 (10%)
21	XAT	2	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.50	18 (33%)
23	CLA	9	314	-	55,63,73	1.62	6 (10%)	64,101,113	1.50	8 (12%)
30	BCR	a	850	-	41,41,41	0.74	0	56,56,56	2.16	14 (25%)
23	CLA	9	311	-	46,54,73	1.77	5 (10%)	53,90,113	1.62	8 (15%)
23	CLA	5	306	1	46,54,73	1.78	6 (13%)	53,90,113	1.55	8 (15%)
23	CLA	b	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	4	306	-	56,64,73	1.61	5 (8%)	65,102,113	1.44	9 (13%)
23	CLA	4	311	-	46,54,73	1.79	6 (13%)	53,90,113	1.51	7 (13%)
23	CLA	a	805	23	55,63,73	1.61	6 (10%)	64,101,113	1.51	8 (12%)
23	CLA	a	836	-	50,58,73	1.70	6 (12%)	58,95,113	1.50	9 (15%)
23	CLA	9	310	-	46,54,73	1.75	5 (10%)	53,90,113	1.64	6 (11%)
21	XAT	4	301	-	39,47,47	0.91	1 (2%)	54,74,74	2.57	19 (35%)

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
23	CLA	1	307	-	1/1/12/20	6/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	4	315	-	1/1/11/20	7/15/93/115	-
23	CLA	3	308	-	1/1/11/20	5/16/94/115	-
23	CLA	a	856	-	1/1/15/20	13/37/115/115	-
21	XAT	2	305	-	-	2/31/93/93	0/4/4/4
23	CLA	5	310	1	1/1/15/20	14/37/115/115	-
23	CLA	b	840	-	1/1/15/20	17/37/115/115	-
23	CLA	6	308	-	1/1/13/20	4/29/107/115	-
21	XAT	2	301	-	-	3/31/93/93	0/4/4/4
23	CLA	a	830	-	1/1/15/20	15/37/115/115	-
21	XAT	3	303	-	-	3/31/93/93	0/4/4/4
25	A1L1F	6	301	-	-	11/43/99/99	0/3/3/3
26	LHG	b	849	23	-	20/35/35/53	-
23	CLA	a	813	-	1/1/12/20	10/24/102/115	-
23	CLA	b	836	-	1/1/13/20	11/29/107/115	-
23	CLA	4	308	-	1/1/12/20	7/19/97/115	-
28	LMG	a	855	-	-	13/29/49/70	0/1/1/1
23	CLA	2	313	7	1/1/10/20	4/8/86/115	-
23	CLA	a	812	23	1/1/14/20	9/34/112/115	-
23	CLA	8	313	-	1/1/11/20	3/15/93/115	-
23	CLA	b	833	-	1/1/13/20	16/29/107/115	-
23	CLA	1	312	8	1/1/12/20	3/22/100/115	-
23	CLA	b	837	-	1/1/15/20	8/37/115/115	-
21	XAT	9	305	-	-	3/31/93/93	0/4/4/4
21	XAT	2	303	-	-	6/31/93/93	0/4/4/4
21	XAT	6	305	-	-	4/31/93/93	0/4/4/4
30	BCR	a	847	-	-	0/29/63/63	0/2/2/2
23	CLA	5	311	-	1/1/11/20	6/15/93/115	-
23	CLA	4	313	4	1/1/11/20	3/13/91/115	-
28	LMG	j	103	-	-	11/27/47/70	0/1/1/1
23	CLA	b	809	-	1/1/15/20	16/37/115/115	-
21	XAT	5	301	-	-	4/31/93/93	0/4/4/4
25	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
30	BCR	f	801	-	-	3/29/63/63	0/2/2/2
23	CLA	a	822	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	8	312	3	1/1/12/20	2/22/100/115	-
23	CLA	6	313	-	1/1/12/20	2/22/100/115	-
23	CLA	9	308	2	1/1/15/20	15/37/115/115	-
23	CLA	a	810	9	1/1/15/20	13/37/115/115	-
23	CLA	b	831	-	1/1/11/20	6/18/96/115	-
21	XAT	8	302	-	-	4/31/93/93	0/4/4/4
23	CLA	a	801	-	1/1/15/20	22/37/115/115	-
22	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
27	DGD	4	317	-	-	10/29/69/95	0/2/2/2
30	BCR	b	844	-	-	2/29/63/63	0/2/2/2
31	SF4	a	851	-	-	-	0/6/5/5
23	CLA	1	306	-	1/1/15/20	15/37/115/115	-
23	CLA	b	806	-	1/1/15/20	19/37/115/115	-
23	CLA	b	832	-	1/1/15/20	13/37/115/115	-
21	XAT	9	303	-	-	4/31/93/93	0/4/4/4
30	BCR	b	846	-	-	0/29/63/63	0/2/2/2
23	CLA	2	312	-	1/1/11/20	4/16/94/115	-
23	CLA	5	308	1	1/1/14/20	7/31/109/115	-
23	CLA	a	811	-	1/1/13/20	8/27/105/115	-
23	CLA	3	314	5	1/1/11/20	7/16/94/115	-
23	CLA	a	808	-	1/1/12/20	3/21/99/115	-
30	BCR	b	845	-	-	6/29/63/63	0/2/2/2
26	LHG	a	846	23	-	16/31/31/53	-
21	XAT	6	303	-	-	5/31/93/93	0/4/4/4
23	CLA	5	313	-	1/1/12/20	0/22/100/115	-
23	CLA	6	314	-	1/1/11/20	6/15/93/115	-
23	CLA	b	816	-	1/1/13/20	4/25/103/115	-
23	CLA	2	307	-	1/1/11/20	6/16/94/115	-
23	CLA	1	313	-	1/1/10/20	3/8/86/115	-
23	CLA	b	819	-	1/1/13/20	3/25/103/115	-
21	XAT	8	301	-	-	3/31/93/93	0/4/4/4
23	CLA	2	310	-	1/1/15/20	14/37/115/115	-
21	XAT	5	305	-	-	1/31/93/93	0/4/4/4
23	CLA	b	820	-	1/1/12/20	7/19/97/115	-
23	CLA	2	316	7	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	i	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	823	-	1/1/12/20	8/23/101/115	-
27	DGD	8	315	23	-	11/29/69/95	0/2/2/2
23	CLA	a	834	-	1/1/15/20	7/37/115/115	-
23	CLA	b	828	-	1/1/15/20	11/37/115/115	-
23	CLA	6	316	6	1/1/11/20	7/15/93/115	-
23	CLA	3	307	5	1/1/11/20	1/13/91/115	-
23	CLA	2	309	-	1/1/11/20	4/15/93/115	-
23	CLA	j	101	16	1/1/10/20	5/10/88/115	-
23	CLA	4	316	-	1/1/13/20	7/25/103/115	-
23	CLA	3	310	-	1/1/13/20	4/27/105/115	-
23	CLA	4	309	-	1/1/15/20	16/37/115/115	-
24	SQD	5	317	23	-	11/30/50/69	0/1/1/1
23	CLA	7	317	-	1/1/11/20	5/13/91/115	-
23	CLA	a	806	-	1/1/15/20	12/37/115/115	-
23	CLA	7	311	-	1/1/11/20	5/15/93/115	-
23	CLA	3	309	5	1/1/13/20	5/27/105/115	-
22	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
23	CLA	a	837	9	1/1/11/20	4/13/91/115	-
23	CLA	b	839	-	1/1/15/20	13/37/115/115	-
23	CLA	b	825	-	1/1/14/20	6/36/114/115	-
23	CLA	7	313	-	1/1/12/20	7/24/102/115	-
23	CLA	a	838	-	1/1/12/20	6/21/99/115	-
26	LHG	9	307	-	-	21/40/40/53	-
21	XAT	2	304	-	-	3/31/93/93	0/4/4/4
23	CLA	f	802	-	1/1/15/20	13/37/115/115	-
23	CLA	9	316	-	1/1/14/20	9/34/112/115	-
23	CLA	a	817	-	1/1/11/20	6/13/91/115	-
23	CLA	b	808	-	1/1/15/20	11/37/115/115	-
23	CLA	9	309	2	1/1/11/20	3/15/93/115	-
23	CLA	a	816	-	1/1/12/20	5/19/97/115	-
23	CLA	a	829	-	1/1/14/20	15/34/112/115	-
23	CLA	9	315	2	1/1/10/20	6/10/88/115	-
22	A1L1G	3	306	-	-	18/29/85/85	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	821	-	1/1/11/20	2/13/91/115	-
23	CLA	b	815	-	1/1/11/20	3/13/91/115	-
23	CLA	8	305	3	1/1/10/20	2/11/89/115	-
23	CLA	h	201	-	1/1/15/20	9/37/115/115	-
30	BCR	a	848	-	-	0/29/63/63	0/2/2/2
23	CLA	4	307	-	1/1/15/20	14/37/115/115	-
23	CLA	7	308	-	1/1/14/20	14/31/109/115	-
23	CLA	b	817	-	1/1/13/20	10/30/108/115	-
30	BCR	b	850	-	-	2/29/63/63	0/2/2/2
31	SF4	c	101	-	-	-	0/6/5/5
23	CLA	5	309	-	1/1/13/20	4/25/103/115	-
23	CLA	b	813	-	1/1/15/20	14/37/115/115	-
21	XAT	8	303	-	-	0/31/93/93	0/4/4/4
21	XAT	9	304	-	-	1/31/93/93	0/4/4/4
23	CLA	a	825	-	1/1/13/20	8/25/103/115	-
21	XAT	7	305	-	-	2/31/93/93	0/4/4/4
23	CLA	a	833	-	1/1/13/20	2/25/103/115	-
21	XAT	3	304	-	-	3/31/93/93	0/4/4/4
23	CLA	5	307	24	1/1/11/20	7/13/91/115	-
23	CLA	6	310	-	1/1/12/20	7/22/100/115	-
25	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
23	CLA	b	824	-	1/1/15/20	14/37/115/115	-
23	CLA	5	314	1	1/1/11/20	5/13/91/115	-
23	CLA	a	809	9	1/1/15/20	15/37/115/115	-
23	CLA	a	827	-	1/1/15/20	8/37/115/115	-
30	BCR	f	804	-	-	4/29/63/63	0/2/2/2
30	BCR	b	848	-	-	2/29/63/63	0/2/2/2
23	CLA	9	313	2	1/1/11/20	9/15/93/115	-
21	XAT	4	302	-	-	3/31/93/93	0/4/4/4
29	PQN	a	843	-	-	5/23/43/43	0/2/2/2
23	CLA	7	310	-	1/1/11/20	6/15/93/115	-
21	XAT	7	303	-	-	8/31/93/93	0/4/4/4
23	CLA	1	305	-	1/1/14/20	10/33/111/115	-
23	CLA	a	804	-	1/1/13/20	10/25/103/115	-
23	CLA	b	841	26	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	XAT	a	853	-	-	5/31/93/93	0/4/4/4
21	XAT	a	854	-	-	7/31/93/93	0/4/4/4
23	CLA	6	307	-	1/1/11/20	1/15/93/115	-
30	BCR	b	847	-	-	1/29/63/63	0/2/2/2
23	CLA	7	312	-	1/1/11/20	3/17/95/115	-
23	CLA	a	818	-	1/1/13/20	11/27/105/115	-
23	CLA	a	835	-	1/1/15/20	12/37/115/115	-
23	CLA	b	818	-	1/1/14/20	14/31/109/115	-
23	CLA	l	202	-	1/1/14/20	6/31/109/115	-
26	LHG	a	845	-	-	27/52/52/53	-
26	LHG	m	101	-	-	28/50/50/53	-
23	CLA	3	312	5	1/1/13/20	9/30/108/115	-
23	CLA	a	852	-	1/1/15/20	17/37/115/115	-
23	CLA	b	807	-	1/1/15/20	12/37/115/115	-
23	CLA	b	822	-	1/1/14/20	7/31/109/115	-
23	CLA	7	306	4	1/1/11/20	10/17/95/115	-
23	CLA	8	311	-	1/1/13/20	8/27/105/115	-
30	BCR	j	102	-	-	4/29/63/63	0/2/2/2
24	SQD	1	315	-	-	19/40/60/69	0/1/1/1
23	CLA	b	801	-	1/1/15/20	20/37/115/115	-
23	CLA	b	802	-	1/1/15/20	18/37/115/115	-
30	BCR	b	852	-	-	5/29/63/63	0/2/2/2
23	CLA	4	305	4	1/1/11/20	7/13/91/115	-
25	A1L1F	1	304	-	-	11/43/99/99	0/3/3/3
23	CLA	4	314	4	1/1/10/20	5/8/86/115	-
23	CLA	4	312	-	1/1/12/20	6/23/101/115	-
23	CLA	7	315	4	1/1/10/20	4/8/86/115	-
23	CLA	3	315	5	1/1/11/20	8/15/93/115	-
23	CLA	a	815	-	1/1/11/20	2/13/91/115	-
23	CLA	1	308	8	1/1/15/20	13/37/115/115	-
23	CLA	8	308	-	1/1/13/20	7/25/103/115	-
23	CLA	a	831	-	1/1/15/20	11/37/115/115	-
23	CLA	7	307	-	1/1/11/20	5/13/91/115	-
31	SF4	c	102	-	-	-	0/6/5/5
23	CLA	5	315	-	1/1/12/20	4/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	6	311	6	1/1/10/20	2/10/88/115	-
23	CLA	b	811	-	1/1/13/20	5/25/101/115	-
23	CLA	b	830	-	1/1/10/20	1/8/86/115	-
23	CLA	b	838	-	1/1/15/20	8/37/115/115	-
21	XAT	1	303	-	-	0/31/93/93	0/4/4/4
23	CLA	a	844	26	1/1/15/20	16/37/115/115	-
23	CLA	5	316	-	1/1/11/20	5/15/93/115	-
23	CLA	1	314	-	1/1/11/20	5/13/91/115	-
23	CLA	b	804	-	1/1/15/20	12/37/115/115	-
23	CLA	b	812	-	1/1/12/20	6/23/101/115	-
23	CLA	l	201	-	1/1/10/20	2/10/88/115	-
21	XAT	3	301	-	-	3/31/93/93	0/4/4/4
21	XAT	7	301	-	-	6/31/93/93	0/4/4/4
21	XAT	7	304	-	-	6/31/93/93	0/4/4/4
30	BCR	b	843	-	-	2/29/63/63	0/2/2/2
23	CLA	a	840	-	1/1/15/20	8/37/115/115	-
23	CLA	9	312	-	1/1/11/20	9/15/93/115	-
23	CLA	b	803	-	1/1/15/20	10/37/115/115	-
23	CLA	6	309	-	1/1/15/20	10/37/115/115	-
23	CLA	b	834	-	1/1/15/20	14/37/115/115	-
25	A1L1F	6	304	-	-	12/39/95/99	0/3/3/3
23	CLA	a	828	-	1/1/15/20	9/37/115/115	-
29	PQN	b	842	-	-	1/23/43/43	0/2/2/2
23	CLA	1	309	8	1/1/11/20	6/15/93/115	-
23	CLA	b	810	-	1/1/15/20	17/37/115/115	-
30	BCR	a	849	-	-	0/29/63/63	0/2/2/2
23	CLA	a	823	-	1/1/11/20	7/18/96/115	-
23	CLA	8	314	-	1/1/10/20	5/8/86/115	-
23	CLA	5	312	-	1/1/12/20	8/21/99/115	-
23	CLA	h	203	-	1/1/13/20	9/25/103/115	-
23	CLA	b	821	-	1/1/12/20	2/21/99/115	-
23	CLA	3	311	-	1/1/12/20	4/19/97/115	-
27	DGD	b	851	-	-	20/46/86/95	0/2/2/2
23	CLA	8	306	27	1/1/11/20	2/15/93/115	-
30	BCR	b	853	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	814	-	1/1/13/20	13/25/103/115	-
21	XAT	6	302	-	-	7/31/93/93	0/4/4/4
23	CLA	l	203	-	1/1/11/20	4/15/93/115	-
21	XAT	5	302	-	-	3/31/93/93	0/4/4/4
23	CLA	a	807	-	1/1/15/20	18/37/115/115	-
23	CLA	a	832	-	1/1/12/20	5/19/97/115	-
23	CLA	a	803	-	1/1/15/20	3/37/115/115	-
23	CLA	b	829	-	1/1/15/20	11/37/115/115	-
23	CLA	a	824	-	1/1/11/20	4/15/93/115	-
22	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
23	CLA	a	826	-	1/1/15/20	9/37/115/115	-
23	CLA	a	802	-	1/1/13/20	7/29/107/115	-
23	CLA	b	805	-	1/1/15/20	16/37/115/115	-
23	CLA	7	314	-	1/1/11/20	4/13/91/115	-
21	XAT	4	304	-	-	4/31/93/93	0/4/4/4
22	A1L1G	5	304	-	-	9/29/85/85	0/3/3/3
25	A1L1F	h	202	-	-	11/43/99/99	1/3/3/3
23	CLA	2	314	-	1/1/13/20	13/27/105/115	-
21	XAT	6	306	-	-	4/31/93/93	0/4/4/4
21	XAT	3	305	-	-	0/31/93/93	0/4/4/4
23	CLA	7	316	-	1/1/12/20	11/21/99/115	-
21	XAT	4	303	-	-	0/31/93/93	0/4/4/4
23	CLA	b	826	-	1/1/15/20	5/37/115/115	-
23	CLA	2	315	-	1/1/10/20	1/10/88/115	-
23	CLA	f	803	13	1/1/12/20	2/22/100/115	-
23	CLA	a	819	-	1/1/12/20	4/24/102/115	-
23	CLA	8	307	3	1/1/15/20	13/37/115/115	-
23	CLA	2	311	-	1/1/13/20	5/29/107/115	-
23	CLA	7	309	-	1/1/11/20	5/15/93/115	-
28	LMG	2	317	-	-	11/30/50/70	0/1/1/1
22	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
30	BCR	i	102	-	-	8/29/63/63	0/2/2/2
23	CLA	8	309	-	1/1/13/20	8/28/106/115	-
23	CLA	1	310	8	1/1/15/20	18/37/115/115	-
23	CLA	a	842	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	835	-	1/1/12/20	8/23/101/115	-
23	CLA	3	313	-	1/1/12/20	1/22/100/115	-
23	CLA	2	306	-	1/1/10/20	2/9/87/115	-
23	CLA	1	311	-	1/1/12/20	6/23/101/115	-
23	CLA	8	310	-	1/1/11/20	5/15/93/115	-
21	XAT	1	302	-	-	0/31/93/93	0/4/4/4
23	CLA	6	315	6	1/1/10/20	3/8/86/115	-
23	CLA	a	839	-	1/1/15/20	15/37/115/115	-
23	CLA	a	841	-	1/1/15/20	15/37/115/115	-
23	CLA	2	308	7	1/1/12/20	5/24/102/115	-
22	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
23	CLA	4	310	-	1/1/11/20	8/15/93/115	-
21	XAT	5	303	-	-	3/31/93/93	0/4/4/4
23	CLA	a	814	-	1/1/15/20	20/37/115/115	-
23	CLA	6	312	6	1/1/12/20	5/21/99/115	-
23	CLA	a	820	-	1/1/15/20	16/37/115/115	-
30	BCR	m	102	-	-	9/29/63/63	0/2/2/2
21	XAT	2	302	-	-	0/31/93/93	0/4/4/4
23	CLA	9	314	-	1/1/13/20	9/25/103/115	-
30	BCR	a	850	-	-	4/29/63/63	0/2/2/2
23	CLA	9	311	-	1/1/11/20	7/15/93/115	-
23	CLA	5	306	1	1/1/11/20	4/15/93/115	-
23	CLA	b	827	-	1/1/15/20	14/37/115/115	-
23	CLA	4	306	-	1/1/13/20	7/27/105/115	-
23	CLA	4	311	-	1/1/11/20	4/15/93/115	-
23	CLA	a	805	23	1/1/13/20	6/25/103/115	-
23	CLA	a	836	-	1/1/12/20	6/19/97/115	-
23	CLA	9	310	-	1/1/11/20	6/15/93/115	-
21	XAT	4	301	-	-	0/31/93/93	0/4/4/4

All (1214) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	312	CLA	C4B-NB	7.98	1.42	1.35
23	a	818	CLA	C4B-NB	7.78	1.42	1.35
23	a	840	CLA	C4B-NB	7.78	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	842	CLA	C4B-NB	7.76	1.42	1.35
23	b	838	CLA	C4B-NB	7.72	1.42	1.35
23	1	309	CLA	C4B-NB	7.71	1.42	1.35
23	2	315	CLA	C4B-NB	7.70	1.42	1.35
23	5	314	CLA	C4B-NB	7.70	1.42	1.35
23	3	315	CLA	C4B-NB	7.69	1.42	1.35
23	4	311	CLA	C4B-NB	7.69	1.42	1.35
23	a	813	CLA	C4B-NB	7.68	1.42	1.35
23	2	314	CLA	C4B-NB	7.68	1.42	1.35
23	6	308	CLA	C4B-NB	7.67	1.42	1.35
23	4	310	CLA	C4B-NB	7.66	1.42	1.35
23	b	841	CLA	C4B-NB	7.65	1.42	1.35
23	6	307	CLA	C4B-NB	7.64	1.42	1.35
23	b	829	CLA	C4B-NB	7.63	1.42	1.35
23	h	201	CLA	C4B-NB	7.63	1.42	1.35
23	b	840	CLA	C4B-NB	7.62	1.42	1.35
29	a	843	PQN	C3-C2	7.62	1.49	1.35
23	a	808	CLA	C4B-NB	7.62	1.42	1.35
23	a	825	CLA	C4B-NB	7.62	1.42	1.35
23	2	312	CLA	C4B-NB	7.61	1.42	1.35
23	4	305	CLA	C4B-NB	7.60	1.42	1.35
23	2	308	CLA	C4B-NB	7.60	1.42	1.35
23	3	311	CLA	C4B-NB	7.60	1.42	1.35
23	6	311	CLA	C4B-NB	7.60	1.42	1.35
23	5	311	CLA	C4B-NB	7.59	1.42	1.35
23	5	306	CLA	C4B-NB	7.58	1.42	1.35
23	f	803	CLA	C4B-NB	7.58	1.42	1.35
23	a	804	CLA	C4B-NB	7.58	1.42	1.35
23	b	835	CLA	C4B-NB	7.58	1.42	1.35
23	4	314	CLA	C4B-NB	7.58	1.42	1.35
23	9	314	CLA	C4B-NB	7.57	1.42	1.35
23	4	306	CLA	C4B-NB	7.57	1.42	1.35
23	a	820	CLA	C4B-NB	7.57	1.42	1.35
23	1	305	CLA	C4B-NB	7.56	1.42	1.35
23	4	313	CLA	C4B-NB	7.55	1.41	1.35
23	4	315	CLA	C4B-NB	7.55	1.41	1.35
23	b	801	CLA	C4B-NB	7.55	1.41	1.35
23	7	311	CLA	C4B-NB	7.55	1.41	1.35
23	b	816	CLA	C4B-NB	7.55	1.41	1.35
23	7	307	CLA	C4B-NB	7.54	1.41	1.35
23	4	316	CLA	C4B-NB	7.54	1.41	1.35
23	a	841	CLA	C4B-NB	7.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	820	CLA	C4B-NB	7.54	1.41	1.35
23	7	315	CLA	C4B-NB	7.53	1.41	1.35
23	2	311	CLA	C4B-NB	7.53	1.41	1.35
23	1	310	CLA	C4B-NB	7.52	1.41	1.35
23	a	805	CLA	C4B-NB	7.52	1.41	1.35
23	4	308	CLA	C4B-NB	7.52	1.41	1.35
23	7	310	CLA	C4B-NB	7.52	1.41	1.35
23	9	309	CLA	C4B-NB	7.52	1.41	1.35
23	a	831	CLA	C4B-NB	7.52	1.41	1.35
23	3	312	CLA	C4B-NB	7.52	1.41	1.35
23	8	313	CLA	C4B-NB	7.51	1.41	1.35
23	a	817	CLA	C4B-NB	7.51	1.41	1.35
23	b	826	CLA	C4B-NB	7.51	1.41	1.35
23	5	307	CLA	C4B-NB	7.50	1.41	1.35
23	7	317	CLA	C4B-NB	7.50	1.41	1.35
23	2	313	CLA	C4B-NB	7.50	1.41	1.35
23	4	309	CLA	C4B-NB	7.50	1.41	1.35
23	6	309	CLA	C4B-NB	7.49	1.41	1.35
23	7	313	CLA	C4B-NB	7.49	1.41	1.35
23	9	316	CLA	C4B-NB	7.49	1.41	1.35
23	2	310	CLA	C4B-NB	7.48	1.41	1.35
23	1	307	CLA	C4B-NB	7.48	1.41	1.35
23	b	833	CLA	C4B-NB	7.48	1.41	1.35
23	3	310	CLA	C4B-NB	7.47	1.41	1.35
23	5	308	CLA	C4B-NB	7.47	1.41	1.35
23	3	307	CLA	C4B-NB	7.47	1.41	1.35
23	1	313	CLA	C4B-NB	7.47	1.41	1.35
23	a	824	CLA	C4B-NB	7.47	1.41	1.35
23	b	828	CLA	C4B-NB	7.47	1.41	1.35
23	2	309	CLA	C4B-NB	7.47	1.41	1.35
23	8	309	CLA	C4B-NB	7.47	1.41	1.35
23	9	311	CLA	C4B-NB	7.46	1.41	1.35
23	2	316	CLA	C4B-NB	7.46	1.41	1.35
23	8	312	CLA	C4B-NB	7.46	1.41	1.35
23	3	308	CLA	C4B-NB	7.46	1.41	1.35
23	a	834	CLA	C4B-NB	7.46	1.41	1.35
23	b	822	CLA	C4B-NB	7.46	1.41	1.35
23	5	316	CLA	C4B-NB	7.46	1.41	1.35
23	1	314	CLA	C4B-NB	7.46	1.41	1.35
23	a	810	CLA	C4B-NB	7.45	1.41	1.35
23	a	829	CLA	C4B-NB	7.45	1.41	1.35
23	2	306	CLA	C4B-NB	7.45	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	827	CLA	C4B-NB	7.45	1.41	1.35
23	5	310	CLA	C4B-NB	7.44	1.41	1.35
23	5	309	CLA	C4B-NB	7.44	1.41	1.35
23	7	306	CLA	C4B-NB	7.44	1.41	1.35
23	b	839	CLA	C4B-NB	7.44	1.41	1.35
23	4	312	CLA	C4B-NB	7.44	1.41	1.35
23	b	818	CLA	C4B-NB	7.43	1.41	1.35
23	b	831	CLA	C4B-NB	7.43	1.41	1.35
23	b	814	CLA	C4B-NB	7.43	1.41	1.35
23	b	834	CLA	C4B-NB	7.43	1.41	1.35
23	8	308	CLA	C4B-NB	7.43	1.41	1.35
23	7	314	CLA	C4B-NB	7.43	1.41	1.35
23	b	803	CLA	C4B-NB	7.42	1.41	1.35
23	a	822	CLA	C4B-NB	7.42	1.41	1.35
23	b	804	CLA	C4B-NB	7.42	1.41	1.35
23	a	852	CLA	C4B-NB	7.42	1.41	1.35
23	b	808	CLA	C4B-NB	7.42	1.41	1.35
23	8	305	CLA	C4B-NB	7.42	1.41	1.35
23	9	315	CLA	C4B-NB	7.42	1.41	1.35
23	b	837	CLA	C4B-NB	7.42	1.41	1.35
23	9	313	CLA	C4B-NB	7.41	1.41	1.35
23	6	312	CLA	C4B-NB	7.41	1.41	1.35
23	b	812	CLA	C4B-NB	7.41	1.41	1.35
23	l	201	CLA	C4B-NB	7.41	1.41	1.35
23	7	309	CLA	C4B-NB	7.40	1.41	1.35
23	1	308	CLA	C4B-NB	7.40	1.41	1.35
23	a	827	CLA	C4B-NB	7.40	1.41	1.35
23	a	823	CLA	C4B-NB	7.40	1.41	1.35
23	6	315	CLA	C4B-NB	7.40	1.41	1.35
23	j	101	CLA	C4B-NB	7.40	1.41	1.35
23	6	314	CLA	C4B-NB	7.39	1.41	1.35
23	f	802	CLA	C4B-NB	7.39	1.41	1.35
23	8	310	CLA	C4B-NB	7.38	1.41	1.35
23	a	836	CLA	C4B-NB	7.38	1.41	1.35
23	6	310	CLA	C4B-NB	7.37	1.41	1.35
23	a	837	CLA	C4B-NB	7.37	1.41	1.35
23	7	308	CLA	C4B-NB	7.37	1.41	1.35
23	3	313	CLA	C4B-NB	7.37	1.41	1.35
23	b	806	CLA	C4B-NB	7.37	1.41	1.35
23	3	314	CLA	C4B-NB	7.36	1.41	1.35
23	a	821	CLA	C4B-NB	7.36	1.41	1.35
23	9	310	CLA	C4B-NB	7.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	306	CLA	C4B-NB	7.35	1.41	1.35
23	a	856	CLA	C4B-NB	7.35	1.41	1.35
23	a	814	CLA	C4B-NB	7.35	1.41	1.35
23	b	802	CLA	C4B-NB	7.34	1.41	1.35
23	h	203	CLA	C4B-NB	7.34	1.41	1.35
23	7	312	CLA	C4B-NB	7.34	1.41	1.35
23	a	803	CLA	C4B-NB	7.34	1.41	1.35
23	b	832	CLA	C4B-NB	7.34	1.41	1.35
23	2	307	CLA	C4B-NB	7.34	1.41	1.35
29	b	842	PQN	C3-C2	7.33	1.48	1.35
23	1	306	CLA	C4B-NB	7.33	1.41	1.35
23	9	312	CLA	C4B-NB	7.33	1.41	1.35
23	b	824	CLA	C4B-NB	7.32	1.41	1.35
23	a	815	CLA	C4B-NB	7.32	1.41	1.35
23	a	816	CLA	C4B-NB	7.32	1.41	1.35
23	9	308	CLA	C4B-NB	7.32	1.41	1.35
23	a	812	CLA	C4B-NB	7.32	1.41	1.35
23	5	315	CLA	C4B-NB	7.31	1.41	1.35
23	b	819	CLA	C4B-NB	7.31	1.41	1.35
23	l	202	CLA	C4B-NB	7.31	1.41	1.35
23	8	314	CLA	C4B-NB	7.31	1.41	1.35
23	8	311	CLA	C4B-NB	7.30	1.41	1.35
23	a	802	CLA	C4B-NB	7.30	1.41	1.35
23	b	807	CLA	C4B-NB	7.30	1.41	1.35
23	a	832	CLA	C4B-NB	7.30	1.41	1.35
23	b	825	CLA	C4B-NB	7.29	1.41	1.35
23	6	316	CLA	C4B-NB	7.29	1.41	1.35
23	a	830	CLA	C4B-NB	7.29	1.41	1.35
23	a	839	CLA	C4B-NB	7.27	1.41	1.35
23	b	821	CLA	C4B-NB	7.27	1.41	1.35
23	6	313	CLA	C4B-NB	7.26	1.41	1.35
23	a	801	CLA	C4B-NB	7.26	1.41	1.35
23	a	833	CLA	C4B-NB	7.26	1.41	1.35
23	3	309	CLA	C4B-NB	7.26	1.41	1.35
23	b	817	CLA	C4B-NB	7.26	1.41	1.35
23	b	823	CLA	C4B-NB	7.25	1.41	1.35
23	b	811	CLA	C4B-NB	7.25	1.41	1.35
23	b	836	CLA	C4B-NB	7.25	1.41	1.35
23	a	811	CLA	C4B-NB	7.25	1.41	1.35
23	b	815	CLA	C4B-NB	7.24	1.41	1.35
23	b	810	CLA	C4B-NB	7.24	1.41	1.35
23	a	835	CLA	C4B-NB	7.23	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	830	CLA	C4B-NB	7.23	1.41	1.35
23	a	807	CLA	C4B-NB	7.23	1.41	1.35
23	b	813	CLA	C4B-NB	7.23	1.41	1.35
23	5	313	CLA	C4B-NB	7.22	1.41	1.35
23	1	311	CLA	C4B-NB	7.22	1.41	1.35
23	l	203	CLA	C4B-NB	7.22	1.41	1.35
23	a	844	CLA	C4B-NB	7.22	1.41	1.35
23	a	819	CLA	C4B-NB	7.22	1.41	1.35
23	a	838	CLA	C4B-NB	7.20	1.41	1.35
23	5	312	CLA	C4B-NB	7.20	1.41	1.35
23	b	809	CLA	C4B-NB	7.20	1.41	1.35
23	b	805	CLA	C4B-NB	7.19	1.41	1.35
23	a	826	CLA	C4B-NB	7.19	1.41	1.35
23	7	316	CLA	C4B-NB	7.17	1.41	1.35
23	4	307	CLA	C4B-NB	7.16	1.41	1.35
23	8	307	CLA	C4B-NB	7.16	1.41	1.35
23	a	809	CLA	C4B-NB	7.14	1.41	1.35
23	a	828	CLA	C4B-NB	7.10	1.41	1.35
23	a	806	CLA	C4B-NB	6.15	1.40	1.35
29	b	842	PQN	C10-C5	4.86	1.48	1.40
29	a	843	PQN	C10-C5	4.74	1.48	1.40
24	5	317	SQD	O8-S	4.65	1.64	1.47
25	h	202	A1L1F	O7-C54	4.58	1.45	1.35
25	9	302	A1L1F	O7-C54	4.58	1.45	1.35
24	1	315	SQD	O8-S	4.56	1.63	1.47
25	8	304	A1L1F	O7-C54	4.52	1.45	1.35
25	1	304	A1L1F	O7-C54	4.51	1.45	1.35
25	6	304	A1L1F	O7-C54	4.49	1.45	1.35
25	6	301	A1L1F	O7-C54	4.43	1.45	1.35
24	1	315	SQD	O48-C23	4.33	1.46	1.33
27	8	315	DGD	O1G-C1A	4.28	1.45	1.33
28	a	855	LMG	O8-C28	4.24	1.45	1.33
24	5	317	SQD	O48-C23	4.24	1.45	1.33
24	1	315	SQD	O47-C7	4.19	1.46	1.34
25	1	304	A1L1F	O13-C45	4.19	1.45	1.33
25	h	202	A1L1F	O13-C45	4.18	1.45	1.33
25	6	304	A1L1F	O13-C45	4.16	1.45	1.33
28	a	855	LMG	O7-C10	4.14	1.46	1.34
28	j	103	LMG	O8-C28	4.12	1.45	1.33
25	6	301	A1L1F	O13-C45	4.10	1.45	1.33
25	8	304	A1L1F	O13-C45	4.09	1.45	1.33
23	a	806	CLA	C4D-ND	-4.08	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	317	SQD	O47-C7	4.08	1.45	1.34
28	2	317	LMG	O8-C28	4.07	1.45	1.33
23	6	315	CLA	C1D-ND	4.07	1.42	1.37
27	4	317	DGD	O1G-C1A	4.04	1.45	1.33
23	a	804	CLA	C1D-ND	4.02	1.42	1.37
27	b	851	DGD	O2G-C1B	4.01	1.45	1.34
23	9	313	CLA	C1D-ND	4.01	1.42	1.37
23	h	201	CLA	C1D-ND	4.00	1.42	1.37
23	3	314	CLA	C1D-ND	4.00	1.42	1.37
28	2	317	LMG	O7-C10	4.00	1.45	1.34
23	6	308	CLA	C1D-ND	4.00	1.42	1.37
23	8	313	CLA	C1D-ND	3.98	1.42	1.37
27	b	851	DGD	O1G-C1A	3.97	1.45	1.33
23	5	309	CLA	C1D-ND	3.96	1.42	1.37
23	2	313	CLA	C1D-ND	3.95	1.42	1.37
23	3	308	CLA	C1D-ND	3.95	1.42	1.37
23	2	306	CLA	C1D-ND	3.95	1.42	1.37
23	7	310	CLA	C1D-ND	3.94	1.42	1.37
25	9	302	A1L1F	O13-C45	3.94	1.44	1.33
23	8	314	CLA	C1D-ND	3.94	1.42	1.37
23	9	312	CLA	C1D-ND	3.93	1.42	1.37
23	b	818	CLA	C1D-ND	3.93	1.42	1.37
23	a	828	CLA	C1D-ND	3.92	1.42	1.37
23	8	309	CLA	C1D-ND	3.92	1.42	1.37
23	6	316	CLA	C1D-ND	3.92	1.42	1.37
23	5	306	CLA	C1D-ND	3.92	1.42	1.37
23	2	307	CLA	C1D-ND	3.91	1.42	1.37
23	7	315	CLA	C1D-ND	3.91	1.42	1.37
23	2	314	CLA	C1D-ND	3.91	1.42	1.37
23	1	203	CLA	C1D-ND	3.91	1.42	1.37
28	j	103	LMG	O7-C10	3.91	1.45	1.34
23	2	315	CLA	C1D-ND	3.90	1.42	1.37
23	3	311	CLA	C1D-ND	3.90	1.42	1.37
23	a	838	CLA	C1D-ND	3.90	1.42	1.37
23	7	306	CLA	C1D-ND	3.90	1.42	1.37
23	a	837	CLA	C1D-ND	3.90	1.42	1.37
23	8	308	CLA	C1D-ND	3.90	1.42	1.37
23	5	315	CLA	C1D-ND	3.90	1.42	1.37
23	b	835	CLA	C1D-ND	3.89	1.42	1.37
23	7	307	CLA	C1D-ND	3.89	1.42	1.37
23	8	310	CLA	C1D-ND	3.89	1.42	1.37
23	8	305	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	840	CLA	C1D-ND	3.88	1.42	1.37
23	7	311	CLA	C1D-ND	3.88	1.42	1.37
23	8	307	CLA	C1D-ND	3.88	1.42	1.37
23	3	315	CLA	C1D-ND	3.88	1.42	1.37
23	l	201	CLA	C1D-ND	3.88	1.42	1.37
25	8	304	A1L1F	C57-C2	-3.88	1.25	1.32
23	4	315	CLA	C1D-ND	3.88	1.42	1.37
23	4	314	CLA	C1D-ND	3.87	1.42	1.37
23	a	815	CLA	C1D-ND	3.87	1.42	1.37
23	b	824	CLA	C1D-ND	3.87	1.42	1.37
22	1	301	A1L1G	C38-C39	3.87	1.40	1.35
23	4	305	CLA	C1D-ND	3.87	1.42	1.37
23	b	820	CLA	C1D-ND	3.87	1.42	1.37
23	9	310	CLA	C1D-ND	3.87	1.42	1.37
23	4	306	CLA	C1D-ND	3.87	1.42	1.37
23	b	840	CLA	C1D-ND	3.87	1.42	1.37
23	1	309	CLA	C1D-ND	3.86	1.42	1.37
23	1	310	CLA	C1D-ND	3.86	1.42	1.37
23	b	806	CLA	C1D-ND	3.86	1.42	1.37
25	h	202	A1L1F	C57-C2	-3.86	1.25	1.32
23	a	814	CLA	C1D-ND	3.86	1.42	1.37
23	2	312	CLA	C1D-ND	3.85	1.42	1.37
23	7	314	CLA	C1D-ND	3.85	1.42	1.37
23	b	813	CLA	C1D-ND	3.85	1.42	1.37
23	1	312	CLA	C1D-ND	3.85	1.42	1.37
23	a	835	CLA	C1D-ND	3.85	1.42	1.37
23	a	844	CLA	C1D-ND	3.85	1.42	1.37
23	4	309	CLA	C1D-ND	3.84	1.42	1.37
23	9	316	CLA	C1D-ND	3.84	1.42	1.37
23	b	836	CLA	C1D-ND	3.84	1.42	1.37
23	1	311	CLA	C1D-ND	3.84	1.42	1.37
23	a	839	CLA	C1D-ND	3.84	1.42	1.37
23	b	826	CLA	C1D-ND	3.84	1.42	1.37
23	j	101	CLA	C1D-ND	3.84	1.42	1.37
23	5	314	CLA	C1D-ND	3.84	1.42	1.37
23	5	312	CLA	C1D-ND	3.83	1.42	1.37
23	1	314	CLA	C1D-ND	3.83	1.42	1.37
23	4	311	CLA	C1D-ND	3.83	1.42	1.37
23	6	309	CLA	C1D-ND	3.83	1.42	1.37
23	a	811	CLA	C1D-ND	3.83	1.42	1.37
23	b	821	CLA	C1D-ND	3.83	1.42	1.37
27	4	317	DGD	O2G-C1B	3.83	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	817	CLA	C1D-ND	3.82	1.42	1.37
23	1	307	CLA	C1D-ND	3.82	1.42	1.37
23	5	310	CLA	C1D-ND	3.82	1.42	1.37
23	9	315	CLA	C1D-ND	3.82	1.42	1.37
23	7	317	CLA	C1D-ND	3.82	1.42	1.37
23	9	314	CLA	C1D-ND	3.82	1.42	1.37
23	7	308	CLA	C1D-ND	3.82	1.42	1.37
23	7	312	CLA	C1D-ND	3.82	1.42	1.37
23	a	831	CLA	C1D-ND	3.81	1.42	1.37
23	6	314	CLA	C1D-ND	3.81	1.42	1.37
23	a	816	CLA	C1D-ND	3.81	1.42	1.37
23	b	804	CLA	C1D-ND	3.81	1.42	1.37
23	b	828	CLA	C1D-ND	3.81	1.42	1.37
23	3	312	CLA	C1D-ND	3.81	1.42	1.37
23	2	309	CLA	C1D-ND	3.81	1.42	1.37
23	a	819	CLA	C1D-ND	3.80	1.42	1.37
23	2	311	CLA	C1D-ND	3.80	1.42	1.37
23	a	825	CLA	C1D-ND	3.80	1.42	1.37
23	4	313	CLA	C1D-ND	3.80	1.42	1.37
23	6	313	CLA	C1D-ND	3.80	1.42	1.37
23	8	306	CLA	C1D-ND	3.80	1.42	1.37
23	7	313	CLA	C1D-ND	3.80	1.42	1.37
23	a	829	CLA	C1D-ND	3.80	1.42	1.37
23	a	809	CLA	C1D-ND	3.79	1.42	1.37
23	b	839	CLA	C1D-ND	3.79	1.42	1.37
23	3	310	CLA	C1D-ND	3.79	1.42	1.37
23	6	311	CLA	C1D-ND	3.79	1.42	1.37
23	b	812	CLA	C1D-ND	3.79	1.42	1.37
23	5	311	CLA	C1D-ND	3.78	1.42	1.37
23	f	802	CLA	C1D-ND	3.78	1.42	1.37
25	9	302	A1L1F	C57-C2	-3.78	1.25	1.32
23	3	309	CLA	C1D-ND	3.78	1.42	1.37
22	1	301	A1L1G	C35-C34	3.78	1.40	1.35
23	5	307	CLA	C1D-ND	3.78	1.42	1.37
23	4	316	CLA	C1D-ND	3.78	1.42	1.37
23	6	307	CLA	C1D-ND	3.78	1.42	1.37
23	b	819	CLA	C1D-ND	3.77	1.42	1.37
23	b	833	CLA	C1D-ND	3.77	1.42	1.37
22	9	301	A1L1G	C35-C34	3.77	1.40	1.35
23	b	810	CLA	C1D-ND	3.77	1.42	1.37
23	a	834	CLA	C1D-ND	3.77	1.42	1.37
23	a	824	CLA	C1D-ND	3.77	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	841	CLA	C1D-ND	3.77	1.42	1.37
23	4	308	CLA	C1D-ND	3.77	1.42	1.37
23	b	838	CLA	C1D-ND	3.77	1.42	1.37
23	3	313	CLA	C1D-ND	3.77	1.42	1.37
23	a	836	CLA	C1D-ND	3.77	1.42	1.37
23	b	817	CLA	C1D-ND	3.77	1.42	1.37
23	a	807	CLA	C1D-ND	3.77	1.42	1.37
23	4	312	CLA	C1D-ND	3.76	1.42	1.37
23	7	316	CLA	C1D-ND	3.76	1.42	1.37
23	b	816	CLA	C1D-ND	3.76	1.42	1.37
23	b	834	CLA	C1D-ND	3.76	1.42	1.37
23	a	826	CLA	C1D-ND	3.76	1.42	1.37
23	5	313	CLA	C1D-ND	3.76	1.42	1.37
23	1	306	CLA	C1D-ND	3.75	1.42	1.37
23	a	813	CLA	C1D-ND	3.75	1.42	1.37
23	b	814	CLA	C1D-ND	3.75	1.42	1.37
23	b	831	CLA	C1D-ND	3.75	1.42	1.37
23	a	841	CLA	C1D-ND	3.75	1.42	1.37
23	a	812	CLA	C1D-ND	3.75	1.42	1.37
23	6	310	CLA	C1D-ND	3.74	1.42	1.37
23	1	305	CLA	C1D-ND	3.74	1.42	1.37
23	a	856	CLA	C1D-ND	3.74	1.42	1.37
23	9	311	CLA	C1D-ND	3.74	1.42	1.37
23	b	829	CLA	C1D-ND	3.74	1.42	1.37
27	8	315	DGD	O2G-C1B	3.73	1.44	1.34
23	f	803	CLA	C1D-ND	3.73	1.42	1.37
23	a	818	CLA	C1D-ND	3.73	1.42	1.37
23	a	830	CLA	C1D-ND	3.73	1.42	1.37
25	6	304	A1L1F	C57-C2	-3.73	1.25	1.32
23	b	827	CLA	C1D-ND	3.72	1.42	1.37
23	2	316	CLA	C1D-ND	3.72	1.42	1.37
23	a	823	CLA	C1D-ND	3.72	1.42	1.37
23	6	312	CLA	C1D-ND	3.72	1.42	1.37
23	9	308	CLA	C1D-ND	3.72	1.42	1.37
23	a	842	CLA	C1D-ND	3.72	1.42	1.37
23	b	807	CLA	C1D-ND	3.71	1.42	1.37
23	4	307	CLA	C1D-ND	3.71	1.42	1.37
23	2	308	CLA	C1D-ND	3.71	1.42	1.37
23	8	311	CLA	C1D-ND	3.71	1.42	1.37
23	a	832	CLA	C1D-ND	3.71	1.42	1.37
23	b	815	CLA	C1D-ND	3.71	1.42	1.37
23	b	801	CLA	C1D-ND	3.71	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	h	203	CLA	C1D-ND	3.71	1.42	1.37
25	6	301	A1L1F	C57-C2	-3.71	1.25	1.32
23	b	837	CLA	C1D-ND	3.71	1.42	1.37
23	b	822	CLA	C1D-ND	3.71	1.42	1.37
23	9	309	CLA	C1D-ND	3.71	1.42	1.37
23	a	852	CLA	C1D-ND	3.71	1.42	1.37
23	a	820	CLA	C1D-ND	3.70	1.42	1.37
23	2	310	CLA	C1D-ND	3.70	1.42	1.37
23	l	202	CLA	C1D-ND	3.70	1.42	1.37
22	9	301	A1L1G	C38-C39	3.70	1.40	1.35
23	a	827	CLA	C1D-ND	3.70	1.42	1.37
30	m	102	BCR	C1-C6	-3.69	1.48	1.53
23	a	822	CLA	C1D-ND	3.68	1.42	1.37
23	a	805	CLA	C1D-ND	3.68	1.42	1.37
22	7	302	A1L1G	C38-C39	3.67	1.40	1.35
23	a	803	CLA	C1D-ND	3.67	1.42	1.37
23	a	808	CLA	C1D-ND	3.67	1.42	1.37
22	3	306	A1L1G	C38-C39	3.67	1.40	1.35
23	a	810	CLA	C1D-ND	3.66	1.42	1.37
23	7	309	CLA	C1D-ND	3.66	1.42	1.37
23	1	313	CLA	C1D-ND	3.66	1.42	1.37
23	a	821	CLA	C1D-ND	3.66	1.42	1.37
23	3	307	CLA	C1D-ND	3.66	1.42	1.37
23	b	809	CLA	C1D-ND	3.66	1.42	1.37
23	b	808	CLA	C1D-ND	3.65	1.42	1.37
22	9	306	A1L1G	C35-C34	3.65	1.40	1.35
23	1	308	CLA	C1D-ND	3.64	1.42	1.37
23	b	805	CLA	C1D-ND	3.64	1.42	1.37
23	5	308	CLA	C1D-ND	3.64	1.42	1.37
23	b	832	CLA	C1D-ND	3.64	1.42	1.37
23	8	312	CLA	C1D-ND	3.64	1.42	1.37
23	5	316	CLA	C1D-ND	3.63	1.42	1.37
22	3	302	A1L1G	C35-C34	3.63	1.40	1.35
23	b	802	CLA	C1D-ND	3.62	1.42	1.37
23	b	825	CLA	C1D-ND	3.62	1.42	1.37
22	3	302	A1L1G	C38-C39	3.61	1.40	1.35
23	b	823	CLA	C1D-ND	3.57	1.42	1.37
23	a	801	CLA	C1D-ND	3.57	1.42	1.37
23	b	811	CLA	C1D-ND	3.56	1.42	1.37
25	1	304	A1L1F	C57-C2	-3.56	1.26	1.32
23	4	310	CLA	C1D-ND	3.54	1.42	1.37
23	b	830	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	802	CLA	C1D-ND	3.53	1.42	1.37
23	b	811	CLA	CAB-C3B	-3.51	1.44	1.51
22	5	304	A1L1G	C38-C39	3.48	1.40	1.35
22	3	302	A1L1G	C42-C44	3.47	1.40	1.35
22	5	304	A1L1G	C35-C34	3.47	1.40	1.35
23	a	833	CLA	C1D-ND	3.46	1.42	1.37
22	3	306	A1L1G	C35-C34	3.46	1.40	1.35
22	9	306	A1L1G	C38-C39	3.46	1.40	1.35
22	7	302	A1L1G	C35-C34	3.43	1.40	1.35
23	4	312	CLA	CHC-C1C	3.33	1.43	1.35
23	7	313	CLA	CHC-C1C	3.31	1.43	1.35
23	a	822	CLA	CHC-C1C	3.29	1.43	1.35
23	b	816	CLA	CHC-C1C	3.28	1.43	1.35
23	9	316	CLA	CHC-C1C	3.28	1.43	1.35
23	a	819	CLA	CHC-C1C	3.25	1.43	1.35
23	a	802	CLA	CHC-C1C	3.25	1.43	1.35
23	b	839	CLA	CHC-C1C	3.25	1.43	1.35
23	9	311	CLA	CHC-C1C	3.24	1.43	1.35
23	8	312	CLA	CHC-C1C	3.24	1.43	1.35
23	b	803	CLA	C1D-ND	3.24	1.41	1.37
23	b	814	CLA	CHC-C1C	3.24	1.43	1.35
23	a	827	CLA	CHC-C1C	3.24	1.43	1.35
23	b	805	CLA	CHC-C1C	3.24	1.43	1.35
23	b	811	CLA	CHC-C1C	3.23	1.43	1.35
23	a	852	CLA	CHC-C1C	3.23	1.43	1.35
23	6	308	CLA	CHC-C1C	3.23	1.43	1.35
23	2	308	CLA	CHC-C1C	3.23	1.43	1.35
23	5	307	CLA	CHC-C1C	3.22	1.43	1.35
23	6	311	CLA	CHC-C1C	3.22	1.43	1.35
23	4	311	CLA	CHC-C1C	3.22	1.43	1.35
23	8	311	CLA	CHC-C1C	3.22	1.43	1.35
23	7	311	CLA	CHC-C1C	3.22	1.43	1.35
23	f	803	CLA	CHC-C1C	3.21	1.43	1.35
23	9	308	CLA	CHC-C1C	3.21	1.43	1.35
23	8	313	CLA	CHC-C1C	3.21	1.43	1.35
23	2	309	CLA	CHC-C1C	3.21	1.43	1.35
23	8	306	CLA	CHC-C1C	3.21	1.43	1.35
23	7	306	CLA	CHC-C1C	3.21	1.43	1.35
23	a	813	CLA	CHC-C1C	3.21	1.43	1.35
23	a	823	CLA	CHC-C1C	3.20	1.43	1.35
23	b	834	CLA	CHC-C1C	3.20	1.43	1.35
23	2	315	CLA	CHC-C1C	3.20	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	312	CLA	CHC-C1C	3.20	1.43	1.35
23	b	825	CLA	CHC-C1C	3.20	1.43	1.35
23	a	818	CLA	CHC-C1C	3.20	1.43	1.35
23	a	856	CLA	CHC-C1C	3.20	1.43	1.35
23	8	314	CLA	CHC-C1C	3.20	1.43	1.35
23	4	313	CLA	CHC-C1C	3.20	1.43	1.35
23	a	820	CLA	CHC-C1C	3.20	1.43	1.35
23	a	837	CLA	CHC-C1C	3.19	1.43	1.35
23	b	828	CLA	CHC-C1C	3.19	1.43	1.35
23	b	804	CLA	CHC-C1C	3.19	1.43	1.35
23	1	308	CLA	CHC-C1C	3.19	1.43	1.35
23	7	314	CLA	CHC-C1C	3.19	1.43	1.35
23	a	842	CLA	CHC-C1C	3.19	1.43	1.35
23	b	832	CLA	CHC-C1C	3.19	1.43	1.35
23	6	313	CLA	CHC-C1C	3.19	1.43	1.35
23	b	836	CLA	CHC-C1C	3.19	1.43	1.35
23	7	312	CLA	CHC-C1C	3.19	1.43	1.35
23	a	804	CLA	CHC-C1C	3.19	1.43	1.35
23	5	313	CLA	CHC-C1C	3.19	1.43	1.35
23	a	809	CLA	CHC-C1C	3.19	1.43	1.35
23	a	832	CLA	CHC-C1C	3.19	1.43	1.35
23	a	841	CLA	CHC-C1C	3.19	1.43	1.35
23	b	815	CLA	CHC-C1C	3.19	1.43	1.35
23	b	813	CLA	CHC-C1C	3.19	1.43	1.35
23	5	316	CLA	CHC-C1C	3.19	1.43	1.35
23	8	305	CLA	CHC-C1C	3.19	1.43	1.35
23	5	312	CLA	CHC-C1C	3.18	1.43	1.35
23	a	826	CLA	CHC-C1C	3.18	1.43	1.35
23	1	310	CLA	CHC-C1C	3.18	1.43	1.35
23	a	833	CLA	CHC-C1C	3.18	1.43	1.35
23	9	314	CLA	CHC-C1C	3.18	1.43	1.35
23	4	314	CLA	CHC-C1C	3.18	1.43	1.35
23	b	822	CLA	CHC-C1C	3.18	1.43	1.35
23	b	831	CLA	CHC-C1C	3.18	1.43	1.35
23	7	308	CLA	CHC-C1C	3.17	1.43	1.35
23	8	309	CLA	CHC-C1C	3.17	1.43	1.35
23	1	312	CLA	CHC-C1C	3.17	1.43	1.35
23	5	315	CLA	CHC-C1C	3.17	1.43	1.35
23	1	307	CLA	CHC-C1C	3.17	1.43	1.35
23	4	309	CLA	CHC-C1C	3.17	1.43	1.35
23	6	314	CLA	CHC-C1C	3.17	1.43	1.35
23	a	839	CLA	CHC-C1C	3.17	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	313	CLA	CHC-C1C	3.17	1.43	1.35
23	3	313	CLA	CHC-C1C	3.17	1.43	1.35
23	4	307	CLA	C4D-ND	-3.17	1.33	1.37
23	b	820	CLA	CHC-C1C	3.17	1.43	1.35
23	a	803	CLA	CHC-C1C	3.17	1.43	1.35
23	7	307	CLA	CHC-C1C	3.16	1.43	1.35
23	b	827	CLA	CHC-C1C	3.16	1.43	1.35
23	a	828	CLA	C4D-ND	-3.16	1.33	1.37
23	a	824	CLA	CHC-C1C	3.16	1.43	1.35
23	4	316	CLA	CHC-C1C	3.16	1.43	1.35
23	b	808	CLA	CHC-C1C	3.16	1.43	1.35
23	9	313	CLA	CHC-C1C	3.16	1.43	1.35
23	3	311	CLA	CHC-C1C	3.16	1.43	1.35
23	b	837	CLA	CHC-C1C	3.16	1.43	1.35
23	b	812	CLA	CHC-C1C	3.16	1.43	1.35
23	h	203	CLA	CHC-C1C	3.16	1.43	1.35
23	2	310	CLA	CHC-C1C	3.16	1.43	1.35
23	7	317	CLA	CHC-C1C	3.16	1.43	1.35
23	a	836	CLA	CHC-C1C	3.16	1.43	1.35
23	2	311	CLA	CHC-C1C	3.16	1.43	1.35
23	1	314	CLA	CHC-C1C	3.16	1.43	1.35
23	b	830	CLA	CHC-C1C	3.16	1.43	1.35
23	9	315	CLA	CHC-C1C	3.15	1.43	1.35
23	a	811	CLA	CHC-C1C	3.15	1.43	1.35
23	l	202	CLA	CHC-C1C	3.15	1.43	1.35
23	a	828	CLA	CHC-C1C	3.15	1.43	1.35
23	5	314	CLA	CHC-C1C	3.15	1.43	1.35
23	a	816	CLA	CHC-C1C	3.15	1.43	1.35
23	f	802	CLA	CHC-C1C	3.15	1.43	1.35
23	b	838	CLA	CHC-C1C	3.15	1.43	1.35
23	3	307	CLA	CHC-C1C	3.15	1.43	1.35
23	1	305	CLA	CHC-C1C	3.15	1.43	1.35
23	3	315	CLA	CHC-C1C	3.15	1.43	1.35
23	2	314	CLA	CHC-C1C	3.15	1.43	1.35
23	5	310	CLA	CHC-C1C	3.15	1.43	1.35
23	a	808	CLA	CHC-C1C	3.15	1.43	1.35
23	a	844	CLA	CHC-C1C	3.15	1.43	1.35
23	b	823	CLA	CHC-C1C	3.15	1.43	1.35
23	l	203	CLA	CHC-C1C	3.15	1.43	1.35
23	a	817	CLA	CHC-C1C	3.15	1.43	1.35
23	2	316	CLA	CHC-C1C	3.15	1.43	1.35
23	3	312	CLA	CHC-C1C	3.15	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	310	CLA	CHC-C1C	3.15	1.43	1.35
23	5	311	CLA	CHC-C1C	3.14	1.43	1.35
23	3	310	CLA	CHC-C1C	3.14	1.43	1.35
23	a	812	CLA	CHC-C1C	3.14	1.43	1.35
23	1	309	CLA	CHC-C1C	3.14	1.43	1.35
23	b	830	CLA	C4D-ND	-3.14	1.33	1.37
23	5	309	CLA	CHC-C1C	3.14	1.43	1.35
23	a	814	CLA	CHC-C1C	3.14	1.43	1.35
23	a	805	CLA	CHC-C1C	3.14	1.43	1.35
23	5	313	CLA	C4D-ND	-3.14	1.33	1.37
23	4	307	CLA	CHC-C1C	3.14	1.43	1.35
23	a	829	CLA	CHC-C1C	3.14	1.43	1.35
23	9	309	CLA	CHC-C1C	3.14	1.43	1.35
23	b	803	CLA	CHC-C1C	3.14	1.43	1.35
23	a	834	CLA	CHC-C1C	3.14	1.43	1.35
23	b	841	CLA	CHC-C1C	3.14	1.43	1.35
23	5	308	CLA	C4D-ND	-3.13	1.33	1.37
23	b	806	CLA	CHC-C1C	3.13	1.43	1.35
23	b	835	CLA	CHC-C1C	3.13	1.43	1.35
23	4	308	CLA	CHC-C1C	3.13	1.43	1.35
23	1	311	CLA	CHC-C1C	3.13	1.43	1.35
23	7	315	CLA	CHC-C1C	3.13	1.43	1.35
30	m	102	BCR	C30-C25	-3.13	1.49	1.53
23	h	201	CLA	CHC-C1C	3.13	1.43	1.35
23	8	307	CLA	CHC-C1C	3.13	1.43	1.35
23	a	815	CLA	CHC-C1C	3.13	1.43	1.35
23	6	316	CLA	CHC-C1C	3.13	1.43	1.35
23	l	201	CLA	CHC-C1C	3.13	1.43	1.35
23	9	312	CLA	CHC-C1C	3.12	1.43	1.35
23	8	310	CLA	CHC-C1C	3.12	1.43	1.35
23	3	309	CLA	CHC-C1C	3.12	1.43	1.35
23	6	307	CLA	CHC-C1C	3.12	1.43	1.35
23	b	821	CLA	CHC-C1C	3.12	1.43	1.35
23	5	306	CLA	CHC-C1C	3.12	1.43	1.35
23	a	810	CLA	CHC-C1C	3.12	1.43	1.35
23	8	307	CLA	C4D-ND	-3.12	1.33	1.37
23	b	817	CLA	C4D-ND	-3.12	1.33	1.37
23	a	838	CLA	CHC-C1C	3.12	1.43	1.35
23	b	817	CLA	CHC-C1C	3.12	1.43	1.35
23	6	309	CLA	CHC-C1C	3.12	1.43	1.35
23	b	824	CLA	CHC-C1C	3.12	1.43	1.35
23	a	830	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	833	CLA	CHC-C1C	3.11	1.42	1.35
23	7	310	CLA	CHC-C1C	3.11	1.42	1.35
23	h	203	CLA	C4D-ND	-3.11	1.33	1.37
23	4	310	CLA	CHC-C1C	3.11	1.42	1.35
23	6	310	CLA	CHC-C1C	3.11	1.42	1.35
23	5	308	CLA	CHC-C1C	3.11	1.42	1.35
23	a	835	CLA	CHC-C1C	3.11	1.42	1.35
23	1	306	CLA	CHC-C1C	3.11	1.42	1.35
23	3	308	CLA	CHC-C1C	3.11	1.42	1.35
23	a	827	CLA	C4D-ND	-3.10	1.33	1.37
23	1	313	CLA	CHC-C1C	3.10	1.42	1.35
23	a	821	CLA	CHC-C1C	3.10	1.42	1.35
23	b	802	CLA	CHC-C1C	3.10	1.42	1.35
23	7	309	CLA	CHC-C1C	3.10	1.42	1.35
23	b	807	CLA	CHC-C1C	3.10	1.42	1.35
23	4	306	CLA	CHC-C1C	3.10	1.42	1.35
23	2	307	CLA	CHC-C1C	3.10	1.42	1.35
23	2	306	CLA	CHC-C1C	3.09	1.42	1.35
23	6	313	CLA	C4D-ND	-3.09	1.33	1.37
23	a	803	CLA	C4D-ND	-3.09	1.33	1.37
23	l	202	CLA	C4D-ND	-3.09	1.33	1.37
23	1	311	CLA	C4D-ND	-3.09	1.33	1.37
23	a	840	CLA	CHC-C1C	3.09	1.42	1.35
23	b	826	CLA	CHC-C1C	3.09	1.42	1.35
23	b	801	CLA	CHC-C1C	3.08	1.42	1.35
23	4	305	CLA	CHC-C1C	3.08	1.42	1.35
23	3	314	CLA	CHC-C1C	3.08	1.42	1.35
23	4	315	CLA	CHC-C1C	3.07	1.42	1.35
23	b	825	CLA	C4D-ND	-3.07	1.33	1.37
23	b	839	CLA	C4D-ND	-3.07	1.33	1.37
23	a	825	CLA	CHC-C1C	3.07	1.42	1.35
23	b	819	CLA	CHC-C1C	3.07	1.42	1.35
23	a	816	CLA	C4D-ND	-3.06	1.33	1.37
23	b	810	CLA	CHC-C1C	3.06	1.42	1.35
23	8	308	CLA	CHC-C1C	3.06	1.42	1.35
23	7	316	CLA	CHC-C1C	3.06	1.42	1.35
23	b	832	CLA	C4D-ND	-3.06	1.33	1.37
23	a	830	CLA	C4D-ND	-3.06	1.33	1.37
23	b	822	CLA	C4D-ND	-3.06	1.33	1.37
23	b	829	CLA	CMB-C2B	-3.06	1.45	1.51
23	a	807	CLA	CHC-C1C	3.06	1.42	1.35
23	3	309	CLA	C4D-ND	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	810	CLA	C4D-ND	-3.05	1.33	1.37
23	b	836	CLA	C4D-ND	-3.05	1.33	1.37
22	9	301	A1L1G	C42-C44	3.05	1.39	1.35
23	6	315	CLA	CHC-C1C	3.04	1.42	1.35
23	a	801	CLA	CHC-C1C	3.04	1.42	1.35
23	9	308	CLA	C4D-ND	-3.04	1.33	1.37
23	l	203	CLA	C4D-ND	-3.04	1.33	1.37
23	9	316	CLA	C4D-ND	-3.04	1.33	1.37
23	b	818	CLA	CHC-C1C	3.03	1.42	1.35
23	a	831	CLA	C4D-ND	-3.03	1.33	1.37
23	7	309	CLA	C4D-ND	-3.03	1.33	1.37
23	j	101	CLA	CHC-C1C	3.03	1.42	1.35
22	7	302	A1L1G	C42-C44	3.03	1.39	1.35
23	8	311	CLA	C4D-ND	-3.02	1.33	1.37
23	b	837	CLA	C4D-ND	-3.02	1.33	1.37
23	a	831	CLA	CMB-C2B	-3.02	1.45	1.51
23	6	310	CLA	C4D-ND	-3.02	1.33	1.37
23	7	313	CLA	C4D-ND	-3.02	1.33	1.37
23	6	312	CLA	CHC-C1C	3.01	1.42	1.35
23	a	829	CLA	C4D-ND	-3.01	1.33	1.37
23	b	807	CLA	C4D-ND	-3.01	1.33	1.37
23	a	856	CLA	C4D-ND	-3.01	1.33	1.37
23	a	852	CLA	C4D-ND	-3.01	1.33	1.37
23	b	841	CLA	C4D-ND	-3.01	1.33	1.37
23	b	813	CLA	C4D-ND	-3.01	1.33	1.37
23	a	819	CLA	C4D-ND	-3.00	1.33	1.37
23	a	824	CLA	C4D-ND	-3.00	1.33	1.37
23	4	311	CLA	C4D-ND	-3.00	1.33	1.37
23	1	310	CLA	C4D-ND	-3.00	1.33	1.37
23	b	833	CLA	C4D-ND	-3.00	1.33	1.37
23	a	807	CLA	C4D-ND	-3.00	1.33	1.37
23	b	828	CLA	C4D-ND	-3.00	1.33	1.37
23	4	312	CLA	C4D-ND	-2.99	1.33	1.37
23	b	819	CLA	C4D-ND	-2.99	1.33	1.37
23	a	808	CLA	C4D-ND	-2.99	1.33	1.37
23	8	312	CLA	C4D-ND	-2.98	1.33	1.37
23	9	315	CLA	C4D-ND	-2.98	1.33	1.37
23	b	826	CLA	C4D-ND	-2.98	1.33	1.37
23	b	809	CLA	CHC-C1C	2.98	1.42	1.35
23	9	311	CLA	C4D-ND	-2.98	1.33	1.37
23	2	309	CLA	C4D-ND	-2.98	1.33	1.37
23	4	309	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	806	CLA	C4D-ND	-2.97	1.33	1.37
23	a	812	CLA	C4D-ND	-2.97	1.33	1.37
23	a	806	CLA	CHC-C1C	2.97	1.42	1.35
23	3	311	CLA	C4D-ND	-2.97	1.33	1.37
23	b	829	CLA	CHC-C1C	2.97	1.42	1.35
23	b	816	CLA	C4D-ND	-2.96	1.33	1.37
23	8	310	CLA	C4D-ND	-2.96	1.33	1.37
23	9	309	CLA	C4D-ND	-2.96	1.33	1.37
23	9	313	CLA	C4D-ND	-2.96	1.33	1.37
23	5	310	CLA	C4D-ND	-2.96	1.33	1.37
23	1	201	CLA	C4D-ND	-2.96	1.33	1.37
23	b	811	CLA	C4D-ND	-2.96	1.33	1.37
23	b	820	CLA	C4D-ND	-2.96	1.33	1.37
23	a	805	CLA	C4D-ND	-2.95	1.33	1.37
23	b	802	CLA	C4D-ND	-2.95	1.33	1.37
23	8	309	CLA	C4D-ND	-2.95	1.33	1.37
23	a	831	CLA	CHC-C1C	2.95	1.42	1.35
23	a	836	CLA	C4D-ND	-2.95	1.33	1.37
23	7	311	CLA	C4D-ND	-2.95	1.33	1.37
23	a	801	CLA	C4D-ND	-2.95	1.33	1.37
23	3	313	CLA	C4D-ND	-2.94	1.33	1.37
23	b	835	CLA	C4D-ND	-2.94	1.33	1.37
24	5	317	SQD	C6-S	-2.94	1.66	1.77
23	9	310	CLA	C4D-ND	-2.94	1.33	1.37
23	b	823	CLA	C4D-ND	-2.94	1.33	1.37
23	2	316	CLA	C4D-ND	-2.94	1.33	1.37
23	b	815	CLA	C4D-ND	-2.94	1.33	1.37
23	4	308	CLA	C4D-ND	-2.93	1.33	1.37
25	9	302	A1L1F	C6-C1	-2.93	1.49	1.54
23	a	834	CLA	C4D-ND	-2.93	1.33	1.37
23	1	308	CLA	C4D-ND	-2.93	1.33	1.37
23	5	314	CLA	C4D-ND	-2.93	1.33	1.37
23	b	824	CLA	C4D-ND	-2.93	1.33	1.37
23	a	814	CLA	C4D-ND	-2.92	1.33	1.37
23	a	841	CLA	C4D-ND	-2.92	1.33	1.37
23	7	310	CLA	C4D-ND	-2.92	1.33	1.37
23	5	309	CLA	C4D-ND	-2.92	1.33	1.37
23	4	316	CLA	C4D-ND	-2.92	1.33	1.37
23	a	832	CLA	C4D-ND	-2.92	1.33	1.37
23	4	315	CLA	C4D-ND	-2.92	1.33	1.37
23	8	306	CLA	C4D-ND	-2.91	1.33	1.37
23	8	313	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	308	CLA	C4D-ND	-2.91	1.33	1.37
23	b	840	CLA	CHC-C1C	2.91	1.42	1.35
23	1	307	CLA	C4D-ND	-2.91	1.33	1.37
23	a	833	CLA	C4D-ND	-2.91	1.33	1.37
23	a	838	CLA	C4D-ND	-2.90	1.33	1.37
23	b	805	CLA	C4D-ND	-2.90	1.33	1.37
23	5	307	CLA	C4D-ND	-2.90	1.33	1.37
23	7	312	CLA	C4D-ND	-2.90	1.33	1.37
23	a	837	CLA	C4D-ND	-2.90	1.33	1.37
23	3	314	CLA	C4D-ND	-2.89	1.33	1.37
23	a	825	CLA	C4D-ND	-2.89	1.33	1.37
24	1	315	SQD	C6-S	-2.89	1.66	1.77
23	7	317	CLA	C4D-ND	-2.89	1.33	1.37
23	1	309	CLA	C4D-ND	-2.89	1.33	1.37
23	5	312	CLA	C4D-ND	-2.89	1.33	1.37
23	7	306	CLA	C4D-ND	-2.89	1.33	1.37
23	b	821	CLA	C4D-ND	-2.89	1.33	1.37
23	7	315	CLA	C4D-ND	-2.89	1.33	1.37
23	6	315	CLA	C4D-ND	-2.89	1.33	1.37
23	7	307	CLA	C4D-ND	-2.89	1.33	1.37
23	a	839	CLA	C4D-ND	-2.89	1.33	1.37
23	1	305	CLA	C4D-ND	-2.89	1.33	1.37
23	9	312	CLA	C4D-ND	-2.88	1.33	1.37
23	b	818	CLA	C4D-ND	-2.88	1.33	1.37
23	6	312	CLA	C4D-ND	-2.88	1.33	1.37
23	7	308	CLA	C4D-ND	-2.88	1.33	1.37
23	a	811	CLA	C4D-ND	-2.88	1.33	1.37
23	5	316	CLA	C4D-ND	-2.88	1.33	1.37
23	6	307	CLA	C4D-ND	-2.88	1.33	1.37
23	4	305	CLA	C4D-ND	-2.88	1.33	1.37
23	8	314	CLA	C4D-ND	-2.88	1.33	1.37
23	a	842	CLA	C4D-ND	-2.88	1.33	1.37
23	b	829	CLA	C4D-ND	-2.88	1.33	1.37
23	b	838	CLA	C4D-ND	-2.88	1.33	1.37
23	a	809	CLA	C4D-ND	-2.88	1.33	1.37
23	b	812	CLA	C4D-ND	-2.87	1.33	1.37
23	f	802	CLA	C4D-ND	-2.87	1.33	1.37
23	3	310	CLA	C4D-ND	-2.87	1.33	1.37
22	1	301	A1L1G	C42-C44	2.87	1.39	1.35
23	a	810	CLA	C4D-ND	-2.87	1.33	1.37
23	6	316	CLA	C4D-ND	-2.86	1.33	1.37
26	a	845	LHG	C26-C25	-2.86	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	306	CLA	C4D-ND	-2.86	1.33	1.37
23	a	813	CLA	C4D-ND	-2.86	1.33	1.37
23	2	310	CLA	C4D-ND	-2.85	1.33	1.37
23	2	314	CLA	C4D-ND	-2.85	1.33	1.37
23	b	804	CLA	C4D-ND	-2.85	1.33	1.37
23	1	313	CLA	C4D-ND	-2.85	1.33	1.37
23	a	826	CLA	C4D-ND	-2.85	1.33	1.37
23	b	834	CLA	C4D-ND	-2.85	1.33	1.37
23	a	804	CLA	C4D-ND	-2.85	1.33	1.37
23	a	802	CLA	C4D-ND	-2.85	1.33	1.37
23	a	815	CLA	C4D-ND	-2.85	1.33	1.37
23	5	311	CLA	C4D-ND	-2.84	1.33	1.37
23	2	311	CLA	C4D-ND	-2.84	1.33	1.37
23	a	817	CLA	C4D-ND	-2.84	1.33	1.37
23	a	823	CLA	C4D-ND	-2.84	1.33	1.37
23	5	315	CLA	C4D-ND	-2.84	1.33	1.37
23	b	809	CLA	C4D-ND	-2.84	1.33	1.37
23	1	312	CLA	C4D-ND	-2.84	1.33	1.37
23	a	835	CLA	C4D-ND	-2.84	1.33	1.37
26	m	101	LHG	C26-C25	-2.84	1.35	1.51
23	8	305	CLA	C4D-ND	-2.84	1.33	1.37
23	b	827	CLA	C4D-ND	-2.84	1.33	1.37
23	a	822	CLA	C4D-ND	-2.83	1.33	1.37
23	4	314	CLA	C4D-ND	-2.83	1.33	1.37
23	2	306	CLA	C4D-ND	-2.83	1.33	1.37
23	b	808	CLA	C4D-ND	-2.83	1.33	1.37
23	3	312	CLA	C4D-ND	-2.83	1.33	1.37
23	b	840	CLA	C4D-ND	-2.83	1.33	1.37
23	f	803	CLA	C4D-ND	-2.82	1.33	1.37
23	4	306	CLA	C4D-ND	-2.82	1.33	1.37
23	6	309	CLA	C4D-ND	-2.82	1.33	1.37
23	2	313	CLA	C4D-ND	-2.82	1.33	1.37
26	b	849	LHG	C26-C25	-2.82	1.35	1.51
23	7	314	CLA	C4D-ND	-2.82	1.33	1.37
23	2	315	CLA	C4D-ND	-2.82	1.33	1.37
23	6	308	CLA	C4D-ND	-2.81	1.33	1.37
23	3	315	CLA	C4D-ND	-2.81	1.33	1.37
23	a	840	CLA	C4D-ND	-2.81	1.33	1.37
26	9	307	LHG	C26-C25	-2.81	1.35	1.51
23	1	314	CLA	C4D-ND	-2.81	1.33	1.37
23	j	101	CLA	C4D-ND	-2.80	1.33	1.37
23	6	314	CLA	C4D-ND	-2.80	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	820	CLA	C4D-ND	-2.80	1.33	1.37
23	8	308	CLA	C4D-ND	-2.80	1.33	1.37
23	a	821	CLA	C4D-ND	-2.80	1.33	1.37
23	a	844	CLA	C4D-ND	-2.80	1.33	1.37
23	b	801	CLA	C4D-ND	-2.80	1.33	1.37
23	6	311	CLA	C4D-ND	-2.79	1.33	1.37
23	h	201	CLA	C4D-ND	-2.79	1.33	1.37
23	9	314	CLA	C4D-ND	-2.79	1.33	1.37
23	a	806	CLA	CMB-C2B	-2.79	1.45	1.51
23	a	818	CLA	C4D-ND	-2.79	1.33	1.37
23	4	313	CLA	C4D-ND	-2.78	1.33	1.37
23	3	307	CLA	C4D-ND	-2.78	1.33	1.37
23	5	306	CLA	C4D-ND	-2.77	1.33	1.37
23	b	814	CLA	C4D-ND	-2.77	1.33	1.37
23	2	307	CLA	C4D-ND	-2.77	1.33	1.37
23	3	308	CLA	C4D-ND	-2.76	1.33	1.37
23	4	310	CLA	C4D-ND	-2.76	1.33	1.37
23	b	819	CLA	CMB-C2B	-2.75	1.45	1.51
23	b	831	CLA	C4D-ND	-2.73	1.33	1.37
23	a	801	CLA	CMB-C2B	-2.73	1.46	1.51
22	5	304	A1L1G	C42-C44	2.72	1.39	1.35
22	9	301	A1L1G	C33-C34	-2.72	1.40	1.45
23	2	312	CLA	C4D-ND	-2.71	1.34	1.37
25	h	202	A1L1F	O15-C20	-2.70	1.42	1.46
25	h	202	A1L1F	C6-C1	-2.68	1.50	1.54
23	b	801	CLA	CMB-C2B	-2.66	1.46	1.51
23	7	316	CLA	C4D-ND	-2.65	1.34	1.37
22	3	306	A1L1G	C40-C39	-2.65	1.40	1.45
22	5	304	A1L1G	C33-C34	-2.63	1.40	1.45
23	2	307	CLA	CMB-C2B	-2.61	1.46	1.51
23	b	840	CLA	CMB-C2B	-2.61	1.46	1.51
22	9	306	A1L1G	C33-C34	-2.60	1.40	1.45
22	3	306	A1L1G	C33-C34	-2.60	1.40	1.45
23	a	806	CLA	C1D-ND	2.60	1.41	1.37
22	3	306	A1L1G	C42-C44	2.60	1.39	1.35
23	a	832	CLA	CMB-C2B	-2.60	1.46	1.51
23	b	818	CLA	CMB-C2B	-2.60	1.46	1.51
23	b	803	CLA	C4D-ND	-2.59	1.34	1.37
23	4	310	CLA	CMB-C2B	-2.59	1.46	1.51
23	b	809	CLA	CMB-C2B	-2.59	1.46	1.51
23	b	817	CLA	CMB-C2B	-2.58	1.46	1.51
23	a	820	CLA	CMB-C2B	-2.57	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	836	CLA	CMB-C2B	-2.57	1.46	1.51
23	8	310	CLA	CMB-C2B	-2.57	1.46	1.51
23	b	835	CLA	CMB-C2B	-2.56	1.46	1.51
23	2	310	CLA	CMB-C2B	-2.55	1.46	1.51
23	b	828	CLA	CMB-C2B	-2.55	1.46	1.51
25	6	301	A1L1F	O15-C20	-2.55	1.42	1.46
23	b	830	CLA	CMB-C2B	-2.54	1.46	1.51
23	a	803	CLA	CMB-C2B	-2.53	1.46	1.51
22	9	306	A1L1G	C42-C44	2.53	1.39	1.35
23	a	802	CLA	CMB-C2B	-2.52	1.46	1.51
23	a	822	CLA	CMB-C2B	-2.52	1.46	1.51
23	a	808	CLA	CMB-C2B	-2.51	1.46	1.51
22	3	302	A1L1G	C33-C34	-2.51	1.40	1.45
22	7	302	A1L1G	C33-C34	-2.51	1.40	1.45
22	5	304	A1L1G	C40-C39	-2.50	1.40	1.45
23	6	313	CLA	CMB-C2B	-2.50	1.46	1.51
23	b	808	CLA	CMB-C2B	-2.50	1.46	1.51
23	4	316	CLA	CMB-C2B	-2.50	1.46	1.51
23	1	203	CLA	CMB-C2B	-2.49	1.46	1.51
23	9	309	CLA	CMB-C2B	-2.49	1.46	1.51
23	7	311	CLA	CMB-C2B	-2.48	1.46	1.51
23	a	818	CLA	CMB-C2B	-2.48	1.46	1.51
23	5	313	CLA	CMB-C2B	-2.48	1.46	1.51
23	b	811	CLA	CMB-C2B	-2.47	1.46	1.51
23	1	201	CLA	CMB-C2B	-2.47	1.46	1.51
23	3	307	CLA	CMB-C2B	-2.47	1.46	1.51
23	a	824	CLA	CMB-C2B	-2.47	1.46	1.51
23	a	837	CLA	CMB-C2B	-2.47	1.46	1.51
23	1	202	CLA	CMB-C2B	-2.46	1.46	1.51
23	1	305	CLA	CMB-C2B	-2.46	1.46	1.51
23	a	856	CLA	CMB-C2B	-2.45	1.46	1.51
22	9	306	A1L1G	C40-C39	-2.45	1.40	1.45
21	9	303	XAT	O4-C5	-2.45	1.42	1.46
23	b	839	CLA	CMB-C2B	-2.45	1.46	1.51
22	1	301	A1L1G	C33-C34	-2.45	1.40	1.45
23	b	824	CLA	CMB-C2B	-2.45	1.46	1.51
23	a	806	CLA	CMD-C2D	-2.45	1.45	1.50
23	6	311	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	825	CLA	CMB-C2B	-2.44	1.46	1.51
23	4	311	CLA	CMB-C2B	-2.44	1.46	1.51
23	6	312	CLA	CMB-C2B	-2.44	1.46	1.51
23	8	308	CLA	CMB-C2B	-2.44	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	815	CLA	CMB-C2B	-2.44	1.46	1.51
23	7	314	CLA	CMB-C2B	-2.43	1.46	1.51
23	7	315	CLA	CMB-C2B	-2.43	1.46	1.51
23	8	314	CLA	CMB-C2B	-2.43	1.46	1.51
23	4	312	CLA	CMB-C2B	-2.43	1.46	1.51
22	3	302	A1L1G	C29-C30	-2.43	1.40	1.45
23	3	308	CLA	CMB-C2B	-2.43	1.46	1.51
23	f	803	CLA	CMB-C2B	-2.43	1.46	1.51
22	7	302	A1L1G	C40-C39	-2.43	1.40	1.45
23	1	309	CLA	CMB-C2B	-2.42	1.46	1.51
23	b	812	CLA	CMB-C2B	-2.42	1.46	1.51
23	a	817	CLA	CMB-C2B	-2.42	1.46	1.51
23	1	306	CLA	CMB-C2B	-2.42	1.46	1.51
23	1	307	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	810	CLA	CMB-C2B	-2.41	1.46	1.51
22	3	302	A1L1G	C40-C39	-2.41	1.40	1.45
23	8	313	CLA	CMB-C2B	-2.41	1.46	1.51
23	2	311	CLA	CMB-C2B	-2.41	1.46	1.51
23	5	314	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	841	CLA	CMB-C2B	-2.41	1.46	1.51
23	j	101	CLA	CMB-C2B	-2.41	1.46	1.51
23	4	309	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	804	CLA	CMB-C2B	-2.41	1.46	1.51
23	9	315	CLA	CMB-C2B	-2.41	1.46	1.51
23	3	311	CLA	CMB-C2B	-2.41	1.46	1.51
23	6	316	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	819	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	842	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	801	CLA	CMD-C2D	-2.41	1.45	1.50
23	7	317	CLA	CMB-C2B	-2.41	1.46	1.51
23	7	307	CLA	CMB-C2B	-2.40	1.46	1.51
23	9	316	CLA	CMB-C2B	-2.40	1.46	1.51
23	a	834	CLA	CMB-C2B	-2.40	1.46	1.51
23	b	827	CLA	CMB-C2B	-2.40	1.46	1.51
23	b	838	CLA	CMB-C2B	-2.40	1.46	1.51
23	a	835	CLA	CMB-C2B	-2.40	1.46	1.51
26	b	849	LHG	O8-C6	-2.40	1.39	1.45
23	b	822	CLA	CMB-C2B	-2.40	1.46	1.51
23	5	307	CLA	CMB-C2B	-2.40	1.46	1.51
23	b	813	CLA	CMB-C2B	-2.40	1.46	1.51
23	a	838	CLA	CMB-C2B	-2.40	1.46	1.51
23	9	308	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	311	CLA	CMB-C2B	-2.40	1.46	1.51
23	3	315	CLA	CMB-C2B	-2.40	1.46	1.51
23	1	310	CLA	CMB-C2B	-2.40	1.46	1.51
23	a	830	CLA	CMC-C2C	-2.39	1.45	1.50
23	9	314	CLA	CMB-C2B	-2.39	1.46	1.51
23	8	306	CLA	CMB-C2B	-2.39	1.46	1.51
23	4	315	CLA	CMB-C2B	-2.39	1.46	1.51
23	5	311	CLA	CMB-C2B	-2.39	1.46	1.51
23	8	312	CLA	CMB-C2B	-2.39	1.46	1.51
23	4	314	CLA	CMB-C2B	-2.39	1.46	1.51
23	7	309	CLA	CMB-C2B	-2.39	1.46	1.51
23	b	837	CLA	CMB-C2B	-2.39	1.46	1.51
23	2	306	CLA	CMB-C2B	-2.39	1.46	1.51
23	f	802	CLA	CMB-C2B	-2.39	1.46	1.51
23	2	316	CLA	CMB-C2B	-2.39	1.46	1.51
23	b	826	CLA	CMB-C2B	-2.39	1.46	1.51
23	b	833	CLA	CMB-C2B	-2.39	1.46	1.51
23	6	309	CLA	CMB-C2B	-2.39	1.46	1.51
23	5	315	CLA	CMB-C2B	-2.39	1.46	1.51
23	b	829	CLA	CMD-C2D	-2.38	1.45	1.50
23	1	308	CLA	CMB-C2B	-2.38	1.46	1.51
23	6	315	CLA	CMB-C2B	-2.38	1.46	1.51
23	1	312	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	836	CLA	CMB-C2B	-2.38	1.46	1.51
23	4	305	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	841	CLA	CMB-C2B	-2.38	1.46	1.51
23	1	313	CLA	CMB-C2B	-2.38	1.46	1.51
23	3	312	CLA	CMB-C2B	-2.38	1.46	1.51
23	7	306	CLA	CMB-C2B	-2.38	1.46	1.51
23	h	203	CLA	CMB-C2B	-2.37	1.46	1.51
23	b	804	CLA	CMB-C2B	-2.37	1.46	1.51
23	a	826	CLA	CMB-C2B	-2.37	1.46	1.51
23	2	314	CLA	CMB-C2B	-2.37	1.46	1.51
23	a	821	CLA	CMB-C2B	-2.37	1.46	1.51
23	5	308	CLA	CMB-C2B	-2.37	1.46	1.51
23	4	308	CLA	CMB-C2B	-2.37	1.46	1.51
23	a	827	CLA	CMB-C2B	-2.37	1.46	1.51
23	7	313	CLA	CMB-C2B	-2.37	1.46	1.51
23	1	311	CLA	CMB-C2B	-2.37	1.46	1.51
23	a	814	CLA	CMB-C2B	-2.37	1.46	1.51
23	b	815	CLA	CMB-C2B	-2.37	1.46	1.51
23	5	309	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	305	CLA	CMB-C2B	-2.37	1.46	1.51
23	3	314	CLA	CMB-C2B	-2.37	1.46	1.51
23	1	314	CLA	CMB-C2B	-2.37	1.46	1.51
23	7	312	CLA	CMB-C2B	-2.37	1.46	1.51
23	2	312	CLA	CMB-C2B	-2.37	1.46	1.51
26	a	846	LHG	O8-C6	-2.36	1.39	1.45
23	a	813	CLA	CMB-C2B	-2.36	1.46	1.51
23	3	313	CLA	CMB-C2B	-2.36	1.46	1.51
23	5	310	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	806	CLA	CMB-C2B	-2.36	1.46	1.51
23	a	806	CLA	C3B-C2B	-2.36	1.37	1.40
23	a	839	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	816	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	820	CLA	CMB-C2B	-2.36	1.46	1.51
23	6	308	CLA	CMB-C2B	-2.36	1.46	1.51
23	h	201	CLA	CMB-C2B	-2.36	1.46	1.51
23	a	806	CLA	CMC-C2C	-2.36	1.45	1.50
26	a	845	LHG	O8-C6	-2.36	1.39	1.45
23	9	312	CLA	CMB-C2B	-2.35	1.46	1.51
26	m	101	LHG	O8-C23	2.35	1.40	1.33
23	4	313	CLA	CMB-C2B	-2.35	1.46	1.51
23	b	834	CLA	CMB-C2B	-2.35	1.46	1.51
26	m	101	LHG	O8-C6	-2.35	1.39	1.45
26	b	849	LHG	O8-C23	2.35	1.40	1.33
23	8	307	CLA	CMB-C2B	-2.35	1.46	1.51
23	6	310	CLA	CMB-C2B	-2.35	1.46	1.51
23	5	316	CLA	CMB-C2B	-2.35	1.46	1.51
23	a	825	CLA	CMB-C2B	-2.35	1.46	1.51
23	7	310	CLA	CMB-C2B	-2.35	1.46	1.51
23	4	306	CLA	CMB-C2B	-2.34	1.46	1.51
23	2	309	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	810	CLA	CMB-C2B	-2.34	1.46	1.51
23	3	310	CLA	CMB-C2B	-2.34	1.46	1.51
23	a	807	CLA	CMB-C2B	-2.34	1.46	1.51
22	9	301	A1L1G	C29-C30	-2.34	1.40	1.45
23	3	309	CLA	CMB-C2B	-2.34	1.46	1.51
23	9	313	CLA	CMB-C2B	-2.34	1.46	1.51
23	a	830	CLA	CMB-C2B	-2.34	1.46	1.51
23	8	309	CLA	CMB-C2B	-2.34	1.46	1.51
23	a	806	CLA	C3B-CAB	-2.34	1.43	1.47
23	8	311	CLA	CMB-C2B	-2.34	1.46	1.51
23	a	852	CLA	CMB-C2B	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	840	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	814	CLA	CMB-C2B	-2.34	1.46	1.51
23	6	307	CLA	CMB-C2B	-2.34	1.46	1.51
23	a	811	CLA	CMB-C2B	-2.33	1.46	1.51
23	2	315	CLA	CMB-C2B	-2.33	1.46	1.51
23	a	812	CLA	CMB-C2B	-2.33	1.46	1.51
23	b	807	CLA	CMB-C2B	-2.33	1.46	1.51
23	4	307	CLA	CMB-C2B	-2.33	1.46	1.51
23	b	831	CLA	CMB-C2B	-2.33	1.46	1.51
25	9	302	A1L1F	O15-C20	-2.33	1.42	1.46
23	a	823	CLA	CMB-C2B	-2.33	1.46	1.51
23	9	310	CLA	CMB-C2B	-2.33	1.46	1.51
23	b	805	CLA	CMB-C2B	-2.33	1.46	1.51
23	a	816	CLA	CMB-C2B	-2.33	1.46	1.51
23	a	844	CLA	CMB-C2B	-2.32	1.46	1.51
23	b	823	CLA	CMB-C2B	-2.32	1.46	1.51
23	4	310	CLA	CMD-C2D	-2.31	1.45	1.50
23	6	314	CLA	CMB-C2B	-2.31	1.46	1.51
23	5	306	CLA	CMB-C2B	-2.31	1.46	1.51
22	1	301	A1L1G	C40-C39	-2.31	1.41	1.45
23	a	828	CLA	CMB-C2B	-2.31	1.46	1.51
23	a	829	CLA	CMB-C2B	-2.31	1.46	1.51
23	b	821	CLA	CMB-C2B	-2.31	1.46	1.51
23	b	832	CLA	CMB-C2B	-2.31	1.46	1.51
23	7	308	CLA	CMB-C2B	-2.31	1.46	1.51
23	a	809	CLA	CMB-C2B	-2.31	1.46	1.51
25	1	304	A1L1F	C6-C1	-2.31	1.50	1.54
23	a	805	CLA	CMB-C2B	-2.30	1.46	1.51
23	2	308	CLA	CMB-C2B	-2.30	1.46	1.51
23	b	802	CLA	CMB-C2B	-2.30	1.46	1.51
26	9	307	LHG	O7-C7	2.30	1.40	1.34
23	a	833	CLA	CMB-C2B	-2.30	1.46	1.51
22	1	301	A1L1G	C29-C30	-2.29	1.40	1.45
23	9	308	CLA	CMC-C2C	-2.29	1.45	1.50
23	2	313	CLA	CMB-C2B	-2.28	1.46	1.51
23	7	316	CLA	CMB-C2B	-2.28	1.46	1.51
22	3	306	A1L1G	C29-C30	-2.28	1.40	1.45
23	b	808	CLA	CMD-C2D	-2.28	1.46	1.50
26	b	849	LHG	O7-C7	2.28	1.40	1.34
26	9	307	LHG	O8-C6	-2.27	1.40	1.45
26	m	101	LHG	O7-C7	2.27	1.40	1.34
26	a	846	LHG	O8-C23	2.27	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	312	CLA	CMB-C2B	-2.27	1.46	1.51
26	a	845	LHG	O7-C7	2.27	1.40	1.34
23	b	822	CLA	CMD-C2D	-2.26	1.46	1.50
26	9	307	LHG	O8-C23	2.26	1.39	1.33
26	a	846	LHG	O7-C5	-2.26	1.40	1.46
22	9	301	A1L1G	C40-C39	-2.26	1.41	1.45
26	a	845	LHG	O8-C23	2.25	1.39	1.33
26	b	849	LHG	O7-C5	-2.24	1.41	1.46
26	a	846	LHG	O7-C7	2.23	1.40	1.34
25	1	304	A1L1F	O15-C20	-2.22	1.43	1.46
23	b	823	CLA	CMD-C2D	-2.22	1.46	1.50
25	6	301	A1L1F	C6-C1	-2.22	1.50	1.54
22	5	304	A1L1G	C29-C30	-2.20	1.40	1.45
23	a	824	CLA	CMD-C2D	-2.19	1.46	1.50
26	a	845	LHG	O7-C5	-2.19	1.41	1.46
23	a	801	CLA	C3B-CAB	-2.19	1.43	1.47
23	3	307	CLA	CMD-C2D	-2.18	1.46	1.50
23	a	801	CLA	CMC-C2C	-2.17	1.46	1.50
23	b	830	CLA	CMD-C2D	-2.17	1.46	1.50
26	9	307	LHG	O7-C5	-2.17	1.41	1.46
23	a	806	CLA	CAA-C2A	-2.16	1.50	1.54
21	2	303	XAT	O4-C5	-2.16	1.43	1.46
23	2	310	CLA	CMD-C2D	-2.16	1.46	1.50
26	m	101	LHG	O7-C5	-2.15	1.41	1.46
23	5	306	CLA	CMD-C2D	-2.15	1.46	1.50
23	7	314	CLA	CMD-C2D	-2.15	1.46	1.50
21	5	303	XAT	O4-C5	-2.15	1.43	1.46
23	b	803	CLA	CMB-C2B	-2.15	1.47	1.51
22	9	306	A1L1G	C29-C30	-2.15	1.40	1.45
23	a	828	CLA	CMC-C2C	-2.15	1.46	1.50
21	5	301	XAT	O24-C25	-2.14	1.43	1.46
23	b	839	CLA	CMD-C2D	-2.14	1.46	1.50
23	9	309	CLA	CMD-C2D	-2.14	1.46	1.50
23	b	802	CLA	CMD-C2D	-2.13	1.46	1.50
23	a	810	CLA	CMD-C2D	-2.13	1.46	1.50
21	9	305	XAT	O4-C5	-2.13	1.43	1.46
27	b	851	DGD	O3D-C3D	-2.13	1.38	1.43
25	8	304	A1L1F	O15-C20	-2.13	1.43	1.46
23	7	316	CLA	CMD-C2D	-2.13	1.46	1.50
23	b	838	CLA	CMD-C2D	-2.13	1.46	1.50
23	a	830	CLA	CMD-C2D	-2.12	1.46	1.50
27	b	851	DGD	C1E-C2E	2.12	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	851	DGD	O4D-C4D	-2.12	1.38	1.43
23	b	811	CLA	CMD-C2D	-2.11	1.46	1.50
21	4	304	XAT	O4-C5	-2.11	1.43	1.46
21	3	305	XAT	O4-C5	-2.11	1.43	1.46
21	1	302	XAT	O4-C5	-2.11	1.43	1.46
23	b	814	CLA	CMD-C2D	-2.11	1.46	1.50
23	b	828	CLA	CMD-C2D	-2.11	1.46	1.50
23	a	804	CLA	CMC-C2C	-2.11	1.46	1.50
21	9	304	XAT	O4-C5	-2.10	1.43	1.46
23	a	816	CLA	CMD-C2D	-2.10	1.46	1.50
23	a	812	CLA	CMD-C2D	-2.10	1.46	1.50
21	3	301	XAT	O4-C5	-2.10	1.43	1.46
23	a	821	CLA	CMD-C2D	-2.10	1.46	1.50
23	a	803	CLA	C3B-CAB	-2.09	1.43	1.47
26	9	307	LHG	P-O6	2.09	1.67	1.59
23	2	316	CLA	CMD-C2D	-2.09	1.46	1.50
23	9	312	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	801	CLA	CMD-C2D	-2.09	1.46	1.50
21	5	301	XAT	O4-C5	-2.09	1.43	1.46
21	a	854	XAT	O4-C5	-2.08	1.43	1.46
26	m	101	LHG	P-O6	2.08	1.67	1.59
23	b	832	CLA	CMD-C2D	-2.07	1.46	1.50
23	a	842	CLA	CMD-C2D	-2.07	1.46	1.50
21	8	303	XAT	O4-C5	-2.07	1.43	1.46
21	2	302	XAT	O4-C5	-2.07	1.43	1.46
26	b	849	LHG	P-O6	2.06	1.67	1.59
23	7	306	CLA	CMD-C2D	-2.06	1.46	1.50
21	1	303	XAT	O4-C5	-2.06	1.43	1.46
21	7	301	XAT	O24-C25	-2.06	1.43	1.46
27	b	851	DGD	O4E-C4E	-2.06	1.38	1.43
21	4	302	XAT	O24-C25	-2.06	1.43	1.46
23	3	315	CLA	CMD-C2D	-2.05	1.46	1.50
23	a	806	CLA	MG-ND	-2.05	2.01	2.05
26	a	845	LHG	P-O6	2.05	1.67	1.59
23	b	834	CLA	CMD-C2D	-2.05	1.46	1.50
23	7	311	CLA	CMD-C2D	-2.05	1.46	1.50
23	a	807	CLA	CMD-C2D	-2.05	1.46	1.50
21	a	853	XAT	O24-C25	-2.05	1.43	1.46
23	l	201	CLA	CMD-C2D	-2.05	1.46	1.50
23	6	307	CLA	CMD-C2D	-2.05	1.46	1.50
23	1	313	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	802	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	314	CLA	CMD-C2D	-2.04	1.46	1.50
27	b	851	DGD	O2D-C2D	-2.04	1.38	1.43
23	a	832	CLA	CMD-C2D	-2.04	1.46	1.50
23	1	305	CLA	CMD-C2D	-2.04	1.46	1.50
21	8	302	XAT	O4-C5	-2.04	1.43	1.46
21	3	304	XAT	O24-C25	-2.04	1.43	1.46
21	6	305	XAT	O4-C5	-2.04	1.43	1.46
21	a	854	XAT	O24-C25	-2.04	1.43	1.46
23	9	316	CLA	CMD-C2D	-2.04	1.46	1.50
23	4	311	CLA	CMD-C2D	-2.04	1.46	1.50
21	5	302	XAT	O4-C5	-2.03	1.43	1.46
21	7	303	XAT	O4-C5	-2.03	1.43	1.46
23	a	819	CLA	CMC-C2C	-2.03	1.46	1.50
25	6	304	A1L1F	O15-C20	-2.03	1.43	1.46
23	6	312	CLA	CMD-C2D	-2.03	1.46	1.50
23	4	313	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	802	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	826	CLA	CMD-C2D	-2.03	1.46	1.50
21	7	304	XAT	O4-C5	-2.03	1.43	1.46
23	3	308	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	815	CLA	CMC-C2C	-2.02	1.46	1.50
23	8	313	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	808	CLA	CMC-C2C	-2.02	1.46	1.50
23	b	821	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	827	CLA	CMD-C2D	-2.02	1.46	1.50
21	3	301	XAT	O24-C25	-2.02	1.43	1.46
21	8	301	XAT	O4-C5	-2.02	1.43	1.46
21	4	301	XAT	O24-C25	-2.02	1.43	1.46
23	3	313	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	852	CLA	CMD-C2D	-2.02	1.46	1.50
23	2	308	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	819	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	827	CLA	CMD-C2D	-2.02	1.46	1.50
23	9	308	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	839	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	820	CLA	CMD-C2D	-2.02	1.46	1.50
22	7	302	A1L1G	C29-C30	-2.02	1.40	1.45
23	a	823	CLA	CMD-C2D	-2.02	1.46	1.50
21	3	304	XAT	O4-C5	-2.02	1.43	1.46
23	1	203	CLA	CMC-C2C	-2.02	1.46	1.50
23	a	818	CLA	CMD-C2D	-2.02	1.46	1.50
21	6	302	XAT	O4-C5	-2.02	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	h	201	CLA	CMD-C2D	-2.02	1.46	1.50
23	2	306	CLA	CMD-C2D	-2.02	1.46	1.50
30	m	102	BCR	C33-C5	-2.02	1.47	1.50
21	6	306	XAT	O24-C25	-2.02	1.43	1.46
23	6	315	CLA	CMD-C2D	-2.01	1.46	1.50
23	8	308	CLA	CMD-C2D	-2.01	1.46	1.50
23	2	314	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	819	CLA	CMD-C2D	-2.01	1.46	1.50
23	l	202	CLA	CMC-C2C	-2.01	1.46	1.50
23	a	809	CLA	CMD-C2D	-2.01	1.46	1.50
23	a	811	CLA	CMD-C2D	-2.01	1.46	1.50
23	5	311	CLA	CMD-C2D	-2.01	1.46	1.50
23	5	309	CLA	CMD-C2D	-2.01	1.46	1.50
23	4	307	CLA	CMD-C2D	-2.01	1.46	1.50
23	h	203	CLA	CMC-C2C	-2.01	1.46	1.50
23	4	314	CLA	CMD-C2D	-2.01	1.46	1.50
23	4	316	CLA	CMD-C2D	-2.01	1.46	1.50
23	4	308	CLA	CMD-C2D	-2.01	1.46	1.50
23	3	309	CLA	CMD-C2D	-2.01	1.46	1.50
23	4	305	CLA	CMD-C2D	-2.01	1.46	1.50
23	8	310	CLA	CMD-C2D	-2.01	1.46	1.50
23	a	836	CLA	CMD-C2D	-2.01	1.46	1.50
23	6	309	CLA	CMD-C2D	-2.01	1.46	1.50
23	2	315	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	825	CLA	CMD-C2D	-2.01	1.46	1.50
23	2	312	CLA	CMD-C2D	-2.01	1.46	1.50
23	a	805	CLA	CMD-C2D	-2.01	1.46	1.50
23	a	813	CLA	CMD-C2D	-2.01	1.46	1.50
23	2	314	CLA	CMC-C2C	-2.00	1.46	1.50
21	4	302	XAT	O4-C5	-2.00	1.43	1.46
23	6	308	CLA	CMD-C2D	-2.00	1.46	1.50
23	b	836	CLA	CMD-C2D	-2.00	1.46	1.50
23	b	803	CLA	CMD-C2D	-2.00	1.46	1.50
23	b	807	CLA	CMD-C2D	-2.00	1.46	1.50
23	b	833	CLA	CMD-C2D	-2.00	1.46	1.50

All (2650) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	9	302	A1L1F	O15-C20-C21	13.14	123.26	113.38
27	4	317	DGD	C6E-C5E-C4E	-9.39	91.00	113.00
25	6	301	A1L1F	O15-C20-C21	8.72	119.94	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	304	A1L1F	O15-C20-C21	8.65	119.88	113.38
25	8	304	A1L1F	O15-C20-C21	8.52	119.78	113.38
25	9	302	A1L1F	C17-C20-C25	-8.46	108.09	122.26
25	6	301	A1L1F	C17-C20-C25	-8.45	108.09	122.26
25	h	202	A1L1F	O15-C20-C21	8.39	119.69	113.38
25	h	202	A1L1F	C17-C20-C25	-8.33	108.30	122.26
25	6	304	A1L1F	C17-C20-C25	-8.26	108.41	122.26
25	8	304	A1L1F	C17-C20-C25	-8.26	108.42	122.26
25	1	304	A1L1F	C17-C20-C25	-8.11	108.67	122.26
25	8	304	A1L1F	C37-C38-C39	-7.85	116.11	127.31
21	6	305	XAT	C18-C5-C4	7.60	122.83	114.28
21	6	303	XAT	C38-C25-C26	-7.41	109.84	122.26
21	9	303	XAT	C38-C25-C24	7.32	122.52	114.28
23	9	310	CLA	C4A-NA-C1A	7.30	109.99	106.71
23	7	314	CLA	C4A-NA-C1A	7.29	109.98	106.71
25	1	304	A1L1F	O15-C20-C21	7.27	118.84	113.38
23	9	313	CLA	C4A-NA-C1A	7.26	109.97	106.71
21	4	304	XAT	C38-C25-C24	7.24	122.43	114.28
23	b	802	CLA	C4A-NA-C1A	7.24	109.96	106.71
23	a	806	CLA	C4A-NA-C1A	7.24	109.96	106.71
21	3	305	XAT	C38-C25-C24	7.22	122.40	114.28
21	1	303	XAT	C38-C25-C24	7.21	122.39	114.28
23	a	835	CLA	C4A-NA-C1A	7.20	109.94	106.71
23	b	840	CLA	C4A-NA-C1A	7.19	109.94	106.71
21	7	304	XAT	C38-C25-C24	7.17	122.35	114.28
21	5	305	XAT	C38-C25-C24	7.15	122.33	114.28
23	l	202	CLA	C4A-NA-C1A	7.15	109.92	106.71
21	9	304	XAT	C38-C25-C24	7.12	122.29	114.28
21	a	854	XAT	C15-C14-C13	-7.11	117.17	127.31
23	a	823	CLA	C4A-NA-C1A	7.08	109.89	106.71
23	9	308	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	a	833	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	4	309	CLA	C4A-NA-C1A	7.05	109.88	106.71
23	b	820	CLA	C4A-NA-C1A	7.05	109.87	106.71
21	7	305	XAT	C38-C25-C24	7.05	122.21	114.28
21	a	853	XAT	C38-C25-C24	7.05	122.21	114.28
21	4	303	XAT	C38-C25-C24	7.04	122.20	114.28
30	f	801	BCR	C24-C23-C22	-7.01	115.64	126.23
21	5	305	XAT	C18-C5-C4	7.01	122.16	114.28
23	b	804	CLA	C4A-NA-C1A	7.00	109.85	106.71
23	b	808	CLA	C4A-NA-C1A	6.99	109.85	106.71
23	b	801	CLA	C4A-NA-C1A	6.99	109.85	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	810	CLA	C4A-NA-C1A	6.98	109.84	106.71
23	6	312	CLA	C4A-NA-C1A	6.94	109.83	106.71
21	3	304	XAT	C38-C25-C24	6.94	122.09	114.28
21	6	302	XAT	C38-C25-C24	6.94	122.09	114.28
23	j	101	CLA	C4A-NA-C1A	6.94	109.83	106.71
23	a	828	CLA	C4A-NA-C1A	6.94	109.82	106.71
21	6	305	XAT	C38-C25-C24	6.94	122.08	114.28
23	1	308	CLA	C4A-NA-C1A	6.93	109.82	106.71
23	7	317	CLA	C4A-NA-C1A	6.93	109.82	106.71
23	4	315	CLA	C4A-NA-C1A	6.93	109.82	106.71
21	8	301	XAT	C38-C25-C24	6.91	122.05	114.28
23	h	201	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	b	821	CLA	C4A-NA-C1A	6.89	109.80	106.71
21	1	302	XAT	C38-C25-C24	6.89	122.03	114.28
21	5	302	XAT	C38-C25-C26	-6.88	110.73	122.26
23	a	801	CLA	C4A-NA-C1A	6.88	109.80	106.71
23	a	821	CLA	C4A-NA-C1A	6.86	109.79	106.71
21	5	305	XAT	C6-C7-C8	-6.85	111.51	125.99
21	2	301	XAT	C18-C5-C6	-6.85	110.79	122.26
23	6	310	CLA	C4A-NA-C1A	6.84	109.78	106.71
23	b	827	CLA	C4A-NA-C1A	6.84	109.78	106.71
23	a	826	CLA	C4A-NA-C1A	6.83	109.78	106.71
21	9	303	XAT	C38-C25-C26	-6.83	110.82	122.26
21	4	304	XAT	C38-C25-C26	-6.82	110.83	122.26
23	b	810	CLA	C4A-NA-C1A	6.82	109.77	106.71
21	8	303	XAT	C38-C25-C24	6.80	121.93	114.28
21	2	304	XAT	C38-C25-C24	6.80	121.93	114.28
23	6	316	CLA	C4A-NA-C1A	6.80	109.76	106.71
21	a	854	XAT	C38-C25-C24	6.79	121.92	114.28
23	b	814	CLA	C4A-NA-C1A	6.79	109.76	106.71
23	f	802	CLA	C4A-NA-C1A	6.79	109.76	106.71
23	3	308	CLA	C4A-NA-C1A	6.78	109.75	106.71
21	4	302	XAT	C38-C25-C24	6.78	121.90	114.28
21	8	301	XAT	C38-C25-C26	-6.77	110.91	122.26
21	3	304	XAT	C38-C25-C26	-6.77	110.92	122.26
23	1	306	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	b	837	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	b	809	CLA	C4A-NA-C1A	6.76	109.75	106.71
23	a	825	CLA	C4A-NA-C1A	6.76	109.75	106.71
23	b	812	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	l	201	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	3	312	CLA	C4A-NA-C1A	6.75	109.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	809	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	b	824	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	8	312	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	4	316	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	2	316	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	4	310	CLA	C4A-NA-C1A	6.74	109.73	106.71
23	a	812	CLA	C4A-NA-C1A	6.74	109.73	106.71
23	b	805	CLA	C4A-NA-C1A	6.74	109.73	106.71
23	7	307	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	a	817	CLA	C4A-NA-C1A	6.73	109.73	106.71
21	8	303	XAT	C18-C5-C6	-6.73	110.98	122.26
23	6	309	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	a	840	CLA	C4A-NA-C1A	6.72	109.73	106.71
23	a	834	CLA	C4A-NA-C1A	6.72	109.73	106.71
23	b	832	CLA	C4A-NA-C1A	6.72	109.73	106.71
21	2	301	XAT	C18-C5-C4	6.72	121.83	114.28
23	3	313	CLA	C4A-NA-C1A	6.71	109.72	106.71
23	a	839	CLA	C4A-NA-C1A	6.71	109.72	106.71
23	6	314	CLA	C4A-NA-C1A	6.71	109.72	106.71
21	9	304	XAT	C38-C25-C26	-6.70	111.03	122.26
23	9	314	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	3	314	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	a	832	CLA	C4A-NA-C1A	6.69	109.72	106.71
23	1	305	CLA	C4A-NA-C1A	6.69	109.71	106.71
23	1	203	CLA	C4A-NA-C1A	6.69	109.71	106.71
21	3	303	XAT	C38-C25-C24	6.69	121.80	114.28
21	8	302	XAT	C38-C25-C24	6.67	121.79	114.28
21	6	302	XAT	C38-C25-C26	-6.67	111.07	122.26
21	6	303	XAT	C38-C25-C24	6.67	121.79	114.28
21	5	305	XAT	C18-C5-C6	-6.67	111.08	122.26
21	7	304	XAT	C18-C5-C6	-6.66	111.09	122.26
23	4	306	CLA	C4A-NA-C1A	6.66	109.70	106.71
21	2	304	XAT	C18-C5-C4	6.66	121.77	114.28
23	2	311	CLA	C4A-NA-C1A	6.66	109.70	106.71
21	3	304	XAT	C18-C5-C6	-6.66	111.10	122.26
23	a	807	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	a	838	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	b	807	CLA	C4A-NA-C1A	6.64	109.69	106.71
21	7	301	XAT	C18-C5-C4	6.64	121.75	114.28
23	5	314	CLA	C4A-NA-C1A	6.64	109.69	106.71
23	3	315	CLA	C4A-NA-C1A	6.64	109.69	106.71
23	6	308	CLA	C4A-NA-C1A	6.63	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	831	CLA	C4A-NA-C1A	6.63	109.69	106.71
21	5	303	XAT	C18-C5-C6	-6.63	111.14	122.26
21	4	301	XAT	C38-C25-C24	6.63	121.74	114.28
21	6	302	XAT	C11-C10-C9	-6.63	117.85	127.31
23	5	311	CLA	C4A-NA-C1A	6.63	109.69	106.71
23	5	307	CLA	C4A-NA-C1A	6.62	109.68	106.71
23	2	314	CLA	C4A-NA-C1A	6.62	109.68	106.71
21	5	301	XAT	C31-C30-C29	-6.62	117.87	127.31
21	7	301	XAT	C18-C5-C6	-6.62	111.17	122.26
23	a	856	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	b	806	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	1	307	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	8	313	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	f	803	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	2	313	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	8	307	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	a	818	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	b	826	CLA	C4A-NA-C1A	6.59	109.67	106.71
30	i	101	BCR	C24-C23-C22	-6.58	116.29	126.23
23	a	805	CLA	C4A-NA-C1A	6.58	109.67	106.71
21	7	303	XAT	C38-C25-C26	-6.58	111.23	122.26
23	b	834	CLA	C4A-NA-C1A	6.58	109.66	106.71
21	5	302	XAT	C38-C25-C24	6.58	121.68	114.28
23	5	309	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	a	804	CLA	C4A-NA-C1A	6.58	109.66	106.71
21	7	304	XAT	C38-C25-C26	-6.57	111.24	122.26
23	5	315	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	a	811	CLA	C4A-NA-C1A	6.57	109.66	106.71
21	a	853	XAT	C38-C25-C26	-6.57	111.25	122.26
23	7	310	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	a	830	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	7	315	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	5	312	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	2	312	CLA	C4A-NA-C1A	6.56	109.66	106.71
21	8	302	XAT	C18-C5-C6	-6.56	111.26	122.26
23	8	305	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	a	837	CLA	C4A-NA-C1A	6.56	109.66	106.71
21	4	302	XAT	C18-C5-C6	-6.56	111.27	122.26
21	3	301	XAT	C18-C5-C4	6.56	121.66	114.28
23	a	841	CLA	C4A-NA-C1A	6.56	109.65	106.71
23	b	833	CLA	C4A-NA-C1A	6.56	109.65	106.71
21	8	302	XAT	C38-C25-C26	-6.55	111.28	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	312	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	4	314	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	a	808	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	7	316	CLA	C4A-NA-C1A	6.55	109.65	106.71
21	6	305	XAT	C38-C25-C26	-6.54	111.30	122.26
21	7	305	XAT	C38-C25-C26	-6.54	111.30	122.26
23	3	311	CLA	C4A-NA-C1A	6.54	109.65	106.71
23	6	311	CLA	C4A-NA-C1A	6.54	109.65	106.71
23	a	842	CLA	C4A-NA-C1A	6.54	109.65	106.71
21	5	305	XAT	C38-C25-C26	-6.54	111.31	122.26
21	7	303	XAT	C38-C25-C24	6.54	121.63	114.28
21	2	303	XAT	C18-C5-C6	-6.54	111.31	122.26
23	7	306	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	a	819	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	4	301	XAT	C18-C5-C4	6.52	121.62	114.28
23	8	309	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	4	313	CLA	C4A-NA-C1A	6.52	109.64	106.71
21	5	301	XAT	C18-C5-C6	-6.52	111.34	122.26
21	7	303	XAT	C18-C5-C6	-6.52	111.34	122.26
21	5	301	XAT	C18-C5-C4	6.51	121.61	114.28
23	4	305	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	6	307	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	a	827	CLA	C4A-NA-C1A	6.50	109.63	106.71
21	8	303	XAT	C18-C5-C4	6.50	121.59	114.28
21	3	305	XAT	C38-C25-C26	-6.50	111.37	122.26
23	b	836	CLA	C4A-NA-C1A	6.50	109.63	106.71
21	6	303	XAT	C18-C5-C6	-6.49	111.38	122.26
21	2	305	XAT	C18-C5-C6	-6.49	111.38	122.26
23	1	313	CLA	C4A-NA-C1A	6.49	109.62	106.71
23	7	311	CLA	C4A-NA-C1A	6.48	109.62	106.71
21	4	302	XAT	C38-C25-C26	-6.48	111.40	122.26
23	5	313	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	3	309	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	b	818	CLA	C4A-NA-C1A	6.48	109.62	106.71
30	a	850	BCR	C24-C23-C22	-6.48	116.45	126.23
21	6	303	XAT	C18-C5-C4	6.47	121.56	114.28
21	2	303	XAT	C38-C25-C26	-6.47	111.41	122.26
23	2	307	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	a	844	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	2	306	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	3	310	CLA	C4A-NA-C1A	6.45	109.61	106.71
23	8	314	CLA	C4A-NA-C1A	6.45	109.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	304	XAT	C38-C25-C26	-6.45	111.45	122.26
23	1	314	CLA	C4A-NA-C1A	6.44	109.60	106.71
23	b	815	CLA	C4A-NA-C1A	6.44	109.60	106.71
21	3	303	XAT	C18-C5-C6	-6.44	111.46	122.26
23	9	312	CLA	C4A-NA-C1A	6.44	109.60	106.71
23	1	312	CLA	C4A-NA-C1A	6.43	109.60	106.71
23	b	839	CLA	C4A-NA-C1A	6.43	109.59	106.71
21	6	306	XAT	C18-C5-C6	-6.42	111.50	122.26
23	8	306	CLA	C4A-NA-C1A	6.42	109.59	106.71
21	5	303	XAT	C26-C27-C28	-6.42	112.42	125.99
23	3	307	CLA	C4A-NA-C1A	6.42	109.59	106.71
21	2	304	XAT	C18-C5-C6	-6.42	111.51	122.26
23	4	307	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	a	813	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	6	315	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	a	816	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	8	311	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	b	813	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	6	302	XAT	C18-C5-C6	-6.41	111.53	122.26
23	5	306	CLA	C4A-NA-C1A	6.40	109.58	106.71
23	5	308	CLA	C4A-NA-C1A	6.40	109.58	106.71
23	7	308	CLA	C4A-NA-C1A	6.40	109.58	106.71
23	a	829	CLA	C4A-NA-C1A	6.40	109.58	106.71
21	1	302	XAT	C38-C25-C26	-6.39	111.55	122.26
23	b	831	CLA	C4A-NA-C1A	6.39	109.58	106.71
21	3	303	XAT	C38-C25-C26	-6.39	111.55	122.26
23	5	310	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	5	316	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	8	308	CLA	C4A-NA-C1A	6.38	109.58	106.71
21	4	304	XAT	C31-C30-C29	-6.38	118.20	127.31
23	a	836	CLA	C4A-NA-C1A	6.38	109.58	106.71
21	a	853	XAT	C18-C5-C6	-6.38	111.57	122.26
21	2	303	XAT	C38-C25-C24	6.37	121.45	114.28
23	a	815	CLA	C4A-NA-C1A	6.37	109.57	106.71
21	3	301	XAT	C18-C5-C6	-6.37	111.59	122.26
23	b	822	CLA	C4A-NA-C1A	6.37	109.57	106.71
21	4	301	XAT	C18-C5-C6	-6.36	111.60	122.26
23	a	814	CLA	C4A-NA-C1A	6.36	109.56	106.71
21	3	305	XAT	C18-C5-C4	6.35	121.43	114.28
21	2	302	XAT	C38-C25-C24	6.35	121.42	114.28
21	1	302	XAT	C18-C5-C4	6.35	121.42	114.28
23	2	315	CLA	C4A-NA-C1A	6.35	109.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	h	203	CLA	C4A-NA-C1A	6.35	109.56	106.71
21	7	305	XAT	C18-C5-C4	6.34	121.41	114.28
21	7	305	XAT	C18-C5-C6	-6.34	111.64	122.26
23	9	311	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	9	316	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	1	309	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	b	819	CLA	C4A-NA-C1A	6.33	109.55	106.71
21	a	853	XAT	C18-C5-C4	6.32	121.39	114.28
21	3	303	XAT	C18-C5-C4	6.32	121.39	114.28
23	a	822	CLA	C4A-NA-C1A	6.31	109.54	106.71
21	1	302	XAT	C18-C5-C6	-6.31	111.68	122.26
21	9	303	XAT	C18-C5-C6	-6.30	111.69	122.26
23	b	823	CLA	C4A-NA-C1A	6.30	109.54	106.71
21	4	303	XAT	C18-C5-C6	-6.30	111.70	122.26
23	2	309	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	b	811	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	7	309	CLA	C4A-NA-C1A	6.30	109.54	106.71
21	6	306	XAT	C38-C25-C26	-6.30	111.70	122.26
23	b	835	CLA	C4A-NA-C1A	6.30	109.54	106.71
21	3	304	XAT	C18-C5-C4	6.29	121.36	114.28
21	4	302	XAT	C18-C5-C4	6.29	121.35	114.28
21	2	302	XAT	C18-C5-C6	-6.29	111.72	122.26
23	4	308	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	1	311	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	b	825	CLA	C4A-NA-C1A	6.28	109.53	106.71
21	4	303	XAT	C38-C25-C26	-6.28	111.73	122.26
21	8	301	XAT	C18-C5-C6	-6.27	111.74	122.26
23	6	313	CLA	C4A-NA-C1A	6.27	109.53	106.71
21	4	304	XAT	C18-C5-C6	-6.26	111.76	122.26
23	2	310	CLA	C4A-NA-C1A	6.26	109.52	106.71
23	b	829	CLA	C4A-NA-C1A	6.26	109.52	106.71
21	4	301	XAT	C38-C25-C26	-6.25	111.78	122.26
23	7	313	CLA	C4A-NA-C1A	6.25	109.52	106.71
21	3	305	XAT	C18-C5-C6	-6.25	111.78	122.26
21	3	301	XAT	C38-C25-C26	-6.25	111.78	122.26
23	a	802	CLA	C4A-NA-C1A	6.25	109.52	106.71
21	1	303	XAT	C18-C5-C6	-6.25	111.79	122.26
21	8	303	XAT	C38-C25-C26	-6.25	111.79	122.26
30	i	101	BCR	C20-C21-C22	-6.25	118.40	127.31
23	a	824	CLA	C4A-NA-C1A	6.25	109.51	106.71
21	a	854	XAT	C38-C25-C26	-6.24	111.80	122.26
21	2	301	XAT	C38-C25-C24	6.24	121.30	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	302	XAT	C11-C10-C9	-6.24	118.41	127.31
23	1	310	CLA	C4A-NA-C1A	6.23	109.51	106.71
23	9	315	CLA	C4A-NA-C1A	6.23	109.50	106.71
23	b	816	CLA	C4A-NA-C1A	6.22	109.50	106.71
21	9	305	XAT	C18-C5-C6	-6.22	111.83	122.26
21	1	303	XAT	C38-C25-C26	-6.22	111.83	122.26
21	6	306	XAT	C18-C5-C4	6.22	121.27	114.28
21	2	302	XAT	C38-C25-C26	-6.21	111.84	122.26
23	b	838	CLA	C4A-NA-C1A	6.20	109.50	106.71
21	6	306	XAT	C38-C25-C24	6.20	121.26	114.28
21	5	302	XAT	C18-C5-C6	-6.20	111.87	122.26
21	3	301	XAT	C38-C25-C24	6.19	121.25	114.28
21	4	303	XAT	C18-C5-C4	6.18	121.24	114.28
21	5	303	XAT	C38-C25-C24	6.18	121.23	114.28
23	4	311	CLA	C4A-NA-C1A	6.17	109.48	106.71
21	6	302	XAT	C18-C5-C4	6.17	121.22	114.28
21	9	305	XAT	C11-C10-C9	-6.16	118.52	127.31
23	9	309	CLA	C4A-NA-C1A	6.15	109.47	106.71
21	1	303	XAT	C18-C5-C4	6.15	121.19	114.28
21	6	305	XAT	C35-C34-C33	-6.14	118.55	127.31
23	a	820	CLA	C4A-NA-C1A	6.12	109.46	106.71
21	2	301	XAT	C38-C25-C26	-6.11	112.02	122.26
23	b	841	CLA	C4A-NA-C1A	6.11	109.45	106.71
21	a	854	XAT	C26-C27-C28	-6.10	113.09	125.99
23	2	308	CLA	C4A-NA-C1A	6.09	109.44	106.71
23	b	817	CLA	C4A-NA-C1A	6.07	109.44	106.71
21	2	305	XAT	C18-C5-C4	6.06	121.10	114.28
23	b	828	CLA	C4A-NA-C1A	6.06	109.43	106.71
21	7	304	XAT	C18-C5-C4	6.05	121.09	114.28
23	b	803	CLA	C4A-NA-C1A	6.05	109.43	106.71
21	4	304	XAT	C18-C5-C4	6.00	121.03	114.28
21	6	303	XAT	C15-C14-C13	-5.99	118.76	127.31
21	2	301	XAT	C31-C30-C29	-5.98	118.77	127.31
30	b	843	BCR	C7-C8-C9	-5.95	117.24	126.23
21	5	305	XAT	C26-C27-C28	-5.95	113.41	125.99
21	2	302	XAT	C18-C5-C4	5.95	120.97	114.28
23	4	312	CLA	C4A-NA-C1A	5.95	109.38	106.71
23	b	830	CLA	C4A-NA-C1A	5.94	109.38	106.71
21	7	301	XAT	C38-C25-C24	5.94	120.96	114.28
21	5	303	XAT	C18-C5-C4	5.93	120.95	114.28
23	a	852	CLA	C4A-NA-C1A	5.92	109.37	106.71
21	7	303	XAT	C18-C5-C4	5.91	120.92	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	8	310	CLA	C4A-NA-C1A	5.91	109.36	106.71
21	8	301	XAT	C18-C5-C4	5.91	120.92	114.28
21	8	302	XAT	C18-C5-C4	5.89	120.90	114.28
30	b	852	BCR	C16-C17-C18	-5.87	118.93	127.31
21	a	853	XAT	C6-C7-C8	-5.85	113.62	125.99
25	8	304	A1L1F	O15-C20-C17	5.84	122.06	115.06
21	5	302	XAT	C18-C5-C4	5.84	120.85	114.28
21	7	301	XAT	C31-C30-C29	-5.83	118.99	127.31
25	h	202	A1L1F	C37-C38-C39	-5.82	119.00	127.31
21	5	303	XAT	C38-C25-C26	-5.80	112.54	122.26
21	9	303	XAT	C18-C5-C4	5.79	120.79	114.28
21	7	301	XAT	C38-C25-C26	-5.79	112.56	122.26
21	2	303	XAT	C18-C5-C4	5.77	120.78	114.28
30	a	850	BCR	C20-C21-C22	-5.76	119.08	127.31
21	5	301	XAT	C35-C34-C33	-5.68	119.20	127.31
25	1	304	A1L1F	O15-C20-C17	5.67	121.85	115.06
21	5	303	XAT	C11-C10-C9	-5.67	119.22	127.31
21	9	304	XAT	C26-C27-C28	-5.65	114.04	125.99
21	5	301	XAT	C38-C25-C24	5.64	120.63	114.28
30	f	801	BCR	C16-C17-C18	-5.63	119.27	127.31
30	b	845	BCR	C24-C23-C22	-5.62	117.74	126.23
30	b	843	BCR	C11-C10-C9	-5.61	119.31	127.31
30	b	845	BCR	C7-C8-C9	-5.56	117.84	126.23
21	6	305	XAT	C31-C30-C29	-5.55	119.39	127.31
21	6	305	XAT	C18-C5-C6	-5.54	112.98	122.26
21	7	305	XAT	C15-C14-C13	-5.52	119.43	127.31
30	b	847	BCR	C16-C17-C18	-5.51	119.45	127.31
25	h	202	A1L1F	O15-C20-C17	5.48	121.62	115.06
21	8	303	XAT	C26-C27-C28	-5.48	114.41	125.99
30	j	102	BCR	C28-C27-C26	-5.46	104.32	114.08
30	f	801	BCR	C20-C21-C22	-5.46	119.51	127.31
21	3	301	XAT	C6-C7-C8	-5.44	114.48	125.99
21	9	303	XAT	C15-C14-C13	-5.44	119.55	127.31
21	3	304	XAT	C35-C34-C33	-5.43	119.56	127.31
25	6	301	A1L1F	O15-C20-C17	5.43	121.56	115.06
21	6	306	XAT	C31-C30-C29	-5.40	119.60	127.31
30	f	804	BCR	C15-C14-C13	-5.40	119.61	127.31
21	a	854	XAT	C18-C5-C6	-5.36	113.28	122.26
21	2	303	XAT	C31-C30-C29	-5.35	119.67	127.31
30	b	845	BCR	C33-C5-C6	-5.35	118.52	124.53
21	6	302	XAT	C15-C14-C13	-5.33	119.70	127.31
21	2	303	XAT	C35-C34-C33	-5.33	119.70	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	301	XAT	C38-C25-C26	-5.32	113.35	122.26
30	b	843	BCR	C3-C4-C5	-5.30	104.62	114.08
21	4	302	XAT	C26-C27-C28	-5.29	114.80	125.99
27	b	851	DGD	O2G-C1B-C2B	5.29	122.91	111.50
23	a	803	CLA	C4A-NA-C1A	5.28	109.08	106.71
30	b	843	BCR	C15-C14-C13	-5.27	119.78	127.31
21	4	304	XAT	C15-C14-C13	-5.27	119.79	127.31
21	2	302	XAT	C35-C34-C33	-5.27	119.79	127.31
21	2	303	XAT	C11-C10-C9	-5.27	119.79	127.31
21	a	854	XAT	C18-C5-C4	5.26	120.20	114.28
21	2	301	XAT	C35-C34-C33	-5.26	119.81	127.31
21	6	302	XAT	C31-C30-C29	-5.25	119.82	127.31
25	6	301	A1L1F	C36-C37-C38	-5.25	112.73	123.47
21	a	854	XAT	C6-C7-C8	-5.24	114.90	125.99
21	2	305	XAT	C31-C30-C29	-5.24	119.83	127.31
30	a	849	BCR	C3-C4-C5	-5.24	104.73	114.08
21	6	306	XAT	C35-C34-C33	-5.23	119.84	127.31
21	4	303	XAT	C26-C27-C28	-5.23	114.93	125.99
21	7	301	XAT	C35-C34-C33	-5.23	119.84	127.31
25	8	304	A1L1F	C41-C42-C44	-5.23	119.85	127.31
21	9	305	XAT	C18-C5-C4	5.22	120.15	114.28
21	2	304	XAT	C6-C7-C8	-5.21	114.98	125.99
30	b	853	BCR	C7-C8-C9	-5.20	118.38	126.23
21	9	303	XAT	C26-C27-C28	-5.20	115.00	125.99
21	a	853	XAT	C26-C27-C28	-5.19	115.02	125.99
21	7	304	XAT	C11-C10-C9	-5.18	119.91	127.31
25	8	304	A1L1F	O7-C54-C56	5.17	120.60	111.09
30	i	102	BCR	C24-C23-C22	-5.12	118.50	126.23
21	8	303	XAT	C15-C14-C13	-5.11	120.01	127.31
30	b	846	BCR	C3-C4-C5	-5.10	104.98	114.08
25	6	304	A1L1F	O15-C20-C17	5.09	121.16	115.06
21	2	305	XAT	C35-C34-C33	-5.07	120.08	127.31
21	1	302	XAT	C35-C34-C33	-5.06	120.09	127.31
30	a	847	BCR	C16-C17-C18	-5.04	120.11	127.31
21	3	305	XAT	C26-C27-C28	-5.04	115.34	125.99
21	8	303	XAT	C6-C7-C8	-5.02	115.38	125.99
21	7	305	XAT	C26-C27-C28	-5.02	115.38	125.99
21	6	302	XAT	C35-C34-C33	-5.00	120.17	127.31
21	5	302	XAT	C26-C27-C28	-5.00	115.42	125.99
21	4	303	XAT	C6-C7-C8	-4.97	115.48	125.99
21	1	302	XAT	C26-C27-C28	-4.97	115.49	125.99
21	3	305	XAT	C6-C7-C8	-4.96	115.50	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	852	BCR	C20-C21-C22	-4.95	120.24	127.31
21	2	301	XAT	C15-C14-C13	-4.95	120.24	127.31
30	b	852	BCR	C11-C10-C9	-4.95	120.24	127.31
30	a	850	BCR	C16-C17-C18	-4.94	120.25	127.31
21	7	303	XAT	C31-C30-C29	-4.91	120.31	127.31
30	f	804	BCR	C11-C10-C9	-4.90	120.32	127.31
21	1	303	XAT	C6-C7-C8	-4.89	115.66	125.99
21	2	305	XAT	C6-C7-C8	-4.88	115.68	125.99
21	4	302	XAT	C11-C10-C9	-4.87	120.35	127.31
21	a	853	XAT	C11-C10-C9	-4.87	120.36	127.31
21	7	304	XAT	C26-C27-C28	-4.87	115.70	125.99
30	a	849	BCR	C16-C17-C18	-4.85	120.38	127.31
30	j	102	BCR	C11-C10-C9	-4.85	120.38	127.31
21	2	301	XAT	C6-C7-C8	-4.85	115.74	125.99
21	5	303	XAT	C15-C14-C13	-4.81	120.44	127.31
21	1	302	XAT	C6-C7-C8	-4.80	115.84	125.99
21	5	305	XAT	C15-C14-C13	-4.80	120.46	127.31
30	i	101	BCR	C16-C17-C18	-4.79	120.47	127.31
21	9	305	XAT	C35-C34-C33	-4.79	120.47	127.31
23	a	831	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
30	b	852	BCR	C38-C26-C25	-4.77	119.17	124.53
30	i	102	BCR	C15-C14-C13	-4.77	120.50	127.31
21	7	301	XAT	C6-C7-C8	-4.76	115.92	125.99
23	b	829	CLA	CMB-C2B-C1B	-4.75	121.17	128.46
21	7	304	XAT	C15-C14-C13	-4.74	120.55	127.31
30	b	850	BCR	C16-C17-C18	-4.73	120.56	127.31
21	7	304	XAT	C35-C34-C33	-4.73	120.56	127.31
30	b	852	BCR	C7-C8-C9	-4.72	119.10	126.23
21	4	301	XAT	C26-C27-C28	-4.72	116.02	125.99
21	8	301	XAT	C26-C27-C28	-4.70	116.05	125.99
21	7	305	XAT	C6-C7-C8	-4.70	116.07	125.99
21	4	301	XAT	C6-C7-C8	-4.68	116.09	125.99
23	b	817	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
21	9	304	XAT	C15-C14-C13	-4.65	120.67	127.31
21	3	303	XAT	C26-C27-C28	-4.65	116.17	125.99
21	9	305	XAT	C38-C25-C24	4.62	119.48	114.28
21	4	301	XAT	C35-C34-C33	-4.62	120.72	127.31
21	3	304	XAT	C6-C7-C8	-4.61	116.25	125.99
21	8	302	XAT	C15-C14-C13	-4.59	120.76	127.31
21	5	302	XAT	C35-C34-C33	-4.59	120.76	127.31
30	b	848	BCR	C16-C17-C18	-4.59	120.77	127.31
21	7	303	XAT	C11-C10-C9	-4.58	120.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	9	302	A1L1F	O7-C54-C56	4.58	119.52	111.09
21	7	301	XAT	C27-C28-C29	-4.57	118.44	125.53
30	b	844	BCR	C11-C10-C9	-4.56	120.80	127.31
21	2	305	XAT	C15-C14-C13	-4.56	120.80	127.31
21	7	303	XAT	C35-C34-C33	-4.55	120.82	127.31
21	4	304	XAT	C26-C27-C28	-4.54	116.39	125.99
30	b	844	BCR	C7-C8-C9	-4.54	119.37	126.23
21	8	302	XAT	C26-C27-C28	-4.53	116.42	125.99
21	8	302	XAT	C35-C34-C33	-4.52	120.86	127.31
25	6	304	A1L1F	O7-C54-C56	4.52	119.40	111.09
21	6	306	XAT	C6-C7-C8	-4.51	116.46	125.99
25	h	202	A1L1F	O7-C54-C56	4.48	119.34	111.09
21	2	302	XAT	C6-C7-C8	-4.48	116.52	125.99
30	a	848	BCR	C16-C17-C18	-4.48	120.92	127.31
21	2	304	XAT	C26-C27-C28	-4.47	116.53	125.99
25	9	302	A1L1F	C36-C35-C34	-4.47	120.93	127.31
21	3	303	XAT	C6-C7-C8	-4.47	116.55	125.99
21	3	305	XAT	C35-C34-C33	-4.46	120.95	127.31
21	7	303	XAT	C26-C27-C28	-4.45	116.58	125.99
23	a	802	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
27	b	851	DGD	O5D-C6D-C5D	-4.43	100.85	109.05
25	6	301	A1L1F	O7-C54-C56	4.43	119.23	111.09
30	a	848	BCR	C15-C14-C13	-4.42	121.00	127.31
30	j	102	BCR	C15-C14-C13	-4.41	121.02	127.31
30	a	849	BCR	C15-C14-C13	-4.40	121.03	127.31
30	b	843	BCR	C16-C17-C18	-4.38	121.05	127.31
28	2	317	LMG	O7-C10-C11	4.37	120.92	111.50
30	b	845	BCR	C16-C17-C18	-4.36	121.08	127.31
25	h	202	A1L1F	C25-C14-C29	-4.35	116.79	125.99
27	4	317	DGD	O6E-C5E-C6E	4.35	117.25	106.44
30	a	850	BCR	C15-C14-C13	-4.35	121.11	127.31
30	b	848	BCR	C33-C5-C6	-4.35	119.65	124.53
21	8	301	XAT	C35-C34-C33	-4.34	121.11	127.31
21	a	853	XAT	C35-C34-C33	-4.33	121.14	127.31
21	3	303	XAT	C35-C34-C33	-4.33	121.14	127.31
25	6	304	A1L1F	C26-C30-C31	-4.31	119.30	124.93
23	b	836	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
21	6	306	XAT	C15-C14-C13	-4.31	121.16	127.31
30	j	102	BCR	C16-C17-C18	-4.30	121.17	127.31
21	3	303	XAT	C15-C14-C13	-4.28	121.19	127.31
23	a	844	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
23	a	833	CLA	CMB-C2B-C1B	-4.28	121.89	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	305	XAT	C35-C34-C33	-4.27	121.21	127.31
21	6	302	XAT	C6-C7-C8	-4.27	116.96	125.99
21	5	301	XAT	C6-C7-C8	-4.27	116.97	125.99
23	4	312	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
21	3	304	XAT	C31-C30-C29	-4.26	121.23	127.31
25	9	302	A1L1F	C14-C29-C30	-4.25	117.97	125.47
23	2	307	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
23	6	314	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
30	b	845	BCR	C15-C14-C13	-4.25	121.25	127.31
23	b	825	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
30	b	844	BCR	C15-C14-C13	-4.24	121.26	127.31
23	8	305	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
25	h	202	A1L1F	C41-C42-C44	-4.23	121.27	127.31
27	4	317	DGD	O2G-C1B-C2B	4.23	120.62	111.50
29	b	842	PQN	C11-C12-C13	-4.23	119.75	126.79
21	9	304	XAT	C18-C5-C4	4.22	119.03	114.28
21	3	301	XAT	C15-C14-C13	-4.22	121.29	127.31
30	f	804	BCR	C24-C23-C22	-4.22	119.86	126.23
22	9	301	A1L1G	C37-C36-C35	4.21	132.10	123.47
23	a	826	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
23	7	308	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
23	8	311	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
30	b	853	BCR	C15-C14-C13	-4.20	121.31	127.31
26	a	845	LHG	O7-C7-C8	4.20	120.56	111.50
23	a	820	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
30	b	847	BCR	C24-C23-C22	-4.20	119.89	126.23
21	2	305	XAT	C38-C25-C24	4.19	119.00	114.28
23	a	809	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
21	7	303	XAT	C15-C14-C13	-4.19	121.33	127.31
21	4	303	XAT	C35-C34-C33	-4.19	121.33	127.31
30	b	850	BCR	C33-C5-C6	-4.18	119.83	124.53
21	6	305	XAT	C27-C28-C29	-4.18	119.04	125.53
23	3	310	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
23	6	309	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
30	b	853	BCR	C33-C5-C6	-4.18	119.83	124.53
30	b	846	BCR	C16-C17-C18	-4.17	121.36	127.31
25	1	304	A1L1F	O7-C54-C56	4.17	118.77	111.09
23	a	823	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
30	i	102	BCR	C20-C21-C22	-4.16	121.37	127.31
30	j	102	BCR	C7-C8-C9	-4.16	119.94	126.23
23	b	814	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
23	a	829	CLA	CMB-C2B-C1B	-4.16	122.07	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	304	A1L1F	C37-C38-C39	-4.16	121.38	127.31
21	4	304	XAT	C35-C34-C33	-4.15	121.38	127.31
23	a	806	CLA	CMB-C2B-C1B	-4.14	122.09	128.46
25	8	304	A1L1F	C41-C40-C39	-4.14	114.78	126.42
25	8	304	A1L1F	C32-C31-C30	-4.14	121.36	127.26
21	7	305	XAT	C11-C10-C9	-4.14	121.40	127.31
23	6	313	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
23	8	308	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
23	1	307	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
30	a	850	BCR	C38-C26-C25	-4.12	119.91	124.53
23	2	308	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
28	a	855	LMG	O7-C10-C11	4.10	120.34	111.50
25	1	304	A1L1F	C17-C20-C21	4.10	118.89	114.28
30	i	102	BCR	C38-C26-C25	-4.10	119.92	124.53
21	3	304	XAT	C15-C14-C13	-4.10	121.46	127.31
23	b	832	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
23	a	816	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
26	b	849	LHG	O7-C7-C8	4.09	120.31	111.50
30	b	847	BCR	C20-C21-C22	-4.09	121.48	127.31
23	9	309	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
30	b	847	BCR	C16-C15-C14	-4.08	115.12	123.47
23	7	316	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
30	f	804	BCR	C7-C8-C9	-4.08	120.08	126.23
23	a	803	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
30	f	801	BCR	C3-C4-C5	-4.07	106.81	114.08
30	b	843	BCR	C28-C27-C26	-4.07	106.81	114.08
30	b	847	BCR	C7-C8-C9	-4.06	120.09	126.23
23	b	810	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
23	5	308	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
23	b	821	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
21	5	301	XAT	C15-C14-C13	-4.04	121.54	127.31
23	a	805	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
21	5	302	XAT	C11-C10-C9	-4.04	121.55	127.31
23	b	809	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
21	4	304	XAT	C6-C7-C8	-4.03	117.48	125.99
30	a	848	BCR	C11-C10-C9	-4.03	121.56	127.31
23	a	804	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
23	a	839	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
23	b	805	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
23	5	312	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
21	7	303	XAT	C6-C7-C8	-4.00	117.54	125.99
30	a	847	BCR	C38-C26-C25	-4.00	120.04	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	826	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
23	8	310	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
23	7	311	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
26	m	101	LHG	O7-C7-C8	3.98	120.08	111.50
25	6	301	A1L1F	C8-O7-C54	-3.98	110.48	117.90
30	b	847	BCR	C15-C14-C13	-3.98	121.63	127.31
30	i	101	BCR	C7-C8-C9	-3.98	120.22	126.23
23	b	806	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
26	a	846	LHG	O7-C7-C8	3.98	120.07	111.50
30	b	847	BCR	C28-C27-C26	-3.98	106.98	114.08
25	6	301	A1L1F	C37-C38-C39	-3.97	121.64	127.31
23	9	312	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
25	8	304	A1L1F	C37-C36-C35	-3.96	115.35	123.47
25	6	304	A1L1F	C36-C35-C34	-3.96	121.65	127.31
30	f	804	BCR	C33-C5-C6	-3.96	120.08	124.53
23	4	307	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
23	8	307	CLA	CMB-C2B-C1B	-3.96	122.39	128.46
23	b	831	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
23	3	309	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
21	9	304	XAT	C18-C5-C6	-3.95	115.64	122.26
21	3	301	XAT	C35-C34-C33	-3.95	121.68	127.31
21	6	303	XAT	C26-C27-C28	-3.95	117.65	125.99
21	2	303	XAT	C15-C14-C13	-3.95	121.68	127.31
21	a	854	XAT	C31-C30-C29	-3.94	121.68	127.31
25	6	304	A1L1F	C37-C38-C39	-3.94	121.68	127.31
30	b	853	BCR	C11-C10-C9	-3.94	121.68	127.31
28	j	103	LMG	O7-C10-C11	3.94	120.00	111.50
23	a	838	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
21	4	304	XAT	C11-C10-C9	-3.94	121.69	127.31
21	1	303	XAT	C26-C27-C28	-3.94	117.67	125.99
23	1	308	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
21	2	302	XAT	C31-C30-C29	-3.93	121.70	127.31
23	a	852	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
21	4	302	XAT	C15-C14-C13	-3.92	121.71	127.31
23	b	816	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
23	7	313	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	a	822	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
23	8	312	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
21	a	853	XAT	C15-C14-C13	-3.91	121.74	127.31
23	2	310	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
23	f	802	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	9	314	CLA	CMB-C2B-C1B	-3.90	122.47	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	813	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
23	b	803	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
30	a	847	BCR	C20-C21-C22	-3.88	121.77	127.31
21	7	301	XAT	C15-C14-C13	-3.88	121.77	127.31
21	2	305	XAT	C27-C28-C29	-3.88	119.51	125.53
23	a	827	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
30	f	804	BCR	C20-C21-C22	-3.88	121.78	127.31
22	3	306	A1L1G	C36-C37-C38	3.87	131.40	123.47
23	b	817	CLA	CMB-C2B-C3B	3.86	131.91	124.68
23	2	312	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
23	4	308	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
23	5	313	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
23	a	815	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
21	2	302	XAT	C15-C14-C13	-3.85	121.82	127.31
30	i	102	BCR	C33-C5-C6	-3.85	120.21	124.53
27	8	315	DGD	O2G-C1B-C2B	3.83	119.77	111.50
30	f	804	BCR	C38-C26-C25	-3.83	120.22	124.53
25	6	304	A1L1F	C17-C20-C21	3.83	118.59	114.28
21	2	302	XAT	C26-C27-C28	-3.83	117.89	125.99
30	b	853	BCR	C16-C17-C18	-3.83	121.84	127.31
23	1	306	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
23	b	815	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
23	7	310	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
22	1	301	A1L1G	C37-C36-C35	3.82	131.30	123.47
23	2	313	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
23	5	315	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
23	l	201	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
23	a	811	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
21	6	306	XAT	C27-C28-C29	-3.80	119.63	125.53
23	h	201	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
30	b	848	BCR	C15-C14-C13	-3.80	121.89	127.31
30	i	102	BCR	C16-C17-C18	-3.79	121.89	127.31
23	a	814	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
23	l	202	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
21	5	302	XAT	C15-C14-C13	-3.79	121.90	127.31
30	a	849	BCR	C28-C27-C26	-3.77	107.34	114.08
23	5	316	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
23	b	824	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
23	a	806	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
30	b	846	BCR	C15-C14-C13	-3.76	121.94	127.31
23	9	308	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
23	7	312	CLA	CMB-C2B-C1B	-3.76	122.68	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	309	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
30	j	102	BCR	C20-C21-C22	-3.76	121.94	127.31
23	b	827	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
23	3	311	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
23	9	310	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
21	1	303	XAT	C35-C34-C33	-3.75	121.95	127.31
23	9	315	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
23	a	812	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
25	h	202	A1L1F	C36-C35-C34	-3.75	121.97	127.31
24	1	315	SQD	O47-C7-C8	3.74	119.57	111.50
23	b	830	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
30	f	804	BCR	C16-C17-C18	-3.74	121.97	127.31
23	b	804	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
21	9	305	XAT	C15-C14-C13	-3.74	121.98	127.31
21	8	301	XAT	C15-C14-C13	-3.74	121.98	127.31
23	1	310	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
25	9	302	A1L1F	O15-C20-C17	3.73	119.53	115.06
30	a	850	BCR	C33-C5-C6	-3.73	120.34	124.53
23	1	311	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
21	2	303	XAT	C26-C27-C28	-3.72	118.12	125.99
23	3	313	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
30	f	801	BCR	C16-C15-C14	-3.72	115.85	123.47
23	a	803	CLA	CMB-C2B-C3B	3.72	131.64	124.68
23	a	830	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
22	9	306	A1L1G	C37-C36-C35	3.71	131.08	123.47
22	5	304	A1L1G	C36-C37-C38	3.71	131.08	123.47
23	7	306	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
21	3	301	XAT	C31-C30-C29	-3.70	122.03	127.31
21	a	854	XAT	C35-C34-C33	-3.70	122.03	127.31
23	a	837	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
21	3	301	XAT	C26-C27-C28	-3.69	118.19	125.99
23	h	203	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
30	b	844	BCR	C3-C4-C5	-3.68	107.51	114.08
25	6	301	A1L1F	C42-C41-C40	-3.68	111.74	123.22
21	2	301	XAT	C27-C28-C29	-3.67	119.84	125.53
23	b	835	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
23	a	821	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
23	a	828	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
30	a	849	BCR	C20-C21-C22	-3.66	122.08	127.31
23	b	836	CLA	CMB-C2B-C3B	3.66	131.53	124.68
23	5	310	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
23	b	820	CLA	CMB-C2B-C1B	-3.66	122.84	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	308	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
23	7	309	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
23	a	826	CLA	CMB-C2B-C3B	3.65	131.52	124.68
23	b	803	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
21	2	303	XAT	C6-C7-C8	-3.65	118.27	125.99
30	b	850	BCR	C7-C8-C9	-3.65	120.72	126.23
21	6	302	XAT	C26-C27-C28	-3.64	118.29	125.99
21	7	304	XAT	C6-C7-C8	-3.64	118.29	125.99
22	7	302	A1L1G	C37-C36-C35	3.64	130.93	123.47
23	b	839	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
23	a	802	CLA	CMB-C2B-C3B	3.64	131.48	124.68
25	9	302	A1L1F	C32-C31-C30	-3.63	122.08	127.26
21	9	305	XAT	C31-C30-C29	-3.63	122.12	127.31
23	b	837	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
21	8	301	XAT	C11-C10-C9	-3.63	122.13	127.31
21	8	301	XAT	C6-C7-C8	-3.62	118.34	125.99
23	b	812	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
21	4	301	XAT	C35-C15-C14	-3.61	116.08	123.47
30	b	847	BCR	C3-C4-C5	-3.61	107.63	114.08
30	a	849	BCR	C11-C10-C9	-3.61	122.17	127.31
23	b	828	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	4	309	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
21	1	302	XAT	C11-C10-C9	-3.59	122.18	127.31
23	7	308	CLA	CMB-C2B-C3B	3.59	131.40	124.68
23	a	808	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	6	310	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	a	844	CLA	CMB-C2B-C3B	3.59	131.39	124.68
23	b	811	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
23	8	309	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
23	8	305	CLA	CMB-C2B-C3B	3.58	131.38	124.68
30	a	847	BCR	C33-C5-C6	-3.58	120.51	124.53
23	6	314	CLA	CMB-C2B-C3B	3.58	131.38	124.68
23	a	829	CLA	CMB-C2B-C3B	3.58	131.37	124.68
22	9	301	A1L1G	C27-C34-C35	-3.58	117.91	122.92
23	1	312	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
23	2	307	CLA	CMB-C2B-C3B	3.57	131.36	124.68
23	b	822	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
23	l	203	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
23	b	807	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
23	a	809	CLA	CMB-C2B-C3B	3.56	131.34	124.68
23	8	311	CLA	CMB-C2B-C3B	3.56	131.34	124.68
23	b	834	CLA	CMB-C2B-C1B	-3.55	123.00	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	303	XAT	C15-C35-C34	-3.55	116.19	123.47
30	i	102	BCR	C3-C4-C5	-3.55	107.73	114.08
23	b	810	CLA	CMB-C2B-C3B	3.55	131.32	124.68
23	8	306	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
22	9	301	A1L1G	C36-C37-C38	3.55	130.75	123.47
21	6	303	XAT	C7-C8-C9	-3.55	120.02	125.53
23	a	835	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	6	304	A1L1F	C32-C31-C30	-3.55	122.21	127.26
23	b	811	CLA	CAB-C3B-C4B	-3.55	123.01	128.46
21	9	303	XAT	C11-C10-C9	-3.55	122.25	127.31
23	a	832	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
30	i	102	BCR	C11-C10-C9	-3.55	122.25	127.31
23	a	833	CLA	CMB-C2B-C3B	3.54	131.31	124.68
23	5	306	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
30	b	844	BCR	C33-C5-C6	-3.54	120.55	124.53
23	b	814	CLA	CMB-C2B-C3B	3.54	131.30	124.68
23	b	818	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
21	9	303	XAT	C35-C34-C33	-3.53	122.27	127.31
23	b	825	CLA	CMB-C2B-C3B	3.53	131.29	124.68
21	6	305	XAT	C15-C14-C13	-3.53	122.27	127.31
30	a	847	BCR	C15-C14-C13	-3.51	122.30	127.31
22	7	302	A1L1G	C36-C37-C38	3.51	130.67	123.47
24	5	317	SQD	O47-C7-C8	3.51	119.07	111.50
22	9	306	A1L1G	C36-C37-C38	3.51	130.67	123.47
23	b	832	CLA	CMB-C2B-C3B	3.51	131.25	124.68
23	a	842	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
21	6	305	XAT	C11-C10-C9	-3.50	122.31	127.31
23	a	823	CLA	CMB-C2B-C3B	3.50	131.24	124.68
23	5	307	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
23	8	308	CLA	CMB-C2B-C3B	3.50	131.22	124.68
23	a	806	CLA	CAA-CBA-CGA	-3.50	103.03	113.25
23	4	312	CLA	CMB-C2B-C3B	3.50	131.22	124.68
23	b	826	CLA	CMB-C2B-C3B	3.49	131.22	124.68
23	a	813	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
23	5	314	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
21	6	303	XAT	C35-C34-C33	-3.49	122.33	127.31
30	i	101	BCR	C33-C5-C6	-3.49	120.61	124.53
23	4	313	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
21	8	302	XAT	C31-C30-C29	-3.49	122.34	127.31
21	4	301	XAT	C11-C10-C9	-3.49	122.34	127.31
30	a	847	BCR	C7-C8-C9	-3.49	120.97	126.23
21	3	303	XAT	C11-C10-C9	-3.48	122.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	803	CLA	CHB-C4A-NA	3.48	129.33	124.51
23	b	808	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	7	302	A1L1G	C27-C34-C35	-3.48	118.04	122.92
21	4	302	XAT	C35-C34-C33	-3.48	122.34	127.31
30	a	848	BCR	C24-C23-C22	-3.48	120.98	126.23
23	a	807	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
21	7	304	XAT	C31-C30-C29	-3.48	122.35	127.31
30	i	101	BCR	C28-C27-C26	-3.47	107.87	114.08
21	2	304	XAT	C31-C30-C29	-3.47	122.35	127.31
30	b	846	BCR	C24-C23-C22	-3.47	120.99	126.23
23	1	309	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
30	a	849	BCR	C4-C5-C6	-3.47	117.69	122.73
30	b	850	BCR	C38-C26-C25	-3.47	120.63	124.53
23	9	316	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
23	3	310	CLA	CMB-C2B-C3B	3.47	131.17	124.68
23	1	305	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
23	a	831	CLA	CMB-C2B-C3B	3.47	131.16	124.68
23	6	309	CLA	CMB-C2B-C3B	3.46	131.16	124.68
23	3	307	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
21	1	303	XAT	C15-C14-C13	-3.46	122.37	127.31
23	5	309	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	6	307	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	4	314	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	9	313	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
23	b	833	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
21	2	305	XAT	C24-C23-C22	-3.46	104.10	110.77
23	2	306	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
23	a	805	CLA	CMB-C2B-C3B	3.46	131.15	124.68
23	2	308	CLA	CMB-C2B-C3B	3.45	131.14	124.68
21	2	304	XAT	C11-C10-C9	-3.45	122.38	127.31
22	9	306	A1L1G	C27-C34-C35	-3.45	118.09	122.92
22	9	306	A1L1G	C28-C39-C38	-3.45	118.09	122.92
22	3	302	A1L1G	C36-C37-C38	3.45	130.54	123.47
23	3	314	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
23	b	823	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
23	a	852	CLA	CMB-C2B-C3B	3.45	131.13	124.68
23	b	838	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
21	6	303	XAT	C31-C30-C29	-3.44	122.39	127.31
23	9	312	CLA	CAA-C2A-C3A	-3.44	103.35	112.78
23	2	314	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
25	9	302	A1L1F	C37-C38-C39	-3.44	122.40	127.31
23	3	315	CLA	CMB-C2B-C1B	-3.44	123.17	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	819	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
23	a	806	CLA	CMB-C2B-C3B	3.44	131.12	124.68
30	a	847	BCR	C24-C23-C22	-3.44	121.04	126.23
23	8	313	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
23	3	308	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
23	9	314	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
23	a	817	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	3	306	A1L1G	C27-C34-C35	-3.43	118.12	122.92
23	a	841	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	4	316	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
23	a	820	CLA	CMB-C2B-C3B	3.42	131.09	124.68
23	a	825	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
22	3	302	A1L1G	C37-C36-C35	3.42	130.49	123.47
23	4	306	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
30	a	849	BCR	C7-C8-C9	-3.42	121.06	126.23
23	9	312	CLA	CMB-C2B-C3B	3.42	131.08	124.68
23	a	819	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	1	301	A1L1G	C28-C39-C38	-3.42	118.13	122.92
26	a	846	LHG	O8-C23-C24	3.42	120.35	111.38
23	6	312	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
23	a	840	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
23	j	101	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
21	5	303	XAT	C6-C7-C8	-3.41	118.77	125.99
23	1	313	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
23	6	313	CLA	CMB-C2B-C3B	3.41	131.06	124.68
23	a	816	CLA	CMB-C2B-C3B	3.41	131.06	124.68
21	3	305	XAT	C15-C14-C13	-3.41	122.44	127.31
22	1	301	A1L1G	C27-C34-C35	-3.41	118.15	122.92
23	7	316	CLA	CMB-C2B-C3B	3.41	131.05	124.68
21	9	304	XAT	C35-C34-C33	-3.41	122.45	127.31
23	4	315	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
23	a	818	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
22	9	301	A1L1G	C28-C39-C38	-3.40	118.16	122.92
22	7	302	A1L1G	C28-C39-C38	-3.40	118.16	122.92
23	4	305	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
30	a	848	BCR	C20-C21-C22	-3.40	122.46	127.31
23	8	314	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
23	4	311	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
22	5	304	A1L1G	C28-C39-C38	-3.40	118.17	122.92
23	6	311	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	2	311	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	2	315	CLA	CMB-C2B-C1B	-3.39	123.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	306	A1L1G	C28-C39-C38	-3.39	118.17	122.92
23	5	311	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	7	317	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	6	316	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	b	805	CLA	CMB-C2B-C3B	3.39	131.02	124.68
23	a	810	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
23	b	821	CLA	CMB-C2B-C3B	3.38	131.01	124.68
23	1	314	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
26	9	307	LHG	O7-C7-C8	3.38	120.23	110.80
23	1	307	CLA	CMB-C2B-C3B	3.38	131.00	124.68
22	3	302	A1L1G	C28-C39-C38	-3.38	118.19	122.92
25	1	304	A1L1F	C8-O7-C54	-3.38	111.60	117.90
23	b	806	CLA	CMB-C2B-C3B	3.38	130.99	124.68
30	a	847	BCR	C11-C10-C9	-3.38	122.49	127.31
23	5	312	CLA	CMB-C2B-C3B	3.37	130.99	124.68
23	b	829	CLA	CMB-C2B-C3B	3.36	130.97	124.68
22	3	302	A1L1G	C27-C34-C35	-3.36	118.21	122.92
23	a	804	CLA	CMB-C2B-C3B	3.36	130.97	124.68
30	b	847	BCR	C10-C11-C12	-3.36	112.73	123.22
23	a	856	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
23	7	307	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
23	b	831	CLA	CMB-C2B-C3B	3.36	130.96	124.68
21	a	853	XAT	C10-C11-C12	-3.36	112.74	123.22
21	8	303	XAT	C30-C31-C32	-3.36	112.75	123.22
23	7	314	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
21	1	303	XAT	C24-C23-C22	-3.35	104.30	110.77
23	5	308	CLA	CMB-C2B-C3B	3.35	130.95	124.68
21	5	302	XAT	C7-C8-C9	-3.35	120.33	125.53
23	f	803	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
23	7	315	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
23	b	813	CLA	CMB-C2B-C3B	3.35	130.94	124.68
23	4	307	CLA	CMB-C2B-C3B	3.34	130.93	124.68
23	b	803	CLA	CMB-C2B-C3B	3.34	130.93	124.68
22	9	301	A1L1G	C33-C34-C35	3.34	124.07	118.94
23	8	307	CLA	CMB-C2B-C3B	3.34	130.93	124.68
30	b	850	BCR	C11-C10-C9	-3.34	122.55	127.31
23	3	309	CLA	CMB-C2B-C3B	3.34	130.92	124.68
25	8	304	A1L1F	C31-C32-C33	-3.34	112.81	123.22
23	a	834	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
30	a	849	BCR	C24-C23-C22	-3.34	121.19	126.23
22	5	304	A1L1G	C27-C34-C35	-3.33	118.25	122.92
23	2	316	CLA	CMB-C2B-C1B	-3.33	123.35	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	843	PQN	C14-C13-C15	3.33	120.87	115.27
23	f	802	CLA	CMB-C2B-C3B	3.33	130.90	124.68
22	5	304	A1L1G	C37-C36-C35	3.33	130.29	123.47
23	b	816	CLA	CMB-C2B-C3B	3.32	130.90	124.68
25	8	304	A1L1F	C14-C29-C30	-3.32	119.61	125.47
23	a	824	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
30	a	847	BCR	C3-C4-C5	-3.32	108.14	114.08
21	5	302	XAT	C6-C7-C8	-3.32	118.97	125.99
21	1	303	XAT	C31-C30-C29	-3.32	122.57	127.31
23	a	838	CLA	CMB-C2B-C3B	3.32	130.88	124.68
23	9	311	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
23	1	308	CLA	CMB-C2B-C3B	3.32	130.88	124.68
22	1	301	A1L1G	C36-C37-C38	3.31	130.26	123.47
21	6	303	XAT	C11-C10-C9	-3.31	122.59	127.31
23	5	313	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
30	i	101	BCR	C15-C14-C13	-3.31	122.59	127.31
23	9	311	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
25	9	302	A1L1F	C25-C14-C29	-3.31	119.00	125.99
23	b	801	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
23	a	839	CLA	CMB-C2B-C3B	3.30	130.86	124.68
25	6	304	A1L1F	C14-C29-C30	-3.30	119.65	125.47
23	a	827	CLA	CMB-C2B-C3B	3.30	130.86	124.68
23	9	309	CLA	CMB-C2B-C3B	3.30	130.85	124.68
27	b	851	DGD	C2G-O2G-C1B	-3.30	109.67	117.79
23	7	313	CLA	CMB-C2B-C3B	3.30	130.84	124.68
23	4	310	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
23	6	315	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
21	5	305	XAT	C24-C23-C22	-3.29	104.42	110.77
22	9	306	A1L1G	C33-C34-C35	3.29	123.99	118.94
21	4	302	XAT	C6-C7-C8	-3.29	119.04	125.99
23	b	841	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
21	9	305	XAT	C38-C25-C26	-3.27	116.77	122.26
21	5	302	XAT	C24-C23-C22	-3.27	104.46	110.77
21	6	305	XAT	C7-C8-C9	-3.27	120.46	125.53
21	5	305	XAT	C4-C3-C2	-3.26	104.47	110.77
30	j	102	BCR	C24-C23-C22	-3.26	121.31	126.23
23	8	312	CLA	CMB-C2B-C3B	3.26	130.78	124.68
21	5	301	XAT	C11-C10-C9	-3.26	122.66	127.31
21	9	304	XAT	C11-C10-C9	-3.25	122.67	127.31
21	3	304	XAT	C26-C27-C28	-3.25	119.12	125.99
23	4	308	CLA	CMB-C2B-C3B	3.25	130.76	124.68
23	9	314	CLA	CMB-C2B-C3B	3.25	130.76	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	h	201	CLA	CMB-C2B-C3B	3.25	130.75	124.68
23	5	315	CLA	CMB-C2B-C3B	3.23	130.73	124.68
23	2	312	CLA	CMB-C2B-C3B	3.23	130.73	124.68
25	h	202	A1L1F	C17-C20-C21	3.23	117.92	114.28
30	a	850	BCR	C7-C8-C9	-3.23	121.35	126.23
23	8	310	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	a	822	CLA	CMB-C2B-C3B	3.23	130.72	124.68
22	1	301	A1L1G	C43-C44-C42	-3.23	118.40	122.92
23	7	311	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	a	815	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	3	312	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
25	1	304	A1L1F	C14-C29-C30	-3.22	119.79	125.47
30	i	101	BCR	C11-C10-C9	-3.22	122.71	127.31
25	h	202	A1L1F	C31-C32-C33	-3.22	113.17	123.22
25	6	301	A1L1F	C25-C14-C29	-3.22	119.19	125.99
23	9	315	CLA	CMB-C2B-C3B	3.22	130.69	124.68
30	b	846	BCR	C20-C21-C22	-3.21	122.72	127.31
23	a	836	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
21	9	305	XAT	C8-C9-C10	3.21	123.87	118.94
23	j	101	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
25	8	304	A1L1F	C26-C30-C31	-3.21	120.74	124.93
30	a	850	BCR	C11-C10-C9	-3.21	122.73	127.31
30	b	853	BCR	C38-C26-C25	-3.20	120.93	124.53
21	4	303	XAT	C15-C14-C13	-3.20	122.74	127.31
25	h	202	A1L1F	C37-C36-C35	-3.20	116.91	123.47
23	2	313	CLA	CMB-C2B-C3B	3.20	130.67	124.68
23	1	306	CLA	CMB-C2B-C3B	3.20	130.67	124.68
23	b	820	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	b	827	CLA	CMB-C2B-C3B	3.20	130.66	124.68
22	1	301	A1L1G	C33-C34-C35	3.20	123.85	118.94
30	b	853	BCR	C24-C23-C22	-3.20	121.40	126.23
23	a	804	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
23	b	808	CLA	O2A-CGA-O1A	-3.20	115.53	123.59
21	a	854	XAT	C10-C11-C12	-3.20	113.25	123.22
30	a	848	BCR	C33-C5-C6	-3.19	120.95	124.53
30	b	852	BCR	C24-C23-C22	-3.18	121.42	126.23
21	a	854	XAT	C11-C10-C9	-3.18	122.77	127.31
21	3	303	XAT	C24-C23-C22	-3.18	104.63	110.77
23	b	840	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
23	b	804	CLA	CMB-C2B-C3B	3.18	130.62	124.68
23	5	316	CLA	CMB-C2B-C3B	3.18	130.62	124.68
23	b	824	CLA	CMB-C2B-C3B	3.17	130.61	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	313	CLA	CMB-C2B-C3B	3.17	130.61	124.68
23	a	830	CLA	CMB-C2B-C3B	3.17	130.61	124.68
30	a	848	BCR	C38-C26-C25	-3.17	120.97	124.53
23	b	815	CLA	CMB-C2B-C3B	3.17	130.61	124.68
22	5	304	A1L1G	C40-C39-C38	3.17	123.80	118.94
22	3	306	A1L1G	C37-C36-C35	3.16	129.96	123.47
23	a	814	CLA	CMB-C2B-C3B	3.16	130.60	124.68
21	6	303	XAT	C24-C23-C22	-3.16	104.66	110.77
23	a	828	CLA	CMB-C2B-C3B	3.16	130.60	124.68
23	7	316	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	a	835	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	7	312	CLA	CMB-C2B-C3B	3.16	130.59	124.68
25	6	301	A1L1F	C26-C30-C31	-3.16	120.80	124.93
21	6	303	XAT	C6-C7-C8	-3.16	119.31	125.99
23	1	310	CLA	CMB-C2B-C3B	3.16	130.59	124.68
21	1	302	XAT	C15-C14-C13	-3.16	122.80	127.31
23	1	313	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	9	308	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	b	809	CLA	CMB-C2B-C3B	3.16	130.59	124.68
21	9	304	XAT	C24-C23-C22	-3.16	104.68	110.77
23	2	309	CLA	CMB-C2B-C3B	3.16	130.58	124.68
21	3	304	XAT	C11-C10-C9	-3.15	122.81	127.31
21	9	303	XAT	C6-C7-C8	-3.15	119.33	125.99
23	9	310	CLA	CMB-C2B-C3B	3.15	130.57	124.68
23	a	818	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
21	4	302	XAT	C24-C23-C22	-3.15	104.70	110.77
21	2	301	XAT	C11-C10-C9	-3.15	122.82	127.31
21	7	305	XAT	C35-C34-C33	-3.15	122.82	127.31
23	a	812	CLA	CMB-C2B-C3B	3.14	130.56	124.68
21	9	303	XAT	C24-C23-C22	-3.14	104.70	110.77
30	b	848	BCR	C10-C11-C12	-3.14	113.41	123.22
23	5	310	CLA	CMB-C2B-C3B	3.14	130.56	124.68
23	a	811	CLA	CMB-C2B-C3B	3.14	130.55	124.68
21	4	303	XAT	C24-C23-C22	-3.14	104.71	110.77
30	b	844	BCR	C16-C17-C18	-3.14	122.83	127.31
23	7	310	CLA	CMB-C2B-C3B	3.14	130.55	124.68
30	a	848	BCR	C3-C4-C5	-3.13	108.48	114.08
22	7	302	A1L1G	C33-C34-C35	3.13	123.75	118.94
22	3	302	A1L1G	C33-C34-C35	3.13	123.74	118.94
23	1	311	CLA	CMB-C2B-C3B	3.13	130.53	124.68
30	b	852	BCR	C33-C5-C6	-3.12	121.02	124.53
23	1	201	CLA	CMB-C2B-C3B	3.12	130.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	301	XAT	C26-C27-C28	-3.11	119.42	125.99
21	a	854	XAT	C35-C15-C14	-3.11	117.10	123.47
23	h	203	CLA	CMB-C2B-C3B	3.11	130.50	124.68
27	4	317	DGD	O1G-C1A-C2A	3.11	121.67	111.91
22	1	301	A1L1G	C40-C39-C38	3.11	123.71	118.94
23	7	306	CLA	CMB-C2B-C3B	3.10	130.49	124.68
23	a	837	CLA	CMB-C2B-C3B	3.10	130.49	124.68
22	7	302	A1L1G	C40-C39-C38	3.10	123.70	118.94
21	8	301	XAT	C24-C23-C22	-3.10	104.78	110.77
22	9	306	A1L1G	C40-C39-C38	3.10	123.70	118.94
23	b	820	CLA	CMB-C2B-C3B	3.10	130.47	124.68
21	9	305	XAT	C24-C23-C22	-3.10	104.79	110.77
23	a	803	CLA	C1B-CHB-C4A	-3.10	123.99	130.12
30	a	849	BCR	C33-C5-C4	3.10	119.56	113.62
30	b	846	BCR	C33-C5-C4	3.09	119.56	113.62
21	7	304	XAT	C24-C23-C22	-3.09	104.81	110.77
30	b	843	BCR	C20-C21-C22	-3.09	122.90	127.31
30	b	846	BCR	C38-C26-C25	-3.08	121.06	124.53
23	b	832	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
23	3	311	CLA	CMB-C2B-C3B	3.08	130.45	124.68
23	3	313	CLA	CMB-C2B-C3B	3.08	130.45	124.68
30	a	849	BCR	C38-C26-C25	-3.08	121.07	124.53
23	1	202	CLA	CMB-C2B-C3B	3.08	130.44	124.68
25	8	304	A1L1F	C25-C14-C29	-3.08	119.49	125.99
23	3	308	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
22	9	301	A1L1G	C40-C39-C38	3.07	123.66	118.94
23	2	310	CLA	CMB-C2B-C3B	3.07	130.42	124.68
21	1	302	XAT	C31-C30-C29	-3.07	122.93	127.31
22	9	306	A1L1G	C43-C44-C42	-3.07	118.63	122.92
23	b	830	CLA	CMB-C2B-C3B	3.07	130.42	124.68
23	b	812	CLA	CMB-C2B-C3B	3.07	130.41	124.68
23	b	808	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	a	821	CLA	CMB-C2B-C3B	3.06	130.41	124.68
23	b	837	CLA	CMB-C2B-C3B	3.06	130.41	124.68
23	a	809	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	a	831	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	8	304	A1L1F	C36-C35-C34	-3.06	122.94	127.31
23	8	308	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
27	8	315	DGD	O1G-C1A-C2A	3.06	121.51	111.91
23	a	852	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
21	6	306	XAT	C26-C27-C28	-3.06	119.53	125.99
30	b	847	BCR	C11-C10-C9	-3.06	122.95	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	304	XAT	C24-C23-C22	-3.06	104.87	110.77
23	4	310	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
30	i	102	BCR	C8-C7-C6	-3.06	118.62	127.20
23	a	801	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
21	4	303	XAT	C35-C15-C14	-3.05	117.22	123.47
23	6	308	CLA	CMB-C2B-C3B	3.05	130.39	124.68
30	b	850	BCR	C15-C14-C13	-3.05	122.95	127.31
23	4	315	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
21	6	306	XAT	C11-C10-C9	-3.05	122.96	127.31
21	3	304	XAT	C4-C3-C2	-3.05	104.89	110.77
22	3	306	A1L1G	C40-C39-C38	3.05	123.61	118.94
25	9	302	A1L1F	C26-C30-C31	-3.04	120.96	124.93
23	4	306	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	h	202	A1L1F	C12-C6-C1	-3.04	107.75	110.47
30	a	848	BCR	C8-C7-C6	-3.04	118.68	127.20
21	2	303	XAT	C19-C9-C10	-3.03	118.67	122.92
21	a	854	XAT	C31-C32-C33	-3.03	117.90	126.42
21	5	302	XAT	C31-C30-C29	-3.03	122.99	127.31
21	9	305	XAT	C19-C9-C10	-3.02	118.69	122.92
23	b	807	CLA	CMB-C2B-C3B	3.02	130.34	124.68
23	l	203	CLA	CMB-C2B-C3B	3.02	130.34	124.68
21	8	302	XAT	C24-C23-C22	-3.02	104.94	110.77
22	7	302	A1L1G	C43-C44-C42	-3.02	118.69	122.92
21	3	305	XAT	C4-C3-C2	-3.02	104.94	110.77
23	7	309	CLA	CMB-C2B-C3B	3.02	130.33	124.68
30	f	801	BCR	C8-C7-C6	-3.02	118.73	127.20
30	b	850	BCR	C16-C15-C14	-3.01	117.30	123.47
25	9	302	A1L1F	C42-C41-C40	-3.01	113.82	123.22
23	b	822	CLA	CMB-C2B-C3B	3.01	130.31	124.68
23	9	310	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
21	6	305	XAT	C35-C15-C14	-3.01	117.31	123.47
23	8	309	CLA	CMB-C2B-C3B	3.01	130.31	124.68
23	b	816	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
23	a	835	CLA	CMB-C2B-C3B	3.00	130.30	124.68
23	b	835	CLA	CMB-C2B-C3B	3.00	130.30	124.68
23	9	313	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
23	b	811	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
21	6	305	XAT	C24-C23-C22	-3.00	104.98	110.77
22	3	306	A1L1G	C43-C44-C42	-2.99	118.73	122.92
23	a	830	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
27	b	851	DGD	O3E-C3E-C2E	-2.99	103.44	110.35
23	b	839	CLA	CMB-C2B-C3B	2.99	130.27	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	301	A1L1F	C17-C20-C21	2.99	117.64	114.28
23	a	807	CLA	CMB-C2B-C3B	2.99	130.27	124.68
21	8	302	XAT	C6-C7-C8	-2.99	119.67	125.99
22	5	304	A1L1G	C33-C34-C35	2.99	123.52	118.94
23	b	807	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
23	4	308	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	2	309	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	b	814	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
21	8	303	XAT	C24-C23-C22	-2.98	105.02	110.77
23	b	835	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
23	1	314	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
23	7	314	CLA	CHB-C4A-NA	2.98	128.63	124.51
22	3	306	A1L1G	C33-C34-C35	2.98	123.51	118.94
23	b	834	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	4	309	CLA	CMB-C2B-C3B	2.97	130.24	124.68
21	5	301	XAT	C31-C32-C33	-2.97	118.07	126.42
23	b	818	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	a	808	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	b	802	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
21	3	305	XAT	C31-C30-C29	-2.97	123.08	127.31
23	6	309	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
30	b	848	BCR	C8-C7-C6	-2.97	118.87	127.20
30	b	844	BCR	C38-C26-C25	-2.96	121.20	124.53
23	b	814	CLA	CHB-C4A-NA	2.96	128.61	124.51
23	6	310	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	a	839	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	3	302	A1L1G	C40-C39-C38	2.96	123.48	118.94
23	7	308	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	a	812	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	4	307	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	9	314	CLA	O2D-CGD-CBD	2.96	116.52	111.27
23	7	313	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
21	7	305	XAT	C4-C3-C2	-2.96	105.06	110.77
23	5	309	CLA	CMB-C2B-C3B	2.96	130.21	124.68
21	9	305	XAT	C27-C28-C29	-2.95	120.94	125.53
23	7	314	CLA	CMB-C2B-C3B	2.95	130.20	124.68
21	3	301	XAT	C4-C3-C2	-2.95	105.08	110.77
23	b	829	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
21	7	303	XAT	C19-C9-C10	-2.94	118.80	122.92
21	4	302	XAT	C30-C31-C32	-2.94	114.03	123.22
21	6	302	XAT	C11-C12-C13	-2.94	118.15	126.42
30	b	846	BCR	C8-C7-C6	-2.94	118.95	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	850	BCR	C28-C27-C26	-2.94	108.83	114.08
23	6	307	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
21	6	302	XAT	C24-C23-C22	-2.94	105.10	110.77
30	b	852	BCR	C16-C15-C14	-2.94	117.46	123.47
21	8	303	XAT	C4-C3-C2	-2.93	105.11	110.77
23	3	309	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
23	b	841	CLA	CMB-C2B-C3B	2.93	130.16	124.68
23	1	311	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	b	840	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	b	838	CLA	CMB-C2B-C3B	2.93	130.16	124.68
22	5	304	A1L1G	C43-C44-C42	-2.93	118.82	122.92
23	6	316	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	b	818	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	b	837	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
21	3	305	XAT	C24-C23-C22	-2.93	105.12	110.77
21	1	302	XAT	C4-C3-C2	-2.93	105.12	110.77
21	4	303	XAT	C4-C3-C2	-2.92	105.13	110.77
23	a	817	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
23	h	201	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
23	8	306	CLA	CMB-C2B-C3B	2.92	130.14	124.68
21	1	302	XAT	C35-C15-C14	-2.92	117.50	123.47
23	b	824	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
21	5	303	XAT	C24-C23-C22	-2.92	105.14	110.77
23	2	313	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	3	308	CLA	CMB-C2B-C3B	2.91	130.13	124.68
23	7	315	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	3	307	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
21	7	305	XAT	C24-C23-C22	-2.91	105.15	110.77
21	2	303	XAT	C4-C3-C2	-2.91	105.15	110.77
23	b	808	CLA	CMB-C2B-C3B	2.91	130.12	124.68
23	b	833	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	9	313	CLA	CMB-C2B-C3B	2.91	130.12	124.68
23	b	826	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	3	314	CLA	CMB-C2B-C3B	2.90	130.11	124.68
21	6	305	XAT	C31-C32-C33	-2.90	118.27	126.42
23	1	312	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	a	813	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	a	820	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	6	311	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	b	804	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
30	b	845	BCR	C38-C26-C25	-2.90	121.28	124.53
23	a	832	CLA	CMB-C2B-C3B	2.89	130.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	828	CLA	CMB-C2B-C3B	2.89	130.09	124.68
23	l	201	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
30	b	850	BCR	C23-C24-C25	-2.89	119.08	127.20
21	5	305	XAT	C5-C4-C3	-2.89	107.03	112.75
23	a	840	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
21	4	301	XAT	C24-C23-C22	-2.89	105.20	110.77
21	2	304	XAT	C24-C23-C22	-2.89	105.20	110.77
23	6	313	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
30	f	801	BCR	C20-C19-C18	-2.89	118.31	126.42
21	7	301	XAT	C4-C3-C2	-2.88	105.20	110.77
23	1	313	CLA	CMB-C2B-C3B	2.88	130.07	124.68
23	1	309	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	3	302	A1L1G	C43-C44-C42	-2.88	118.89	122.92
23	4	311	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	2	307	CLA	CHB-C4A-NA	2.88	128.49	124.51
23	6	316	CLA	CMB-C2B-C3B	2.88	130.06	124.68
23	2	314	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	7	312	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	6	308	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	4	313	CLA	CMB-C2B-C3B	2.87	130.05	124.68
25	8	304	A1L1F	C17-C20-C21	2.87	117.51	114.28
21	4	301	XAT	C4-C3-C2	-2.87	105.23	110.77
23	b	823	CLA	CMB-C2B-C3B	2.87	130.05	124.68
23	1	305	CLA	CMB-C2B-C3B	2.87	130.05	124.68
30	a	848	BCR	C7-C8-C9	-2.87	121.90	126.23
21	5	303	XAT	C35-C34-C33	-2.87	123.22	127.31
23	2	310	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	b	846	BCR	C4-C5-C6	-2.87	118.57	122.73
23	5	316	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
21	1	302	XAT	C24-C23-C22	-2.87	105.23	110.77
23	b	817	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	5	308	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	8	311	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	4	314	CLA	CMB-C2B-C3B	2.86	130.04	124.68
24	5	317	SQD	C44-O6-C1	-2.86	108.15	113.74
23	5	310	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	8	310	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	3	312	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	2	316	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	b	805	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
30	f	801	BCR	C33-C5-C6	-2.86	121.32	124.53
21	6	305	XAT	O4-C5-C4	2.86	115.53	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	307	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	7	310	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	b	833	CLA	CMB-C2B-C3B	2.85	130.02	124.68
30	b	847	BCR	C33-C5-C6	-2.85	121.32	124.53
23	a	810	CLA	CMB-C2B-C3B	2.85	130.02	124.68
21	5	305	XAT	C19-C9-C8	2.85	122.57	118.08
30	b	848	BCR	C15-C16-C17	-2.85	117.63	123.47
23	6	310	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	a	825	CLA	CMB-C2B-C3B	2.85	130.01	124.68
23	a	819	CLA	CMB-C2B-C3B	2.85	130.01	124.68
23	9	312	CLA	CHB-C4A-NA	2.85	128.45	124.51
21	9	304	XAT	C15-C35-C34	-2.85	117.64	123.47
23	a	823	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	9	301	A1L1G	C43-C44-C42	-2.85	118.94	122.92
30	b	845	BCR	C34-C9-C10	-2.85	118.94	122.92
21	a	854	XAT	C24-C23-C22	-2.85	105.28	110.77
23	8	306	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
23	7	307	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	a	811	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	a	841	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	5	306	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	3	313	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	5	311	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	8	313	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	4	316	CLA	CMB-C2B-C3B	2.84	129.99	124.68
21	1	303	XAT	C4-C3-C2	-2.84	105.29	110.77
23	a	825	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	b	803	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
23	b	838	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	a	826	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	a	853	XAT	C4-C3-C2	-2.83	105.30	110.77
23	a	827	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	b	827	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	9	315	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	1	307	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	a	802	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	a	833	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
25	8	304	A1L1F	C11-C1-C6	2.83	122.50	119.70
23	3	311	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	8	312	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
21	3	303	XAT	C4-C3-C2	-2.83	105.31	110.77
21	9	303	XAT	C15-C35-C34	-2.82	117.69	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	816	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	j	101	CLA	CMB-C2B-C3B	2.82	129.96	124.68
23	8	313	CLA	CMB-C2B-C3B	2.82	129.96	124.68
21	2	305	XAT	C11-C10-C9	-2.82	123.28	127.31
22	1	301	A1L1G	C20-C21-C22	-2.82	107.17	112.75
23	a	813	CLA	CMB-C2B-C3B	2.82	129.95	124.68
23	a	837	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	1	305	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	a	836	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	b	848	BCR	C21-C20-C19	-2.82	114.43	123.22
23	5	307	CLA	CMB-C2B-C3B	2.82	129.95	124.68
23	b	839	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	6	314	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	6	315	CLA	CMB-C2B-C3B	2.81	129.94	124.68
21	2	304	XAT	C4-C3-C2	-2.81	105.34	110.77
27	4	317	DGD	O5E-C6E-C5E	-2.81	101.64	111.29
23	3	307	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	a	841	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	5	313	CLA	O2D-CGD-CBD	2.81	116.26	111.27
23	b	841	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	4	305	CLA	CMB-C2B-C3B	2.81	129.93	124.68
23	2	311	CLA	CMB-C2B-C3B	2.81	129.93	124.68
30	b	845	BCR	C20-C21-C22	-2.81	123.31	127.31
30	b	845	BCR	C37-C22-C21	-2.81	118.99	122.92
21	8	303	XAT	C11-C10-C9	-2.80	123.31	127.31
21	5	301	XAT	C4-C3-C2	-2.80	105.36	110.77
30	b	843	BCR	C33-C5-C4	2.80	119.00	113.62
23	1	306	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	9	314	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
23	2	306	CLA	CMB-C2B-C3B	2.80	129.92	124.68
23	9	311	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	1	314	CLA	CMB-C2B-C3B	2.80	129.92	124.68
23	8	314	CLA	CMB-C2B-C3B	2.80	129.92	124.68
21	6	305	XAT	C26-C27-C28	-2.80	120.08	125.99
23	a	842	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	5	314	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	f	803	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	3	315	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	2	308	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	a	805	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	a	815	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
29	b	842	PQN	C16-C15-C13	-2.79	106.13	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	8	305	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	b	821	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	b	828	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	a	828	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	a	844	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	b	819	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	a	832	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	b	815	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	a	817	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	a	821	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	7	306	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	7	315	CLA	CMB-C2B-C3B	2.79	129.89	124.68
23	9	316	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	1	304	A1L1F	C20-C21-C22	-2.79	107.24	112.75
21	9	304	XAT	C4-C3-C2	-2.78	105.39	110.77
21	3	304	XAT	C24-C23-C22	-2.78	105.39	110.77
23	8	307	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	1	308	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	1	202	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
21	4	303	XAT	C11-C10-C9	-2.78	123.34	127.31
21	2	301	XAT	C4-C3-C2	-2.78	105.40	110.77
23	a	834	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	7	317	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	9	308	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	2	315	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	4	304	XAT	C4-C3-C2	-2.78	105.41	110.77
23	4	312	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
30	b	844	BCR	C21-C20-C19	-2.78	114.55	123.22
23	a	803	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	3	315	CLA	CMB-C2B-C3B	2.78	129.87	124.68
21	7	305	XAT	C15-C35-C34	-2.78	117.79	123.47
23	5	314	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
30	j	102	BCR	C38-C26-C27	2.77	118.94	113.62
23	5	309	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
27	b	851	DGD	O1G-C1A-C2A	2.77	120.61	111.91
23	b	811	CLA	CMB-C2B-C3B	2.77	130.11	124.69
23	3	314	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	1	310	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
27	b	851	DGD	C6D-O5D-C1E	2.77	119.14	113.74
21	4	301	XAT	C31-C30-C29	-2.77	123.36	127.31
23	h	203	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	6	311	CLA	CMB-C2B-C3B	2.77	129.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	831	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
21	9	304	XAT	C30-C31-C32	-2.77	114.59	123.22
23	b	810	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	4	311	CLA	CMB-C2B-C3B	2.76	129.85	124.68
23	a	840	CLA	CMB-C2B-C3B	2.76	129.85	124.68
23	8	309	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	9	312	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	6	312	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	b	801	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	b	823	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	6	307	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	2	316	CLA	CMB-C2B-C3B	2.76	129.84	124.68
25	1	304	A1L1F	C36-C35-C34	-2.76	123.37	127.31
21	5	301	XAT	C26-C27-C28	-2.76	120.16	125.99
23	a	856	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	8	314	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
30	a	850	BCR	C38-C26-C27	2.75	118.91	113.62
25	h	202	A1L1F	C26-C30-C31	-2.75	121.33	124.93
23	7	317	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	4	313	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	5	315	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
28	2	317	LMG	O8-C28-C29	2.75	120.53	111.91
30	b	843	BCR	C24-C23-C22	-2.75	122.08	126.23
23	2	314	CLA	CMB-C2B-C3B	2.75	129.82	124.68
23	9	311	CLA	CMB-C2B-C3B	2.75	129.82	124.68
23	5	311	CLA	CMB-C2B-C3B	2.75	129.82	124.68
23	4	315	CLA	CMB-C2B-C3B	2.75	129.82	124.68
21	6	303	XAT	C15-C35-C34	-2.75	117.85	123.47
25	8	304	A1L1F	O7-C54-O55	-2.75	117.51	122.96
25	1	304	A1L1F	C26-O13-C45	2.74	121.79	115.68
21	2	301	XAT	C24-C23-C22	-2.74	105.47	110.77
23	f	802	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
23	4	306	CLA	CMB-C2B-C3B	2.74	129.81	124.68
21	3	303	XAT	C31-C30-C29	-2.74	123.40	127.31
23	b	822	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	a	820	CLA	C1-C2-C3	-2.74	121.31	126.04
23	f	803	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	4	305	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
30	b	850	BCR	C24-C23-C22	-2.74	122.10	126.23
30	a	849	BCR	C2-C1-C6	2.74	114.69	110.48
23	2	312	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
21	2	302	XAT	C35-C15-C14	-2.73	117.87	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	315	CLA	CAA-C2A-C3A	-2.73	109.72	116.10
23	b	830	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
23	b	825	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	3	312	CLA	CMB-C2B-C3B	2.73	129.79	124.68
23	a	824	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	b	843	BCR	C38-C26-C25	-2.73	121.46	124.53
23	a	819	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
21	3	301	XAT	C10-C11-C12	-2.73	114.70	123.22
21	2	305	XAT	C38-C25-C26	-2.73	117.69	122.26
23	a	807	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	i	101	BCR	C20-C19-C18	-2.73	118.75	126.42
23	a	838	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	2	315	CLA	CMB-C2B-C3B	2.72	129.77	124.68
23	7	307	CLA	CMB-C2B-C3B	2.72	129.77	124.68
28	a	855	LMG	O8-C28-C29	2.72	120.45	111.91
23	9	310	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	8	304	A1L1F	O13-C45-C47	2.72	120.44	111.91
23	a	829	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
21	3	305	XAT	C35-C15-C14	-2.72	117.91	123.47
23	b	801	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	b	812	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
30	b	843	BCR	C23-C24-C25	-2.72	119.58	127.20
23	a	841	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
30	b	845	BCR	C11-C10-C9	-2.71	123.44	127.31
30	j	102	BCR	C23-C24-C25	-2.71	119.59	127.20
21	2	305	XAT	C4-C3-C2	-2.71	105.54	110.77
21	8	303	XAT	C39-C29-C28	2.71	122.35	118.08
21	1	303	XAT	C10-C11-C12	-2.71	114.76	123.22
23	a	835	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	9	302	A1L1F	O13-C45-C47	2.71	120.41	111.91
23	a	808	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
23	6	312	CLA	CMB-C2B-C3B	2.71	129.74	124.68
23	4	312	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
21	9	304	XAT	C7-C8-C9	-2.70	121.33	125.53
21	7	301	XAT	C11-C10-C9	-2.70	123.45	127.31
23	3	312	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
23	b	809	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
21	a	853	XAT	C24-C23-C22	-2.70	105.56	110.77
29	b	842	PQN	C2M-C2-C3	-2.70	120.00	124.40
21	a	853	XAT	C15-C35-C34	-2.70	117.95	123.47
23	b	819	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
21	2	301	XAT	C31-C32-C33	-2.70	118.84	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	317	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	5	306	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
23	7	311	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
21	2	302	XAT	C24-C23-C22	-2.70	105.57	110.77
21	8	301	XAT	C7-C8-C9	-2.70	121.35	125.53
25	h	202	A1L1F	O13-C45-C47	2.70	120.37	111.91
21	6	306	XAT	C4-C3-C2	-2.70	105.57	110.77
30	b	843	BCR	C4-C5-C6	-2.70	118.82	122.73
23	l	202	CLA	CHB-C4A-NA	2.69	128.24	124.51
23	l	203	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
30	b	852	BCR	C20-C19-C18	-2.69	118.85	126.42
23	5	315	CLA	CHB-C4A-NA	2.69	128.23	124.51
21	8	303	XAT	C35-C34-C33	-2.69	123.47	127.31
23	a	804	CLA	C1-C2-C3	-2.69	121.40	126.04
30	b	847	BCR	C35-C13-C12	2.69	122.31	118.08
23	b	836	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
24	1	315	SQD	O48-C23-C24	2.69	120.34	111.91
21	a	853	XAT	C31-C30-C29	-2.68	123.48	127.31
23	a	814	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
21	5	303	XAT	C4-C3-C2	-2.68	105.59	110.77
23	b	811	CLA	CAB-C3B-C2B	2.68	129.94	124.69
25	h	202	A1L1F	C8-O7-C54	-2.68	112.90	117.90
21	3	301	XAT	C19-C9-C8	2.68	122.30	118.08
30	b	846	BCR	C10-C11-C12	-2.68	114.86	123.22
23	1	312	CLA	CMB-C2B-C3B	2.68	129.69	124.68
23	9	309	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	4	314	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	5	317	SQD	O48-C23-C24	2.68	120.31	111.91
23	b	806	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	a	822	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
30	i	101	BCR	C29-C30-C25	2.68	114.60	110.48
21	6	302	XAT	C4-C3-C2	-2.68	105.61	110.77
23	h	201	CLA	C1-C2-C3	-2.67	121.42	126.04
26	m	101	LHG	O8-C23-C24	2.67	120.30	111.91
21	4	303	XAT	C31-C30-C29	-2.67	123.50	127.31
23	h	201	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	4	307	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
21	3	301	XAT	C24-C23-C22	-2.67	105.62	110.77
30	f	801	BCR	C33-C5-C4	2.67	118.74	113.62
23	4	316	CLA	CHB-C4A-NA	2.67	128.20	124.51
21	a	853	XAT	C31-C32-C33	-2.66	118.93	126.42
21	4	304	XAT	C31-C32-C33	-2.66	118.94	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	850	BCR	C20-C21-C22	-2.66	123.51	127.31
30	b	843	BCR	C2-C1-C6	2.66	114.58	110.48
23	a	805	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	a	826	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	4	314	CLA	CHB-C4A-NA	2.66	128.18	124.51
30	b	846	BCR	C7-C8-C9	-2.65	122.22	126.23
21	6	305	XAT	C6-C7-C8	-2.65	120.38	125.99
23	a	821	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	5	301	XAT	C39-C29-C30	-2.65	119.21	122.92
23	6	315	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
21	3	301	XAT	C27-C28-C29	-2.65	121.42	125.53
21	5	305	XAT	C10-C11-C12	-2.65	114.95	123.22
23	b	818	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
23	b	819	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
30	a	847	BCR	C16-C15-C14	-2.64	118.06	123.47
23	4	309	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
23	b	824	CLA	CHB-C4A-NA	2.64	128.17	124.51
21	5	305	XAT	C8-C9-C10	-2.64	114.89	118.94
25	6	301	AI1F	O13-C45-C47	2.64	120.19	111.91
21	4	302	XAT	C4-C3-C2	-2.64	105.67	110.77
21	a	854	XAT	O4-C5-C4	2.64	115.36	113.38
23	a	834	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
21	7	304	XAT	C4-C3-C2	-2.64	105.68	110.77
23	1	314	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	4	304	XAT	C7-C8-C9	-2.63	121.44	125.53
27	b	851	DGD	C1E-O6E-C5E	2.63	118.86	113.69
21	4	302	XAT	C39-C29-C28	2.63	122.23	118.08
30	b	850	BCR	C28-C27-C26	-2.63	109.37	114.08
23	2	313	CLA	CAA-C2A-C3A	-2.63	109.95	116.10
23	b	826	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
23	1	306	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	9	311	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
23	a	814	CLA	CHB-C4A-NA	2.63	128.14	124.51
21	7	303	XAT	C24-C23-C22	-2.62	105.70	110.77
23	a	824	CLA	CMB-C2B-C3B	2.62	129.58	124.68
23	4	316	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
21	4	301	XAT	C15-C14-C13	-2.62	123.57	127.31
21	2	305	XAT	C31-C32-C33	-2.62	119.06	126.42
23	a	809	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	a	819	CLA	CHB-C4A-NA	2.62	128.13	124.51
21	5	302	XAT	C35-C15-C14	-2.62	118.11	123.47
23	5	307	CLA	O2D-CGD-O1D	-2.62	118.72	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	305	XAT	O4-C5-C4	2.62	115.35	113.38
21	9	303	XAT	C30-C31-C32	-2.62	115.05	123.22
21	8	302	XAT	C4-C3-C2	-2.62	105.72	110.77
23	b	830	CLA	CAA-C2A-C3A	-2.62	109.99	116.10
21	2	304	XAT	C15-C14-C13	-2.61	123.58	127.31
23	a	832	CLA	CHB-C4A-NA	2.61	128.13	124.51
30	f	801	BCR	C10-C11-C12	-2.61	115.06	123.22
23	a	833	CLA	CHB-C4A-NA	2.61	128.13	124.51
23	b	834	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
21	4	304	XAT	C39-C29-C30	-2.61	119.26	122.92
23	3	315	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	6	316	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	a	807	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	b	805	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	a	849	BCR	C16-C15-C14	-2.61	118.13	123.47
23	j	101	CLA	CHB-C4A-NA	2.61	128.12	124.51
21	5	301	XAT	C27-C28-C29	-2.61	121.48	125.53
23	b	841	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
21	6	303	XAT	C4-C3-C2	-2.61	105.74	110.77
23	4	310	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	b	810	CLA	CHB-C4A-NA	2.61	128.12	124.51
21	5	305	XAT	C31-C30-C29	-2.61	123.59	127.31
30	i	102	BCR	C28-C27-C26	-2.60	109.43	114.08
30	m	102	BCR	C15-C16-C17	-2.60	118.14	123.47
23	1	309	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
25	h	202	A1L1F	C20-C21-C22	-2.60	107.60	112.75
23	4	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	9	307	LHG	O8-C23-C24	2.60	120.06	111.91
30	b	850	BCR	C21-C20-C19	-2.60	115.11	123.22
23	a	810	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	7	309	CLA	O2D-CGD-O1D	-2.60	118.19	124.09
21	2	304	XAT	C35-C15-C14	-2.60	118.16	123.47
23	4	314	CLA	CAA-C2A-C3A	-2.60	110.04	116.10
28	j	103	LMG	O8-C28-C29	2.59	120.05	111.91
25	h	202	A1L1F	C29-C30-C31	-2.59	115.00	118.93
23	9	316	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
23	a	852	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
23	b	817	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	a	802	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
23	b	801	CLA	CMB-C2B-C3B	2.59	129.52	124.68
21	7	303	XAT	C4-C3-C2	-2.59	105.78	110.77
23	b	820	CLA	C1-C2-C3	-2.59	122.57	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	308	CLA	C1-C2-C3	-2.58	121.57	126.04
23	a	842	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
30	b	846	BCR	C2-C1-C6	2.58	114.46	110.48
23	a	825	CLA	CHB-C4A-NA	2.58	128.09	124.51
26	b	849	LHG	O8-C23-C24	2.58	120.02	111.91
26	a	845	LHG	O8-C23-C24	2.58	120.01	111.91
23	5	314	CLA	CHB-C4A-NA	2.58	128.08	124.51
30	m	102	BCR	C33-C5-C6	-2.58	121.63	124.53
23	8	312	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	9	309	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
30	m	102	BCR	C27-C26-C25	2.58	126.48	122.73
23	a	829	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
30	j	102	BCR	C33-C5-C6	-2.58	121.63	124.53
25	1	304	A1L1F	O13-C45-C47	2.58	120.00	111.91
23	3	312	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
23	3	310	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
21	6	306	XAT	C24-C23-C22	-2.58	105.80	110.77
23	a	856	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	8	311	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
23	3	308	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	b	847	BCR	C38-C26-C25	-2.57	121.64	124.53
23	b	816	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
23	b	808	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	b	853	BCR	C20-C21-C22	-2.57	123.64	127.31
25	1	304	A1L1F	C26-C30-C31	-2.57	121.57	124.93
23	5	307	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	8	302	XAT	C19-C9-C10	-2.57	119.32	122.92
23	f	802	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	2	311	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
23	2	313	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	b	817	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
23	b	825	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
23	2	308	CLA	C1B-CHB-C4A	-2.57	125.04	130.12
23	b	808	CLA	C1B-CHB-C4A	-2.57	125.04	130.12
21	8	301	XAT	C4-C3-C2	-2.56	105.82	110.77
21	6	302	XAT	C27-C28-C29	-2.56	121.55	125.53
23	b	813	CLA	CHB-C4A-NA	2.56	128.06	124.51
23	2	311	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	b	829	CLA	C2D-C1D-ND	-2.56	108.22	110.10
23	a	801	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
23	9	313	CLA	CHB-C4A-NA	2.56	128.06	124.51
23	2	307	CLA	C1B-CHB-C4A	-2.56	125.04	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	309	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	b	836	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	2	302	XAT	C4-C3-C2	-2.56	105.83	110.77
30	b	848	BCR	C24-C23-C22	-2.56	122.37	126.23
30	a	849	BCR	C23-C24-C25	-2.56	120.02	127.20
23	1	308	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	5	312	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
21	8	302	XAT	C11-C12-C13	-2.55	119.24	126.42
23	l	203	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	a	804	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	a	818	CLA	CMB-C2B-C3B	2.55	129.45	124.68
23	b	804	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	9	303	XAT	C4-C3-C2	-2.55	105.85	110.77
23	a	814	CLA	CHD-C1D-ND	-2.55	122.11	124.45
23	1	312	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	b	847	BCR	C8-C7-C6	-2.55	120.05	127.20
30	b	848	BCR	C34-C9-C8	2.55	122.09	118.08
21	8	301	XAT	C31-C30-C29	-2.55	123.68	127.31
23	8	307	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	7	313	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
23	8	311	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	b	813	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	2	306	CLA	O2D-CGD-O1D	-2.54	118.32	124.09
23	7	307	CLA	CHB-C4A-NA	2.54	128.02	124.51
30	b	853	BCR	C34-C9-C10	-2.54	119.37	122.92
23	f	803	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	6	302	XAT	C19-C9-C10	-2.54	119.37	122.92
23	l	201	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	3	314	CLA	CHB-C4A-NA	2.54	128.02	124.51
30	b	852	BCR	C15-C14-C13	-2.53	123.69	127.31
30	i	102	BCR	C38-C26-C27	2.53	118.48	113.62
23	b	812	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	b	820	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	a	827	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
21	9	303	XAT	C7-C8-C9	-2.53	121.60	125.53
23	5	313	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	4	305	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	b	821	CLA	CHB-C4A-NA	2.53	128.01	124.51
30	b	848	BCR	C20-C21-C22	-2.53	123.70	127.31
23	a	820	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
30	b	847	BCR	C33-C5-C4	2.53	118.48	113.62
23	5	312	CLA	C1B-CHB-C4A	-2.53	125.11	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	306	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	4	310	CLA	CMB-C2B-C3B	2.53	129.41	124.68
23	8	308	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	9	308	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
23	a	806	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
23	h	201	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
23	a	831	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
23	2	312	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	1	315	SQD	O8-S-C6	2.53	109.77	105.74
23	a	808	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	a	810	CLA	CHB-C4A-NA	2.53	128.00	124.51
30	b	844	BCR	C24-C23-C22	-2.52	122.42	126.23
23	b	829	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
23	4	306	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	7	316	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	b	831	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	7	315	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	l	202	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
23	a	802	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	6	311	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	b	837	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	a	822	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
23	3	313	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	a	806	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	a	840	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	b	802	CLA	CMB-C2B-C3B	2.52	129.38	124.68
23	3	307	CLA	CHB-C4A-NA	2.52	127.99	124.51
23	8	314	CLA	CAA-C2A-C3A	-2.52	110.23	116.10
23	b	802	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
23	b	835	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
23	a	811	CLA	CHB-C4A-NA	2.51	127.99	124.51
24	5	317	SQD	O7-S-C6	2.51	109.93	106.94
21	2	302	XAT	C11-C10-C9	-2.51	123.72	127.31
23	b	834	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	a	838	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	8	304	A1L1F	C12-C6-C1	-2.51	108.22	110.47
21	1	303	XAT	C35-C15-C14	-2.51	118.33	123.47
23	4	313	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	a	812	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	5	316	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	6	310	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	a	822	CLA	CHB-C4A-NA	2.51	127.98	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	855	LMG	C8-O7-C10	-2.51	111.62	117.79
21	5	305	XAT	C15-C35-C34	-2.51	118.34	123.47
30	f	801	BCR	C2-C1-C6	2.50	114.34	110.48
23	5	311	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	6	312	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	3	309	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	b	806	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	a	836	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	b	838	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	a	832	CLA	C1-C2-C3	-2.50	122.71	126.75
23	7	306	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	8	301	XAT	C35-C15-C14	-2.50	118.36	123.47
23	a	836	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	4	315	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	5	313	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
25	6	304	A1L1F	O13-C45-C47	2.50	119.74	111.91
23	a	823	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	6	314	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	1	310	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
25	6	301	A1L1F	C31-C32-C33	-2.49	115.44	123.22
23	1	307	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	a	817	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	a	841	CLA	C1-C2-C3	-2.49	121.74	126.04
21	7	301	XAT	C35-C15-C14	-2.49	118.38	123.47
23	b	819	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	9	308	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	7	311	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	9	302	A1L1F	C36-C37-C38	-2.49	118.38	123.47
23	a	818	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	a	841	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
23	6	309	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	a	827	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	5	305	XAT	C39-C29-C28	2.49	121.99	118.08
30	i	102	BCR	C15-C16-C17	-2.49	118.38	123.47
23	b	820	CLA	O2D-CGD-CBD	2.49	115.68	111.27
21	6	302	XAT	C31-C32-C33	-2.48	119.44	126.42
21	7	304	XAT	C19-C9-C10	-2.48	119.44	122.92
23	2	314	CLA	CHB-C4A-NA	2.48	127.95	124.51
23	2	306	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	b	851	DGD	O2G-C1B-O1B	-2.48	117.71	123.70
30	b	844	BCR	C15-C16-C17	-2.48	118.39	123.47
30	f	804	BCR	C15-C16-C17	-2.48	118.39	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	834	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
23	1	310	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	8	313	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	h	203	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	7	313	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	a	816	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	b	842	PQN	C14-C13-C15	2.48	119.44	115.27
23	1	309	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	a	806	CLA	O1D-CGD-CBD	2.47	129.55	124.48
23	a	802	CLA	C1-C2-C3	-2.47	121.76	126.04
23	b	807	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	b	822	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	6	307	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	a	815	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	b	803	CLA	CHD-C1D-ND	-2.47	122.18	124.45
22	9	301	A1L1G	C20-C21-C22	-2.47	107.86	112.75
30	b	853	BCR	C28-C27-C26	-2.47	109.66	114.08
30	i	102	BCR	C33-C5-C4	2.47	118.36	113.62
21	5	303	XAT	C19-C9-C10	-2.47	119.46	122.92
23	a	835	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
30	b	846	BCR	C21-C20-C19	-2.47	115.52	123.22
23	a	820	CLA	CHB-C4A-NA	2.47	127.92	124.51
30	b	848	BCR	C38-C26-C25	-2.47	121.76	124.53
30	b	843	BCR	C15-C16-C17	-2.46	118.43	123.47
21	5	302	XAT	C4-C3-C2	-2.46	106.02	110.77
23	a	812	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	b	807	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	8	303	XAT	C28-C29-C30	-2.46	115.17	118.94
23	8	309	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	a	828	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	8	314	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	b	839	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	a	809	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
21	5	301	XAT	C35-C15-C14	-2.46	118.44	123.47
30	b	847	BCR	C39-C30-C25	-2.46	106.31	110.30
23	a	805	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
30	j	102	BCR	C15-C16-C17	-2.46	118.44	123.47
23	b	831	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
23	5	309	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	6	315	CLA	CHB-C4A-NA	2.45	127.91	124.51
23	8	305	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	a	839	CLA	CHB-C4A-NA	2.45	127.90	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	305	XAT	C30-C31-C32	-2.45	115.57	123.22
23	a	837	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	7	308	CLA	CHB-C4A-NA	2.45	127.89	124.51
25	h	202	A1L1F	C41-C40-C39	-2.45	119.55	126.42
30	j	102	BCR	C27-C26-C25	-2.45	119.18	122.73
23	4	311	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	b	828	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
30	b	853	BCR	C21-C20-C19	-2.44	115.59	123.22
23	a	830	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	5	310	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	3	311	CLA	C1-C2-C3	-2.44	122.80	126.75
25	6	304	A1L1F	C25-C14-C29	-2.44	120.83	125.99
23	b	840	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	h	203	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	2	316	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	l	203	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	b	813	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	8	308	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	1	313	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	l	202	CLA	CHD-C1D-ND	-2.44	122.22	124.45
23	9	309	CLA	CHB-C4A-NA	2.43	127.88	124.51
21	7	304	XAT	C11-C12-C13	-2.43	119.58	126.42
23	a	856	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	b	815	CLA	CHB-C4A-NA	2.43	127.88	124.51
23	b	835	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	7	305	XAT	C31-C30-C29	-2.43	123.84	127.31
23	a	834	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	b	816	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	a	848	BCR	C33-C5-C4	2.43	118.28	113.62
25	6	304	A1L1F	C42-C41-C40	-2.43	115.65	123.22
23	4	307	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	3	304	XAT	C31-C32-C33	-2.42	119.61	126.42
23	a	804	CLA	O2D-CGD-CBD	2.42	115.58	111.27
23	a	837	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
25	h	202	A1L1F	C27-C34-C33	2.42	121.89	118.08
23	2	315	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	a	807	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	7	314	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
25	1	304	A1L1F	C27-C34-C33	2.42	121.89	118.08
23	4	312	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	2	311	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	9	305	XAT	C35-C15-C14	-2.42	118.52	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	810	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
23	b	830	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
23	5	315	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
23	6	313	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	9	314	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	9	311	CLA	O2D-CGD-CBD	2.41	115.56	111.27
30	a	850	BCR	C8-C7-C6	-2.41	120.42	127.20
23	9	315	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	b	833	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	b	843	BCR	C21-C20-C19	-2.41	115.70	123.22
25	8	304	A1L1F	C28-C39-C38	-2.41	119.55	122.92
23	a	803	CLA	CHD-C1D-ND	-2.41	122.24	124.45
30	b	850	BCR	C33-C5-C4	2.41	118.24	113.62
23	b	802	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	4	311	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	7	310	CLA	CHB-C4A-NA	2.41	127.84	124.51
21	5	303	XAT	C31-C30-C29	-2.41	123.88	127.31
23	8	307	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
30	j	102	BCR	C38-C26-C25	-2.41	121.83	124.53
23	3	310	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	b	811	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	a	832	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
21	8	302	XAT	C7-C8-C9	-2.40	121.80	125.53
23	b	837	CLA	CHD-C1D-ND	-2.40	122.25	124.45
23	8	312	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	a	813	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	a	836	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
30	b	845	BCR	C28-C27-C26	-2.40	109.79	114.08
23	5	316	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	8	310	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	a	814	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	4	308	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	b	833	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	3	306	A1L1G	C17-C20-C21	2.40	116.98	114.28
23	a	840	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	b	827	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
30	f	804	BCR	C28-C27-C26	-2.40	109.79	114.08
21	4	301	XAT	C10-C11-C12	-2.40	115.73	123.22
23	6	313	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	8	310	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	a	856	CLA	CHB-C4A-NA	2.40	127.82	124.51
23	1	313	CLA	C1B-CHB-C4A	-2.39	125.37	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	308	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	7	303	XAT	C8-C9-C10	2.39	122.61	118.94
21	2	303	XAT	C8-C9-C10	2.39	122.61	118.94
25	6	304	A1L1F	C11-C1-C6	2.39	122.07	119.70
23	7	308	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	3	311	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	a	818	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	4	311	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	1	201	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	5	308	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	3	309	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	b	809	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	b	852	BCR	C36-C18-C17	-2.39	119.58	122.92
23	b	805	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
21	9	304	XAT	C39-C29-C28	2.39	121.84	118.08
23	b	832	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	6	303	XAT	C11-C12-C13	-2.39	119.71	126.42
23	a	810	CLA	C1-C2-C3	-2.39	121.91	126.04
30	a	850	BCR	C10-C11-C12	-2.39	115.77	123.22
23	b	816	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	b	825	CLA	CHB-C4A-NA	2.39	127.81	124.51
30	b	850	BCR	C8-C7-C6	-2.39	120.50	127.20
23	8	306	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	7	314	CLA	C2A-C1A-CHA	2.39	128.03	123.86
23	4	316	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
23	a	808	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
23	1	305	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	2	309	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	9	316	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	3	308	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
28	j	103	LMG	C8-O7-C10	-2.38	111.93	117.79
21	2	303	XAT	C24-C23-C22	-2.38	106.17	110.77
23	a	835	CLA	O2D-CGD-CBD	2.38	115.50	111.27
23	a	804	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	b	818	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	b	834	CLA	CHD-C1D-ND	-2.38	122.27	124.45
30	a	850	BCR	C16-C15-C14	-2.38	118.60	123.47
23	7	312	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	b	827	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	a	825	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	b	811	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	1	311	CLA	CHB-C4A-NA	2.38	127.80	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	312	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	a	842	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	a	811	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	b	837	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	6	310	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	h	202	A1L1F	C23-C22-C21	-2.37	106.19	110.77
23	a	816	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	4	308	CLA	CHB-C4A-NA	2.37	127.79	124.51
30	a	847	BCR	C23-C24-C25	-2.37	120.54	127.20
21	3	305	XAT	C10-C11-C12	-2.37	115.82	123.22
25	6	304	A1L1F	C31-C32-C33	-2.37	115.82	123.22
23	a	812	CLA	CHD-C1D-ND	-2.37	122.28	124.45
25	h	202	A1L1F	O7-C54-O55	-2.37	118.25	122.96
23	6	309	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	b	846	BCR	C33-C5-C6	-2.37	121.87	124.53
23	9	316	CLA	CHB-C4A-NA	2.37	127.79	124.51
21	7	304	XAT	O4-C5-C4	2.37	115.16	113.38
21	5	301	XAT	C40-C33-C34	-2.37	119.61	122.92
23	b	830	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	a	834	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
30	b	843	BCR	C29-C30-C25	2.37	114.12	110.48
23	5	308	CLA	CHB-C4A-NA	2.37	127.78	124.51
23	b	822	CLA	CHB-C4A-NA	2.37	127.78	124.51
23	7	312	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
23	3	310	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	a	828	CLA	C1-C2-C3	-2.36	121.95	126.04
21	3	303	XAT	C30-C31-C32	-2.36	115.84	123.22
30	b	844	BCR	C28-C27-C26	-2.36	109.86	114.08
30	i	101	BCR	C37-C22-C21	-2.36	119.61	122.92
23	9	315	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
30	b	850	BCR	C10-C11-C12	-2.36	115.85	123.22
23	a	801	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	9	312	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	5	305	XAT	C25-C24-C23	-2.36	108.08	112.75
23	b	815	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	2	304	XAT	C35-C34-C33	-2.36	123.94	127.31
23	a	806	CLA	C5-C3-C2	-2.36	116.35	121.12
23	1	308	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	b	824	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	f	802	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	a	833	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	b	839	CLA	C1B-CHB-C4A	-2.35	125.45	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	848	BCR	C15-C16-C17	-2.35	118.65	123.47
23	b	820	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
21	7	301	XAT	C31-C32-C33	-2.35	119.81	126.42
23	f	803	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	b	806	CLA	C1-C2-C3	-2.35	121.97	126.04
25	8	304	A1L1F	C23-C22-C21	-2.35	106.23	110.77
23	1	313	CLA	CAA-C2A-C3A	-2.35	110.61	116.10
23	7	309	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
25	9	302	A1L1F	O7-C54-O55	-2.35	118.29	122.96
21	4	302	XAT	O4-C5-C4	2.35	115.15	113.38
23	3	313	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	7	311	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	9	311	CLA	CHD-C1D-ND	-2.35	122.30	124.45
21	4	301	XAT	C30-C31-C32	-2.35	115.89	123.22
23	b	823	CLA	CHB-C4A-NA	2.35	127.76	124.51
30	b	844	BCR	C33-C5-C4	2.35	118.13	113.62
21	2	302	XAT	O4-C5-C4	2.35	115.15	113.38
23	a	826	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
23	4	312	CLA	CHD-C1D-ND	-2.35	122.30	124.45
23	1	311	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	6	304	A1L1F	O7-C54-O55	-2.35	118.30	122.96
23	5	310	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
21	6	306	XAT	C31-C32-C33	-2.35	119.83	126.42
23	a	841	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
23	4	310	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
23	a	839	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
21	7	303	XAT	O4-C5-C4	2.34	115.14	113.38
27	8	315	DGD	C2G-O2G-C1B	-2.34	112.02	117.79
30	b	844	BCR	C23-C24-C25	-2.34	120.62	127.20
23	b	832	CLA	CHD-C1D-ND	-2.34	122.30	124.45
21	5	303	XAT	O4-C5-C4	2.34	115.14	113.38
23	1	309	CLA	CHD-C1D-ND	-2.34	122.30	124.45
23	8	313	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	b	846	BCR	C16-C15-C14	-2.34	118.68	123.47
23	b	804	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	6	304	A1L1F	C5-C6-C1	-2.34	108.38	110.47
23	a	828	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
23	7	309	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	a	831	CLA	CHB-C4A-NA	2.34	127.75	124.51
30	a	847	BCR	C33-C5-C4	2.34	118.11	113.62
23	a	819	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
30	f	804	BCR	C3-C4-C5	-2.34	109.91	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	9	313	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
23	b	809	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
29	a	843	PQN	C11-C12-C13	-2.34	122.90	126.79
23	b	801	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
23	a	806	CLA	C6-C5-C3	-2.33	107.33	113.45
23	7	311	CLA	CHD-C1D-ND	-2.33	122.31	124.45
23	9	310	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
23	a	844	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	b	836	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	a	801	CLA	CMB-C2B-C3B	2.33	129.03	124.68
23	b	812	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
23	8	306	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
23	4	314	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	7	302	A1L1G	C17-C20-C21	2.33	116.90	114.28
21	9	304	XAT	O4-C5-C4	2.32	115.13	113.38
30	b	853	BCR	C15-C16-C17	-2.32	118.71	123.47
23	2	314	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
21	6	303	XAT	O24-C25-C38	2.32	117.84	115.06
21	1	303	XAT	C27-C28-C29	-2.32	121.93	125.53
23	b	818	CLA	CHD-C1D-ND	-2.32	122.32	124.45
23	a	810	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	a	836	CLA	C1-C2-C3	-2.32	123.00	126.75
23	a	815	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
25	1	304	A1L1F	C31-C32-C33	-2.32	115.98	123.22
23	6	312	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	5	303	XAT	C15-C35-C34	-2.32	118.73	123.47
23	5	311	CLA	CHD-C1D-ND	-2.32	122.33	124.45
23	b	841	CLA	CHB-C4A-NA	2.31	127.71	124.51
23	2	313	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
23	b	835	CLA	CHD-C1D-ND	-2.31	122.33	124.45
23	5	307	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	7	314	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	7	309	CLA	CHD-C1D-ND	-2.31	122.33	124.45
23	1	309	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	j	101	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	a	805	CLA	CHD-C1D-ND	-2.31	122.33	124.45
30	a	848	BCR	C10-C11-C12	-2.31	116.02	123.22
23	3	314	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	b	806	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	a	816	CLA	C1-C2-C3	-2.31	123.02	126.75
21	5	302	XAT	O4-C5-C4	2.31	115.11	113.38
23	a	824	CLA	CHB-C4A-NA	2.31	127.70	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	843	BCR	C38-C26-C27	2.31	118.05	113.62
23	7	310	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
30	b	843	BCR	C11-C12-C13	-2.31	119.94	126.42
25	6	301	A1L1F	C14-C29-C30	-2.31	121.41	125.47
30	f	804	BCR	C11-C12-C13	-2.30	119.94	126.42
23	2	312	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
23	2	315	CLA	CHB-C4A-NA	2.30	127.70	124.51
23	4	313	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	a	823	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	7	316	CLA	O2D-CGD-CBD	2.30	115.36	111.27
23	b	840	CLA	CMB-C2B-C3B	2.30	128.98	124.68
23	6	315	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	b	831	CLA	CHD-C1D-ND	-2.30	122.34	124.45
21	2	301	XAT	C10-C11-C12	-2.30	116.04	123.22
23	4	309	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
30	m	102	BCR	C8-C7-C6	-2.30	120.75	127.20
21	8	303	XAT	C40-C33-C32	2.29	121.69	118.08
23	3	315	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
23	a	842	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
23	a	827	CLA	CHD-C1D-ND	-2.29	122.35	124.45
23	b	825	CLA	CHD-C1D-ND	-2.29	122.35	124.45
21	9	303	XAT	C39-C29-C28	2.29	121.69	118.08
25	6	301	A1L1F	C36-C35-C34	-2.29	124.04	127.31
23	8	314	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	i	101	BCR	C16-C15-C14	-2.29	118.78	123.47
21	a	854	XAT	C19-C9-C8	2.29	121.69	118.08
23	7	306	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	1	312	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	1	305	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	8	309	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
21	a	853	XAT	C39-C29-C28	2.29	121.68	118.08
23	7	313	CLA	CHD-C1D-ND	-2.29	122.35	124.45
23	b	814	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	5	313	CLA	CHD-C1D-ND	-2.29	122.35	124.45
23	a	830	CLA	C1-C2-C3	-2.29	122.09	126.04
21	3	304	XAT	C27-C28-C29	-2.28	121.98	125.53
21	2	302	XAT	C10-C11-C12	-2.28	116.09	123.22
23	6	307	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
23	a	815	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	1	314	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
23	b	802	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	1	307	CLA	C1B-CHB-C4A	-2.28	125.60	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	311	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	1	305	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	a	820	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	b	809	CLA	C1-C2-C3	-2.28	122.10	126.04
23	a	810	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
23	5	314	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	7	313	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
30	b	852	BCR	C23-C24-C25	-2.28	120.80	127.20
23	4	305	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	b	823	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	6	316	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	b	826	CLA	CHB-C4A-NA	2.28	127.66	124.51
23	2	306	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	3	307	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
23	5	311	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
21	8	302	XAT	O4-C5-C4	2.27	115.09	113.38
23	6	311	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
23	a	821	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
30	j	102	BCR	C34-C9-C10	-2.27	119.74	122.92
23	5	315	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	b	803	CLA	C3C-C4C-NC	-2.27	108.02	110.57
23	b	832	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	2	304	XAT	C20-C13-C12	2.27	121.65	118.08
30	a	848	BCR	C16-C15-C14	-2.27	118.83	123.47
23	2	310	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
25	6	301	A1L1F	O7-C54-O55	-2.27	118.46	122.96
23	4	309	CLA	O2A-CGA-O1A	-2.27	117.88	123.59
30	b	853	BCR	C23-C24-C25	-2.27	120.84	127.20
23	a	813	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
23	1	306	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
23	4	306	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	b	838	CLA	CHB-C4A-NA	2.26	127.64	124.51
23	a	844	CLA	CHB-C4A-NA	2.26	127.64	124.51
25	1	304	A1L1F	C37-C36-C35	-2.26	118.85	123.47
21	8	302	XAT	C8-C9-C10	2.26	122.41	118.94
23	b	821	CLA	C1-C2-C3	-2.26	122.14	126.04
21	5	302	XAT	O24-C25-C38	2.26	117.76	115.06
23	a	824	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	8	308	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
21	2	303	XAT	O4-C5-C4	2.26	115.08	113.38
23	a	805	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	7	315	CLA	C1B-CHB-C4A	-2.26	125.65	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	302	XAT	O4-C5-C4	2.26	115.08	113.38
30	b	848	BCR	C35-C13-C12	2.26	121.63	118.08
25	1	304	A1L1F	O7-C54-O55	-2.25	118.48	122.96
23	8	309	CLA	C1-C2-C3	-2.25	122.14	126.04
21	8	301	XAT	O4-C5-C4	2.25	115.08	113.38
23	a	822	CLA	CHD-C1D-ND	-2.25	122.38	124.45
30	b	847	BCR	C21-C20-C19	-2.25	116.19	123.22
30	b	847	BCR	C38-C26-C27	2.25	117.94	113.62
21	7	301	XAT	C26-C27-C28	-2.25	121.23	125.99
23	5	306	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	a	838	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	8	308	CLA	C1-C2-C3	-2.25	122.15	126.04
30	m	102	BCR	C24-C23-C22	-2.25	122.83	126.23
23	a	817	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
21	3	301	XAT	C15-C35-C34	-2.25	118.86	123.47
25	6	301	A1L1F	C23-C22-C21	-2.25	106.43	110.77
30	f	801	BCR	C28-C27-C26	-2.25	110.06	114.08
21	6	303	XAT	C20-C13-C14	-2.25	119.77	122.92
23	b	821	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
30	b	850	BCR	C37-C22-C23	2.25	121.62	118.08
25	6	301	A1L1F	C32-C31-C30	-2.25	124.06	127.26
25	9	302	A1L1F	C26-O13-C45	2.24	120.67	115.68
30	a	849	BCR	C38-C26-C27	2.24	117.93	113.62
22	1	301	A1L1G	C14-C29-C30	-2.24	121.52	125.47
23	a	813	CLA	CHD-C1D-ND	-2.24	122.39	124.45
23	a	827	CLA	CAA-C2A-C1A	-2.24	104.63	111.97
30	f	801	BCR	C34-C9-C8	2.24	121.61	118.08
23	6	308	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	8	305	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
30	b	846	BCR	C11-C10-C9	-2.24	124.11	127.31
23	4	308	CLA	CHD-C1D-ND	-2.24	122.40	124.45
21	3	304	XAT	C40-C33-C34	-2.24	119.79	122.92
23	b	808	CLA	O2D-CGD-CBD	2.24	115.25	111.27
23	7	316	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
24	1	315	SQD	O9-S-C6	2.24	109.60	106.94
21	7	301	XAT	C24-C23-C22	-2.24	106.45	110.77
23	a	806	CLA	CHD-C1D-ND	-2.24	122.40	124.45
30	a	848	BCR	C21-C20-C19	-2.23	116.25	123.22
21	2	303	XAT	C40-C33-C34	-2.23	119.80	122.92
22	1	301	A1L1G	C17-C20-C21	2.23	116.79	114.28
23	2	316	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	9	301	A1L1G	C14-C29-C30	-2.23	121.54	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	305	XAT	C19-C9-C8	2.23	121.59	118.08
30	b	847	BCR	C34-C9-C8	2.23	121.59	118.08
23	4	307	CLA	CHD-C1D-ND	-2.23	122.41	124.45
21	8	301	XAT	C30-C31-C32	-2.23	116.27	123.22
23	b	805	CLA	CHD-C1D-ND	-2.23	122.41	124.45
23	a	829	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	2	310	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	4	304	XAT	C15-C35-C34	-2.22	118.92	123.47
23	1	311	CLA	CHD-C1D-ND	-2.22	122.41	124.45
23	6	314	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
30	b	845	BCR	C33-C5-C4	2.22	117.89	113.62
21	6	306	XAT	C35-C15-C14	-2.22	118.92	123.47
22	9	301	A1L1G	C29-C30-C31	2.22	122.30	118.93
21	8	302	XAT	O24-C25-C38	2.22	117.72	115.06
23	7	317	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	b	841	CLA	CHD-C1D-ND	-2.22	122.41	124.45
23	7	312	CLA	CHD-C1D-ND	-2.22	122.41	124.45
23	b	803	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	9	302	A1L1F	C20-C21-C22	-2.22	108.36	112.75
23	7	307	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
30	a	849	BCR	C21-C20-C19	-2.22	116.30	123.22
23	5	308	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
23	4	315	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	b	836	CLA	CAC-C3C-C4C	2.22	127.69	124.81
24	5	317	SQD	C45-O47-C7	-2.22	112.33	117.79
21	5	303	XAT	C11-C12-C13	-2.22	120.19	126.42
23	a	820	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
21	2	305	XAT	C15-C35-C34	-2.21	118.94	123.47
23	a	841	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	b	829	CLA	CHB-C4A-NA	2.21	127.57	124.51
30	b	847	BCR	C23-C24-C25	-2.21	120.99	127.20
23	2	311	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
30	a	850	BCR	C20-C19-C18	-2.21	120.21	126.42
30	b	852	BCR	C38-C26-C27	2.21	117.86	113.62
23	a	818	CLA	O2D-CGD-CBD	2.21	115.19	111.27
30	b	853	BCR	C29-C30-C25	2.21	113.88	110.48
25	9	302	A1L1F	C23-C22-C21	-2.21	106.51	110.77
30	b	853	BCR	C39-C30-C25	-2.20	106.72	110.30
21	5	301	XAT	O4-C5-C4	2.20	115.04	113.38
23	2	309	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
21	8	302	XAT	C20-C13-C14	-2.20	119.84	122.92
23	a	819	CLA	O2A-CGA-O1A	-2.20	118.03	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	9	302	A1L1F	C31-C32-C33	-2.20	116.35	123.22
23	3	311	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
23	a	836	CLA	CHD-C1D-ND	-2.20	122.43	124.45
21	1	303	XAT	O4-C5-C4	2.20	115.03	113.38
24	5	317	SQD	O9-S-C6	2.20	109.55	106.94
21	2	303	XAT	C39-C29-C30	-2.20	119.85	122.92
21	9	303	XAT	O4-C5-C4	2.20	115.03	113.38
23	2	308	CLA	CHB-C4A-NA	2.20	127.55	124.51
21	3	301	XAT	C8-C9-C10	-2.20	115.57	118.94
21	1	303	XAT	C19-C9-C8	2.20	121.54	118.08
30	f	801	BCR	C15-C14-C13	-2.20	124.18	127.31
23	l	201	CLA	CHD-C1D-ND	-2.20	122.44	124.45
23	5	312	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
21	7	301	XAT	C39-C29-C30	-2.19	119.85	122.92
21	3	305	XAT	C19-C9-C8	2.19	121.53	118.08
30	f	801	BCR	C35-C13-C12	2.19	121.53	118.08
21	6	302	XAT	C20-C13-C14	-2.19	119.85	122.92
21	a	853	XAT	O24-C25-C38	2.19	117.68	115.06
21	5	302	XAT	C30-C31-C32	-2.19	116.38	123.22
23	a	825	CLA	CHD-C1D-ND	-2.19	122.44	124.45
23	a	852	CLA	CHD-C1D-ND	-2.19	122.44	124.45
23	b	821	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
21	3	303	XAT	O24-C25-C38	2.19	117.68	115.06
23	b	828	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	b	813	CLA	C1-C2-C3	-2.19	122.26	126.04
23	b	837	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
22	7	302	A1L1G	C20-C21-C22	-2.19	108.42	112.75
23	1	312	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
23	a	806	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
21	3	303	XAT	C15-C35-C34	-2.18	119.00	123.47
23	b	833	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	b	850	BCR	C35-C13-C12	2.18	121.52	118.08
21	6	303	XAT	O4-C5-C4	2.18	115.02	113.38
25	6	304	A1L1F	C36-C37-C38	-2.18	119.01	123.47
30	a	848	BCR	C23-C24-C25	-2.18	121.08	127.20
23	a	839	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	a	834	CLA	C1-C2-C3	-2.18	122.28	126.04
23	8	309	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	b	844	BCR	C36-C18-C19	2.18	121.51	118.08
21	2	303	XAT	C31-C32-C33	-2.18	120.30	126.42
23	a	830	CLA	CHB-C4A-NA	2.18	127.52	124.51
21	4	304	XAT	O4-C5-C4	2.18	115.02	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	804	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
21	4	302	XAT	O24-C25-C38	2.18	117.66	115.06
23	b	804	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
21	7	305	XAT	C30-C31-C32	-2.17	116.43	123.22
23	3	313	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	8	301	XAT	O24-C25-C38	2.17	117.66	115.06
23	a	833	CLA	C1-C2-C3	-2.17	122.28	126.04
30	b	845	BCR	C7-C6-C5	-2.17	116.20	121.46
21	7	305	XAT	C39-C29-C28	2.17	121.50	118.08
23	8	311	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	a	831	CLA	O2D-CGD-CBD	2.17	115.13	111.27
23	h	203	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	7	304	XAT	O24-C25-C38	2.17	117.66	115.06
23	8	312	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	b	803	CLA	O1D-CGD-CBD	2.17	128.92	124.48
23	5	310	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	3	306	A1L1G	C20-C21-C22	-2.17	108.46	112.75
23	7	312	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	a	808	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	f	803	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	a	854	XAT	C40-C33-C32	2.17	121.49	118.08
27	b	851	DGD	O3D-C3D-C4D	-2.16	105.34	110.35
30	i	101	BCR	C23-C22-C21	2.16	122.26	118.94
23	b	812	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	b	839	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	b	836	CLA	C1-C2-C3	-2.16	122.30	126.04
21	9	303	XAT	O24-C25-C38	2.16	117.65	115.06
23	a	801	CLA	CHB-C4A-NA	2.16	127.50	124.51
21	5	303	XAT	C20-C13-C14	-2.16	119.90	122.92
25	6	304	A1L1F	C20-C21-C22	-2.16	108.48	112.75
21	2	301	XAT	C39-C29-C30	-2.16	119.90	122.92
23	8	310	CLA	CHD-C1D-ND	-2.16	122.47	124.45
30	b	844	BCR	C11-C12-C13	-2.16	120.36	126.42
23	7	308	CLA	CHD-C1D-ND	-2.16	122.47	124.45
30	b	844	BCR	C37-C22-C23	2.16	121.47	118.08
21	8	303	XAT	O4-C5-C18	2.15	117.64	115.06
23	5	316	CLA	CHD-C1D-ND	-2.15	122.47	124.45
23	6	310	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
23	a	829	CLA	CHD-C1D-ND	-2.15	122.47	124.45
21	9	305	XAT	C5-C4-C3	2.15	117.01	112.75
21	6	306	XAT	O4-C5-C4	2.15	115.00	113.38
23	3	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	309	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	b	840	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
23	8	308	CLA	O2D-CGD-CBD	2.15	115.09	111.27
23	8	307	CLA	CHD-C1D-ND	-2.15	122.48	124.45
21	6	305	XAT	C10-C11-C12	-2.15	116.51	123.22
21	6	302	XAT	O24-C25-C38	2.15	117.63	115.06
23	3	313	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
21	7	305	XAT	O4-C5-C18	2.15	117.63	115.06
23	a	844	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	a	831	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
30	a	849	BCR	C10-C11-C12	-2.15	116.52	123.22
30	b	848	BCR	C37-C22-C23	2.15	121.46	118.08
23	b	828	CLA	CHD-C1D-ND	-2.15	122.48	124.45
30	b	846	BCR	C34-C9-C8	2.14	121.46	118.08
21	5	305	XAT	O24-C25-C38	2.14	117.62	115.06
23	8	305	CLA	CHD-C1D-ND	-2.14	122.48	124.45
21	9	304	XAT	C10-C11-C12	-2.14	116.53	123.22
30	a	849	BCR	C8-C7-C6	-2.14	121.19	127.20
21	2	303	XAT	O4-C5-C18	2.14	117.62	115.06
21	4	301	XAT	C20-C13-C12	2.14	121.45	118.08
21	2	305	XAT	O4-C5-C4	2.14	114.99	113.38
30	b	853	BCR	C3-C4-C5	-2.14	110.25	114.08
21	7	304	XAT	C25-C24-C23	-2.14	108.52	112.75
21	4	304	XAT	O24-C25-C38	2.14	117.62	115.06
29	a	843	PQN	C2M-C2-C3	-2.14	120.91	124.40
21	5	303	XAT	O24-C25-C26	-2.14	57.19	58.96
30	a	847	BCR	C38-C26-C27	2.14	117.72	113.62
21	3	303	XAT	C39-C29-C28	2.14	121.44	118.08
30	b	847	BCR	C29-C30-C25	2.14	113.77	110.48
21	2	304	XAT	O24-C25-C38	2.13	117.61	115.06
23	a	844	CLA	C1-C2-C3	-2.13	122.35	126.04
23	1	308	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
21	7	303	XAT	O24-C25-C38	2.13	117.61	115.06
21	a	853	XAT	O4-C5-C4	2.13	114.98	113.38
30	j	102	BCR	C3-C4-C5	-2.13	110.27	114.08
21	3	303	XAT	C35-C15-C14	-2.13	119.11	123.47
23	a	816	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	a	856	CLA	CHD-C1D-ND	-2.13	122.49	124.45
21	4	301	XAT	C39-C29-C28	2.13	121.44	118.08
23	a	812	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	1	301	A1L1G	C29-C30-C31	2.13	122.16	118.93
23	a	806	CLA	C6-C7-C8	-2.13	109.03	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	9	314	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	7	316	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	b	810	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	a	834	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	f	802	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
28	2	317	LMG	C8-O7-C10	-2.13	112.55	117.79
30	m	102	BCR	C15-C14-C13	-2.13	124.27	127.31
21	6	305	XAT	C40-C33-C34	-2.13	119.94	122.92
30	j	102	BCR	C16-C15-C14	-2.13	119.12	123.47
23	5	313	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
21	4	302	XAT	C7-C8-C9	-2.12	122.23	125.53
23	a	839	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	4	312	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	9	316	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	4	305	CLA	CHD-C1D-ND	-2.12	122.50	124.45
30	b	846	BCR	C23-C24-C25	-2.12	121.25	127.20
23	b	823	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
21	2	304	XAT	C10-C11-C12	-2.12	116.60	123.22
30	a	847	BCR	C8-C7-C6	-2.12	121.25	127.20
23	4	306	CLA	O2D-CGD-CBD	2.12	115.03	111.27
23	b	807	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	b	840	CLA	C1-C2-C3	-2.12	122.38	126.04
30	a	848	BCR	C34-C9-C8	2.12	121.41	118.08
21	3	303	XAT	O4-C5-C4	2.12	114.97	113.38
23	b	821	CLA	CHD-C1D-ND	-2.11	122.51	124.45
30	b	853	BCR	C37-C22-C23	2.11	121.41	118.08
21	6	306	XAT	O24-C25-C38	2.11	117.59	115.06
21	2	305	XAT	O4-C5-C18	2.11	117.59	115.06
21	a	854	XAT	O24-C25-C38	2.11	117.59	115.06
23	b	820	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
30	b	843	BCR	C33-C5-C6	-2.11	122.16	124.53
21	3	301	XAT	O4-C5-C18	2.11	117.59	115.06
30	f	804	BCR	C35-C13-C14	-2.11	119.97	122.92
23	a	807	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	3	315	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	b	829	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	4	310	CLA	O2D-CGD-CBD	2.11	115.01	111.27
23	b	829	CLA	C1-C2-C3	-2.11	122.40	126.04
23	3	311	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	a	809	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	a	838	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
21	7	305	XAT	O24-C25-C38	2.10	117.58	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	306	CLA	C1-C2-C3	-2.10	122.40	126.04
23	a	837	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	4	307	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	b	801	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	b	816	CLA	C1-C2-C3	-2.10	122.41	126.04
21	9	305	XAT	C31-C32-C33	-2.10	120.51	126.42
30	b	852	BCR	C32-C1-C6	-2.10	106.89	110.30
30	i	101	BCR	C10-C11-C12	-2.10	116.66	123.22
23	9	316	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
30	b	846	BCR	C15-C16-C17	-2.10	119.17	123.47
21	4	303	XAT	O4-C5-C18	2.10	117.57	115.06
23	a	824	CLA	CHD-C1D-ND	-2.10	122.53	124.45
23	b	822	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	b	839	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	4	307	CLA	O2D-CGD-CBD	2.10	115.00	111.27
30	b	843	BCR	C37-C22-C23	2.10	121.38	118.08
25	9	302	A1L1F	C17-C20-C21	2.10	116.64	114.28
23	b	823	CLA	C1-C2-C3	-2.10	122.42	126.04
23	a	811	CLA	CHD-C1D-ND	-2.10	122.53	124.45
23	b	819	CLA	CHD-C1D-ND	-2.10	122.53	124.45
21	8	303	XAT	O24-C25-C38	2.10	117.57	115.06
21	7	301	XAT	C10-C11-C12	-2.10	116.68	123.22
23	5	312	CLA	CHD-C1D-ND	-2.10	122.53	124.45
23	b	838	CLA	C1-C2-C3	-2.10	122.42	126.04
23	9	308	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	a	844	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	a	832	CLA	CHD-C1D-ND	-2.09	122.53	124.45
28	2	317	LMG	C4-C3-C2	-2.09	107.17	110.82
23	b	806	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
21	7	303	XAT	C15-C35-C34	-2.09	119.19	123.47
30	j	102	BCR	C29-C30-C25	2.09	113.70	110.48
21	5	305	XAT	O4-C5-C18	2.09	117.56	115.06
23	2	308	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
21	3	304	XAT	O4-C5-C18	2.09	117.56	115.06
21	3	303	XAT	C10-C11-C12	-2.09	116.70	123.22
23	3	309	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	h	202	A1L1F	C26-O13-C45	2.09	120.32	115.68
21	9	304	XAT	O24-C25-C38	2.09	117.56	115.06
21	7	304	XAT	C8-C9-C10	2.09	122.14	118.94
23	4	308	CLA	C1-C2-C3	-2.09	123.38	126.75
23	a	829	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
23	a	834	CLA	CHD-C1D-ND	-2.09	122.54	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	304	XAT	O4-C5-C4	2.09	114.95	113.38
30	a	849	BCR	C15-C16-C17	-2.09	119.20	123.47
23	8	309	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
21	3	303	XAT	O4-C5-C18	2.08	117.55	115.06
21	4	304	XAT	O4-C5-C18	2.08	117.55	115.06
23	9	312	CLA	CHD-C1D-ND	-2.08	122.54	124.45
30	b	848	BCR	C23-C24-C25	-2.08	121.35	127.20
23	b	819	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
30	b	845	BCR	C8-C9-C10	2.08	122.14	118.94
23	b	841	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
21	6	303	XAT	C27-C28-C29	-2.08	122.30	125.53
23	b	804	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	3	301	XAT	O24-C25-C38	2.08	117.55	115.06
21	3	305	XAT	O24-C25-C38	2.08	117.55	115.06
23	1	306	CLA	CAC-C3C-C4C	2.08	127.51	124.81
23	2	315	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	7	301	XAT	O4-C5-C18	2.08	117.55	115.06
23	a	852	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	b	812	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	5	309	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
30	b	852	BCR	C34-C9-C10	-2.08	120.01	122.92
21	4	301	XAT	O4-C5-C4	2.08	114.94	113.38
23	2	308	CLA	CHD-C1D-ND	-2.08	122.55	124.45
25	6	301	A1L1F	C5-C6-C1	-2.07	108.61	110.47
25	6	301	A1L1F	C12-C6-C1	-2.07	108.61	110.47
21	5	303	XAT	C30-C31-C32	-2.07	116.74	123.22
23	a	827	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
21	2	301	XAT	O24-C25-C38	2.07	117.54	115.06
23	4	309	CLA	CHD-C1D-ND	-2.07	122.55	124.45
21	5	305	XAT	C35-C15-C14	-2.07	119.23	123.47
21	7	305	XAT	C7-C8-C9	-2.07	122.31	125.53
21	2	304	XAT	C15-C35-C34	-2.07	119.23	123.47
21	2	303	XAT	O24-C25-C38	2.07	117.54	115.06
21	9	303	XAT	C11-C12-C13	-2.07	120.60	126.42
23	6	307	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	7	313	CLA	C1-C2-C3	-2.07	122.46	126.04
21	5	302	XAT	O4-C5-C18	2.07	117.54	115.06
23	a	804	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	a	856	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
21	4	302	XAT	C35-C15-C14	-2.07	119.24	123.47
23	5	306	CLA	CHD-C1D-ND	-2.07	122.55	124.45
21	9	304	XAT	C31-C30-C29	-2.07	124.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	303	XAT	O4-C5-C18	2.07	117.53	115.06
21	6	305	XAT	O24-C25-C38	2.07	117.53	115.06
30	b	845	BCR	C16-C15-C14	-2.07	119.24	123.47
23	b	801	CLA	CHD-C1D-ND	-2.07	122.56	124.45
27	8	315	DGD	O2G-C1B-O1B	-2.07	118.71	123.70
23	1	312	CLA	CHD-C1D-ND	-2.07	122.56	124.45
21	2	304	XAT	O4-C5-C18	2.06	117.53	115.06
23	b	830	CLA	CMA-C3A-C2A	-2.06	111.28	116.10
23	b	838	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
21	2	301	XAT	O4-C5-C4	2.06	114.93	113.38
21	5	301	XAT	C28-C29-C30	2.06	122.11	118.94
21	6	306	XAT	O4-C5-C18	2.06	117.53	115.06
21	1	302	XAT	O24-C25-C38	2.06	117.53	115.06
21	7	304	XAT	C20-C13-C14	-2.06	120.03	122.92
25	8	304	A1L1F	C20-C21-C22	-2.06	108.67	112.75
23	5	308	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	b	811	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	b	820	CLA	CHD-C1D-ND	-2.06	122.56	124.45
30	a	847	BCR	C28-C27-C26	-2.06	110.40	114.08
21	5	302	XAT	C39-C29-C28	2.06	121.33	118.08
27	b	851	DGD	O5E-C6E-C5E	-2.06	104.22	111.29
21	a	854	XAT	C20-C13-C14	-2.06	120.04	122.92
23	a	822	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
21	3	305	XAT	O4-C5-C18	2.06	117.52	115.06
23	a	836	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
21	3	304	XAT	O24-C25-C38	2.06	117.52	115.06
23	2	312	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	a	809	CLA	O2D-CGD-CBD	2.06	114.92	111.27
23	4	313	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	b	835	CLA	C1-C2-C3	-2.05	122.49	126.04
23	8	312	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	1	310	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	f	803	CLA	C1-C2-C3	-2.05	122.49	126.04
23	b	807	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
23	4	315	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	6	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	4	316	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
21	8	302	XAT	O4-C5-C18	2.05	117.52	115.06
21	9	304	XAT	C40-C33-C32	2.05	121.31	118.08
23	3	313	CLA	C1-C2-C3	-2.05	122.50	126.04
23	6	313	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
30	b	853	BCR	C33-C5-C4	2.05	117.56	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	h	203	CLA	O2D-CGD-CBD	2.05	114.91	111.27
23	a	818	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	6	304	A1L1F	C12-C6-C1	-2.05	108.64	110.47
21	4	303	XAT	C19-C9-C8	2.05	121.30	118.08
21	1	302	XAT	O4-C5-C18	2.05	117.51	115.06
23	8	313	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	2	314	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	b	813	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	f	802	CLA	C1-C2-C3	-2.05	122.50	126.04
23	a	825	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	a	840	CLA	C1-C2-C3	-2.05	122.50	126.04
21	2	302	XAT	C27-C28-C29	-2.05	122.36	125.53
23	1	311	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
21	4	301	XAT	O24-C25-C38	2.05	117.51	115.06
21	3	304	XAT	C35-C15-C14	-2.04	119.28	123.47
23	3	308	CLA	O2D-CGD-CBD	2.04	114.90	111.27
25	8	304	A1L1F	C27-C34-C33	2.04	121.30	118.08
23	b	833	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
23	b	824	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	b	829	CLA	O2D-CGD-CBD	2.04	114.90	111.27
21	1	303	XAT	O24-C25-C38	2.04	117.50	115.06
21	9	305	XAT	C11-C12-C13	-2.04	120.68	126.42
23	2	310	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
21	6	306	XAT	C10-C11-C12	-2.04	116.85	123.22
23	9	309	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	1	311	CLA	O2D-CGD-CBD	2.04	114.89	111.27
21	2	304	XAT	C30-C31-C32	-2.04	116.86	123.22
23	8	311	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	b	817	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	7	315	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	b	803	CLA	CAC-C3C-C4C	2.04	127.45	124.81
30	b	846	BCR	C28-C27-C26	-2.04	110.44	114.08
23	a	832	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	b	831	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	f	804	BCR	C21-C20-C19	-2.04	116.86	123.22
23	3	310	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	b	827	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	a	847	BCR	C20-C19-C18	-2.04	120.69	126.42
23	a	823	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	a	838	CLA	C1-C2-C3	-2.04	122.52	126.04
23	a	808	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
21	2	302	XAT	O24-C25-C38	2.03	117.49	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	h	203	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	8	306	CLA	CHD-C1D-ND	-2.03	122.58	124.45
21	5	301	XAT	O4-C5-C18	2.03	117.49	115.06
21	2	305	XAT	C10-C11-C12	-2.03	116.87	123.22
30	f	804	BCR	C34-C9-C10	-2.03	120.08	122.92
23	1	310	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	a	814	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	3	308	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
21	1	303	XAT	C11-C10-C9	-2.03	124.41	127.31
21	8	301	XAT	C39-C29-C28	2.03	121.28	118.08
23	1	307	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	5	317	SQD	O8-S-C6	2.03	108.97	105.74
23	5	315	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	l	203	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	1	303	XAT	O4-C5-C18	2.03	117.48	115.06
23	9	313	CLA	CHD-C1D-ND	-2.03	122.59	124.45
30	b	848	BCR	C33-C5-C4	2.03	117.51	113.62
21	9	303	XAT	C19-C9-C8	2.03	121.27	118.08
23	9	308	CLA	CHD-C1D-ND	-2.03	122.59	124.45
30	b	846	BCR	C35-C13-C12	2.02	121.27	118.08
21	6	302	XAT	C39-C29-C30	-2.02	120.09	122.92
23	9	308	CLA	C1-C2-C3	-2.02	122.54	126.04
30	f	804	BCR	C8-C7-C6	-2.02	121.52	127.20
23	1	306	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
21	2	304	XAT	C40-C33-C32	2.02	121.26	118.08
23	b	840	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
21	a	854	XAT	C39-C29-C28	2.02	121.26	118.08
23	a	811	CLA	C1-C2-C3	-2.02	122.55	126.04
23	2	307	CLA	C2A-C1A-CHA	2.02	127.39	123.86
21	7	301	XAT	C19-C9-C8	2.02	121.26	118.08
21	1	303	XAT	C20-C13-C12	2.02	121.26	118.08
30	f	804	BCR	C33-C5-C4	2.02	117.50	113.62
23	b	802	CLA	O2D-CGD-CBD	2.02	114.86	111.27
23	b	814	CLA	C1-C2-C3	-2.02	122.55	126.04
21	2	302	XAT	C19-C9-C8	2.02	121.26	118.08
21	2	301	XAT	C19-C9-C8	2.02	121.26	118.08
23	a	801	CLA	O1D-CGD-CBD	2.02	128.61	124.48
23	a	830	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	2	313	CLA	CHD-C1D-ND	-2.02	122.60	124.45
21	7	304	XAT	C31-C32-C33	-2.02	120.75	126.42
21	9	305	XAT	C7-C8-C9	-2.02	122.40	125.53
23	a	833	CLA	O2A-CGA-O1A	-2.02	118.50	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	312	CLA	C1-C2-C3	-2.02	122.56	126.04
30	a	848	BCR	C28-C27-C26	-2.02	110.48	114.08
23	b	809	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
21	3	305	XAT	C20-C13-C12	2.02	121.25	118.08
21	7	304	XAT	O4-C5-C18	2.02	117.47	115.06
23	b	816	CLA	O2D-CGD-CBD	2.01	114.85	111.27
23	b	809	CLA	CHD-C1D-ND	-2.01	122.60	124.45
23	a	809	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
21	8	301	XAT	O4-C5-C18	2.01	117.47	115.06
23	b	807	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	9	306	A1L1G	C20-C21-C22	2.01	116.73	112.75
25	1	304	A1L1F	C25-C14-C29	-2.01	121.74	125.99
23	b	810	CLA	C1-C2-C3	-2.01	122.56	126.04
21	7	305	XAT	C11-C12-C13	-2.01	120.77	126.42
23	b	830	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	a	811	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	a	821	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
23	8	307	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	4	306	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	1	308	CLA	CHD-C1D-ND	-2.01	122.61	124.45
30	b	845	BCR	C1-C6-C7	2.01	121.46	115.78
30	b	843	BCR	C16-C15-C14	-2.01	119.36	123.47
23	3	314	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	5	306	CLA	C2D-C1D-ND	-2.01	108.62	110.10
23	b	827	CLA	C1-C2-C3	-2.01	122.57	126.04
30	b	847	BCR	C2-C1-C6	2.01	113.57	110.48
23	b	824	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	b	814	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	b	803	CLA	O2D-CGD-CBD	2.01	114.83	111.27
23	2	307	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
23	a	815	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
21	3	301	XAT	O4-C5-C4	2.00	114.89	113.38
23	9	315	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	a	842	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	b	817	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	4	306	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
30	b	848	BCR	C8-C9-C10	-2.00	115.87	118.94
23	b	815	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	b	802	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
21	1	302	XAT	C30-C31-C32	-2.00	116.97	123.22
23	b	817	CLA	C1-C2-C3	-2.00	122.58	126.04
23	a	802	CLA	CHD-C1D-ND	-2.00	122.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	816	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (188) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	5	306	CLA	ND
23	5	307	CLA	ND
23	5	308	CLA	ND
23	5	309	CLA	ND
23	5	310	CLA	ND
23	5	311	CLA	ND
23	5	312	CLA	ND
23	5	313	CLA	ND
23	5	314	CLA	ND
23	5	315	CLA	ND
23	5	316	CLA	ND
23	9	308	CLA	ND
23	9	309	CLA	ND
23	9	310	CLA	ND
23	9	311	CLA	ND
23	9	312	CLA	ND
23	9	313	CLA	ND
23	9	314	CLA	ND
23	9	315	CLA	ND
23	9	316	CLA	ND
23	8	305	CLA	ND
23	8	306	CLA	ND
23	8	307	CLA	ND
23	8	308	CLA	ND
23	8	309	CLA	ND
23	8	310	CLA	ND
23	8	311	CLA	ND
23	8	312	CLA	ND
23	8	313	CLA	ND
23	8	314	CLA	ND
23	4	305	CLA	ND
23	4	306	CLA	ND
23	4	307	CLA	ND
23	4	308	CLA	ND
23	4	309	CLA	ND
23	4	310	CLA	ND
23	4	311	CLA	ND

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Mol	Chain	Res	Type	Atom
23	4	312	CLA	ND
23	4	313	CLA	ND
23	4	314	CLA	ND
23	4	315	CLA	ND
23	4	316	CLA	ND
23	3	307	CLA	ND
23	3	308	CLA	ND
23	3	309	CLA	ND
23	3	310	CLA	ND
23	3	311	CLA	ND
23	3	312	CLA	ND
23	3	313	CLA	ND
23	3	314	CLA	ND
23	3	315	CLA	ND
23	6	307	CLA	ND
23	6	308	CLA	ND
23	6	309	CLA	ND
23	6	310	CLA	ND
23	6	311	CLA	ND
23	6	312	CLA	ND
23	6	313	CLA	ND
23	6	314	CLA	ND
23	6	315	CLA	ND
23	6	316	CLA	ND
23	2	306	CLA	ND
23	2	307	CLA	ND
23	2	308	CLA	ND
23	2	309	CLA	ND
23	2	310	CLA	ND
23	2	311	CLA	ND
23	2	312	CLA	ND
23	2	313	CLA	ND
23	2	314	CLA	ND
23	2	315	CLA	ND
23	2	316	CLA	ND
23	7	306	CLA	ND
23	7	307	CLA	ND
23	7	308	CLA	ND
23	7	309	CLA	ND
23	7	310	CLA	ND
23	7	311	CLA	ND
23	7	312	CLA	ND

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Mol	Chain	Res	Type	Atom
23	7	313	CLA	ND
23	7	314	CLA	ND
23	7	315	CLA	ND
23	7	316	CLA	ND
23	7	317	CLA	ND
23	1	305	CLA	ND
23	1	306	CLA	ND
23	1	307	CLA	ND
23	1	308	CLA	ND
23	1	309	CLA	ND
23	1	310	CLA	ND
23	1	311	CLA	ND
23	1	312	CLA	ND
23	1	313	CLA	ND
23	1	314	CLA	ND
23	a	801	CLA	ND
23	a	802	CLA	ND
23	a	803	CLA	ND
23	a	804	CLA	ND
23	a	805	CLA	ND
23	a	806	CLA	ND
23	a	807	CLA	ND
23	a	808	CLA	ND
23	a	809	CLA	ND
23	a	810	CLA	ND
23	a	811	CLA	ND
23	a	812	CLA	ND
23	a	813	CLA	ND
23	a	814	CLA	ND
23	a	815	CLA	ND
23	a	816	CLA	ND
23	a	817	CLA	ND
23	a	818	CLA	ND
23	a	819	CLA	ND
23	a	820	CLA	ND
23	a	821	CLA	ND
23	a	822	CLA	ND
23	a	823	CLA	ND
23	a	824	CLA	ND
23	a	825	CLA	ND
23	a	826	CLA	ND
23	a	827	CLA	ND

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Mol	Chain	Res	Type	Atom
23	a	828	CLA	ND
23	a	829	CLA	ND
23	a	830	CLA	ND
23	a	831	CLA	ND
23	a	832	CLA	ND
23	a	833	CLA	ND
23	a	834	CLA	ND
23	a	835	CLA	ND
23	a	836	CLA	ND
23	a	837	CLA	ND
23	a	838	CLA	ND
23	a	839	CLA	ND
23	a	840	CLA	ND
23	a	841	CLA	ND
23	a	842	CLA	ND
23	a	844	CLA	ND
23	a	852	CLA	ND
23	a	856	CLA	ND
23	b	801	CLA	ND
23	b	802	CLA	ND
23	b	803	CLA	ND
23	b	804	CLA	ND
23	b	805	CLA	ND
23	b	806	CLA	ND
23	b	807	CLA	ND
23	b	808	CLA	ND
23	b	809	CLA	ND
23	b	810	CLA	ND
23	b	811	CLA	ND
23	b	812	CLA	ND
23	b	813	CLA	ND
23	b	814	CLA	ND
23	b	815	CLA	ND
23	b	816	CLA	ND
23	b	817	CLA	ND
23	b	818	CLA	ND
23	b	819	CLA	ND
23	b	820	CLA	ND
23	b	821	CLA	ND
23	b	822	CLA	ND
23	b	823	CLA	ND
23	b	824	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	825	CLA	ND
23	b	826	CLA	ND
23	b	827	CLA	ND
23	b	828	CLA	ND
23	b	829	CLA	ND
23	b	830	CLA	ND
23	b	831	CLA	ND
23	b	832	CLA	ND
23	b	833	CLA	ND
23	b	834	CLA	ND
23	b	835	CLA	ND
23	b	836	CLA	ND
23	b	837	CLA	ND
23	b	838	CLA	ND
23	b	839	CLA	ND
23	b	840	CLA	ND
23	b	841	CLA	ND
23	f	802	CLA	ND
23	f	803	CLA	ND
23	h	201	CLA	ND
23	h	203	CLA	ND
23	j	101	CLA	ND
23	l	201	CLA	ND
23	l	202	CLA	ND
23	l	203	CLA	ND

All (2078) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	5	301	XAT	C27-C28-C29-C30
21	5	301	XAT	C27-C28-C29-C39
21	5	303	XAT	O4-C6-C7-C8
21	5	303	XAT	C7-C8-C9-C10
21	5	303	XAT	C7-C8-C9-C19
21	9	303	XAT	O4-C6-C7-C8
21	9	304	XAT	O24-C26-C27-C28
21	9	305	XAT	O4-C6-C7-C8
21	9	305	XAT	C7-C8-C9-C10
21	9	305	XAT	C7-C8-C9-C19
21	8	301	XAT	C7-C8-C9-C19
21	8	302	XAT	O4-C6-C7-C8
21	8	302	XAT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	8	302	XAT	C7-C8-C9-C19
21	4	302	XAT	O4-C6-C7-C8
21	4	302	XAT	C7-C8-C9-C10
21	4	302	XAT	C7-C8-C9-C19
21	4	304	XAT	O24-C26-C27-C28
21	3	301	XAT	O4-C6-C7-C8
21	3	301	XAT	C27-C28-C29-C30
21	3	301	XAT	C27-C28-C29-C39
21	3	303	XAT	C27-C28-C29-C30
21	3	303	XAT	C27-C28-C29-C39
21	3	304	XAT	O24-C26-C27-C28
21	3	304	XAT	C27-C28-C29-C30
21	3	304	XAT	C27-C28-C29-C39
21	6	302	XAT	O24-C26-C27-C28
21	6	302	XAT	C27-C28-C29-C30
21	6	302	XAT	C27-C28-C29-C39
21	6	303	XAT	O4-C6-C7-C8
21	6	305	XAT	O24-C26-C27-C28
21	6	305	XAT	C27-C28-C29-C30
21	6	305	XAT	C27-C28-C29-C39
21	6	306	XAT	C27-C28-C29-C30
21	6	306	XAT	C27-C28-C29-C39
21	2	303	XAT	O4-C6-C7-C8
21	2	303	XAT	O24-C26-C27-C28
21	2	303	XAT	C27-C28-C29-C30
21	2	303	XAT	C27-C28-C29-C39
21	2	305	XAT	C25-C26-C27-C28
21	7	301	XAT	O4-C6-C7-C8
21	7	301	XAT	C27-C28-C29-C30
21	7	301	XAT	C27-C28-C29-C39
21	7	303	XAT	O4-C6-C7-C8
21	7	303	XAT	O24-C26-C27-C28
21	7	303	XAT	C27-C28-C29-C30
21	7	303	XAT	C27-C28-C29-C39
21	7	304	XAT	O4-C6-C7-C8
21	7	304	XAT	C11-C12-C13-C14
21	7	304	XAT	C11-C12-C13-C20
21	a	853	XAT	O4-C6-C7-C8
21	a	853	XAT	C7-C8-C9-C10
21	a	853	XAT	C7-C8-C9-C19
21	a	853	XAT	O24-C26-C27-C28
21	a	854	XAT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	a	854	XAT	C7-C8-C9-C19
21	a	854	XAT	C11-C12-C13-C14
21	a	854	XAT	C11-C12-C13-C20
21	a	854	XAT	C27-C28-C29-C30
21	a	854	XAT	C27-C28-C29-C39
22	5	304	A1L1G	C26-C30-C31-C32
22	5	304	A1L1G	C31-C32-C33-C34
22	5	304	A1L1G	C32-C33-C34-C27
22	5	304	A1L1G	C32-C33-C34-C35
22	5	304	A1L1G	C41-C42-C44-C2
22	5	304	A1L1G	C41-C42-C44-C43
22	9	301	A1L1G	O13-C26-C30-C29
22	9	301	A1L1G	C26-C30-C31-C32
22	9	301	A1L1G	C31-C32-C33-C34
22	9	301	A1L1G	C28-C39-C40-C41
22	9	301	A1L1G	C38-C39-C40-C41
22	9	301	A1L1G	C39-C40-C41-C42
22	9	306	A1L1G	C45-C2-C44-C42
22	9	306	A1L1G	C45-C2-C44-C43
22	9	306	A1L1G	C29-C14-C25-C24
22	9	306	A1L1G	C25-C14-C29-C30
22	9	306	A1L1G	C35-C36-C37-C38
22	9	306	A1L1G	C37-C38-C39-C28
22	9	306	A1L1G	C37-C38-C39-C40
22	3	302	A1L1G	C25-C14-C29-C30
22	3	302	A1L1G	C14-C29-C30-C26
22	3	302	A1L1G	C26-C30-C31-C32
22	3	302	A1L1G	C29-C30-C31-C32
22	3	302	A1L1G	C41-C42-C44-C2
22	3	302	A1L1G	C41-C42-C44-C43
22	3	306	A1L1G	C45-C2-C44-C42
22	3	306	A1L1G	C45-C2-C44-C43
22	3	306	A1L1G	O13-C26-C30-C29
22	3	306	A1L1G	C37-C38-C39-C28
22	3	306	A1L1G	C37-C38-C39-C40
22	3	306	A1L1G	C39-C40-C41-C42
22	3	306	A1L1G	C41-C42-C44-C2
22	3	306	A1L1G	C41-C42-C44-C43
22	7	302	A1L1G	C45-C2-C44-C42
22	7	302	A1L1G	C29-C14-C25-C24
22	7	302	A1L1G	C35-C36-C37-C38
22	7	302	A1L1G	C37-C38-C39-C28

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Mol	Chain	Res	Type	Atoms
22	7	302	A1L1G	C37-C38-C39-C40
22	7	302	A1L1G	C39-C40-C41-C42
22	7	302	A1L1G	C41-C42-C44-C2
22	7	302	A1L1G	C41-C42-C44-C43
22	1	301	A1L1G	C45-C2-C44-C42
22	1	301	A1L1G	C45-C2-C44-C43
22	1	301	A1L1G	O13-C26-C30-C29
22	1	301	A1L1G	C27-C34-C35-C36
22	1	301	A1L1G	C33-C34-C35-C36
22	1	301	A1L1G	C35-C36-C37-C38
22	1	301	A1L1G	C28-C39-C40-C41
22	1	301	A1L1G	C38-C39-C40-C41
22	1	301	A1L1G	C39-C40-C41-C42
23	5	308	CLA	CHA-CBD-CGD-O1D
23	5	308	CLA	CHA-CBD-CGD-O2D
23	5	309	CLA	CBD-CGD-O2D-CED
23	5	310	CLA	CHA-CBD-CGD-O1D
23	5	310	CLA	CHA-CBD-CGD-O2D
23	5	310	CLA	CAD-CBD-CGD-O1D
23	5	310	CLA	CAD-CBD-CGD-O2D
23	5	311	CLA	CBD-CGD-O2D-CED
23	5	315	CLA	C1A-C2A-CAA-CBA
23	5	315	CLA	C3A-C2A-CAA-CBA
23	5	316	CLA	CBD-CGD-O2D-CED
23	5	316	CLA	O1D-CGD-O2D-CED
23	9	308	CLA	CBD-CGD-O2D-CED
23	9	310	CLA	CHA-CBD-CGD-O1D
23	9	310	CLA	CHA-CBD-CGD-O2D
23	9	311	CLA	CHA-CBD-CGD-O1D
23	9	311	CLA	CHA-CBD-CGD-O2D
23	9	311	CLA	CBD-CGD-O2D-CED
23	9	311	CLA	O1D-CGD-O2D-CED
23	9	313	CLA	C2A-CAA-CBA-CGA
23	9	314	CLA	CHA-CBD-CGD-O1D
23	9	314	CLA	CHA-CBD-CGD-O2D
23	9	315	CLA	CHA-CBD-CGD-O1D
23	9	315	CLA	CHA-CBD-CGD-O2D
23	9	315	CLA	CBD-CGD-O2D-CED
23	8	307	CLA	CHA-CBD-CGD-O1D
23	8	307	CLA	CHA-CBD-CGD-O2D
23	8	311	CLA	C2-C3-C5-C6
23	8	311	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	4	305	CLA	C1A-C2A-CAA-CBA
23	4	306	CLA	CHA-CBD-CGD-O2D
23	4	308	CLA	CHA-CBD-CGD-O1D
23	4	308	CLA	CHA-CBD-CGD-O2D
23	4	308	CLA	CBD-CGD-O2D-CED
23	4	309	CLA	C1A-C2A-CAA-CBA
23	4	310	CLA	CBA-CGA-O2A-C1
23	4	310	CLA	CBD-CGD-O2D-CED
23	4	311	CLA	C1A-C2A-CAA-CBA
23	4	311	CLA	C3A-C2A-CAA-CBA
23	4	312	CLA	CHA-CBD-CGD-O1D
23	4	312	CLA	CHA-CBD-CGD-O2D
23	4	314	CLA	CHA-CBD-CGD-O1D
23	4	314	CLA	CHA-CBD-CGD-O2D
23	4	315	CLA	C2A-CAA-CBA-CGA
23	4	315	CLA	CBD-CGD-O2D-CED
23	4	316	CLA	CBD-CGD-O2D-CED
23	3	309	CLA	CHA-CBD-CGD-O1D
23	3	309	CLA	CHA-CBD-CGD-O2D
23	3	310	CLA	C2-C3-C5-C6
23	3	310	CLA	C4-C3-C5-C6
23	3	312	CLA	C1A-C2A-CAA-CBA
23	3	315	CLA	C1A-C2A-CAA-CBA
23	6	309	CLA	C6-C7-C8-C9
23	6	310	CLA	CHA-CBD-CGD-O1D
23	6	310	CLA	CHA-CBD-CGD-O2D
23	6	311	CLA	C1A-C2A-CAA-CBA
23	6	311	CLA	C3A-C2A-CAA-CBA
23	6	314	CLA	CBD-CGD-O2D-CED
23	6	315	CLA	CBD-CGD-O2D-CED
23	6	316	CLA	C1A-C2A-CAA-CBA
23	2	307	CLA	CBD-CGD-O2D-CED
23	2	308	CLA	CHA-CBD-CGD-O1D
23	2	308	CLA	CHA-CBD-CGD-O2D
23	2	309	CLA	CBD-CGD-O2D-CED
23	2	312	CLA	CBD-CGD-O2D-CED
23	2	313	CLA	CBD-CGD-O2D-CED
23	7	306	CLA	C3A-C2A-CAA-CBA
23	7	306	CLA	CBD-CGD-O2D-CED
23	7	307	CLA	CBD-CGD-O2D-CED
23	7	310	CLA	CBA-CGA-O2A-C1
23	7	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	7	313	CLA	CHA-CBD-CGD-O1D
23	7	313	CLA	CHA-CBD-CGD-O2D
23	7	314	CLA	CBD-CGD-O2D-CED
23	7	315	CLA	CHA-CBD-CGD-O1D
23	7	315	CLA	CBD-CGD-O2D-CED
23	7	316	CLA	C1A-C2A-CAA-CBA
23	7	316	CLA	C3A-C2A-CAA-CBA
23	1	305	CLA	CHA-CBD-CGD-O1D
23	1	305	CLA	CHA-CBD-CGD-O2D
23	1	305	CLA	C11-C10-C8-C9
23	1	307	CLA	O1A-CGA-O2A-C1
23	1	310	CLA	CBD-CGD-O2D-CED
23	1	311	CLA	CHA-CBD-CGD-O1D
23	1	311	CLA	CHA-CBD-CGD-O2D
23	1	313	CLA	CBD-CGD-O2D-CED
23	1	314	CLA	C1A-C2A-CAA-CBA
23	1	314	CLA	C3A-C2A-CAA-CBA
23	a	801	CLA	CHA-CBD-CGD-O1D
23	a	801	CLA	CHA-CBD-CGD-O2D
23	a	801	CLA	CBD-CGD-O2D-CED
23	a	805	CLA	C1A-C2A-CAA-CBA
23	a	805	CLA	C3A-C2A-CAA-CBA
23	a	806	CLA	CHA-CBD-CGD-O1D
23	a	806	CLA	CHA-CBD-CGD-O2D
23	a	806	CLA	O2A-C1-C2-C3
23	a	809	CLA	C1A-C2A-CAA-CBA
23	a	809	CLA	C3A-C2A-CAA-CBA
23	a	811	CLA	CHA-CBD-CGD-O1D
23	a	811	CLA	CHA-CBD-CGD-O2D
23	a	811	CLA	CBD-CGD-O2D-CED
23	a	817	CLA	C2A-CAA-CBA-CGA
23	a	818	CLA	C1A-C2A-CAA-CBA
23	a	818	CLA	C3A-C2A-CAA-CBA
23	a	818	CLA	CHA-CBD-CGD-O1D
23	a	818	CLA	CHA-CBD-CGD-O2D
23	a	819	CLA	C3A-C2A-CAA-CBA
23	a	820	CLA	C1A-C2A-CAA-CBA
23	a	820	CLA	C3A-C2A-CAA-CBA
23	a	823	CLA	C1A-C2A-CAA-CBA
23	a	823	CLA	C3A-C2A-CAA-CBA
23	a	825	CLA	CHA-CBD-CGD-O1D
23	a	825	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	a	829	CLA	C1A-C2A-CAA-CBA
23	a	829	CLA	CBD-CGD-O2D-CED
23	a	831	CLA	C2-C3-C5-C6
23	a	831	CLA	C4-C3-C5-C6
23	a	832	CLA	C1A-C2A-CAA-CBA
23	a	832	CLA	C3A-C2A-CAA-CBA
23	a	838	CLA	C1A-C2A-CAA-CBA
23	a	838	CLA	C2-C3-C5-C6
23	a	838	CLA	C4-C3-C5-C6
23	a	839	CLA	C2-C3-C5-C6
23	a	839	CLA	C4-C3-C5-C6
23	a	840	CLA	CHA-CBD-CGD-O1D
23	a	840	CLA	CHA-CBD-CGD-O2D
23	a	841	CLA	CHA-CBD-CGD-O1D
23	a	841	CLA	CHA-CBD-CGD-O2D
23	a	844	CLA	CHA-CBD-CGD-O1D
23	a	844	CLA	CHA-CBD-CGD-O2D
23	a	856	CLA	C1A-C2A-CAA-CBA
23	b	802	CLA	CHA-CBD-CGD-O1D
23	b	802	CLA	CHA-CBD-CGD-O2D
23	b	802	CLA	CBD-CGD-O2D-CED
23	b	803	CLA	CBD-CGD-O2D-CED
23	b	804	CLA	C2A-CAA-CBA-CGA
23	b	805	CLA	C1A-C2A-CAA-CBA
23	b	805	CLA	C3A-C2A-CAA-CBA
23	b	805	CLA	CHA-CBD-CGD-O1D
23	b	805	CLA	CHA-CBD-CGD-O2D
23	b	805	CLA	CAD-CBD-CGD-O1D
23	b	809	CLA	C1A-C2A-CAA-CBA
23	b	809	CLA	C2A-CAA-CBA-CGA
23	b	810	CLA	C1A-C2A-CAA-CBA
23	b	810	CLA	CHA-CBD-CGD-O1D
23	b	810	CLA	CHA-CBD-CGD-O2D
23	b	810	CLA	CAD-CBD-CGD-O1D
23	b	812	CLA	C1A-C2A-CAA-CBA
23	b	812	CLA	C2-C3-C5-C6
23	b	812	CLA	C4-C3-C5-C6
23	b	814	CLA	C1A-C2A-CAA-CBA
23	b	814	CLA	CBD-CGD-O2D-CED
23	b	817	CLA	C3A-C2A-CAA-CBA
23	b	818	CLA	C1A-C2A-CAA-CBA
23	b	818	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	b	820	CLA	C1A-C2A-CAA-CBA
23	b	820	CLA	C3A-C2A-CAA-CBA
23	b	820	CLA	CHA-CBD-CGD-O1D
23	b	820	CLA	CHA-CBD-CGD-O2D
23	b	823	CLA	CHA-CBD-CGD-O1D
23	b	823	CLA	CHA-CBD-CGD-O2D
23	b	826	CLA	CHA-CBD-CGD-O1D
23	b	826	CLA	CHA-CBD-CGD-O2D
23	b	828	CLA	C1A-C2A-CAA-CBA
23	b	828	CLA	C3A-C2A-CAA-CBA
23	b	832	CLA	C1A-C2A-CAA-CBA
23	b	832	CLA	C3A-C2A-CAA-CBA
23	b	833	CLA	C1A-C2A-CAA-CBA
23	b	833	CLA	C2-C3-C5-C6
23	b	833	CLA	C4-C3-C5-C6
23	b	834	CLA	C1A-C2A-CAA-CBA
23	b	834	CLA	C3A-C2A-CAA-CBA
23	b	834	CLA	C11-C12-C13-C14
23	b	835	CLA	CBD-CGD-O2D-CED
23	b	837	CLA	CHA-CBD-CGD-O1D
23	b	837	CLA	CHA-CBD-CGD-O2D
23	b	840	CLA	C1A-C2A-CAA-CBA
23	b	840	CLA	C3A-C2A-CAA-CBA
23	b	840	CLA	CHA-CBD-CGD-O1D
23	b	840	CLA	CHA-CBD-CGD-O2D
23	b	840	CLA	CAD-CBD-CGD-O1D
23	b	840	CLA	CBD-CGD-O2D-CED
23	h	201	CLA	C1A-C2A-CAA-CBA
23	j	101	CLA	CAD-CBD-CGD-O1D
23	j	101	CLA	CAD-CBD-CGD-O2D
23	j	101	CLA	CBD-CGD-O2D-CED
23	l	201	CLA	CHA-CBD-CGD-O1D
23	l	201	CLA	CHA-CBD-CGD-O2D
23	l	202	CLA	CHA-CBD-CGD-O1D
23	l	202	CLA	CHA-CBD-CGD-O2D
23	l	202	CLA	C6-C7-C8-C9
24	5	317	SQD	O49-C7-O47-C45
24	5	317	SQD	C8-C7-O47-C45
24	5	317	SQD	C5-C6-S-O7
24	5	317	SQD	C5-C6-S-O8
24	5	317	SQD	C5-C6-S-O9
24	1	315	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
24	1	315	SQD	C5-C6-S-O7
24	1	315	SQD	C5-C6-S-O8
24	1	315	SQD	C5-C6-S-O9
25	9	302	A1L1F	C4-C8-O7-C54
25	9	302	A1L1F	O13-C26-C30-C31
25	8	304	A1L1F	C32-C33-C34-C27
25	8	304	A1L1F	C32-C33-C34-C35
25	8	304	A1L1F	C56-C54-O7-C8
25	8	304	A1L1F	O55-C54-O7-C8
25	6	304	A1L1F	C14-C29-C30-C31
25	1	304	A1L1F	C32-C33-C34-C27
25	1	304	A1L1F	C32-C33-C34-C35
25	1	304	A1L1F	C28-C39-C40-C41
25	1	304	A1L1F	C38-C39-C40-C41
25	h	202	A1L1F	C56-C54-O7-C8
25	h	202	A1L1F	O55-C54-O7-C8
26	9	307	LHG	C3-O3-P-O4
26	9	307	LHG	C3-O3-P-O5
26	9	307	LHG	C3-O3-P-O6
26	9	307	LHG	O9-C7-O7-C5
26	9	307	LHG	C8-C7-O7-C5
26	a	845	LHG	O1-C1-C2-C3
26	a	845	LHG	C3-O3-P-O4
26	a	845	LHG	C4-O6-P-O3
26	a	845	LHG	C4-O6-P-O5
26	a	845	LHG	O6-C4-C5-O7
26	a	845	LHG	O7-C5-C6-O8
26	a	846	LHG	O1-C1-C2-C3
26	a	846	LHG	O6-C4-C5-O7
26	b	849	LHG	O1-C1-C2-C3
26	b	849	LHG	C1-C2-C3-O3
26	b	849	LHG	O2-C2-C3-O3
26	b	849	LHG	C3-O3-P-O5
26	b	849	LHG	C4-O6-P-O3
26	b	849	LHG	C4-O6-P-O4
26	b	849	LHG	C4-O6-P-O5
26	m	101	LHG	C1-C2-C3-O3
26	m	101	LHG	C3-O3-P-O4
26	m	101	LHG	O9-C7-O7-C5
26	m	101	LHG	C8-C7-O7-C5
27	8	315	DGD	C2B-C1B-O2G-C2G
27	8	315	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
27	8	315	DGD	O6E-C1E-O5D-C6D
27	4	317	DGD	C2B-C1B-O2G-C2G
27	4	317	DGD	O1B-C1B-O2G-C2G
27	4	317	DGD	C2E-C1E-O5D-C6D
27	4	317	DGD	O6E-C1E-O5D-C6D
28	2	317	LMG	O1-C7-C8-O7
28	a	855	LMG	C11-C10-O7-C8
28	j	103	LMG	O9-C10-O7-C8
28	j	103	LMG	C11-C10-O7-C8
30	a	850	BCR	C23-C24-C25-C26
30	b	843	BCR	C7-C8-C9-C10
30	b	843	BCR	C7-C8-C9-C34
30	b	845	BCR	C1-C6-C7-C8
30	b	845	BCR	C5-C6-C7-C8
30	i	101	BCR	C21-C22-C23-C24
30	i	101	BCR	C37-C22-C23-C24
30	j	102	BCR	C7-C8-C9-C10
30	j	102	BCR	C7-C8-C9-C34
30	m	102	BCR	C1-C6-C7-C8
30	m	102	BCR	C7-C8-C9-C34
30	m	102	BCR	C21-C22-C23-C24
30	m	102	BCR	C37-C22-C23-C24
25	9	302	A1L1F	C56-C54-O7-C8
25	9	302	A1L1F	O55-C54-O7-C8
25	6	304	A1L1F	C56-C54-O7-C8
23	5	311	CLA	O1D-CGD-O2D-CED
23	9	315	CLA	O1D-CGD-O2D-CED
23	4	308	CLA	O1D-CGD-O2D-CED
23	2	314	CLA	O1D-CGD-O2D-CED
23	7	314	CLA	O1D-CGD-O2D-CED
25	6	304	A1L1F	O55-C54-O7-C8
23	9	308	CLA	O1D-CGD-O2D-CED
23	6	315	CLA	O1D-CGD-O2D-CED
23	2	307	CLA	O1D-CGD-O2D-CED
23	2	309	CLA	O1D-CGD-O2D-CED
23	2	313	CLA	O1D-CGD-O2D-CED
23	7	307	CLA	O1D-CGD-O2D-CED
23	1	313	CLA	O1D-CGD-O2D-CED
23	a	812	CLA	O1D-CGD-O2D-CED
23	b	802	CLA	O1D-CGD-O2D-CED
23	b	835	CLA	O1D-CGD-O2D-CED
23	5	314	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	9	316	CLA	CBD-CGD-O2D-CED
23	8	306	CLA	CBD-CGD-O2D-CED
23	4	305	CLA	CBD-CGD-O2D-CED
23	6	313	CLA	CBD-CGD-O2D-CED
23	2	314	CLA	CBD-CGD-O2D-CED
23	1	309	CLA	CBD-CGD-O2D-CED
23	a	812	CLA	CBD-CGD-O2D-CED
23	8	308	CLA	O1A-CGA-O2A-C1
23	4	309	CLA	O1A-CGA-O2A-C1
23	a	806	CLA	O1A-CGA-O2A-C1
23	b	814	CLA	O1A-CGA-O2A-C1
25	6	304	A1L1F	O46-C45-O13-C26
26	m	101	LHG	O10-C23-O8-C6
28	2	317	LMG	O10-C28-O8-C9
23	7	310	CLA	O1A-CGA-O2A-C1
23	4	315	CLA	O1D-CGD-O2D-CED
23	7	315	CLA	O1D-CGD-O2D-CED
23	b	803	CLA	O1D-CGD-O2D-CED
23	5	309	CLA	O1D-CGD-O2D-CED
23	4	316	CLA	O1D-CGD-O2D-CED
23	2	312	CLA	O1D-CGD-O2D-CED
23	7	306	CLA	O1D-CGD-O2D-CED
23	a	801	CLA	O1D-CGD-O2D-CED
23	a	811	CLA	O1D-CGD-O2D-CED
23	a	829	CLA	O1D-CGD-O2D-CED
23	b	814	CLA	O1D-CGD-O2D-CED
23	b	840	CLA	O1D-CGD-O2D-CED
23	j	101	CLA	O1D-CGD-O2D-CED
23	8	308	CLA	CBA-CGA-O2A-C1
23	1	307	CLA	CBA-CGA-O2A-C1
23	a	806	CLA	CBA-CGA-O2A-C1
23	b	814	CLA	CBA-CGA-O2A-C1
25	6	304	A1L1F	C47-C45-O13-C26
26	m	101	LHG	C24-C23-O8-C6
23	5	306	CLA	CBD-CGD-O2D-CED
23	5	307	CLA	CBD-CGD-O2D-CED
23	5	310	CLA	CBD-CGD-O2D-CED
23	9	312	CLA	CBD-CGD-O2D-CED
23	9	314	CLA	CBD-CGD-O2D-CED
23	8	309	CLA	CBD-CGD-O2D-CED
23	3	308	CLA	CBD-CGD-O2D-CED
23	6	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	2	316	CLA	CBD-CGD-O2D-CED
23	7	308	CLA	CBD-CGD-O2D-CED
23	7	310	CLA	CBD-CGD-O2D-CED
23	a	804	CLA	CBD-CGD-O2D-CED
23	a	814	CLA	CBD-CGD-O2D-CED
23	b	805	CLA	CBD-CGD-O2D-CED
23	b	819	CLA	CBD-CGD-O2D-CED
23	b	836	CLA	CBD-CGD-O2D-CED
23	h	203	CLA	CBD-CGD-O2D-CED
23	2	310	CLA	O1A-CGA-O2A-C1
23	2	311	CLA	O1A-CGA-O2A-C1
23	7	312	CLA	O1A-CGA-O2A-C1
23	a	805	CLA	O1A-CGA-O2A-C1
23	a	818	CLA	O1A-CGA-O2A-C1
23	b	821	CLA	O1A-CGA-O2A-C1
23	f	802	CLA	O1A-CGA-O2A-C1
25	6	301	A1L1F	O46-C45-O13-C26
26	b	849	LHG	O10-C23-O8-C6
27	8	315	DGD	O1A-C1A-O1G-C1G
28	a	855	LMG	O10-C28-O8-C9
23	4	310	CLA	O1A-CGA-O2A-C1
23	7	311	CLA	O1A-CGA-O2A-C1
23	1	310	CLA	O1D-CGD-O2D-CED
25	6	301	A1L1F	C56-C54-O7-C8
23	4	310	CLA	O1D-CGD-O2D-CED
23	6	314	CLA	O1D-CGD-O2D-CED
23	4	306	CLA	CBD-CGD-O2D-CED
23	6	312	CLA	CBD-CGD-O2D-CED
23	a	818	CLA	CBD-CGD-O2D-CED
23	a	837	CLA	CBD-CGD-O2D-CED
27	8	315	DGD	O1B-C1B-O2G-C2G
28	a	855	LMG	O9-C10-O7-C8
23	6	316	CLA	CBA-CGA-O2A-C1
23	1	309	CLA	CBA-CGA-O2A-C1
25	1	304	A1L1F	C56-C54-O7-C8
23	1	309	CLA	O1A-CGA-O2A-C1
23	1	203	CLA	O1A-CGA-O2A-C1
23	3	312	CLA	C3-C5-C6-C7
23	2	310	CLA	C3-C5-C6-C7
23	2	311	CLA	C3-C5-C6-C7
23	2	314	CLA	C3-C5-C6-C7
23	7	308	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	a	810	CLA	C3-C5-C6-C7
23	a	852	CLA	C3-C5-C6-C7
23	b	804	CLA	C3-C5-C6-C7
23	b	806	CLA	C3-C5-C6-C7
23	b	808	CLA	C3-C5-C6-C7
23	2	310	CLA	CBA-CGA-O2A-C1
23	2	311	CLA	CBA-CGA-O2A-C1
23	7	312	CLA	CBA-CGA-O2A-C1
23	a	805	CLA	CBA-CGA-O2A-C1
23	a	818	CLA	CBA-CGA-O2A-C1
23	a	836	CLA	CBA-CGA-O2A-C1
23	b	821	CLA	CBA-CGA-O2A-C1
23	b	823	CLA	CBA-CGA-O2A-C1
23	f	802	CLA	CBA-CGA-O2A-C1
25	6	301	A1L1F	C47-C45-O13-C26
28	2	317	LMG	C29-C28-O8-C9
28	a	855	LMG	C29-C28-O8-C9
25	1	304	A1L1F	O55-C54-O7-C8
23	1	309	CLA	O1D-CGD-O2D-CED
23	3	309	CLA	CBD-CGD-O2D-CED
23	3	315	CLA	CBD-CGD-O2D-CED
23	b	810	CLA	CBD-CGD-O2D-CED
23	7	306	CLA	O1A-CGA-O2A-C1
23	6	316	CLA	O1A-CGA-O2A-C1
23	9	309	CLA	CBA-CGA-O2A-C1
23	l	203	CLA	CBA-CGA-O2A-C1
23	a	813	CLA	C4-C3-C5-C6
23	a	825	CLA	C4-C3-C5-C6
23	b	828	CLA	C4-C3-C5-C6
23	b	823	CLA	CBD-CGD-O2D-CED
23	b	827	CLA	CBD-CGD-O2D-CED
23	9	311	CLA	C2A-CAA-CBA-CGA
23	9	312	CLA	C2A-CAA-CBA-CGA
23	7	317	CLA	C2A-CAA-CBA-CGA
23	a	825	CLA	C2A-CAA-CBA-CGA
23	a	842	CLA	C2A-CAA-CBA-CGA
23	b	820	CLA	C2A-CAA-CBA-CGA
23	b	834	CLA	C2A-CAA-CBA-CGA
23	b	839	CLA	C2A-CAA-CBA-CGA
23	9	308	CLA	C3-C5-C6-C7
23	8	308	CLA	C3-C5-C6-C7
23	1	307	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	1	310	CLA	C3-C5-C6-C7
23	b	818	CLA	C3-C5-C6-C7
23	4	309	CLA	CBA-CGA-O2A-C1
23	1	305	CLA	CBA-CGA-O2A-C1
23	a	807	CLA	CBA-CGA-O2A-C1
23	a	811	CLA	CBA-CGA-O2A-C1
23	b	805	CLA	CBA-CGA-O2A-C1
23	b	810	CLA	CBA-CGA-O2A-C1
23	b	818	CLA	CBA-CGA-O2A-C1
26	9	307	LHG	C24-C23-O8-C6
26	b	849	LHG	C24-C23-O8-C6
27	8	315	DGD	C2A-C1A-O1G-C1G
28	j	103	LMG	C29-C28-O8-C9
28	j	103	LMG	C12-C13-C14-C15
23	6	313	CLA	O1D-CGD-O2D-CED
23	7	317	CLA	CBD-CGD-O2D-CED
23	a	841	CLA	CBD-CGD-O2D-CED
28	j	103	LMG	C4-C5-C6-O5
23	5	312	CLA	O1A-CGA-O2A-C1
23	1	305	CLA	O1A-CGA-O2A-C1
23	a	811	CLA	O1A-CGA-O2A-C1
23	a	812	CLA	O1A-CGA-O2A-C1
23	a	820	CLA	O1A-CGA-O2A-C1
23	b	805	CLA	O1A-CGA-O2A-C1
23	b	818	CLA	O1A-CGA-O2A-C1
28	j	103	LMG	O10-C28-O8-C9
22	9	301	A1L1G	C30-C31-C32-C33
22	9	301	A1L1G	C40-C41-C42-C44
22	3	302	A1L1G	C30-C31-C32-C33
22	7	302	A1L1G	C30-C31-C32-C33
25	8	304	A1L1F	C30-C31-C32-C33
25	6	301	A1L1F	C36-C37-C38-C39
23	4	307	CLA	CBD-CGD-O2D-CED
23	a	807	CLA	CBD-CGD-O2D-CED
23	a	810	CLA	CBD-CGD-O2D-CED
23	a	834	CLA	CBD-CGD-O2D-CED
23	a	835	CLA	CBD-CGD-O2D-CED
23	b	841	CLA	CBD-CGD-O2D-CED
23	9	316	CLA	O1D-CGD-O2D-CED
23	8	306	CLA	O1D-CGD-O2D-CED
26	9	307	LHG	O2-C2-C3-O3
26	a	845	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
26	m	101	LHG	O2-C2-C3-O3
23	7	306	CLA	CBA-CGA-O2A-C1
23	a	812	CLA	CBA-CGA-O2A-C1
23	b	840	CLA	CBA-CGA-O2A-C1
23	a	836	CLA	O1A-CGA-O2A-C1
23	b	823	CLA	O1A-CGA-O2A-C1
26	9	307	LHG	O10-C23-O8-C6
23	4	305	CLA	O1D-CGD-O2D-CED
23	9	312	CLA	CBA-CGA-O2A-C1
23	6	314	CLA	CBA-CGA-O2A-C1
23	5	312	CLA	CBD-CGD-O2D-CED
23	b	822	CLA	CBD-CGD-O2D-CED
23	b	840	CLA	O1A-CGA-O2A-C1
25	9	302	A1L1F	C47-C48-C49-C50
26	a	845	LHG	C12-C13-C14-C15
28	2	317	LMG	C29-C30-C31-C32
27	b	851	DGD	O6E-C5E-C6E-O5E
23	5	310	CLA	C3-C5-C6-C7
23	a	807	CLA	C3-C5-C6-C7
23	a	835	CLA	C3-C5-C6-C7
23	5	312	CLA	CBA-CGA-O2A-C1
23	6	309	CLA	CBA-CGA-O2A-C1
23	a	820	CLA	CBA-CGA-O2A-C1
26	a	845	LHG	C28-C29-C30-C31
23	a	807	CLA	O1A-CGA-O2A-C1
23	b	810	CLA	O1A-CGA-O2A-C1
23	8	313	CLA	CBA-CGA-O2A-C1
23	1	312	CLA	C3-C5-C6-C7
23	9	312	CLA	O1A-CGA-O2A-C1
23	a	825	CLA	C2-C3-C5-C6
23	5	311	CLA	C2A-CAA-CBA-CGA
23	4	310	CLA	C2A-CAA-CBA-CGA
23	b	801	CLA	C2A-CAA-CBA-CGA
23	b	826	CLA	C2A-CAA-CBA-CGA
23	5	314	CLA	O1D-CGD-O2D-CED
28	a	855	LMG	O6-C5-C6-O5
28	j	103	LMG	O6-C5-C6-O5
23	6	309	CLA	O1A-CGA-O2A-C1
23	9	309	CLA	O1A-CGA-O2A-C1
23	7	316	CLA	CBA-CGA-O2A-C1
26	a	845	LHG	C23-C24-C25-C26
23	a	804	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	b	805	CLA	O1D-CGD-O2D-CED
23	9	312	CLA	O1D-CGD-O2D-CED
23	9	314	CLA	O1D-CGD-O2D-CED
23	8	309	CLA	O1D-CGD-O2D-CED
23	7	310	CLA	O1D-CGD-O2D-CED
23	6	308	CLA	CBD-CGD-O2D-CED
26	9	307	LHG	C1-C2-C3-O3
26	a	845	LHG	C1-C2-C3-O3
23	b	836	CLA	O1D-CGD-O2D-CED
23	h	203	CLA	O1D-CGD-O2D-CED
23	5	309	CLA	CBA-CGA-O2A-C1
23	8	311	CLA	CBA-CGA-O2A-C1
23	3	311	CLA	CBA-CGA-O2A-C1
23	a	809	CLA	CBA-CGA-O2A-C1
23	a	839	CLA	CBA-CGA-O2A-C1
23	a	856	CLA	CBA-CGA-O2A-C1
23	b	820	CLA	CBA-CGA-O2A-C1
23	b	826	CLA	CBA-CGA-O2A-C1
23	b	834	CLA	CBA-CGA-O2A-C1
23	h	201	CLA	CBA-CGA-O2A-C1
23	4	314	CLA	CBD-CGD-O2D-CED
23	b	806	CLA	CBD-CGD-O2D-CED
23	h	201	CLA	CBD-CGD-O2D-CED
28	a	855	LMG	C4-C5-C6-O5
23	5	306	CLA	O1D-CGD-O2D-CED
22	5	304	A1L1G	C40-C41-C42-C44
25	8	304	A1L1F	C40-C41-C42-C44
23	a	807	CLA	C5-C6-C7-C8
23	a	810	CLA	C13-C15-C16-C17
23	9	316	CLA	C8-C10-C11-C12
23	8	307	CLA	C5-C6-C7-C8
23	b	808	CLA	C5-C6-C7-C8
26	a	846	LHG	O2-C2-C3-O3
28	a	855	LMG	C28-C29-C30-C31
23	8	311	CLA	O1A-CGA-O2A-C1
23	a	809	CLA	O1A-CGA-O2A-C1
23	a	856	CLA	O1A-CGA-O2A-C1
23	a	813	CLA	C2-C3-C5-C6
23	9	316	CLA	C11-C10-C8-C9
23	9	316	CLA	C11-C12-C13-C14
23	8	307	CLA	C11-C10-C8-C9
23	8	311	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	2	310	CLA	C11-C12-C13-C14
23	1	306	CLA	C6-C7-C8-C9
23	1	306	CLA	C11-C12-C13-C14
23	1	310	CLA	C14-C13-C15-C16
23	a	829	CLA	C11-C10-C8-C9
23	b	801	CLA	C11-C10-C8-C9
23	b	801	CLA	C14-C13-C15-C16
23	b	804	CLA	C11-C10-C8-C9
23	b	818	CLA	C11-C10-C8-C9
23	b	824	CLA	C6-C7-C8-C9
23	b	829	CLA	C14-C13-C15-C16
23	b	839	CLA	C6-C7-C8-C9
23	f	802	CLA	C11-C12-C13-C14
23	2	316	CLA	O1D-CGD-O2D-CED
23	b	806	CLA	C15-C16-C17-C18
23	2	310	CLA	C2A-CAA-CBA-CGA
23	7	310	CLA	C2A-CAA-CBA-CGA
23	h	203	CLA	C2A-CAA-CBA-CGA
21	6	303	XAT	C7-C8-C9-C19
21	6	303	XAT	C11-C12-C13-C20
21	2	301	XAT	C27-C28-C29-C39
21	2	304	XAT	C7-C8-C9-C19
22	3	306	A1L1G	C28-C39-C40-C41
22	7	302	A1L1G	C32-C33-C34-C27
25	8	304	A1L1F	C28-C39-C40-C41
30	b	852	BCR	C7-C8-C9-C34
30	i	102	BCR	C7-C8-C9-C34
30	i	102	BCR	C37-C22-C23-C24
21	6	303	XAT	C7-C8-C9-C10
21	2	301	XAT	C27-C28-C29-C30
22	3	306	A1L1G	C38-C39-C40-C41
30	b	852	BCR	C7-C8-C9-C10
30	i	102	BCR	C7-C8-C9-C10
30	i	102	BCR	C21-C22-C23-C24
23	a	814	CLA	O1D-CGD-O2D-CED
25	1	304	A1L1F	C49-C50-C51-C52
27	b	851	DGD	C1A-C2A-C3A-C4A
23	3	311	CLA	O1A-CGA-O2A-C1
23	b	820	CLA	O1A-CGA-O2A-C1
23	h	201	CLA	O1A-CGA-O2A-C1
23	a	809	CLA	C5-C6-C7-C8
23	b	801	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	6	301	A1L1F	O55-C54-O7-C8
23	9	313	CLA	CBA-CGA-O2A-C1
23	4	315	CLA	CBA-CGA-O2A-C1
23	2	312	CLA	CBA-CGA-O2A-C1
23	b	839	CLA	CBA-CGA-O2A-C1
23	2	310	CLA	C15-C16-C17-C18
23	a	834	CLA	C15-C16-C17-C18
23	b	832	CLA	C13-C15-C16-C17
23	b	834	CLA	C13-C15-C16-C17
23	5	310	CLA	O1D-CGD-O2D-CED
23	5	309	CLA	O1A-CGA-O2A-C1
23	b	826	CLA	O1A-CGA-O2A-C1
23	8	310	CLA	CBD-CGD-O2D-CED
22	3	302	A1L1G	C35-C36-C37-C38
23	5	310	CLA	C13-C15-C16-C17
23	9	308	CLA	C5-C6-C7-C8
23	9	316	CLA	C10-C11-C12-C13
23	4	307	CLA	C10-C11-C12-C13
23	1	306	CLA	C8-C10-C11-C12
23	a	802	CLA	C5-C6-C7-C8
23	a	809	CLA	C8-C10-C11-C12
23	a	814	CLA	C13-C15-C16-C17
23	a	830	CLA	C13-C15-C16-C17
23	a	831	CLA	C5-C6-C7-C8
23	b	808	CLA	C8-C10-C11-C12
23	b	841	CLA	C13-C15-C16-C17
23	l	202	CLA	C10-C11-C12-C13
26	a	846	LHG	C7-C8-C9-C10
26	b	849	LHG	C7-C8-C9-C10
28	a	855	LMG	C10-C11-C12-C13
23	f	802	CLA	CBD-CGD-O2D-CED
23	1	306	CLA	C5-C6-C7-C8
23	b	813	CLA	C15-C16-C17-C18
23	b	829	CLA	C8-C10-C11-C12
23	b	823	CLA	C3-C5-C6-C7
23	3	308	CLA	O1D-CGD-O2D-CED
23	6	310	CLA	O1D-CGD-O2D-CED
23	b	819	CLA	O1D-CGD-O2D-CED
23	a	807	CLA	C15-C16-C17-C18
23	a	841	CLA	C5-C6-C7-C8
23	b	814	CLA	C5-C6-C7-C8
23	b	837	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	1	304	A1L1F	C45-C47-C48-C49
23	a	852	CLA	CBD-CGD-O2D-CED
23	7	306	CLA	O2A-C1-C2-C3
23	7	309	CLA	O2A-C1-C2-C3
23	6	312	CLA	O1D-CGD-O2D-CED
23	a	837	CLA	O1D-CGD-O2D-CED
23	1	310	CLA	C11-C10-C8-C7
23	a	801	CLA	C12-C13-C15-C16
23	a	809	CLA	C12-C13-C15-C16
23	a	828	CLA	C12-C13-C15-C16
23	a	831	CLA	C11-C10-C8-C7
23	a	844	CLA	C12-C13-C15-C16
23	b	807	CLA	C12-C13-C15-C16
23	a	801	CLA	C3-C5-C6-C7
23	a	839	CLA	O1A-CGA-O2A-C1
23	b	834	CLA	O1A-CGA-O2A-C1
25	6	301	A1L1F	C34-C35-C36-C37
23	b	827	CLA	CBA-CGA-O2A-C1
23	a	830	CLA	C2A-CAA-CBA-CGA
23	5	307	CLA	O1D-CGD-O2D-CED
23	7	308	CLA	O1D-CGD-O2D-CED
23	9	308	CLA	C8-C10-C11-C12
23	1	306	CLA	C15-C16-C17-C18
23	5	306	CLA	CBA-CGA-O2A-C1
23	a	826	CLA	CBD-CGD-O2D-CED
23	a	841	CLA	C15-C16-C17-C18
23	a	818	CLA	O1D-CGD-O2D-CED
22	5	304	A1L1G	C39-C40-C41-C42
22	9	306	A1L1G	C39-C40-C41-C42
22	3	302	A1L1G	C39-C40-C41-C42
22	7	302	A1L1G	C31-C32-C33-C34
23	6	309	CLA	C10-C11-C12-C13
23	a	801	CLA	C8-C10-C11-C12
23	a	828	CLA	C13-C15-C16-C17
23	a	828	CLA	C15-C16-C17-C18
23	a	831	CLA	C15-C16-C17-C18
23	b	841	CLA	C10-C11-C12-C13
23	f	802	CLA	C13-C15-C16-C17
23	h	203	CLA	C5-C6-C7-C8
23	4	306	CLA	O1D-CGD-O2D-CED
23	2	312	CLA	O1A-CGA-O2A-C1
23	7	316	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	7	308	CLA	C10-C11-C12-C13
23	b	837	CLA	C8-C10-C11-C12
29	b	842	PQN	C23-C25-C26-C27
23	3	315	CLA	O1D-CGD-O2D-CED
23	a	852	CLA	C8-C10-C11-C12
23	b	801	CLA	C13-C15-C16-C17
23	b	827	CLA	C13-C15-C16-C17
23	f	802	CLA	C5-C6-C7-C8
23	l	202	CLA	C8-C10-C11-C12
26	a	845	LHG	C3-O3-P-O6
26	b	849	LHG	C3-O3-P-O6
23	7	313	CLA	C3-C5-C6-C7
23	4	316	CLA	CBA-CGA-O2A-C1
23	a	816	CLA	CBA-CGA-O2A-C1
23	a	852	CLA	CBA-CGA-O2A-C1
23	b	831	CLA	CBA-CGA-O2A-C1
23	a	839	CLA	C13-C15-C16-C17
23	b	801	CLA	C8-C10-C11-C12
23	b	810	CLA	O1D-CGD-O2D-CED
23	7	308	CLA	C4-C3-C5-C6
23	1	308	CLA	C4-C3-C5-C6
27	b	851	DGD	C4E-C5E-C6E-O5E
23	8	313	CLA	O1A-CGA-O2A-C1
23	6	314	CLA	O1A-CGA-O2A-C1
23	7	316	CLA	C2C-C3C-CAC-CBC
23	5	307	CLA	C2A-CAA-CBA-CGA
23	1	314	CLA	C2A-CAA-CBA-CGA
23	b	828	CLA	C2A-CAA-CBA-CGA
23	a	801	CLA	C16-C17-C18-C20
23	b	810	CLA	C16-C17-C18-C20
23	4	312	CLA	C3-C5-C6-C7
23	a	814	CLA	CBA-CGA-O2A-C1
23	a	838	CLA	CBA-CGA-O2A-C1
22	9	306	A1L1G	C40-C41-C42-C44
26	a	845	LHG	C11-C10-C9-C8
27	4	317	DGD	C3B-C4B-C5B-C6B
27	b	851	DGD	C9B-CAB-CBB-CCB
23	3	309	CLA	O1D-CGD-O2D-CED
23	a	841	CLA	O1D-CGD-O2D-CED
23	a	836	CLA	CBD-CGD-O2D-CED
24	1	315	SQD	C8-C7-O47-C45
23	9	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	a	824	CLA	CBA-CGA-O2A-C1
23	b	824	CLA	C5-C6-C7-C8
23	b	829	CLA	C10-C11-C12-C13
23	b	840	CLA	C5-C6-C7-C8
22	9	301	A1L1G	C41-C42-C44-C43
22	9	306	A1L1G	C41-C42-C44-C43
22	3	302	A1L1G	C37-C38-C39-C28
22	3	306	A1L1G	C27-C34-C35-C36
26	9	307	LHG	C34-C35-C36-C37
23	b	823	CLA	O1D-CGD-O2D-CED
23	b	834	CLA	C16-C17-C18-C19
23	b	841	CLA	C16-C17-C18-C20
23	a	833	CLA	CBA-CGA-O2A-C1
23	a	844	CLA	CBA-CGA-O2A-C1
26	9	307	LHG	C31-C32-C33-C34
26	a	845	LHG	C27-C28-C29-C30
24	1	315	SQD	O49-C7-O47-C45
23	a	856	CLA	C5-C6-C7-C8
26	9	307	LHG	C28-C29-C30-C31
26	a	845	LHG	C13-C14-C15-C16
23	b	827	CLA	O1D-CGD-O2D-CED
23	b	839	CLA	O1A-CGA-O2A-C1
26	9	307	LHG	C27-C28-C29-C30
23	a	834	CLA	O1D-CGD-O2D-CED
23	a	835	CLA	O1D-CGD-O2D-CED
22	5	304	A1L1G	C29-C30-C31-C32
22	9	301	A1L1G	C29-C30-C31-C32
22	9	306	A1L1G	C29-C30-C31-C32
26	m	101	LHG	C9-C10-C11-C12
25	9	302	A1L1F	C45-C47-C48-C49
23	7	317	CLA	O1D-CGD-O2D-CED
22	9	301	A1L1G	C41-C42-C44-C2
22	9	306	A1L1G	C41-C42-C44-C2
22	3	302	A1L1G	C37-C38-C39-C40
22	3	306	A1L1G	C33-C34-C35-C36
24	1	315	SQD	C24-C23-O48-C46
23	4	316	CLA	O1A-CGA-O2A-C1
23	a	816	CLA	O1A-CGA-O2A-C1
23	a	852	CLA	O1A-CGA-O2A-C1
23	4	309	CLA	C4-C3-C5-C6
23	b	840	CLA	C4-C3-C5-C6
23	1	308	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	806	CLA	C2-C3-C5-C6
23	b	828	CLA	C2-C3-C5-C6
22	9	306	A1L1G	C14-C29-C30-C31
22	3	302	A1L1G	C14-C29-C30-C31
23	a	828	CLA	C14-C13-C15-C16
23	a	839	CLA	C6-C7-C8-C9
23	a	840	CLA	C14-C13-C15-C16
23	b	825	CLA	C11-C10-C8-C9
28	2	317	LMG	C28-C29-C30-C31
23	5	316	CLA	C2C-C3C-CAC-CBC
26	m	101	LHG	C11-C12-C13-C14
27	4	317	DGD	C2B-C3B-C4B-C5B
27	b	851	DGD	C4A-C5A-C6A-C7A
23	a	814	CLA	C10-C11-C12-C13
23	a	814	CLA	C2A-CAA-CBA-CGA
23	b	831	CLA	C2A-CAA-CBA-CGA
23	b	841	CLA	O1D-CGD-O2D-CED
23	b	827	CLA	O1A-CGA-O2A-C1
21	9	303	XAT	C7-C8-C9-C19
21	2	303	XAT	C7-C8-C9-C19
22	9	301	A1L1G	C32-C33-C34-C27
22	3	302	A1L1G	C32-C33-C34-C27
30	a	850	BCR	C37-C22-C23-C24
30	f	801	BCR	C37-C22-C23-C24
27	b	851	DGD	C3B-C4B-C5B-C6B
21	9	303	XAT	C7-C8-C9-C10
21	8	301	XAT	C7-C8-C9-C10
21	2	303	XAT	C7-C8-C9-C10
21	7	304	XAT	C7-C8-C9-C10
22	9	301	A1L1G	C32-C33-C34-C35
22	3	302	A1L1G	C32-C33-C34-C35
25	8	304	A1L1F	C38-C39-C40-C41
30	a	850	BCR	C21-C22-C23-C24
30	f	801	BCR	C21-C22-C23-C24
23	b	827	CLA	C8-C10-C11-C12
29	a	843	PQN	C25-C26-C27-C28
26	m	101	LHG	C28-C29-C30-C31
25	8	304	A1L1F	C45-C47-C48-C49
23	a	814	CLA	O1A-CGA-O2A-C1
23	4	307	CLA	C16-C17-C18-C20
23	b	810	CLA	C16-C17-C18-C19
23	b	811	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	f	802	CLA	C16-C17-C18-C19
23	f	802	CLA	C16-C17-C18-C20
23	a	827	CLA	C8-C10-C11-C12
23	a	841	CLA	C8-C10-C11-C12
23	b	805	CLA	C15-C16-C17-C18
23	b	808	CLA	C10-C11-C12-C13
23	b	836	CLA	C5-C6-C7-C8
23	h	201	CLA	C10-C11-C12-C13
23	6	316	CLA	CBD-CGD-O2D-CED
24	1	315	SQD	C11-C10-C9-C8
26	m	101	LHG	C14-C15-C16-C17
23	a	814	CLA	C5-C6-C7-C8
25	9	302	A1L1F	C48-C49-C50-C51
25	1	304	A1L1F	C47-C48-C49-C50
25	h	202	A1L1F	C47-C48-C49-C50
23	4	307	CLA	O1D-CGD-O2D-CED
23	a	807	CLA	O1D-CGD-O2D-CED
23	a	810	CLA	O1D-CGD-O2D-CED
23	9	310	CLA	C3A-C2A-CAA-CBA
23	9	313	CLA	C3A-C2A-CAA-CBA
23	4	309	CLA	C3A-C2A-CAA-CBA
23	3	312	CLA	C3A-C2A-CAA-CBA
23	3	314	CLA	C3A-C2A-CAA-CBA
23	2	306	CLA	C3A-C2A-CAA-CBA
23	7	311	CLA	C3A-C2A-CAA-CBA
23	a	807	CLA	C3A-C2A-CAA-CBA
23	a	838	CLA	C3A-C2A-CAA-CBA
23	a	856	CLA	C3A-C2A-CAA-CBA
23	b	809	CLA	C3A-C2A-CAA-CBA
23	b	812	CLA	C3A-C2A-CAA-CBA
23	b	814	CLA	C3A-C2A-CAA-CBA
23	f	803	CLA	C3A-C2A-CAA-CBA
23	h	201	CLA	C3A-C2A-CAA-CBA
23	b	831	CLA	O1A-CGA-O2A-C1
23	b	801	CLA	C16-C17-C18-C20
23	b	811	CLA	C6-C7-C8-C10
27	b	851	DGD	C2B-C3B-C4B-C5B
27	b	851	DGD	C4B-C5B-C6B-C7B
23	3	314	CLA	CBD-CGD-O2D-CED
22	9	301	A1L1G	C35-C36-C37-C38
22	3	306	A1L1G	C35-C36-C37-C38
30	m	102	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	b	816	CLA	CBA-CGA-O2A-C1
23	4	309	CLA	C2-C3-C5-C6
23	a	828	CLA	C2-C3-C5-C6
23	b	840	CLA	C2-C3-C5-C6
23	b	833	CLA	CBD-CGD-O2D-CED
26	a	845	LHG	O1-C1-C2-O2
26	a	846	LHG	O1-C1-C2-O2
26	b	849	LHG	O1-C1-C2-O2
23	b	834	CLA	C16-C17-C18-C20
23	b	807	CLA	C5-C6-C7-C8
23	9	308	CLA	CBA-CGA-O2A-C1
23	a	833	CLA	O1A-CGA-O2A-C1
23	a	838	CLA	O1A-CGA-O2A-C1
23	a	844	CLA	O1A-CGA-O2A-C1
24	1	315	SQD	O10-C23-O48-C46
23	a	818	CLA	C2-C1-O2A-CGA
23	9	313	CLA	O1A-CGA-O2A-C1
23	b	807	CLA	C3-C5-C6-C7
30	a	850	BCR	C23-C24-C25-C30
30	b	844	BCR	C1-C6-C7-C8
30	b	844	BCR	C5-C6-C7-C8
30	b	853	BCR	C1-C6-C7-C8
30	i	102	BCR	C23-C24-C25-C26
30	i	102	BCR	C23-C24-C25-C30
30	m	102	BCR	C5-C6-C7-C8
26	9	307	LHG	C30-C31-C32-C33
23	a	823	CLA	CBA-CGA-O2A-C1
23	b	806	CLA	CBA-CGA-O2A-C1
23	b	836	CLA	CBA-CGA-O2A-C1
23	a	809	CLA	C13-C15-C16-C17
23	b	829	CLA	C15-C16-C17-C18
23	b	833	CLA	C8-C10-C11-C12
23	b	839	CLA	C15-C16-C17-C18
26	a	845	LHG	C26-C27-C28-C29
23	2	314	CLA	C11-C10-C8-C9
23	4	315	CLA	O1A-CGA-O2A-C1
23	a	840	CLA	C13-C15-C16-C17
23	b	804	CLA	C13-C15-C16-C17
23	1	310	CLA	C4-C3-C5-C6
23	a	807	CLA	C4-C3-C5-C6
23	a	828	CLA	C4-C3-C5-C6
23	3	312	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	1	305	CLA	C11-C10-C8-C7
23	1	308	CLA	C11-C10-C8-C7
23	a	801	CLA	C11-C12-C13-C15
23	a	826	CLA	C11-C10-C8-C7
23	a	829	CLA	C11-C10-C8-C7
23	a	839	CLA	C6-C7-C8-C10
23	a	840	CLA	C12-C13-C15-C16
23	a	852	CLA	C11-C12-C13-C15
23	b	806	CLA	C11-C12-C13-C15
23	b	809	CLA	C11-C10-C8-C7
23	b	810	CLA	C2-C3-C5-C6
23	b	838	CLA	C11-C12-C13-C15
23	9	308	CLA	O1A-CGA-O2A-C1
23	b	803	CLA	C2C-C3C-CAC-CBC
23	b	809	CLA	C5-C6-C7-C8
25	6	304	A1L1F	C4-C8-O7-C54
28	2	317	LMG	C10-C11-C12-C13
23	a	825	CLA	CBA-CGA-O2A-C1
23	b	824	CLA	CBA-CGA-O2A-C1
23	4	307	CLA	C15-C16-C17-C18
23	b	832	CLA	C15-C16-C17-C18
27	b	851	DGD	CAB-CBB-CCB-CDB
23	a	811	CLA	C11-C10-C8-C7
24	1	315	SQD	C7-C8-C9-C10
23	a	806	CLA	C13-C15-C16-C17
27	b	851	DGD	C6A-C7A-C8A-C9A
23	4	306	CLA	C3-C5-C6-C7
23	b	816	CLA	O1A-CGA-O2A-C1
27	4	317	DGD	O6D-C1D-O3G-C3G
23	8	307	CLA	C15-C16-C17-C18
23	5	312	CLA	O1D-CGD-O2D-CED
27	8	315	DGD	C2B-C3B-C4B-C5B
26	a	846	LHG	C8-C7-O7-C5
27	b	851	DGD	C2B-C1B-O2G-C2G
26	b	849	LHG	O6-C4-C5-O7
22	9	306	A1L1G	C31-C32-C33-C34
23	9	313	CLA	CBD-CGD-O2D-CED
23	a	808	CLA	CBD-CGD-O2D-CED
26	a	846	LHG	O9-C7-O7-C5
23	2	308	CLA	C3-C5-C6-C7
27	4	317	DGD	O1G-C1G-C2G-O2G
23	b	841	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	b	808	CLA	C15-C16-C17-C18
23	b	806	CLA	C4-C3-C5-C6
23	b	810	CLA	C4-C3-C5-C6
23	8	310	CLA	CBA-CGA-O2A-C1
23	3	315	CLA	CBA-CGA-O2A-C1
23	7	308	CLA	C2-C3-C5-C6
23	a	804	CLA	C2-C3-C5-C6
23	b	802	CLA	C2-C3-C5-C6
23	4	307	CLA	C11-C12-C13-C14
23	3	312	CLA	C6-C7-C8-C9
23	2	310	CLA	C14-C13-C15-C16
23	1	308	CLA	C11-C10-C8-C9
23	1	310	CLA	C11-C10-C8-C9
23	a	801	CLA	C11-C12-C13-C14
23	a	807	CLA	C14-C13-C15-C16
23	a	814	CLA	C11-C10-C8-C9
23	a	826	CLA	C11-C10-C8-C9
23	a	831	CLA	C11-C10-C8-C9
23	a	852	CLA	C11-C12-C13-C14
23	b	806	CLA	C11-C12-C13-C14
23	b	806	CLA	C14-C13-C15-C16
23	b	809	CLA	C11-C10-C8-C9
23	b	818	CLA	C6-C7-C8-C9
23	b	822	CLA	C6-C7-C8-C9
23	b	824	CLA	C11-C10-C8-C9
23	b	825	CLA	C6-C7-C8-C9
23	b	838	CLA	C11-C12-C13-C14
23	8	308	CLA	C2A-CAA-CBA-CGA
23	a	806	CLA	C2A-CAA-CBA-CGA
23	a	810	CLA	C2A-CAA-CBA-CGA
23	b	832	CLA	C2A-CAA-CBA-CGA
23	7	316	CLA	C4C-C3C-CAC-CBC
21	5	302	XAT	C7-C8-C9-C19
21	7	304	XAT	C7-C8-C9-C19
22	9	306	A1L1G	C32-C33-C34-C27
25	h	202	A1L1F	C28-C39-C40-C41
23	4	307	CLA	C13-C15-C16-C17
23	b	809	CLA	C10-C11-C12-C13
23	a	823	CLA	O1A-CGA-O2A-C1
23	b	806	CLA	O1A-CGA-O2A-C1
23	5	307	CLA	C1A-C2A-CAA-CBA
23	9	310	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	9	313	CLA	C1A-C2A-CAA-CBA
23	4	312	CLA	C1A-C2A-CAA-CBA
23	3	314	CLA	C1A-C2A-CAA-CBA
23	2	306	CLA	C1A-C2A-CAA-CBA
23	7	306	CLA	C1A-C2A-CAA-CBA
23	7	311	CLA	C1A-C2A-CAA-CBA
23	7	313	CLA	C1A-C2A-CAA-CBA
23	1	306	CLA	C1A-C2A-CAA-CBA
23	a	807	CLA	C1A-C2A-CAA-CBA
23	a	817	CLA	C1A-C2A-CAA-CBA
23	a	819	CLA	C1A-C2A-CAA-CBA
23	a	825	CLA	C1A-C2A-CAA-CBA
23	b	816	CLA	C1A-C2A-CAA-CBA
23	b	817	CLA	C1A-C2A-CAA-CBA
23	b	838	CLA	C1A-C2A-CAA-CBA
23	f	803	CLA	C1A-C2A-CAA-CBA
23	a	801	CLA	C16-C17-C18-C19
23	b	801	CLA	C16-C17-C18-C19
26	m	101	LHG	C29-C30-C31-C32
25	h	202	A1L1F	C40-C41-C42-C44
23	b	822	CLA	O1D-CGD-O2D-CED
23	5	306	CLA	O1A-CGA-O2A-C1
23	1	305	CLA	C8-C10-C11-C12
23	a	844	CLA	C10-C11-C12-C13
26	m	101	LHG	C3-O3-P-O6
23	7	313	CLA	C5-C6-C7-C8
25	9	302	A1L1F	C49-C50-C51-C52
23	b	813	CLA	C3-C5-C6-C7
23	b	806	CLA	O1D-CGD-O2D-CED
23	5	316	CLA	C4C-C3C-CAC-CBC
23	b	836	CLA	O1A-CGA-O2A-C1
23	b	829	CLA	C13-C15-C16-C17
26	a	845	LHG	O6-C4-C5-C6
27	b	851	DGD	CBB-CCB-CDB-CEB
23	a	812	CLA	C10-C11-C12-C13
23	a	806	CLA	C16-C17-C18-C19
23	4	314	CLA	O1D-CGD-O2D-CED
26	m	101	LHG	C12-C13-C14-C15
23	b	835	CLA	C4-C3-C5-C6
23	b	836	CLA	C2C-C3C-CAC-CBC
25	h	202	A1L1F	C4-C8-O7-C54
23	b	824	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	a	822	CLA	C2A-CAA-CBA-CGA
23	a	820	CLA	C16-C17-C18-C20
23	b	814	CLA	C6-C7-C8-C10
23	h	201	CLA	O1D-CGD-O2D-CED
23	a	839	CLA	C3-C5-C6-C7
23	b	801	CLA	C3-C5-C6-C7
26	a	845	LHG	C4-C5-C6-O8
26	b	849	LHG	C4-C5-C6-O8
27	4	317	DGD	O1G-C1G-C2G-C3G
23	a	820	CLA	C8-C10-C11-C12
23	a	829	CLA	C10-C11-C12-C13
23	6	308	CLA	O1D-CGD-O2D-CED
25	1	304	A1L1F	C50-C51-C52-C53
27	b	851	DGD	C3A-C4A-C5A-C6A
28	j	103	LMG	C13-C14-C15-C16
25	6	301	A1L1F	C50-C51-C52-C53
26	m	101	LHG	C11-C10-C9-C8
23	5	311	CLA	CAA-CBA-CGA-O2A
23	8	310	CLA	O1D-CGD-O2D-CED
25	6	304	A1L1F	C45-C47-C48-C49
26	b	849	LHG	C8-C7-O7-C5
23	a	856	CLA	C10-C11-C12-C13
29	a	843	PQN	C23-C25-C26-C27
23	a	804	CLA	C4-C3-C5-C6
23	a	820	CLA	C4-C3-C5-C6
23	b	802	CLA	C4-C3-C5-C6
23	b	813	CLA	C4-C3-C5-C6
23	a	844	CLA	C16-C17-C18-C19
23	8	307	CLA	CBA-CGA-O2A-C1
25	h	202	A1L1F	C48-C49-C50-C51
23	1	311	CLA	CBD-CGD-O2D-CED
23	1	308	CLA	C13-C15-C16-C17
23	b	840	CLA	C13-C15-C16-C17
28	a	855	LMG	C14-C15-C16-C17
23	9	314	CLA	C3-C5-C6-C7
23	a	852	CLA	O1D-CGD-O2D-CED
23	f	802	CLA	O1D-CGD-O2D-CED
23	a	829	CLA	C8-C10-C11-C12
27	b	851	DGD	CCB-CDB-CEB-CFB
23	a	835	CLA	CBA-CGA-O2A-C1
23	a	825	CLA	O1A-CGA-O2A-C1
23	3	315	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	b	818	CLA	C11-C12-C13-C14
23	1	310	CLA	C5-C6-C7-C8
23	b	837	CLA	C2C-C3C-CAC-CBC
23	8	314	CLA	CBD-CGD-O2D-CED
26	a	845	LHG	C7-C8-C9-C10
23	1	308	CLA	C15-C16-C17-C18
23	a	810	CLA	C5-C6-C7-C8
23	a	826	CLA	C15-C16-C17-C18
27	4	317	DGD	C2D-C1D-O3G-C3G
25	6	301	A1L1F	C47-C48-C49-C50
23	b	803	CLA	C15-C16-C17-C18
23	a	801	CLA	C4-C3-C5-C6
23	4	307	CLA	C12-C13-C15-C16
23	6	309	CLA	C11-C10-C8-C7
23	1	306	CLA	C6-C7-C8-C10
23	a	807	CLA	C12-C13-C15-C16
23	a	809	CLA	C6-C7-C8-C10
23	a	810	CLA	C12-C13-C15-C16
23	a	812	CLA	C6-C7-C8-C10
23	a	820	CLA	C2-C3-C5-C6
23	a	822	CLA	C6-C7-C8-C10
23	a	830	CLA	C12-C13-C15-C16
23	a	841	CLA	C11-C10-C8-C7
23	a	844	CLA	C11-C12-C13-C15
23	b	802	CLA	C12-C13-C15-C16
23	b	806	CLA	C11-C10-C8-C7
23	b	806	CLA	C12-C13-C15-C16
23	b	810	CLA	C11-C12-C13-C15
23	b	813	CLA	C2-C3-C5-C6
23	b	818	CLA	C6-C7-C8-C10
23	b	822	CLA	C6-C7-C8-C10
23	b	824	CLA	C11-C10-C8-C7
23	b	825	CLA	C6-C7-C8-C10
23	b	827	CLA	C6-C7-C8-C10
23	b	828	CLA	C12-C13-C15-C16
23	b	834	CLA	C11-C12-C13-C15
23	b	839	CLA	C6-C7-C8-C10
23	f	802	CLA	C11-C12-C13-C15
23	4	316	CLA	C3-C5-C6-C7
23	7	308	CLA	C11-C10-C8-C9
23	a	807	CLA	C11-C12-C13-C14
23	a	809	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	a	810	CLA	C14-C13-C15-C16
23	a	822	CLA	C6-C7-C8-C9
23	a	827	CLA	C11-C10-C8-C9
23	a	830	CLA	C14-C13-C15-C16
23	a	835	CLA	C6-C7-C8-C9
23	a	841	CLA	C11-C10-C8-C9
23	a	842	CLA	C11-C12-C13-C14
23	a	844	CLA	C11-C10-C8-C9
23	a	844	CLA	C11-C12-C13-C14
23	a	844	CLA	C14-C13-C15-C16
23	b	801	CLA	C11-C12-C13-C14
23	b	802	CLA	C6-C7-C8-C9
23	b	802	CLA	C11-C10-C8-C9
23	b	807	CLA	C11-C10-C8-C9
23	b	810	CLA	C11-C12-C13-C14
23	b	828	CLA	C11-C12-C13-C14
23	b	833	CLA	C6-C7-C8-C9
23	b	837	CLA	C14-C13-C15-C16
25	h	202	A1L1F	C3-C8-O7-C54
26	9	307	LHG	C25-C26-C27-C28
23	4	306	CLA	CBA-CGA-O2A-C1
23	a	841	CLA	CBA-CGA-O2A-C1
23	a	812	CLA	C8-C10-C11-C12
21	7	303	XAT	C7-C8-C9-C19
22	3	306	A1L1G	C32-C33-C34-C27
23	a	844	CLA	C16-C17-C18-C20
23	b	814	CLA	C6-C7-C8-C9
21	4	304	XAT	C27-C28-C29-C30
26	b	849	LHG	C9-C10-C11-C12
23	a	836	CLA	O1D-CGD-O2D-CED
23	b	827	CLA	C15-C16-C17-C18
23	9	310	CLA	O1A-CGA-O2A-C1
23	a	824	CLA	O1A-CGA-O2A-C1
23	8	307	CLA	O1A-CGA-O2A-C1
27	b	851	DGD	C2A-C1A-O1G-C1G
23	a	826	CLA	O1D-CGD-O2D-CED
23	b	804	CLA	C16-C17-C18-C20
26	b	849	LHG	O6-C4-C5-C6
23	b	834	CLA	C3-C5-C6-C7
23	h	203	CLA	C3-C5-C6-C7
23	a	844	CLA	C15-C16-C17-C18
23	b	833	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	a	852	CLA	C4-C3-C5-C6
23	b	839	CLA	C4-C3-C5-C6
23	a	801	CLA	C2-C3-C5-C6
23	a	807	CLA	C2-C3-C5-C6
23	b	806	CLA	C10-C11-C12-C13
27	b	851	DGD	O1B-C1B-O2G-C2G
23	a	811	CLA	C11-C10-C8-C9
23	b	832	CLA	C3-C5-C6-C7
23	a	805	CLA	C6-C7-C8-C9
23	a	819	CLA	C2A-CAA-CBA-CGA
23	3	314	CLA	CBA-CGA-O2A-C1
23	1	306	CLA	CBA-CGA-O2A-C1
23	1	310	CLA	CBA-CGA-O2A-C1
23	b	828	CLA	CBA-CGA-O2A-C1
26	m	101	LHG	C2-C3-O3-P
23	4	310	CLA	C3A-C2A-CAA-CBA
23	3	315	CLA	C3A-C2A-CAA-CBA
23	2	314	CLA	C3A-C2A-CAA-CBA
23	a	829	CLA	C3A-C2A-CAA-CBA
23	b	810	CLA	C3A-C2A-CAA-CBA
23	b	833	CLA	C3A-C2A-CAA-CBA
23	b	812	CLA	C5-C6-C7-C8
26	a	845	LHG	C34-C35-C36-C37
23	a	805	CLA	C6-C7-C8-C10
23	a	831	CLA	CBA-CGA-O2A-C1
23	b	811	CLA	CBA-CGA-O2A-C1
23	a	830	CLA	C5-C6-C7-C8
23	b	801	CLA	C5-C6-C7-C8
24	1	315	SQD	O6-C44-C45-C46
26	a	846	LHG	C4-C5-C6-O8
28	2	317	LMG	O1-C7-C8-C9
25	6	301	A1L1F	C48-C49-C50-C51
23	b	836	CLA	C3-C5-C6-C7
26	9	307	LHG	C33-C34-C35-C36
27	b	851	DGD	C7A-C8A-C9A-CAA
23	b	818	CLA	C11-C12-C13-C15
23	6	316	CLA	O1D-CGD-O2D-CED
23	3	314	CLA	O1D-CGD-O2D-CED
23	a	827	CLA	C3-C5-C6-C7
23	7	314	CLA	C2A-CAA-CBA-CGA
23	a	809	CLA	C2A-CAA-CBA-CGA
23	4	316	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	a	803	CLA	C15-C16-C17-C18
28	j	103	LMG	C28-C29-C30-C31
23	9	314	CLA	CBA-CGA-O2A-C1
23	a	835	CLA	O1A-CGA-O2A-C1
23	a	820	CLA	C16-C17-C18-C19
23	4	306	CLA	O1A-CGA-O2A-C1
23	a	806	CLA	CBD-CGD-O2D-CED
23	4	307	CLA	C16-C17-C18-C19
23	a	806	CLA	C16-C17-C18-C20
23	b	827	CLA	C16-C17-C18-C20
23	b	822	CLA	C10-C11-C12-C13
22	9	301	A1L1G	O13-C26-C30-C31
26	b	849	LHG	O9-C7-O7-C5
23	a	840	CLA	C4-C3-C5-C6
23	7	308	CLA	C2-C1-O2A-CGA
25	1	304	A1L1F	C14-C29-C30-C31
23	b	802	CLA	C13-C15-C16-C17
23	b	805	CLA	C10-C11-C12-C13
23	9	308	CLA	C11-C10-C8-C9
23	4	309	CLA	C11-C10-C8-C9
23	1	306	CLA	C11-C10-C8-C9
23	1	310	CLA	C6-C7-C8-C9
23	a	814	CLA	C11-C12-C13-C14
23	a	840	CLA	C11-C10-C8-C9
23	a	852	CLA	C6-C7-C8-C9
23	a	852	CLA	C11-C10-C8-C9
23	b	803	CLA	C6-C7-C8-C9
23	b	805	CLA	C6-C7-C8-C9
23	b	809	CLA	C6-C7-C8-C9
23	b	824	CLA	C11-C12-C13-C14
23	b	838	CLA	C14-C13-C15-C16
23	b	839	CLA	C11-C12-C13-C14
23	5	310	CLA	C5-C6-C7-C8
23	1	310	CLA	C16-C17-C18-C20
30	b	848	BCR	C5-C6-C7-C8
30	b	852	BCR	C23-C24-C25-C26
30	b	852	BCR	C23-C24-C25-C30
30	b	853	BCR	C5-C6-C7-C8
30	f	804	BCR	C23-C24-C25-C26
30	i	102	BCR	C1-C6-C7-C8
30	i	102	BCR	C5-C6-C7-C8
23	b	809	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	4	304	XAT	C27-C28-C29-C39
21	7	303	XAT	C7-C8-C9-C10
22	9	306	A1L1G	C26-C30-C31-C32
22	7	302	A1L1G	C32-C33-C34-C35
23	2	315	CLA	C1A-C2A-CAA-CBA
23	j	101	CLA	C1A-C2A-CAA-CBA
23	4	309	CLA	C15-C16-C17-C18
23	a	856	CLA	C8-C10-C11-C12
23	9	308	CLA	C16-C17-C18-C20
23	1	306	CLA	C16-C17-C18-C20
23	b	806	CLA	C5-C6-C7-C8
23	b	828	CLA	C5-C6-C7-C8
23	9	313	CLA	O1D-CGD-O2D-CED
26	a	846	LHG	O6-C4-C5-C6
26	m	101	LHG	O6-C4-C5-C6
26	9	307	LHG	C32-C33-C34-C35
28	a	855	LMG	C12-C13-C14-C15
23	9	308	CLA	C11-C12-C13-C15
23	9	316	CLA	C11-C10-C8-C7
23	8	307	CLA	C11-C10-C8-C7
23	8	309	CLA	C11-C10-C8-C7
23	4	309	CLA	C11-C10-C8-C7
23	1	308	CLA	C11-C12-C13-C15
23	a	801	CLA	C6-C7-C8-C10
23	a	802	CLA	C6-C7-C8-C10
23	a	807	CLA	C11-C12-C13-C15
23	a	814	CLA	C6-C7-C8-C10
23	a	814	CLA	C11-C12-C13-C15
23	a	820	CLA	C11-C12-C13-C15
23	a	827	CLA	C11-C10-C8-C7
23	a	829	CLA	C6-C7-C8-C10
23	a	835	CLA	C6-C7-C8-C10
23	a	840	CLA	C2-C3-C5-C6
23	a	842	CLA	C11-C12-C13-C15
23	a	844	CLA	C11-C10-C8-C7
23	b	801	CLA	C11-C12-C13-C15
23	b	802	CLA	C6-C7-C8-C10
23	b	802	CLA	C11-C10-C8-C7
23	b	807	CLA	C11-C10-C8-C7
23	b	809	CLA	C6-C7-C8-C10
23	b	813	CLA	C11-C10-C8-C7
23	b	824	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	b	829	CLA	C12-C13-C15-C16
23	b	833	CLA	C6-C7-C8-C10
23	b	837	CLA	C12-C13-C15-C16
23	b	838	CLA	C12-C13-C15-C16
23	b	839	CLA	C12-C13-C15-C16
24	1	315	SQD	C9-C10-C11-C12
23	a	842	CLA	C8-C10-C11-C12
22	9	306	A1L1G	C30-C31-C32-C33
22	3	306	A1L1G	C40-C41-C42-C44
22	7	302	A1L1G	C34-C35-C36-C37
23	b	804	CLA	C16-C17-C18-C19
23	a	827	CLA	C5-C6-C7-C8
28	2	317	LMG	C31-C32-C33-C34
23	a	841	CLA	O1A-CGA-O2A-C1
23	a	808	CLA	O1D-CGD-O2D-CED
22	7	302	A1L1G	C45-C2-C44-C43
23	5	315	CLA	CAD-CBD-CGD-O2D
23	9	309	CLA	CAD-CBD-CGD-O2D
23	8	313	CLA	CAD-CBD-CGD-O2D
23	3	310	CLA	CAD-CBD-CGD-O2D
23	6	315	CLA	CAD-CBD-CGD-O2D
23	7	306	CLA	CAD-CBD-CGD-O2D
23	7	311	CLA	CAD-CBD-CGD-O2D
23	a	808	CLA	CAD-CBD-CGD-O2D
23	a	810	CLA	CAD-CBD-CGD-O2D
23	a	815	CLA	CAD-CBD-CGD-O2D
23	a	821	CLA	CAD-CBD-CGD-O2D
23	a	824	CLA	CAD-CBD-CGD-O2D
23	a	832	CLA	CAD-CBD-CGD-O2D
23	a	842	CLA	CAD-CBD-CGD-O2D
23	a	852	CLA	CAD-CBD-CGD-O2D
23	a	856	CLA	CAD-CBD-CGD-O2D
23	b	805	CLA	CAD-CBD-CGD-O2D
23	b	811	CLA	CAD-CBD-CGD-O2D
23	b	825	CLA	CAD-CBD-CGD-O2D
23	b	830	CLA	CAD-CBD-CGD-O2D
23	b	834	CLA	CAD-CBD-CGD-O2D
23	b	839	CLA	CAD-CBD-CGD-O2D
23	b	840	CLA	CAD-CBD-CGD-O2D
25	8	304	A1L1F	C57-C2-C44-C43
28	a	855	LMG	C9-C8-O7-C10
23	a	841	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	b	839	CLA	C13-C15-C16-C17
23	4	312	CLA	CBA-CGA-O2A-C1
23	9	308	CLA	C16-C17-C18-C19
26	a	845	LHG	C9-C10-C11-C12
28	2	317	LMG	C33-C34-C35-C36
27	8	315	DGD	C1G-C2G-C3G-O3G
23	7	313	CLA	CBD-CGD-O2D-CED
23	b	811	CLA	O1A-CGA-O2A-C1
23	6	310	CLA	C2A-CAA-CBA-CGA
23	2	307	CLA	C2A-CAA-CBA-CGA
23	2	314	CLA	C2A-CAA-CBA-CGA
23	2	310	CLA	C16-C17-C18-C19
23	b	809	CLA	C16-C17-C18-C19
23	8	308	CLA	CHA-CBD-CGD-O1D
23	8	308	CLA	CHA-CBD-CGD-O2D
23	8	309	CLA	CHA-CBD-CGD-O1D
23	8	309	CLA	CHA-CBD-CGD-O2D
23	8	314	CLA	CHA-CBD-CGD-O1D
23	8	314	CLA	CHA-CBD-CGD-O2D
23	4	306	CLA	CHA-CBD-CGD-O1D
23	3	308	CLA	CHA-CBD-CGD-O1D
23	3	308	CLA	CHA-CBD-CGD-O2D
23	6	309	CLA	CHA-CBD-CGD-O1D
23	6	309	CLA	CHA-CBD-CGD-O2D
23	2	313	CLA	CHA-CBD-CGD-O1D
23	7	308	CLA	CHA-CBD-CGD-O1D
23	7	308	CLA	CHA-CBD-CGD-O2D
23	7	315	CLA	CHA-CBD-CGD-O2D
23	7	316	CLA	CHA-CBD-CGD-O1D
23	7	316	CLA	CHA-CBD-CGD-O2D
23	a	809	CLA	CHA-CBD-CGD-O1D
23	a	809	CLA	CHA-CBD-CGD-O2D
23	a	814	CLA	CHA-CBD-CGD-O1D
23	a	814	CLA	CHA-CBD-CGD-O2D
23	a	823	CLA	CHA-CBD-CGD-O1D
23	a	828	CLA	CHA-CBD-CGD-O1D
23	a	831	CLA	CHA-CBD-CGD-O1D
23	a	831	CLA	CHA-CBD-CGD-O2D
23	a	837	CLA	CHA-CBD-CGD-O1D
23	a	839	CLA	CHA-CBD-CGD-O1D
23	a	839	CLA	CHA-CBD-CGD-O2D
23	b	803	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	803	CLA	CHA-CBD-CGD-O2D
23	b	808	CLA	CHA-CBD-CGD-O1D
23	b	808	CLA	CHA-CBD-CGD-O2D
23	b	814	CLA	CHA-CBD-CGD-O1D
23	b	829	CLA	CHA-CBD-CGD-O1D
23	b	829	CLA	CHA-CBD-CGD-O2D
23	b	835	CLA	CHA-CBD-CGD-O1D
23	b	835	CLA	CHA-CBD-CGD-O2D
23	b	836	CLA	CHA-CBD-CGD-O1D
23	3	314	CLA	O1A-CGA-O2A-C1
23	b	828	CLA	O1A-CGA-O2A-C1
27	b	851	DGD	O1A-C1A-O1G-C1G
23	7	312	CLA	O2A-C1-C2-C3
27	8	315	DGD	O2G-C2G-C3G-O3G
23	9	316	CLA	CBA-CGA-O2A-C1
23	1	306	CLA	O1A-CGA-O2A-C1
23	1	310	CLA	O1A-CGA-O2A-C1
23	a	831	CLA	O1A-CGA-O2A-C1
23	b	833	CLA	O1D-CGD-O2D-CED
23	b	817	CLA	C10-C11-C12-C13
23	9	314	CLA	O1A-CGA-O2A-C1
23	1	310	CLA	C2-C3-C5-C6
28	a	855	LMG	C31-C32-C33-C34
23	1	308	CLA	C11-C12-C13-C14
23	a	807	CLA	C11-C10-C8-C9
23	a	829	CLA	C6-C7-C8-C9
23	b	832	CLA	C14-C13-C15-C16
23	4	312	CLA	O1A-CGA-O2A-C1
23	a	852	CLA	C2A-CAA-CBA-CGA
23	b	807	CLA	C2A-CAA-CBA-CGA
21	6	302	XAT	C7-C8-C9-C19
21	5	302	XAT	C7-C8-C9-C10
21	6	302	XAT	C7-C8-C9-C10
25	h	202	A1L1F	C38-C39-C40-C41
23	1	306	CLA	C3-C5-C6-C7
23	3	311	CLA	C1A-C2A-CAA-CBA
23	2	314	CLA	C1A-C2A-CAA-CBA
23	a	824	CLA	C1A-C2A-CAA-CBA
23	b	813	CLA	C1A-C2A-CAA-CBA
23	b	823	CLA	C1A-C2A-CAA-CBA
23	1	308	CLA	CBD-CGD-O2D-CED
23	1	307	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	2	304	XAT	C33-C34-C35-C15
23	8	314	CLA	O1D-CGD-O2D-CED
26	m	101	LHG	C4-O6-P-O3
23	a	806	CLA	O1D-CGD-O2D-CED
23	2	314	CLA	C4-C3-C5-C6
23	a	830	CLA	C8-C10-C11-C12
23	8	311	CLA	C3-C5-C6-C7
26	9	307	LHG	C2-C3-O3-P
23	b	835	CLA	C2-C3-C5-C6
26	a	845	LHG	C3-O3-P-O5
26	a	846	LHG	C4-O6-P-O5
26	m	101	LHG	C3-O3-P-O5
26	m	101	LHG	C4-O6-P-O5
23	2	310	CLA	C16-C17-C18-C20
23	1	310	CLA	C16-C17-C18-C19
23	3	311	CLA	C2A-CAA-CBA-CGA
25	8	304	A1L1F	C47-C48-C49-C50
23	b	807	CLA	C16-C17-C18-C20
24	1	315	SQD	C13-C14-C15-C16
26	a	846	LHG	C10-C11-C12-C13
23	5	312	CLA	C2-C3-C5-C6
23	9	313	CLA	CAD-CBD-CGD-O1D
23	9	315	CLA	CAD-CBD-CGD-O1D
23	8	309	CLA	CAD-CBD-CGD-O1D
23	8	314	CLA	CAD-CBD-CGD-O1D
23	4	314	CLA	CAD-CBD-CGD-O1D
23	6	310	CLA	CAD-CBD-CGD-O1D
23	6	312	CLA	C2-C3-C5-C6
23	1	313	CLA	CAD-CBD-CGD-O1D
23	a	806	CLA	CAD-CBD-CGD-O1D
23	a	814	CLA	CAD-CBD-CGD-O1D
23	a	828	CLA	CAD-CBD-CGD-O1D
23	a	839	CLA	CAD-CBD-CGD-O1D
23	a	844	CLA	CAD-CBD-CGD-O1D
23	b	832	CLA	CAD-CBD-CGD-O1D
23	b	836	CLA	CAD-CBD-CGD-O1D
23	b	837	CLA	CAD-CBD-CGD-O1D
23	f	802	CLA	CAD-CBD-CGD-O1D
25	6	304	A1L1F	O13-C26-C30-C31
23	9	308	CLA	C10-C11-C12-C13
23	b	841	CLA	C15-C16-C17-C18
23	4	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	5	308	CLA	C11-C10-C8-C7
23	8	307	CLA	C6-C7-C8-C10
23	6	309	CLA	C6-C7-C8-C10
23	6	316	CLA	C3A-C2A-CAA-CBA
23	2	310	CLA	C11-C12-C13-C15
23	a	842	CLA	C12-C13-C15-C16
23	b	801	CLA	C11-C10-C8-C7
23	b	801	CLA	C12-C13-C15-C16
23	b	805	CLA	C11-C12-C13-C15
23	b	827	CLA	C11-C10-C8-C7
23	b	829	CLA	C11-C12-C13-C15
23	b	832	CLA	C12-C13-C15-C16
26	m	101	LHG	O6-C4-C5-O7
29	a	843	PQN	C22-C23-C25-C26
23	a	834	CLA	C5-C6-C7-C8
23	b	818	CLA	C8-C10-C11-C12
23	b	824	CLA	C8-C10-C11-C12
23	8	309	CLA	C2A-CAA-CBA-CGA
23	1	308	CLA	C16-C17-C18-C19
24	5	317	SQD	C44-C45-C46-O48
24	5	317	SQD	O47-C45-C46-O48
24	1	315	SQD	O6-C44-C45-O47
26	a	846	LHG	O7-C5-C6-O8
26	b	849	LHG	O7-C5-C6-O8
23	b	814	CLA	C3-C5-C6-C7
23	9	316	CLA	O1A-CGA-O2A-C1
23	1	311	CLA	CBA-CGA-O2A-C1
23	b	804	CLA	CBA-CGA-O2A-C1
23	8	310	CLA	O1A-CGA-O2A-C1
26	m	101	LHG	C10-C11-C12-C13
23	5	310	CLA	C6-C7-C8-C9
23	9	308	CLA	C11-C12-C13-C14
23	8	309	CLA	C11-C10-C8-C9
23	4	307	CLA	C14-C13-C15-C16
23	2	311	CLA	C11-C10-C8-C9
23	a	801	CLA	C6-C7-C8-C9
23	a	802	CLA	C6-C7-C8-C9
23	a	807	CLA	C6-C7-C8-C9
23	a	809	CLA	C6-C7-C8-C9
23	a	814	CLA	C6-C7-C8-C9
23	a	820	CLA	C11-C12-C13-C14
23	a	842	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	803	CLA	C11-C12-C13-C14
23	b	813	CLA	C11-C10-C8-C9
23	b	839	CLA	C14-C13-C15-C16
23	2	308	CLA	C6-C7-C8-C9
23	b	840	CLA	C2C-C3C-CAC-CBC
23	3	315	CLA	O1A-CGA-O2A-C1
23	3	308	CLA	CAA-CBA-CGA-O2A
23	a	809	CLA	C10-C11-C12-C13
22	9	306	A1L1G	C32-C33-C34-C35
22	1	301	A1L1G	C37-C38-C39-C28
23	b	832	CLA	C2C-C3C-CAC-CBC
23	b	802	CLA	C3-C5-C6-C7
26	m	101	LHG	C13-C14-C15-C16
23	7	308	CLA	C8-C10-C11-C12
23	b	827	CLA	C10-C11-C12-C13
23	8	307	CLA	C16-C17-C18-C20
23	a	823	CLA	C1-C2-C3-C4
23	b	831	CLA	C1-C2-C3-C4
23	a	801	CLA	CAA-CBA-CGA-O2A
24	1	315	SQD	C46-C45-O47-C7
23	4	316	CLA	C2A-CAA-CBA-CGA
23	1	305	CLA	C2A-CAA-CBA-CGA
23	1	308	CLA	C2A-CAA-CBA-CGA
23	a	813	CLA	C2A-CAA-CBA-CGA
23	a	821	CLA	C2A-CAA-CBA-CGA
23	b	824	CLA	C2A-CAA-CBA-CGA
23	b	827	CLA	C2A-CAA-CBA-CGA
23	5	312	CLA	C2-C1-O2A-CGA
23	6	309	CLA	C2-C1-O2A-CGA
23	6	312	CLA	C2-C1-O2A-CGA
23	7	306	CLA	C2-C1-O2A-CGA
23	a	816	CLA	C2-C1-O2A-CGA
23	a	822	CLA	C2-C1-O2A-CGA
23	b	809	CLA	C2-C1-O2A-CGA
24	5	317	SQD	C7-C8-C9-C10
23	b	822	CLA	C3-C5-C6-C7
23	1	311	CLA	O1D-CGD-O2D-CED
23	1	311	CLA	O1A-CGA-O2A-C1
23	b	804	CLA	O1A-CGA-O2A-C1
23	h	203	CLA	C4-C3-C5-C6
23	a	856	CLA	CBD-CGD-O2D-CED
23	1	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	b	848	BCR	C1-C6-C7-C8
30	f	804	BCR	C23-C24-C25-C30
23	b	839	CLA	C2-C3-C5-C6
26	b	849	LHG	C25-C26-C27-C28
23	b	817	CLA	CBA-CGA-O2A-C1
23	a	830	CLA	C16-C17-C18-C19
23	b	807	CLA	C16-C17-C18-C19
23	b	817	CLA	O1A-CGA-O2A-C1
23	a	839	CLA	C15-C16-C17-C18
26	9	307	LHG	C4-O6-P-O3
26	a	846	LHG	C3-O3-P-O6
26	a	846	LHG	C4-O6-P-O3
23	b	801	CLA	O1A-CGA-O2A-C1
23	b	802	CLA	C16-C17-C18-C20
23	a	841	CLA	C4-C3-C5-C6
23	4	307	CLA	C11-C12-C13-C15
23	2	311	CLA	C11-C10-C8-C7
23	b	825	CLA	C11-C10-C8-C7
23	f	802	CLA	C6-C7-C8-C10
23	a	801	CLA	C14-C13-C15-C16
23	a	812	CLA	C6-C7-C8-C9
23	b	802	CLA	C14-C13-C15-C16
23	b	827	CLA	C11-C10-C8-C9
23	b	828	CLA	C14-C13-C15-C16
29	a	843	PQN	C24-C23-C25-C26
21	5	301	XAT	C29-C30-C31-C32
22	3	302	A1L1G	C36-C37-C38-C39
30	m	102	BCR	C13-C14-C15-C16
23	b	801	CLA	CBA-CGA-O2A-C1
23	5	308	CLA	C8-C10-C11-C12
23	a	830	CLA	C15-C16-C17-C18
23	a	856	CLA	C15-C16-C17-C18
23	h	201	CLA	C13-C15-C16-C17
23	9	314	CLA	C2A-CAA-CBA-CGA
21	7	303	XAT	C11-C12-C13-C20
23	5	316	CLA	CAA-CBA-CGA-O2A
21	6	303	XAT	C11-C12-C13-C14
22	3	306	A1L1G	C32-C33-C34-C35
23	8	312	CLA	CBD-CGD-O2D-CED
23	2	314	CLA	C11-C10-C8-C7
26	a	846	LHG	C1-C2-C3-O3
23	2	314	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	827	CLA	C16-C17-C18-C19
23	a	813	CLA	CBA-CGA-O2A-C1
23	a	813	CLA	O1A-CGA-O2A-C1
23	8	305	CLA	CBD-CGD-O2D-CED
23	4	309	CLA	CBD-CGD-O2D-CED
23	a	832	CLA	CBD-CGD-O2D-CED
23	3	312	CLA	CBA-CGA-O2A-C1
23	b	840	CLA	C16-C17-C18-C20
23	5	311	CLA	CAA-CBA-CGA-O1A
21	6	306	XAT	C29-C30-C31-C32
21	7	301	XAT	C29-C30-C31-C32
21	a	853	XAT	C9-C10-C11-C12
22	3	302	A1L1G	C40-C41-C42-C44
23	a	820	CLA	C13-C15-C16-C17
23	a	856	CLA	O1D-CGD-O2D-CED
23	7	313	CLA	O1D-CGD-O2D-CED
23	a	812	CLA	C3-C5-C6-C7
26	a	845	LHG	C25-C26-C27-C28
23	b	813	CLA	C10-C11-C12-C13
23	a	810	CLA	C2-C1-O2A-CGA
23	a	814	CLA	C2-C1-O2A-CGA
23	a	839	CLA	C16-C17-C18-C20
23	6	310	CLA	C3-C5-C6-C7
23	8	305	CLA	O1D-CGD-O2D-CED
23	5	310	CLA	C2A-CAA-CBA-CGA
23	8	307	CLA	C2A-CAA-CBA-CGA
23	2	309	CLA	C2A-CAA-CBA-CGA
23	7	306	CLA	C2A-CAA-CBA-CGA
23	a	803	CLA	C2A-CAA-CBA-CGA
23	b	808	CLA	C2A-CAA-CBA-CGA
23	b	810	CLA	C2A-CAA-CBA-CGA
27	b	851	DGD	O2G-C2G-C3G-O3G
25	9	302	A1L1F	C3-C8-O7-C54
23	2	310	CLA	C3A-C2A-CAA-CBA
23	b	813	CLA	C3A-C2A-CAA-CBA
23	b	831	CLA	C3A-C2A-CAA-CBA
28	2	317	LMG	O9-C10-O7-C8
22	3	306	A1L1G	C30-C31-C32-C33
23	8	312	CLA	O1D-CGD-O2D-CED
23	a	802	CLA	C4-C3-C5-C6
23	5	308	CLA	C11-C10-C8-C9
23	1	310	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	a	822	CLA	C11-C10-C8-C9
23	a	829	CLA	C11-C12-C13-C14
23	a	831	CLA	C6-C7-C8-C9
23	a	844	CLA	C6-C7-C8-C9
23	a	856	CLA	C11-C10-C8-C9
23	b	807	CLA	C6-C7-C8-C9
23	a	830	CLA	C16-C17-C18-C20
30	b	845	BCR	C11-C10-C9-C34
30	b	845	BCR	C20-C21-C22-C37
30	b	853	BCR	C11-C10-C9-C34
30	f	804	BCR	C35-C13-C14-C15
23	3	315	CLA	CAA-CBA-CGA-O1A
23	a	832	CLA	O1D-CGD-O2D-CED
23	8	307	CLA	C16-C17-C18-C19
23	1	308	CLA	C16-C17-C18-C20
23	a	801	CLA	CBA-CGA-O2A-C1
23	b	841	CLA	CBA-CGA-O2A-C1
27	8	315	DGD	O6D-C1D-O3G-C3G
26	a	845	LHG	C14-C15-C16-C17
21	7	301	XAT	C7-C8-C9-C19
23	5	307	CLA	CAA-CBA-CGA-O1A
23	4	310	CLA	C1A-C2A-CAA-CBA
23	4	315	CLA	C1A-C2A-CAA-CBA
23	2	310	CLA	C1A-C2A-CAA-CBA
23	2	316	CLA	C1A-C2A-CAA-CBA
23	b	815	CLA	C1A-C2A-CAA-CBA
23	b	835	CLA	C1A-C2A-CAA-CBA
26	m	101	LHG	C15-C16-C17-C18
23	a	807	CLA	C11-C10-C8-C7
23	a	814	CLA	C11-C10-C8-C7
23	a	852	CLA	C12-C13-C15-C16
23	3	312	CLA	O1A-CGA-O2A-C1
23	4	313	CLA	CAA-CBA-CGA-O2A
23	a	817	CLA	CAA-CBA-CGA-O1A
28	a	855	LMG	C11-C12-C13-C14
23	b	840	CLA	C4C-C3C-CAC-CBC
23	1	305	CLA	C3-C5-C6-C7
23	5	308	CLA	C2A-CAA-CBA-CGA
23	h	201	CLA	C8-C10-C11-C12
23	a	801	CLA	O1A-CGA-O2A-C1
23	b	841	CLA	O1A-CGA-O2A-C1
23	a	817	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	b	817	CLA	CBD-CGD-O2D-CED
23	4	309	CLA	C13-C15-C16-C17
23	4	313	CLA	CAA-CBA-CGA-O1A
23	1	307	CLA	C6-C7-C8-C9
23	a	852	CLA	C2-C3-C5-C6
23	4	309	CLA	O1D-CGD-O2D-CED
30	b	845	BCR	C11-C10-C9-C8
30	b	845	BCR	C20-C21-C22-C23
30	b	853	BCR	C11-C10-C9-C8
30	f	804	BCR	C12-C13-C14-C15
23	4	305	CLA	C2A-CAA-CBA-CGA
23	5	311	CLA	CBA-CGA-O2A-C1
22	9	301	A1L1G	C34-C35-C36-C37
22	7	302	A1L1G	C36-C37-C38-C39
22	1	301	A1L1G	C40-C41-C42-C44
28	2	317	LMG	C11-C10-O7-C8
23	5	314	CLA	CAA-CBA-CGA-O1A
23	a	830	CLA	C4-C3-C5-C6
23	a	839	CLA	C2-C1-O2A-CGA
23	a	802	CLA	C2-C3-C5-C6
23	a	841	CLA	C2-C3-C5-C6
23	b	817	CLA	O1D-CGD-O2D-CED
23	b	807	CLA	C14-C13-C15-C16
23	5	307	CLA	CAA-CBA-CGA-O2A
23	5	312	CLA	C4-C3-C5-C6
23	6	307	CLA	C2A-CAA-CBA-CGA
23	a	839	CLA	C2A-CAA-CBA-CGA
23	a	842	CLA	O1A-CGA-O2A-C1
30	b	850	BCR	C23-C24-C25-C30
30	j	102	BCR	C1-C6-C7-C8
30	m	102	BCR	C23-C24-C25-C30
24	1	315	SQD	C15-C16-C17-C18
23	a	819	CLA	CAA-CBA-CGA-O2A
23	b	836	CLA	C4C-C3C-CAC-CBC
23	a	830	CLA	O1A-CGA-O2A-C1
25	h	202	A1L1F	C36-C37-C38-C39
21	2	304	XAT	C7-C8-C9-C10
21	a	854	XAT	C31-C32-C33-C34
23	9	312	CLA	CAA-CBA-CGA-O2A
27	b	851	DGD	C1B-C2B-C3B-C4B
23	a	852	CLA	C10-C11-C12-C13
23	a	813	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	7	307	CLA	CAA-CBA-CGA-O2A
23	a	804	CLA	O1A-CGA-O2A-C1
23	5	308	CLA	C11-C12-C13-C14
23	b	813	CLA	C16-C17-C18-C19
23	2	314	CLA	O1A-CGA-O2A-C1
23	5	314	CLA	CAA-CBA-CGA-O2A
23	7	307	CLA	CAA-CBA-CGA-O1A
23	1	314	CLA	CAA-CBA-CGA-O2A
23	9	308	CLA	C2A-CAA-CBA-CGA
23	a	826	CLA	C13-C15-C16-C17
23	a	830	CLA	CBA-CGA-O2A-C1
23	a	842	CLA	CBA-CGA-O2A-C1
23	7	317	CLA	CAA-CBA-CGA-O2A
23	b	807	CLA	C4-C3-C5-C6
23	a	852	CLA	C11-C10-C8-C7
23	4	307	CLA	C3-C5-C6-C7
23	b	813	CLA	C5-C6-C7-C8
21	8	302	XAT	C9-C10-C11-C12
27	8	315	DGD	C2D-C1D-O3G-C3G
25	6	304	A1L1F	C3-C8-O7-C54
23	1	314	CLA	CAA-CBA-CGA-O1A
23	4	308	CLA	CAA-CBA-CGA-O2A
23	1	306	CLA	C16-C17-C18-C19
23	a	804	CLA	CBA-CGA-O2A-C1
23	5	315	CLA	C4-C3-C5-C6
23	b	810	CLA	C8-C10-C11-C12
28	j	103	LMG	C11-C12-C13-C14
23	a	830	CLA	C2-C3-C5-C6
25	h	202	A1L1F	C14-C29-C30-C31
23	a	804	CLA	C6-C7-C8-C9
26	m	101	LHG	C35-C36-C37-C38
23	8	307	CLA	C6-C7-C8-C9
23	4	307	CLA	C6-C7-C8-C9
23	6	309	CLA	C11-C10-C8-C9
23	a	801	CLA	C11-C10-C8-C9
23	b	805	CLA	C11-C12-C13-C14
23	b	829	CLA	C11-C12-C13-C14
23	b	813	CLA	C13-C15-C16-C17
23	4	305	CLA	C3A-C2A-CAA-CBA
23	2	316	CLA	C3A-C2A-CAA-CBA
23	1	310	CLA	C3A-C2A-CAA-CBA
23	b	808	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	b	838	CLA	CAA-CBA-CGA-O2A
23	5	307	CLA	CAD-CBD-CGD-O2D
23	5	312	CLA	CAD-CBD-CGD-O2D
23	9	312	CLA	CAD-CBD-CGD-O2D
23	8	310	CLA	CAD-CBD-CGD-O2D
23	8	311	CLA	CAD-CBD-CGD-O2D
23	4	310	CLA	CAD-CBD-CGD-O2D
23	3	314	CLA	CAD-CBD-CGD-O2D
23	6	312	CLA	CAD-CBD-CGD-O2D
23	2	316	CLA	CAD-CBD-CGD-O2D
23	7	307	CLA	CAD-CBD-CGD-O2D
23	1	307	CLA	CAD-CBD-CGD-O2D
23	1	309	CLA	CAD-CBD-CGD-O2D
23	a	827	CLA	CAD-CBD-CGD-O2D
23	a	829	CLA	CAD-CBD-CGD-O2D
23	b	812	CLA	CAD-CBD-CGD-O2D
23	b	813	CLA	CAD-CBD-CGD-O2D
23	b	816	CLA	CAD-CBD-CGD-O2D
23	b	838	CLA	CAD-CBD-CGD-O2D
23	l	203	CLA	CAD-CBD-CGD-O2D
23	b	818	CLA	C2A-CAA-CBA-CGA
23	a	818	CLA	CAA-CBA-CGA-O2A
23	b	802	CLA	C10-C11-C12-C13
23	a	835	CLA	C4-C3-C5-C6
23	b	834	CLA	C4-C3-C5-C6
23	7	317	CLA	CAA-CBA-CGA-O1A
23	b	807	CLA	C2-C3-C5-C6
23	b	801	CLA	CAA-CBA-CGA-O2A
23	l	203	CLA	CAA-CBA-CGA-O2A
30	f	801	BCR	C17-C18-C19-C20
21	5	301	XAT	O4-C6-C7-C8
21	5	302	XAT	O4-C6-C7-C8
21	5	305	XAT	O24-C26-C27-C28
21	9	303	XAT	O24-C26-C27-C28
21	8	301	XAT	O24-C26-C27-C28
21	4	304	XAT	O4-C6-C7-C8
21	3	303	XAT	O4-C6-C7-C8
21	6	305	XAT	O4-C6-C7-C8
21	6	306	XAT	O4-C6-C7-C8
21	2	301	XAT	O4-C6-C7-C8
21	2	305	XAT	O24-C26-C27-C28
21	7	305	XAT	O4-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	7	305	XAT	O24-C26-C27-C28
22	3	302	A1L1G	C29-C14-C25-O15
24	1	315	SQD	O47-C7-C8-C9
23	b	834	CLA	C15-C16-C17-C18
23	4	308	CLA	O2A-C1-C2-C3
23	3	310	CLA	O2A-C1-C2-C3
23	2	314	CLA	O2A-C1-C2-C3
23	1	305	CLA	O2A-C1-C2-C3
23	a	826	CLA	O2A-C1-C2-C3
23	b	817	CLA	O2A-C1-C2-C3
23	b	832	CLA	O2A-C1-C2-C3
23	4	307	CLA	C2A-CAA-CBA-CGA
23	2	308	CLA	C2A-CAA-CBA-CGA
29	a	843	PQN	C18-C20-C21-C22
23	9	313	CLA	CAA-CBA-CGA-O2A
23	a	836	CLA	CAA-CBA-CGA-O2A
23	4	305	CLA	CAA-CBA-CGA-O2A
21	7	304	XAT	C9-C10-C11-C12
23	5	314	CLA	CHA-CBD-CGD-O1D
23	4	309	CLA	CHA-CBD-CGD-O1D
23	4	313	CLA	CHA-CBD-CGD-O2D
23	6	314	CLA	CHA-CBD-CGD-O2D
23	2	307	CLA	CHA-CBD-CGD-O1D
23	2	307	CLA	CHA-CBD-CGD-O2D
23	2	310	CLA	CHA-CBD-CGD-O1D
23	2	310	CLA	CHA-CBD-CGD-O2D
23	2	313	CLA	CHA-CBD-CGD-O2D
23	a	802	CLA	CHA-CBD-CGD-O1D
23	a	802	CLA	CHA-CBD-CGD-O2D
23	a	804	CLA	CHA-CBD-CGD-O1D
23	a	804	CLA	CHA-CBD-CGD-O2D
23	a	816	CLA	CHA-CBD-CGD-O1D
23	a	817	CLA	CHA-CBD-CGD-O1D
23	a	817	CLA	CHA-CBD-CGD-O2D
23	a	820	CLA	CHA-CBD-CGD-O1D
23	a	820	CLA	CHA-CBD-CGD-O2D
23	a	823	CLA	CHA-CBD-CGD-O2D
23	a	828	CLA	CHA-CBD-CGD-O2D
23	a	830	CLA	CHA-CBD-CGD-O1D
23	a	830	CLA	CHA-CBD-CGD-O2D
23	a	837	CLA	CHA-CBD-CGD-O2D
23	b	801	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	801	CLA	CHA-CBD-CGD-O2D
23	b	804	CLA	CHA-CBD-CGD-O1D
23	b	804	CLA	CHA-CBD-CGD-O2D
23	b	814	CLA	CHA-CBD-CGD-O2D
23	b	815	CLA	CHA-CBD-CGD-O1D
23	b	815	CLA	CHA-CBD-CGD-O2D
23	b	824	CLA	CHA-CBD-CGD-O1D
23	b	824	CLA	CHA-CBD-CGD-O2D
23	b	833	CLA	CHA-CBD-CGD-O2D
23	b	836	CLA	CHA-CBD-CGD-O2D
25	6	304	A1L1F	O13-C45-C47-C48
25	9	302	A1L1F	C50-C51-C52-C53
23	2	314	CLA	CBA-CGA-O2A-C1
23	a	835	CLA	C2-C3-C5-C6
23	a	827	CLA	C10-C11-C12-C13
23	a	810	CLA	CAA-CBA-CGA-O2A
23	b	806	CLA	CAA-CBA-CGA-O2A
23	h	203	CLA	CAA-CBA-CGA-O2A
26	9	307	LHG	O7-C5-C6-O8
23	4	311	CLA	O1A-CGA-O2A-C1
23	b	802	CLA	CAA-CBA-CGA-O2A
23	b	806	CLA	C16-C17-C18-C19
23	b	824	CLA	C10-C11-C12-C13
23	9	308	CLA	C11-C10-C8-C7
23	8	311	CLA	C6-C7-C8-C10
23	1	310	CLA	C12-C13-C15-C16
23	a	801	CLA	C11-C10-C8-C7
23	a	835	CLA	C11-C12-C13-C15
23	b	809	CLA	C2-C3-C5-C6
22	3	306	A1L1G	C14-C29-C30-C31
23	1	306	CLA	CAA-CBA-CGA-O2A
23	1	309	CLA	CAA-CBA-CGA-O2A
23	a	829	CLA	CAA-CBA-CGA-O2A
23	b	808	CLA	CAA-CBA-CGA-O2A
23	b	817	CLA	CAA-CBA-CGA-O2A
23	b	832	CLA	CAA-CBA-CGA-O2A
23	6	308	CLA	C6-C7-C8-C9
23	a	834	CLA	C11-C12-C13-C14
23	f	802	CLA	C6-C7-C8-C9
23	1	312	CLA	CAA-CBA-CGA-O2A
26	a	845	LHG	O8-C23-C24-C25
23	b	838	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	5	317	SQD	C4-C5-C6-S
25	9	302	A1L1F	O13-C26-C30-C29
25	6	304	A1L1F	O13-C26-C30-C29
23	a	829	CLA	C2A-CAA-CBA-CGA
23	a	841	CLA	C2A-CAA-CBA-CGA
21	6	302	XAT	C31-C32-C33-C40
23	4	308	CLA	CAA-CBA-CGA-O1A
23	a	818	CLA	CAA-CBA-CGA-O1A
26	m	101	LHG	O1-C1-C2-C3
25	8	304	A1L1F	C3-C8-O7-C54
23	b	833	CLA	CAA-CBA-CGA-O2A
23	b	801	CLA	CAA-CBA-CGA-O1A
23	b	809	CLA	CAA-CBA-CGA-O1A
23	b	817	CLA	CAA-CBA-CGA-O1A
24	1	315	SQD	O49-C7-C8-C9
21	6	302	XAT	C31-C32-C33-C34
21	7	301	XAT	C7-C8-C9-C10
30	i	101	BCR	C17-C18-C19-C20
23	9	311	CLA	C1A-C2A-CAA-CBA
23	9	312	CLA	C1A-C2A-CAA-CBA
23	1	310	CLA	C1A-C2A-CAA-CBA
23	a	803	CLA	C1A-C2A-CAA-CBA
23	a	804	CLA	C1A-C2A-CAA-CBA
23	a	814	CLA	C1A-C2A-CAA-CBA
23	a	815	CLA	C1A-C2A-CAA-CBA
23	b	822	CLA	C1A-C2A-CAA-CBA
23	b	825	CLA	C1A-C2A-CAA-CBA
23	b	831	CLA	C1A-C2A-CAA-CBA
23	b	819	CLA	C6-C7-C8-C9
23	a	827	CLA	C2-C1-O2A-CGA
23	a	829	CLA	C2-C1-O2A-CGA
23	b	806	CLA	C2-C1-O2A-CGA
23	b	835	CLA	C2-C1-O2A-CGA
23	4	305	CLA	CAA-CBA-CGA-O1A
28	j	103	LMG	C7-C8-C9-O8
26	m	101	LHG	C30-C31-C32-C33
23	b	802	CLA	C5-C6-C7-C8
23	b	833	CLA	C10-C11-C12-C13
26	m	101	LHG	C27-C28-C29-C30
23	7	309	CLA	CBA-CGA-O2A-C1
25	6	301	A1L1F	O13-C45-C47-C48
23	h	203	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	803	CLA	C4C-C3C-CAC-CBC
23	a	826	CLA	C10-C11-C12-C13
26	a	846	LHG	C3-O3-P-O5
23	b	808	CLA	CAA-CBA-CGA-O1A
23	b	832	CLA	CAA-CBA-CGA-O1A
25	6	304	A1L1F	O46-C45-C47-C48
23	3	312	CLA	CAA-CBA-CGA-O2A
30	b	850	BCR	C23-C24-C25-C26
30	b	852	BCR	C1-C6-C7-C8
30	j	102	BCR	C5-C6-C7-C8
30	m	102	BCR	C23-C24-C25-C26
23	1	312	CLA	CAA-CBA-CGA-O1A
23	a	836	CLA	CAA-CBA-CGA-O1A
23	b	806	CLA	CAA-CBA-CGA-O1A
23	h	203	CLA	CAA-CBA-CGA-O1A
23	b	813	CLA	CBD-CGD-O2D-CED
23	b	803	CLA	CAA-CBA-CGA-O2A
23	9	315	CLA	C2C-C3C-CAC-CBC
23	7	308	CLA	C2A-CAA-CBA-CGA
23	7	309	CLA	O1A-CGA-O2A-C1
23	a	813	CLA	CBD-CGD-O2D-CED
23	3	313	CLA	C4-C3-C5-C6
23	a	810	CLA	C16-C17-C18-C20
23	a	814	CLA	C16-C17-C18-C19
23	b	809	CLA	C16-C17-C18-C20
23	4	309	CLA	CAD-CBD-CGD-O1D
23	4	315	CLA	CAD-CBD-CGD-O1D
23	3	307	CLA	CAD-CBD-CGD-O1D
23	2	309	CLA	CAD-CBD-CGD-O1D
23	7	316	CLA	C2-C3-C5-C6
23	a	816	CLA	CAD-CBD-CGD-O1D
23	b	814	CLA	CAD-CBD-CGD-O1D
23	b	818	CLA	CAD-CBD-CGD-O1D
24	5	317	SQD	O5-C5-C6-S
26	9	307	LHG	C6-C5-O7-C7
25	9	302	A1L1F	O46-C45-O13-C26
23	b	804	CLA	C11-C12-C13-C14
23	b	805	CLA	C11-C10-C8-C9
23	b	833	CLA	C11-C10-C8-C9
23	a	820	CLA	CBD-CGD-O2D-CED
23	b	833	CLA	C3-C5-C6-C7
23	9	314	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	6	316	CLA	CAA-CBA-CGA-O2A
23	7	308	CLA	CAA-CBA-CGA-O2A
23	7	316	CLA	CAA-CBA-CGA-O2A
23	a	813	CLA	CAA-CBA-CGA-O2A
24	5	317	SQD	C10-C11-C12-C13
23	4	309	CLA	C8-C10-C11-C12
23	a	834	CLA	C10-C11-C12-C13
23	b	824	CLA	C15-C16-C17-C18
23	a	820	CLA	O1D-CGD-O2D-CED
23	3	309	CLA	C2A-CAA-CBA-CGA
23	4	309	CLA	CAA-CBA-CGA-O2A
23	7	309	CLA	CAA-CBA-CGA-O2A
23	a	826	CLA	CAA-CBA-CGA-O2A
23	a	856	CLA	CAA-CBA-CGA-O2A
23	5	310	CLA	C15-C16-C17-C18
23	a	801	CLA	C5-C6-C7-C8
23	a	810	CLA	CAA-CBA-CGA-O1A
23	a	813	CLA	O1D-CGD-O2D-CED
23	8	308	CLA	C4-C3-C5-C6
23	b	809	CLA	C4-C3-C5-C6
23	9	311	CLA	C3A-C2A-CAA-CBA
23	9	312	CLA	C3A-C2A-CAA-CBA
23	6	308	CLA	C6-C7-C8-C10
23	7	309	CLA	CHA-CBD-CGD-O1D
23	1	306	CLA	C3A-C2A-CAA-CBA
23	a	834	CLA	C11-C12-C13-C15
23	b	804	CLA	C11-C12-C13-C15
23	b	818	CLA	C11-C10-C8-C7
23	1	202	CLA	C6-C7-C8-C10
23	3	312	CLA	CAA-CBA-CGA-O1A
23	a	813	CLA	CAA-CBA-CGA-O1A
23	b	833	CLA	CAA-CBA-CGA-O1A
23	5	310	CLA	CAA-CBA-CGA-O2A
23	2	307	CLA	CAA-CBA-CGA-O2A
23	7	310	CLA	CAA-CBA-CGA-O2A
23	a	835	CLA	CAA-CBA-CGA-O2A
21	7	303	XAT	C11-C12-C13-C14
30	b	847	BCR	C7-C8-C9-C10
24	1	315	SQD	C12-C13-C14-C15
23	b	829	CLA	O1A-CGA-O2A-C1
23	7	308	CLA	CAA-CBA-CGA-O1A
23	7	316	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	a	835	CLA	CAA-CBA-CGA-O1A
25	6	301	A1L1F	O46-C45-C47-C48
25	9	302	A1L1F	C47-C45-O13-C26
23	6	314	CLA	CAA-CBA-CGA-O2A
26	a	845	LHG	O10-C23-C24-C25
23	5	310	CLA	CAA-CBA-CGA-O1A
23	7	314	CLA	CAA-CBA-CGA-O2A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	h	202	A1L1F	C1-C11-C3-C4-C6-C8

234 monomers are involved in 806 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	315	CLA	1	0
23	3	308	CLA	2	0
23	a	856	CLA	23	0
21	2	305	XAT	4	0
23	5	310	CLA	6	0
23	b	840	CLA	5	0
23	6	308	CLA	5	0
21	2	301	XAT	3	0
23	a	830	CLA	7	0
21	3	303	XAT	2	0
25	6	301	A1L1F	2	0
26	b	849	LHG	2	0
23	a	813	CLA	1	0
23	b	836	CLA	5	0
23	4	308	CLA	3	0
28	a	855	LMG	10	0
23	a	812	CLA	2	0
21	2	303	XAT	11	0
23	8	313	CLA	3	0
23	1	312	CLA	2	0
21	9	305	XAT	3	0
23	b	833	CLA	5	0
23	b	837	CLA	7	0
21	6	305	XAT	3	0
30	a	847	BCR	3	0
23	5	311	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	313	CLA	1	0
28	j	103	LMG	6	0
23	b	809	CLA	1	0
21	5	301	XAT	4	0
25	8	304	A1L1F	2	0
30	f	801	BCR	24	0
23	a	822	CLA	5	0
23	8	312	CLA	2	0
23	6	313	CLA	1	0
23	9	308	CLA	5	0
23	a	810	CLA	9	0
21	8	302	XAT	6	0
22	9	301	A1L1G	2	0
23	a	801	CLA	6	0
23	b	831	CLA	1	0
27	4	317	DGD	11	0
30	b	844	BCR	2	0
23	1	306	CLA	5	0
23	b	806	CLA	5	0
23	b	832	CLA	11	0
21	9	303	XAT	6	0
30	b	846	BCR	2	0
23	5	308	CLA	7	0
23	a	808	CLA	1	0
30	b	845	BCR	6	0
26	a	846	LHG	2	0
21	6	303	XAT	10	0
23	5	313	CLA	3	0
23	6	314	CLA	1	0
23	b	816	CLA	4	0
23	b	819	CLA	1	0
21	8	301	XAT	3	0
21	5	305	XAT	5	0
23	2	310	CLA	3	0
23	b	820	CLA	2	0
23	2	316	CLA	2	0
30	i	101	BCR	4	0
23	b	823	CLA	6	0
27	8	315	DGD	2	0
23	a	834	CLA	7	0
23	b	828	CLA	3	0
23	j	101	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	316	CLA	7	0
23	4	309	CLA	4	0
24	5	317	SQD	1	0
23	a	806	CLA	10	0
23	7	311	CLA	3	0
23	3	309	CLA	1	0
22	9	306	A1L1G	1	0
23	a	837	CLA	1	0
23	b	839	CLA	15	0
23	b	825	CLA	3	0
23	7	313	CLA	4	0
23	a	838	CLA	1	0
26	9	307	LHG	1	0
21	2	304	XAT	3	0
23	f	802	CLA	1	0
23	9	316	CLA	12	0
23	b	808	CLA	3	0
23	9	309	CLA	1	0
23	a	816	CLA	2	0
23	a	829	CLA	7	0
23	9	315	CLA	1	0
23	8	305	CLA	4	0
23	h	201	CLA	5	0
30	a	848	BCR	5	0
23	4	307	CLA	6	0
23	7	308	CLA	7	0
23	b	817	CLA	8	0
30	b	850	BCR	4	0
23	5	309	CLA	1	0
23	b	813	CLA	6	0
21	8	303	XAT	6	0
21	9	304	XAT	7	0
23	a	825	CLA	5	0
21	7	305	XAT	2	0
23	a	833	CLA	11	0
21	3	304	XAT	4	0
25	9	302	A1L1F	1	0
23	b	824	CLA	6	0
23	a	809	CLA	2	0
23	a	827	CLA	3	0
30	f	804	BCR	7	0
30	b	848	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	9	313	CLA	2	0
21	4	302	XAT	9	0
29	a	843	PQN	4	0
23	7	310	CLA	1	0
21	7	303	XAT	12	0
21	a	854	XAT	3	0
21	a	853	XAT	4	0
23	a	804	CLA	2	0
23	b	841	CLA	4	0
30	b	847	BCR	6	0
23	7	312	CLA	1	0
23	a	818	CLA	12	0
23	a	835	CLA	4	0
23	b	818	CLA	3	0
23	l	202	CLA	9	0
26	a	845	LHG	3	0
26	m	101	LHG	2	0
23	3	312	CLA	1	0
23	a	852	CLA	4	0
23	b	807	CLA	2	0
23	b	822	CLA	5	0
23	7	306	CLA	2	0
23	8	311	CLA	3	0
30	j	102	BCR	14	0
24	1	315	SQD	3	0
23	b	801	CLA	16	0
23	b	802	CLA	3	0
30	b	852	BCR	12	0
23	4	305	CLA	2	0
25	1	304	A1L1F	11	0
23	4	314	CLA	1	0
23	4	312	CLA	3	0
23	7	315	CLA	2	0
23	1	308	CLA	4	0
23	8	308	CLA	2	0
23	a	831	CLA	5	0
23	7	307	CLA	2	0
31	c	102	SF4	3	0
23	5	315	CLA	3	0
23	b	811	CLA	2	0
23	b	830	CLA	5	0
23	b	838	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	303	XAT	4	0
23	a	844	CLA	17	0
23	5	316	CLA	1	0
21	7	301	XAT	3	0
21	3	301	XAT	4	0
21	7	304	XAT	11	0
23	b	804	CLA	3	0
23	b	812	CLA	5	0
23	l	201	CLA	1	0
30	b	843	BCR	4	0
23	a	840	CLA	6	0
23	9	312	CLA	4	0
23	b	803	CLA	4	0
23	6	309	CLA	2	0
23	b	834	CLA	4	0
25	6	304	A1L1F	3	0
23	a	828	CLA	5	0
29	b	842	PQN	6	0
23	b	810	CLA	22	0
30	a	849	BCR	4	0
23	a	823	CLA	3	0
23	8	314	CLA	1	0
23	5	312	CLA	1	0
23	h	203	CLA	2	0
23	b	821	CLA	3	0
23	3	311	CLA	1	0
27	b	851	DGD	6	0
23	8	306	CLA	1	0
30	b	853	BCR	16	0
23	b	814	CLA	3	0
21	6	302	XAT	3	0
21	5	302	XAT	6	0
23	a	807	CLA	4	0
22	7	302	A1L1G	2	0
23	a	803	CLA	13	0
23	a	832	CLA	2	0
23	a	824	CLA	1	0
23	b	829	CLA	4	0
23	a	826	CLA	8	0
23	a	802	CLA	14	0
23	b	805	CLA	2	0
21	4	304	XAT	6	0

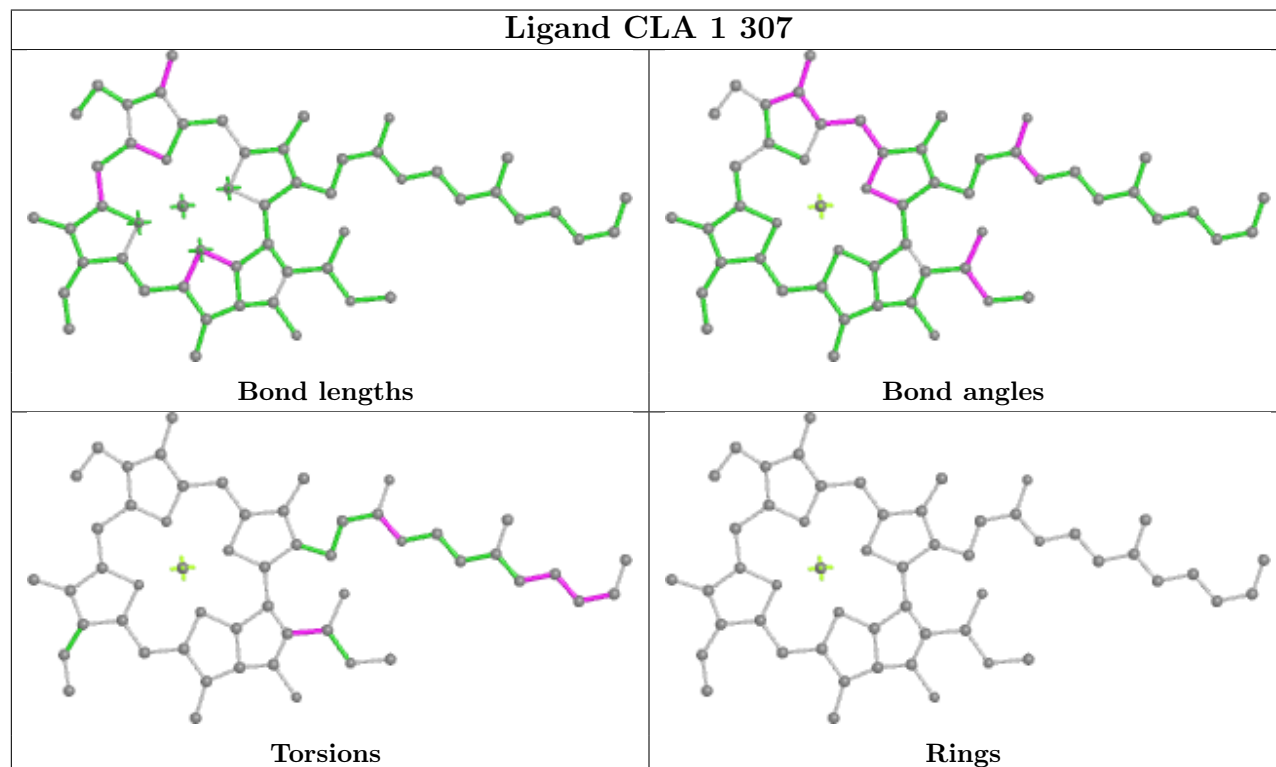
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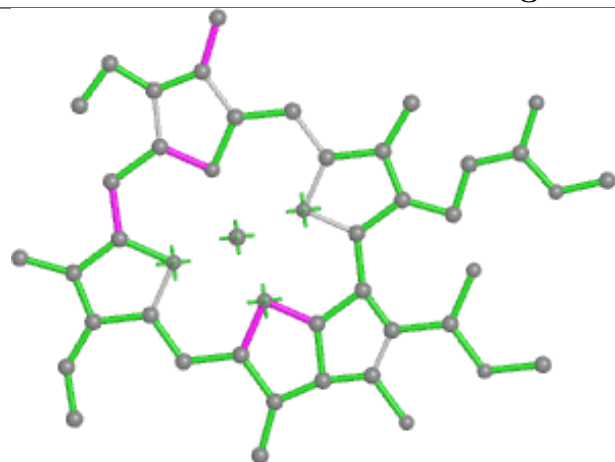
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	304	A1L1G	1	0
23	7	314	CLA	3	0
25	h	202	A1L1F	4	0
23	2	314	CLA	1	0
21	6	306	XAT	2	0
21	3	305	XAT	4	0
23	7	316	CLA	1	0
21	4	303	XAT	3	0
23	b	826	CLA	5	0
23	f	803	CLA	1	0
23	a	819	CLA	5	0
23	8	307	CLA	5	0
28	2	317	LMG	3	0
30	i	102	BCR	13	0
23	a	842	CLA	4	0
23	b	835	CLA	1	0
23	3	313	CLA	3	0
23	1	311	CLA	4	0
23	8	310	CLA	1	0
21	1	302	XAT	3	0
23	6	315	CLA	3	0
23	a	839	CLA	3	0
23	a	841	CLA	17	0
23	2	308	CLA	4	0
22	1	301	A1L1G	1	0
21	5	303	XAT	9	0
23	4	310	CLA	2	0
23	a	814	CLA	3	0
23	a	820	CLA	6	0
21	2	302	XAT	3	0
23	9	314	CLA	7	0
30	a	850	BCR	2	0
23	9	311	CLA	2	0
23	5	306	CLA	2	0
23	b	827	CLA	4	0
23	4	306	CLA	1	0
23	4	311	CLA	1	0
23	a	805	CLA	1	0
23	9	310	CLA	1	0
21	4	301	XAT	6	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

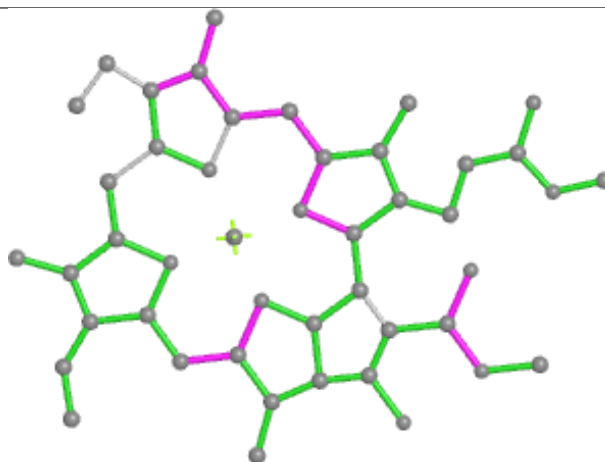
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



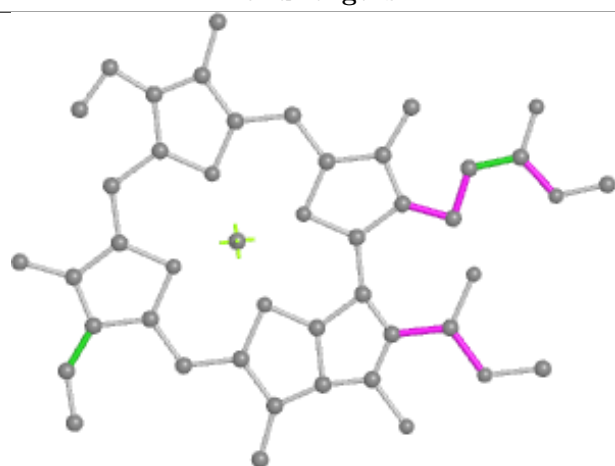
Ligand CLA 4 315



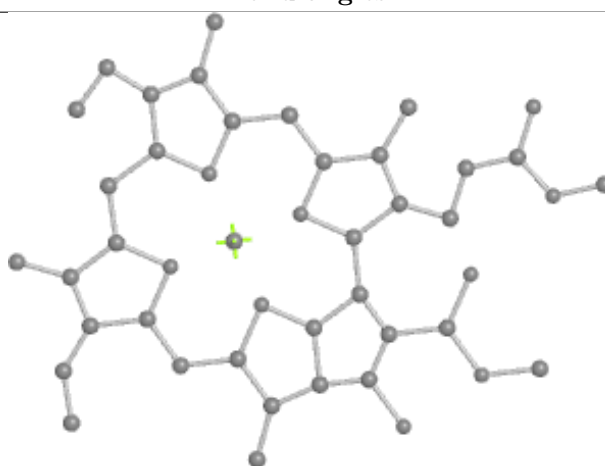
Bond lengths



Bond angles

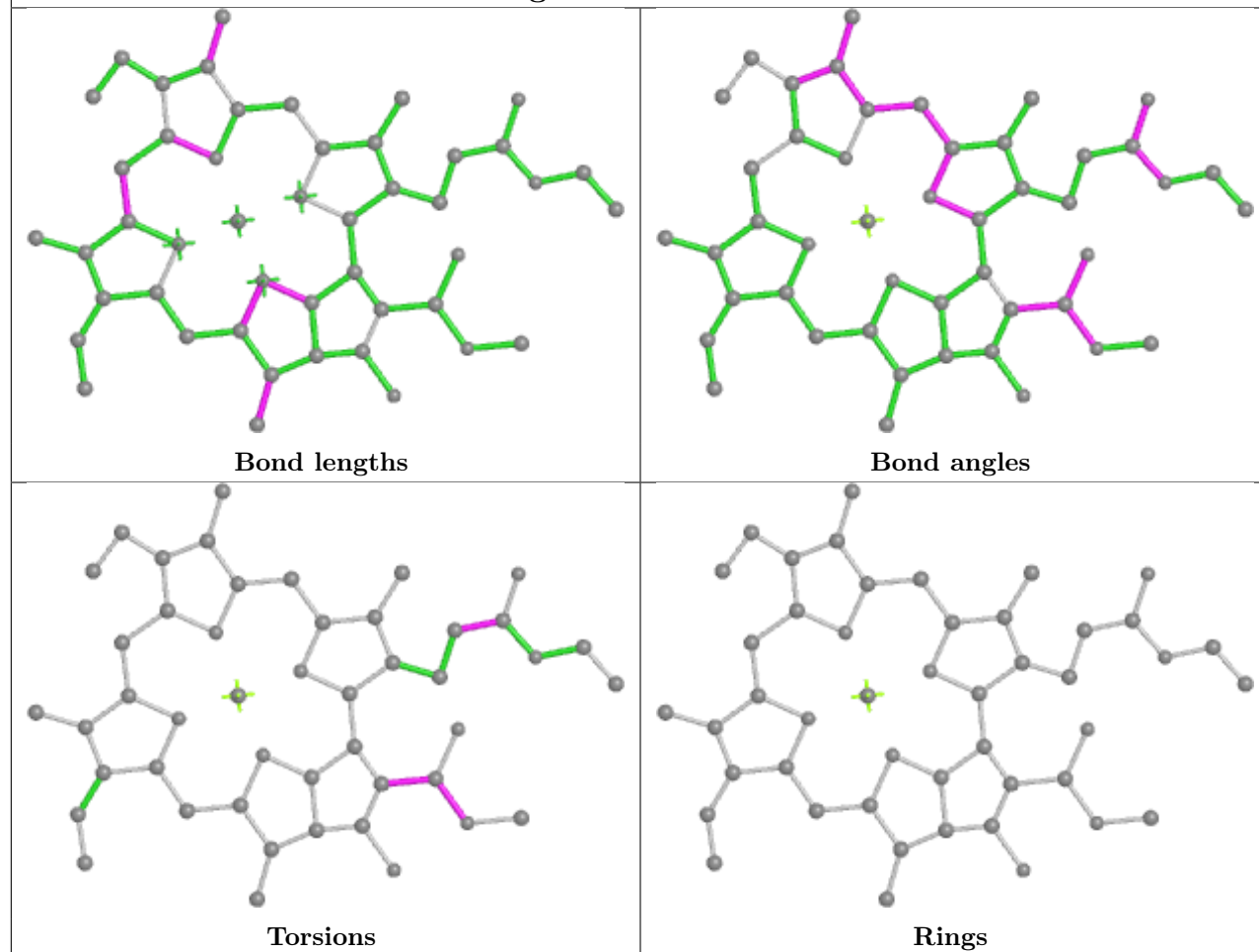


Torsions

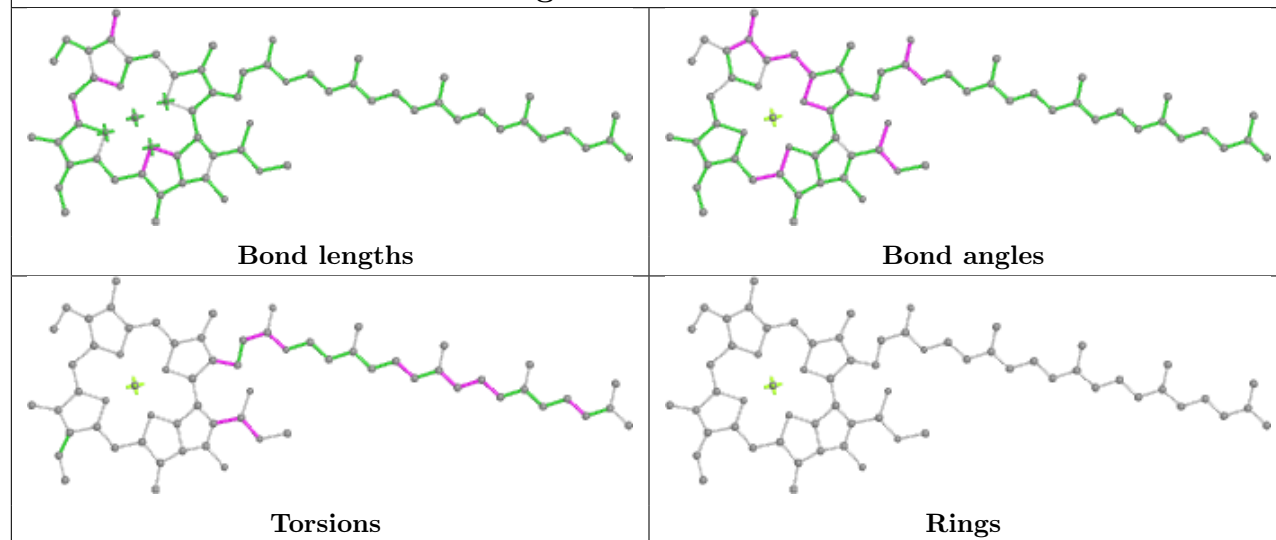


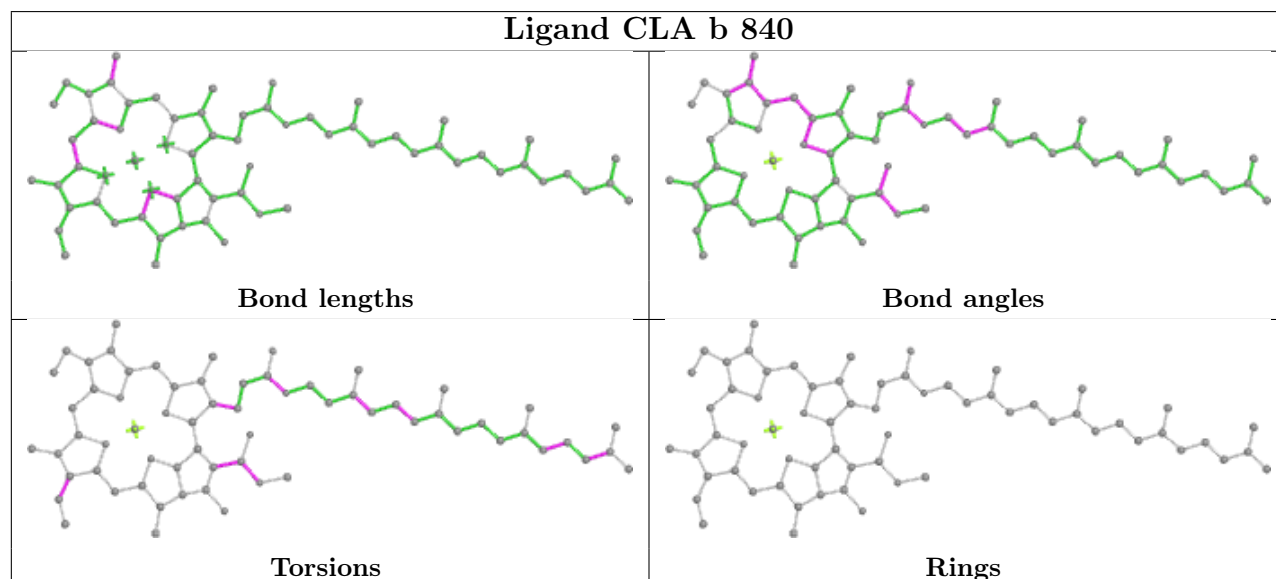
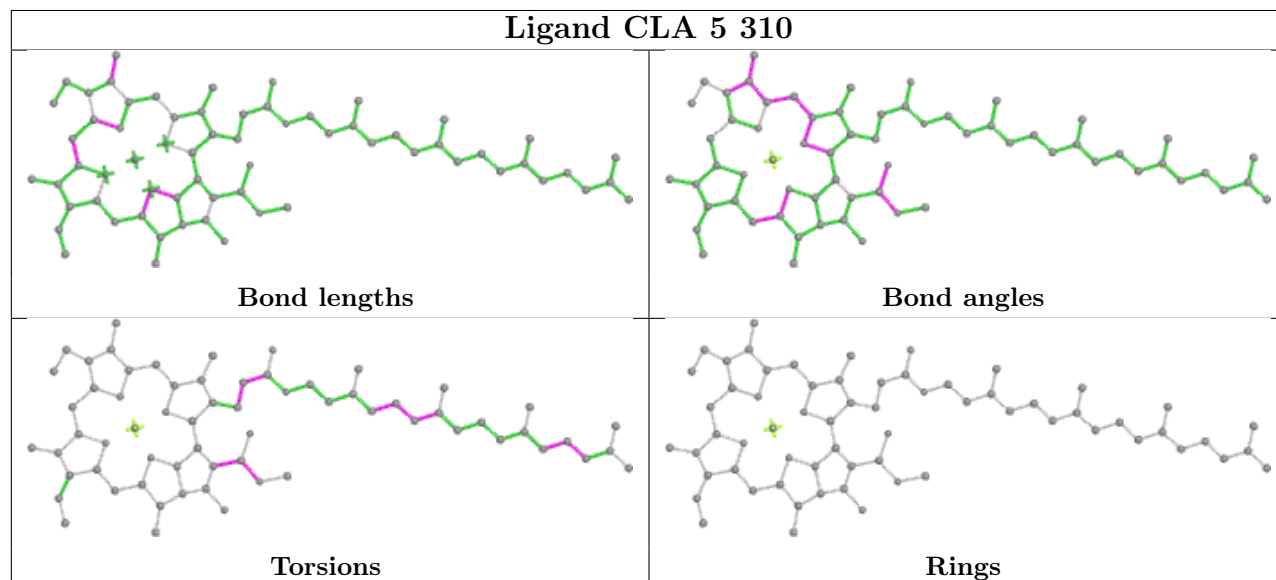
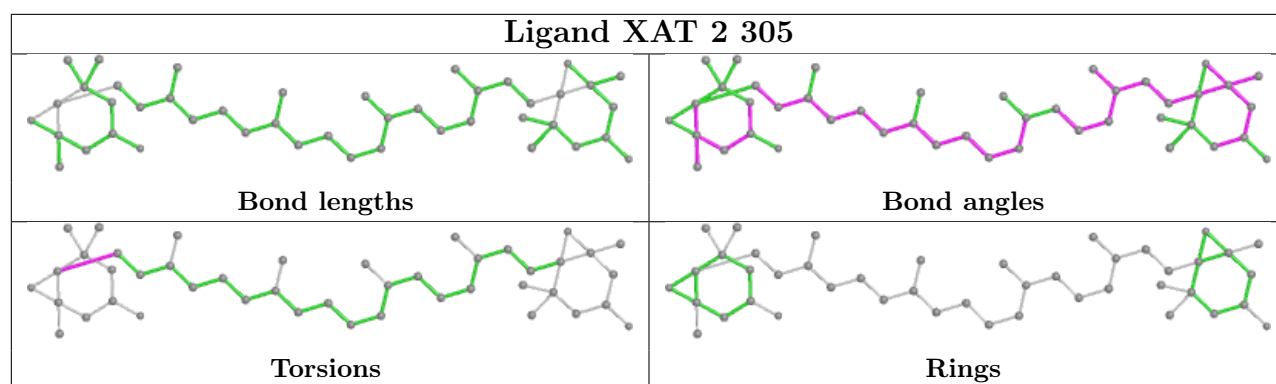
Rings

Ligand CLA 3 308

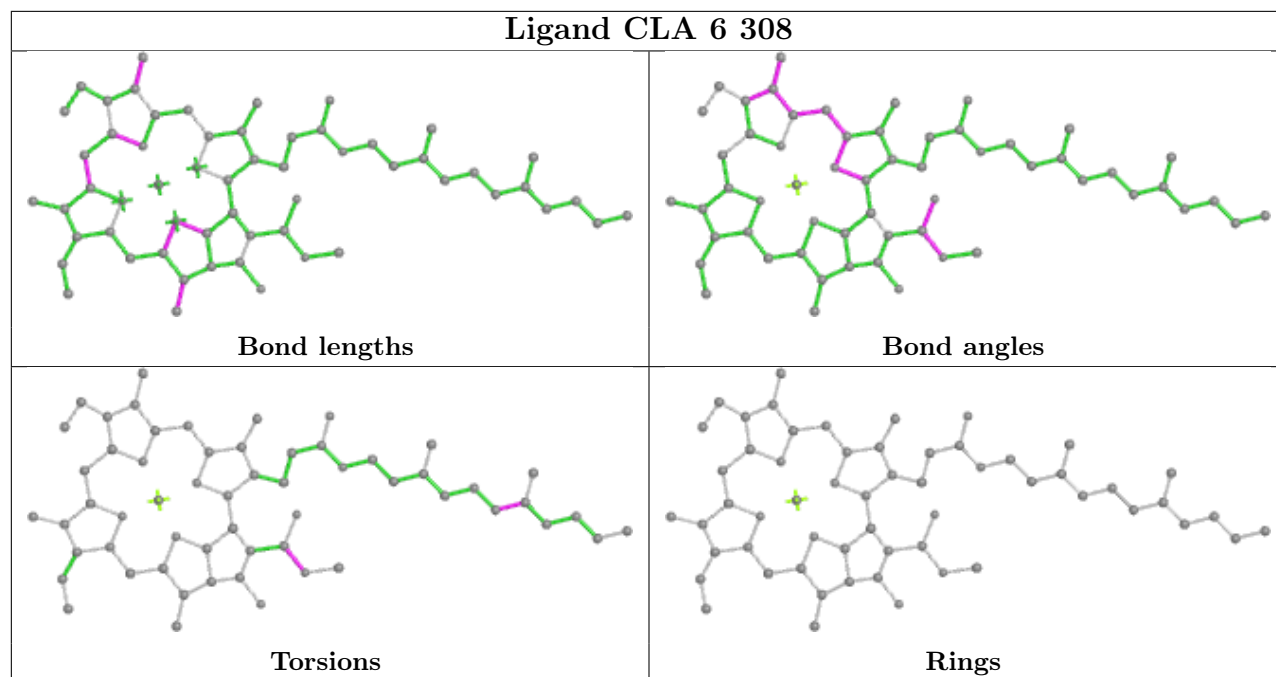


Ligand CLA a 856

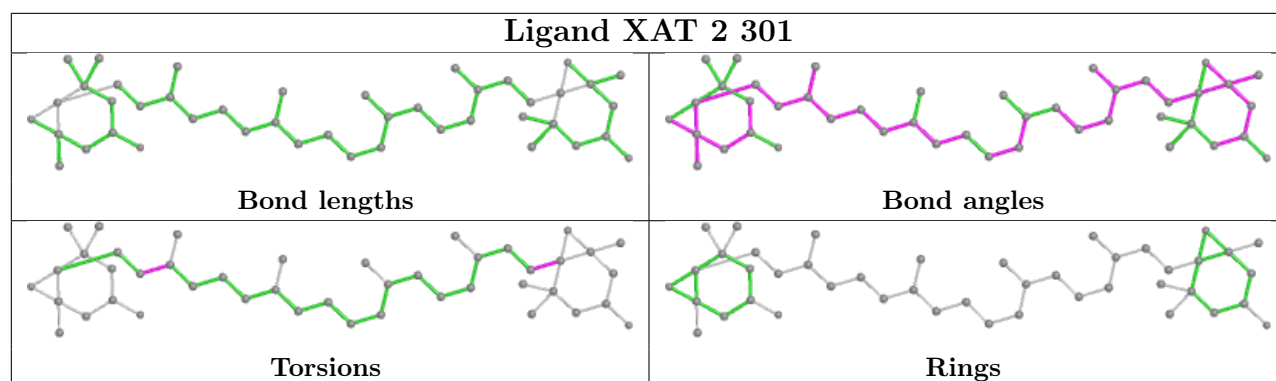




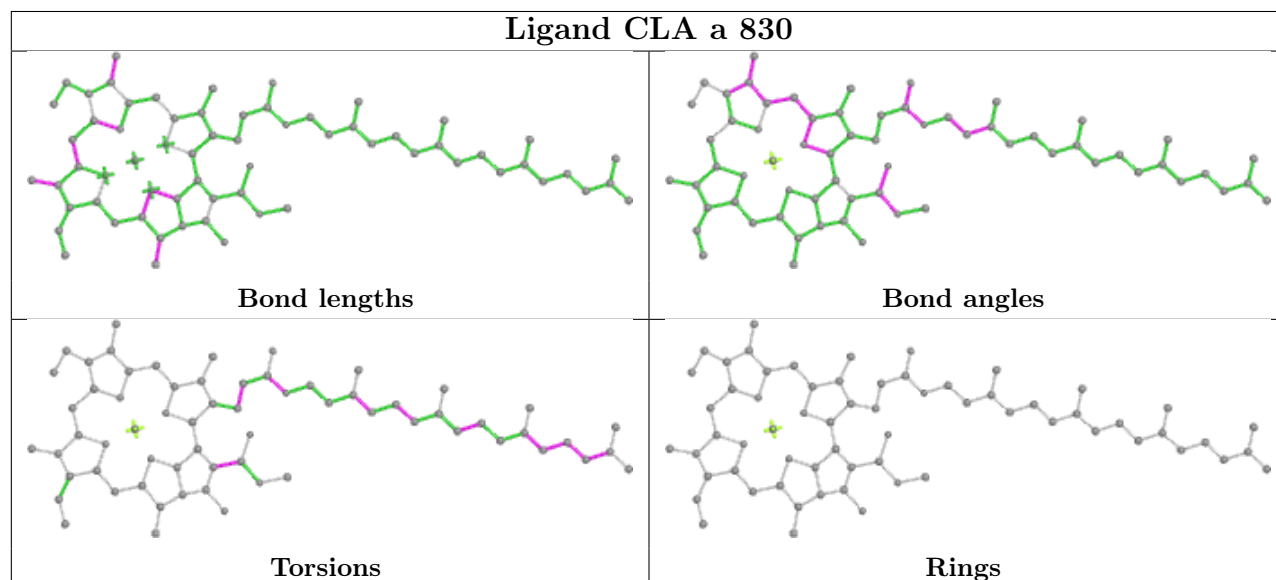
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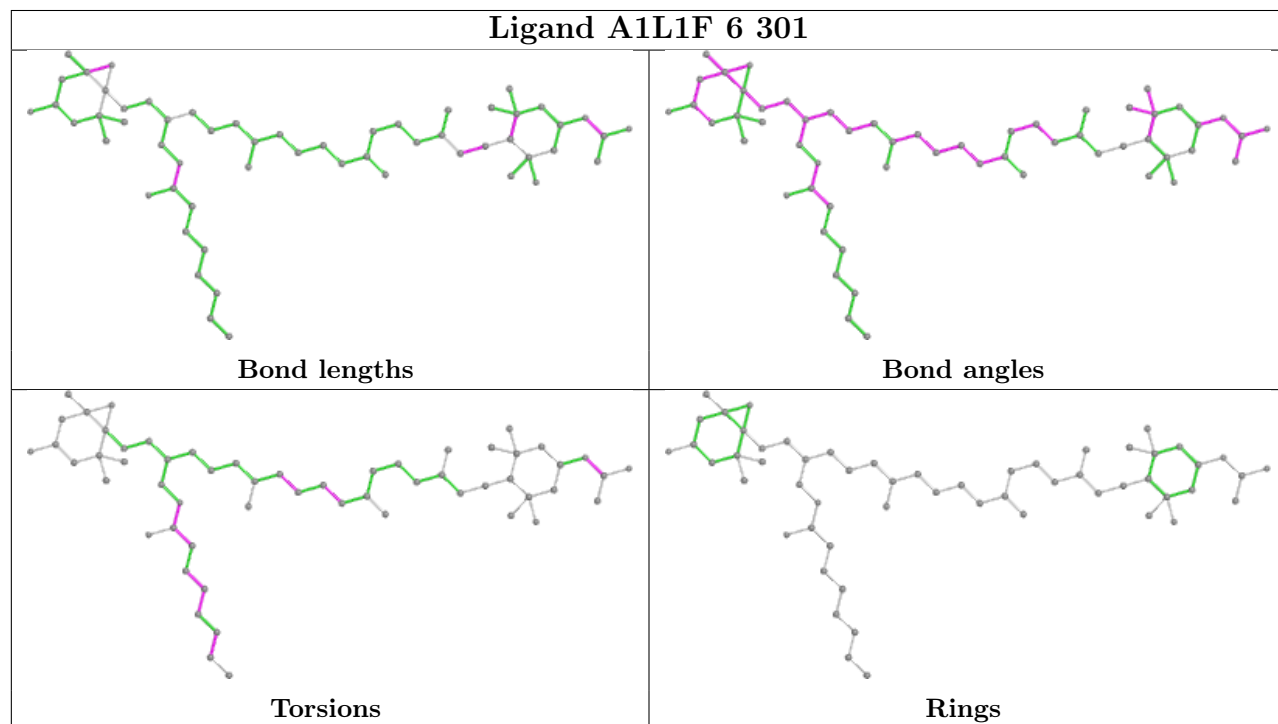
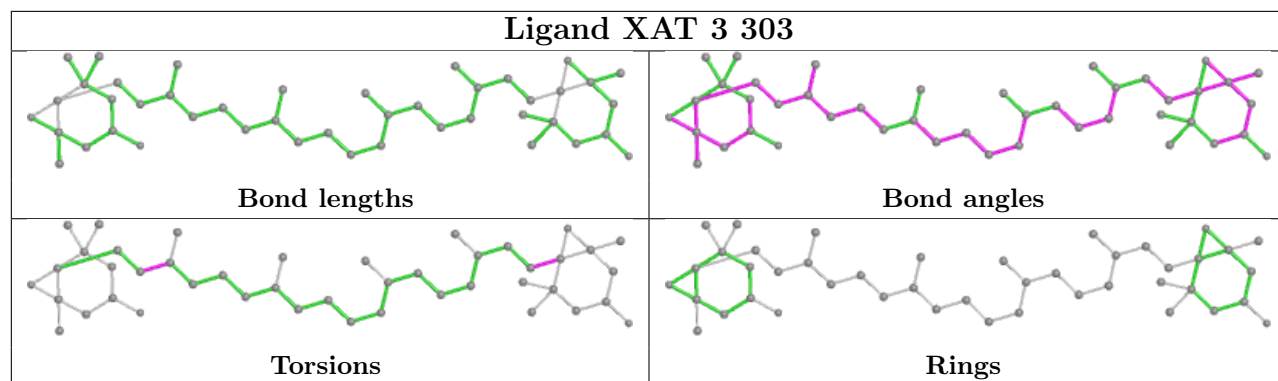


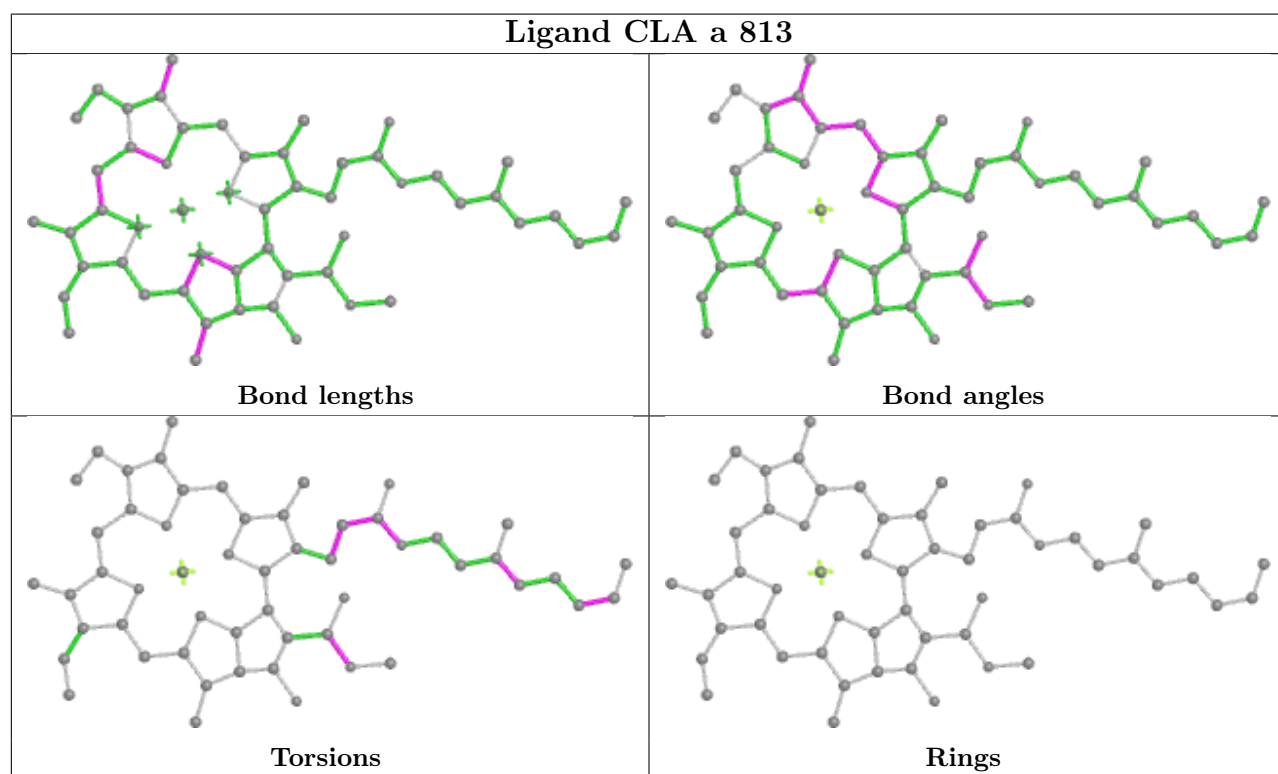
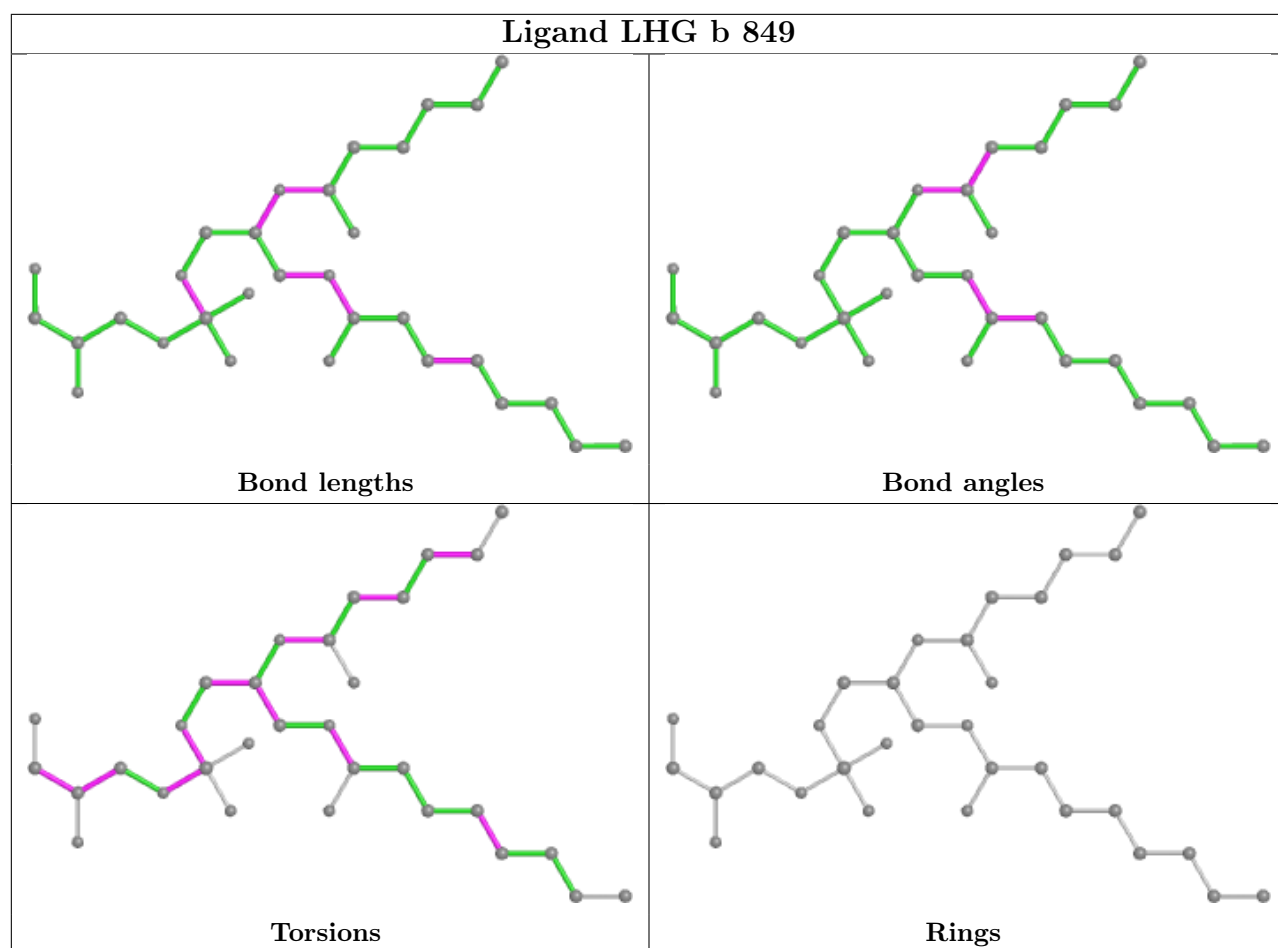
Ligand XAT 2 301



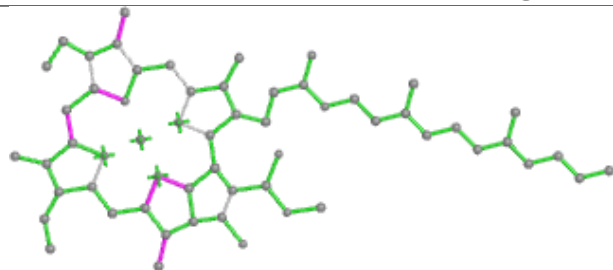
Ligand CLA a 830



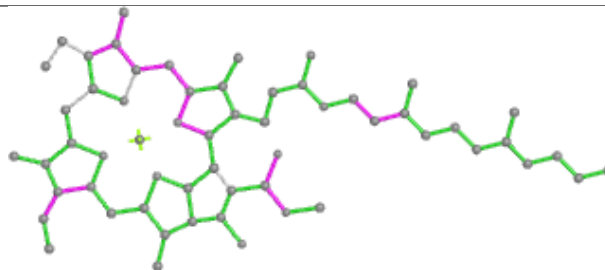




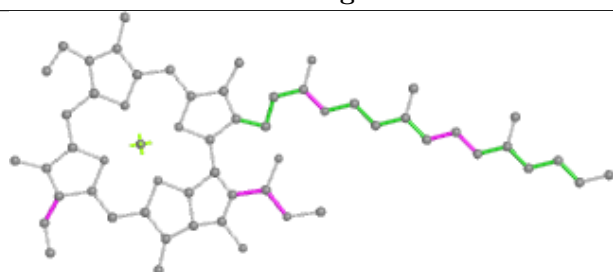
Ligand CLA b 836



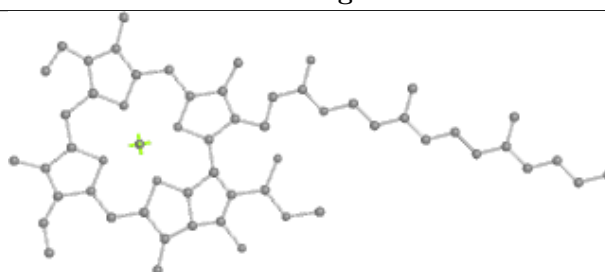
Bond lengths



Bond angles

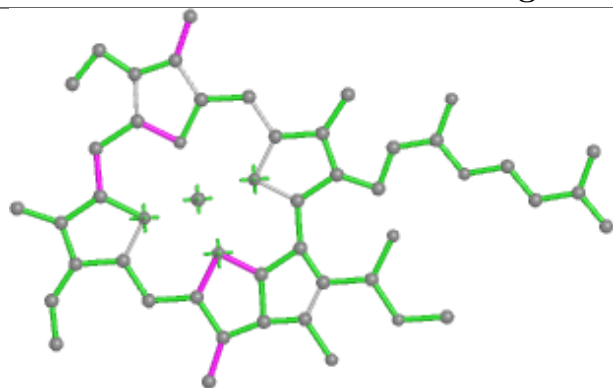


Torsions

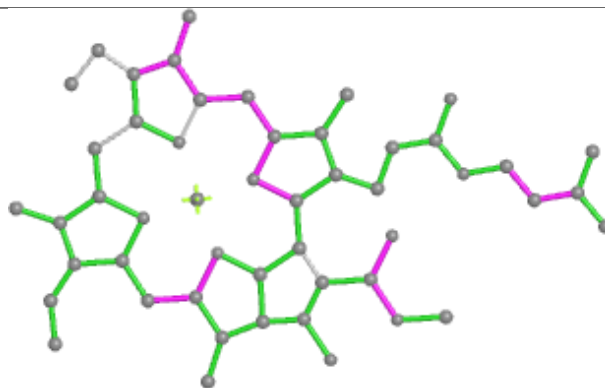


Rings

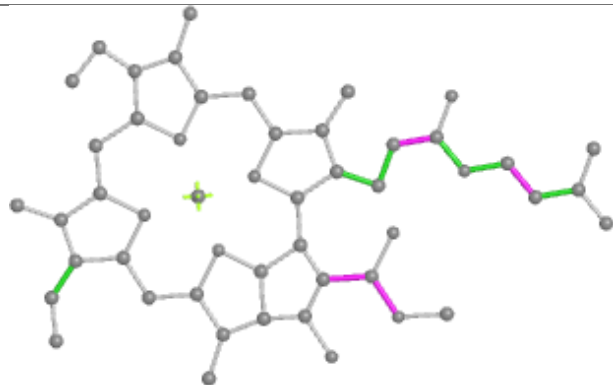
Ligand CLA 4 308



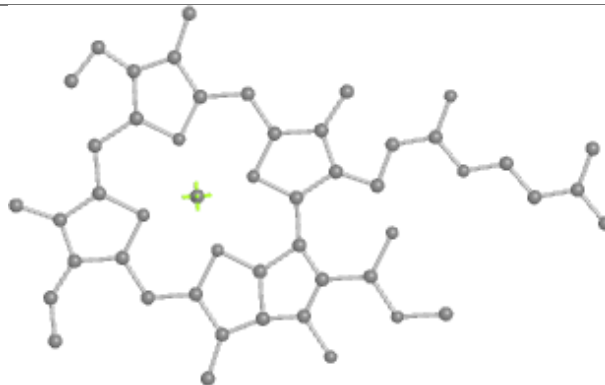
Bond lengths



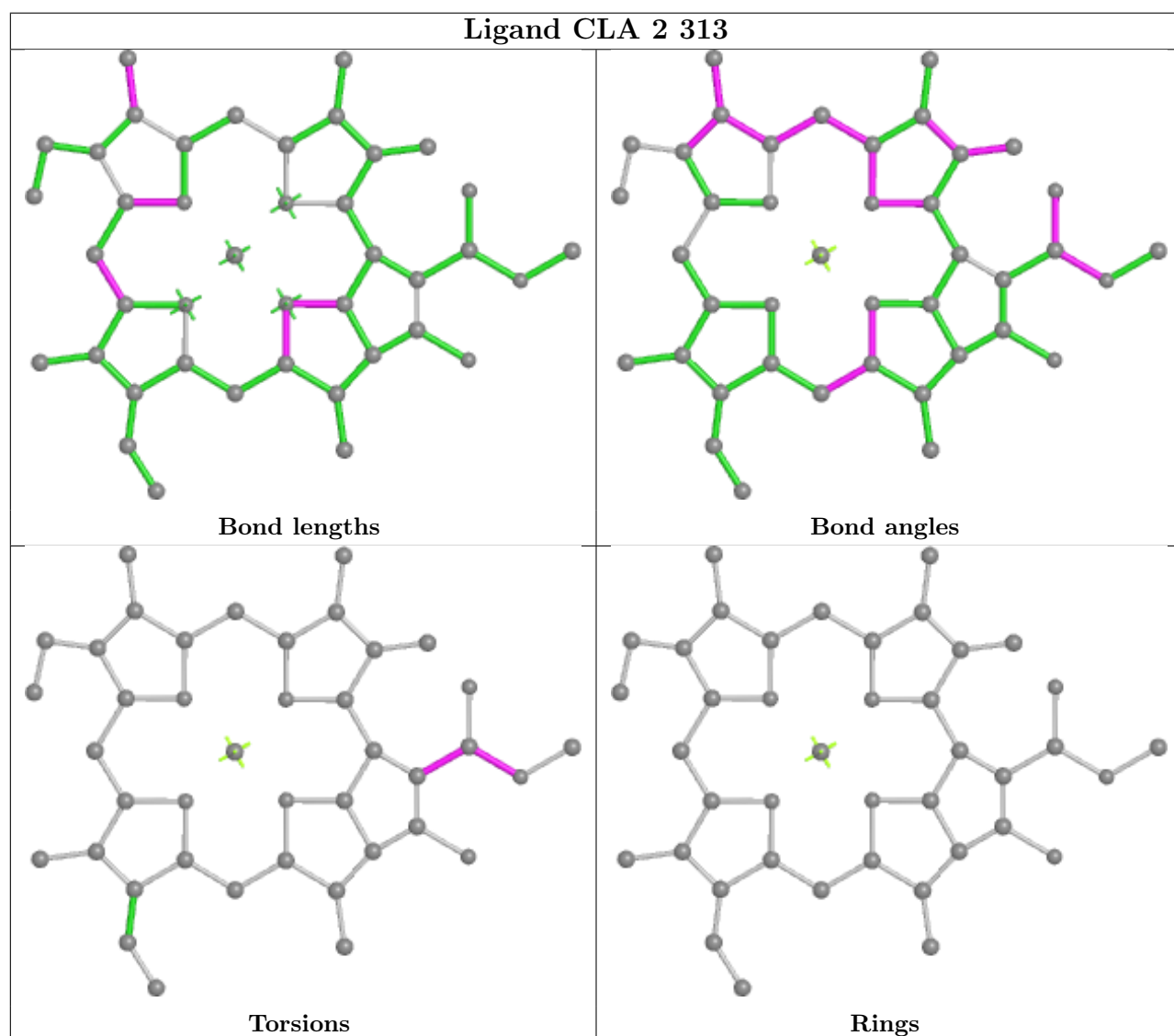
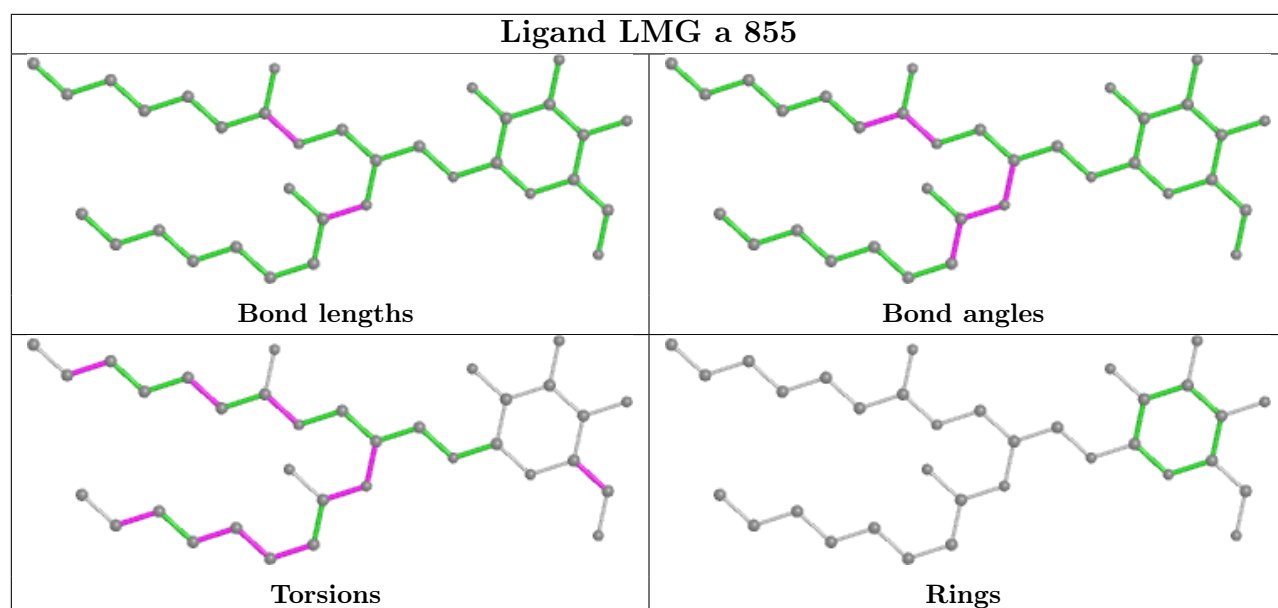
Bond angles

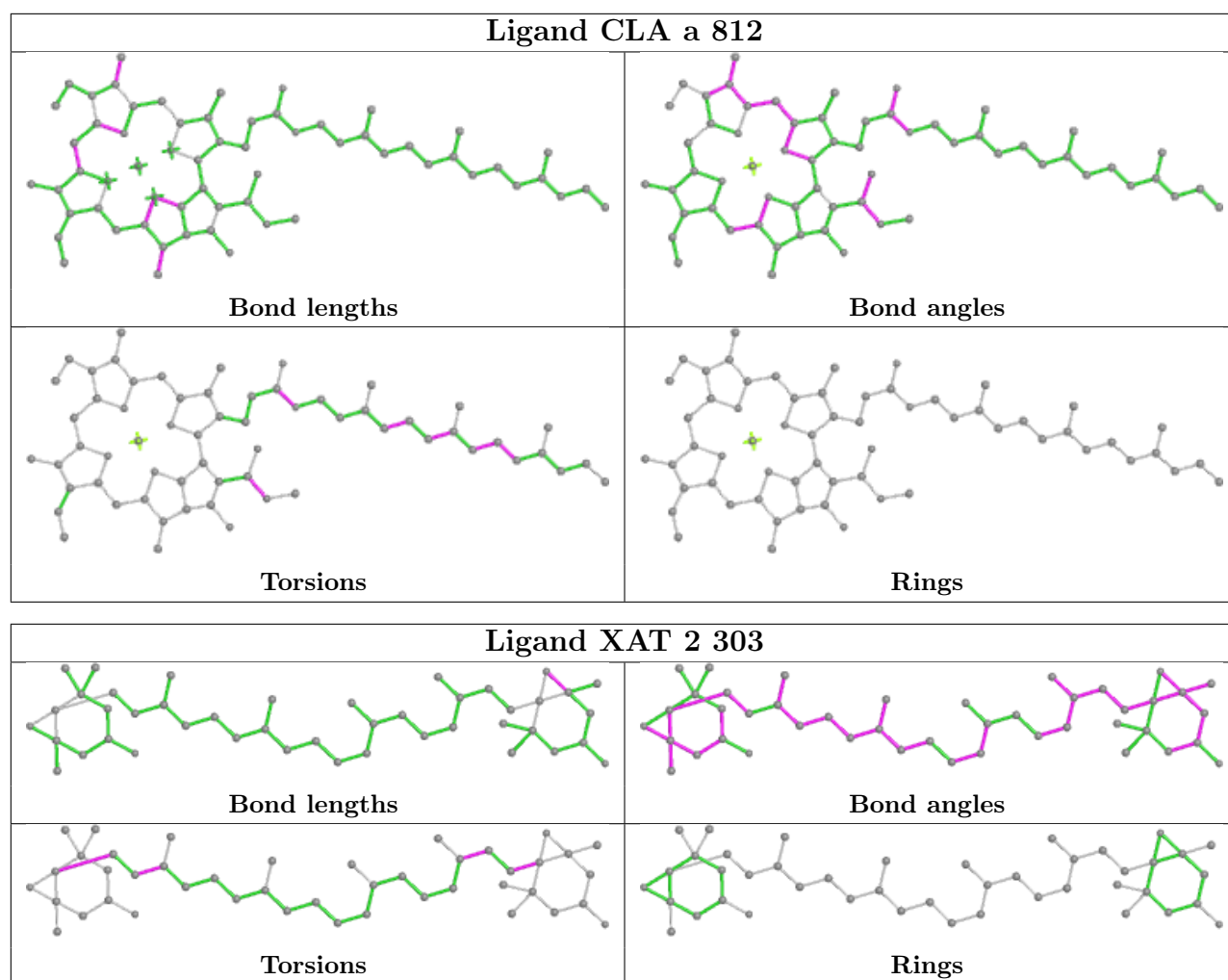


Torsions

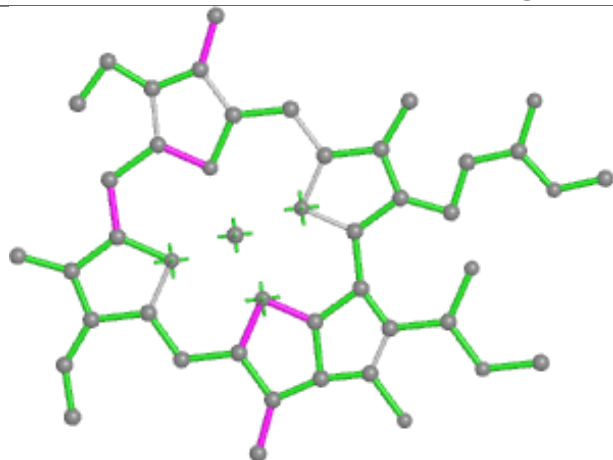


Rings

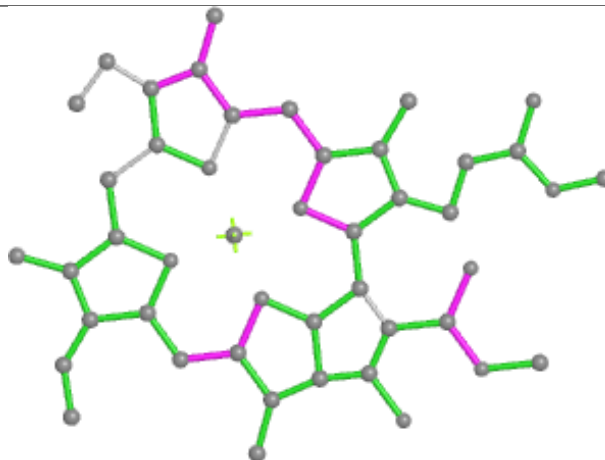




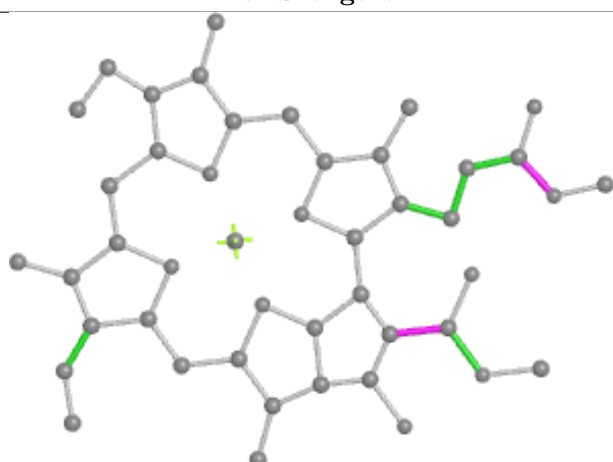
Ligand CLA 8 313



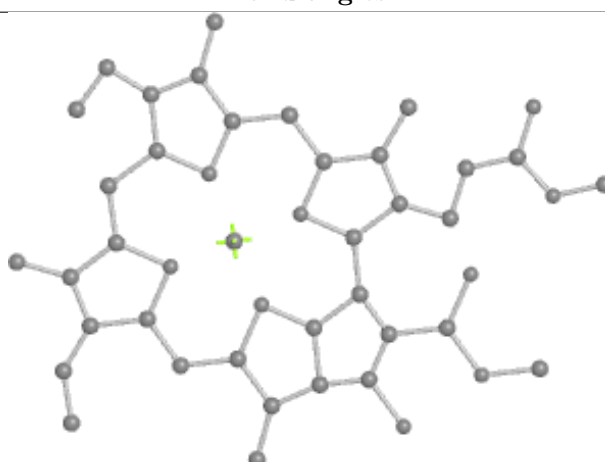
Bond lengths



Bond angles

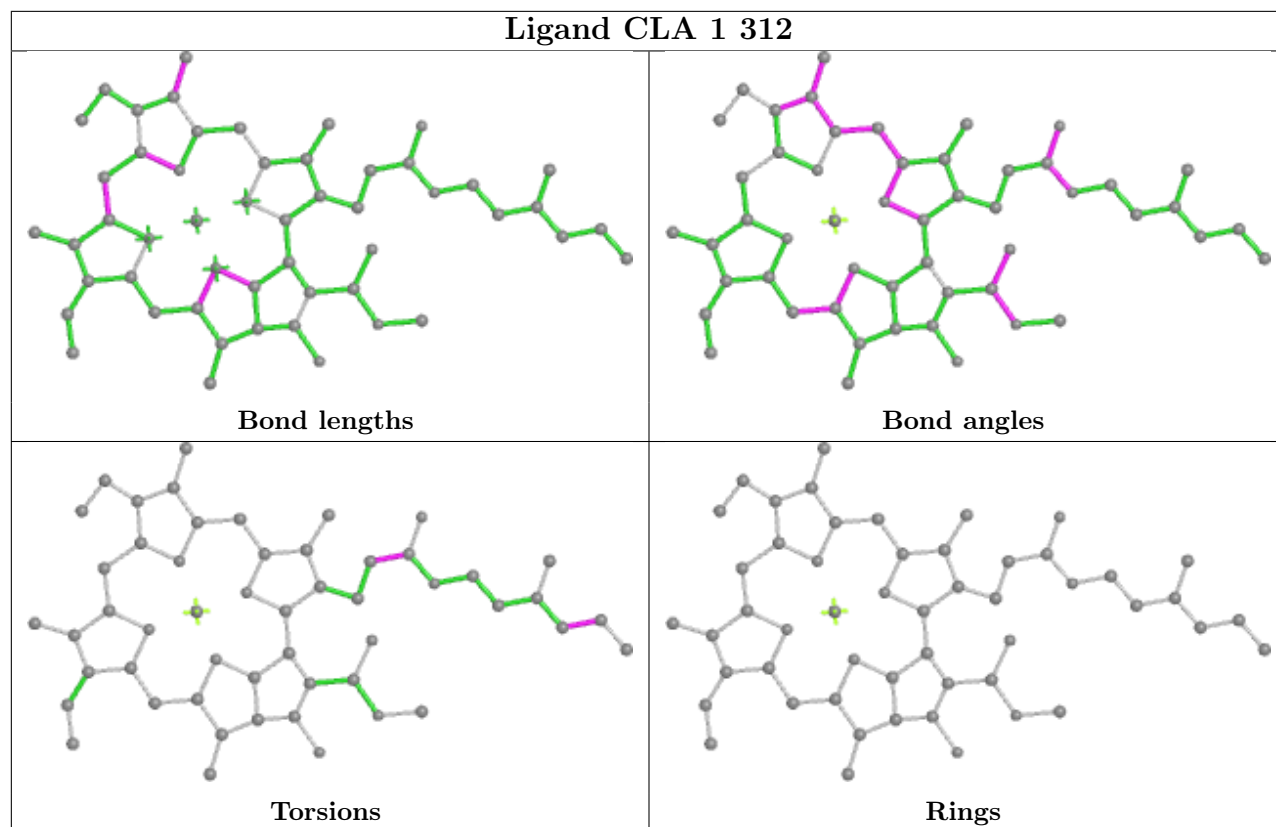


Torsions

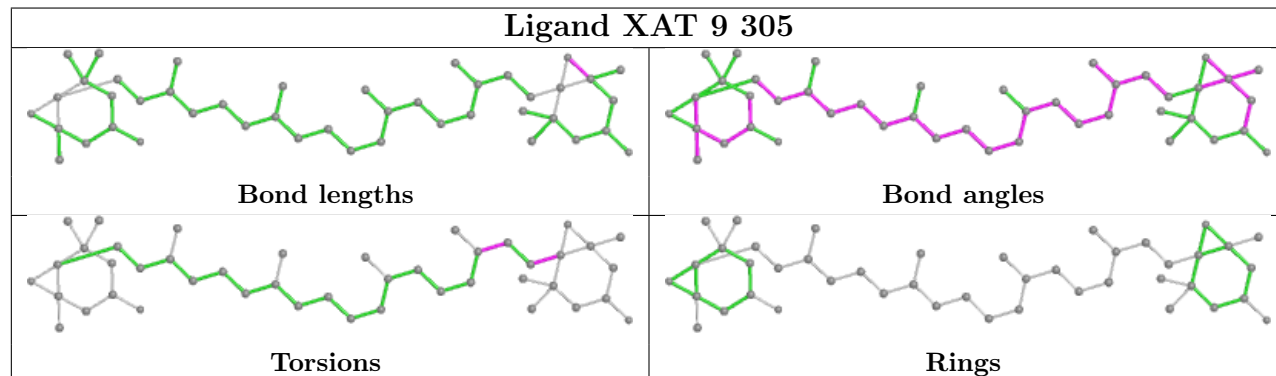


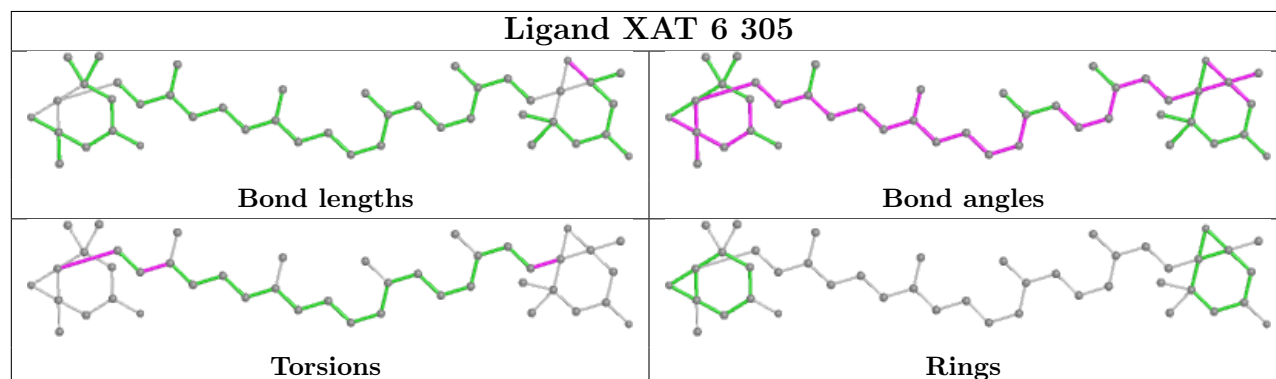
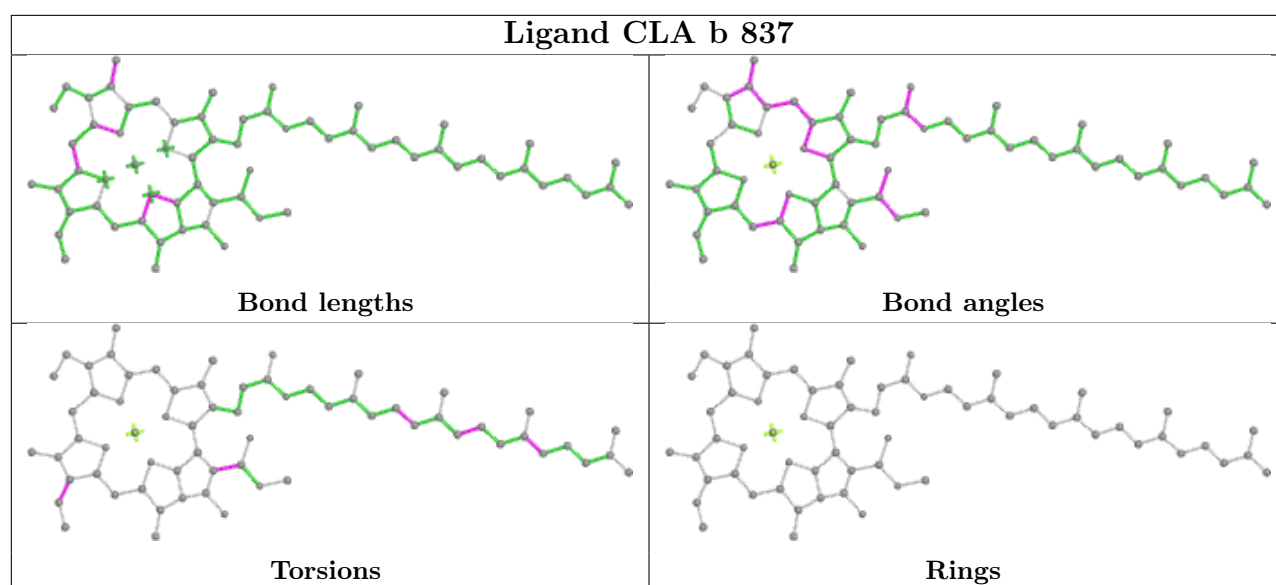
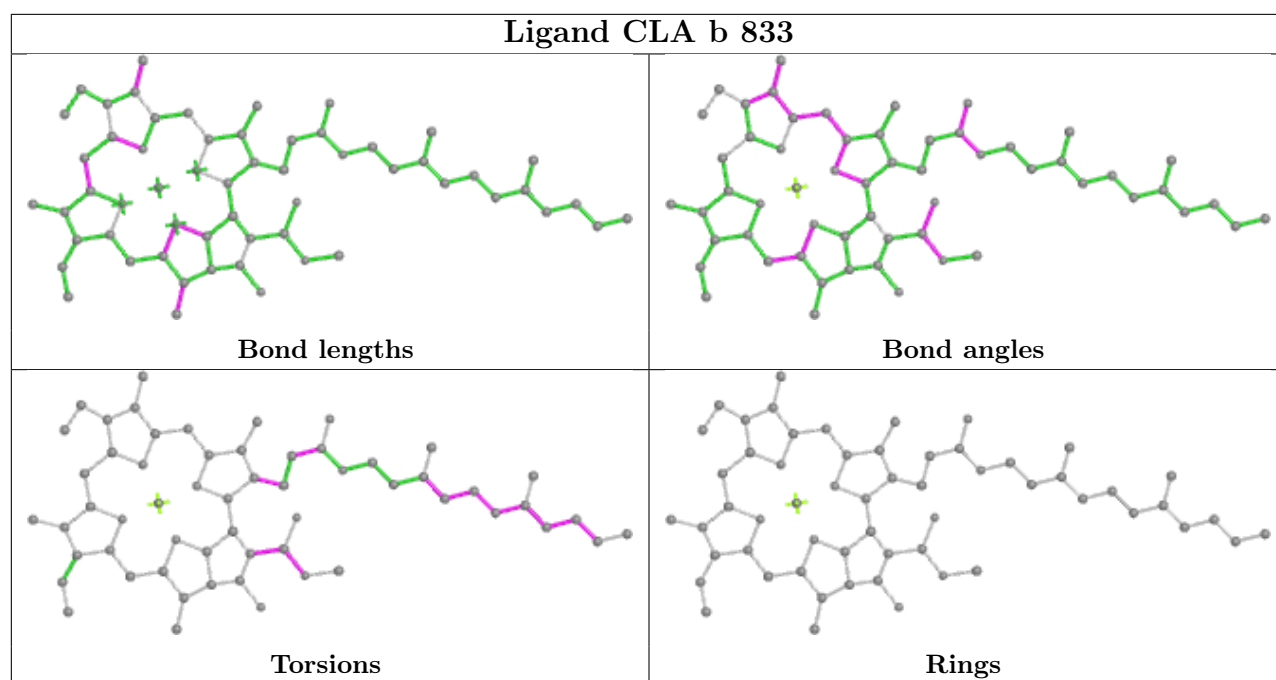
Rings

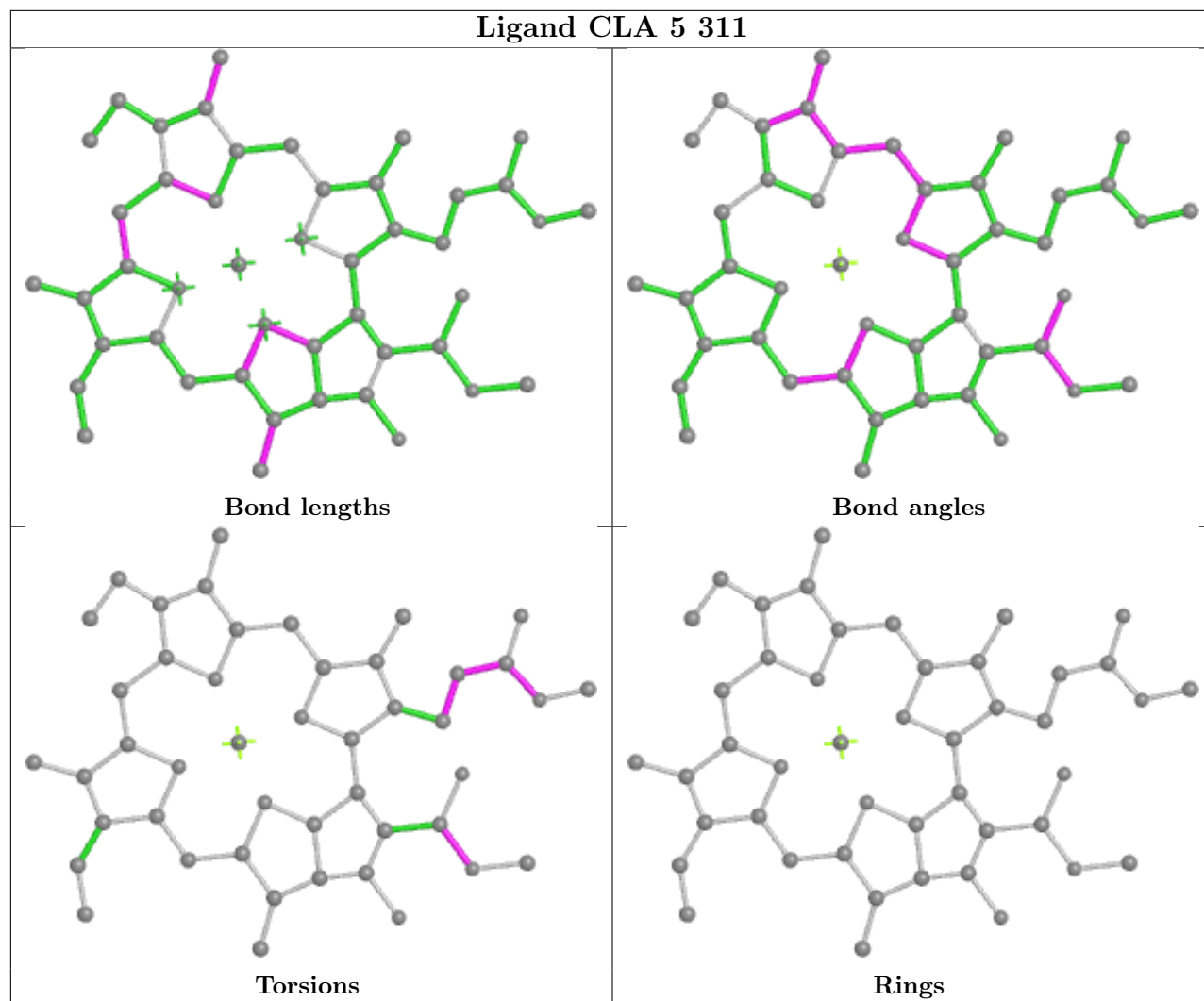
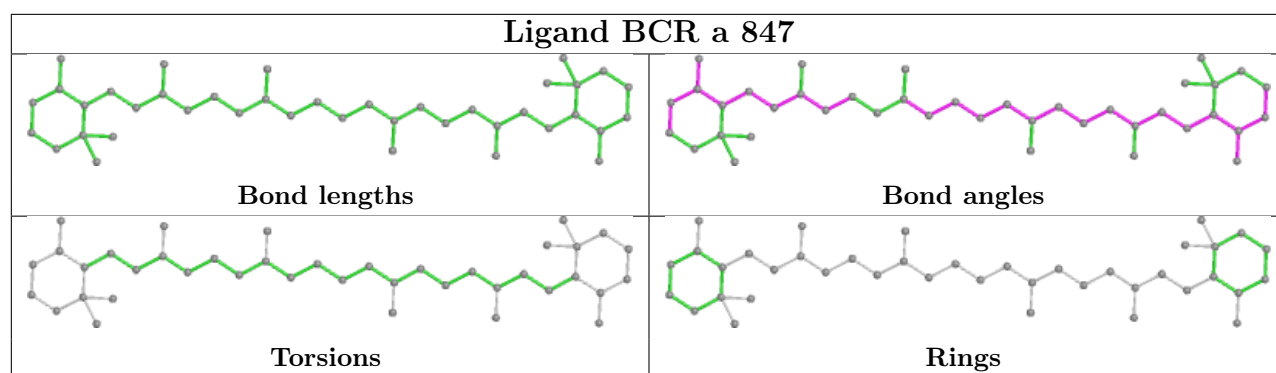
Ligand CLA 1 312



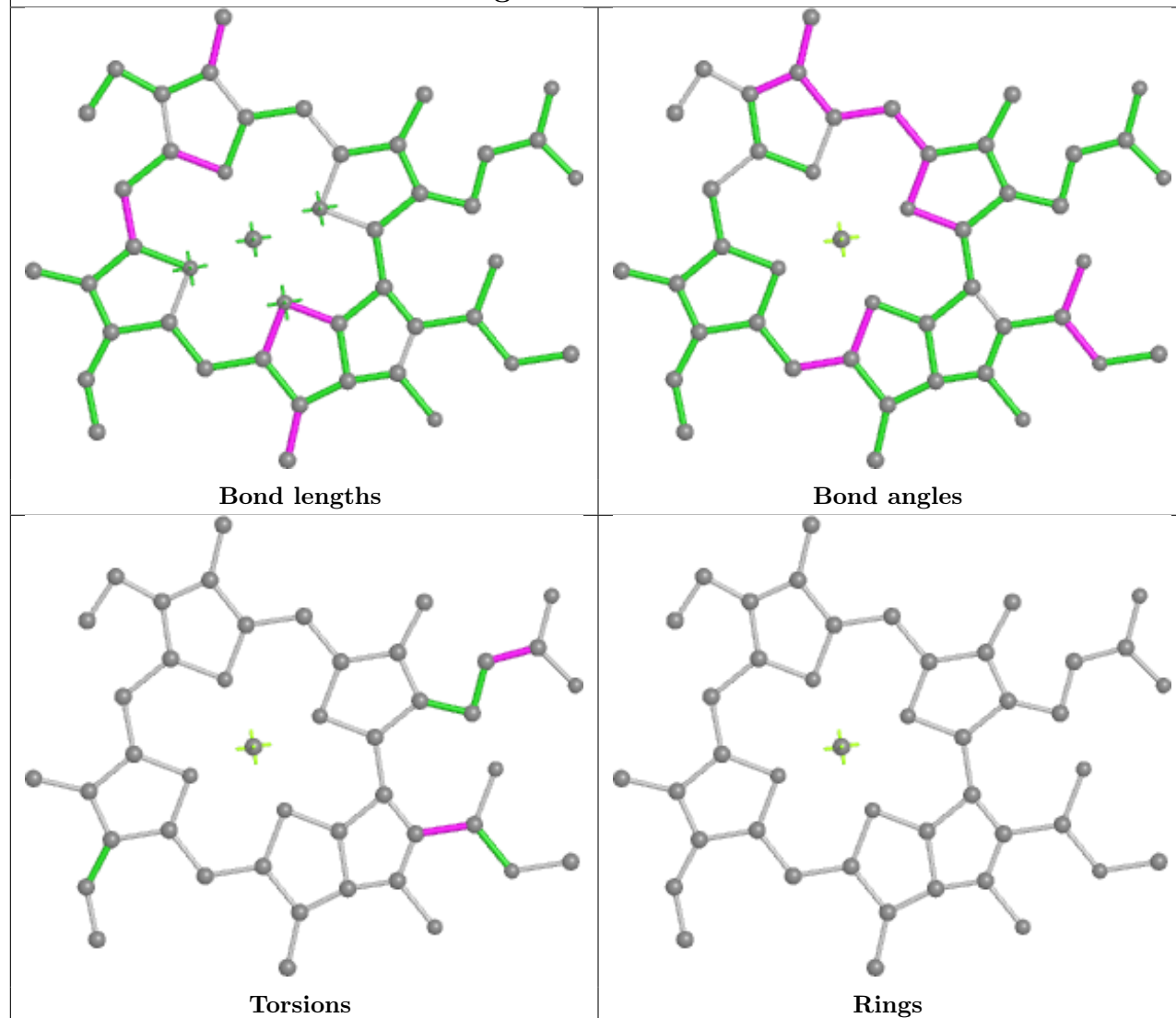
Ligand XAT 9 305



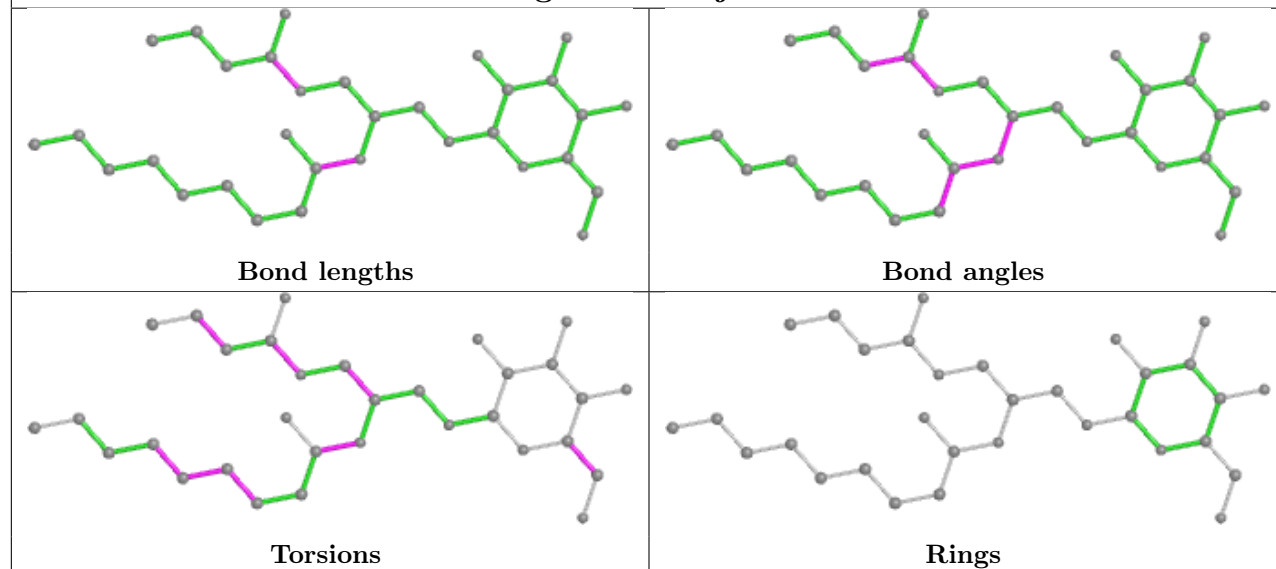


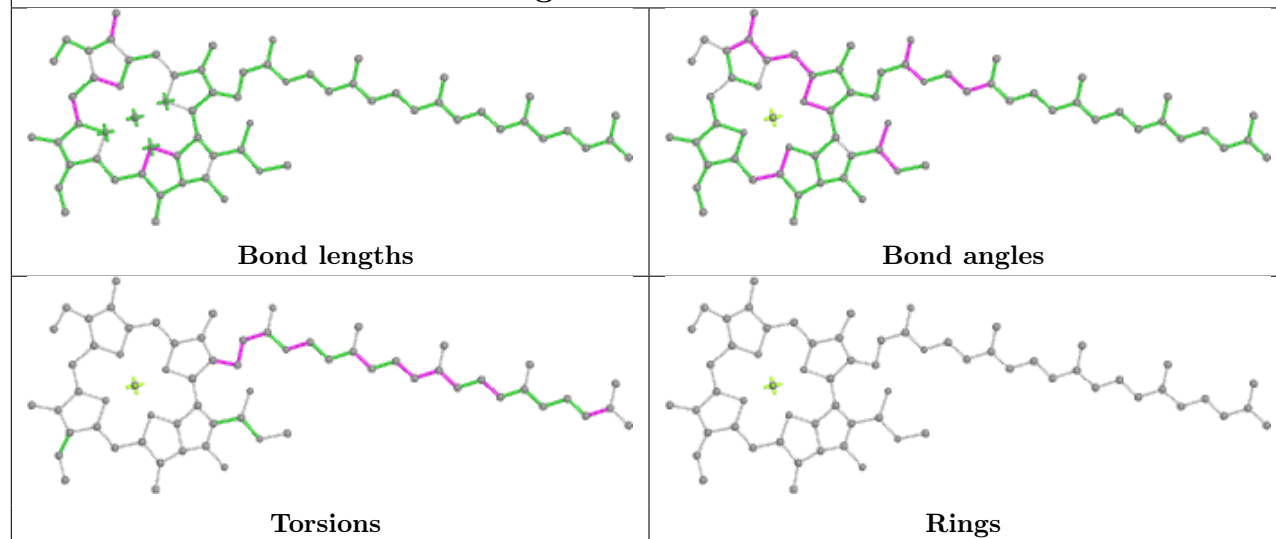
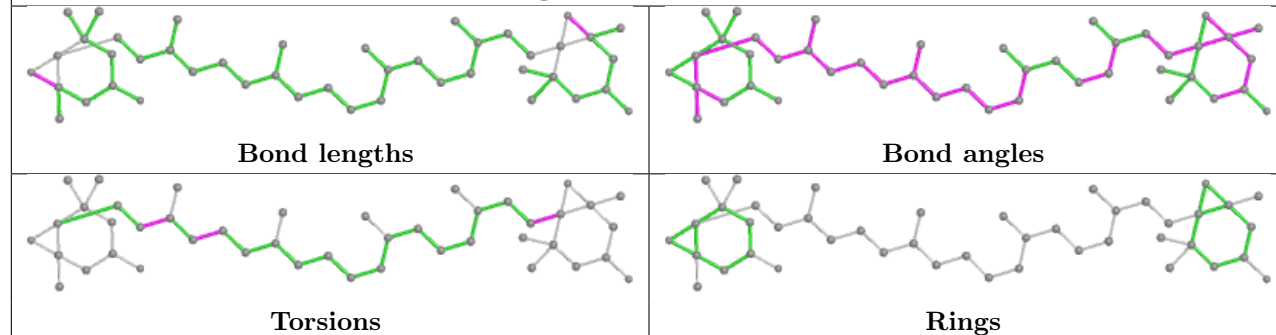
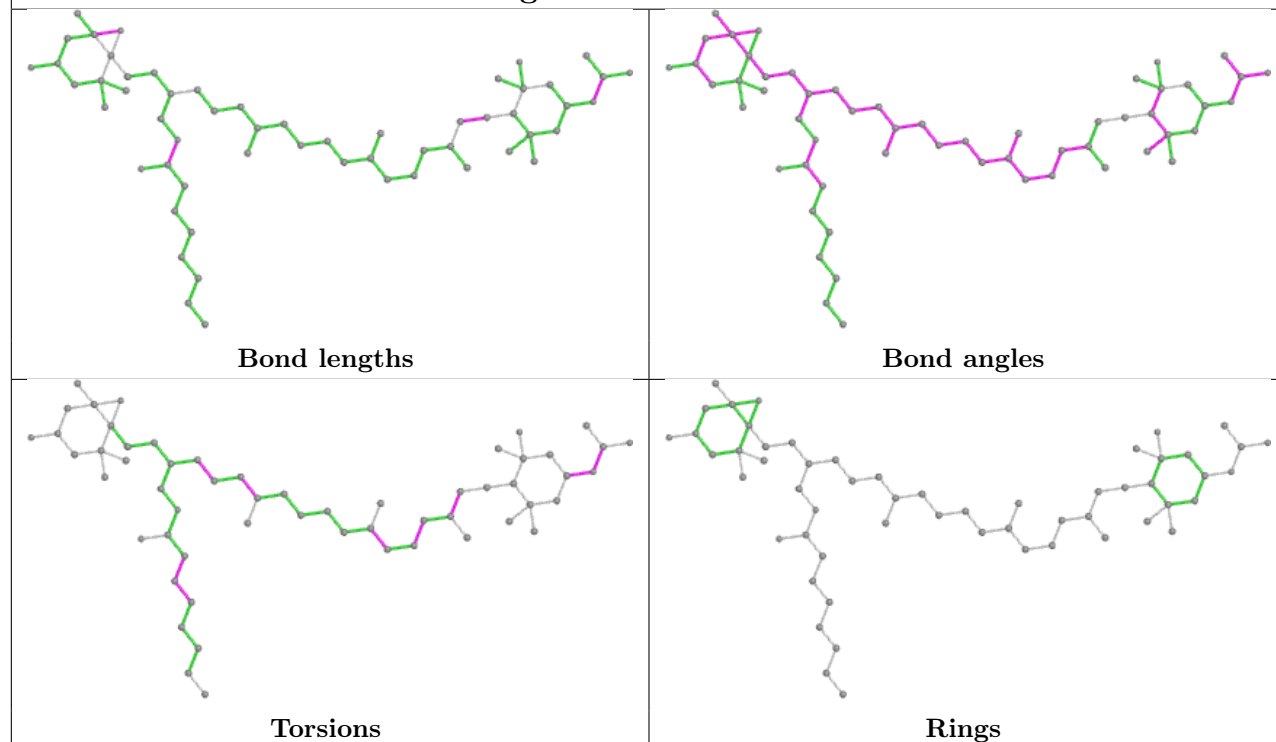


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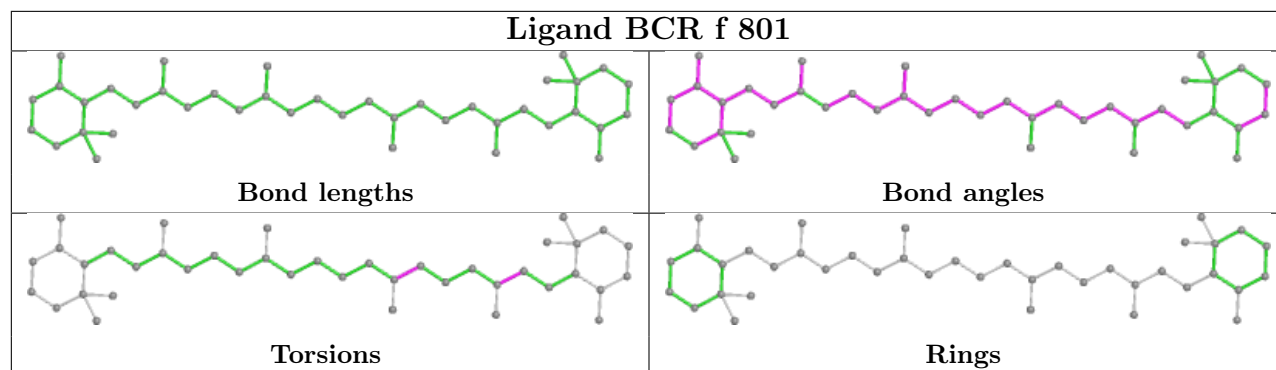


Ligand LMG j 103

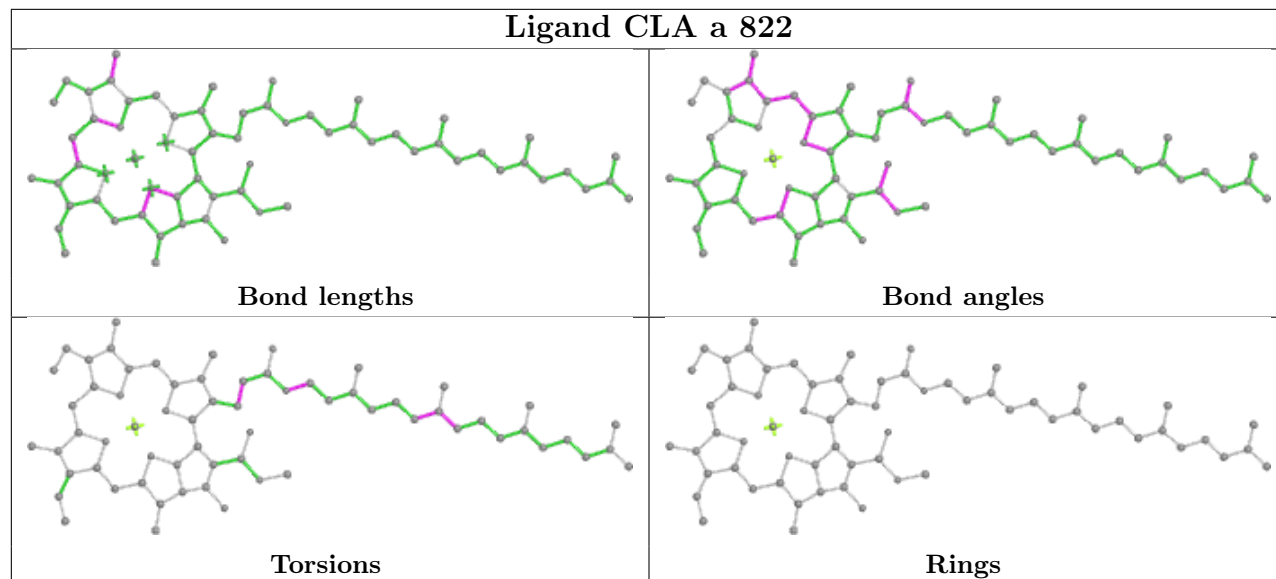


Ligand CLA b 809**Ligand XAT 5 301****Ligand A1L1F 8 304**

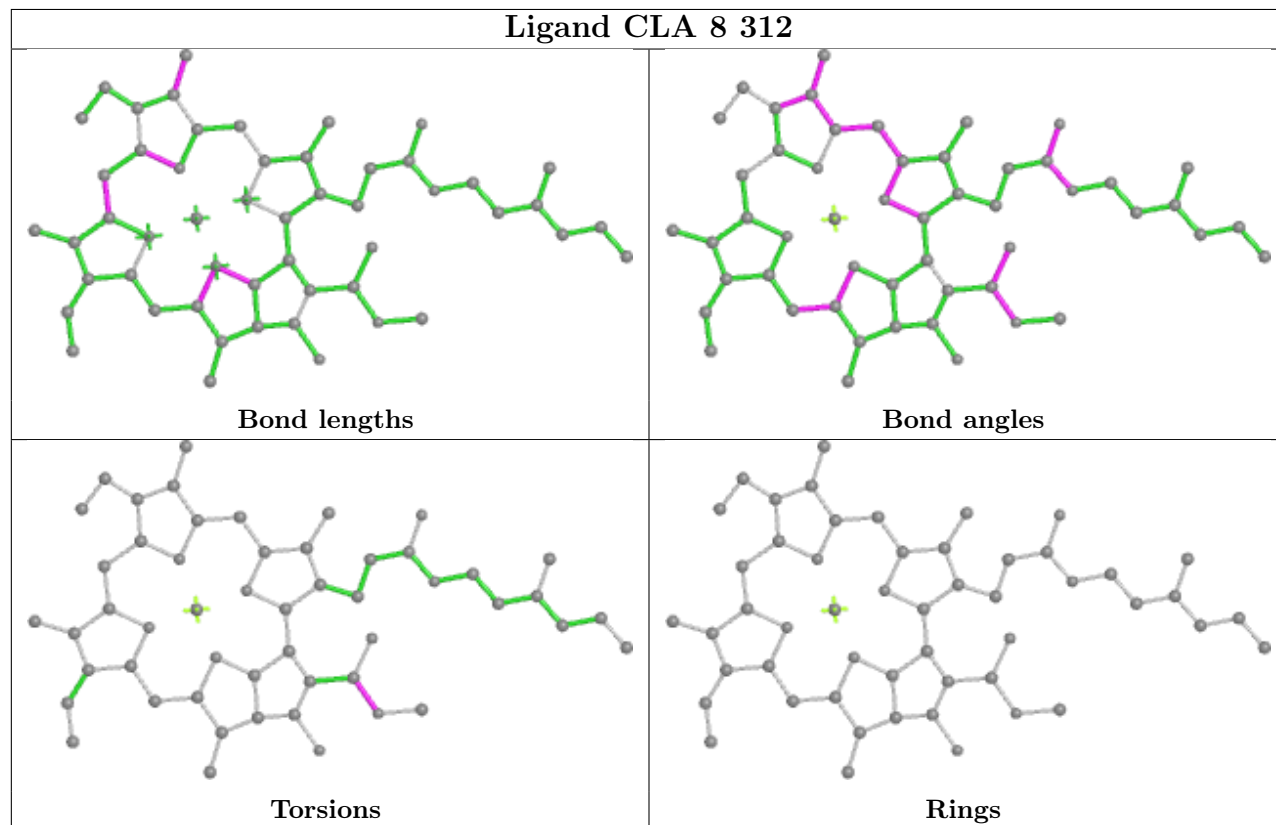
Ligand BCR f 801

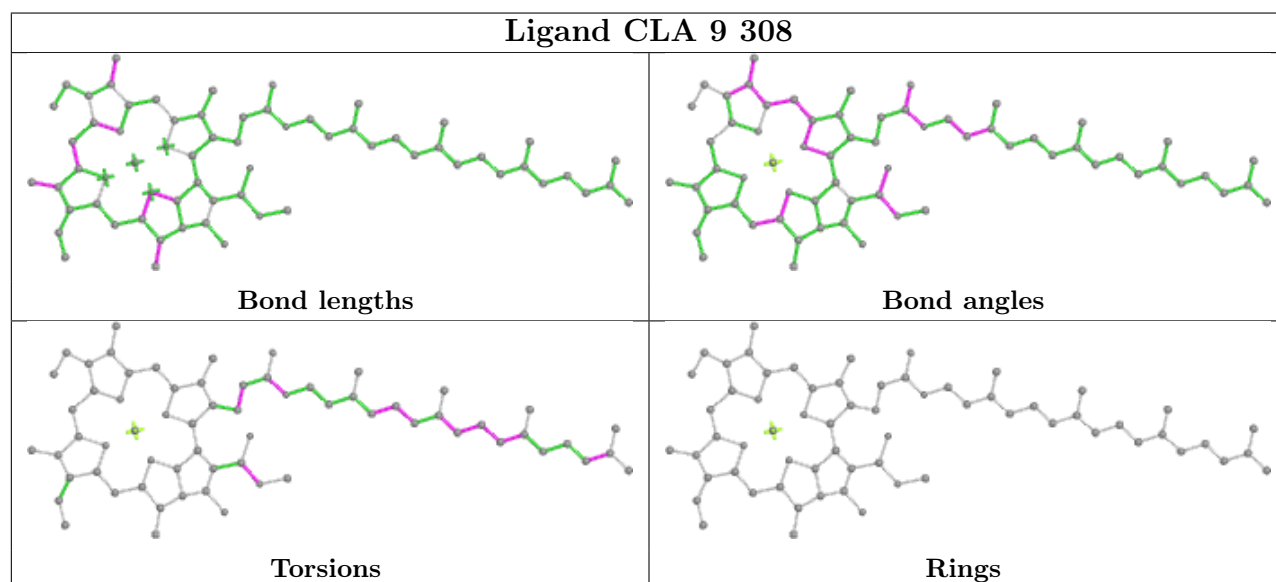
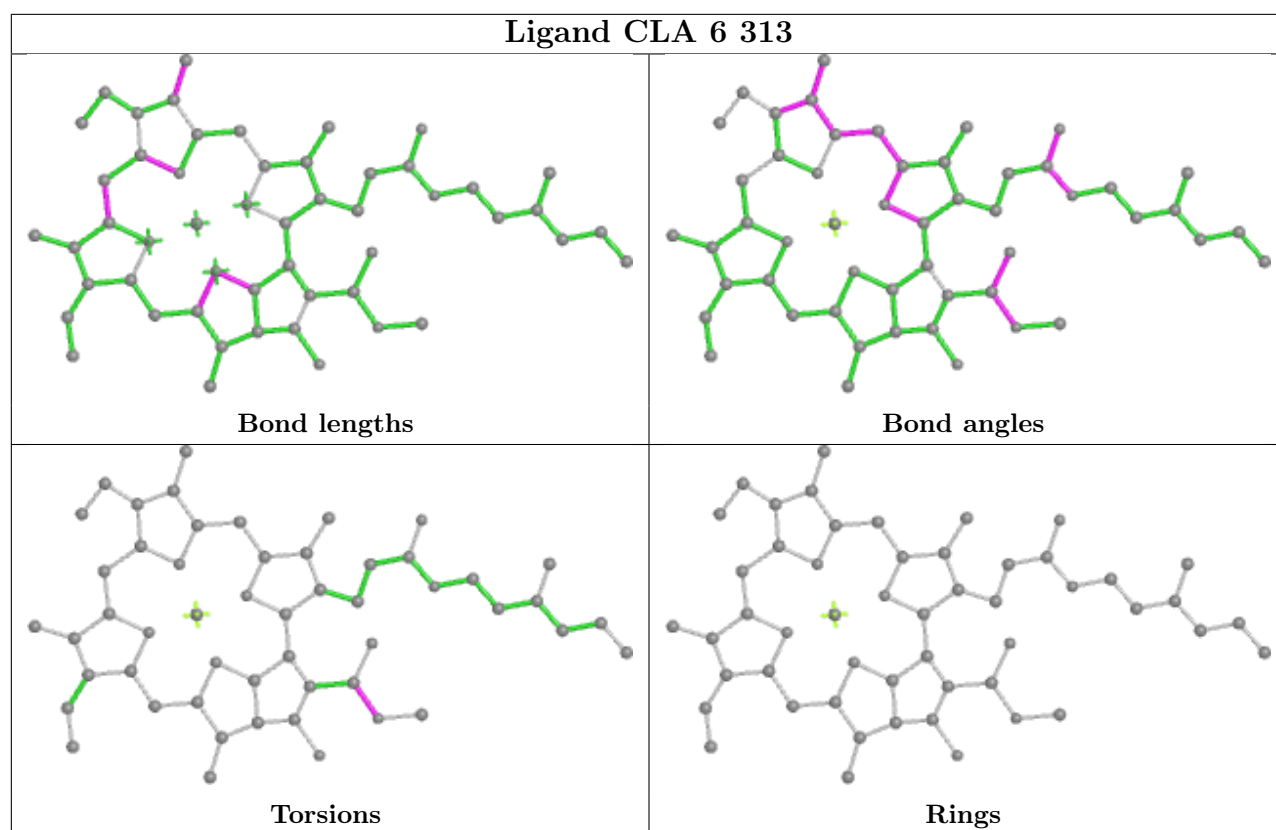


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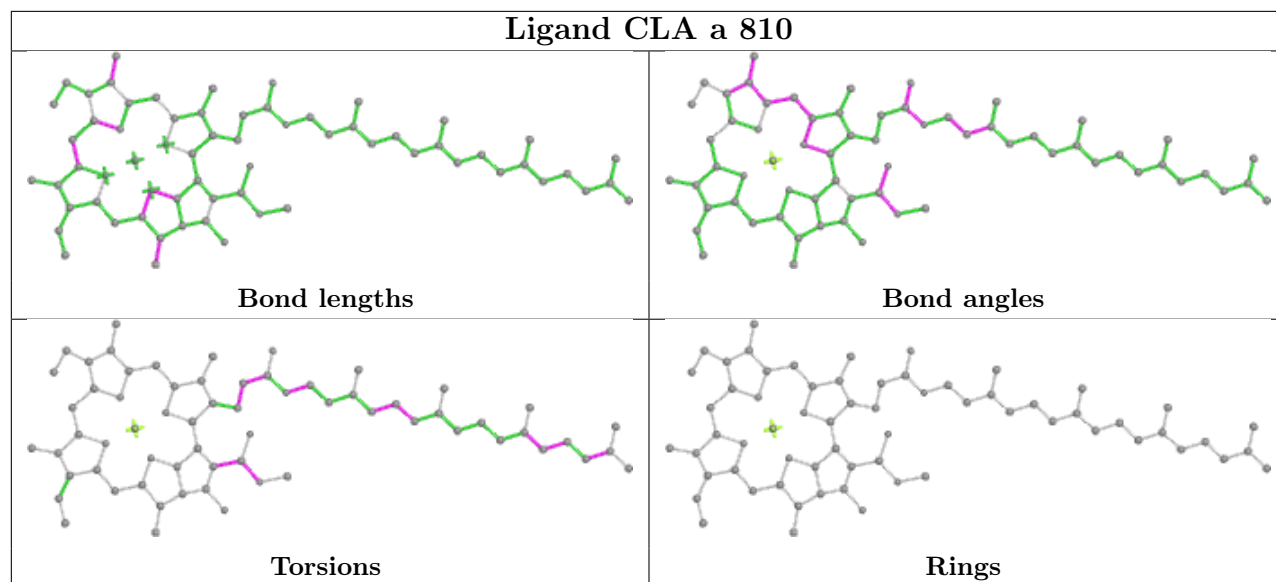


Ligand CLA 8 312

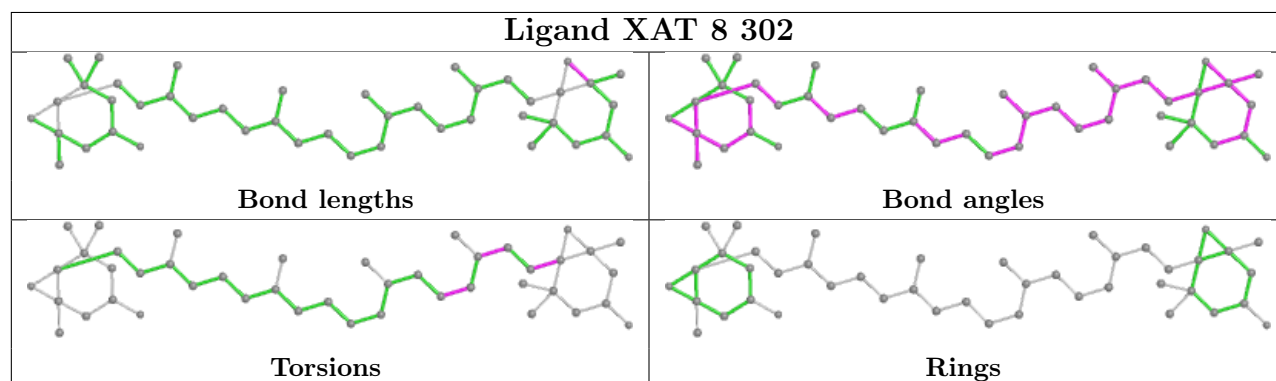




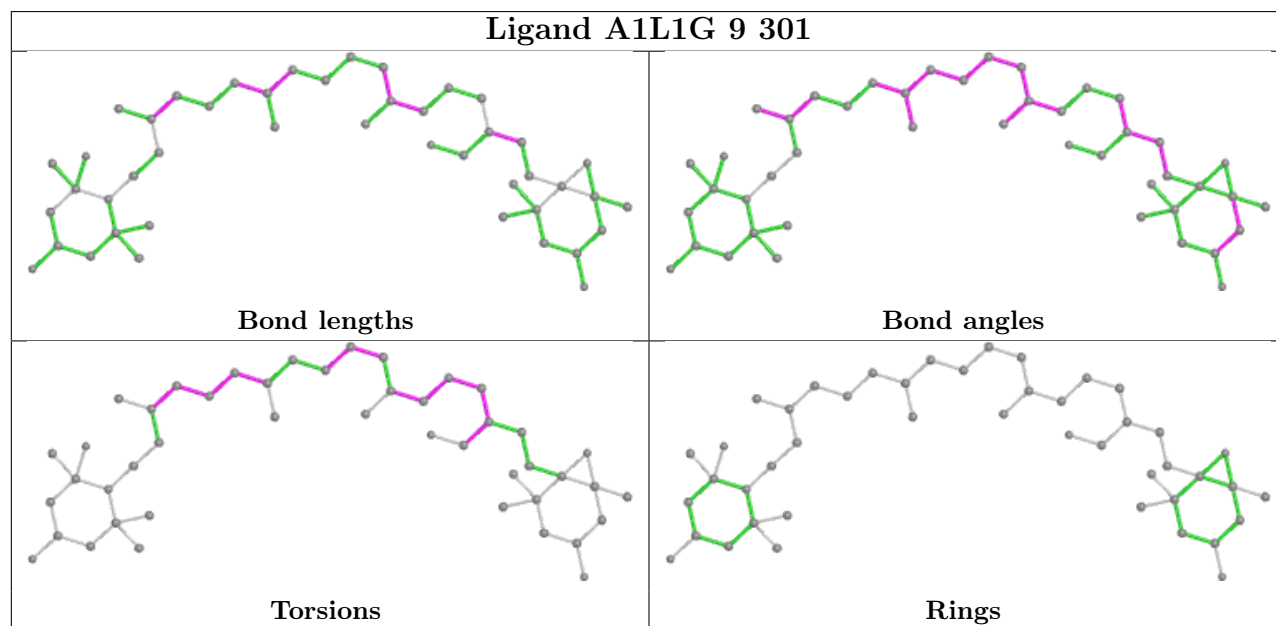
Ligand CLA a 810



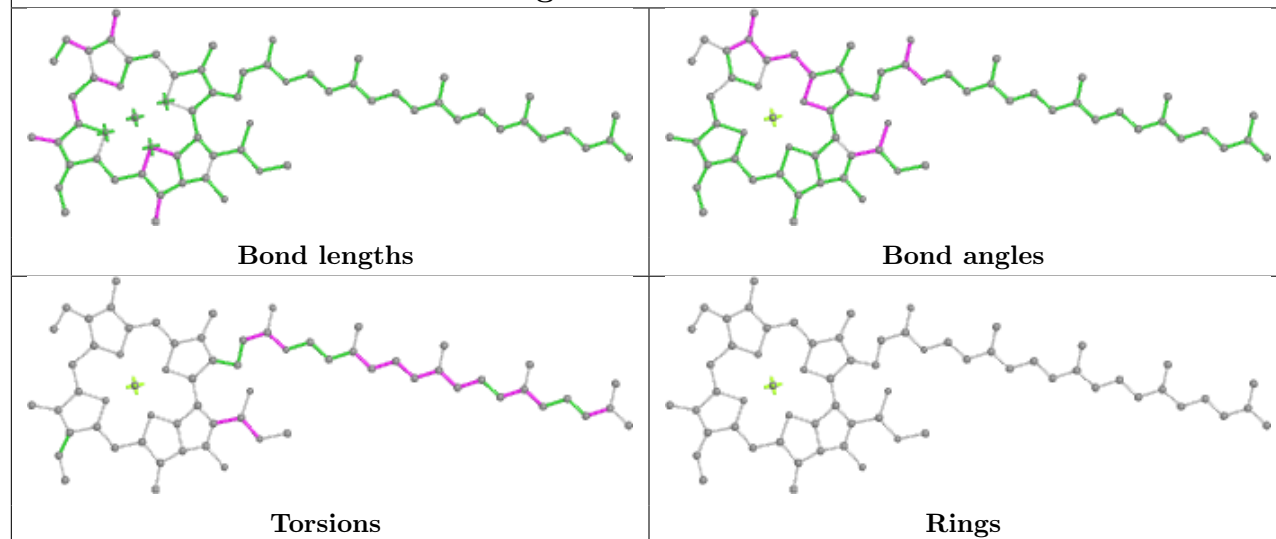
Ligand XAT 8 302



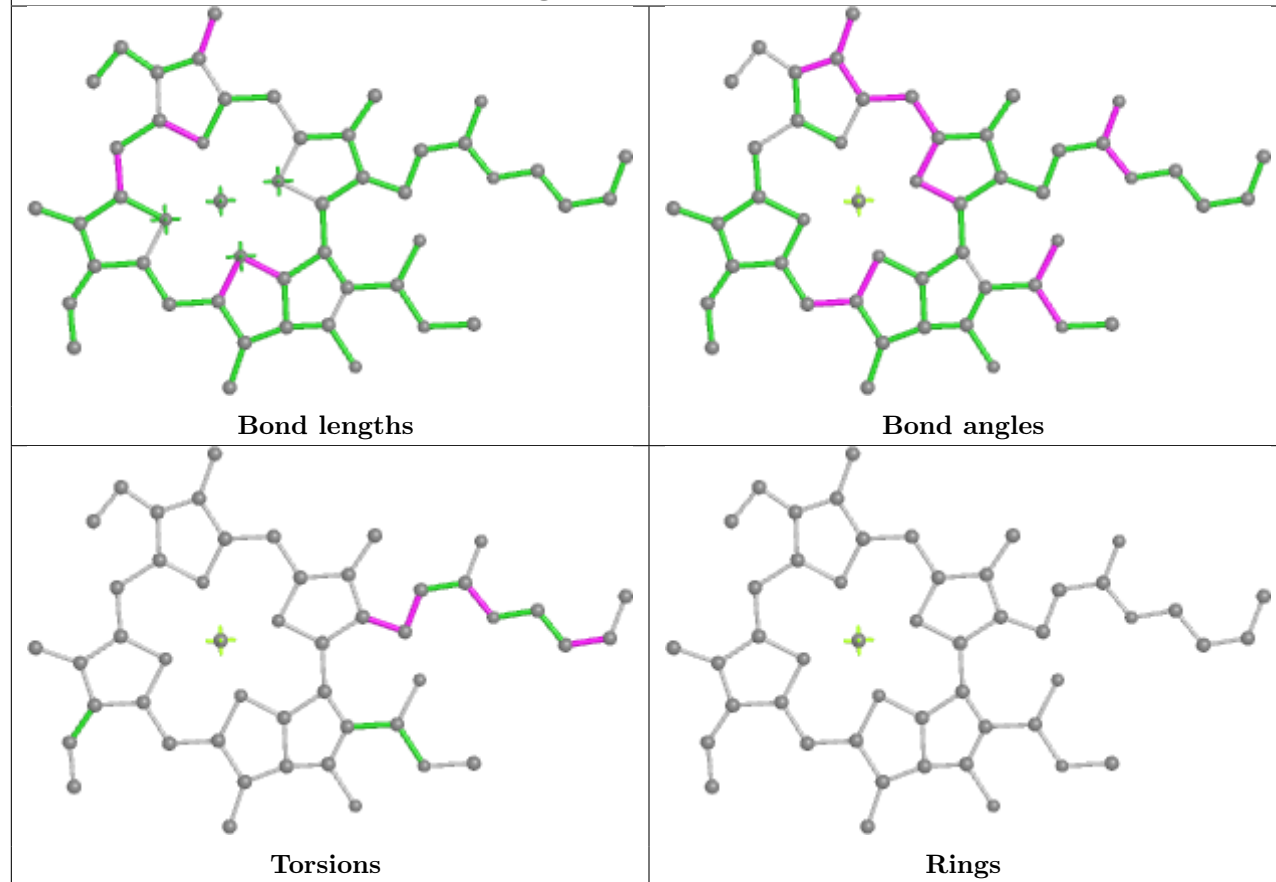
Ligand A1L1G 9 301



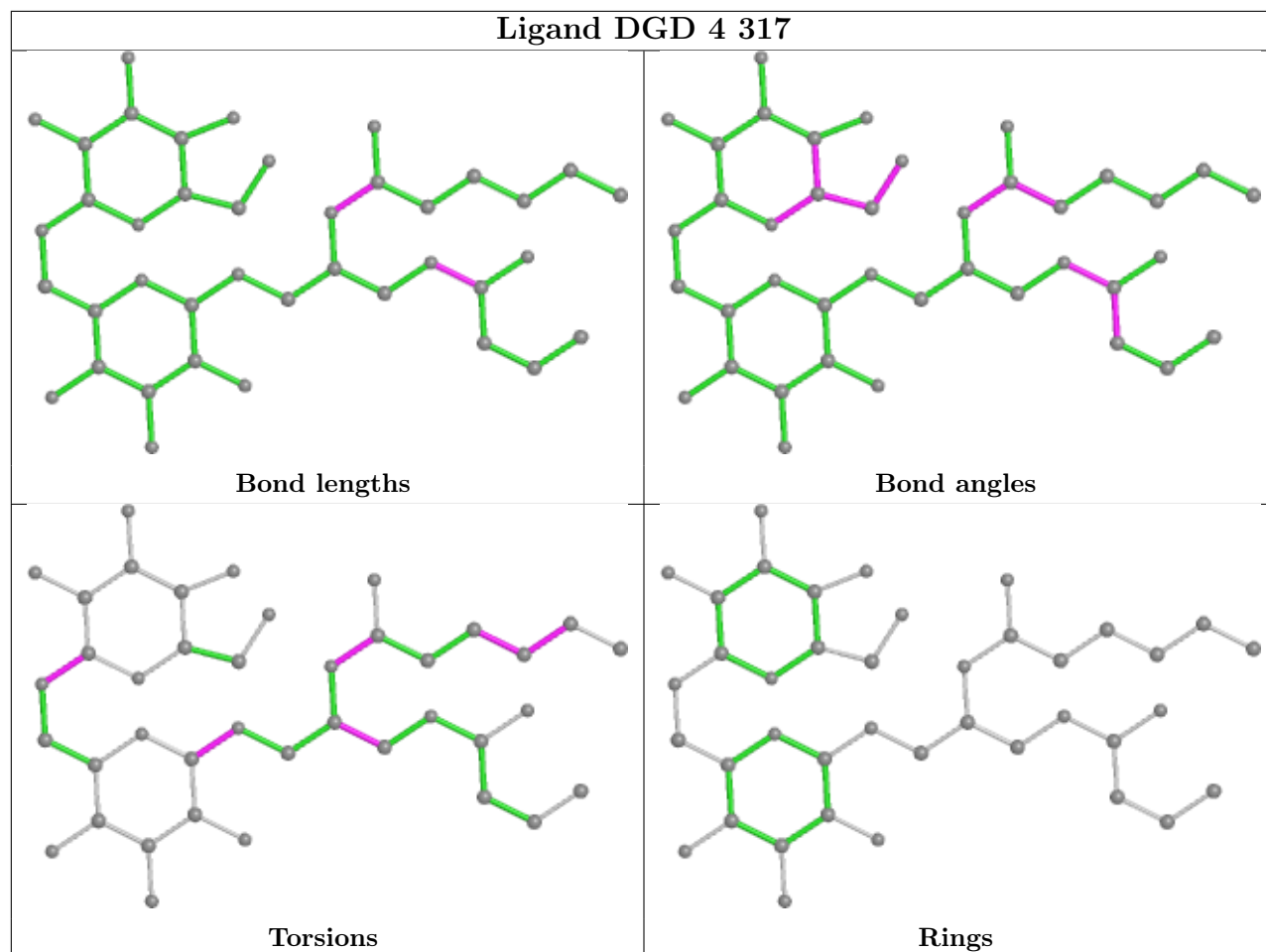
Ligand CLA a 801



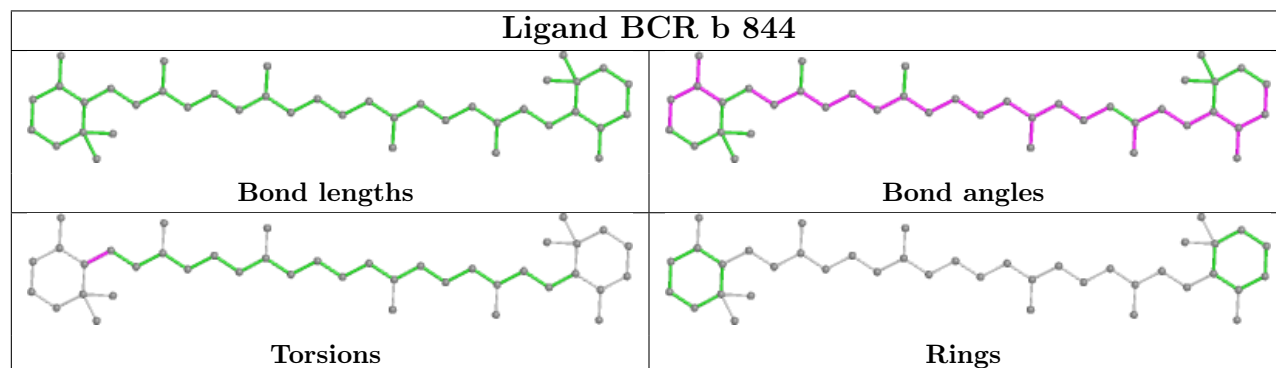
Ligand CLA b 831



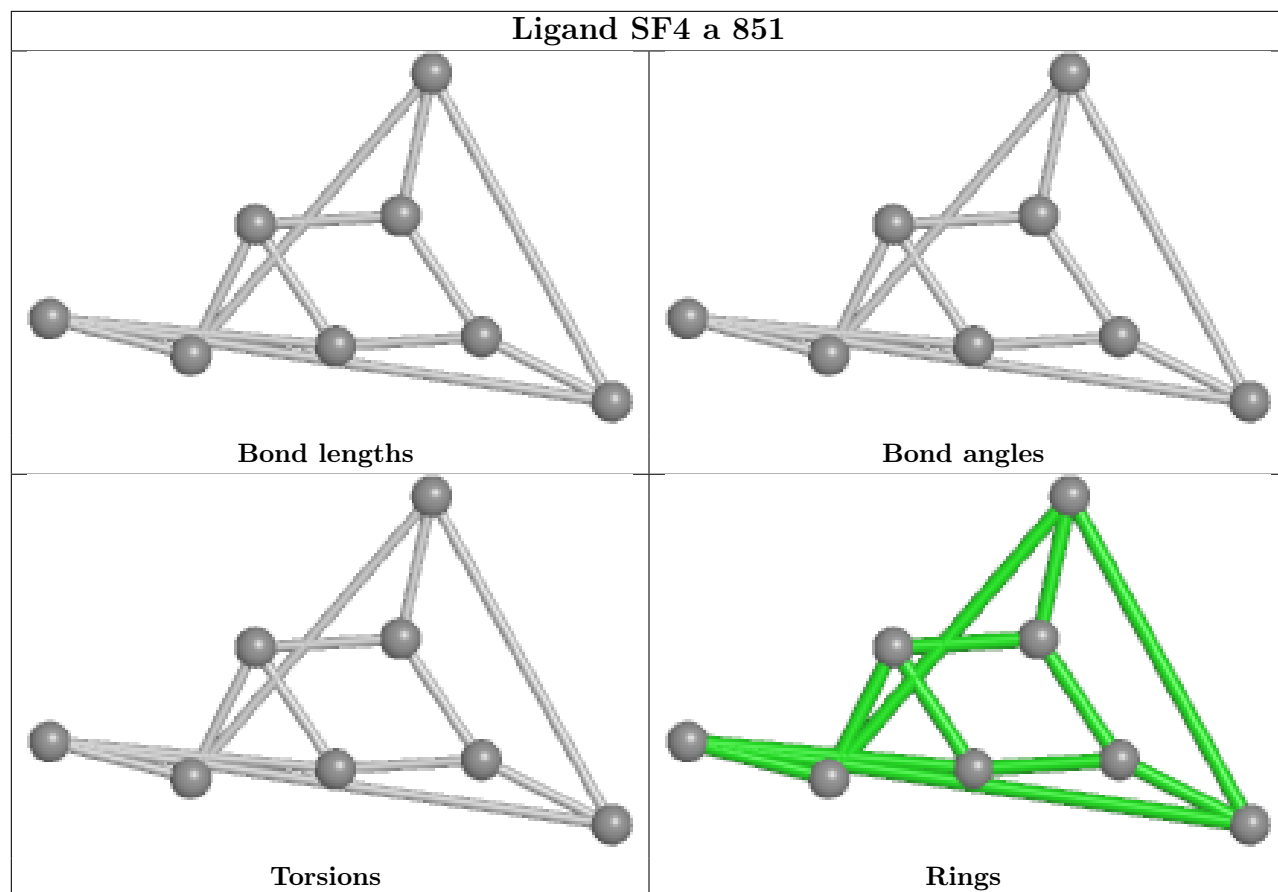
Ligand DGD 4 317



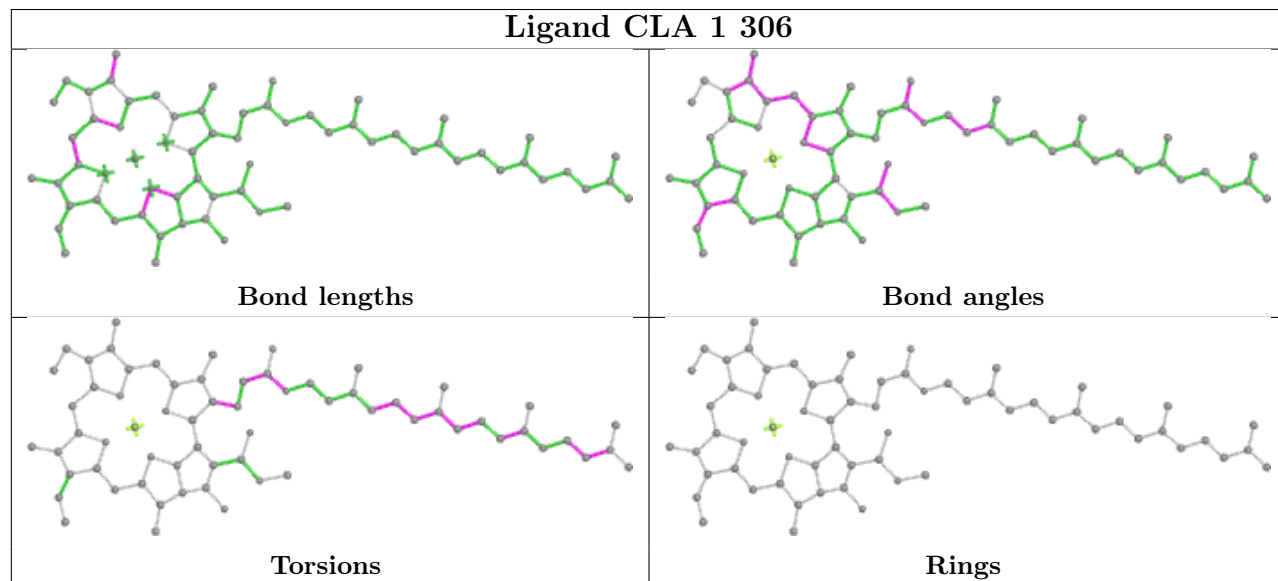
Ligand BCR b 844

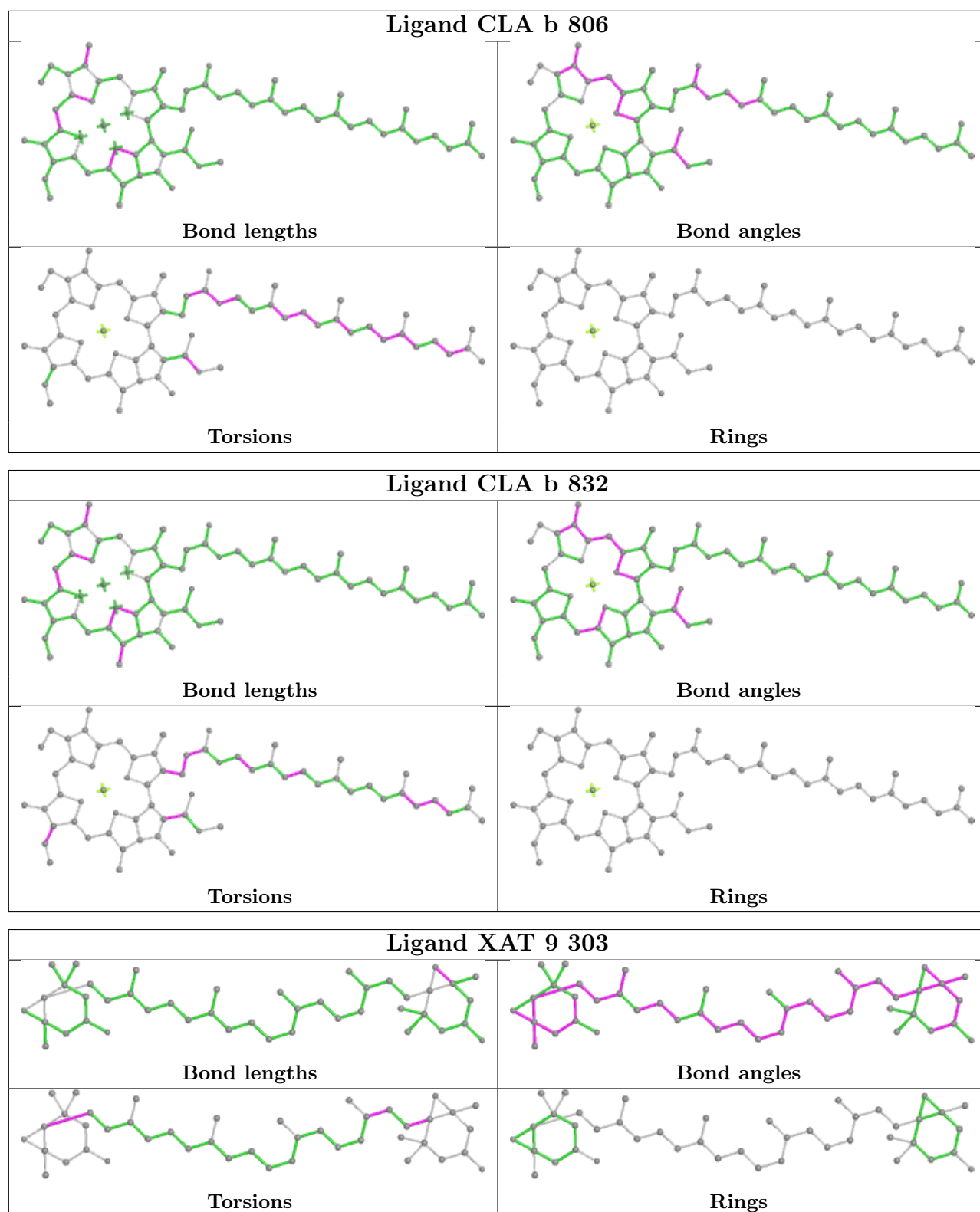


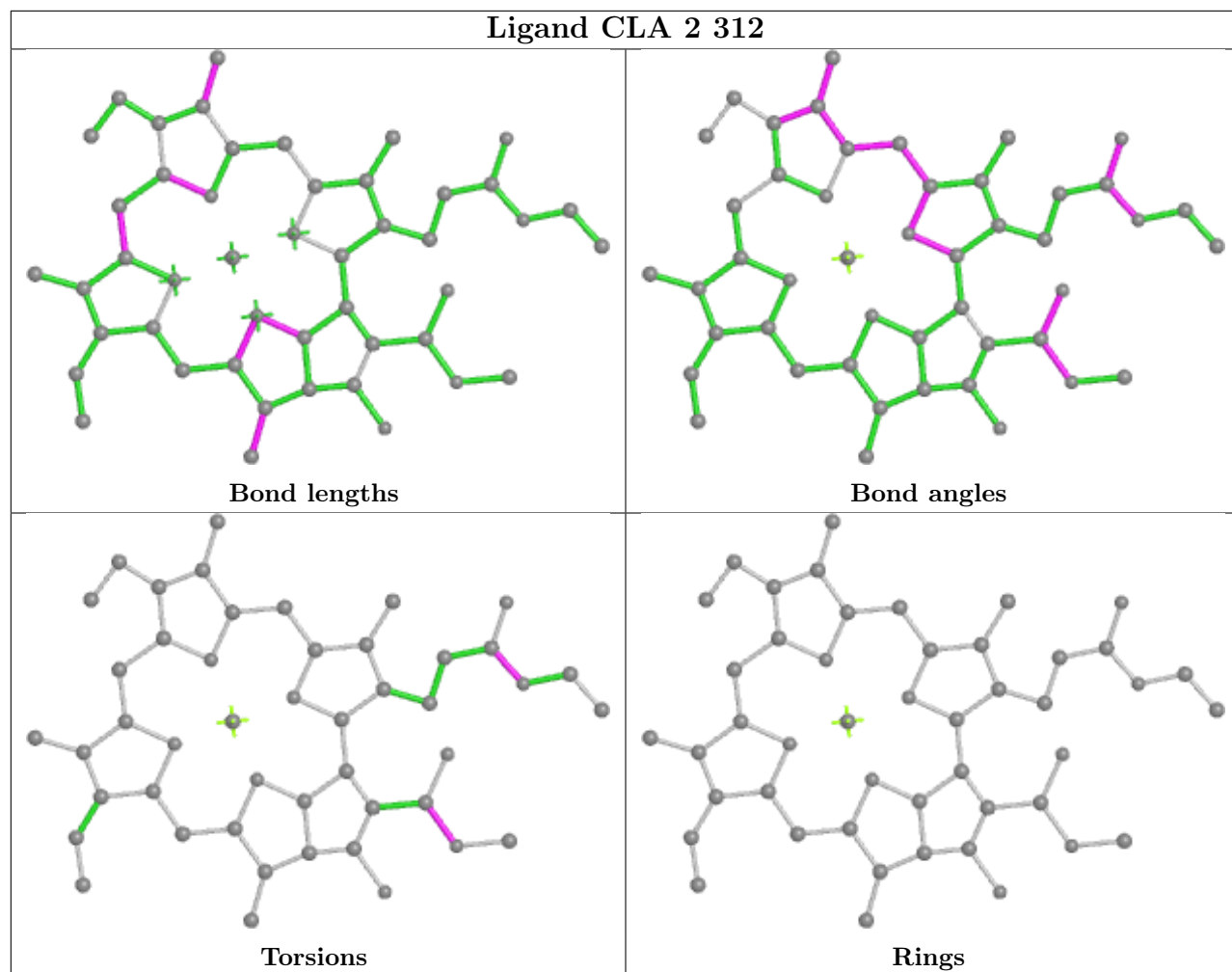
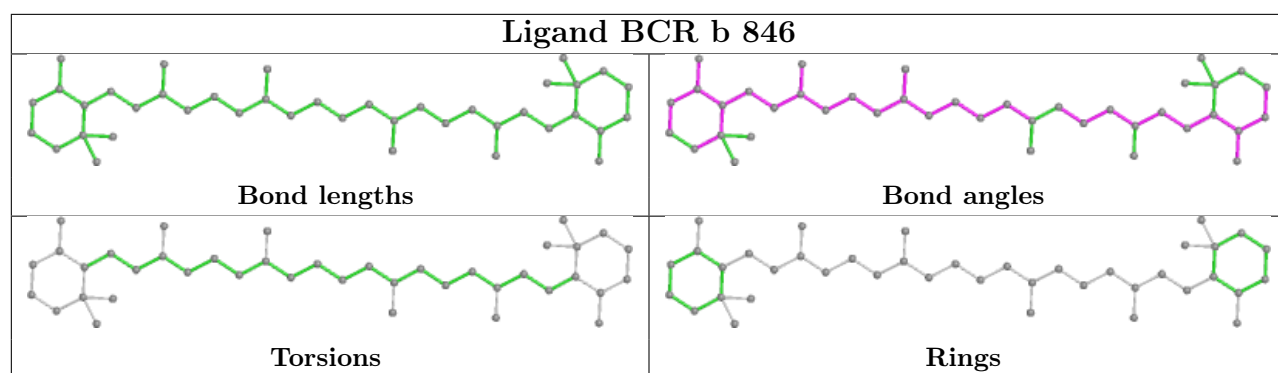
Ligand SF4 a 851



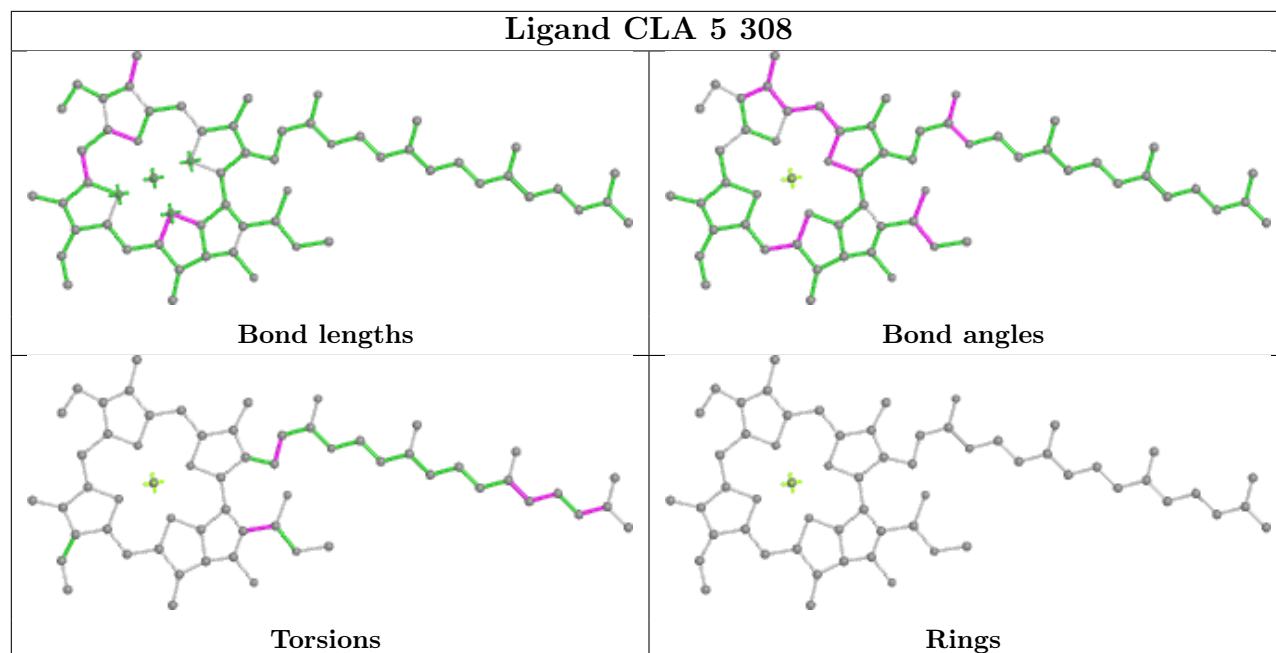
Ligand CLA 1 306



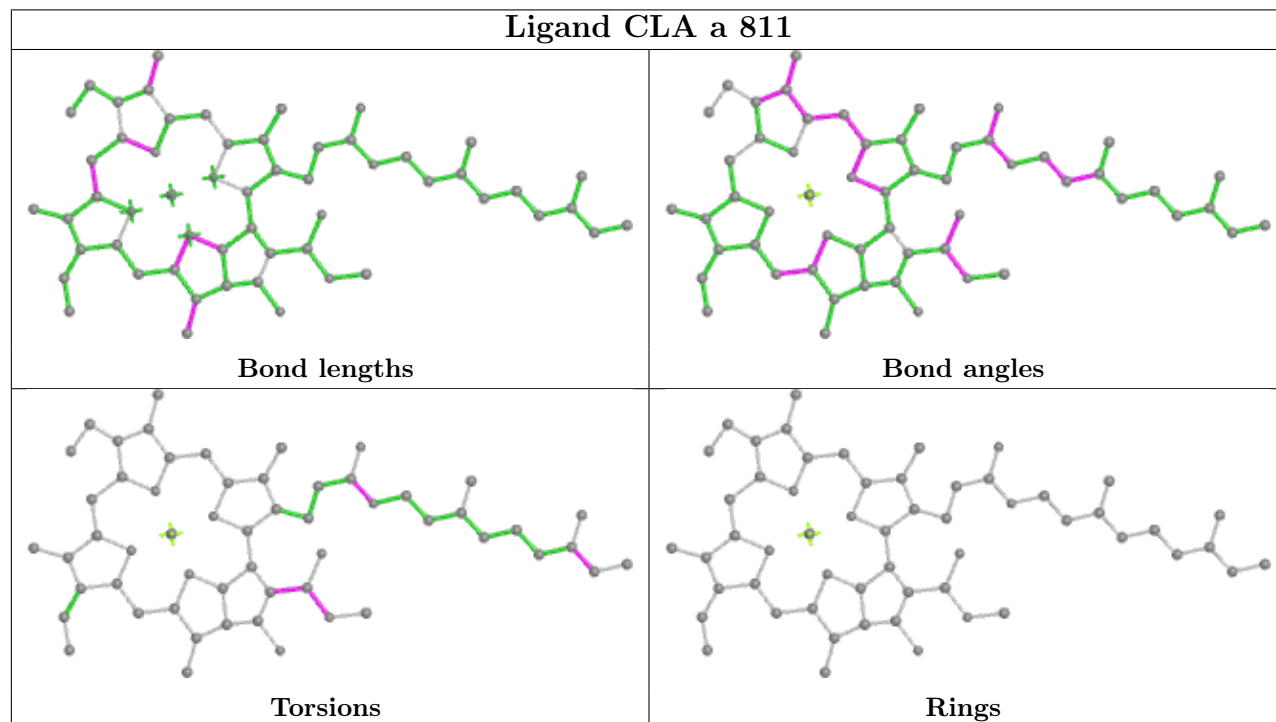




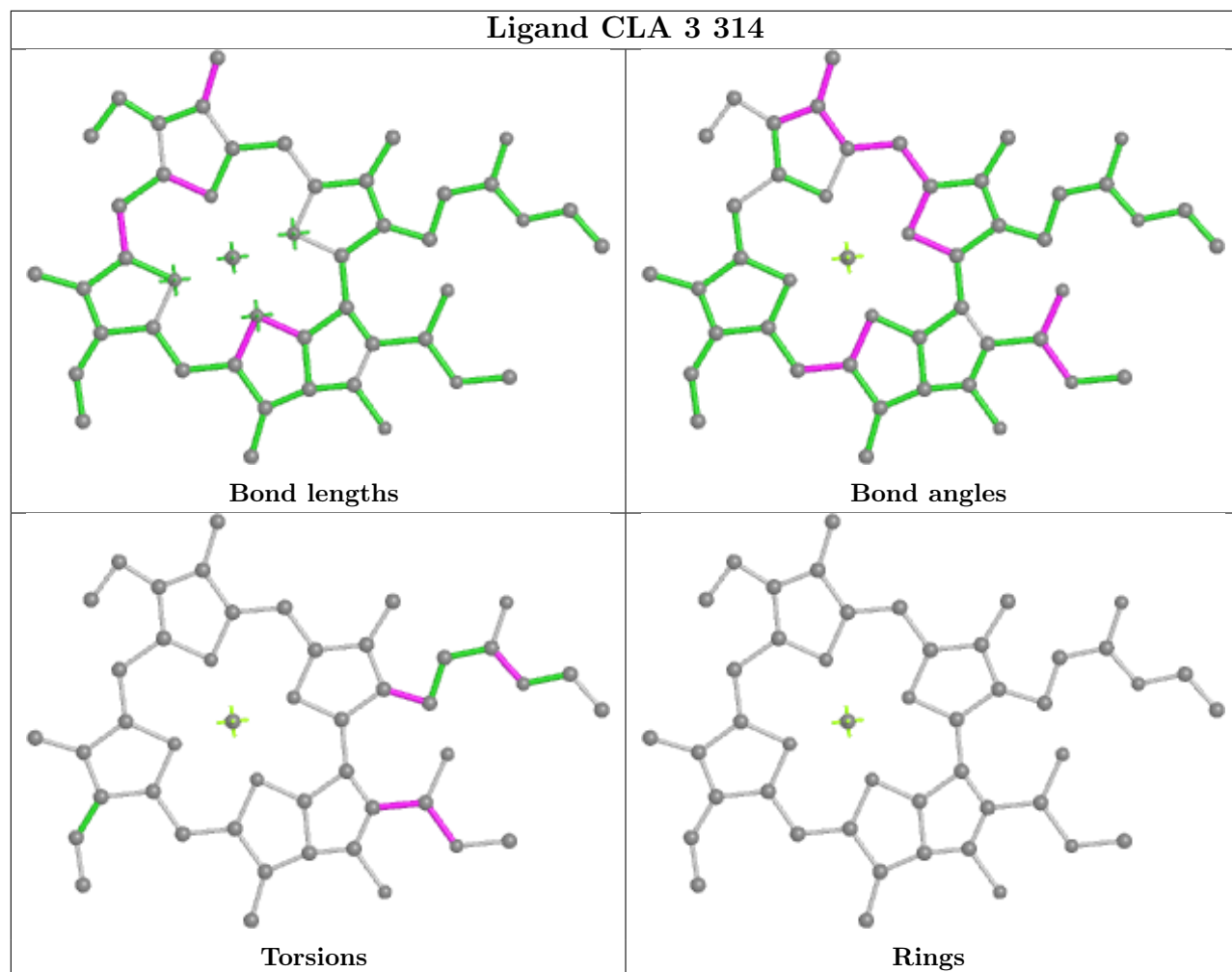
Ligand CLA 5 308

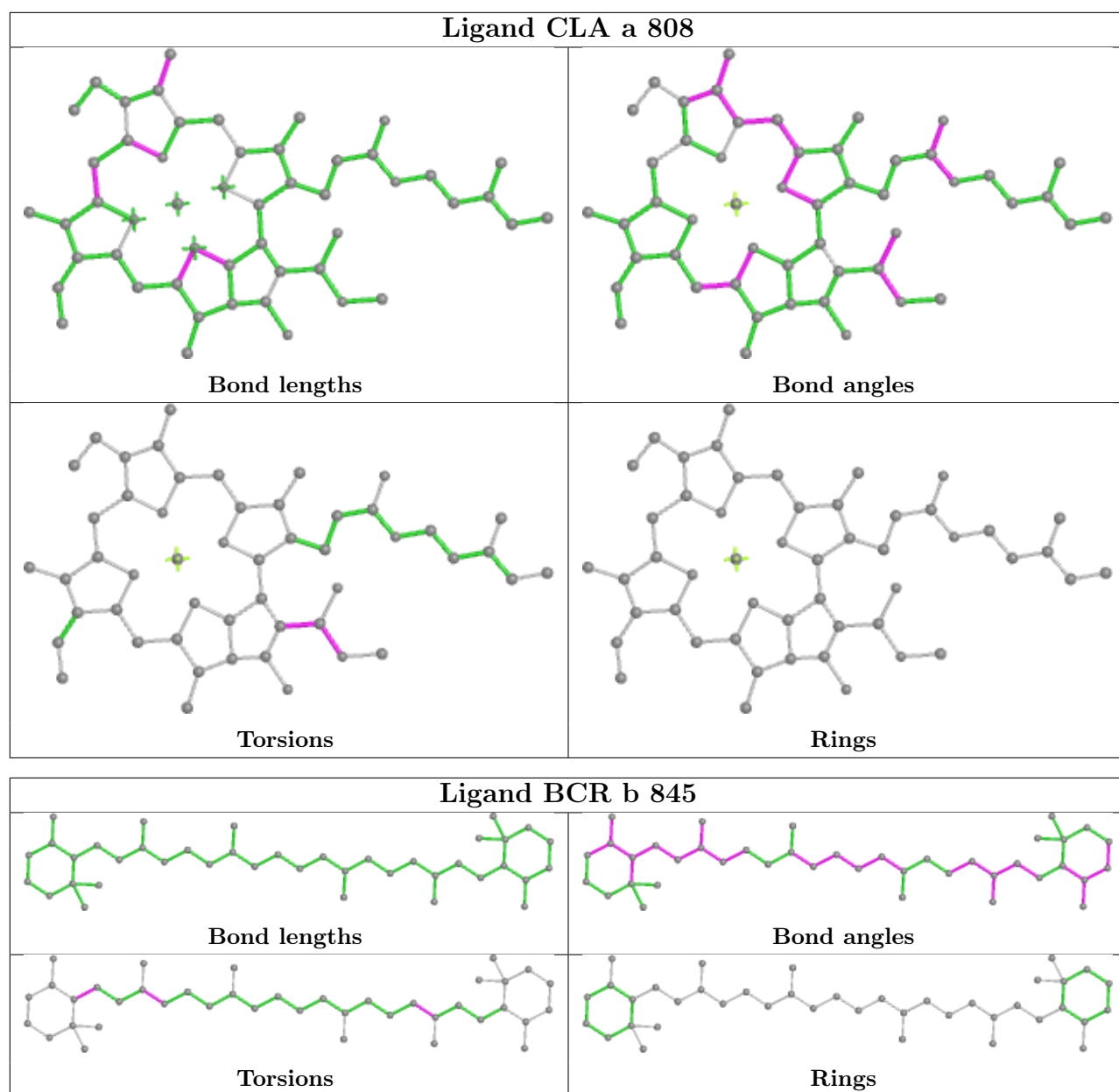


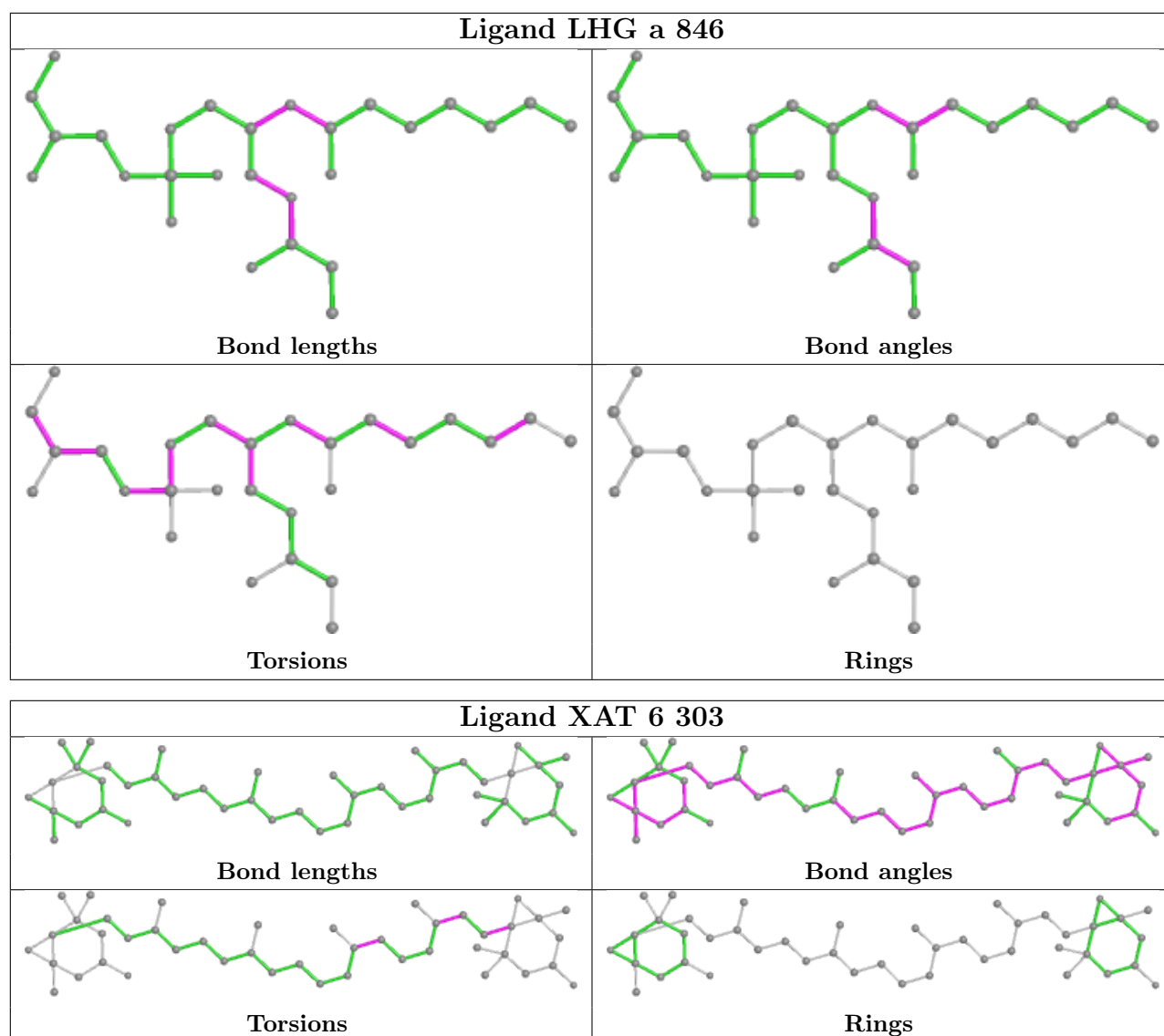
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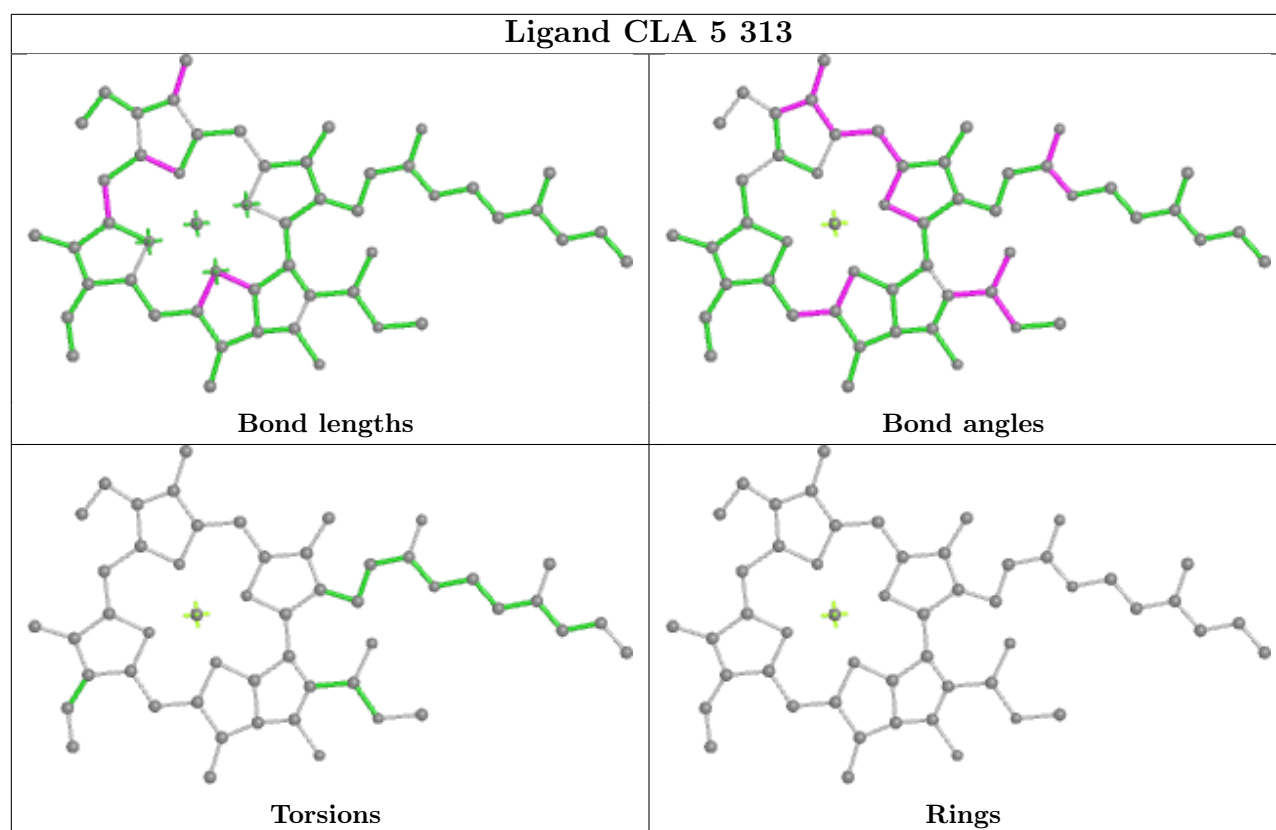


Ligand CLA 3 314

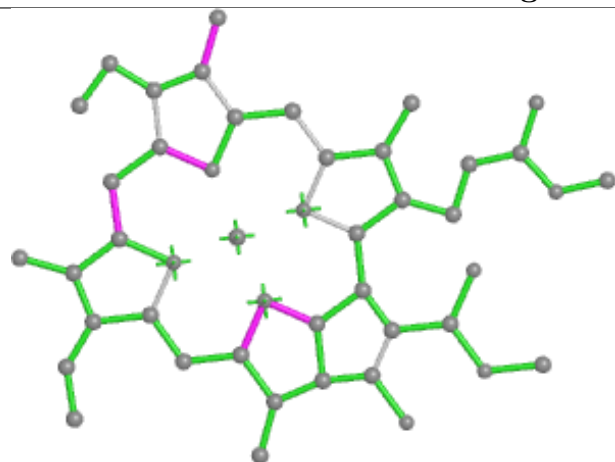




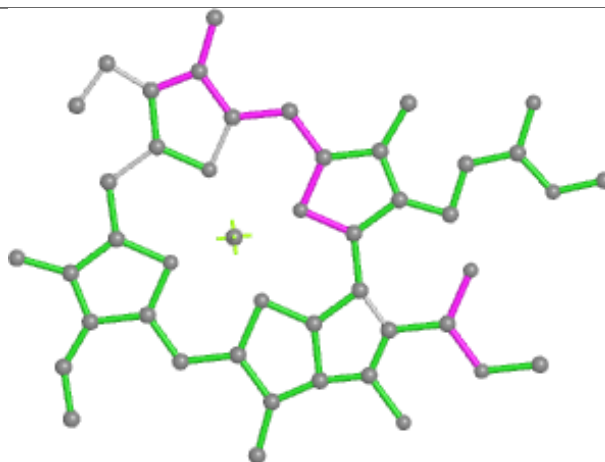




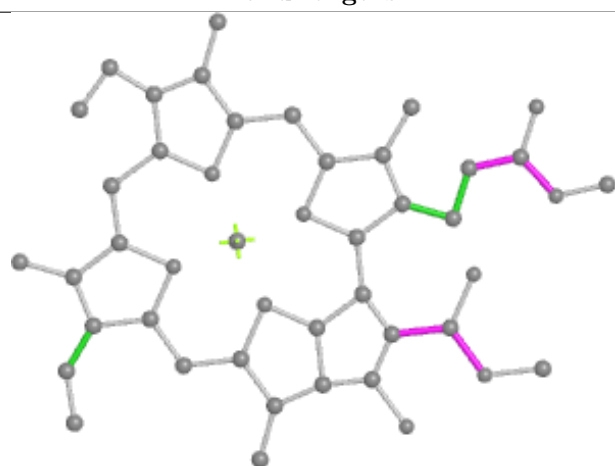
Ligand CLA 6 314



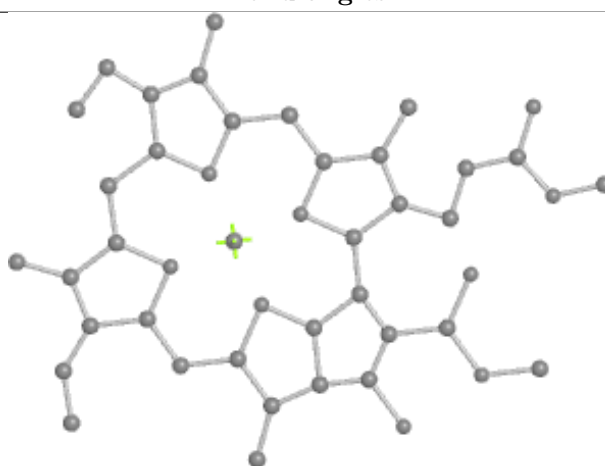
Bond lengths



Bond angles

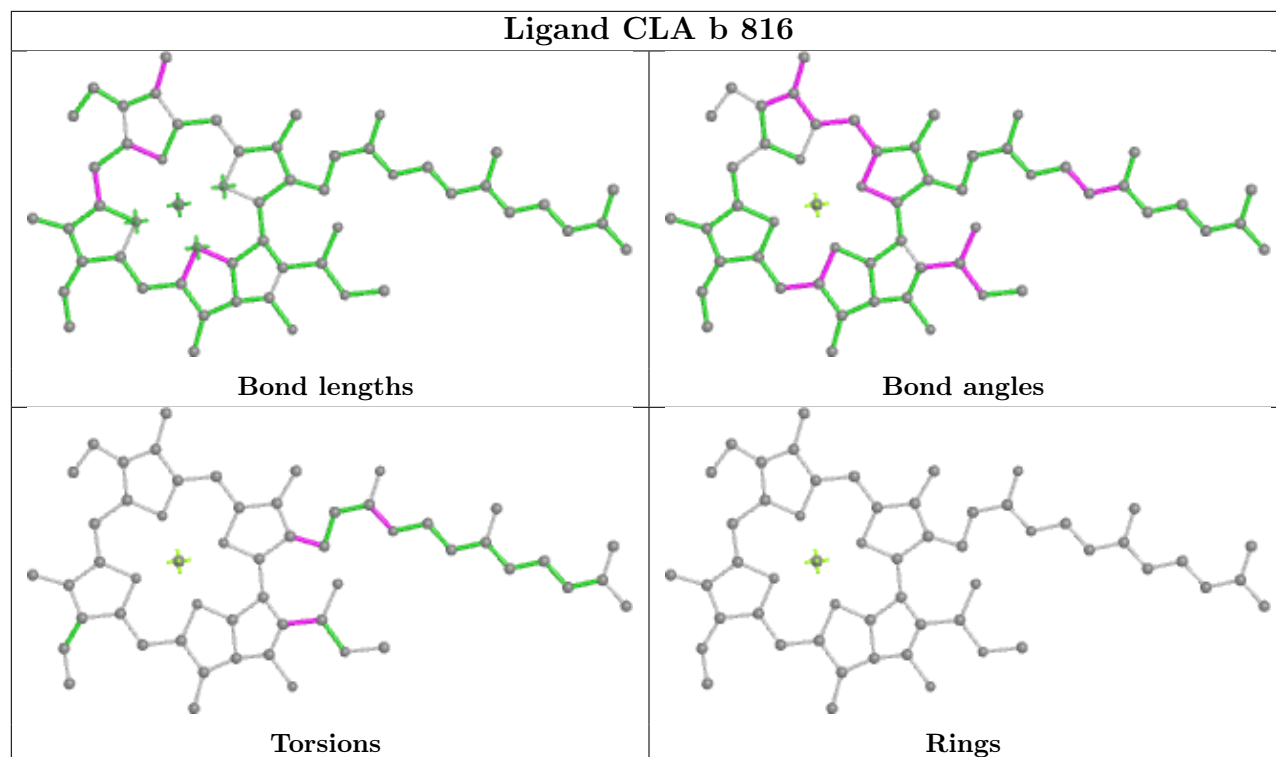


Torsions

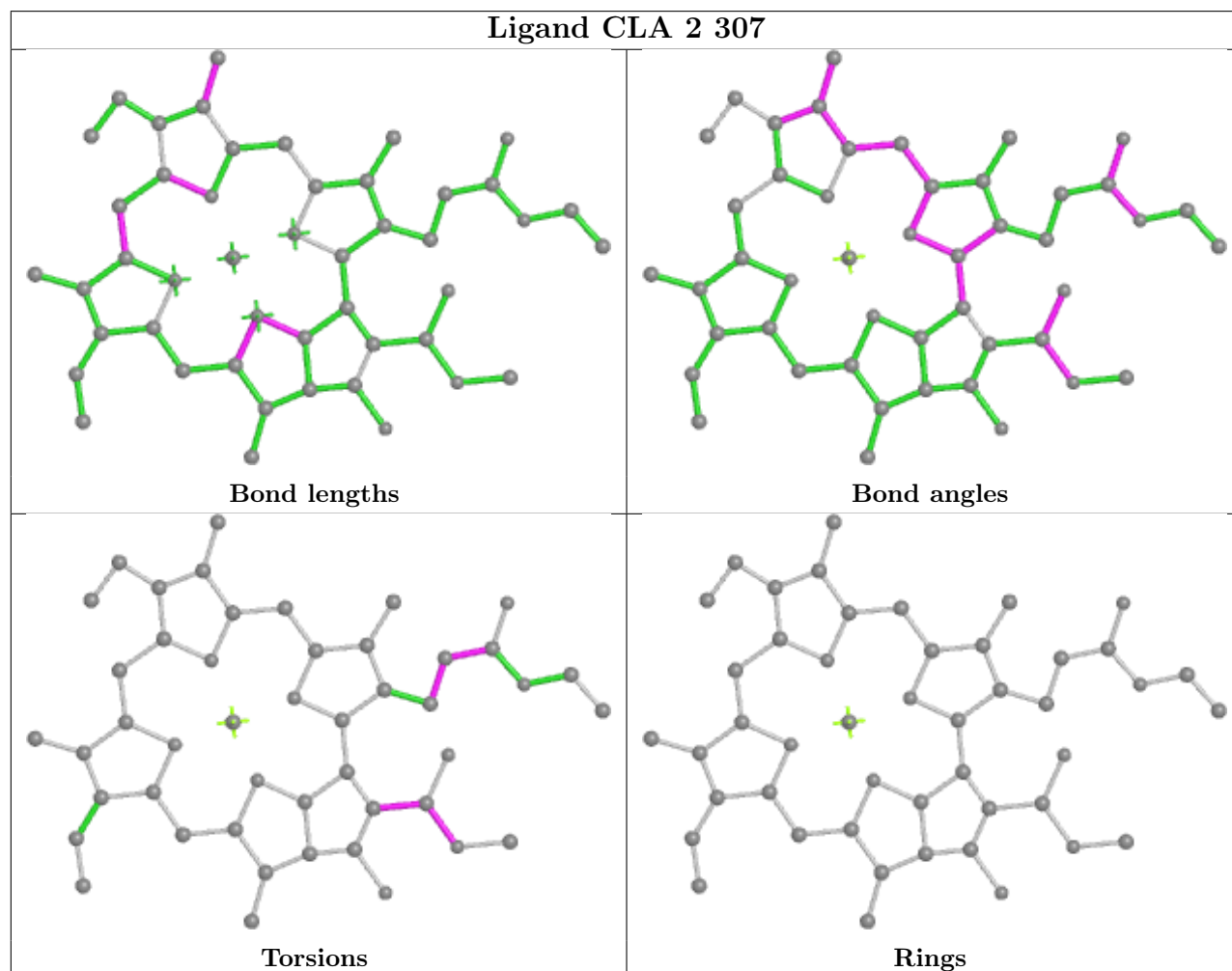


Rings

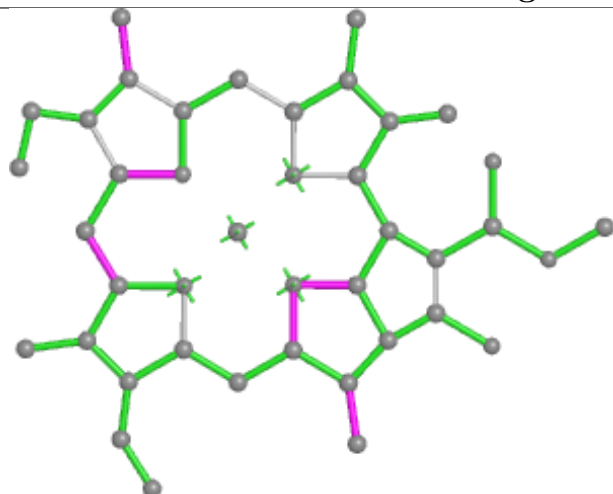
Ligand CLA b 816



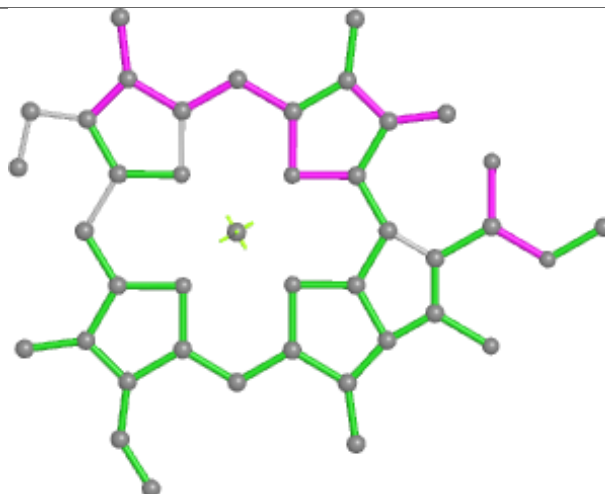
Ligand CLA 2 307



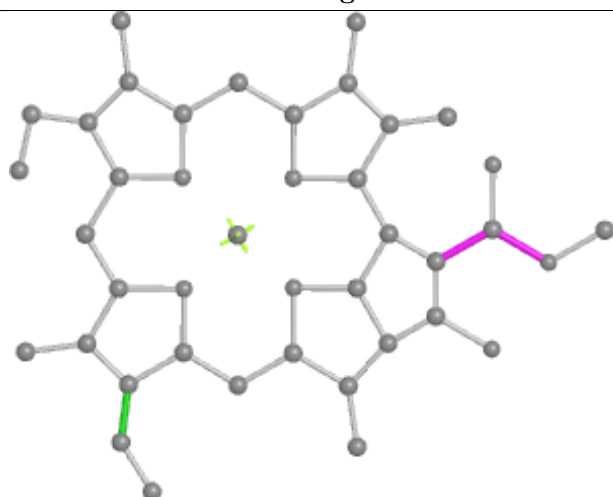
Ligand CLA 1 313



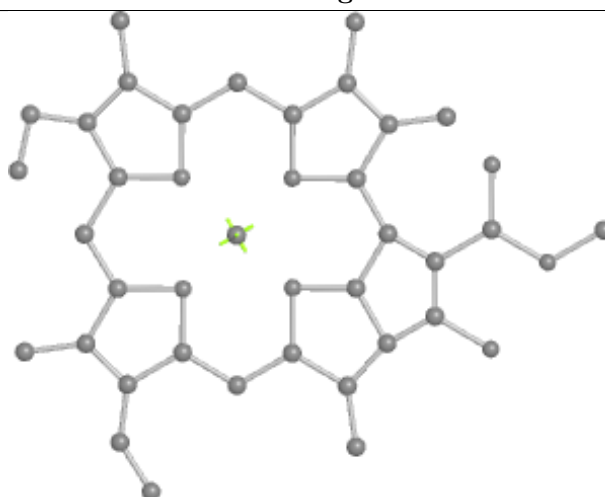
Bond lengths



Bond angles

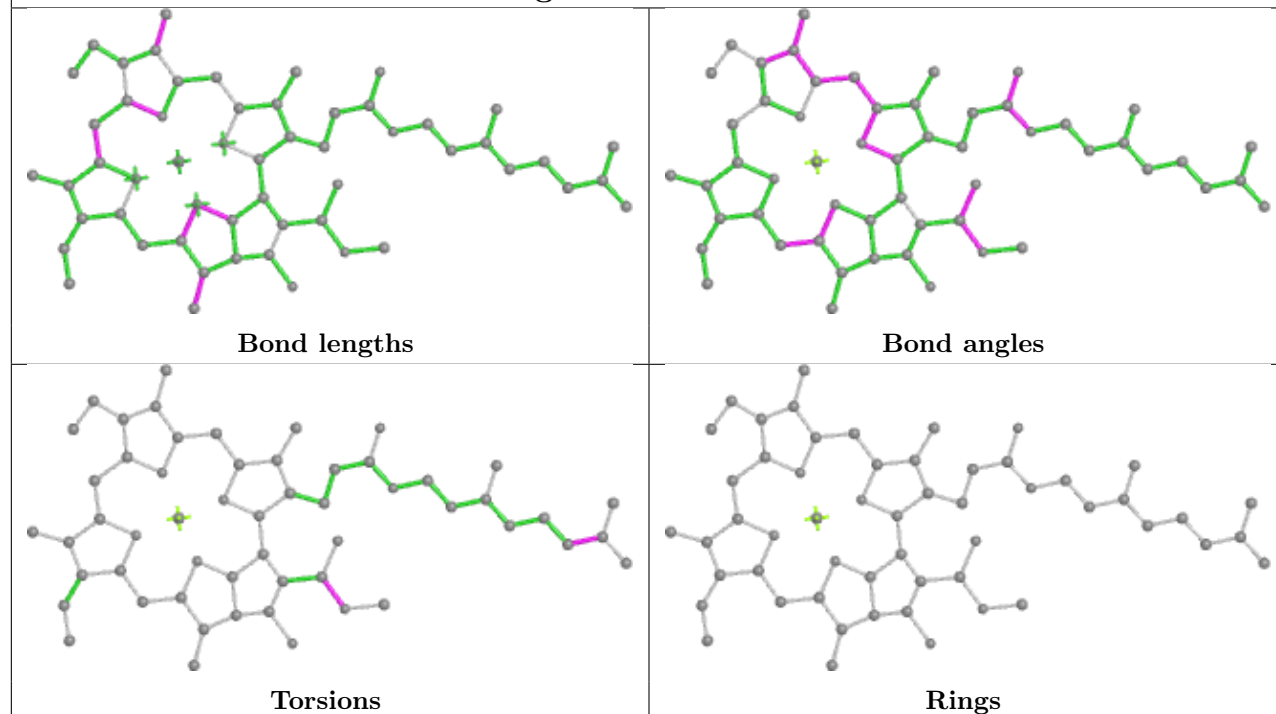


Torsions

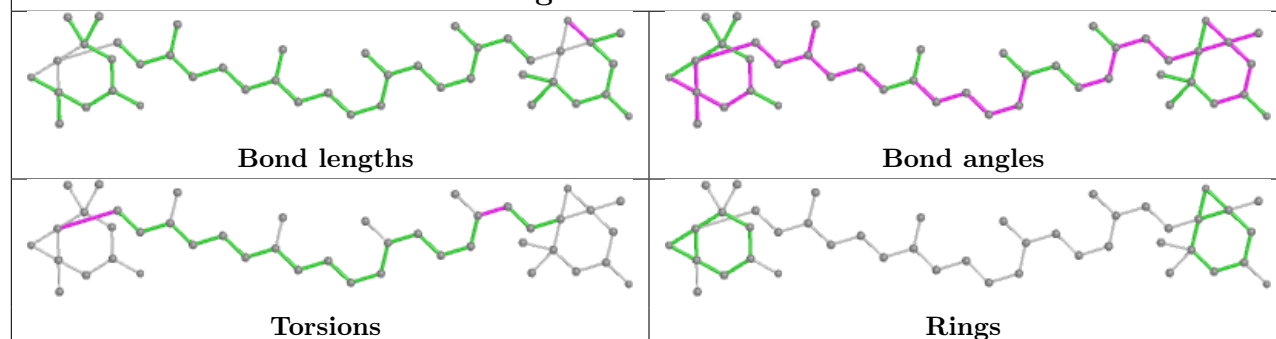


Rings

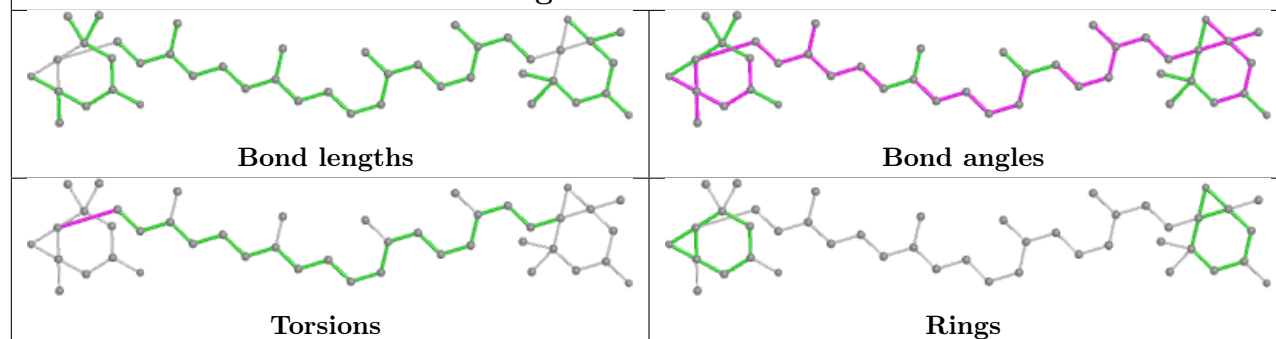
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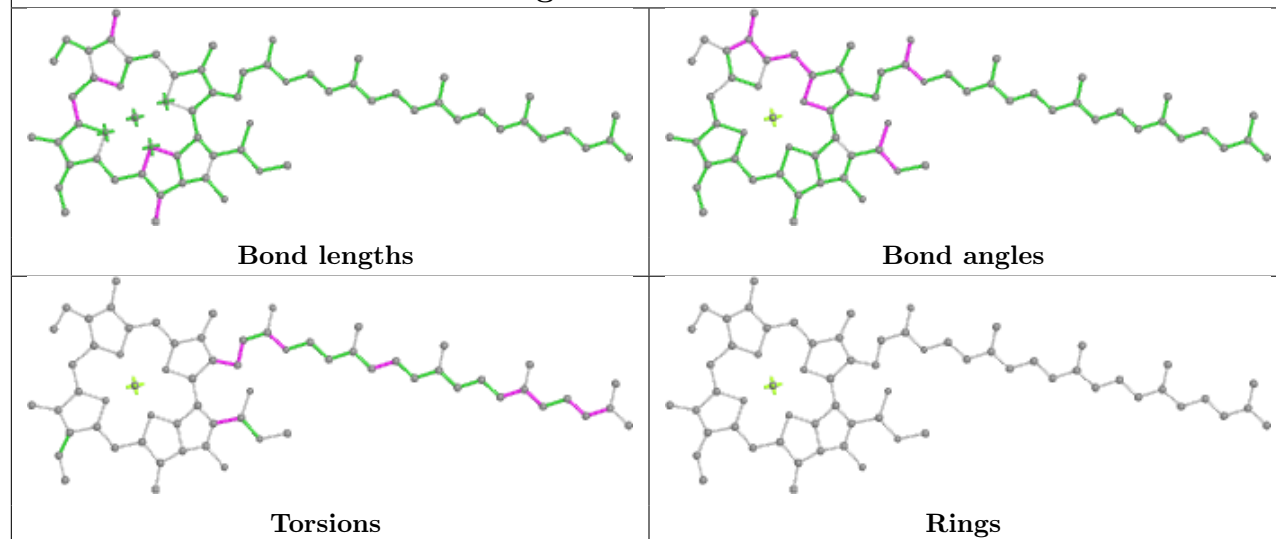
Ligand XAT 8 301



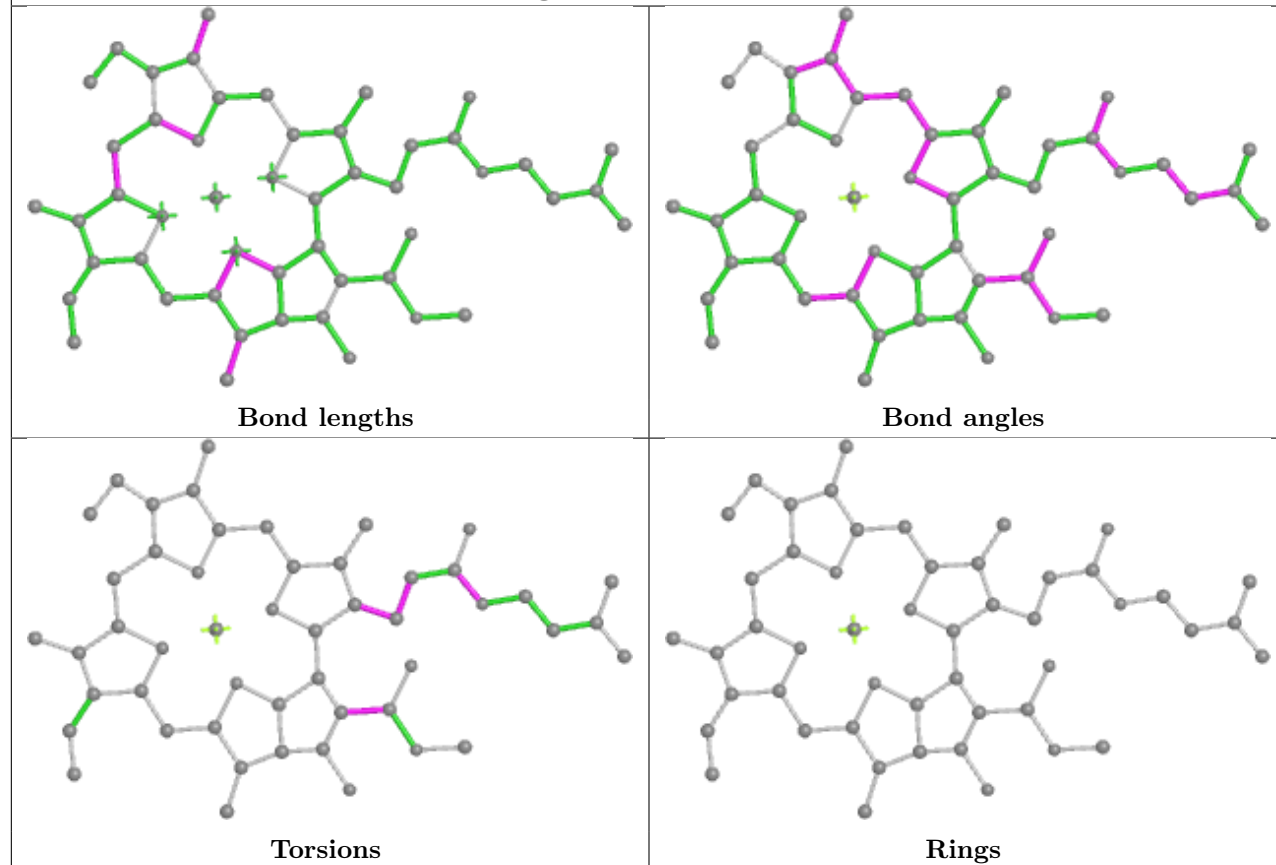
Ligand XAT 5 305



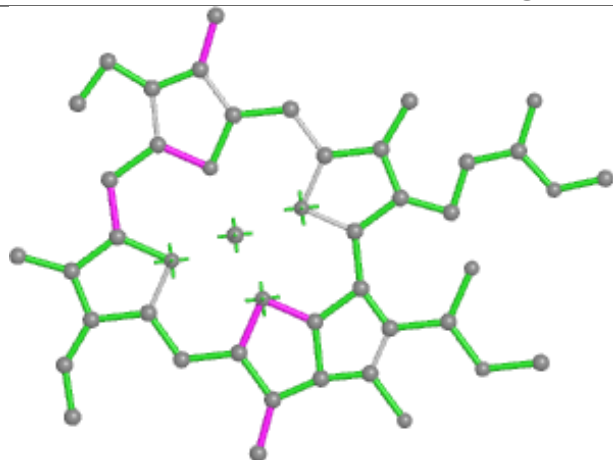
Ligand CLA 2 310



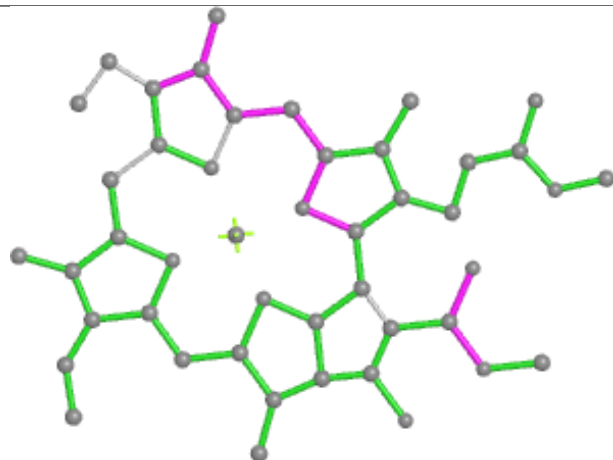
Ligand CLA b 820



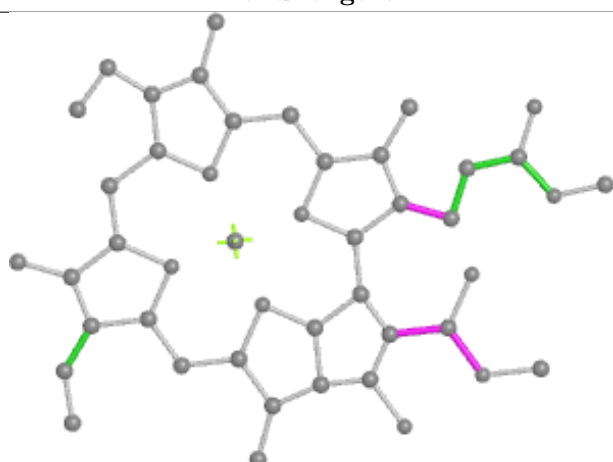
Ligand CLA 2 316



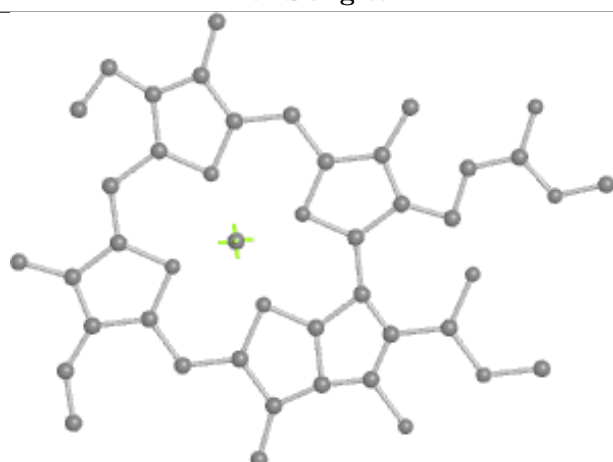
Bond lengths



Bond angles

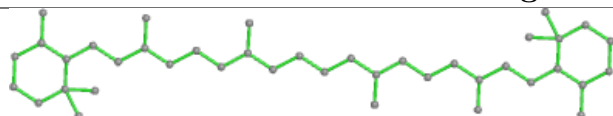


Torsions

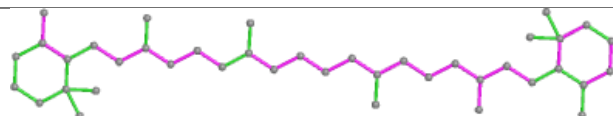


Rings

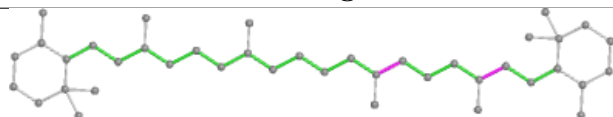
Ligand BCR i 101



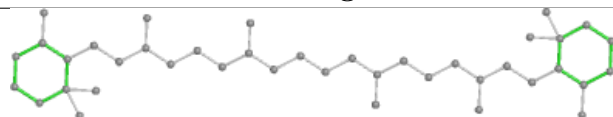
Bond lengths



Bond angles

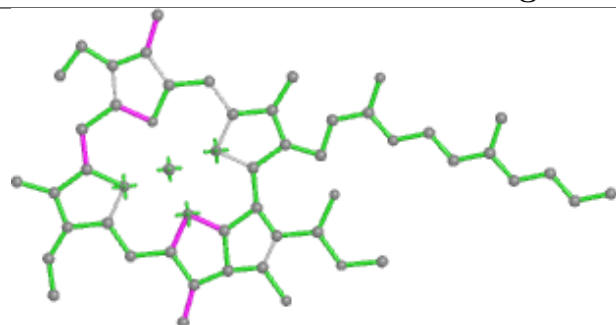


Torsions

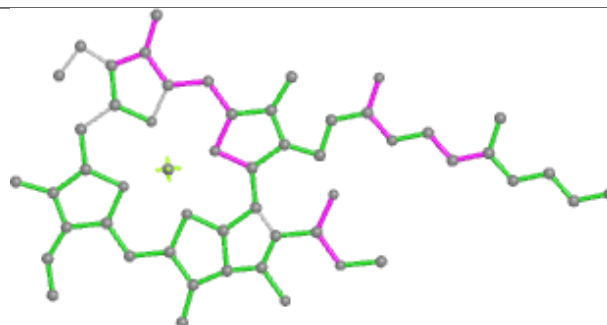


Rings

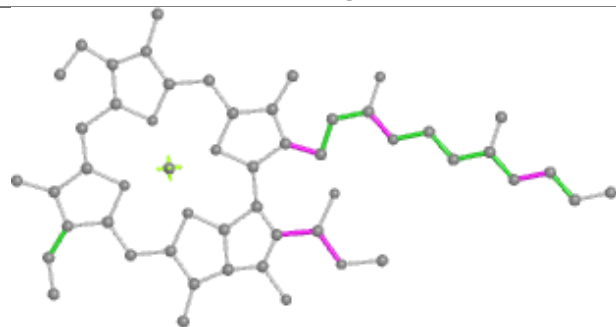
Ligand CLA b 823



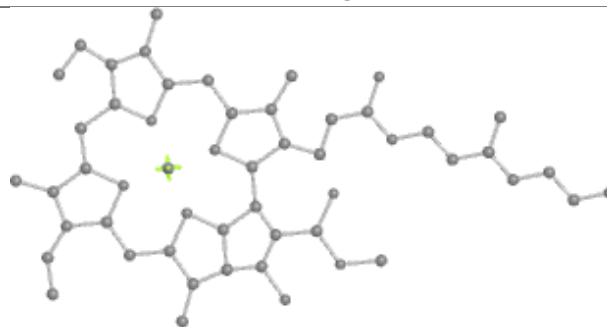
Bond lengths



Bond angles

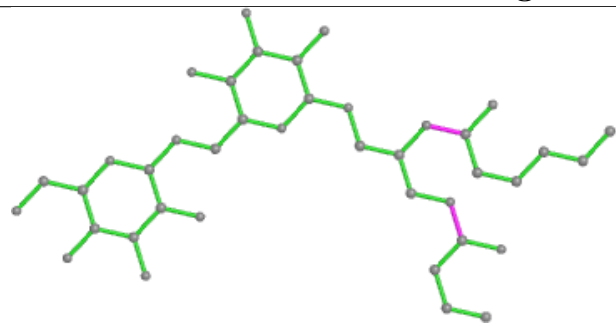


Torsions

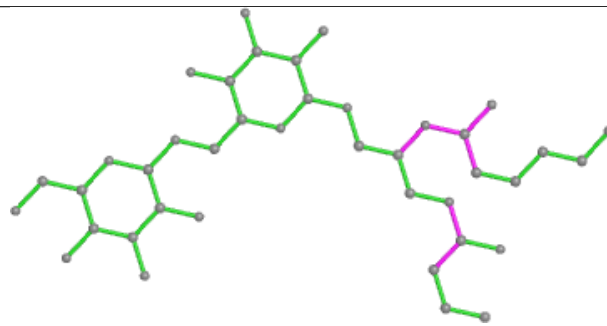


Rings

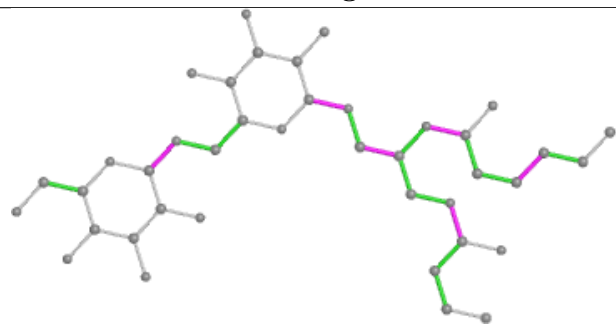
Ligand DGD 8 315



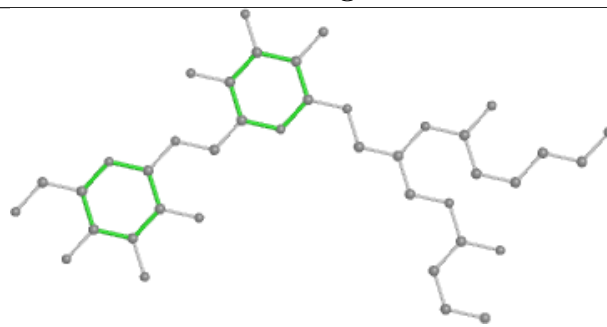
Bond lengths



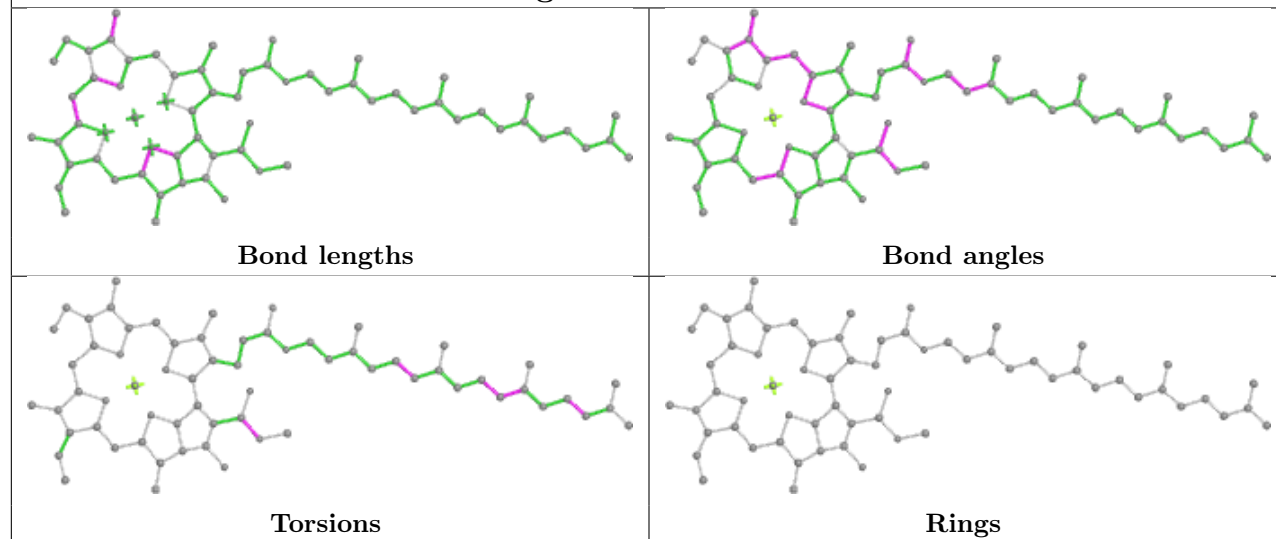
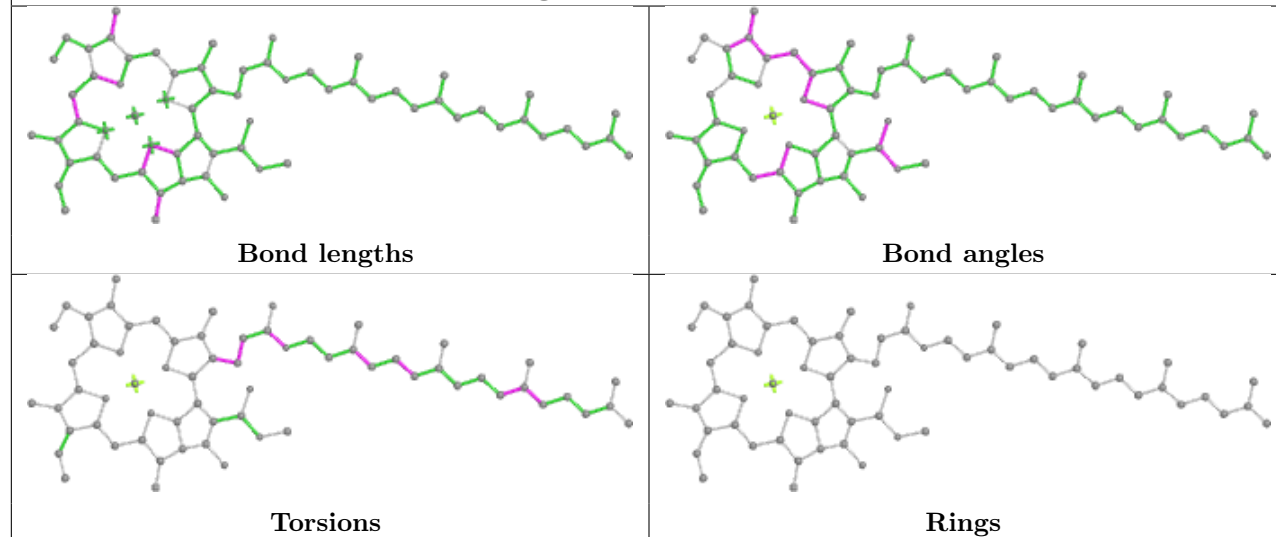
Bond angles



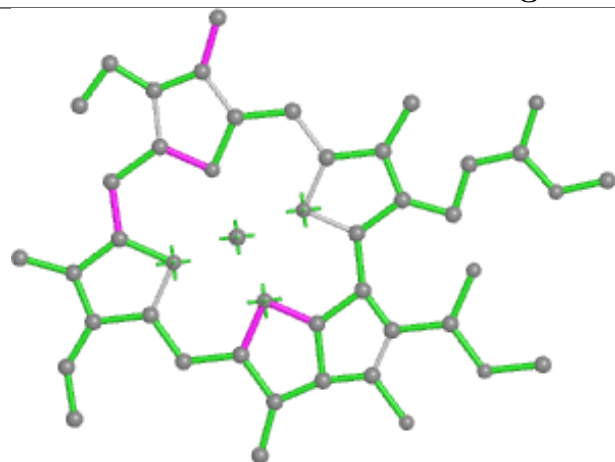
Torsions



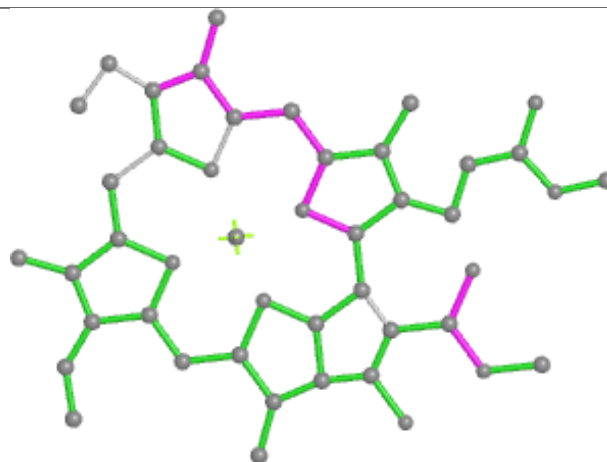
Rings

Ligand CLA a 834**Ligand CLA b 828**

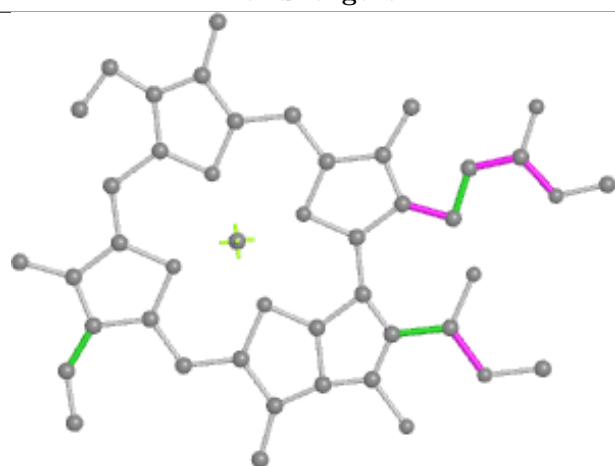
Ligand CLA 6 316



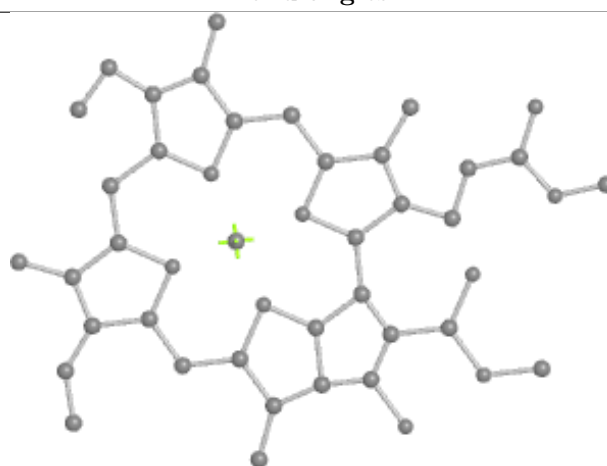
Bond lengths



Bond angles

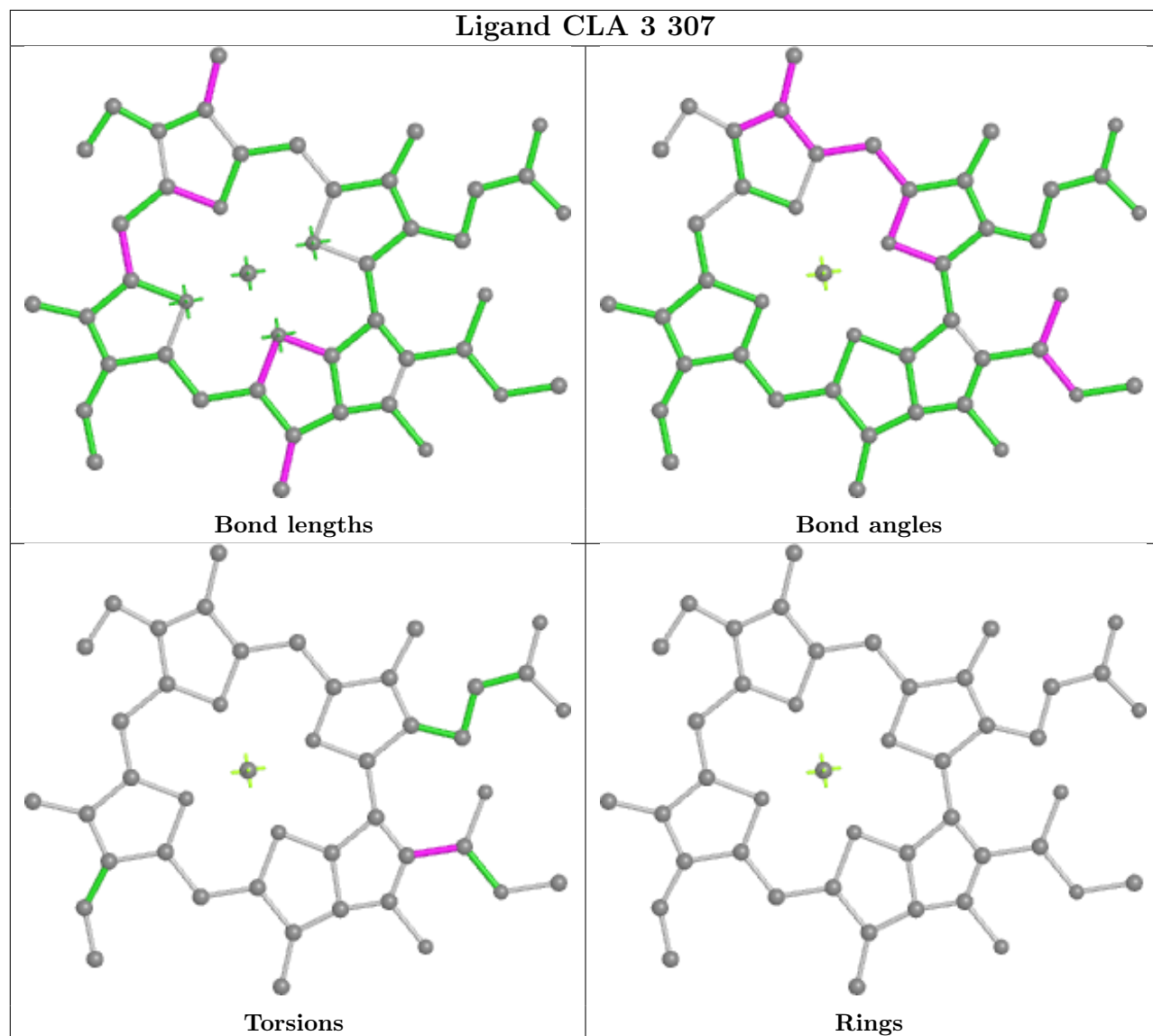


Torsions

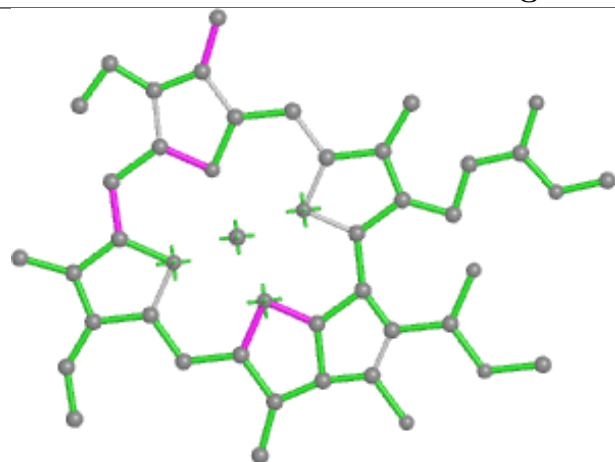


Rings

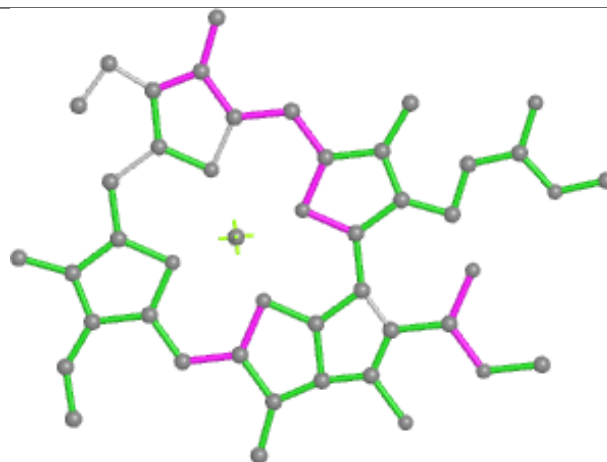
Ligand CLA 3 307



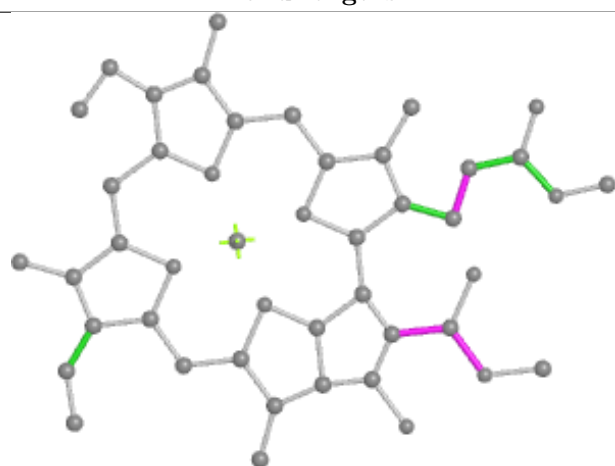
Ligand CLA 2 309



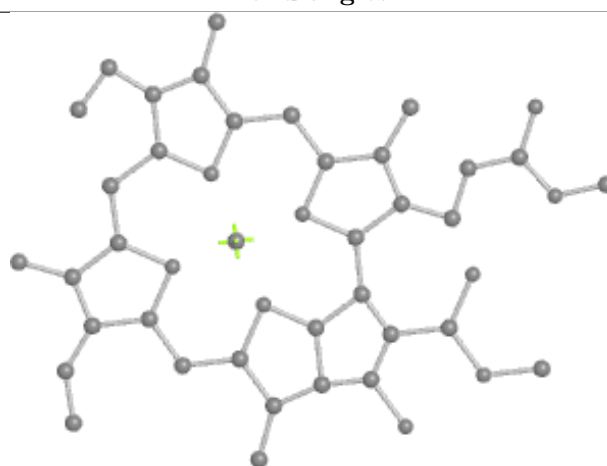
Bond lengths



Bond angles

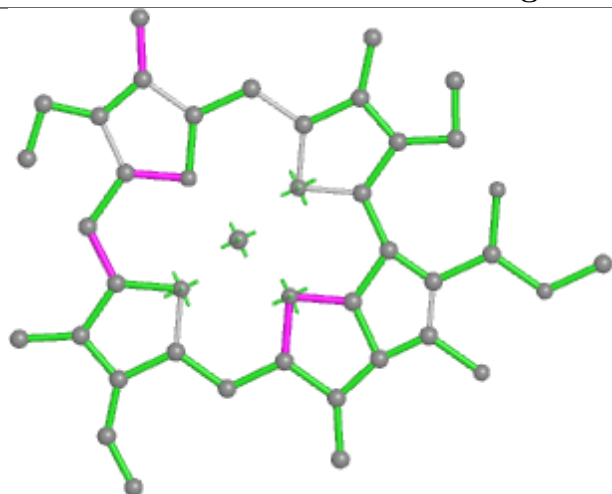


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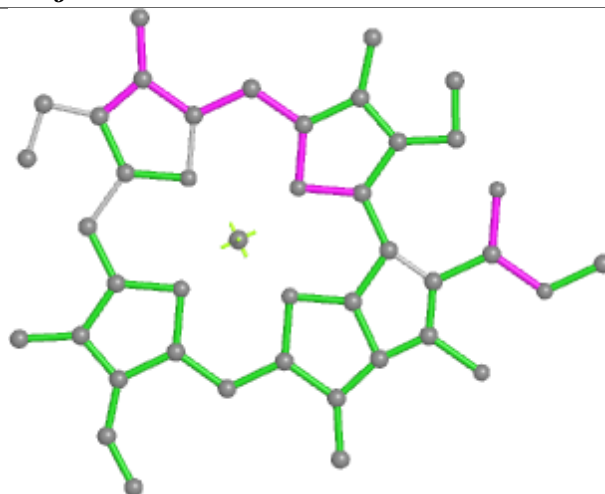


Rings

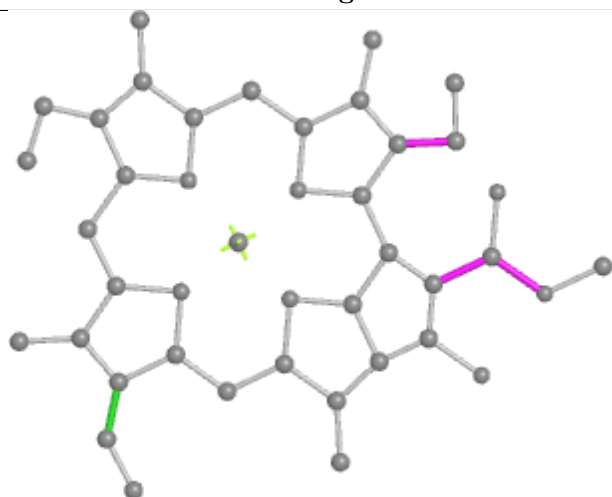
Ligand CLA j 101



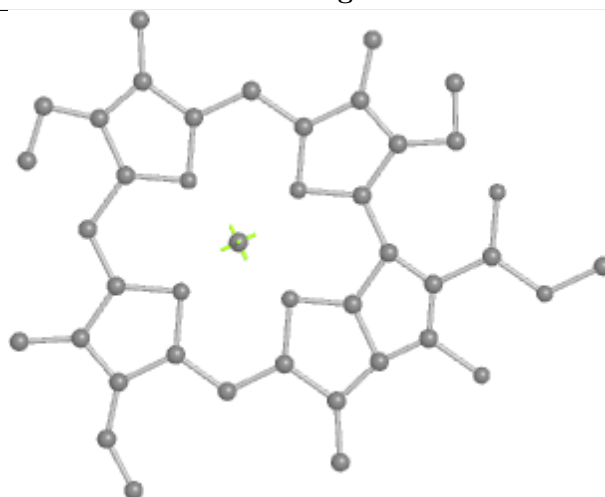
Bond lengths



Bond angles

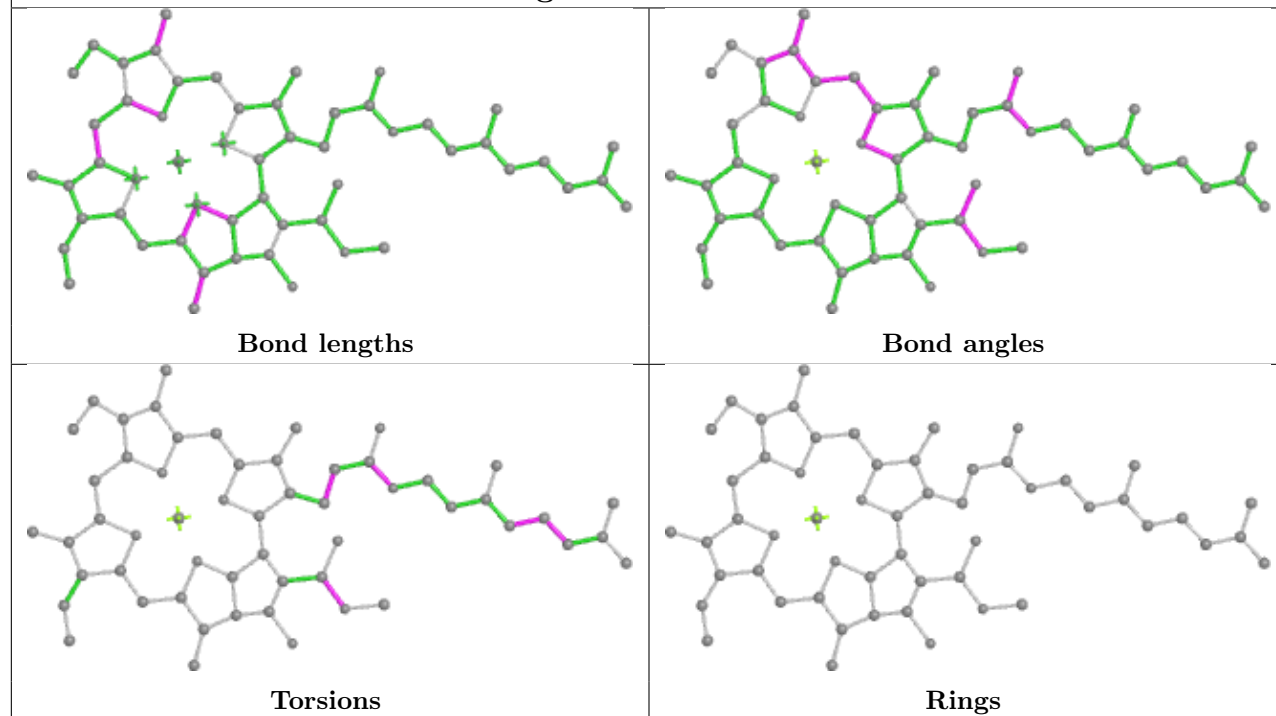


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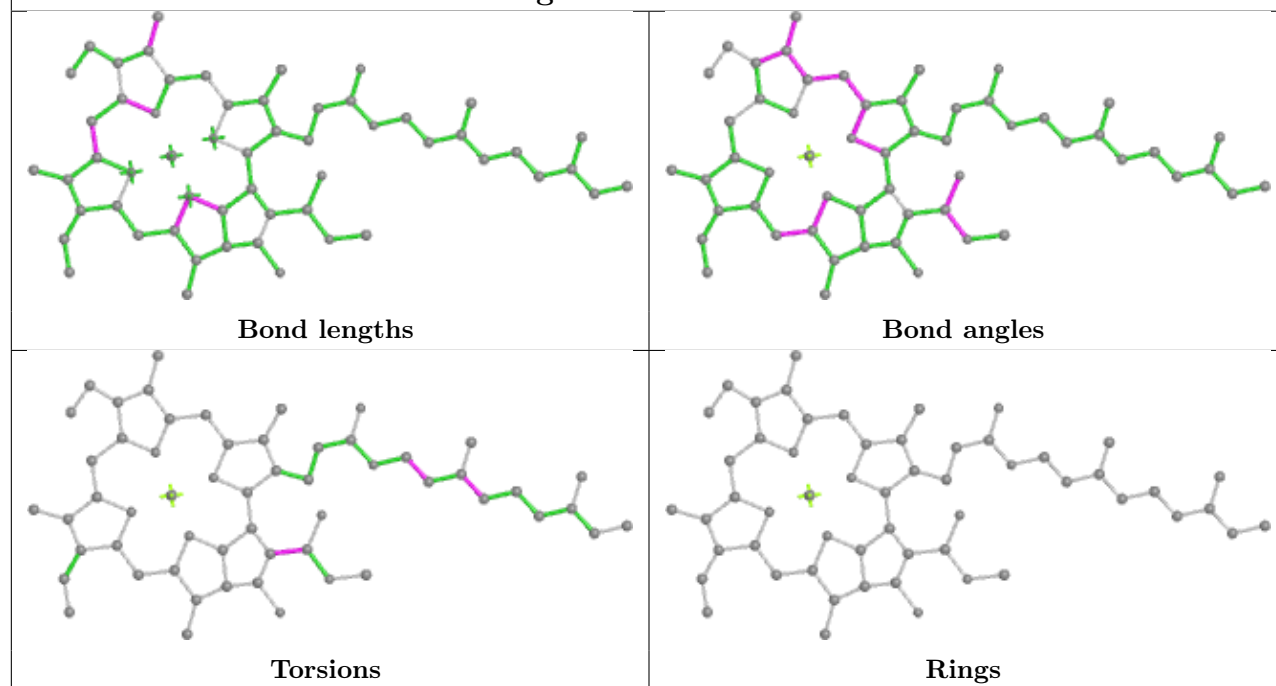


Rings

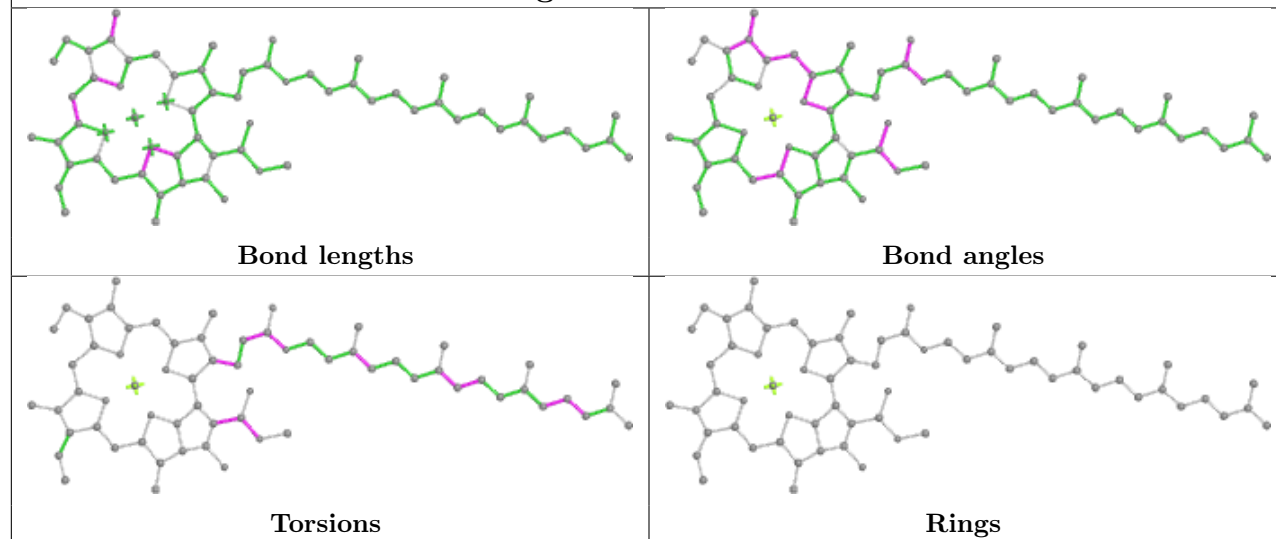
Ligand CLA 4 316



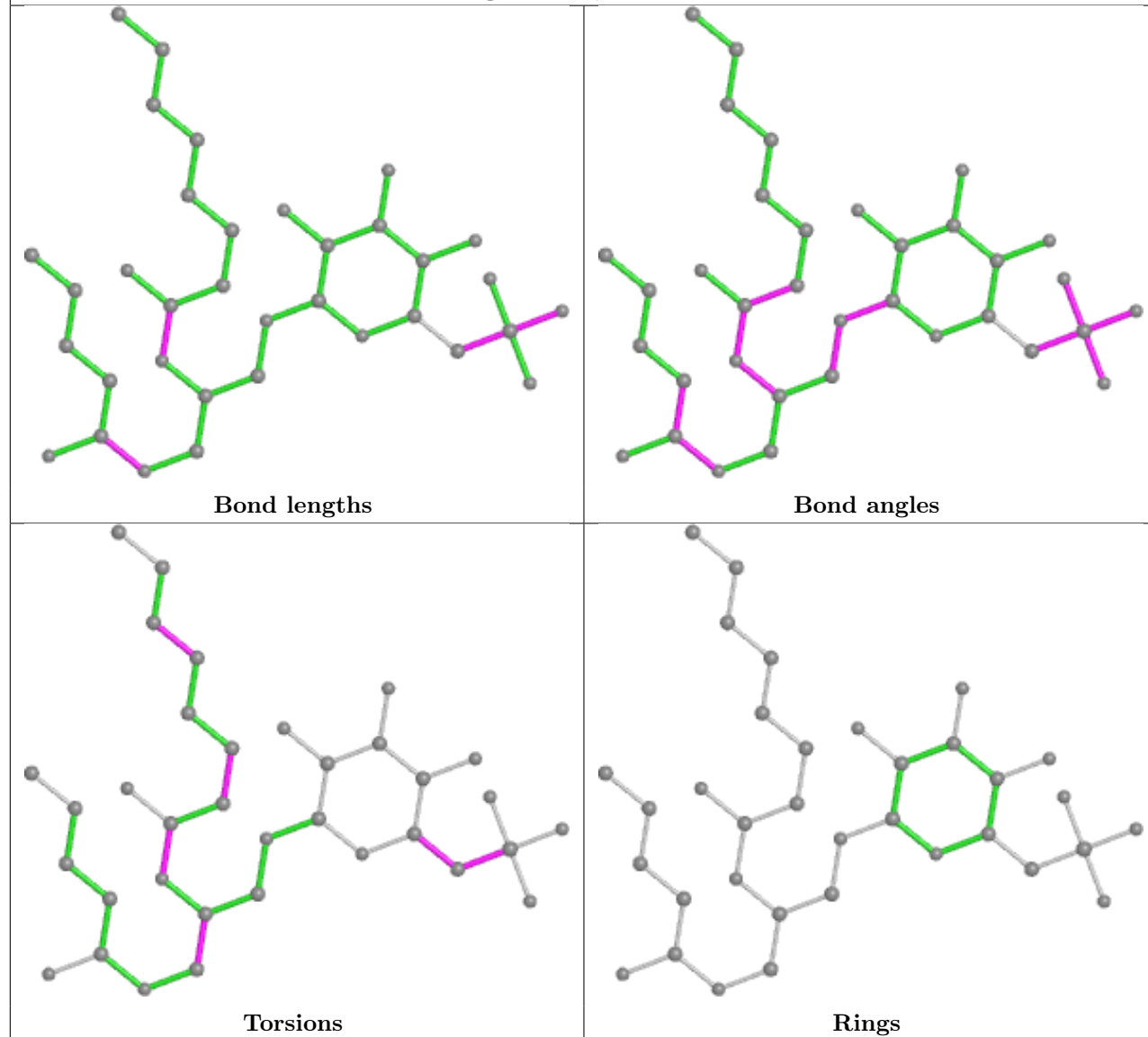
Ligand CLA 3 310



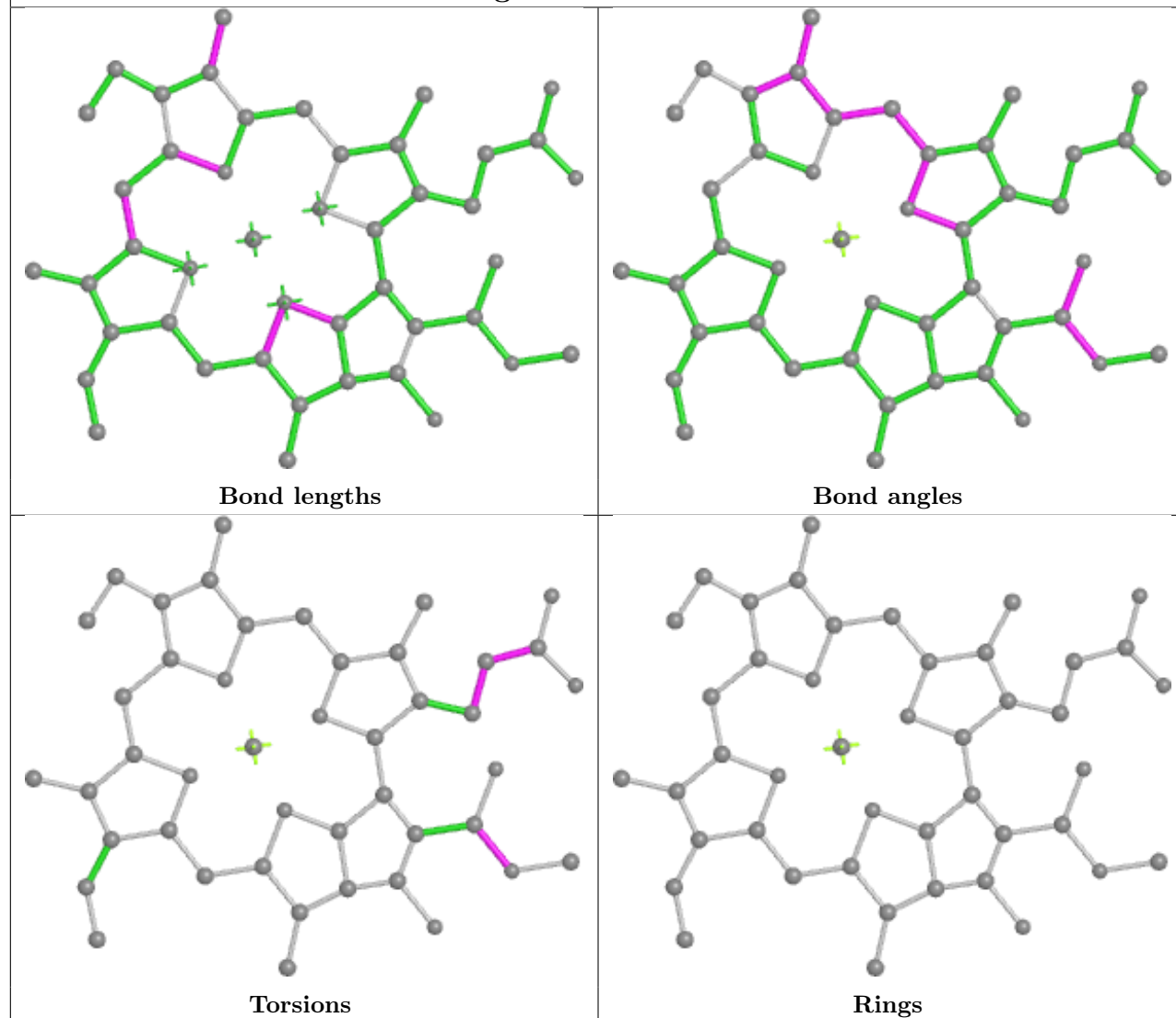
Ligand CLA 4 309



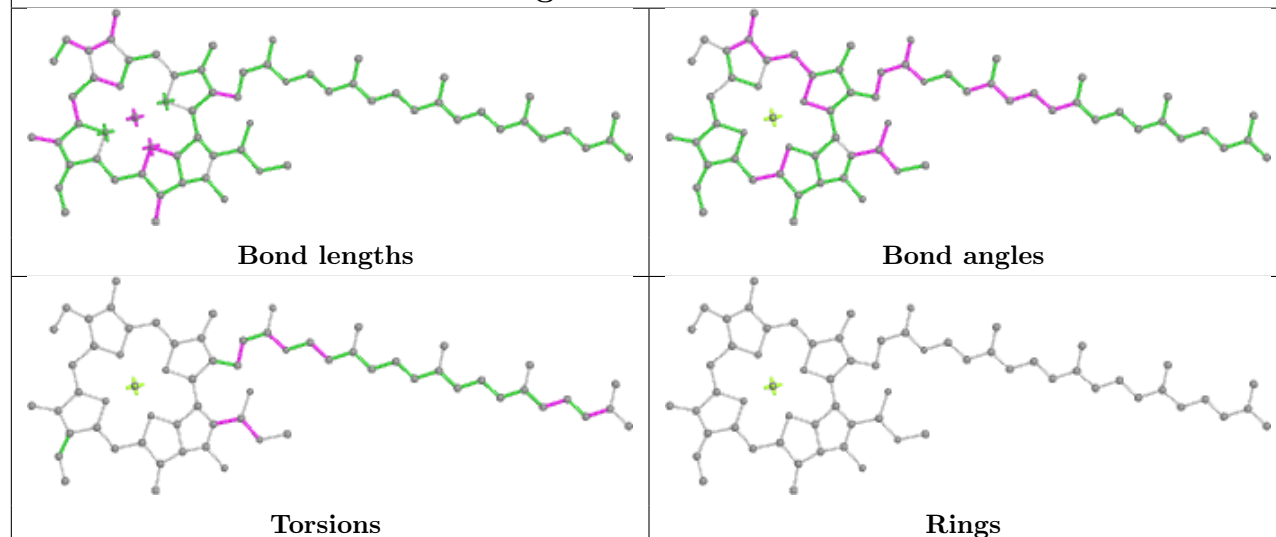
Ligand SQD 5 317



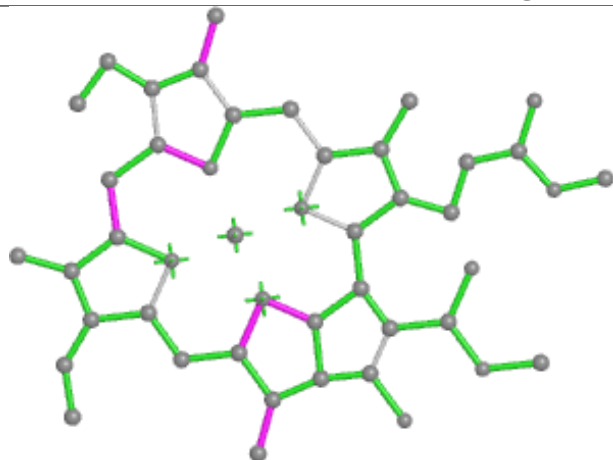
Ligand CLA 7 317



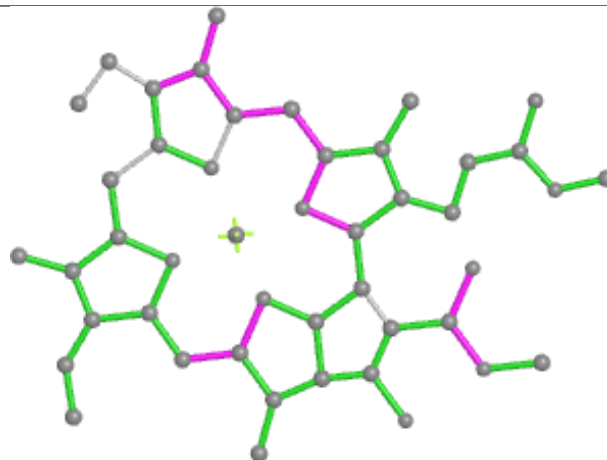
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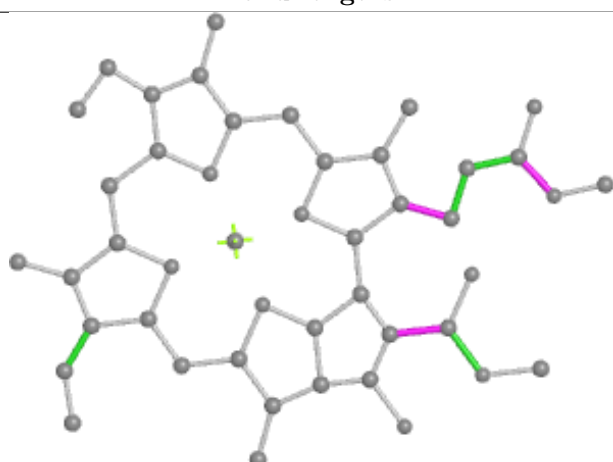
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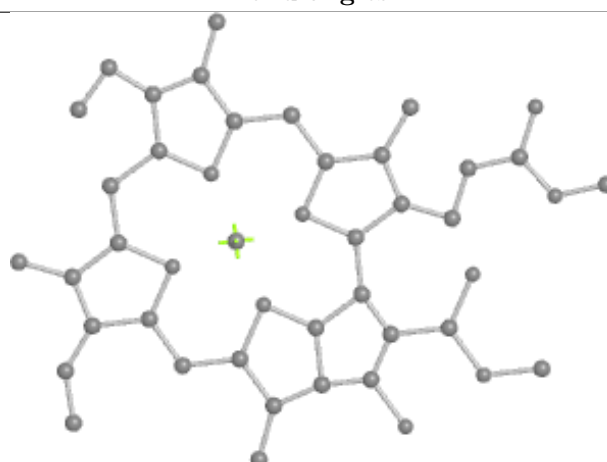
Bond lengths



Bond angles

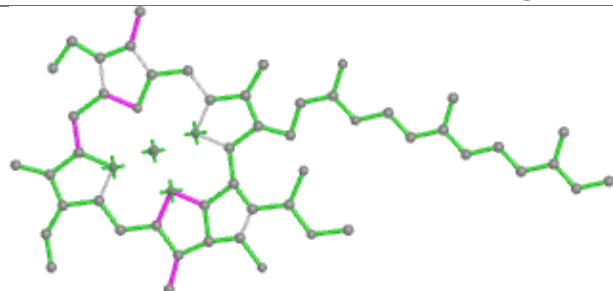


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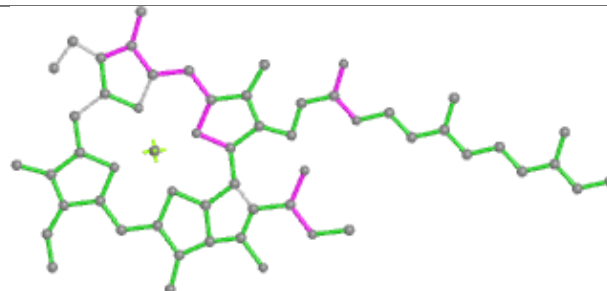


Rings

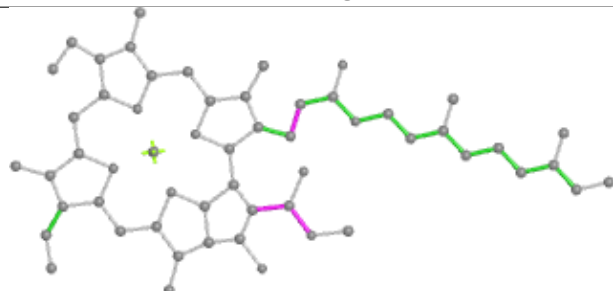
Ligand CLA 3 309



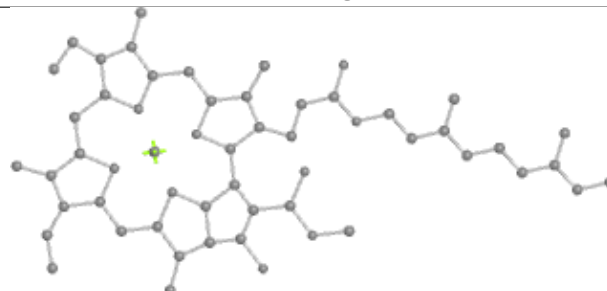
Bond lengths



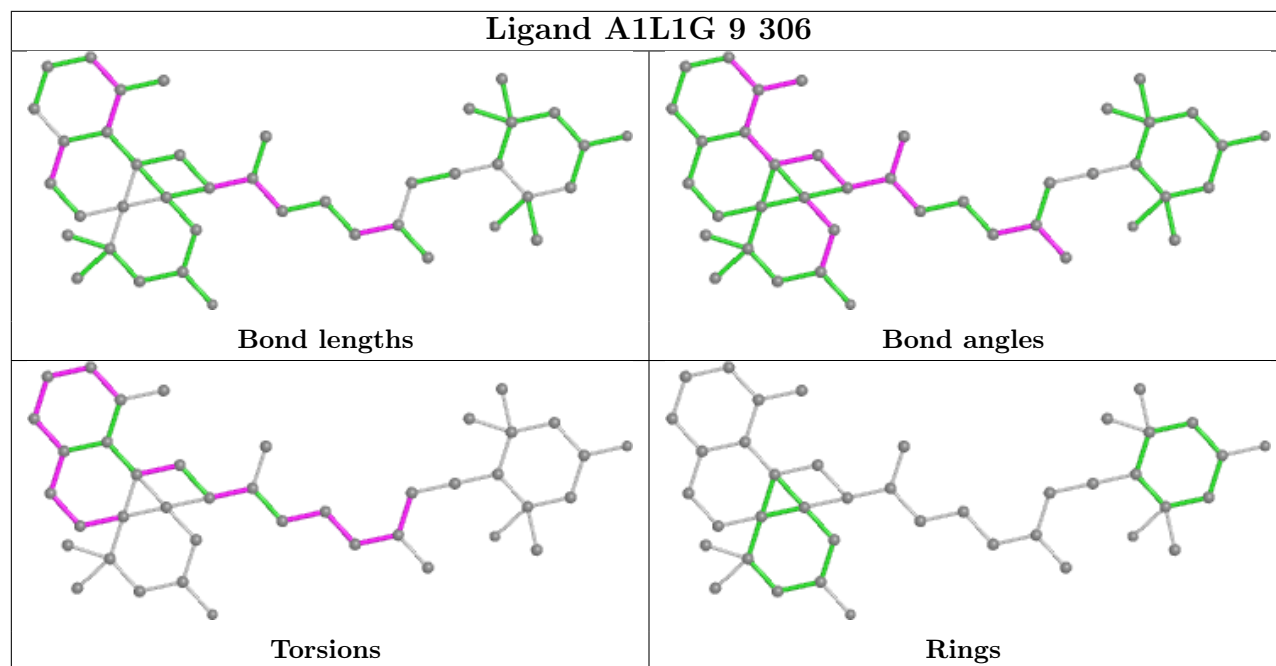
Bond angles



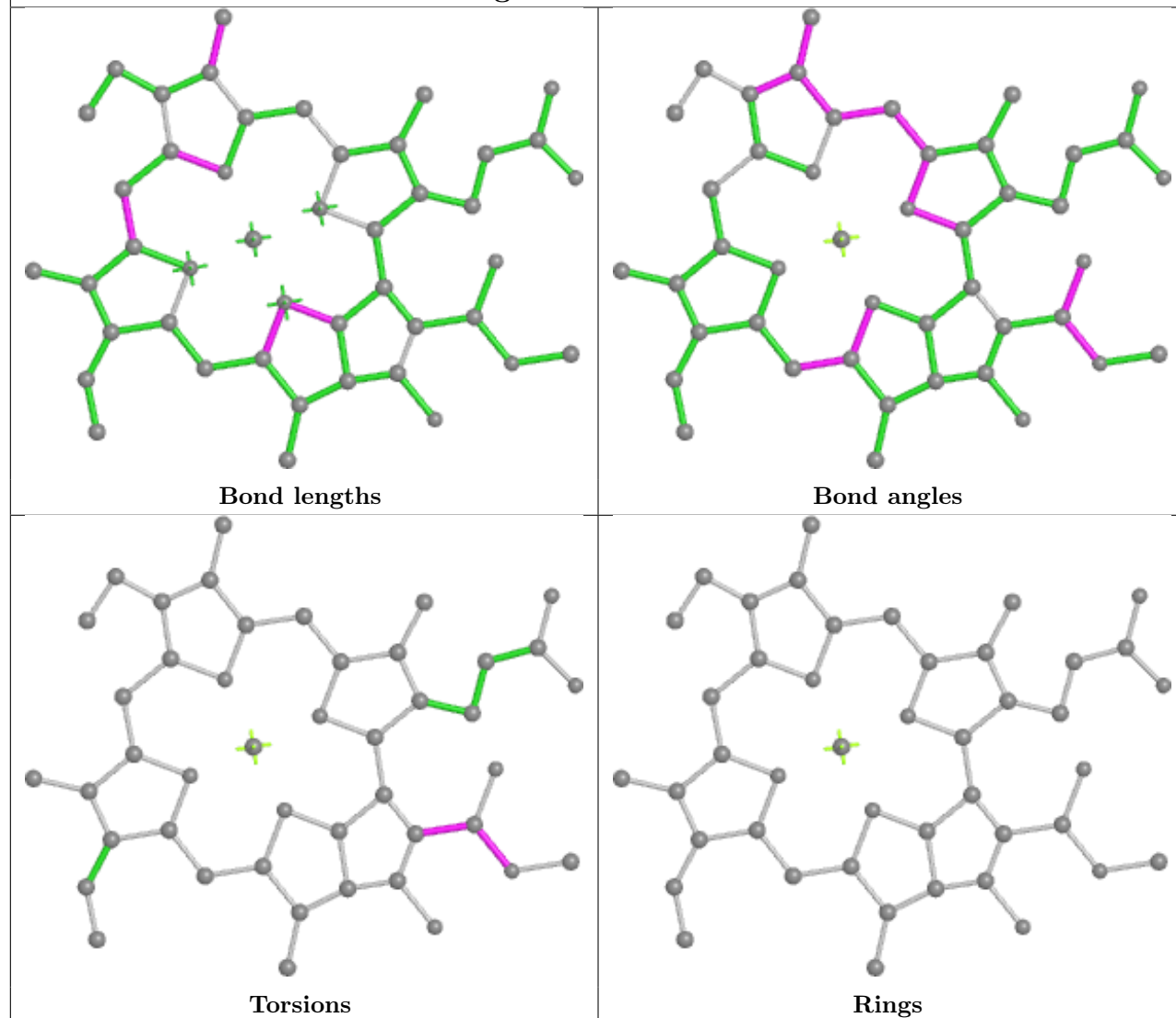
Torsions



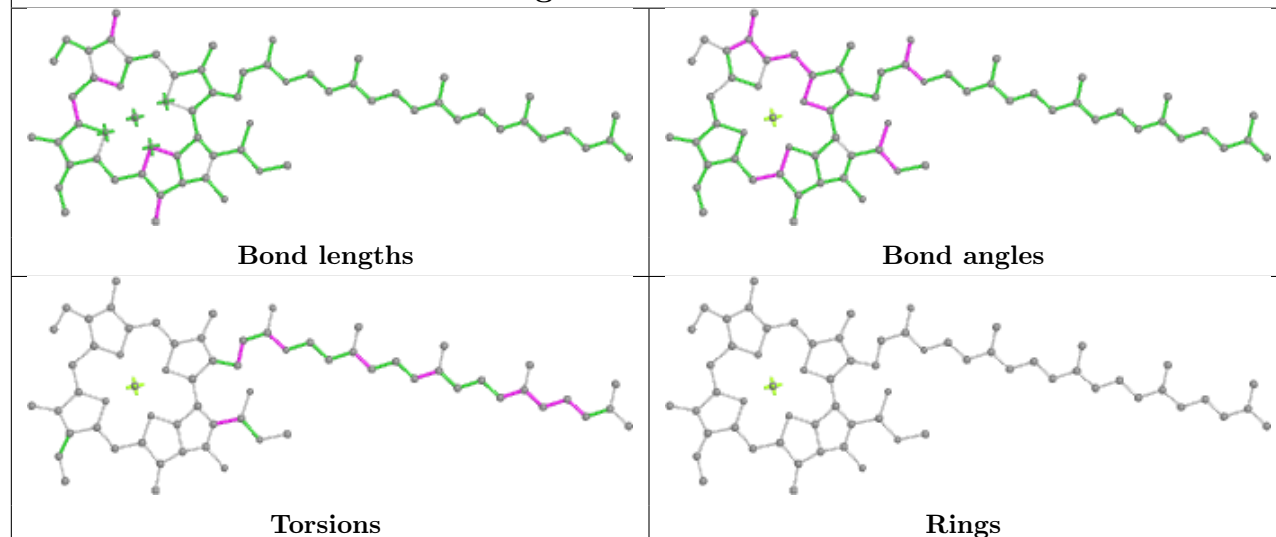
Rings

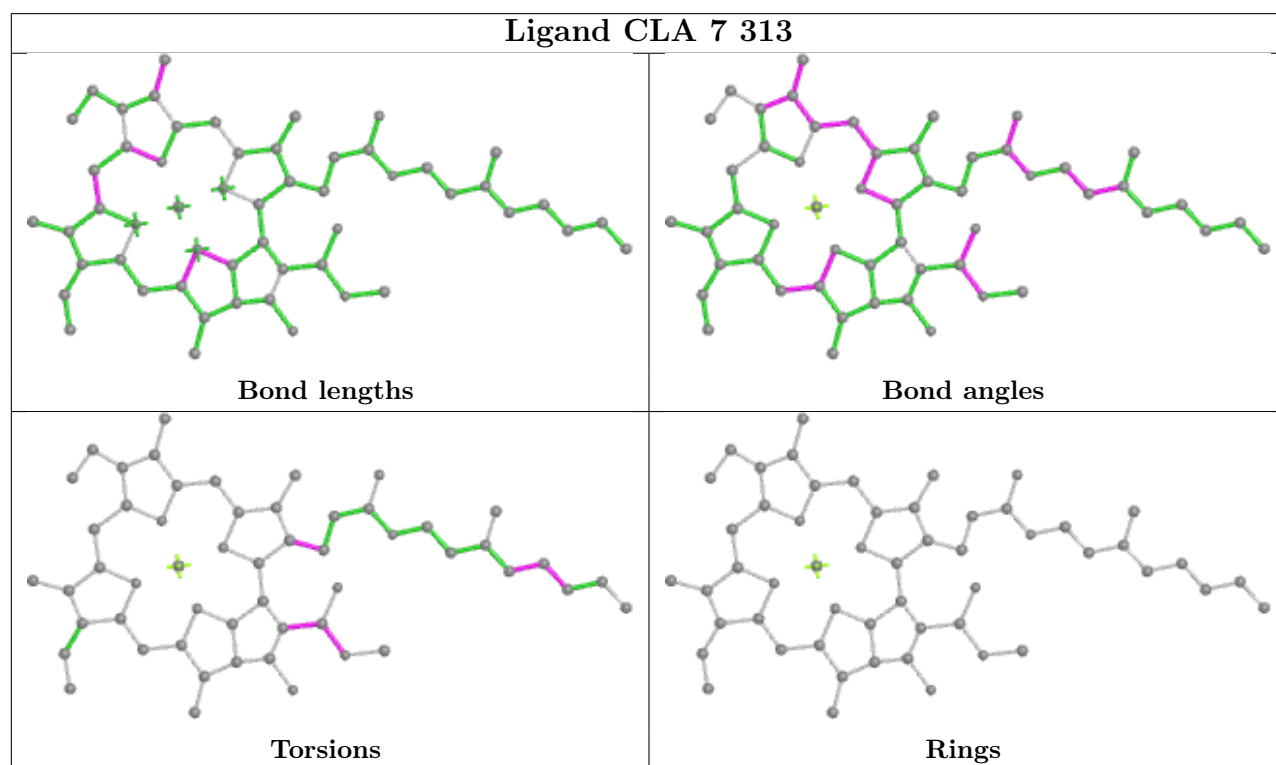
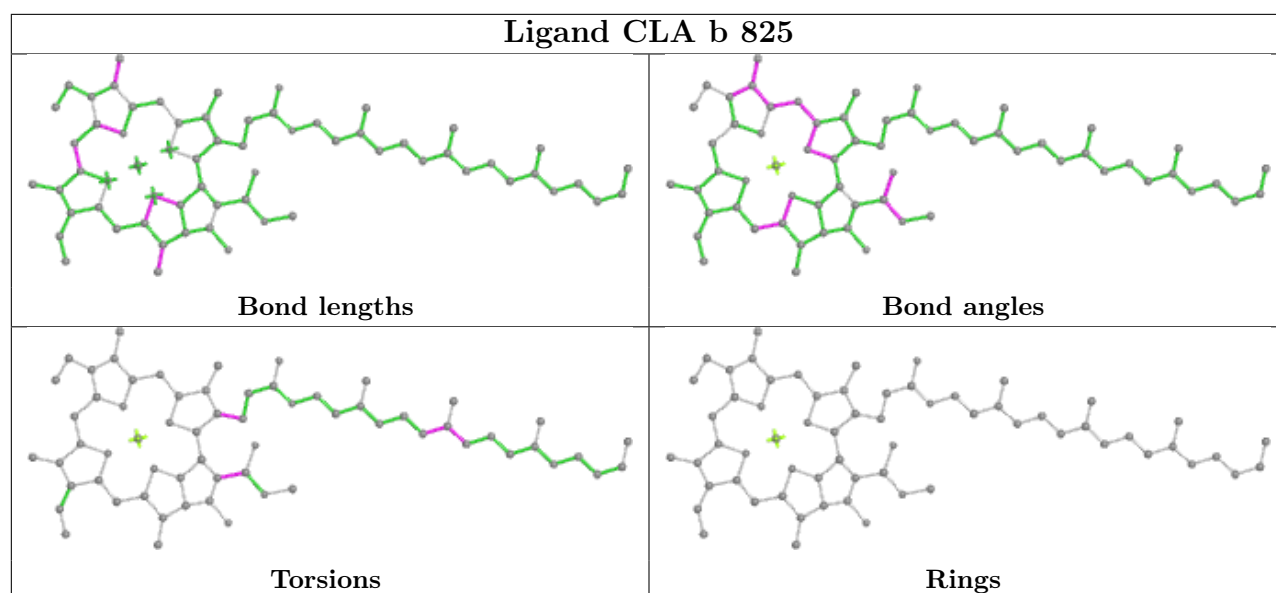


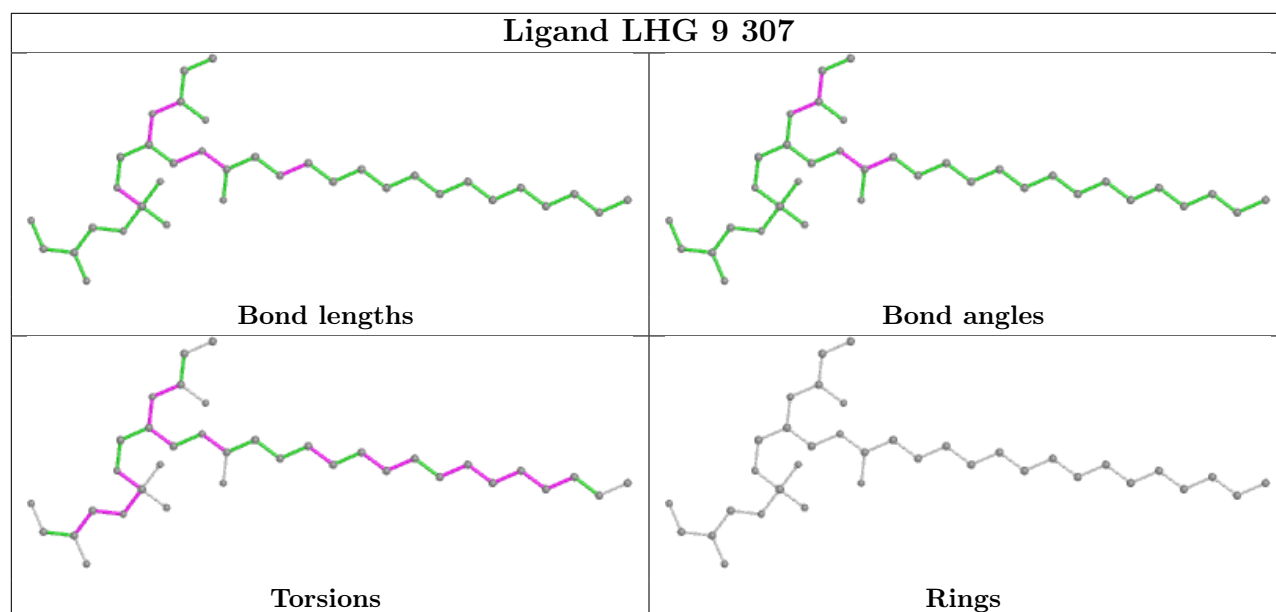
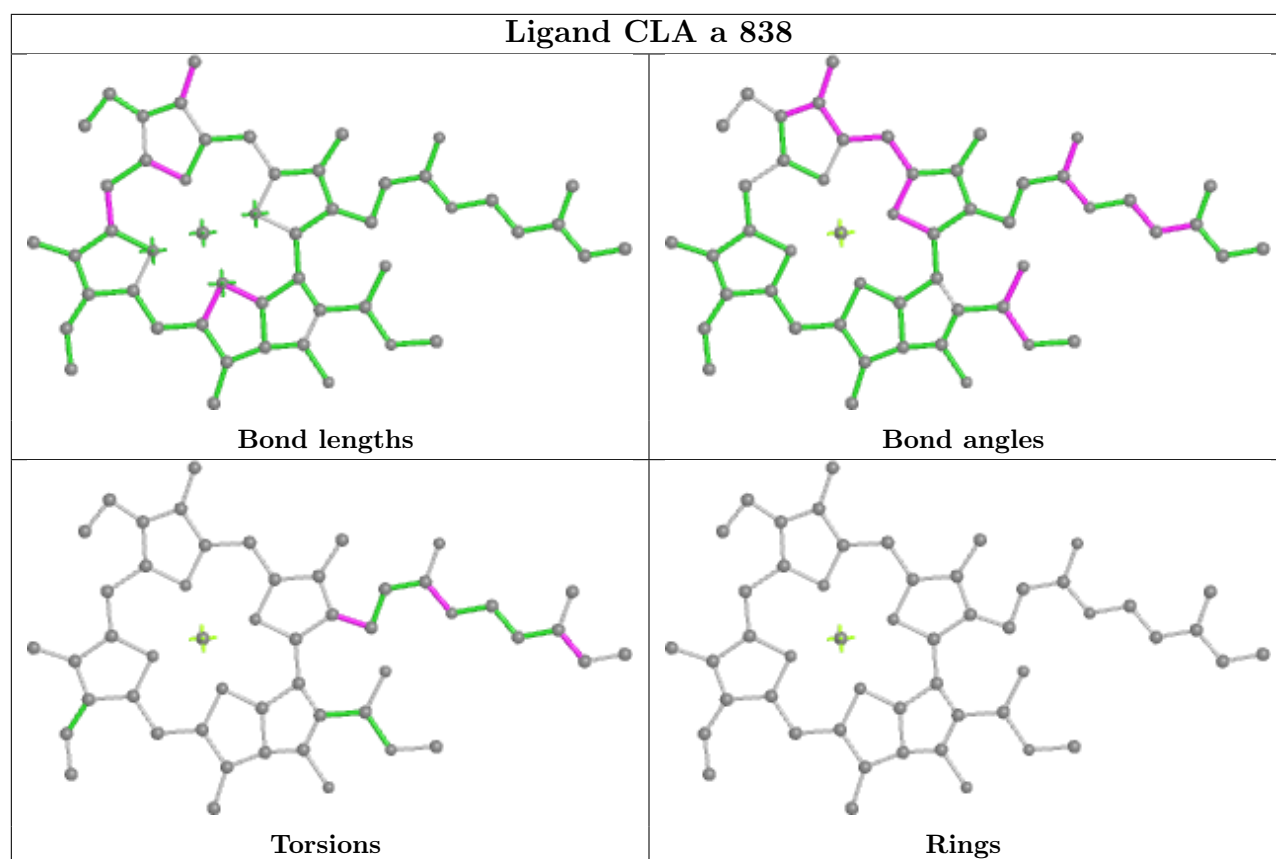
Ligand CLA a 837

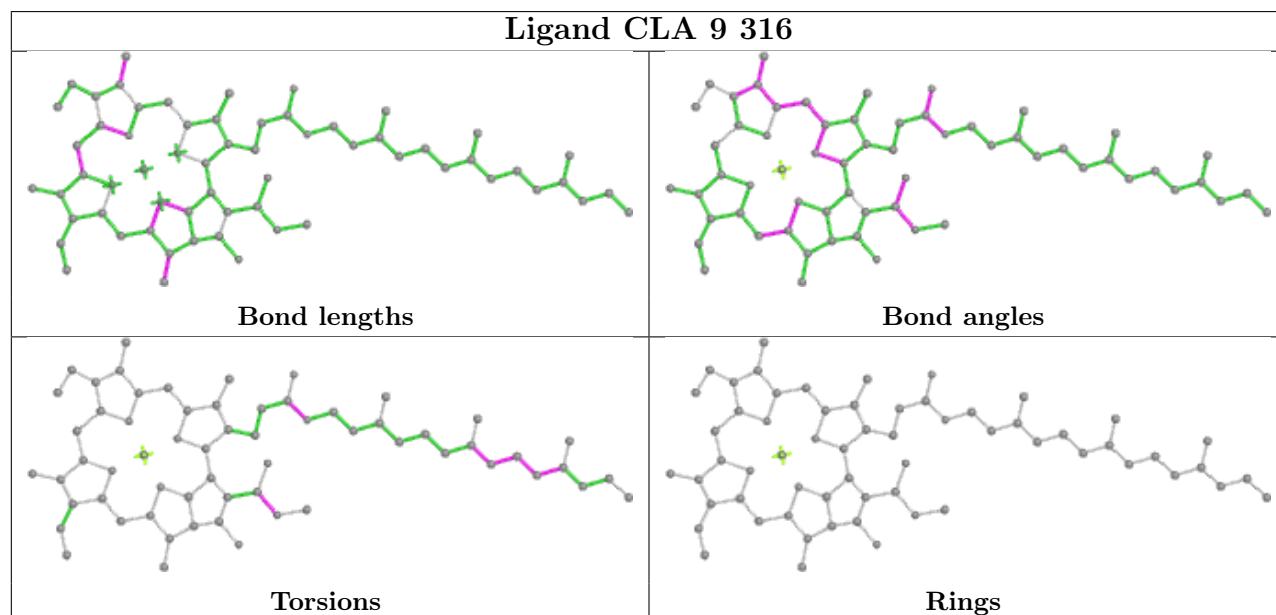
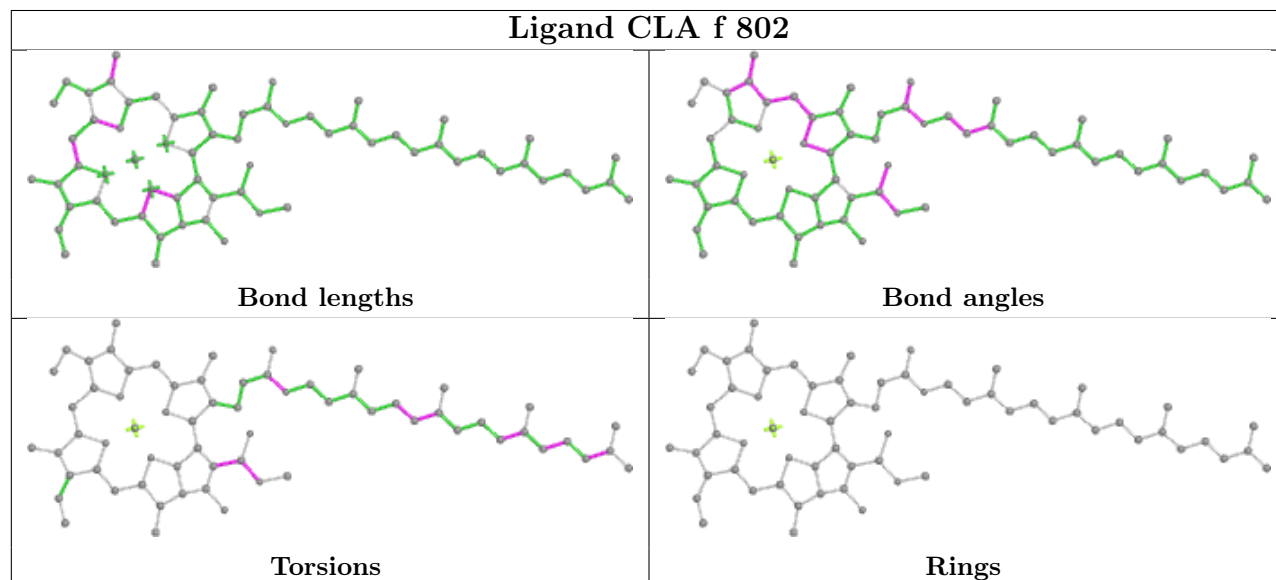
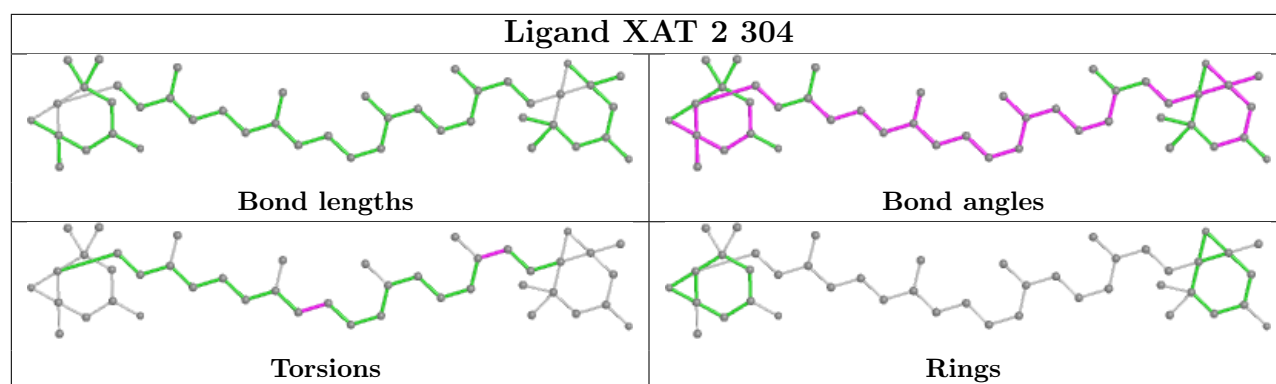


Ligand CLA b 839

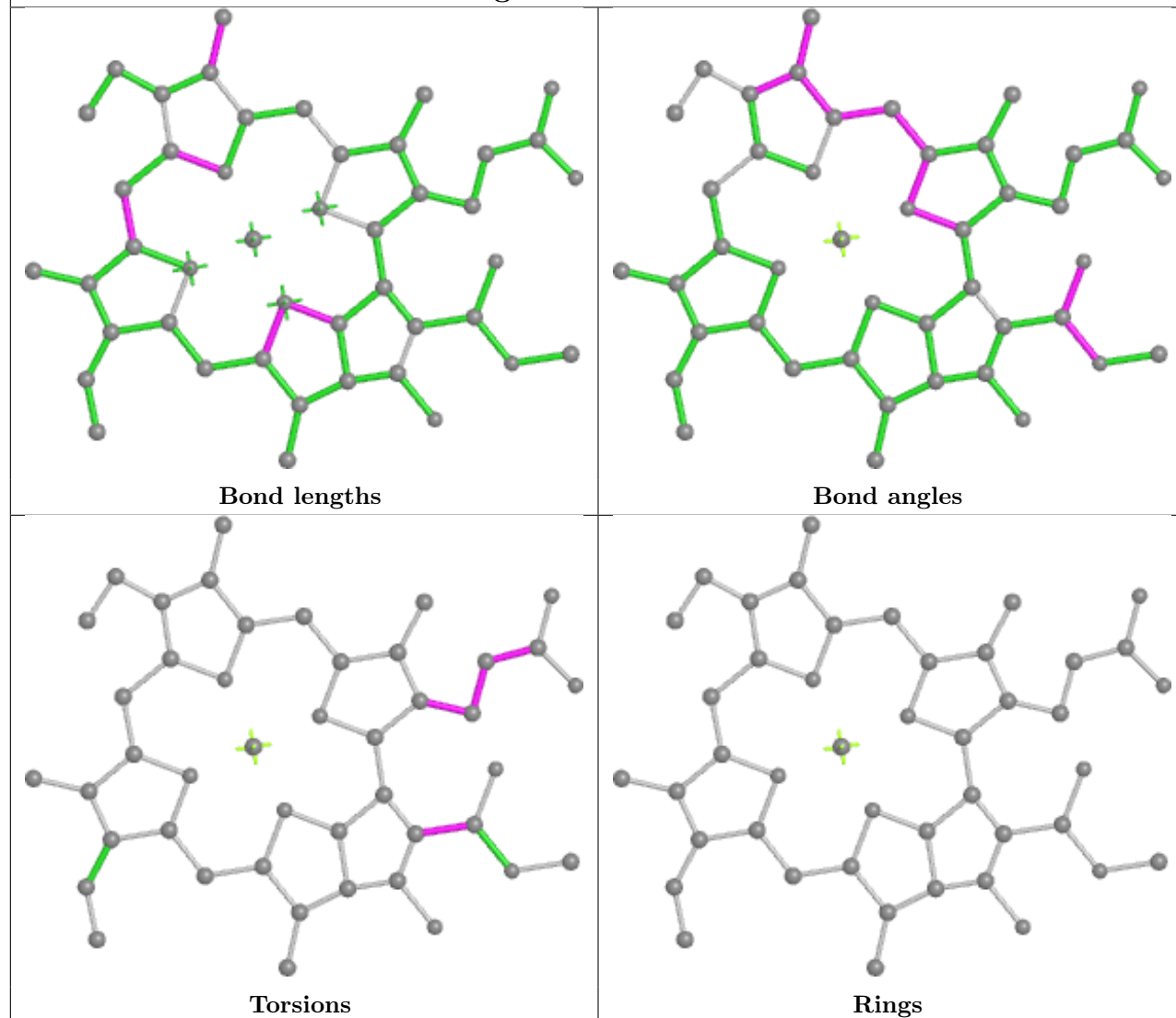




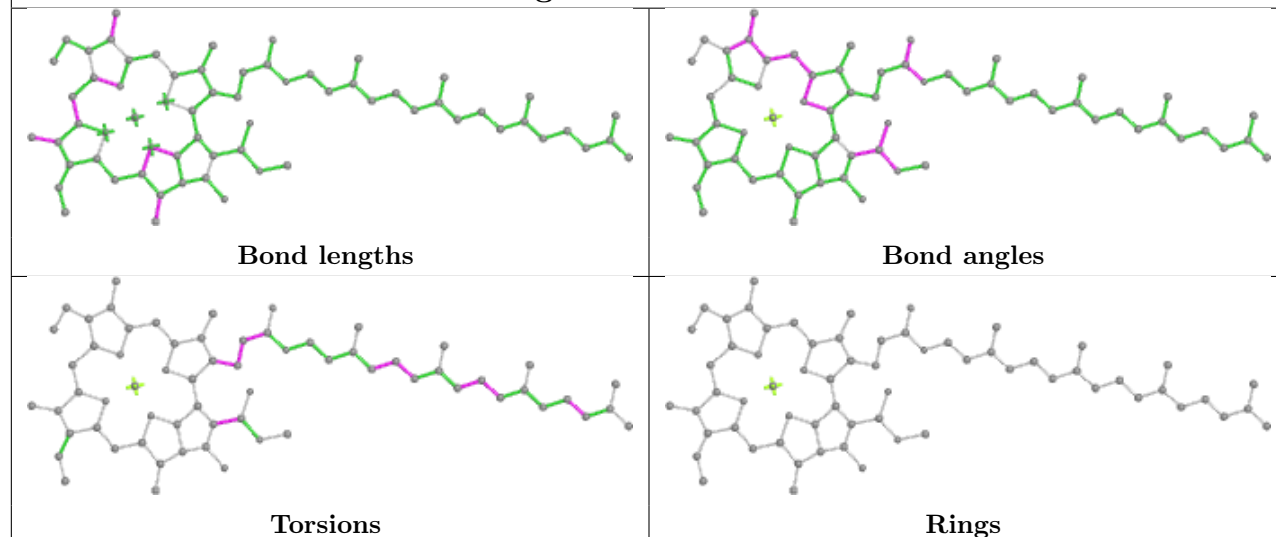




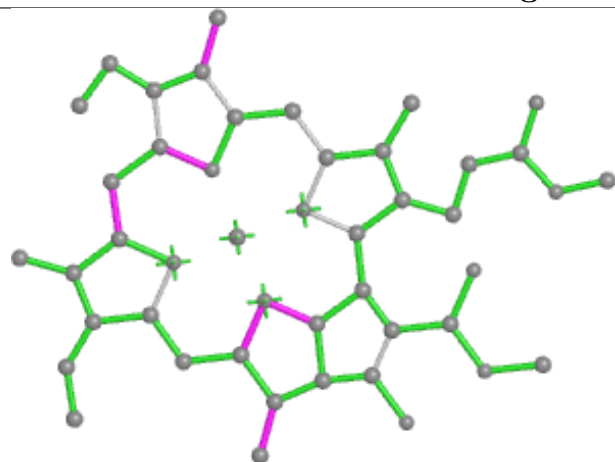
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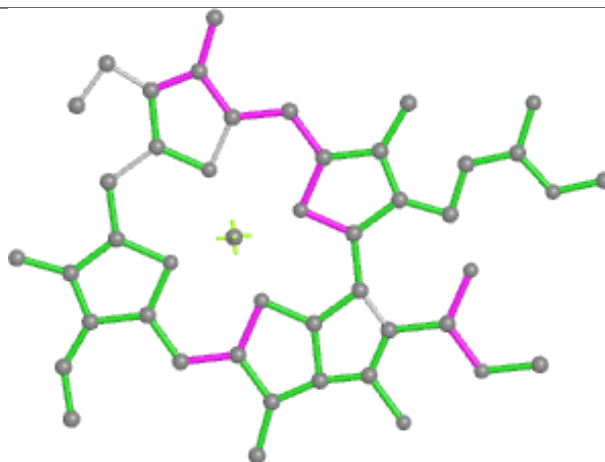
Ligand CLA b 808



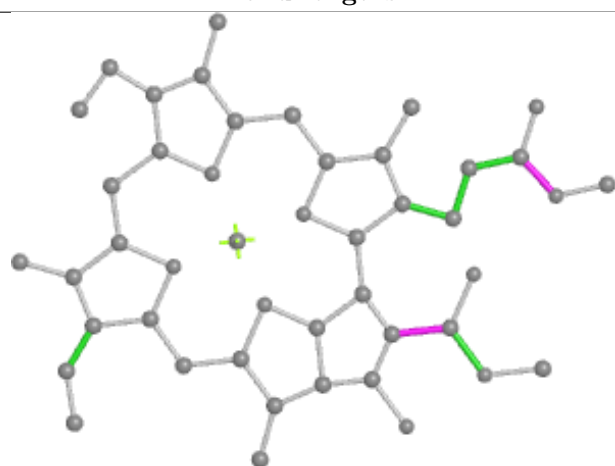
Ligand CLA 9 309



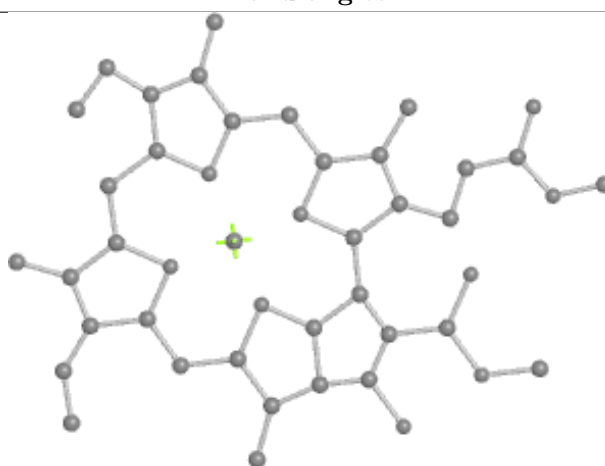
Bond lengths



Bond angles

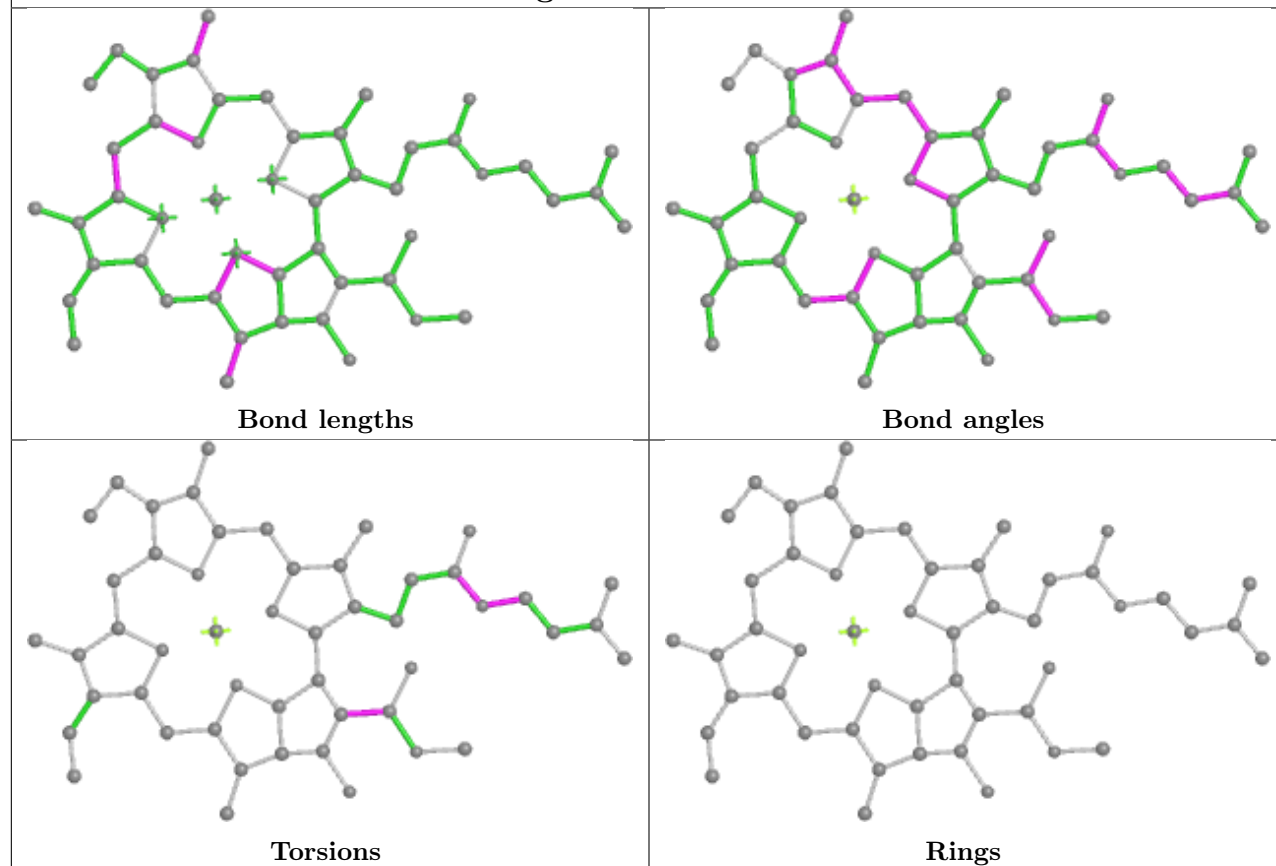


Torsions

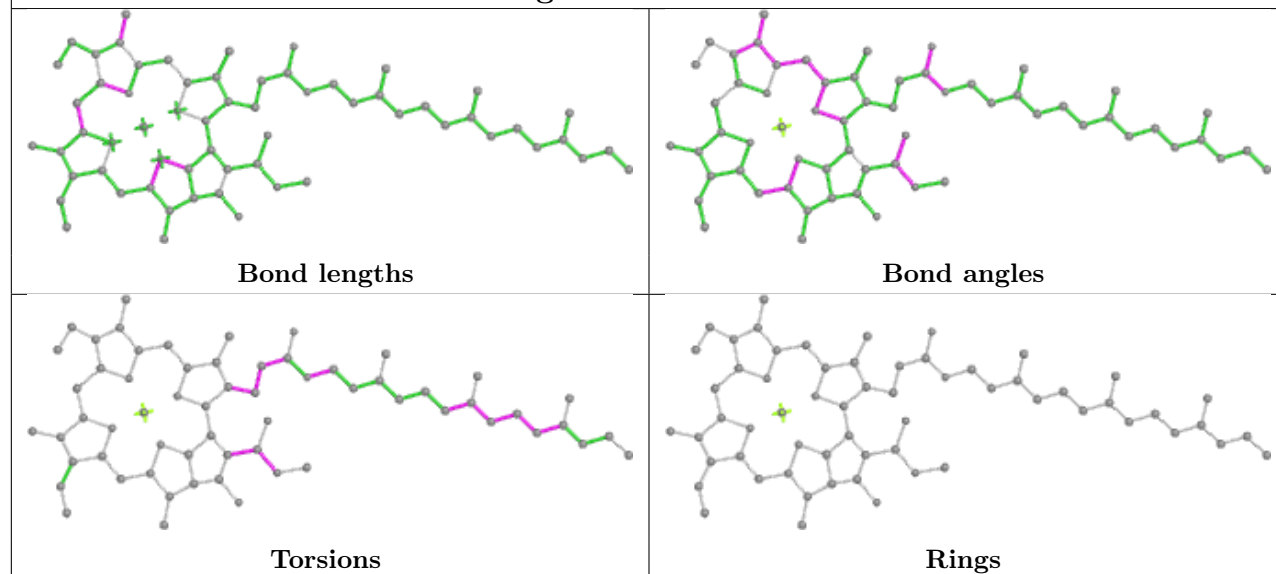


Rings

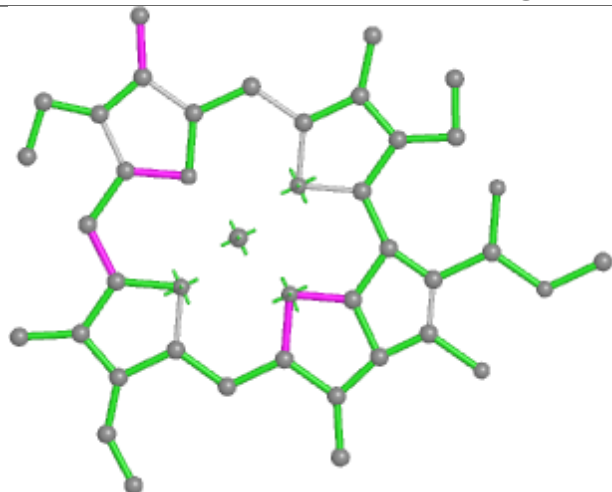
Ligand CLA a 816



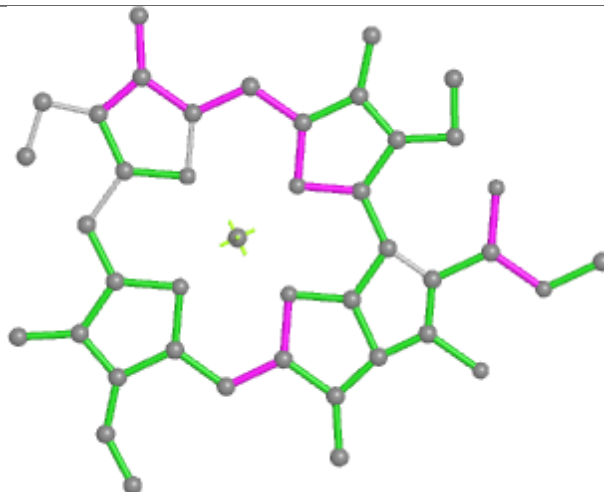
Ligand CLA a 829



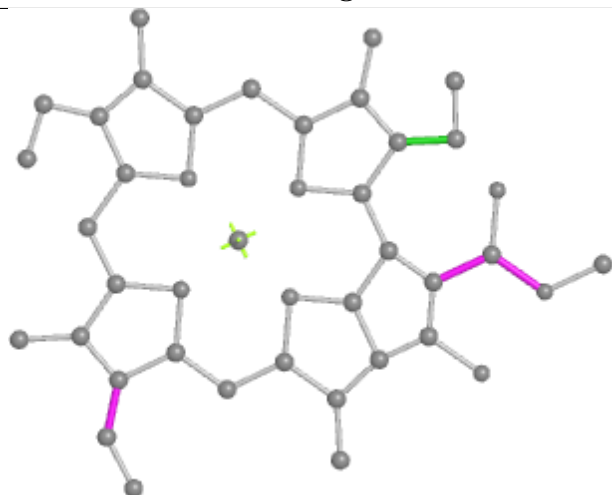
Ligand CLA 9 315



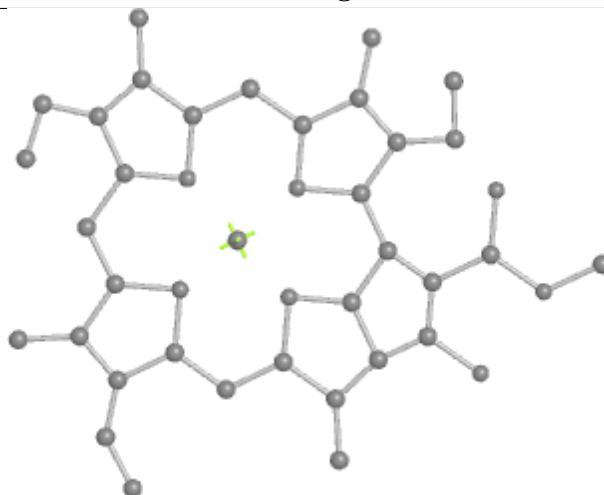
Bond lengths



Bond angles

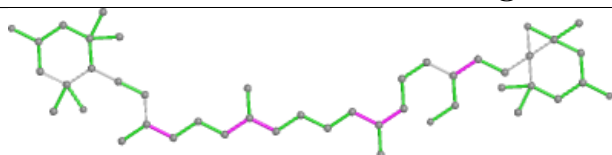


Torsions

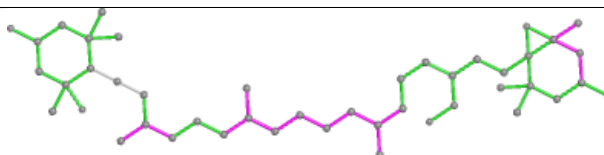


Rings

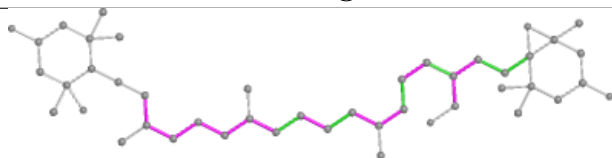
Ligand A1L1G 3 306



Bond lengths



Bond angles

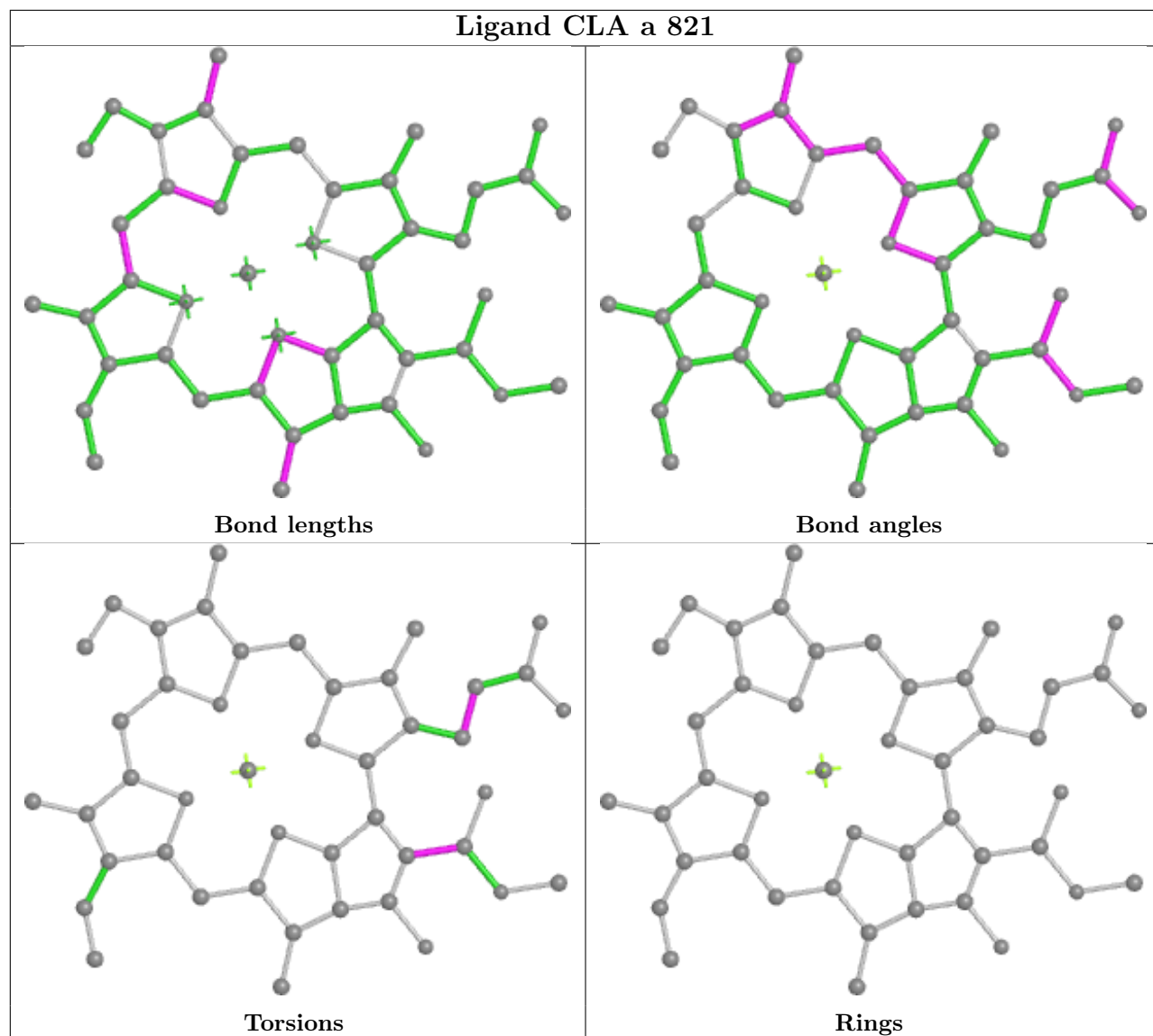


Torsions

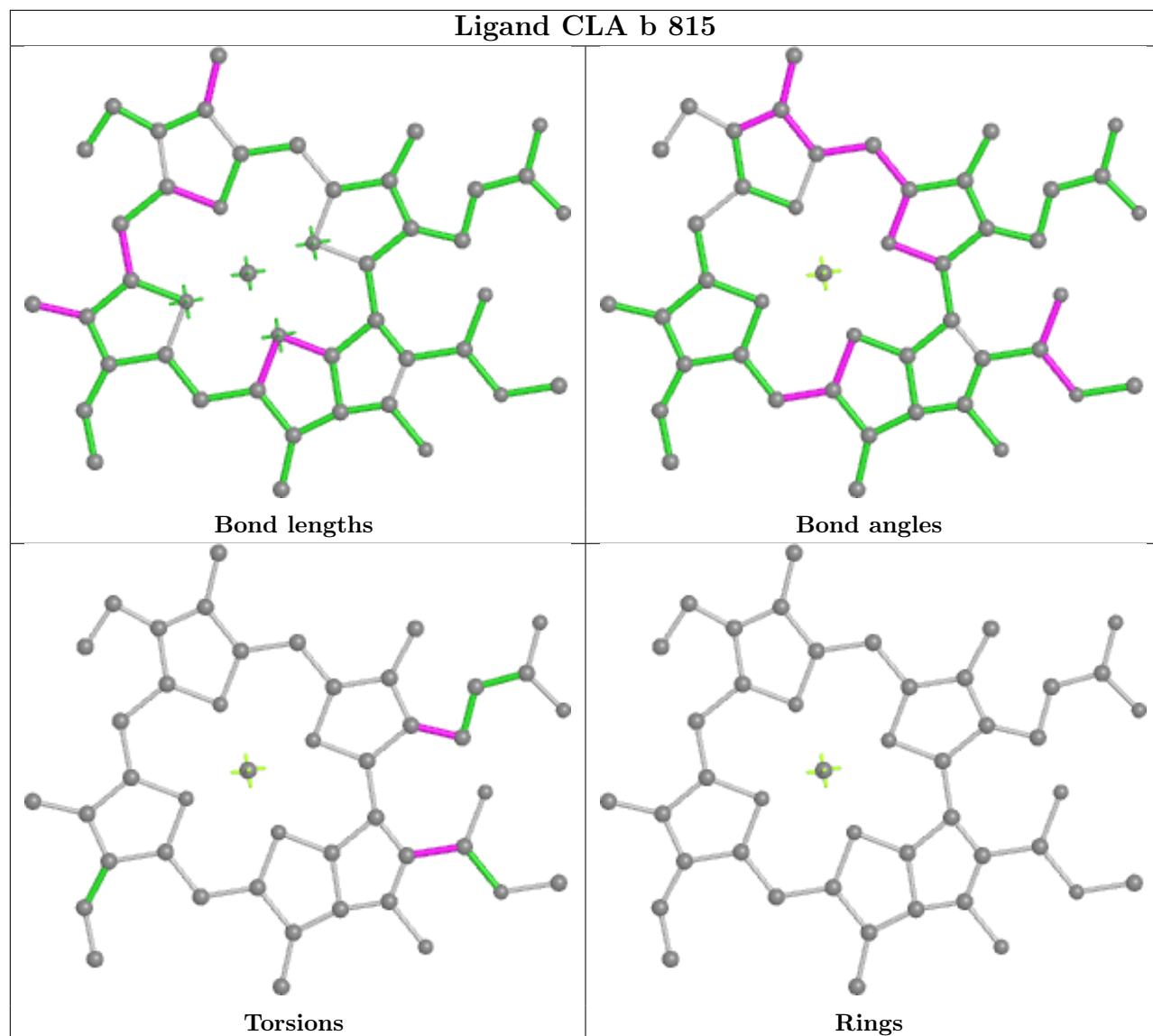


Rings

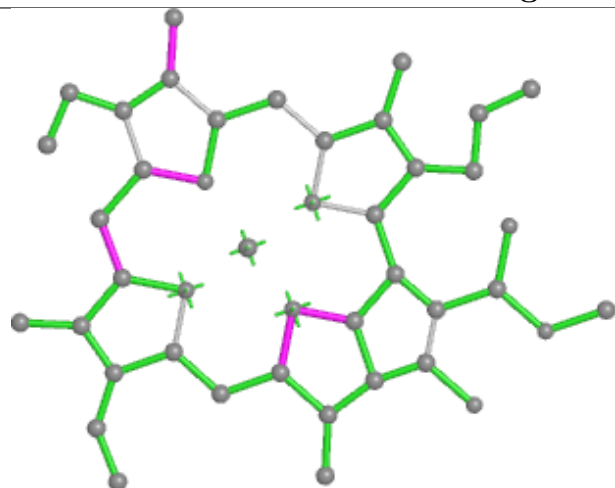
Ligand CLA a 821



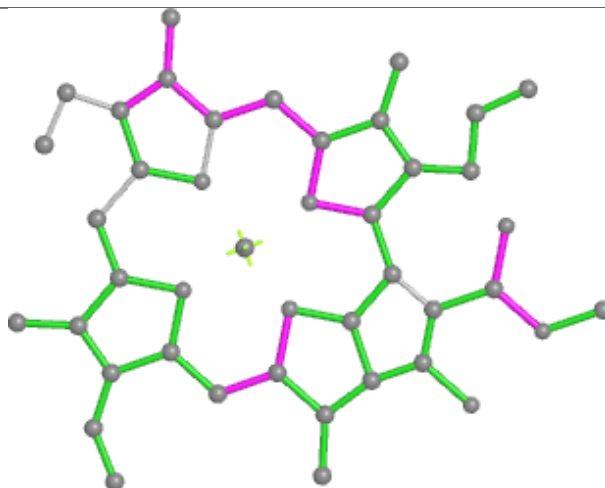
Ligand CLA b 815



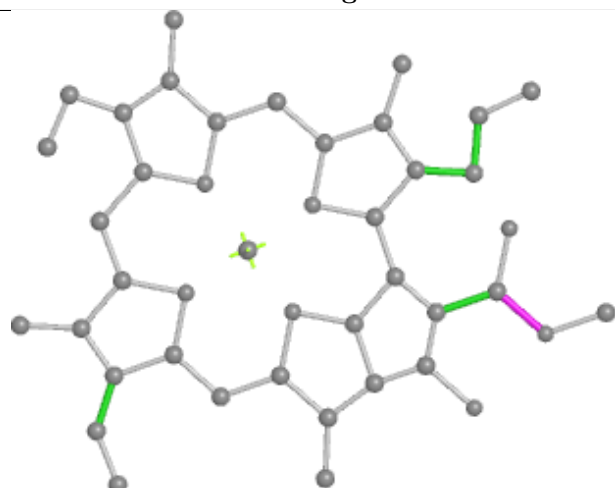
Ligand CLA 8 305



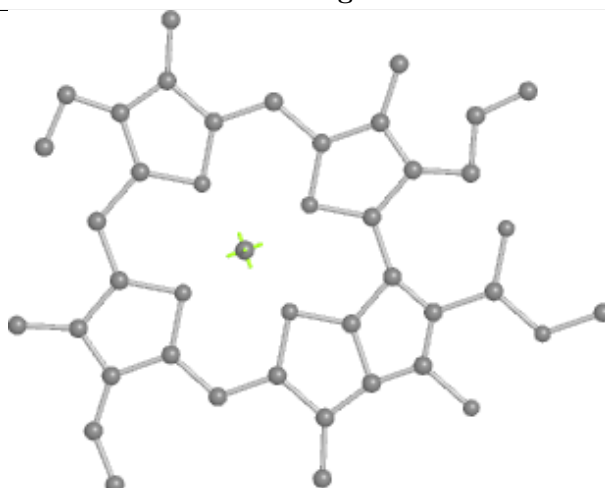
Bond lengths



Bond angles

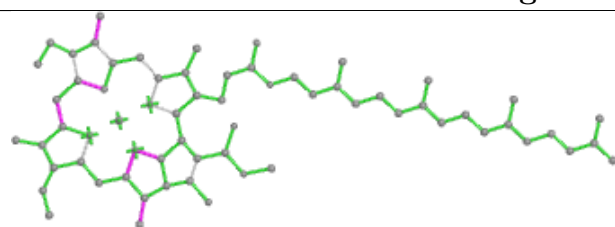


Torsions

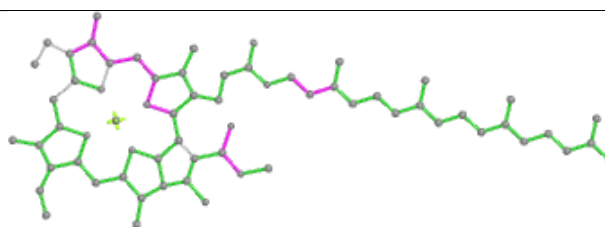


Rings

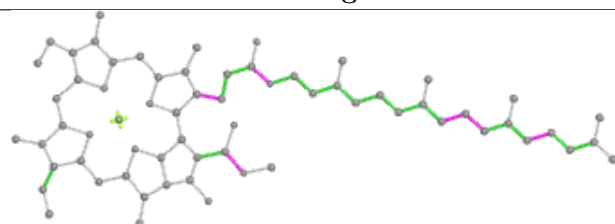
Ligand CLA h 201



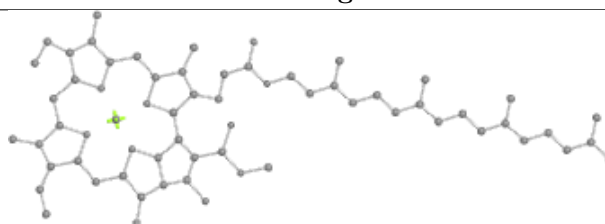
Bond lengths



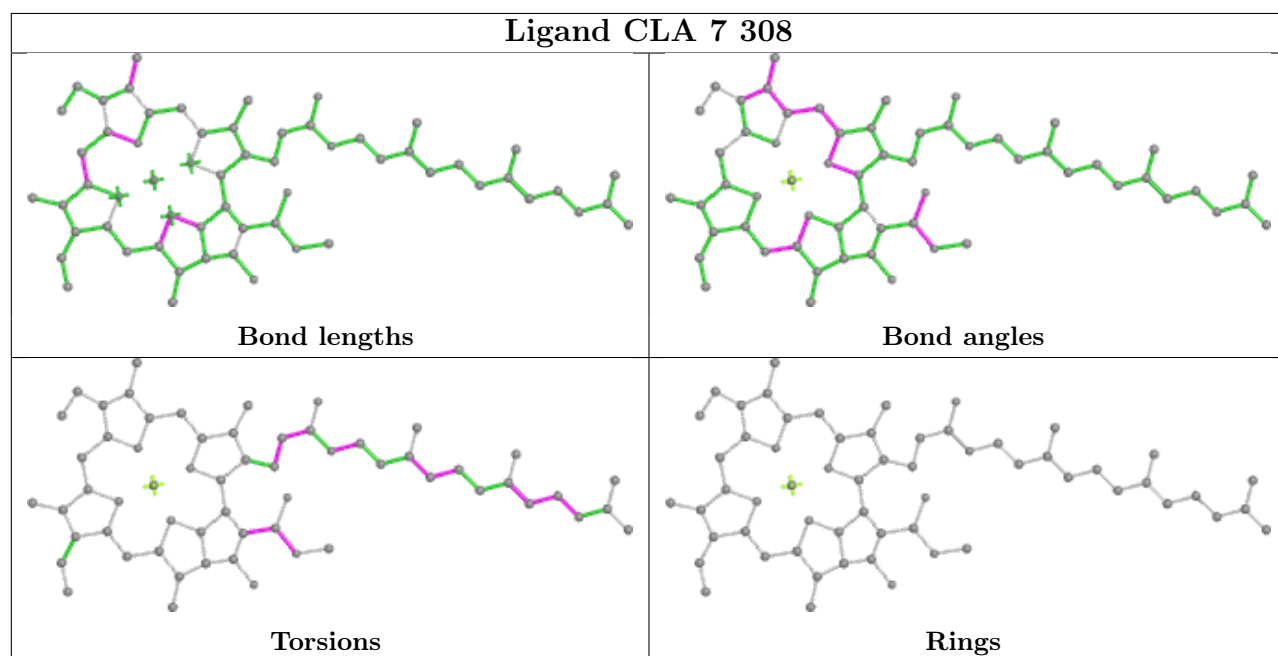
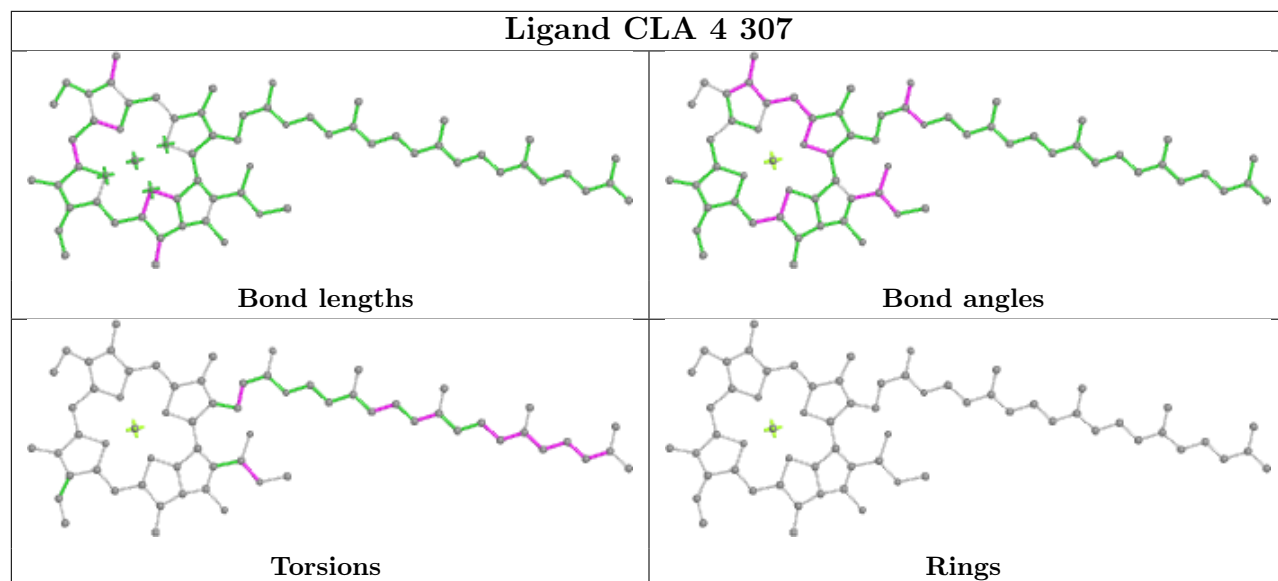
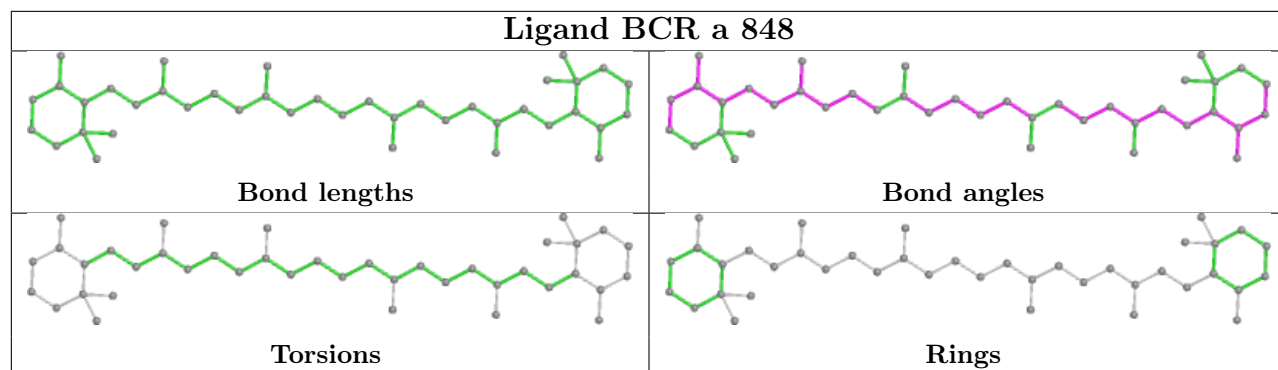
Bond angles



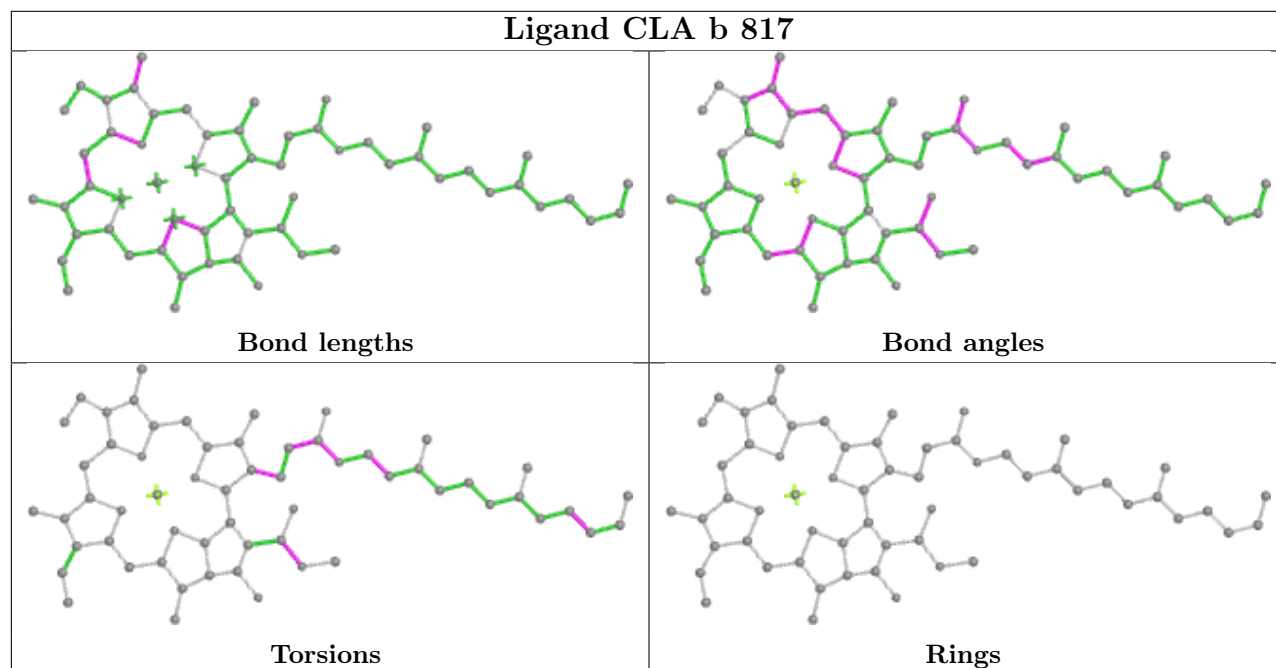
Torsions



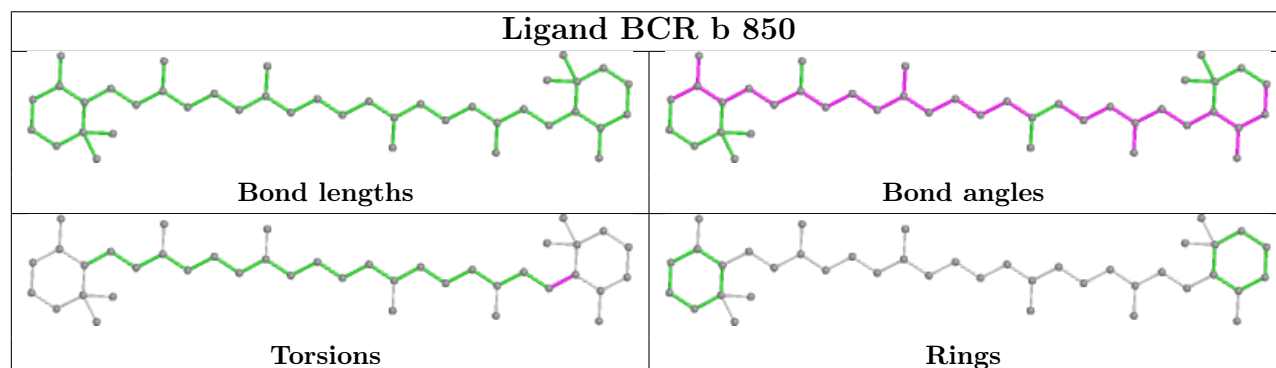
Rings



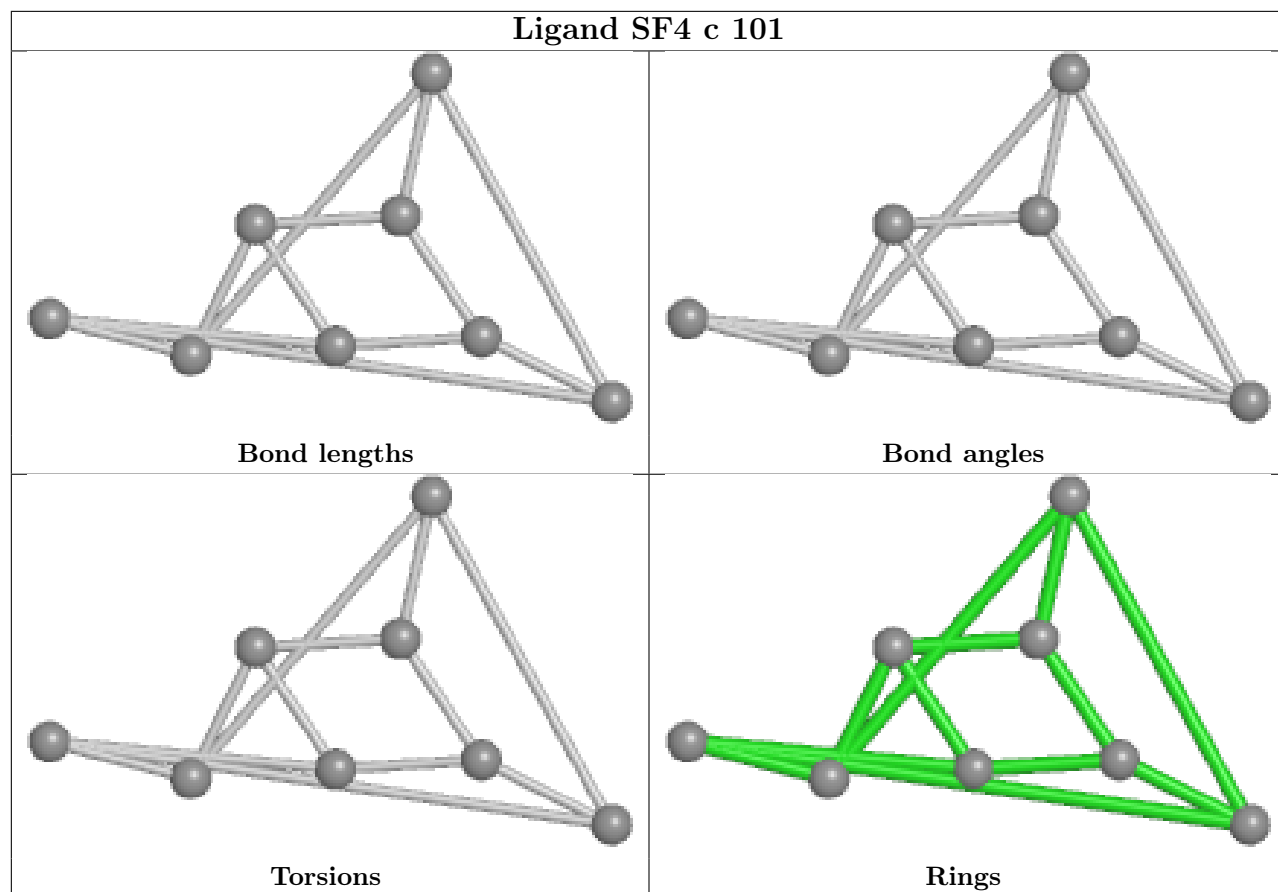
Ligand CLA b 817



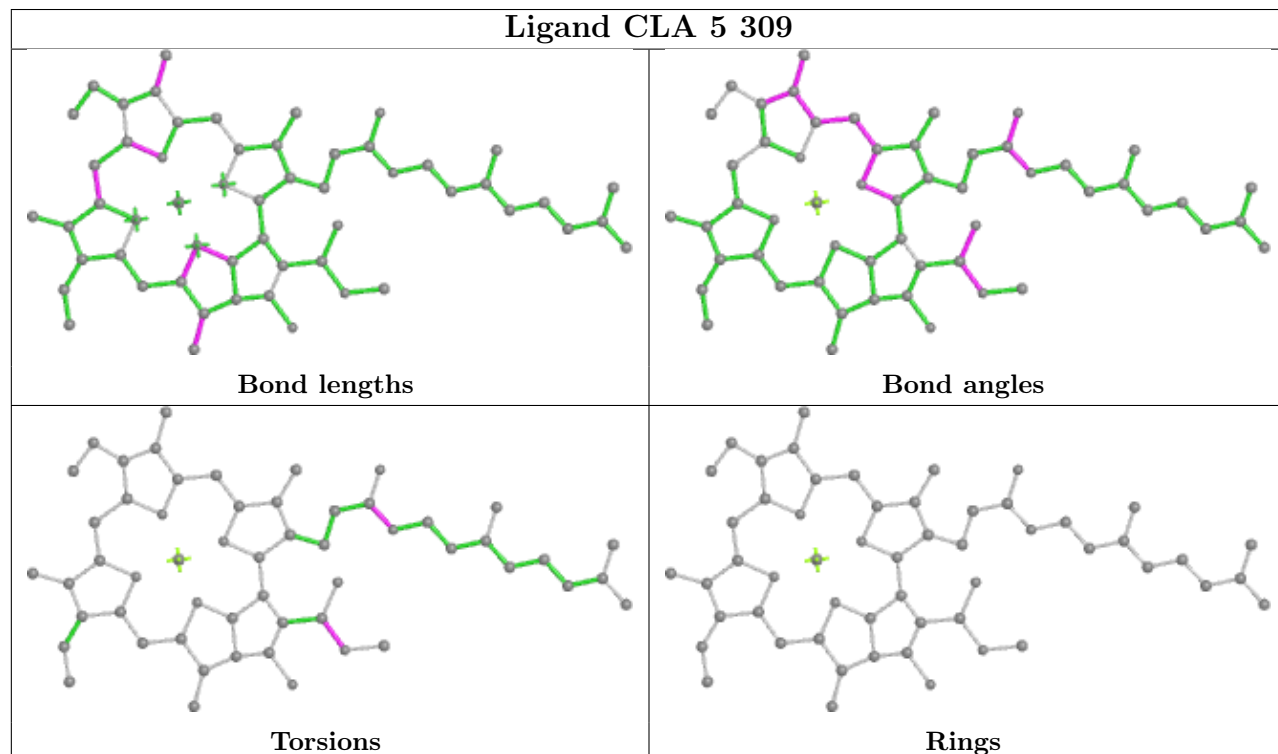
Ligand BCR b 850

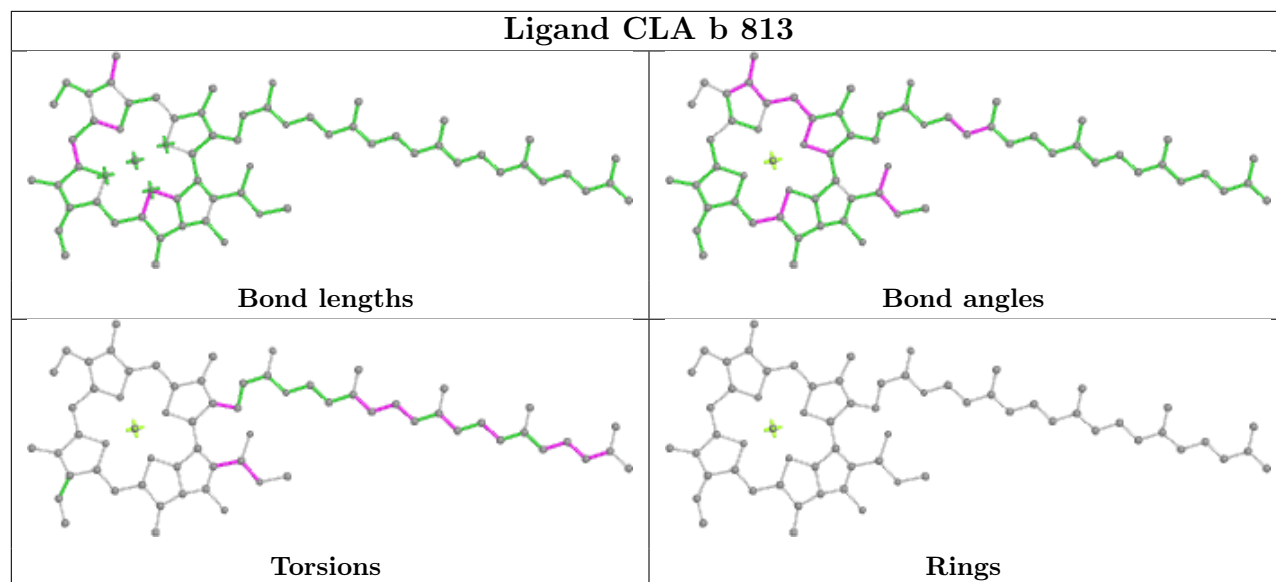
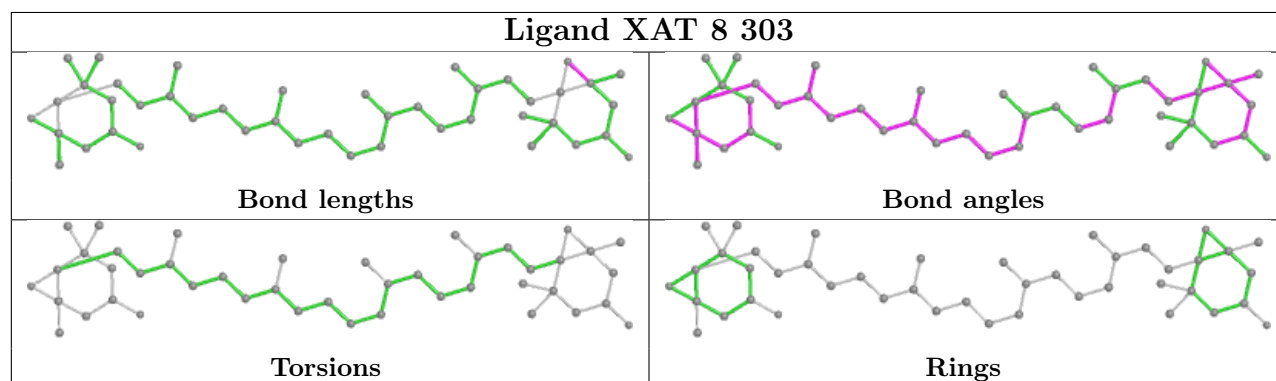
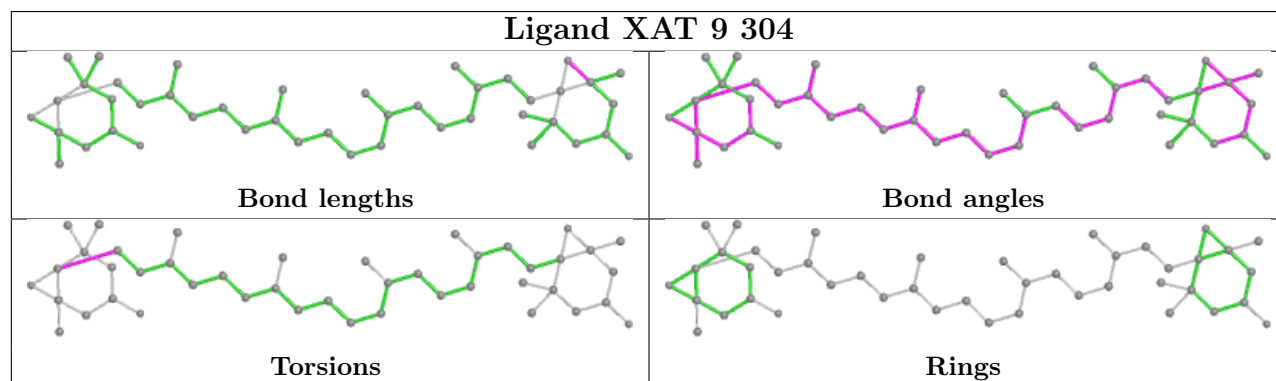


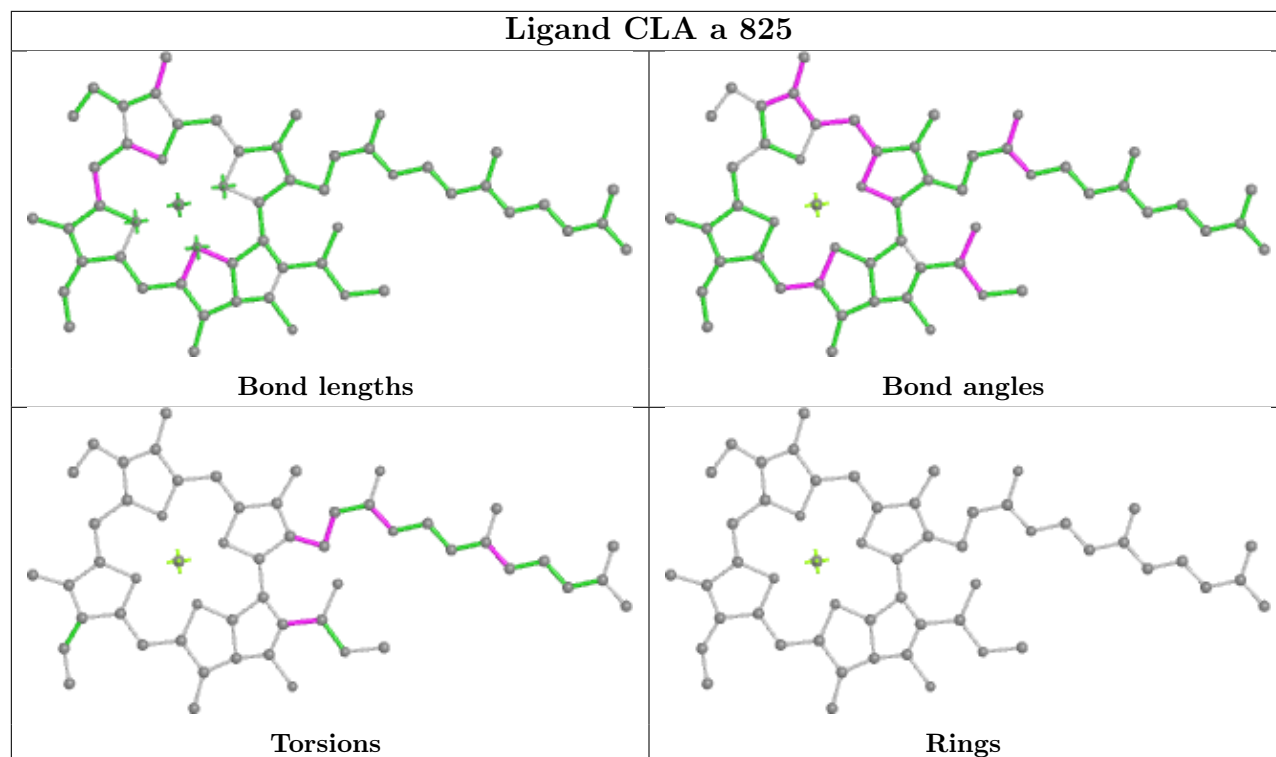
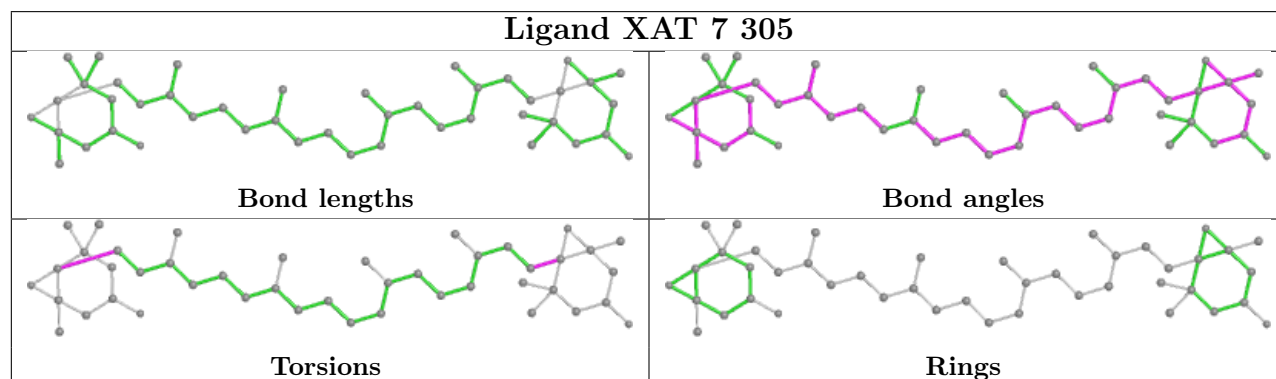
Ligand SF4 c 101

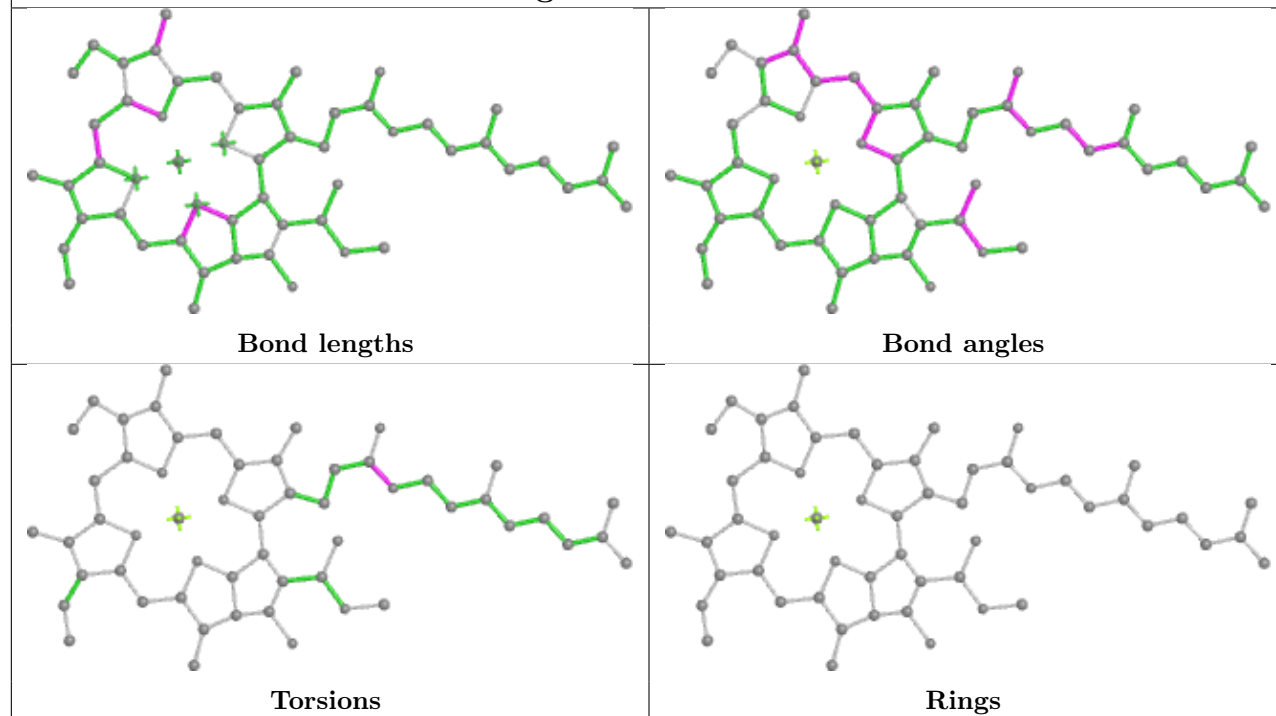
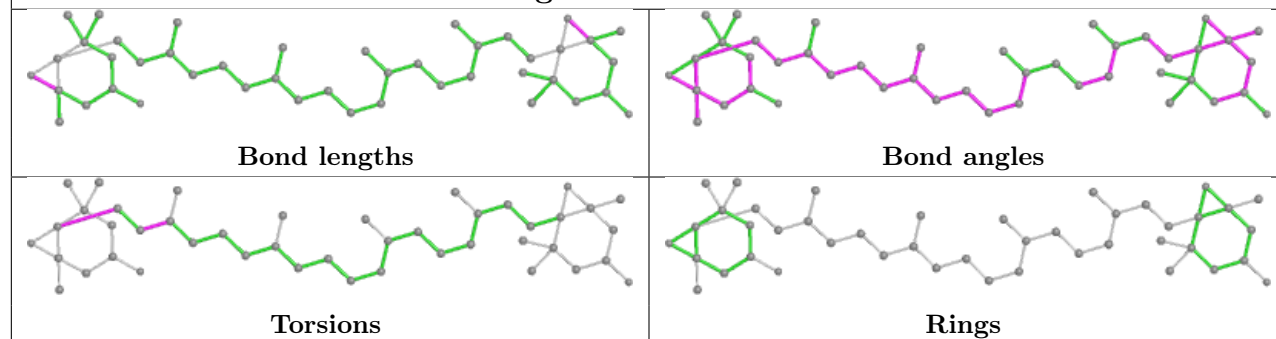


Ligand CLA 5 309

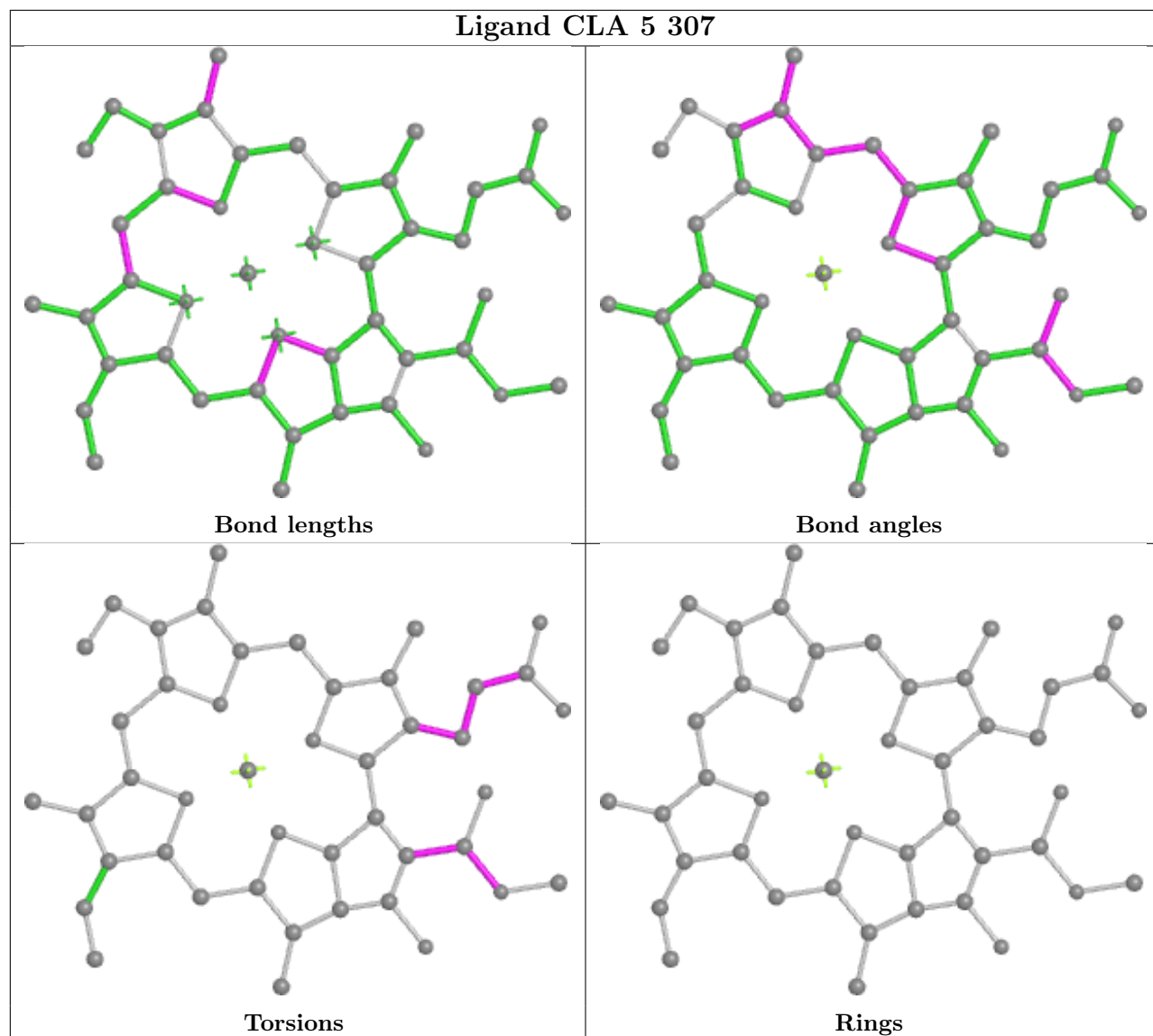


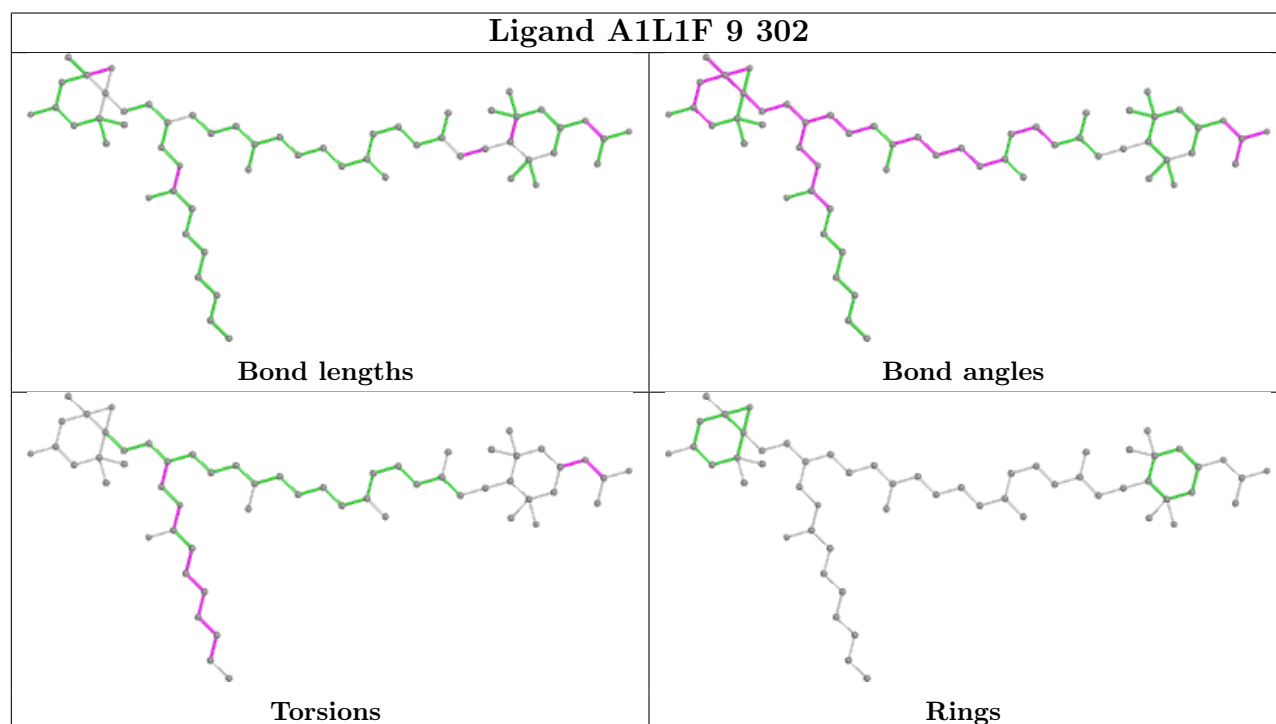
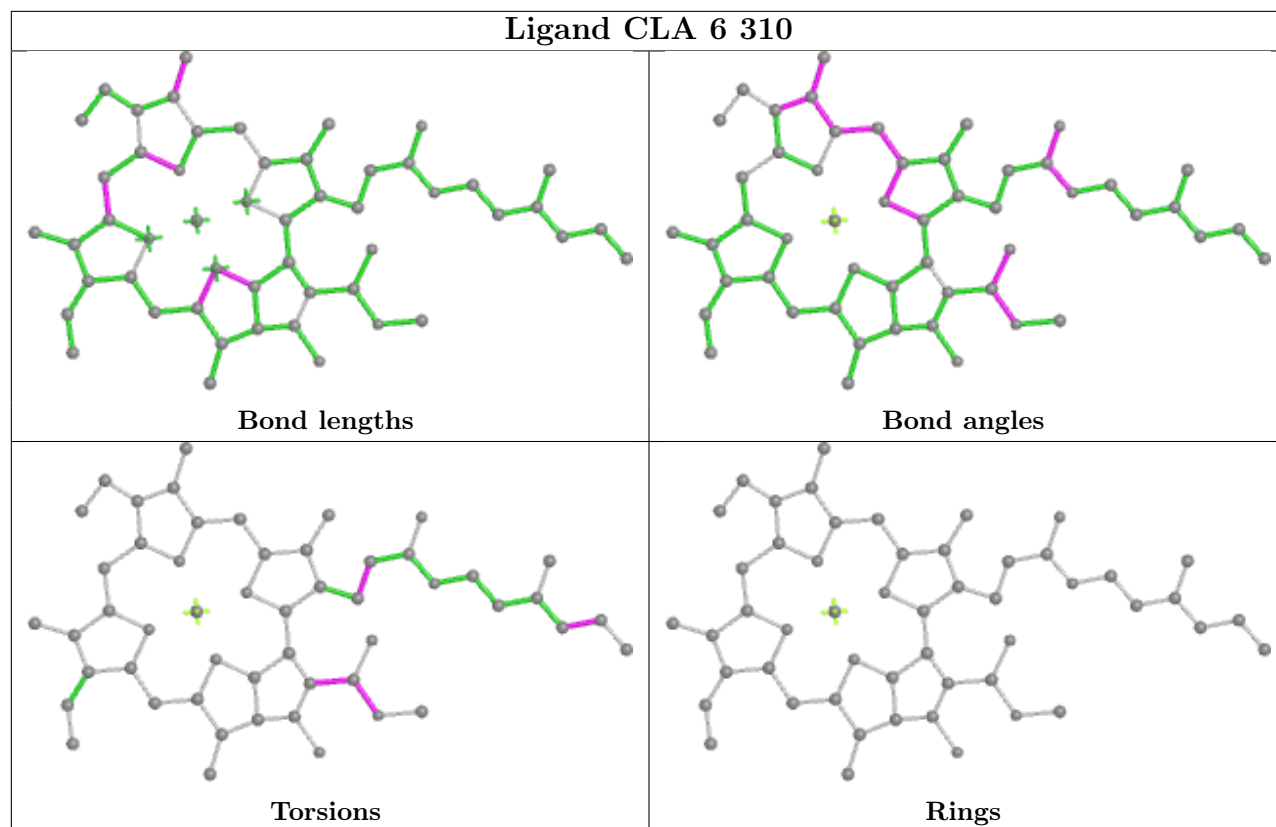
Ligand CLA b 813**Ligand XAT 8 303****Ligand XAT 9 304**

Ligand CLA a 825**Ligand XAT 7 305**

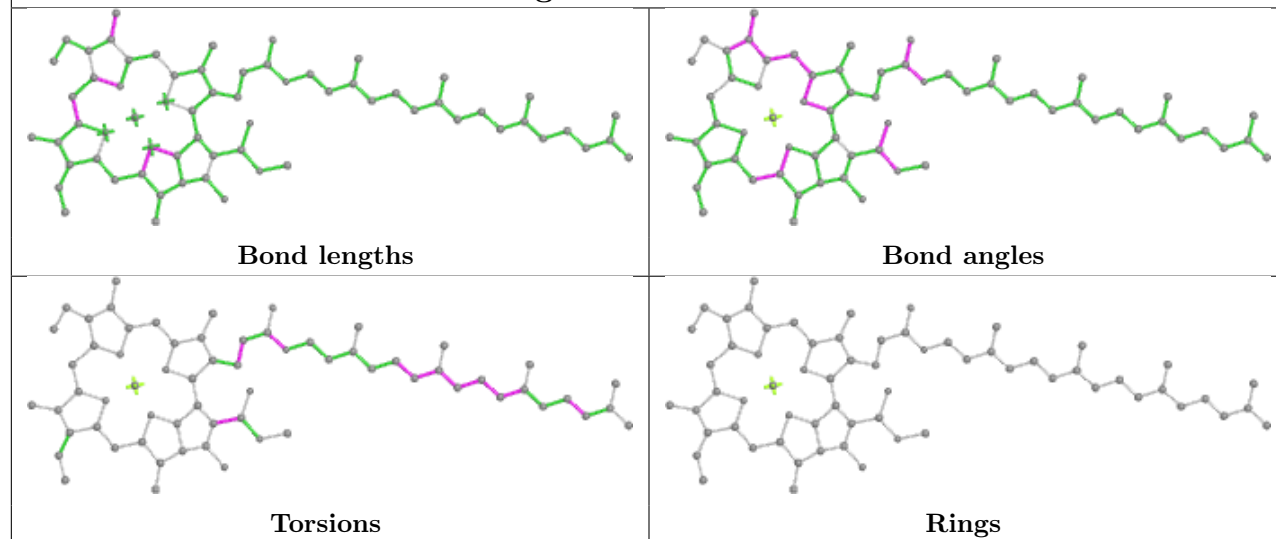
Ligand CLA a 833**Ligand XAT 3 304**

Ligand CLA 5 307

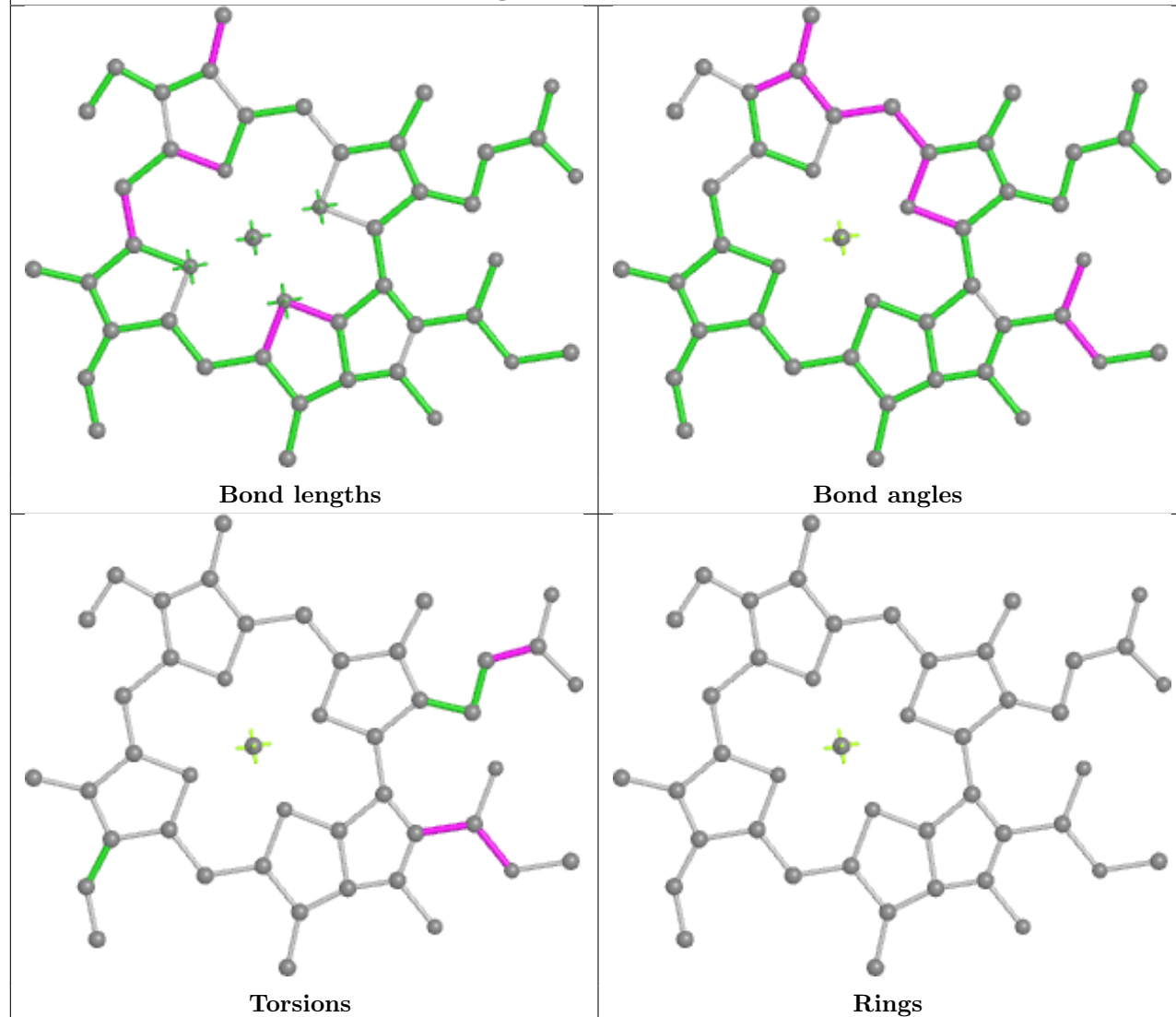




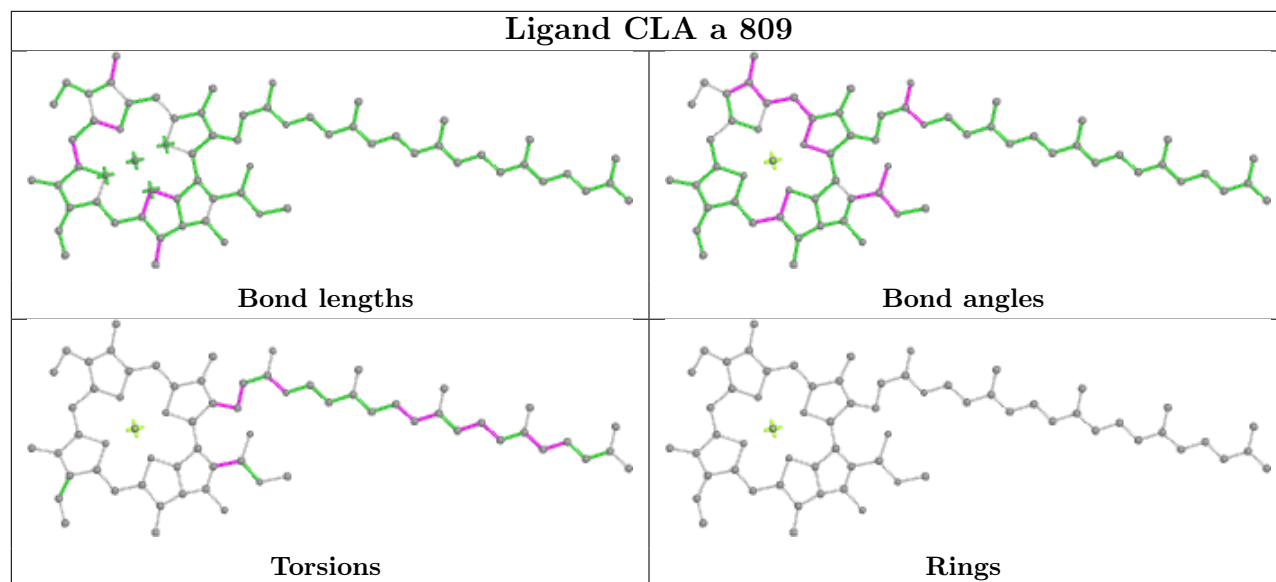
Ligand CLA b 824



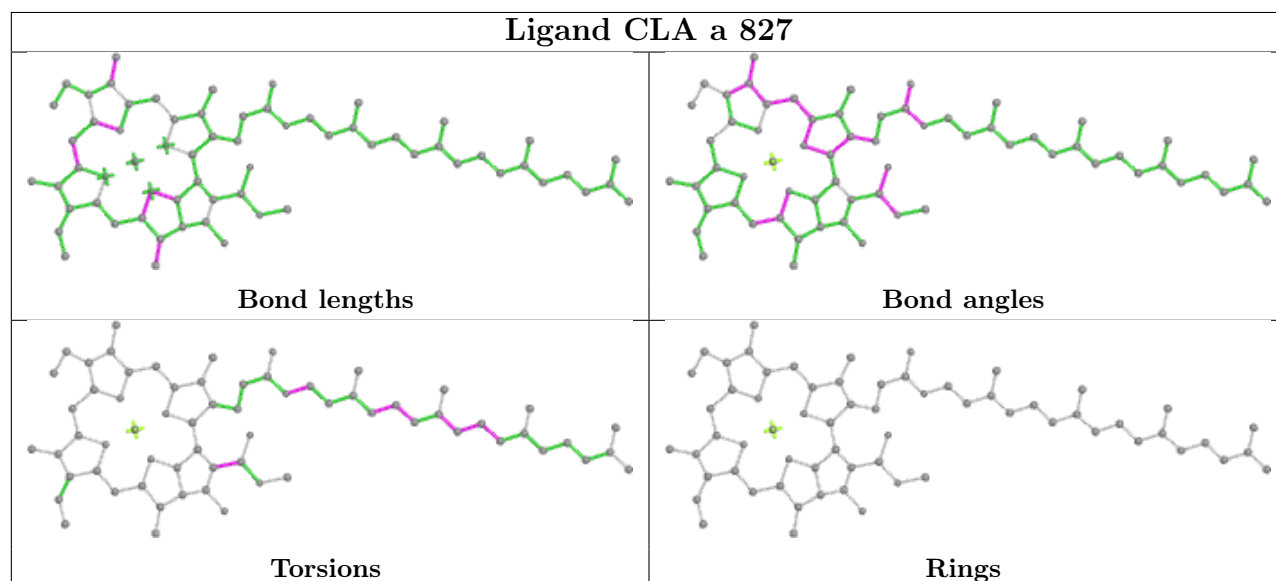
Ligand CLA 5 314



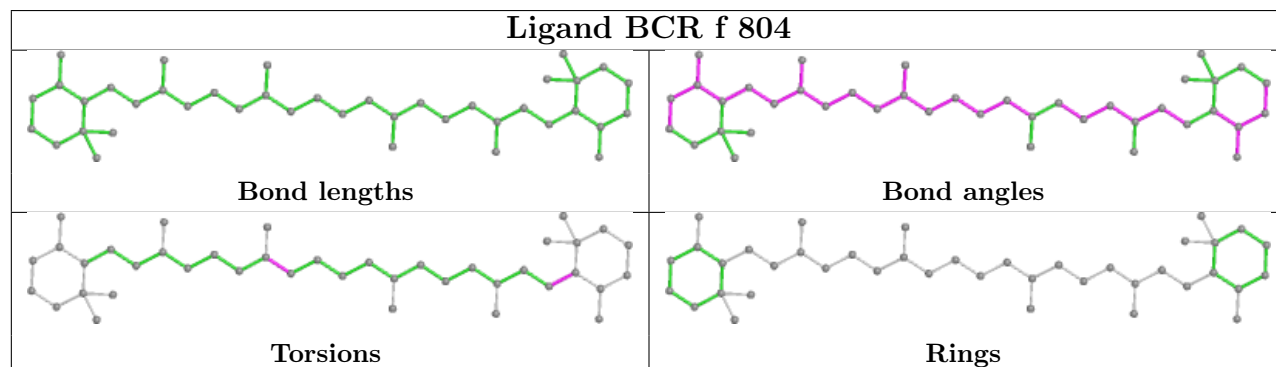
Ligand CLA a 809

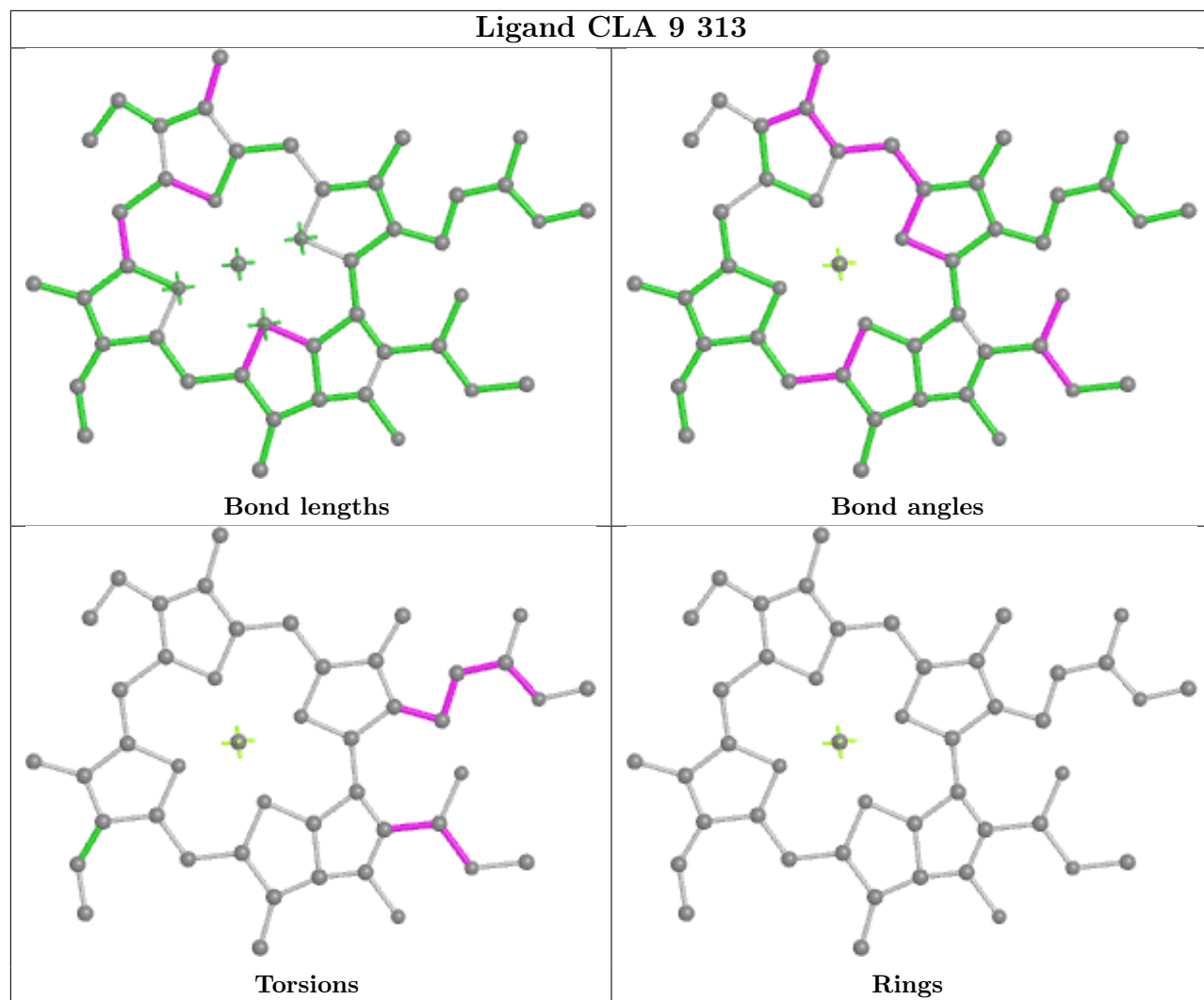
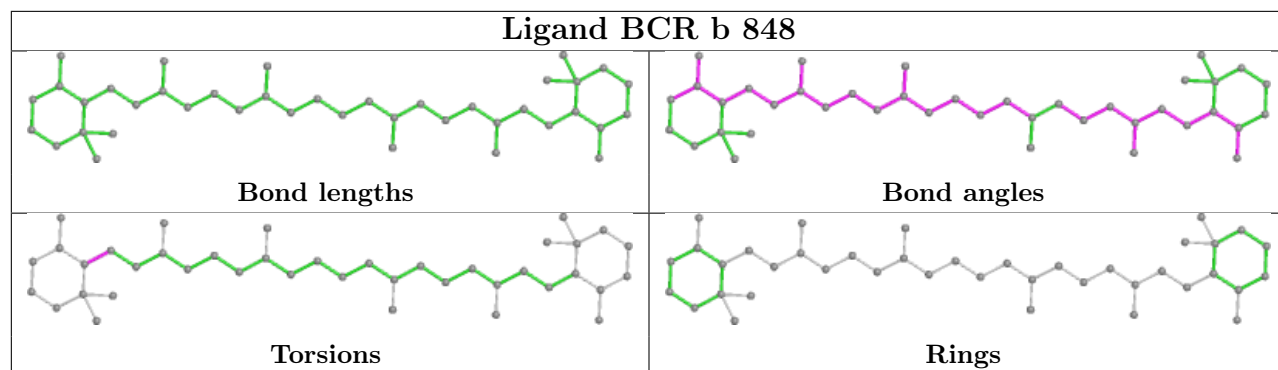


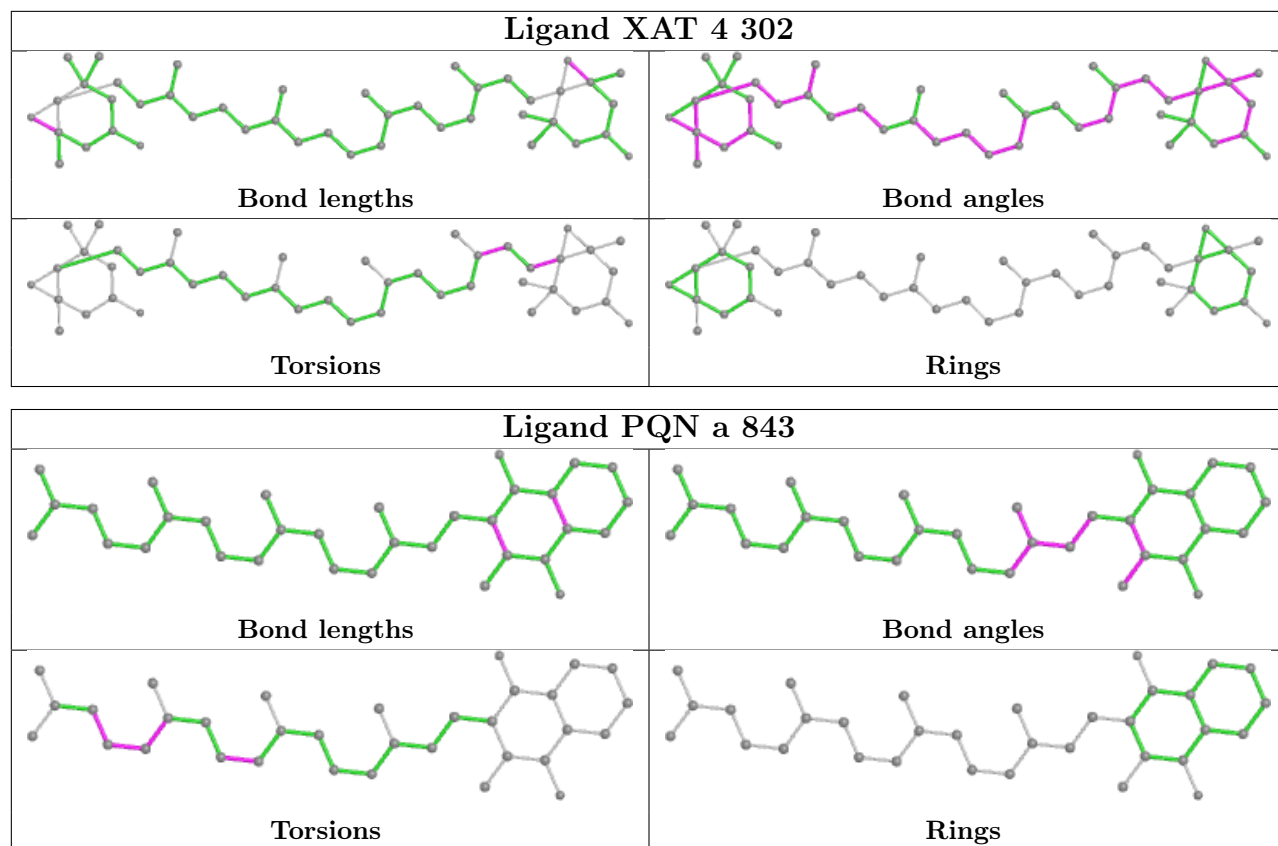
Ligand CLA a 827



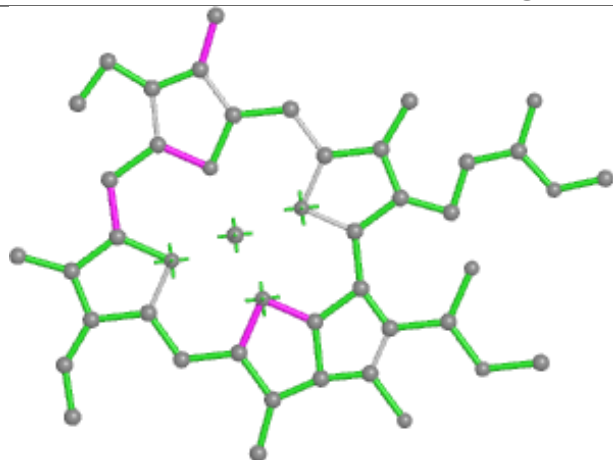
Ligand BCR f 804



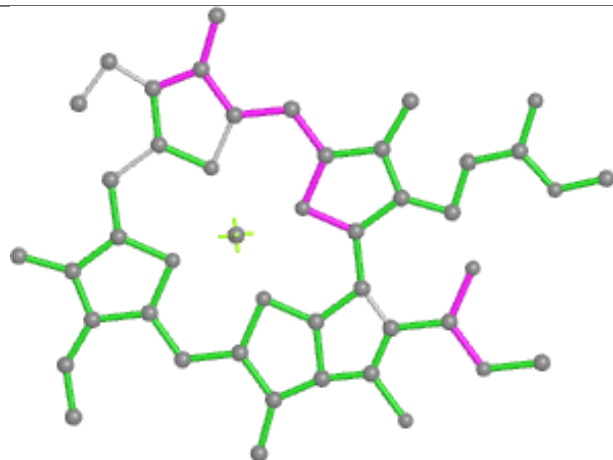




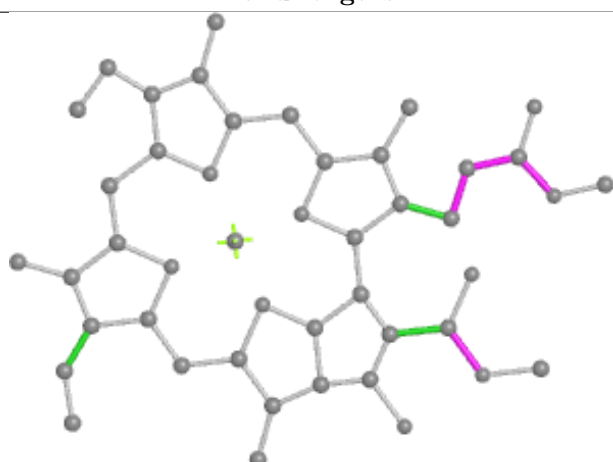
Ligand CLA 7 310



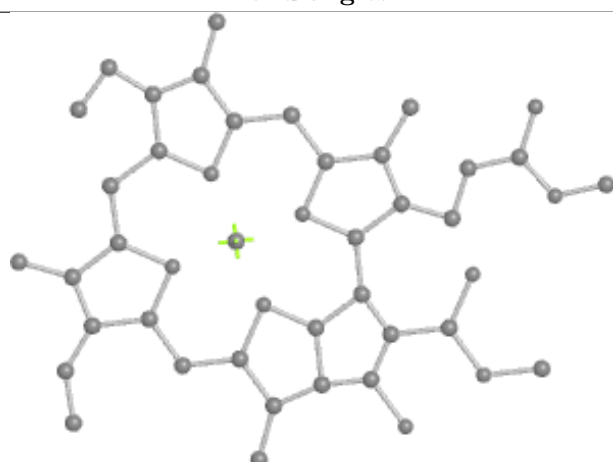
Bond lengths



Bond angles

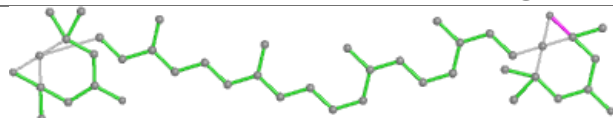


Torsions

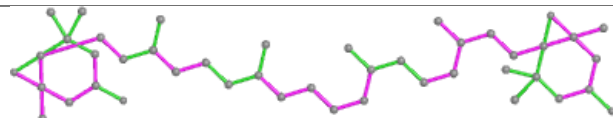


Rings

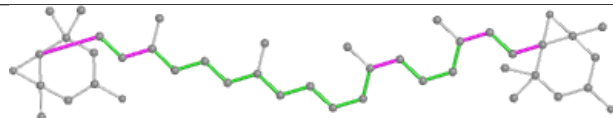
Ligand XAT 7 303



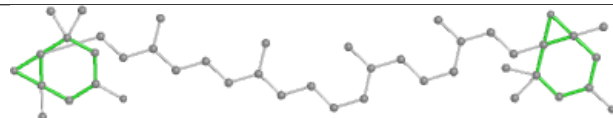
Bond lengths



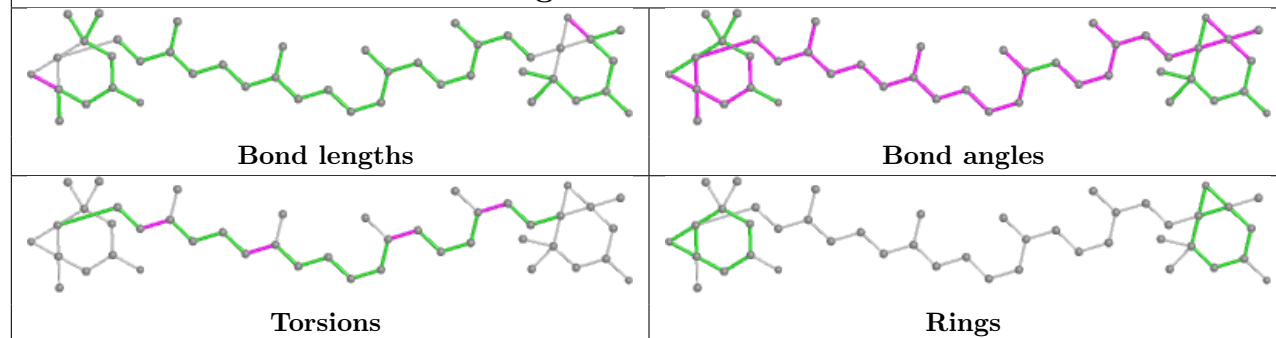
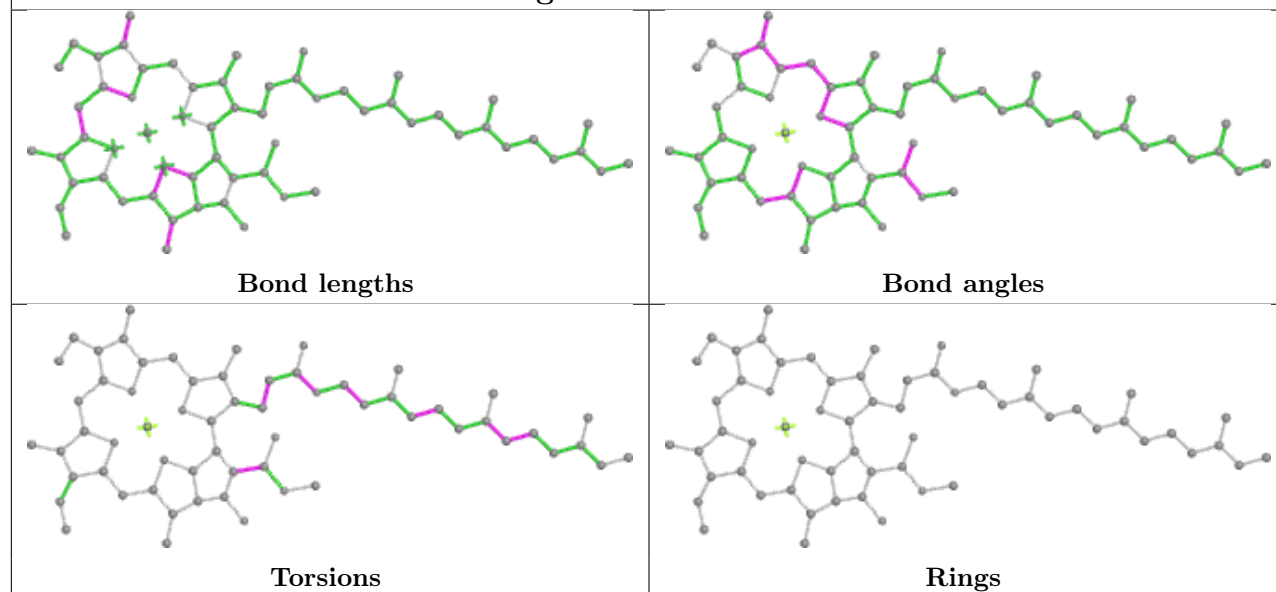
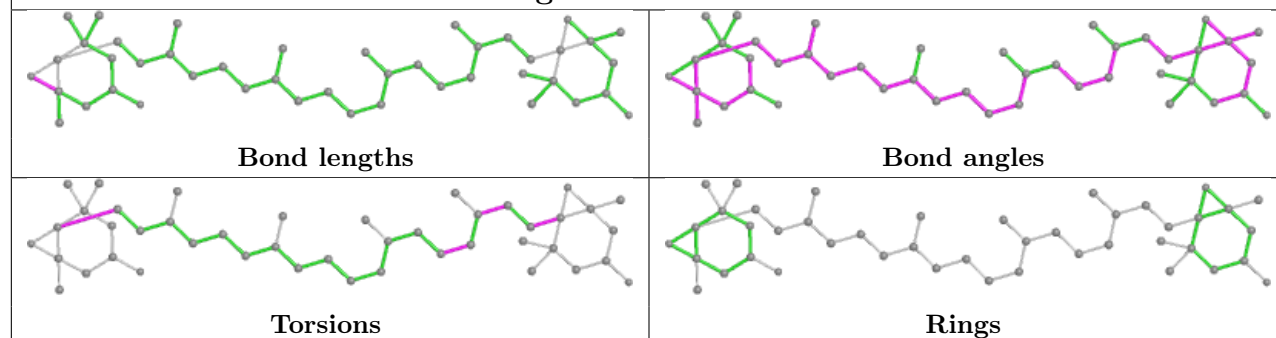
Bond angles



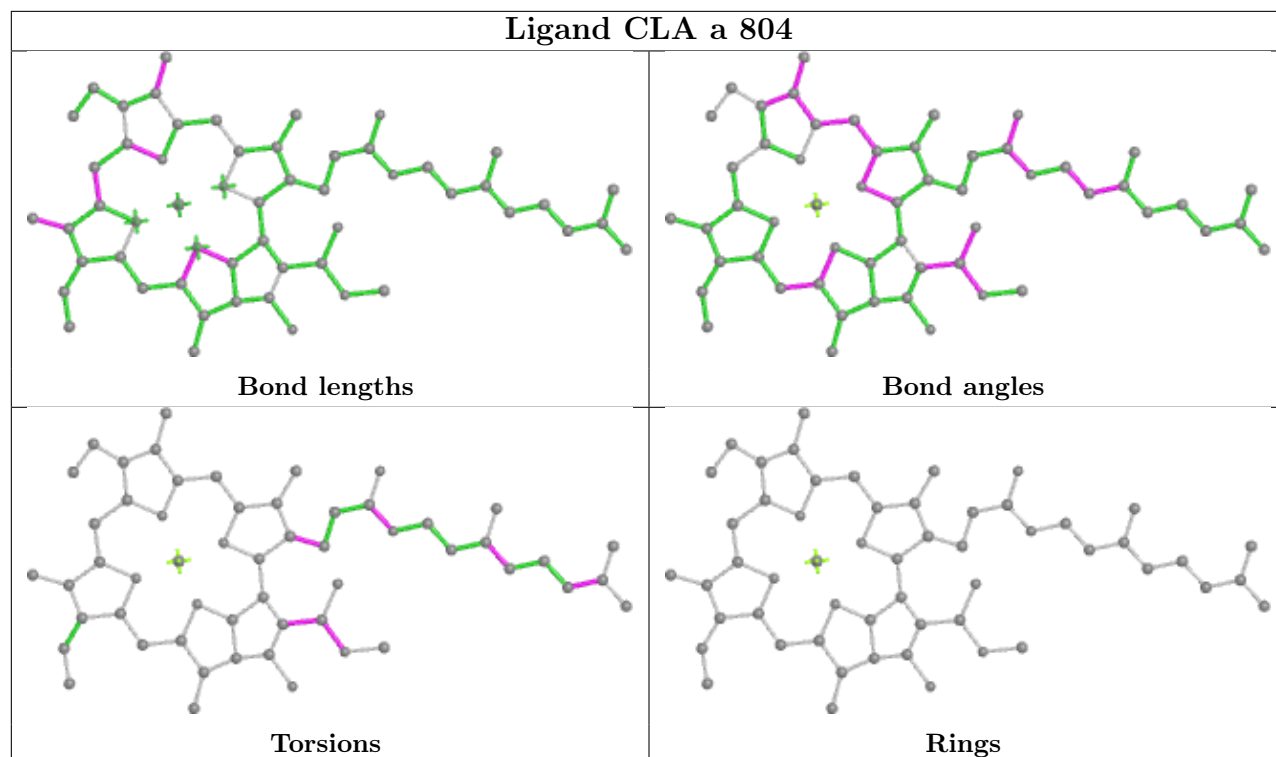
Torsions



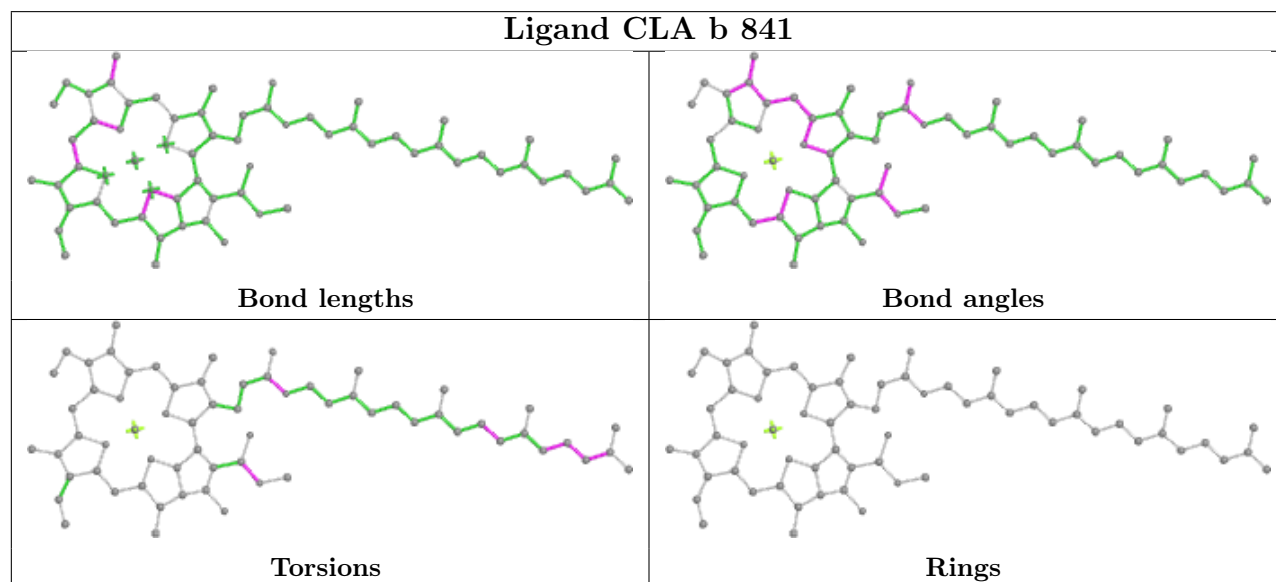
Rings

Ligand XAT a 854**Ligand CLA 1 305****Ligand XAT a 853**

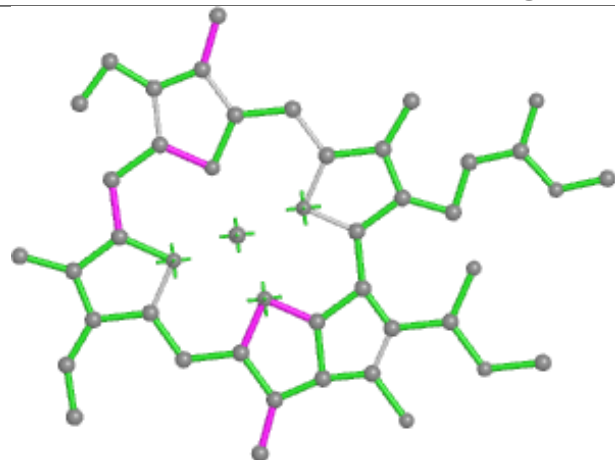
Ligand CLA a 804



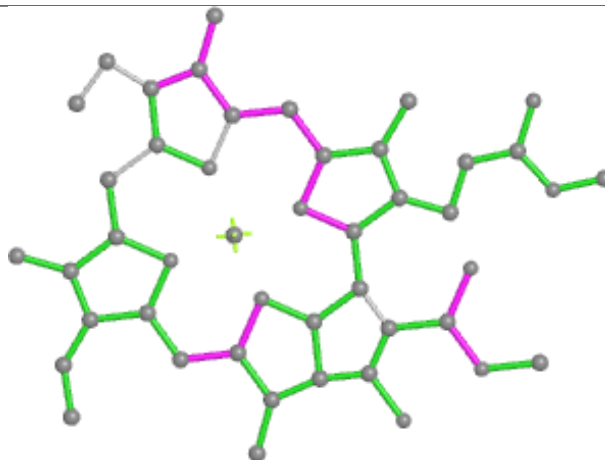
Ligand CLA b 841



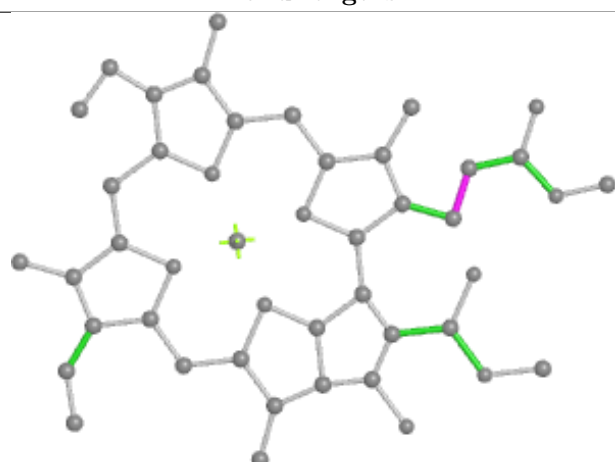
Ligand CLA 6 307



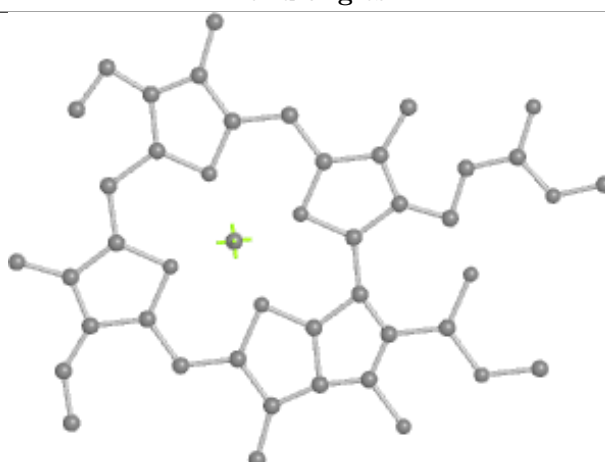
Bond lengths



Bond angles

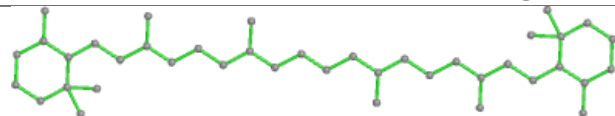


Torsions

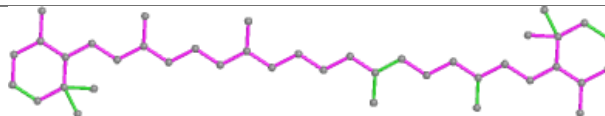


Rings

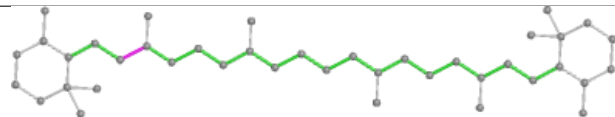
Ligand BCR b 847



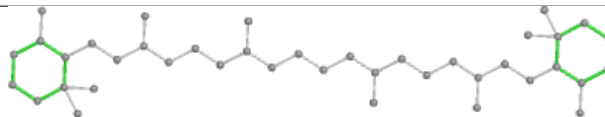
Bond lengths



Bond angles

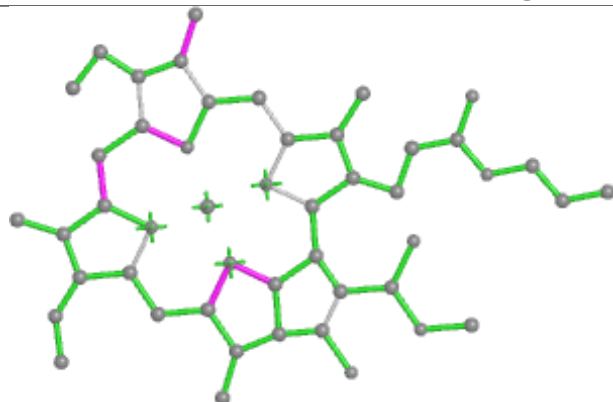


Torsions

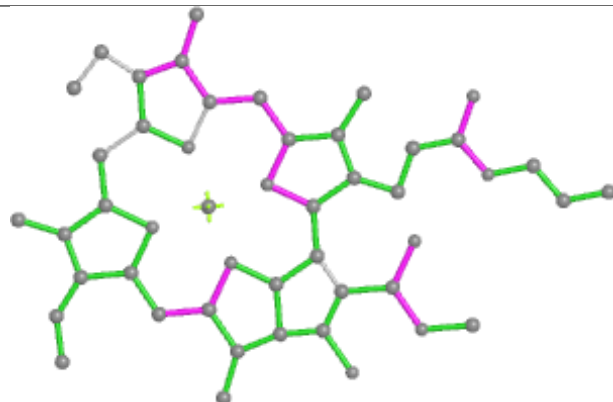


Rings

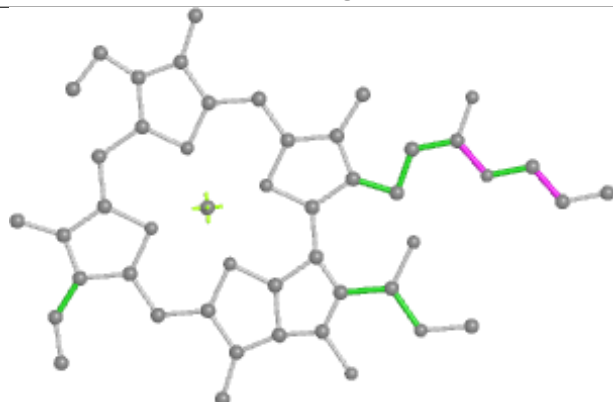
Ligand CLA 7 312



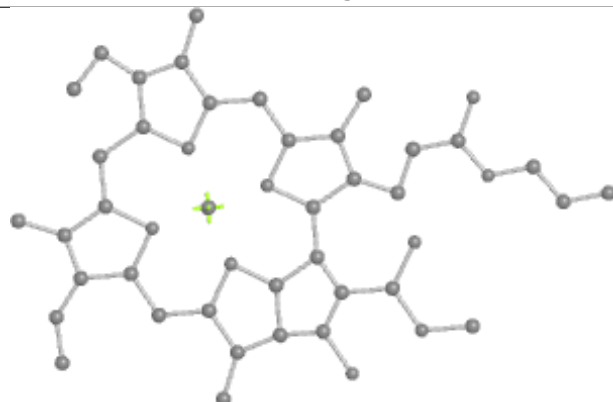
Bond lengths



Bond angles

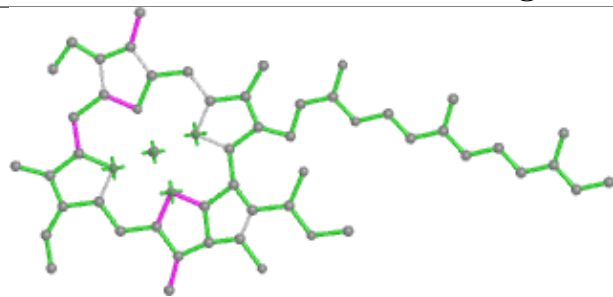


Torsions

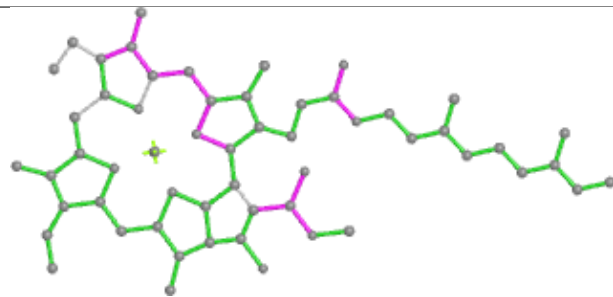


Rings

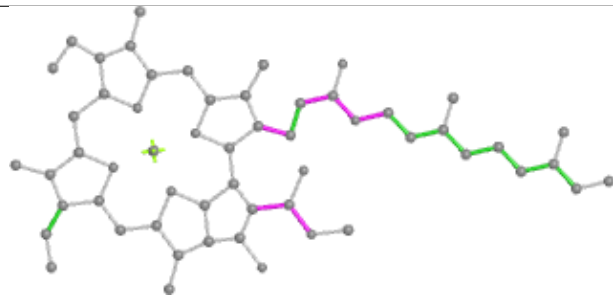
Ligand CLA a 818



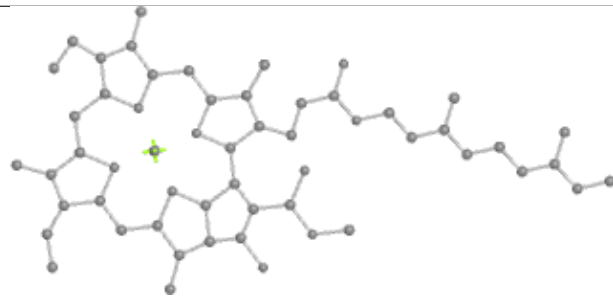
Bond lengths



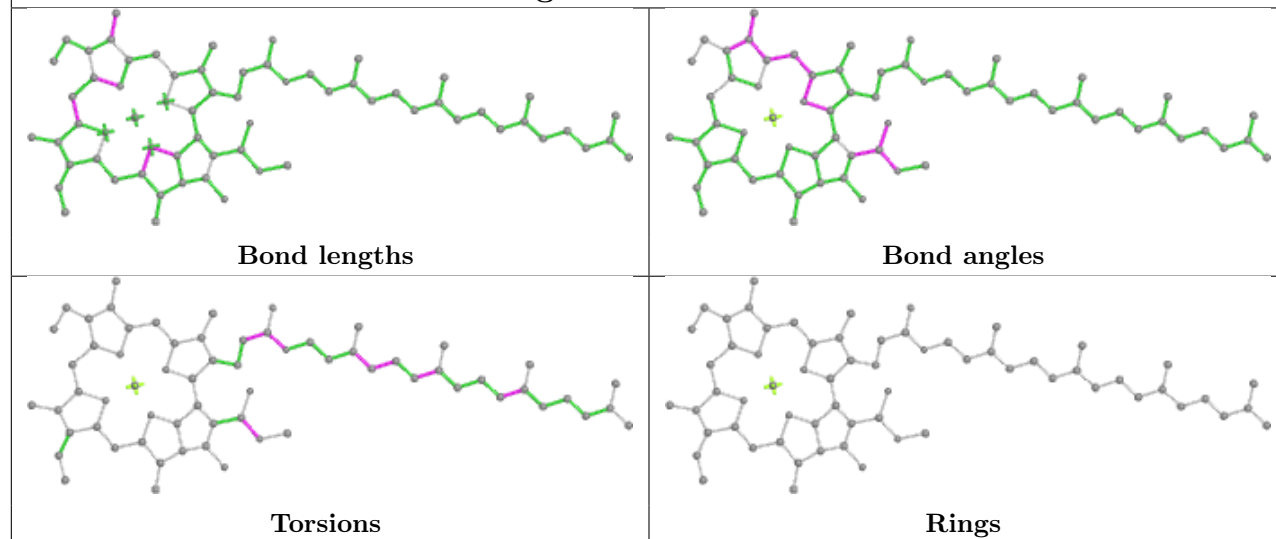
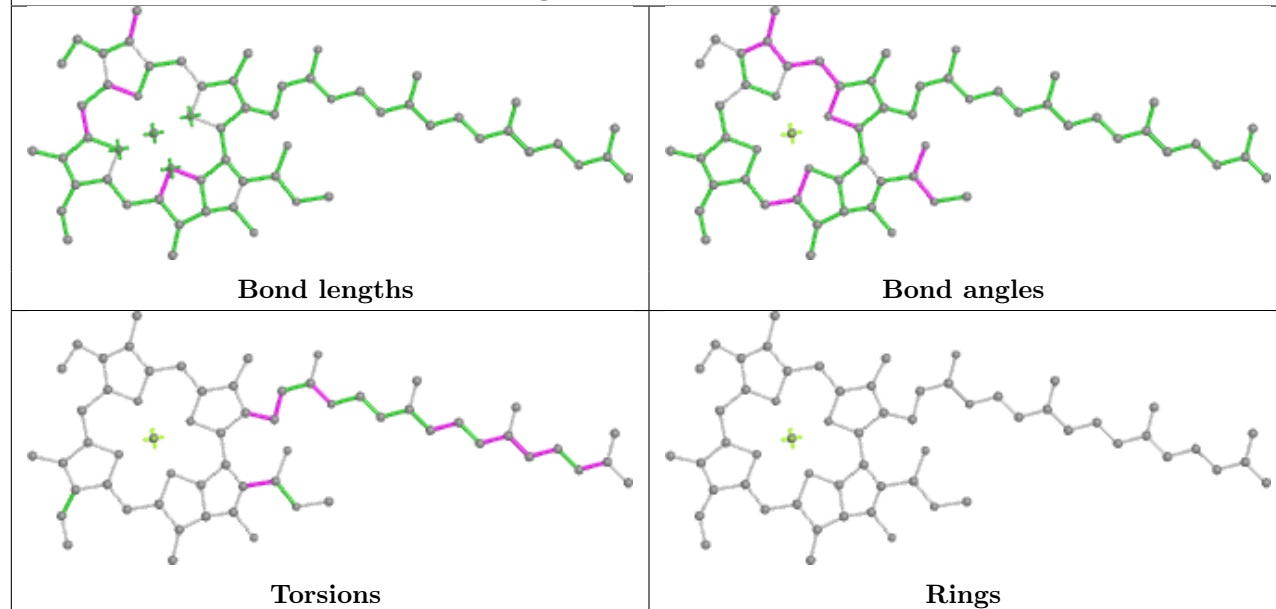
Bond angles

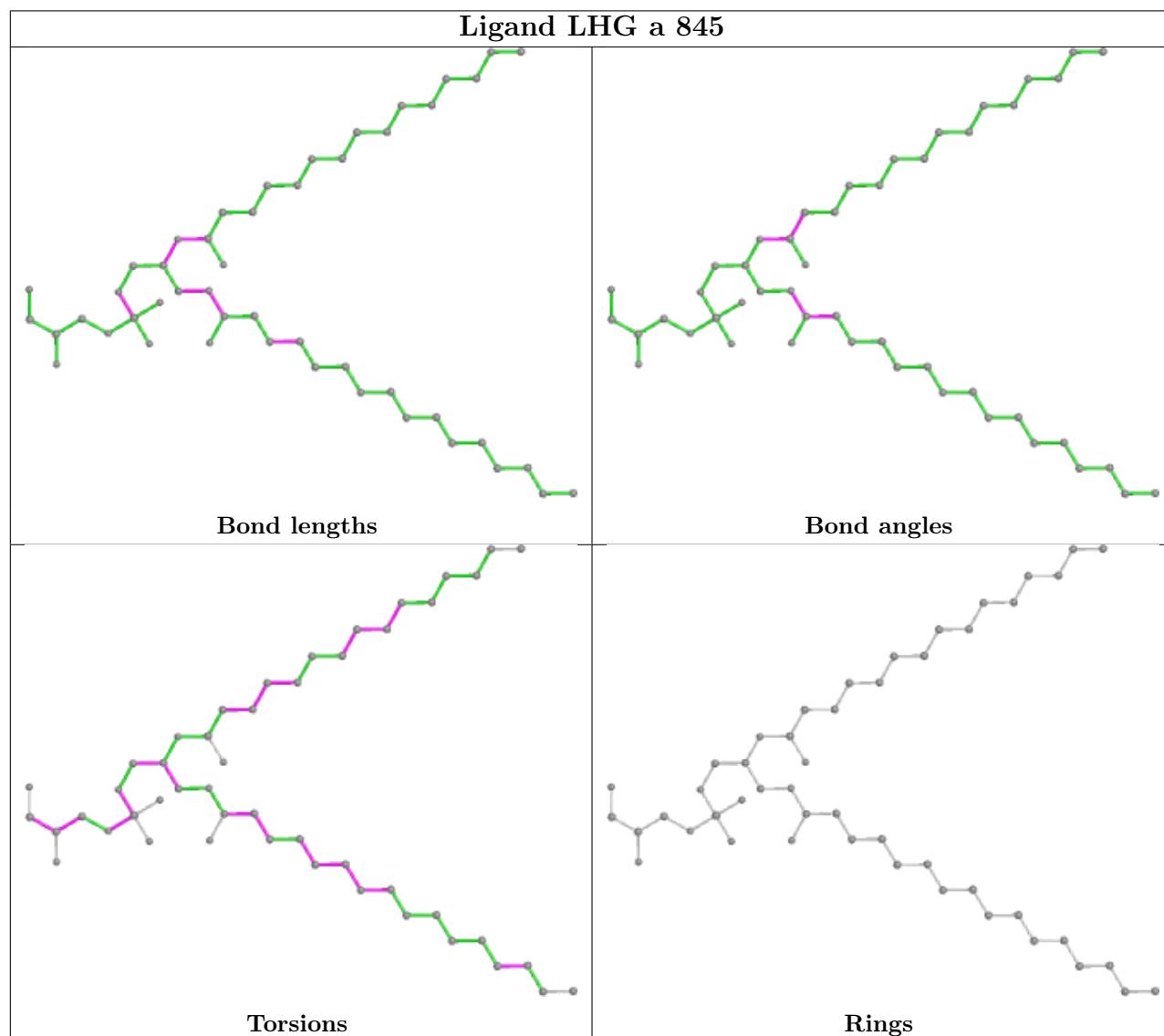
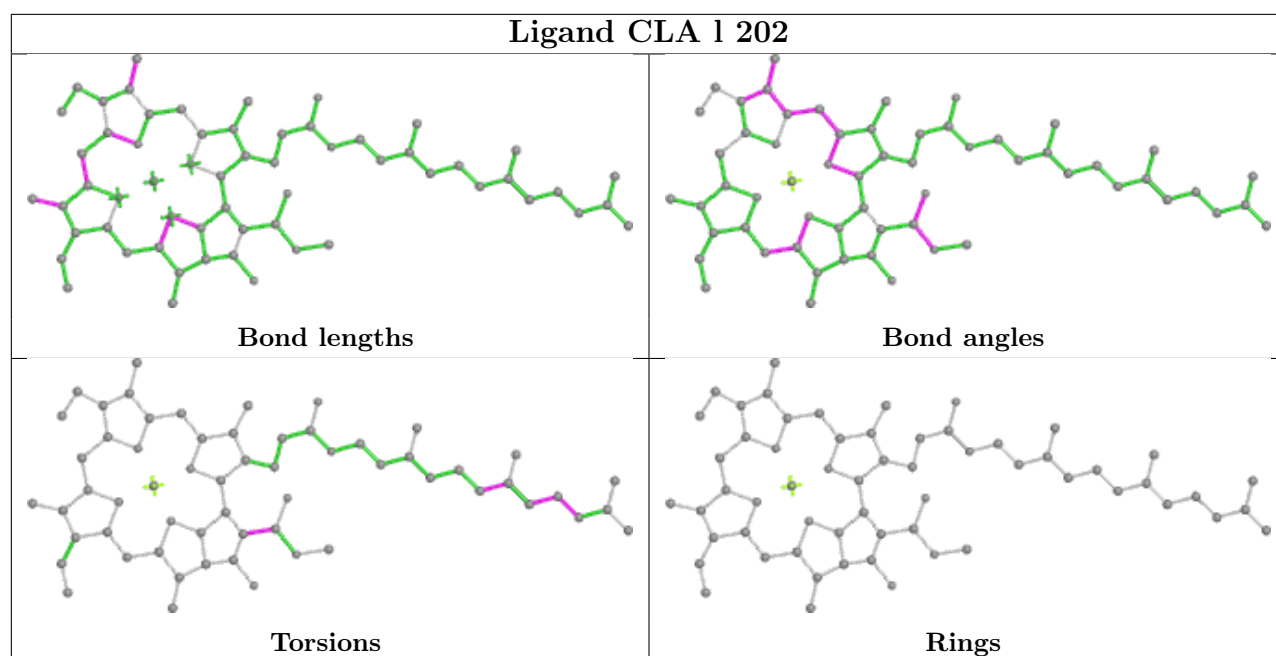


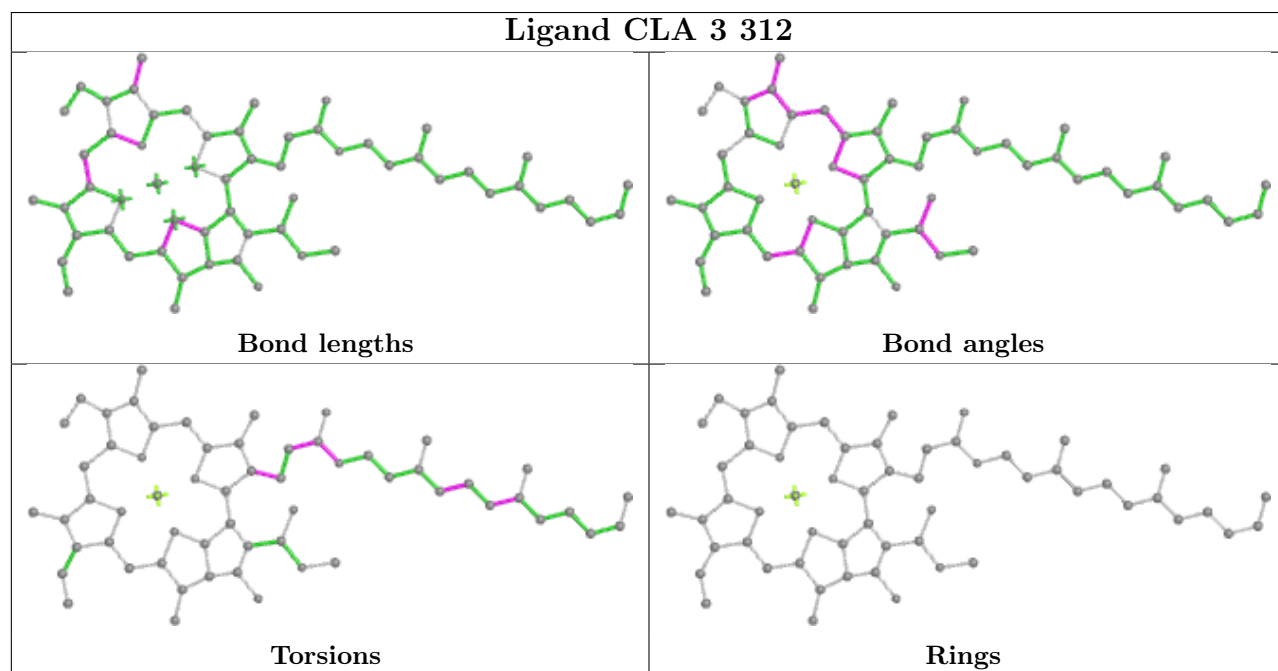
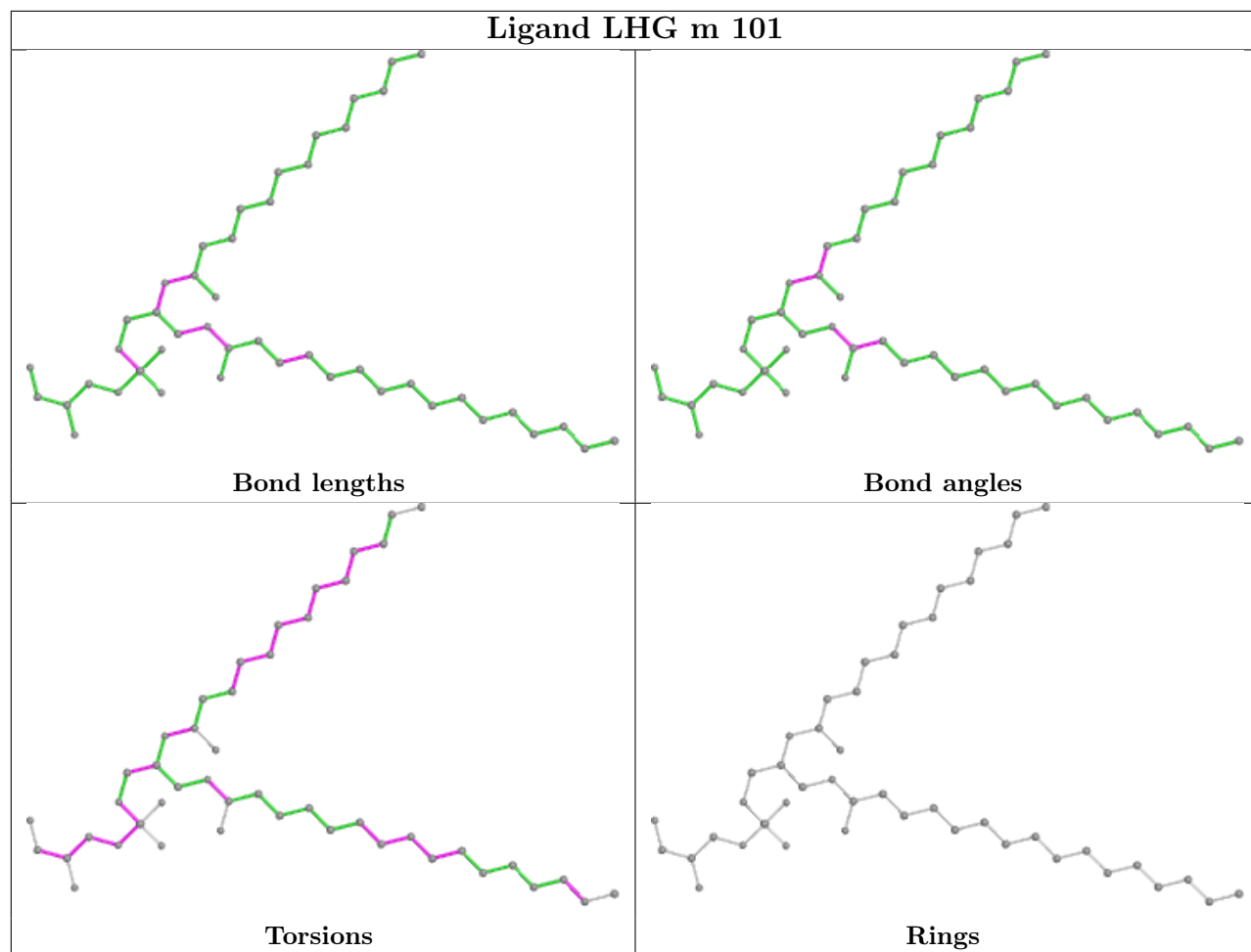
Torsions

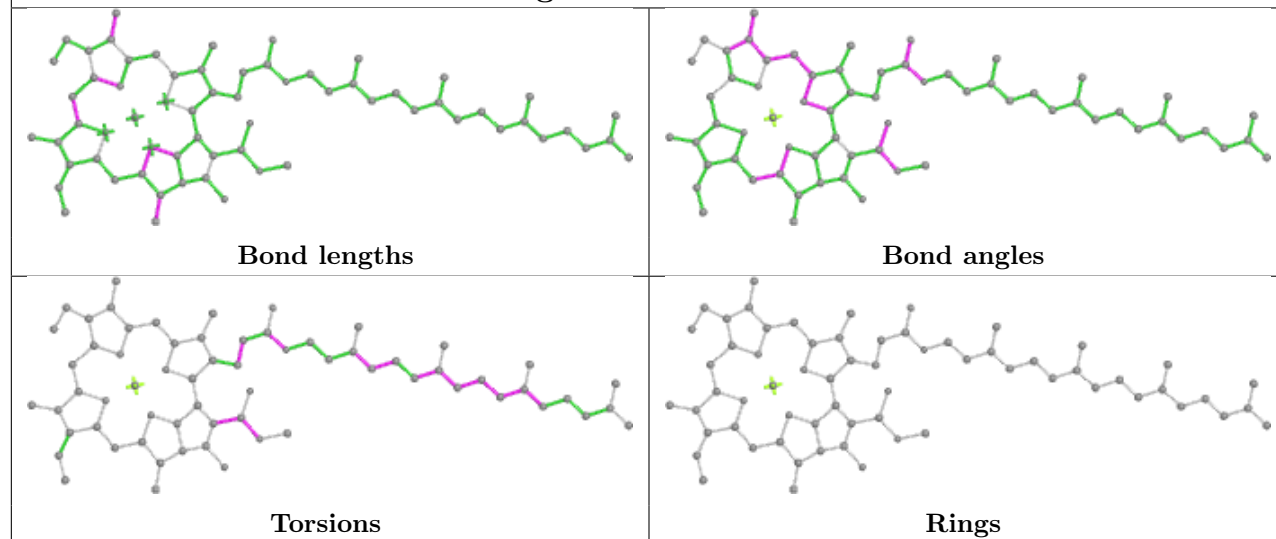
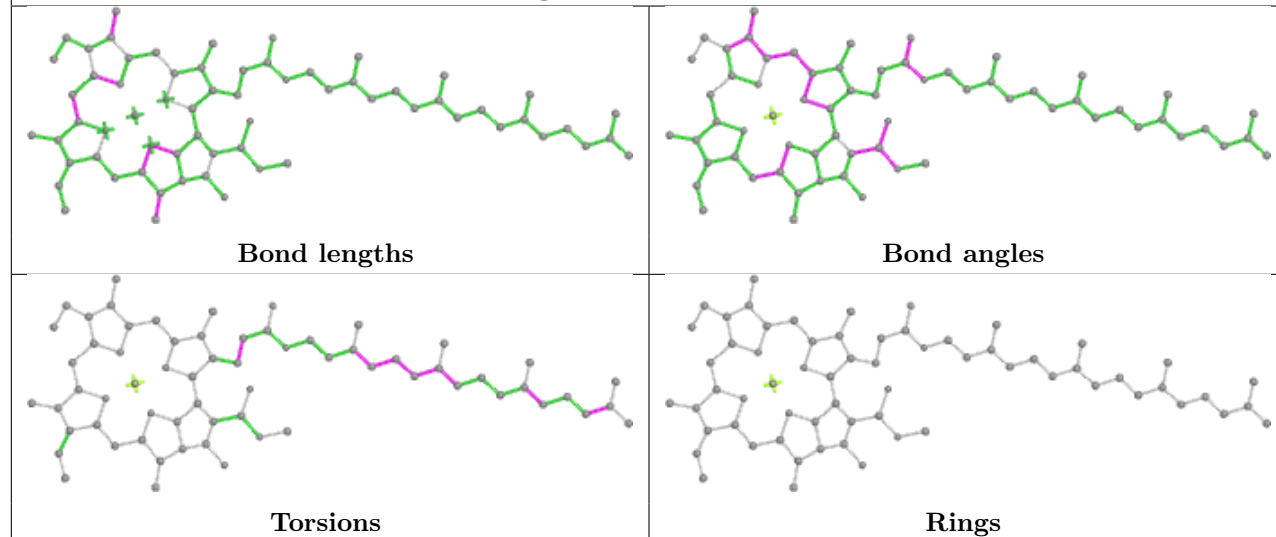


Rings

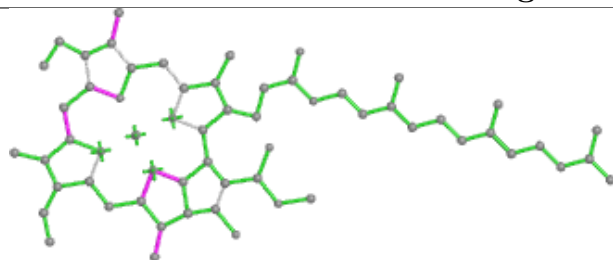
Ligand CLA a 835**Ligand CLA b 818**



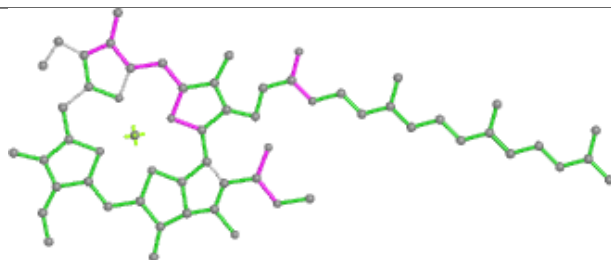


Ligand CLA a 852**Ligand CLA b 807**

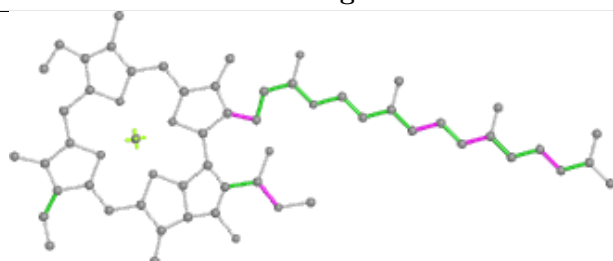
Ligand CLA b 822



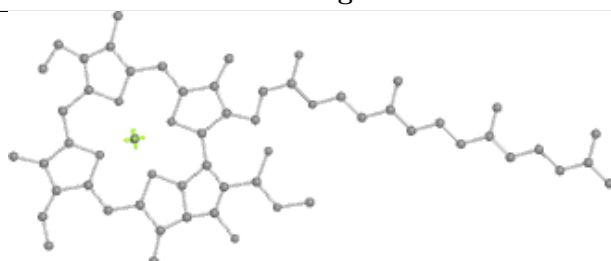
Bond lengths



Bond angles

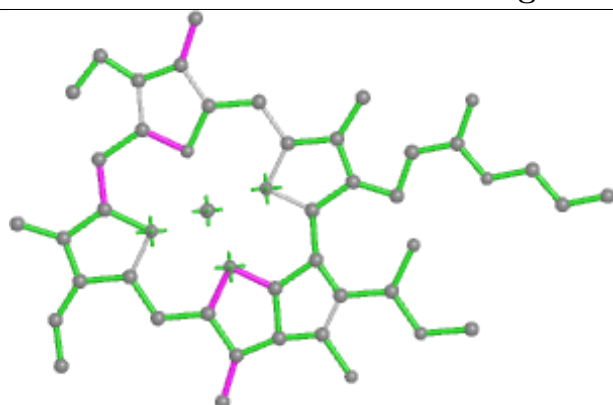


Torsions

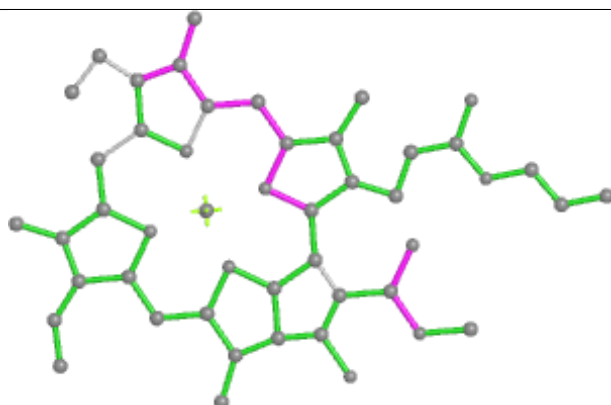


Rings

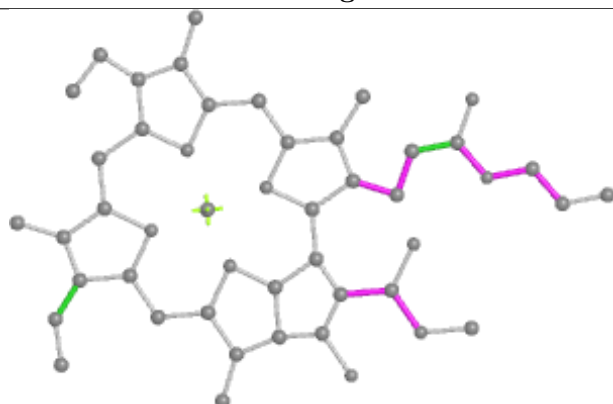
Ligand CLA 7 306



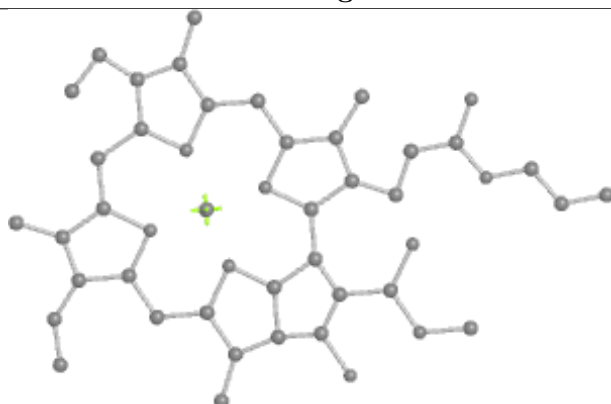
Bond lengths



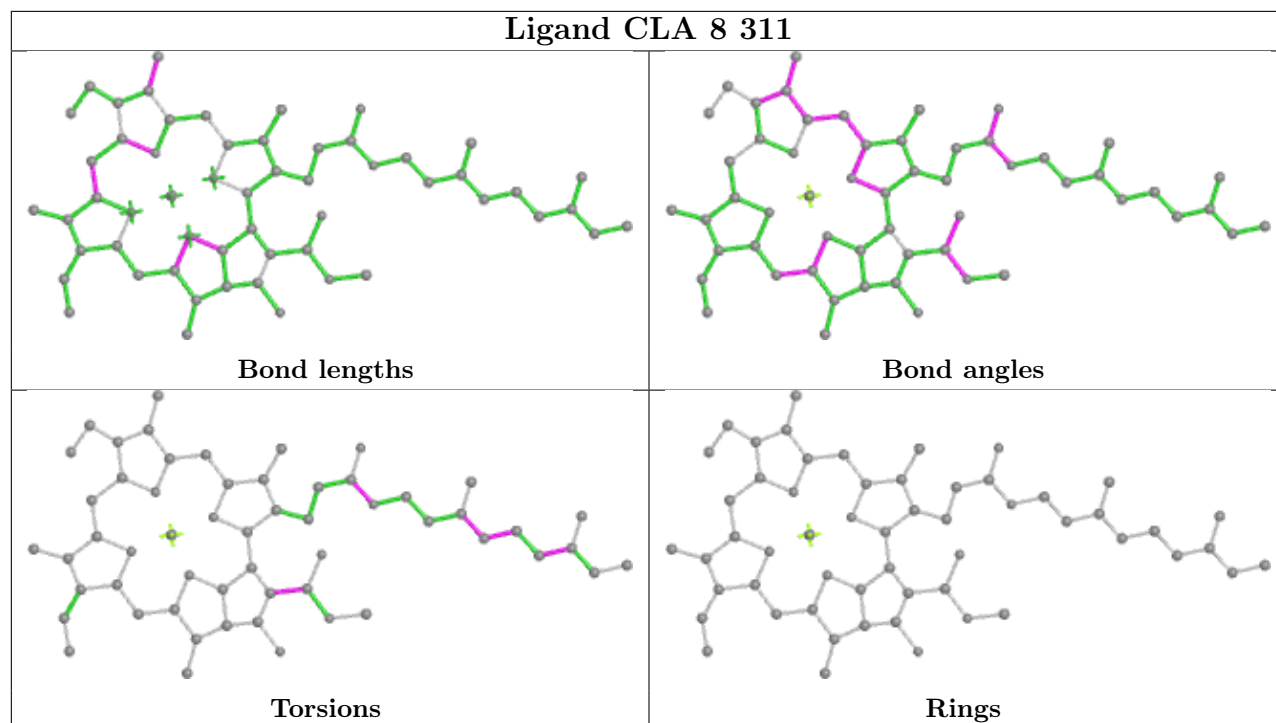
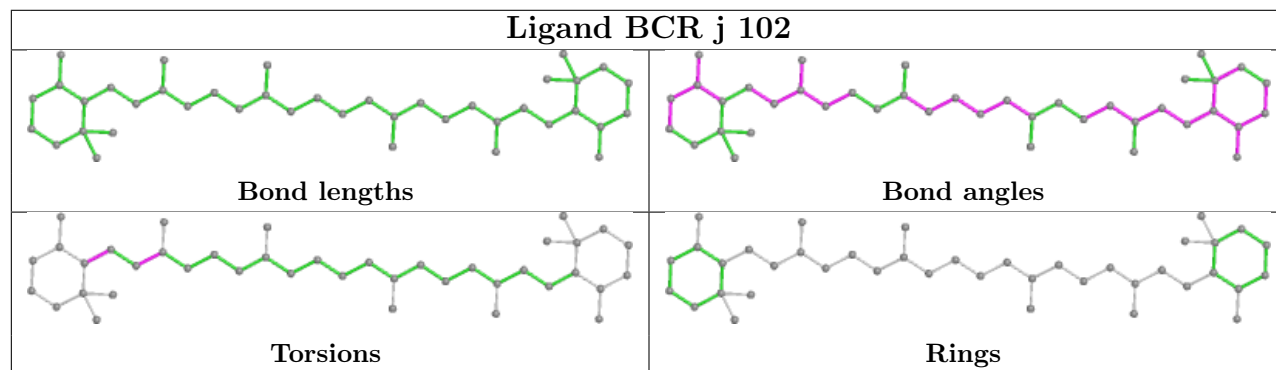
Bond angles

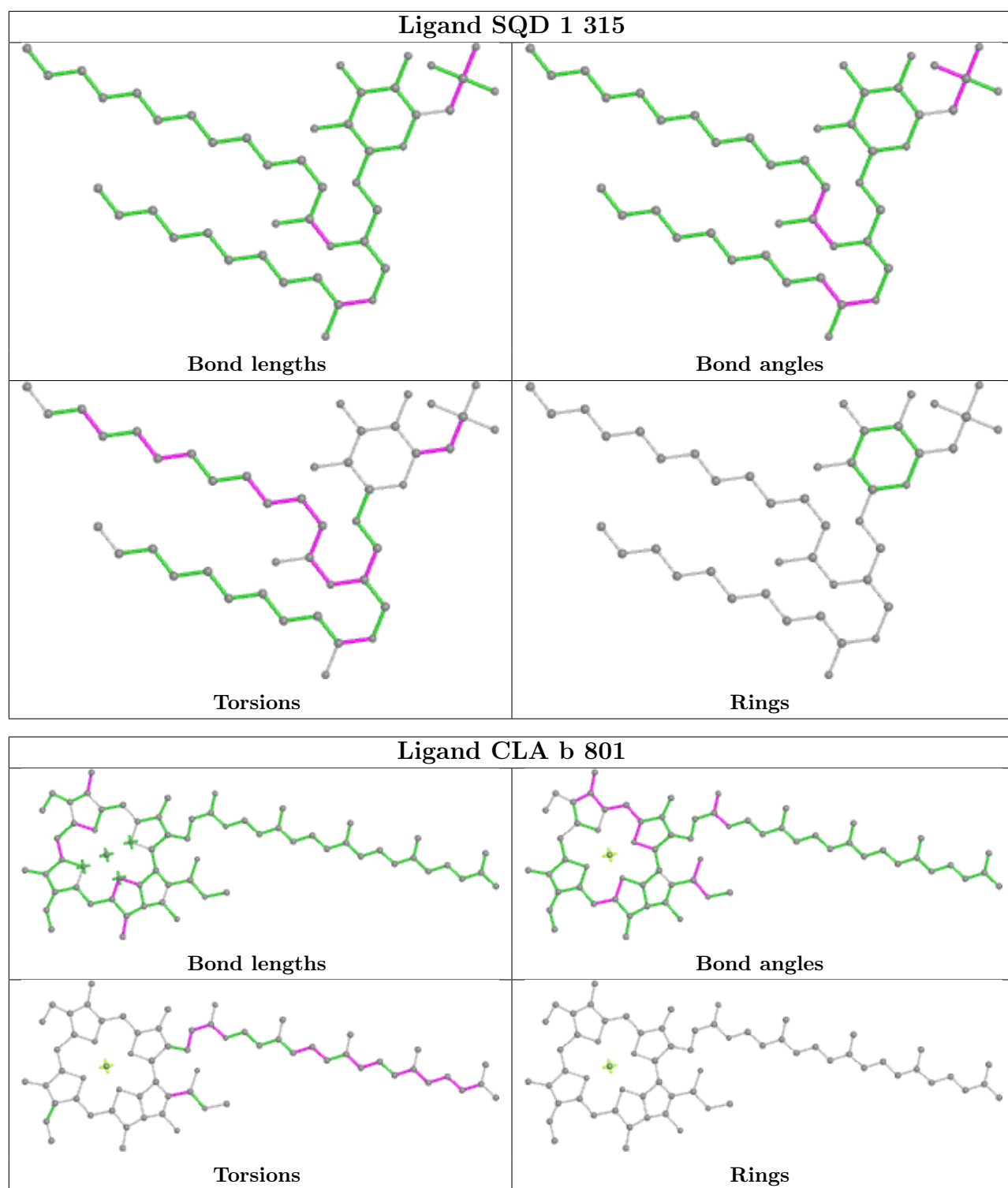


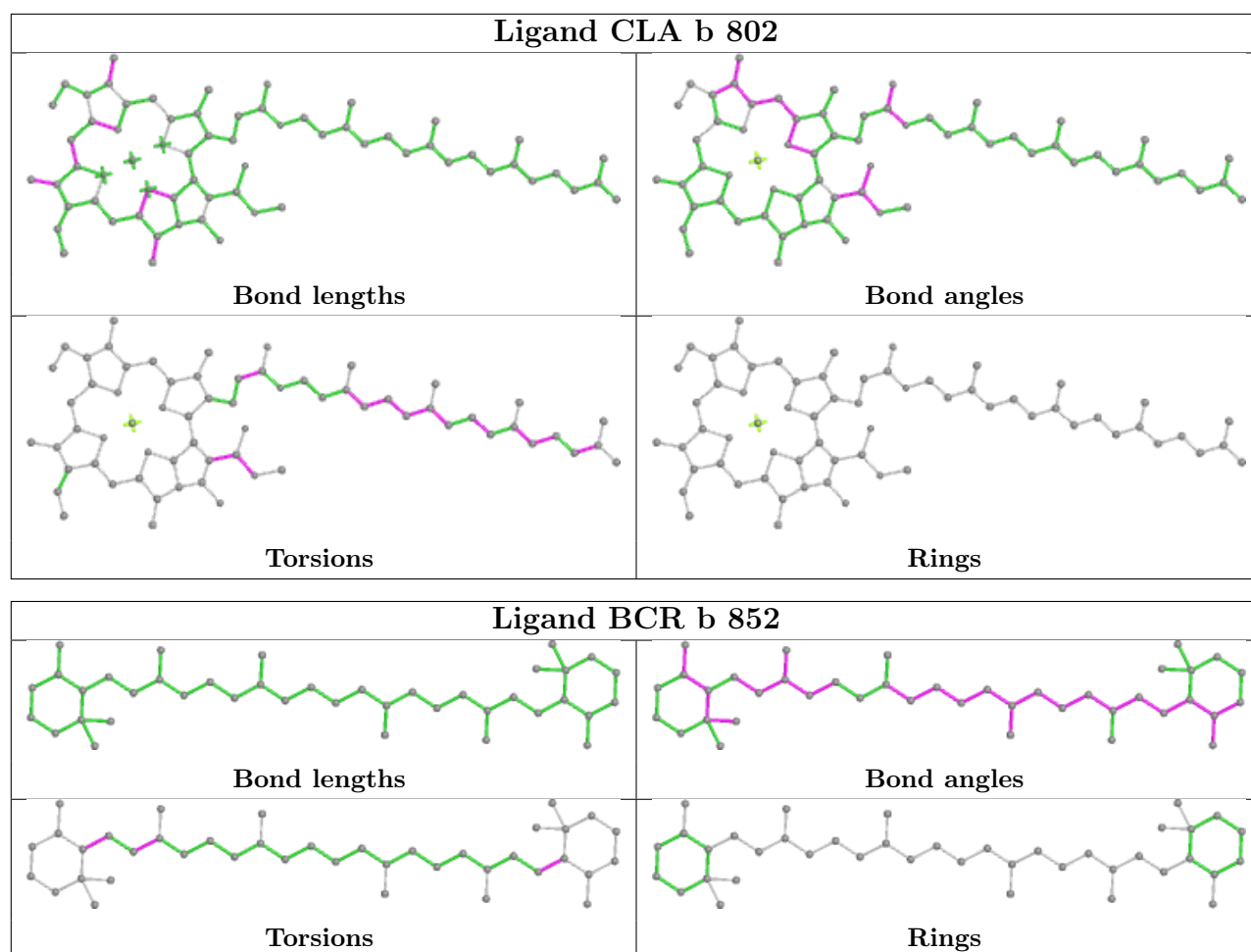
Torsions



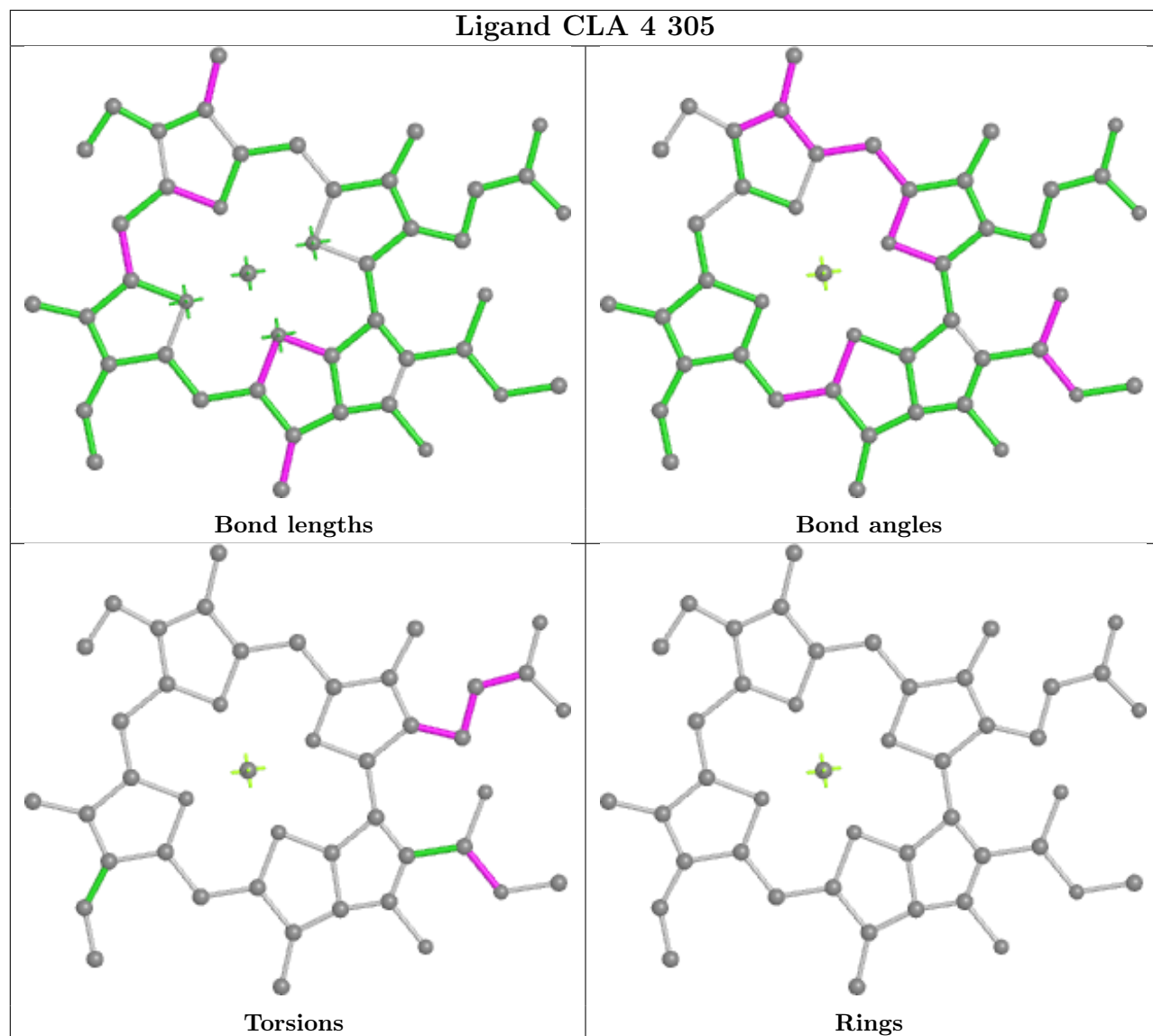
Rings

Ligand CLA 8 311**Ligand BCR j 102**

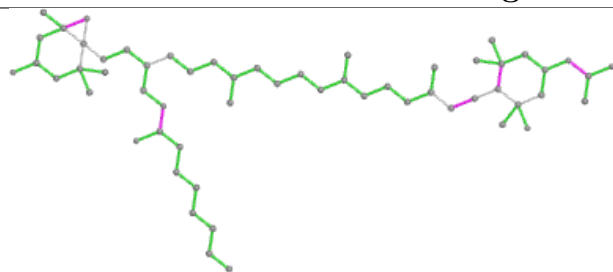




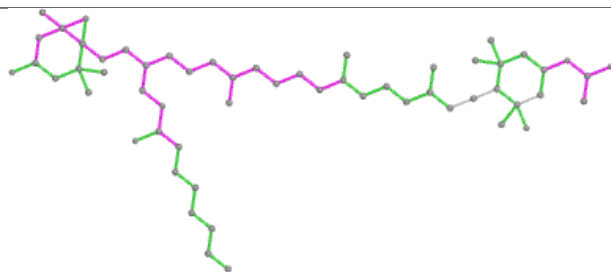
Ligand CLA 4 305



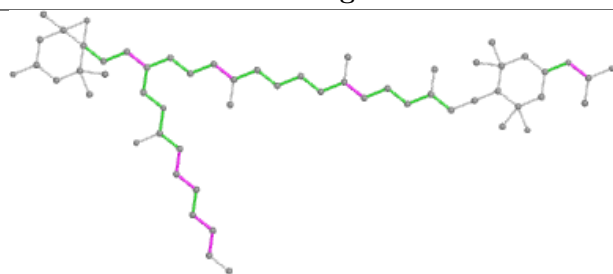
Ligand A1L1F 1 304



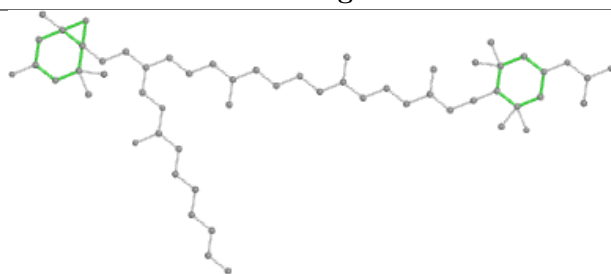
Bond lengths



Bond angles

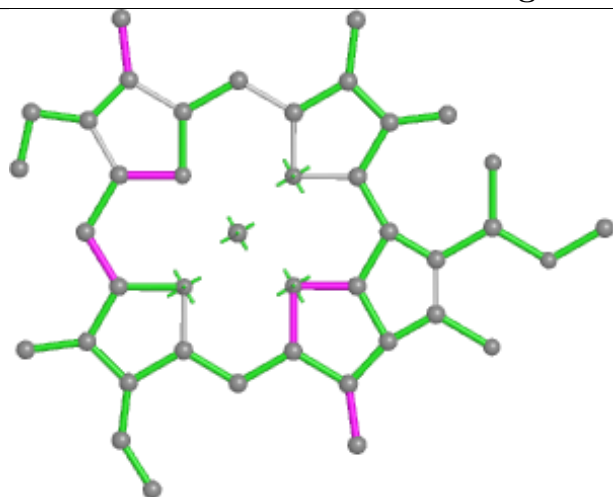


Torsions

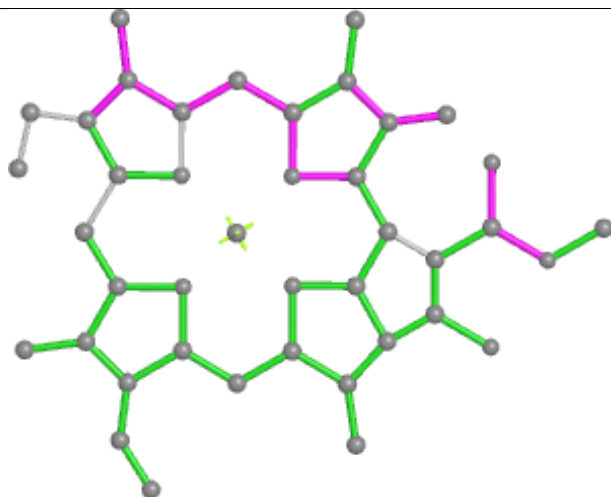


Rings

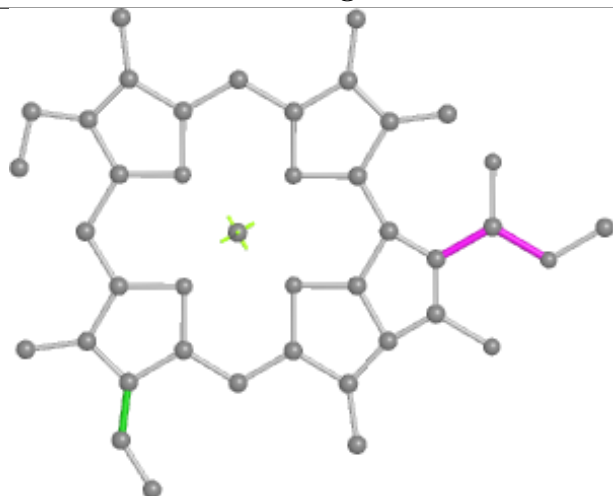
Ligand CLA 4 314



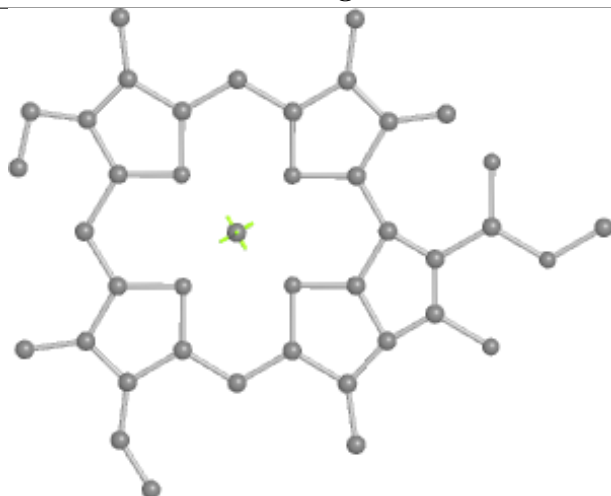
Bond lengths



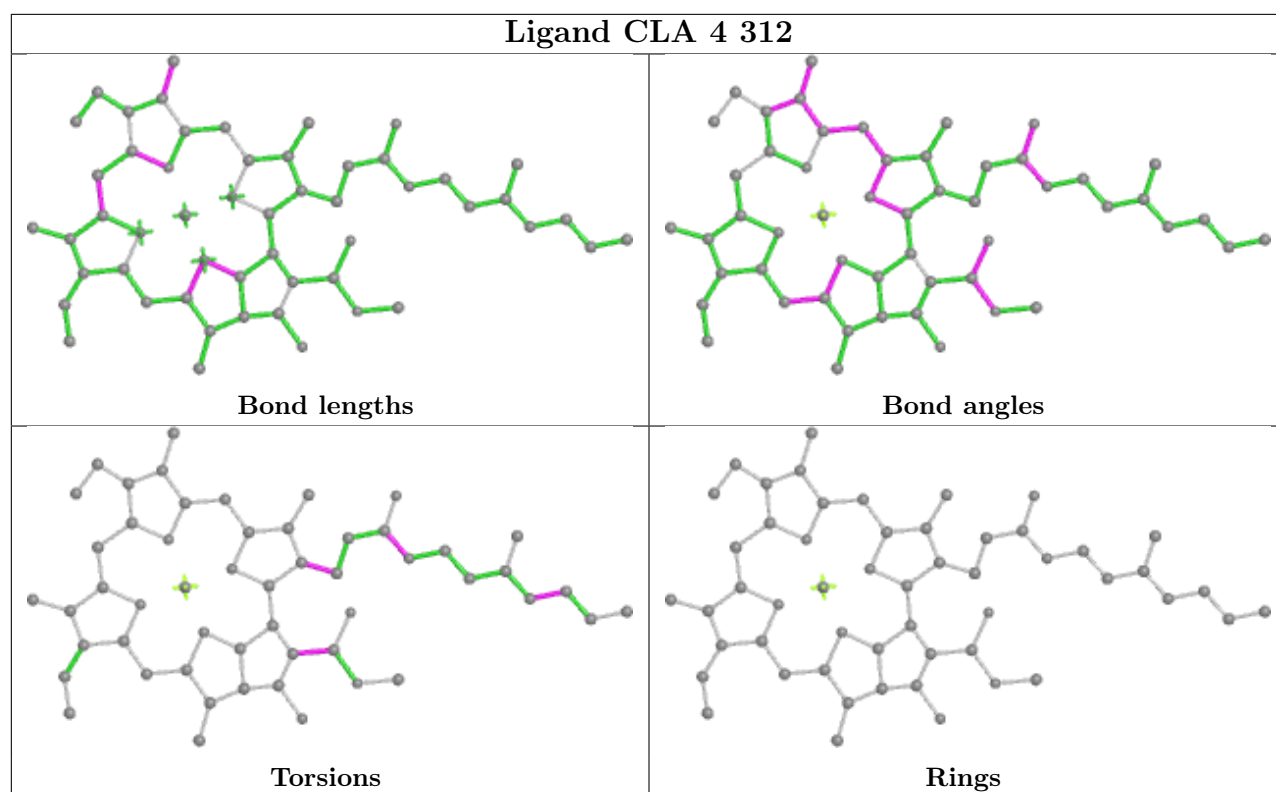
Bond angles



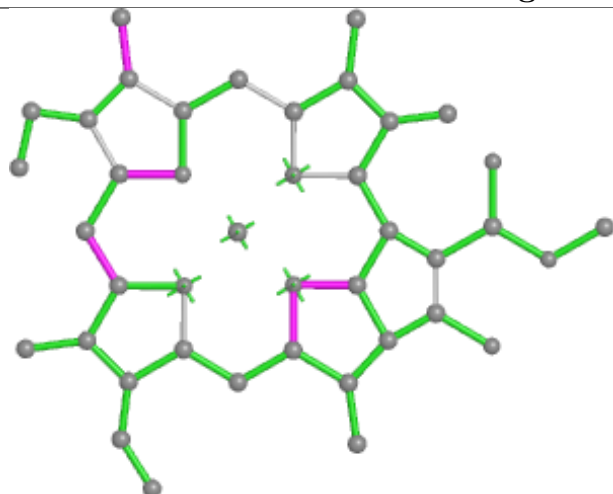
Torsions



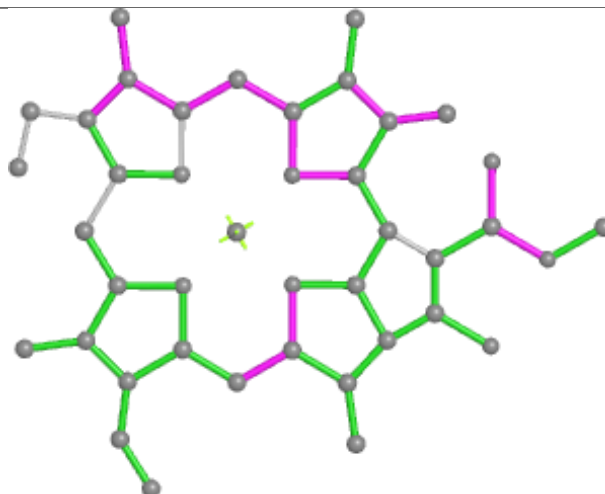
Rings



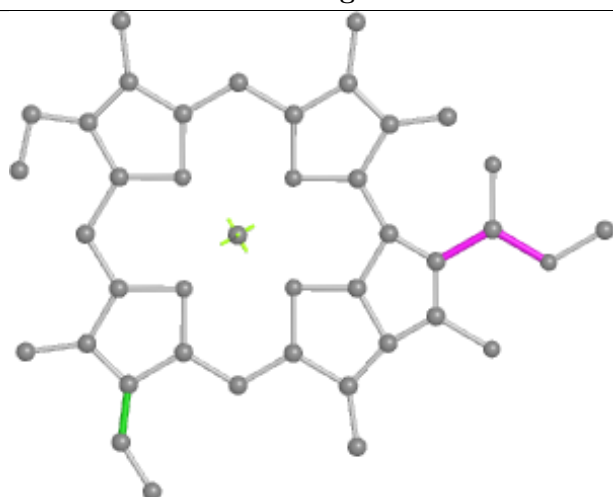
Ligand CLA 7 315



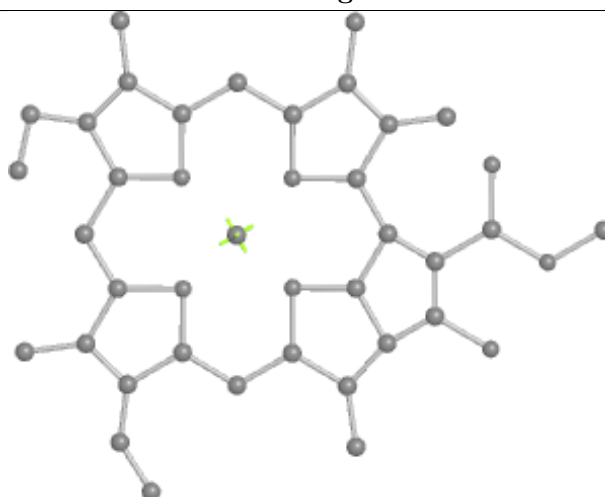
Bond lengths



Bond angles

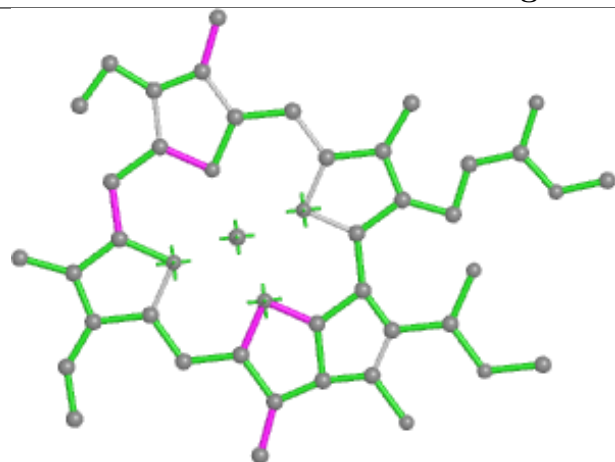


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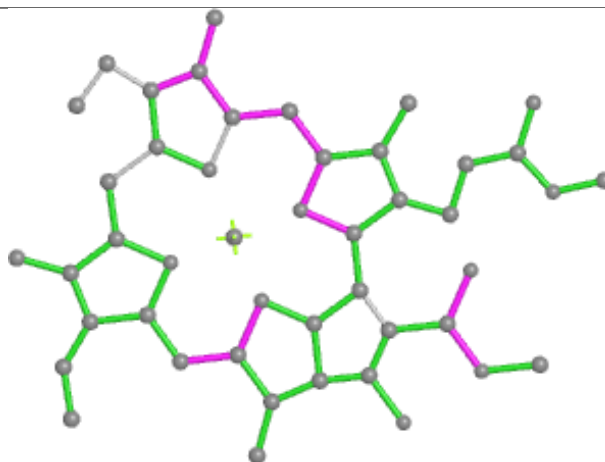


Rings

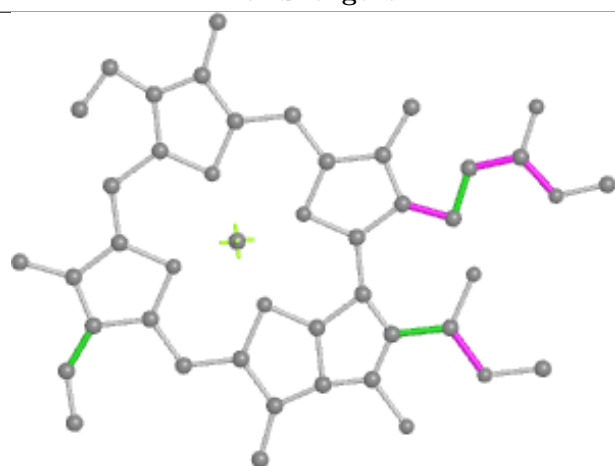
Ligand CLA 3 315



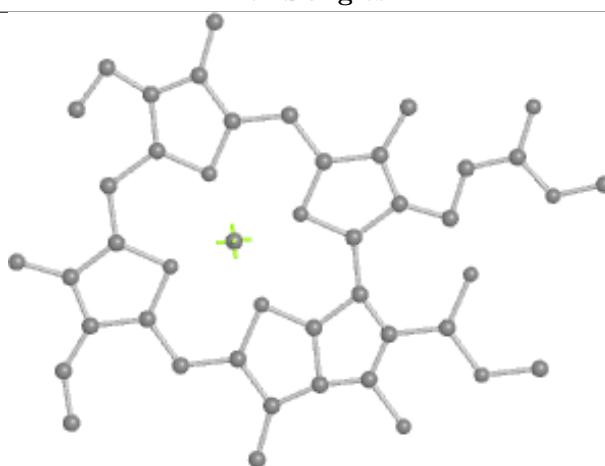
Bond lengths



Bond angles

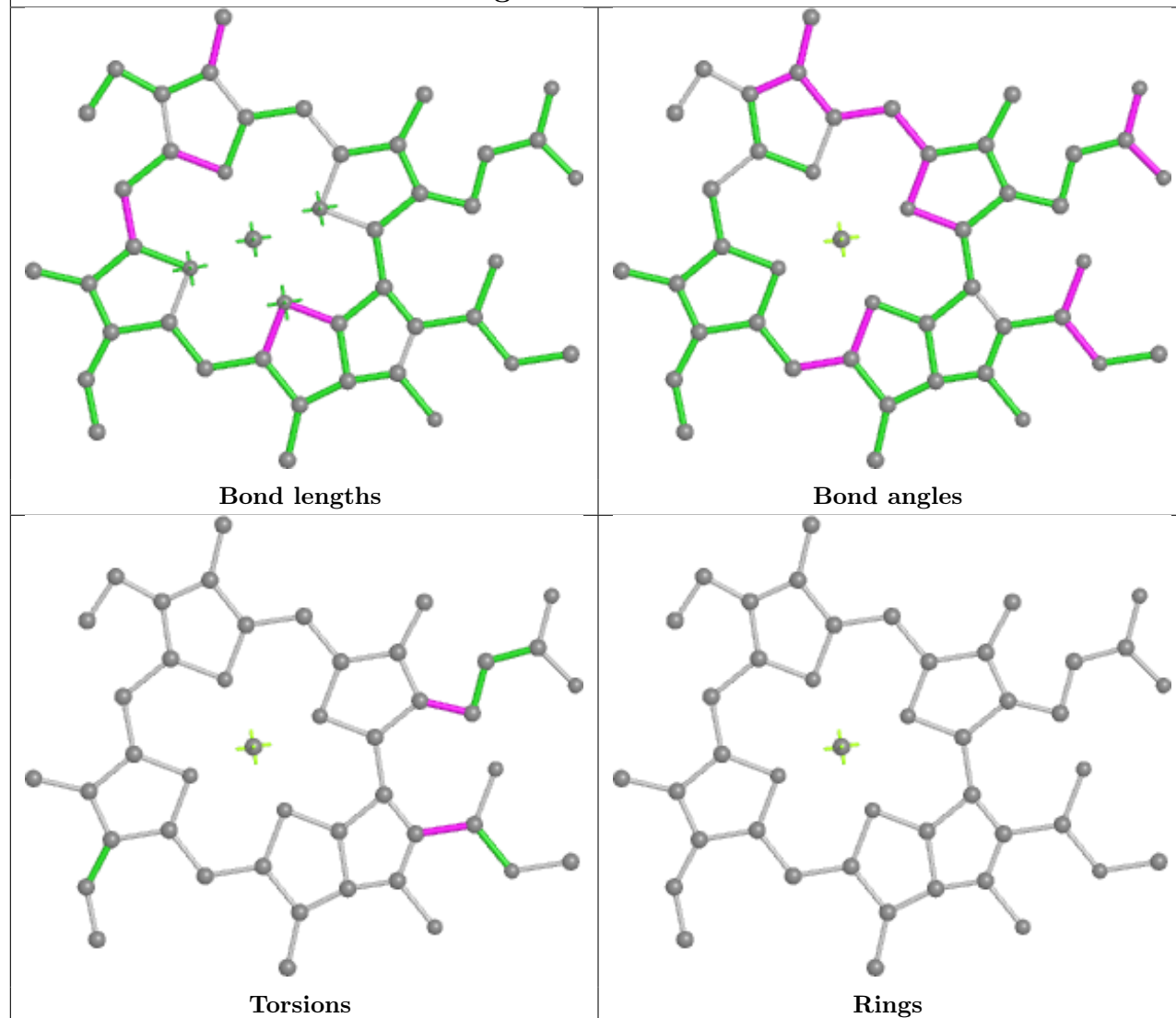


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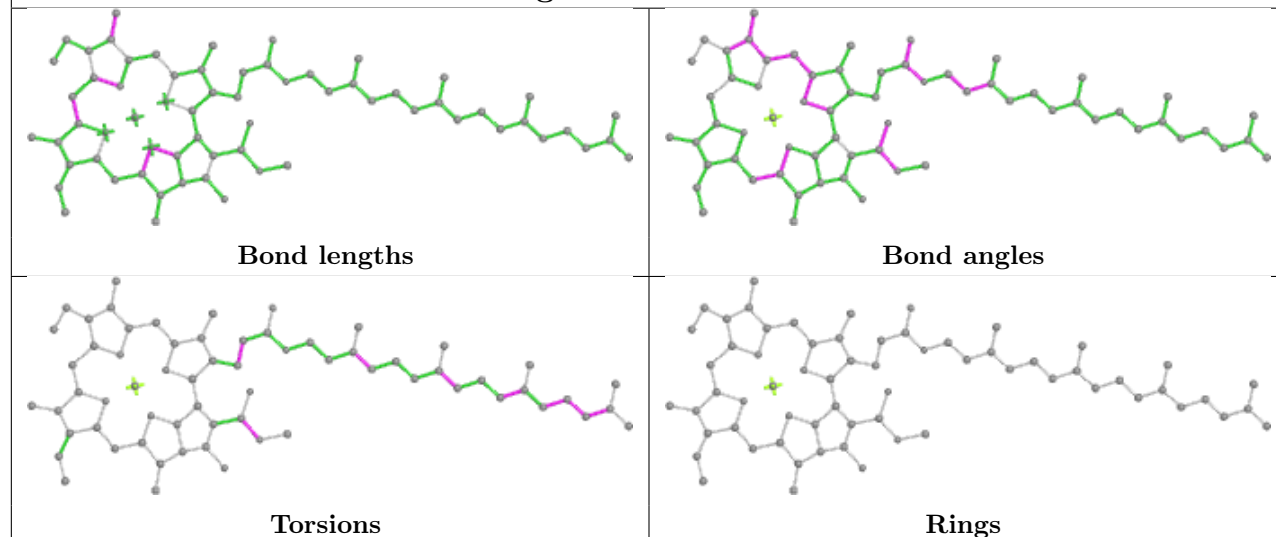


Rings

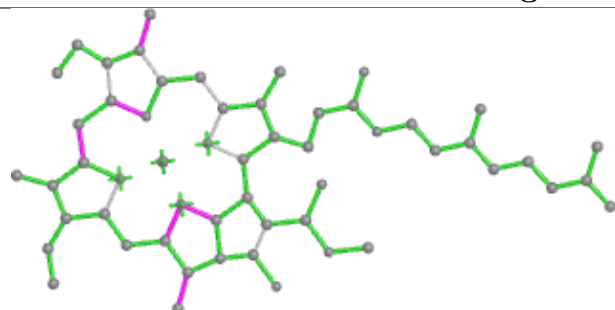
Ligand CLA a 815



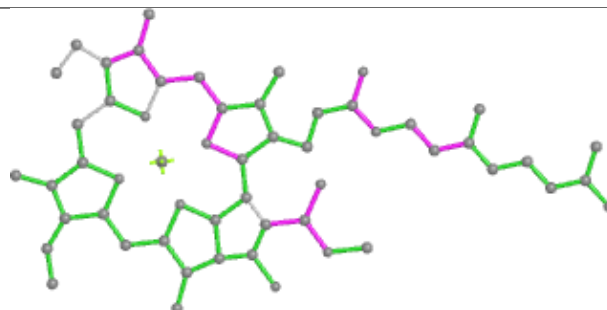
Ligand CLA 1 308



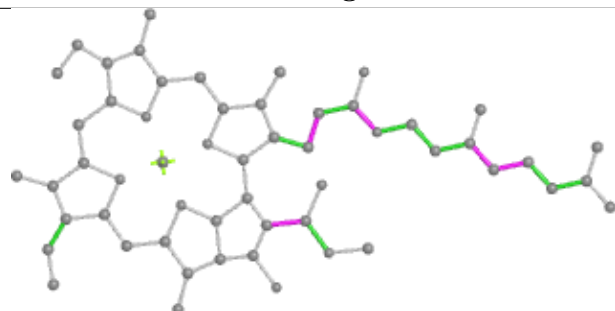
Ligand CLA 8 308



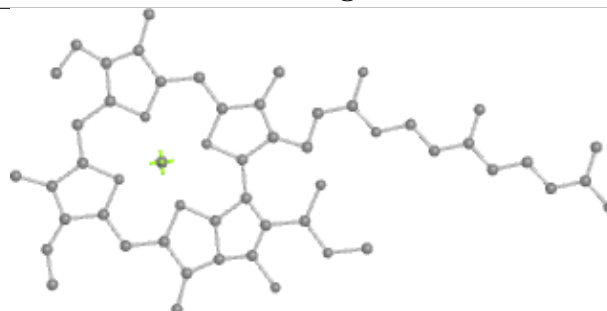
Bond lengths



Bond angles

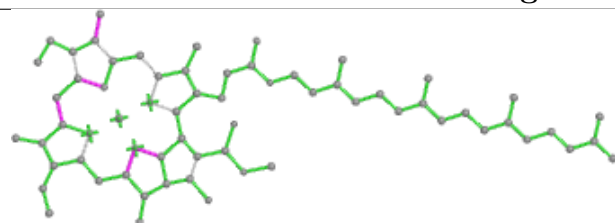


Torsions

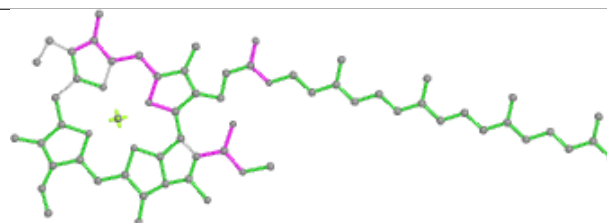


Rings

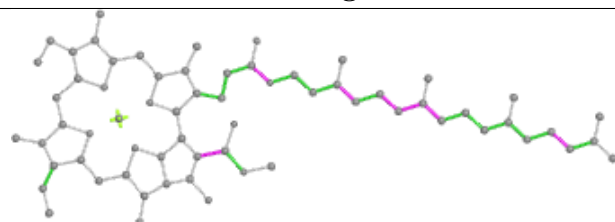
Ligand CLA a 831



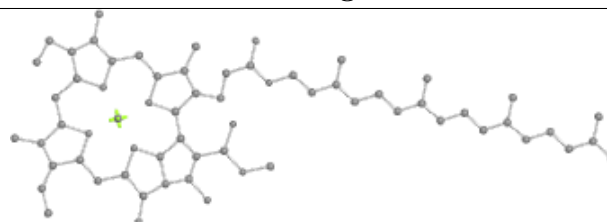
Bond lengths



Bond angles

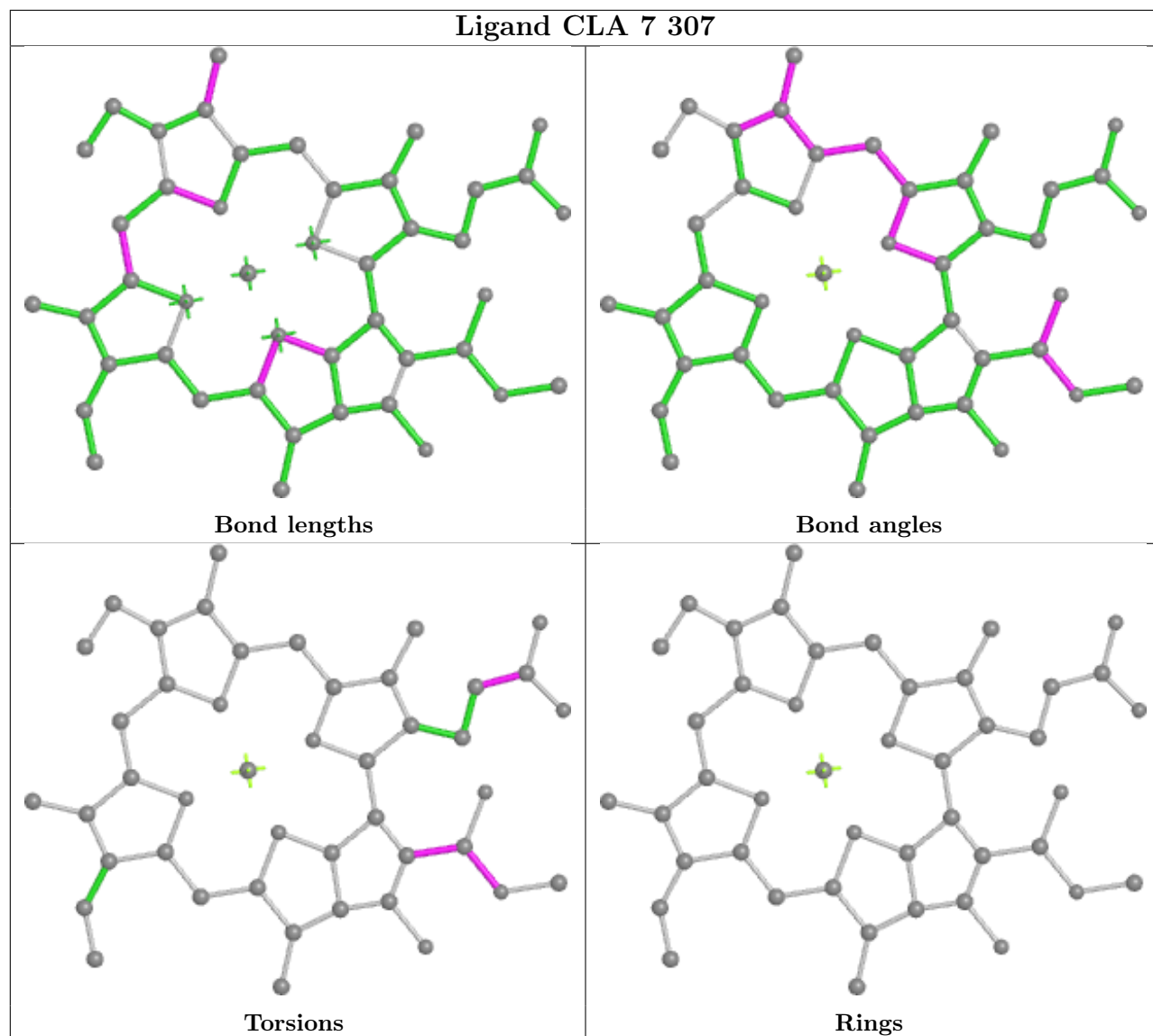


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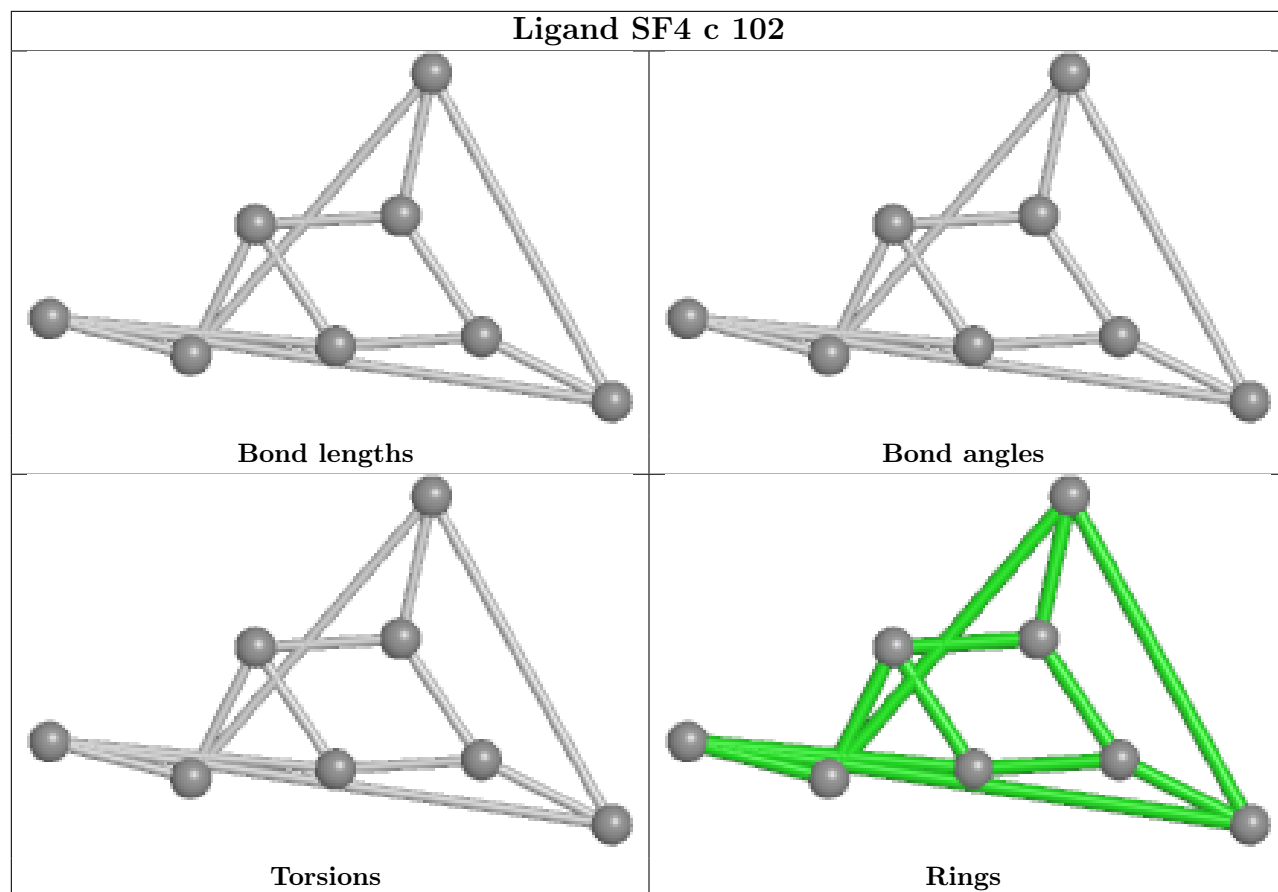


Rings

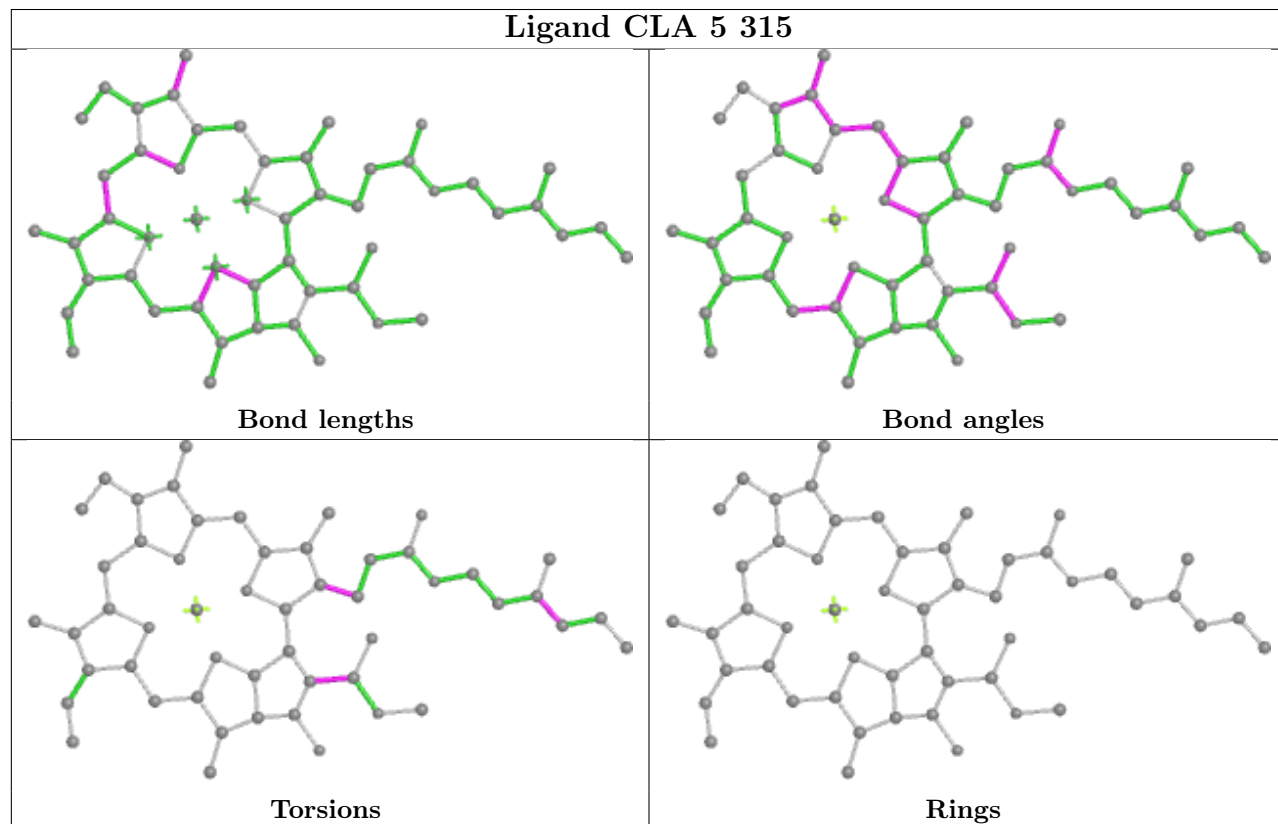
Ligand CLA 7 307



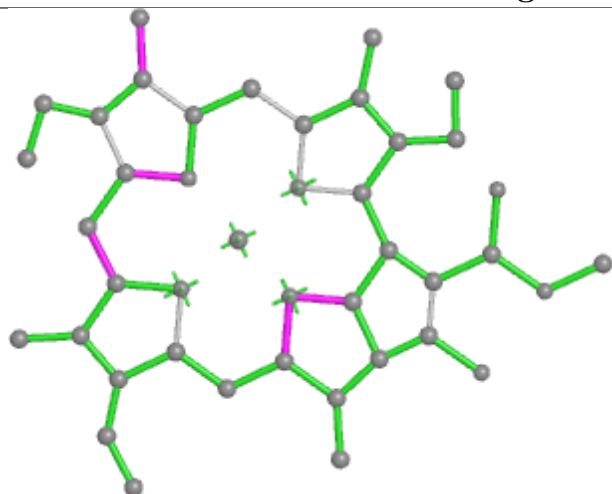
Ligand SF4 c 102



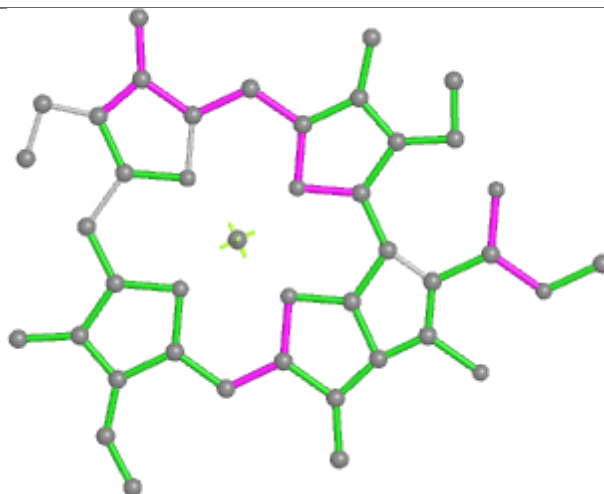
Ligand CLA 5 315



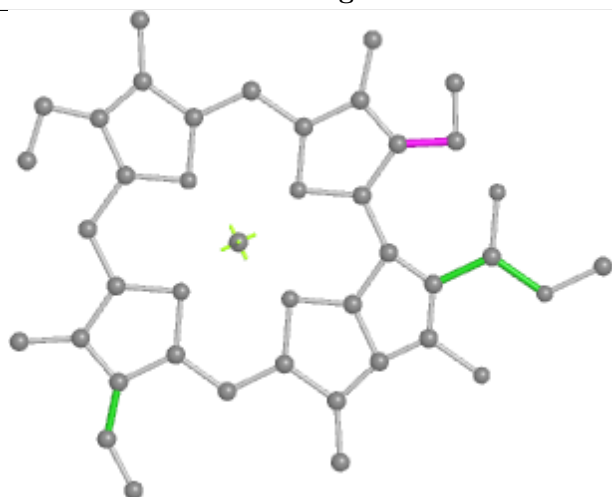
Ligand CLA 6 311



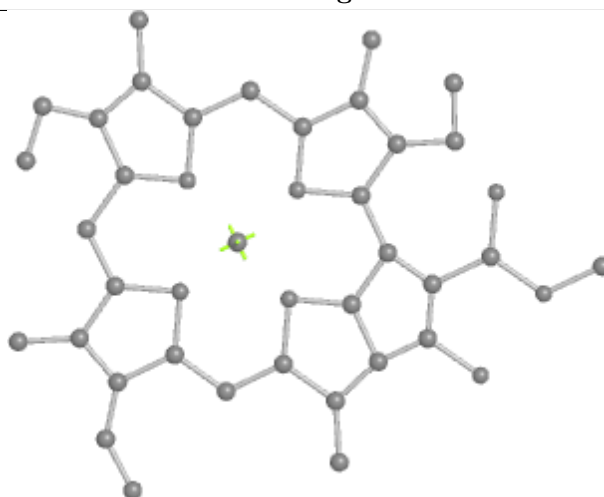
Bond lengths



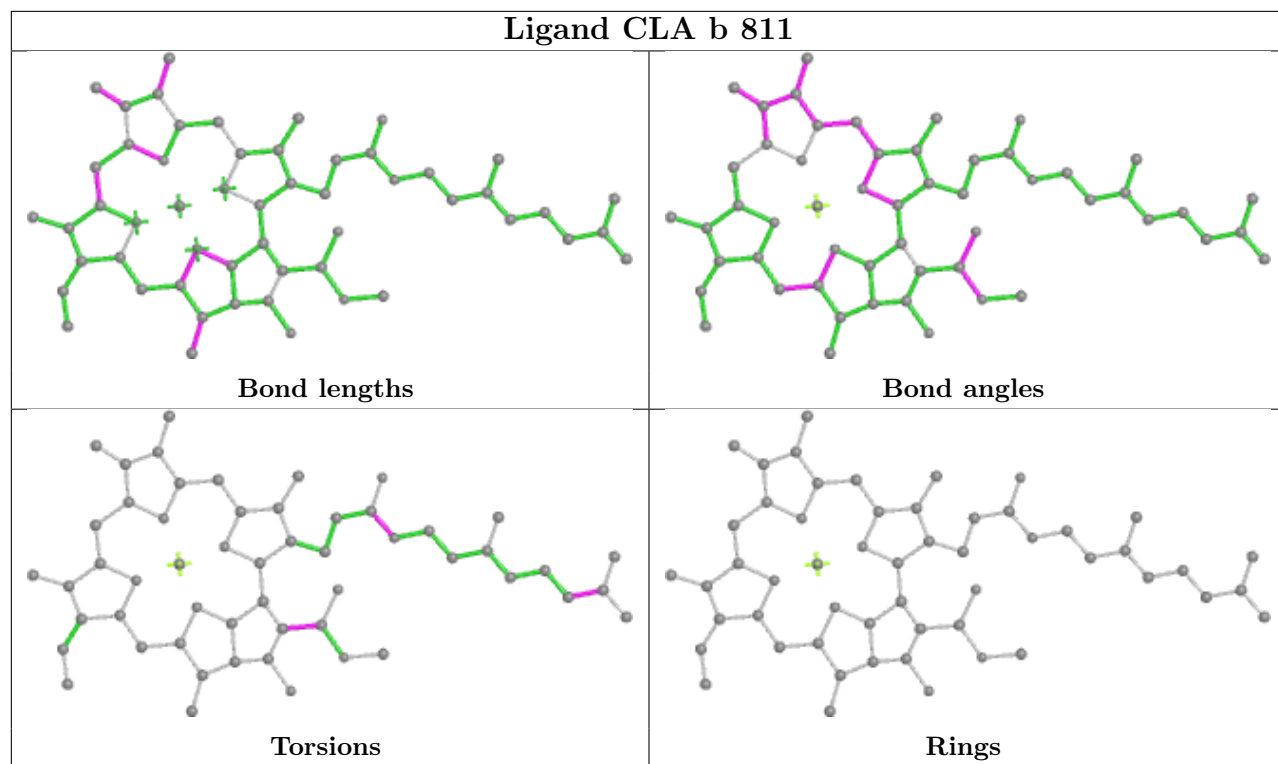
Bond angles



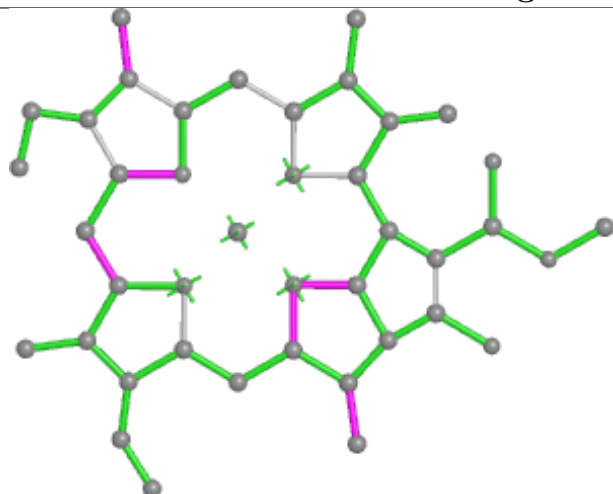
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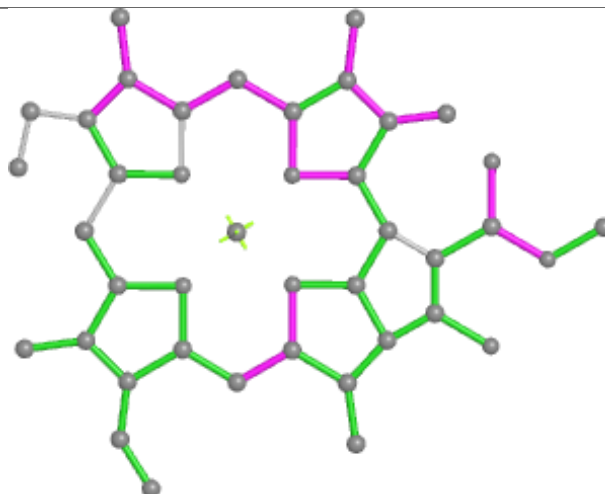
Rings



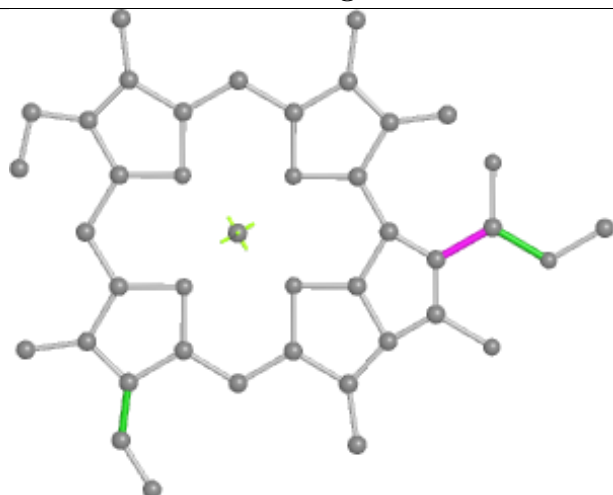
Ligand CLA b 830



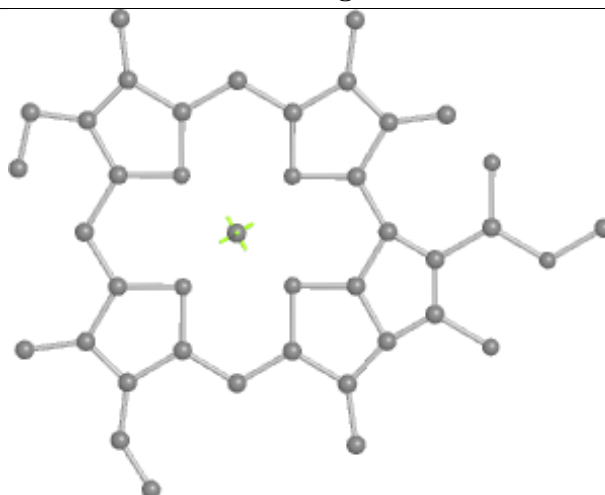
Bond lengths



Bond angles

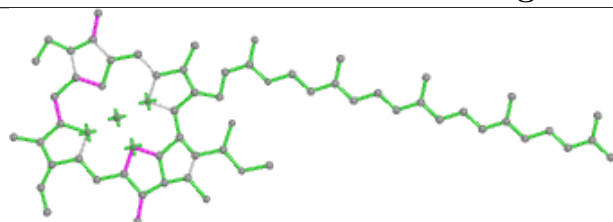


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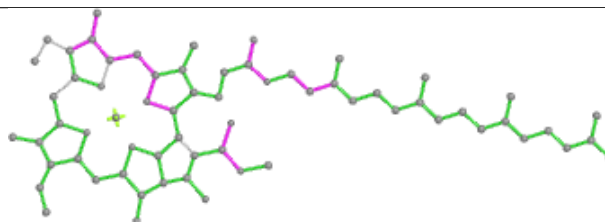


Rings

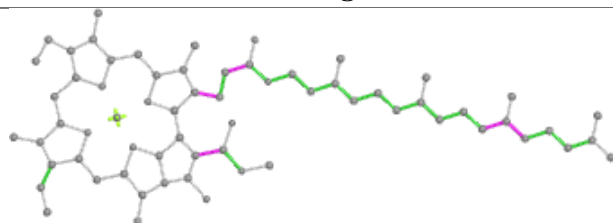
Ligand CLA b 838



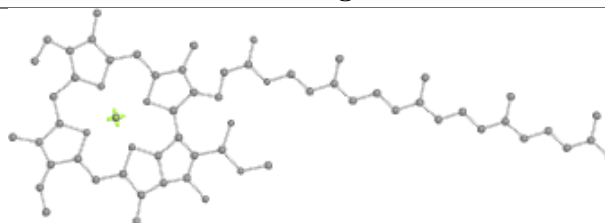
Bond lengths



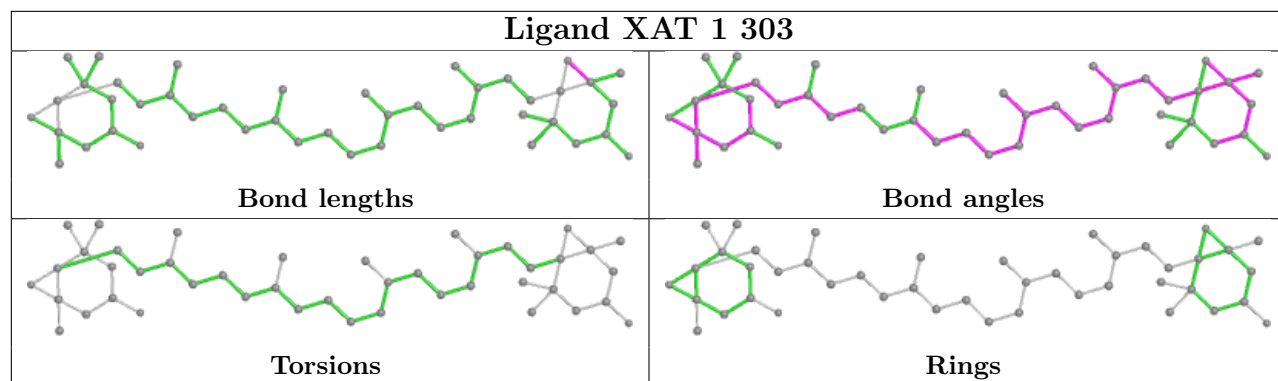
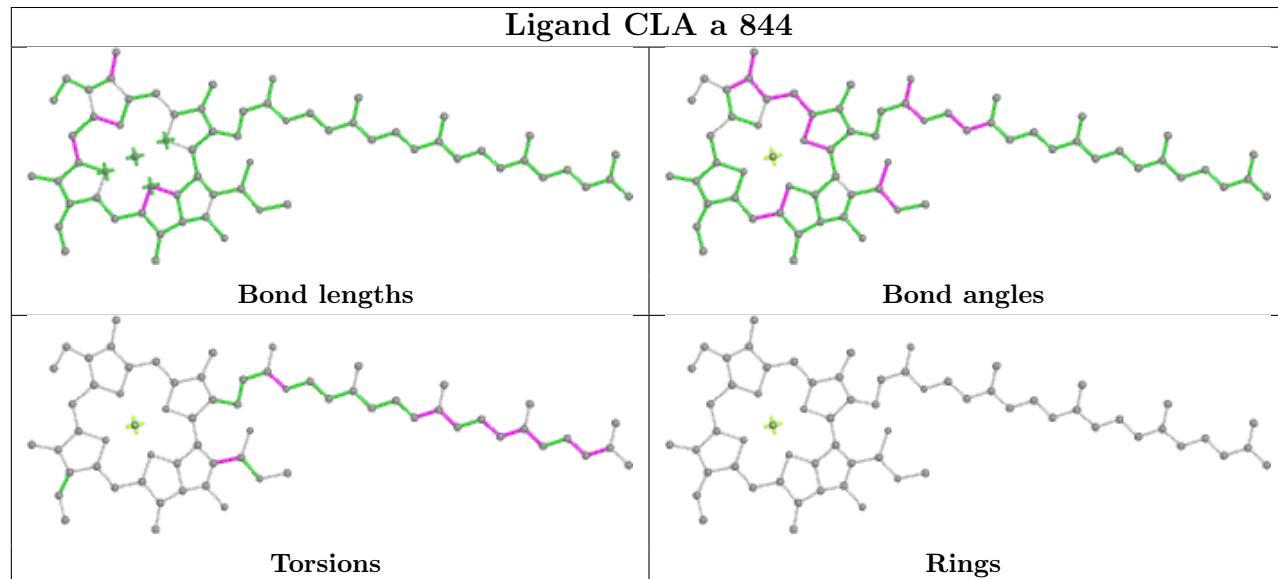
Bond angles



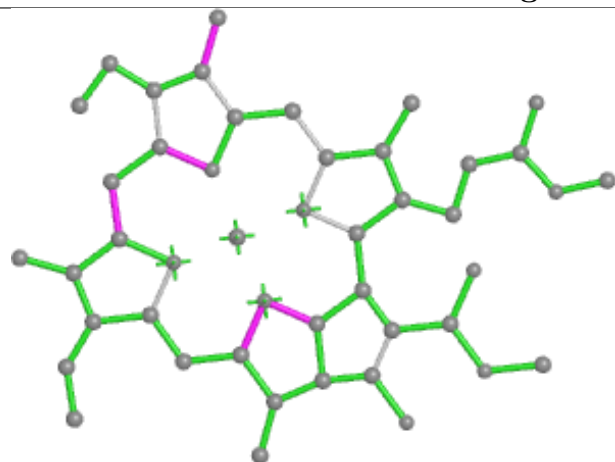
Torsions



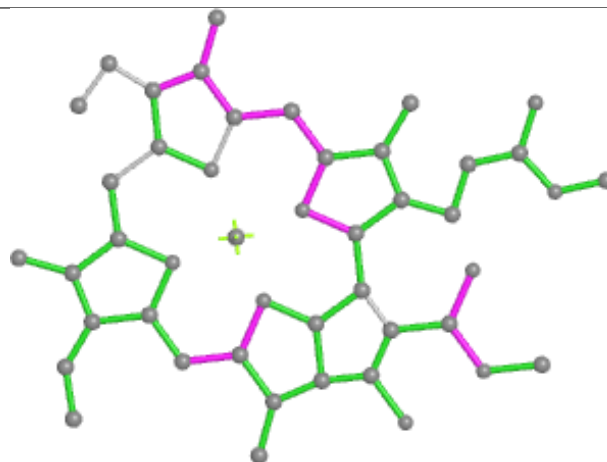
Rings

Ligand XAT 1 303**Ligand CLA a 844**

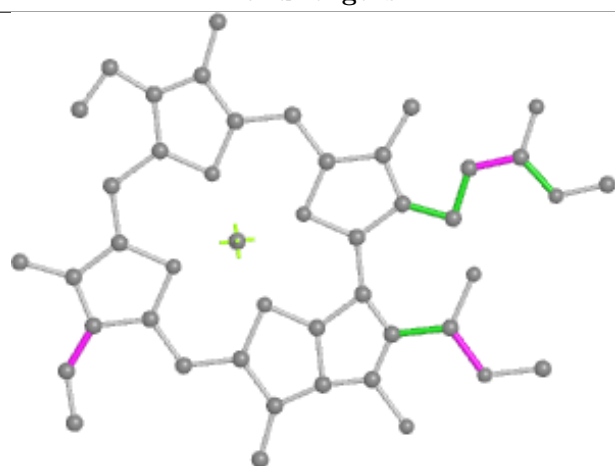
Ligand CLA 5 316



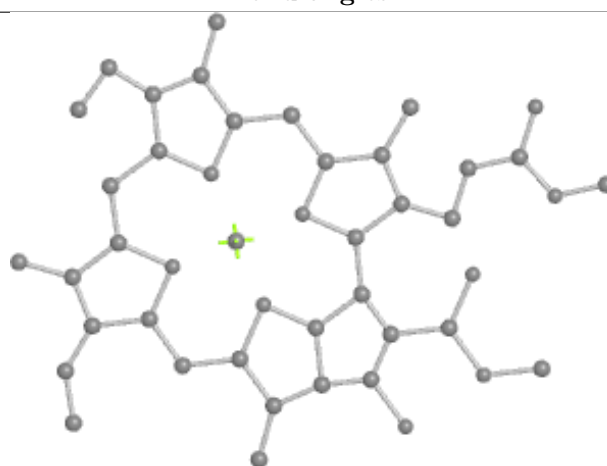
Bond lengths



Bond angles

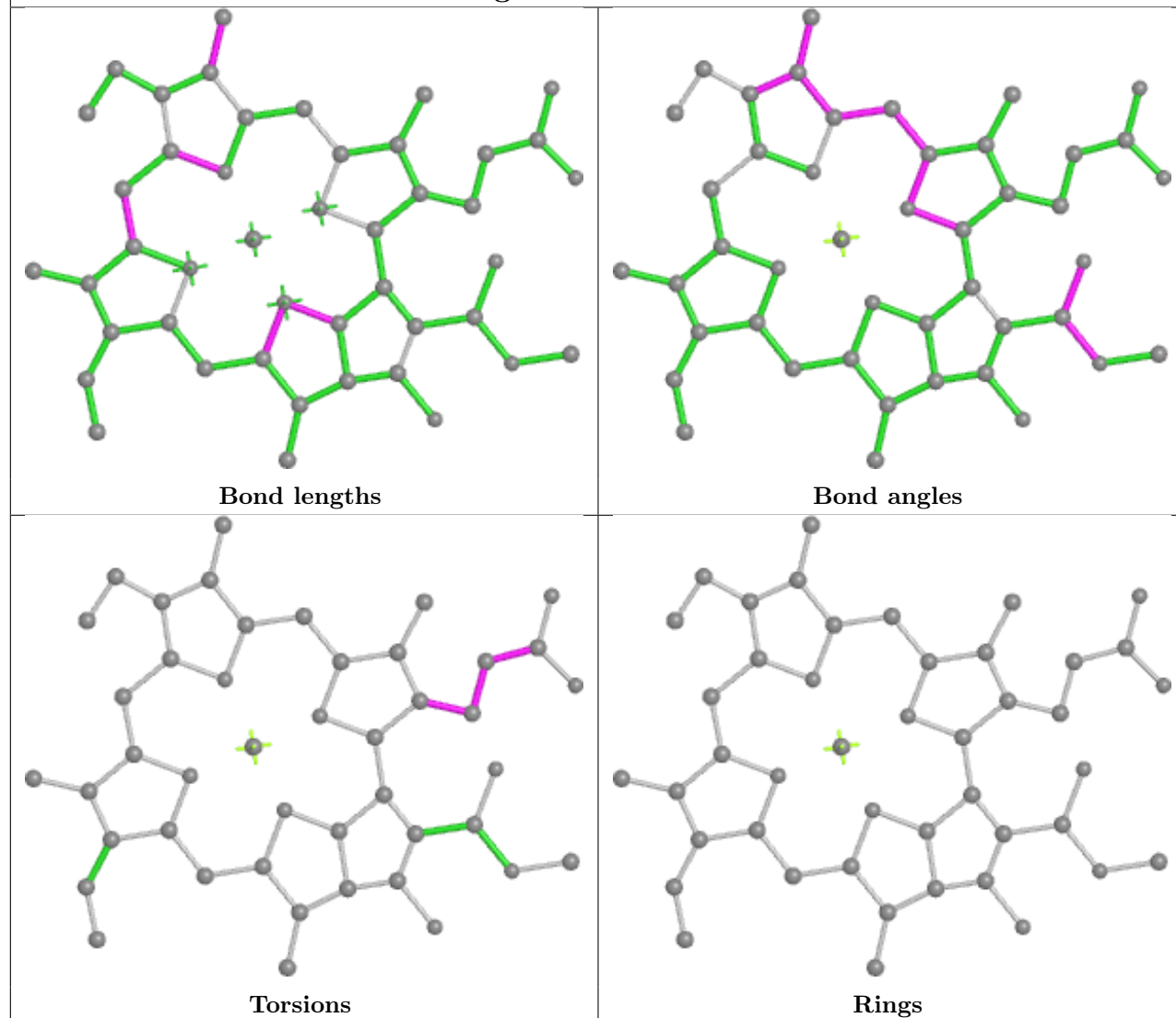


Torsions

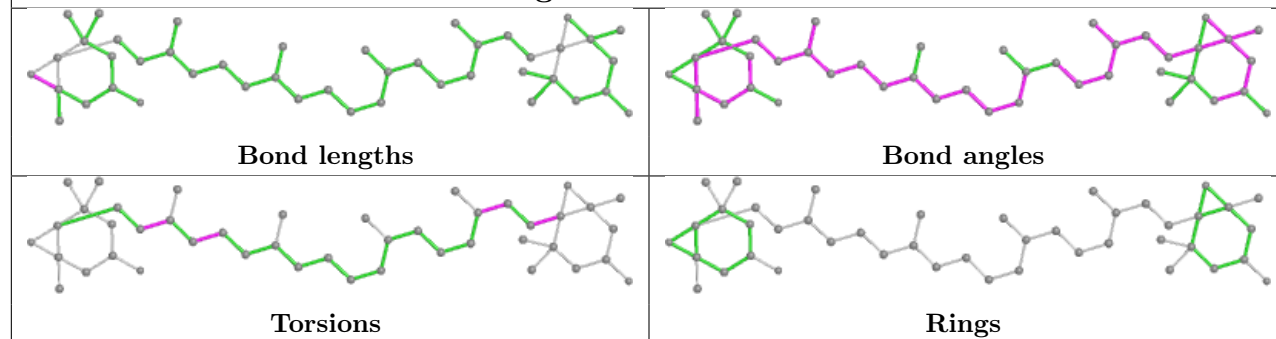


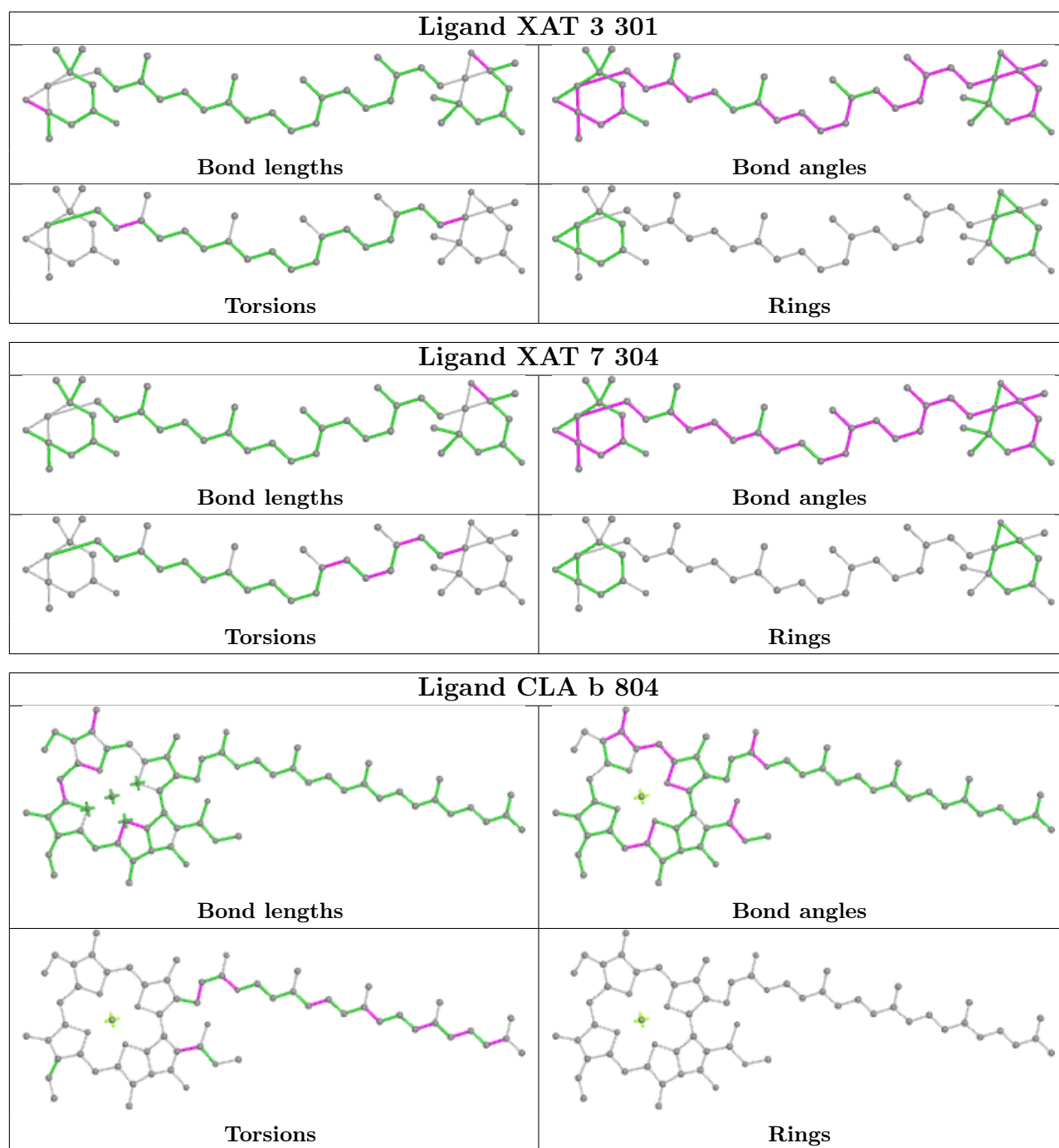
Rings

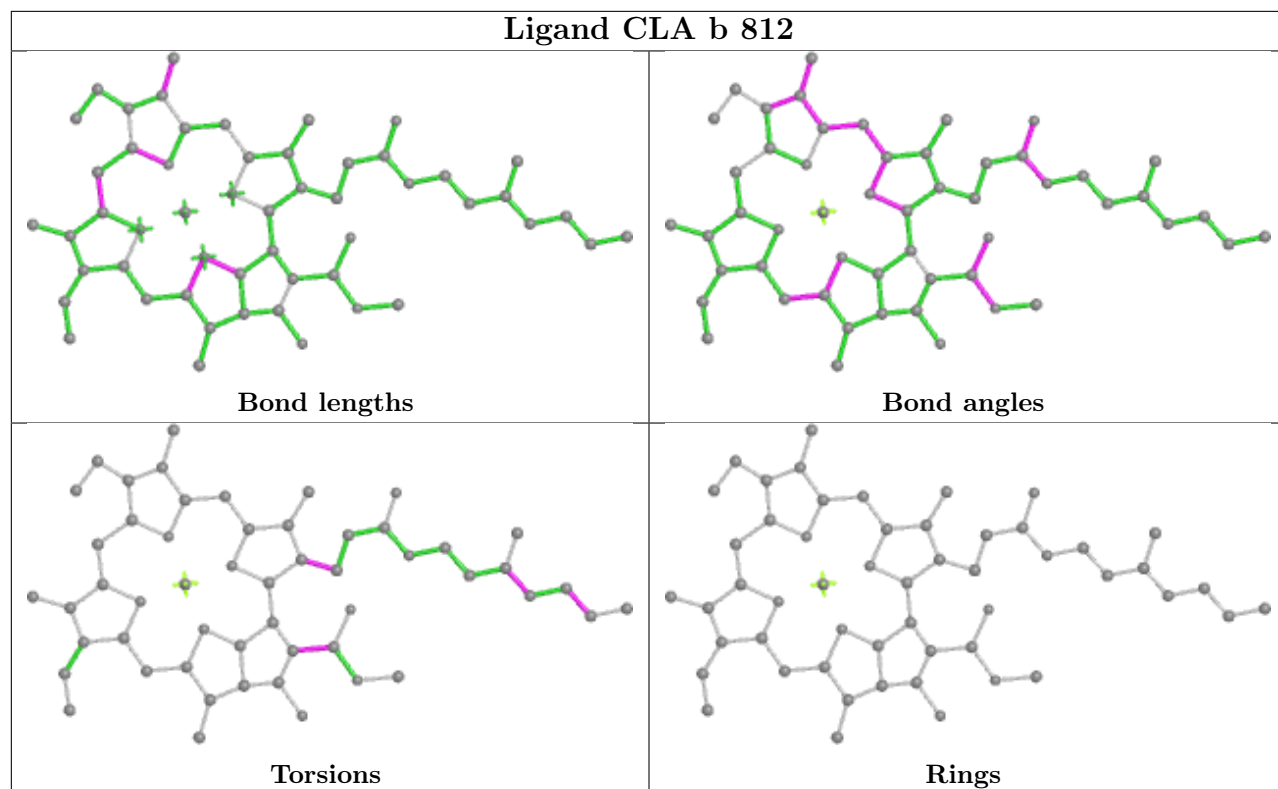
Ligand CLA 1 314



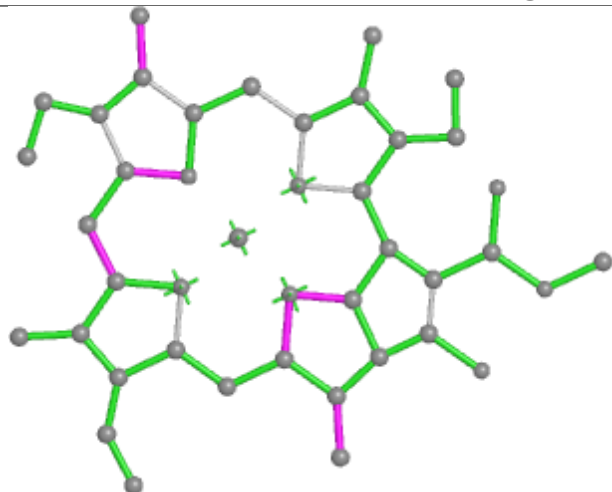
Ligand XAT 7 301



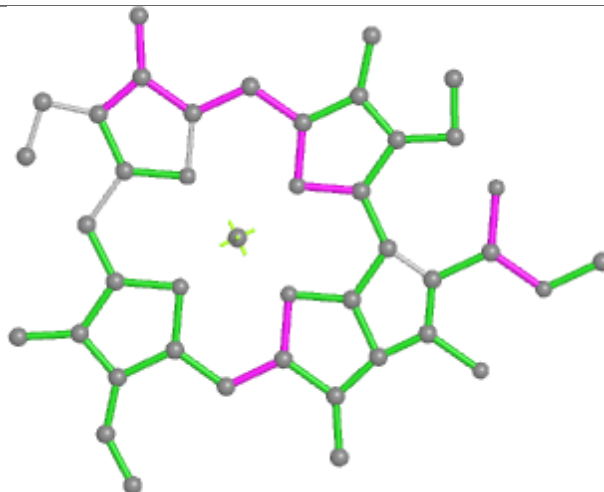




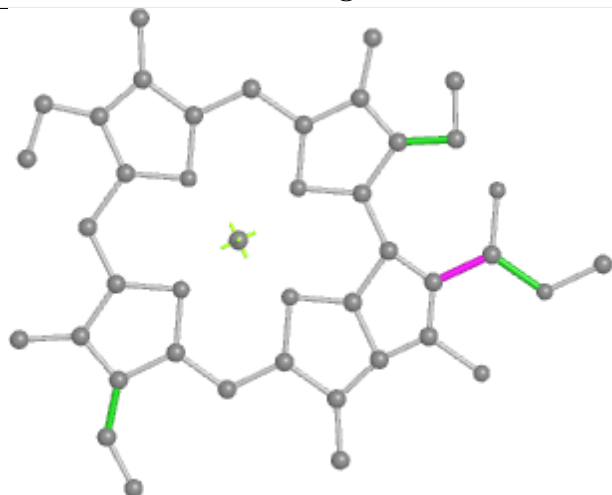
Ligand CLA l 201



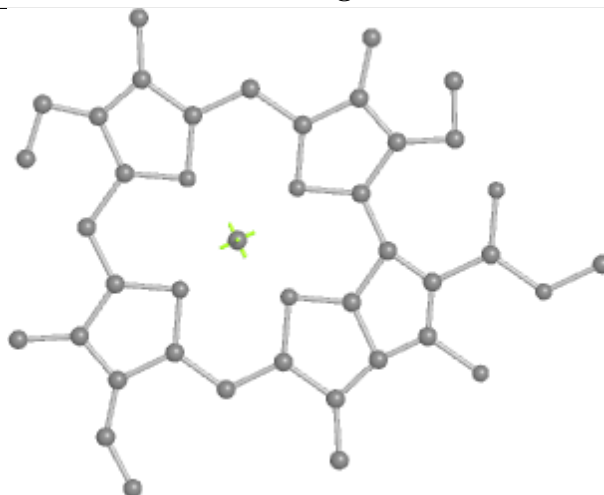
Bond lengths



Bond angles

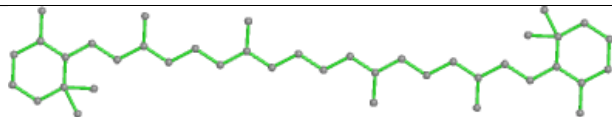


Torsions

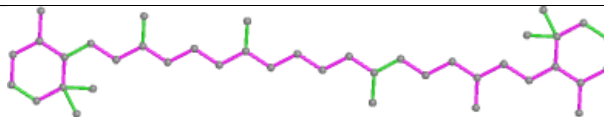


Rings

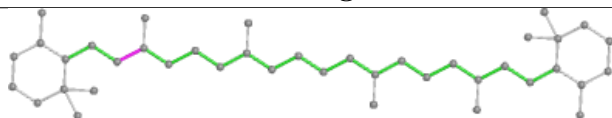
Ligand BCR b 843



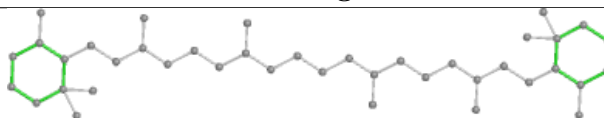
Bond lengths



Bond angles

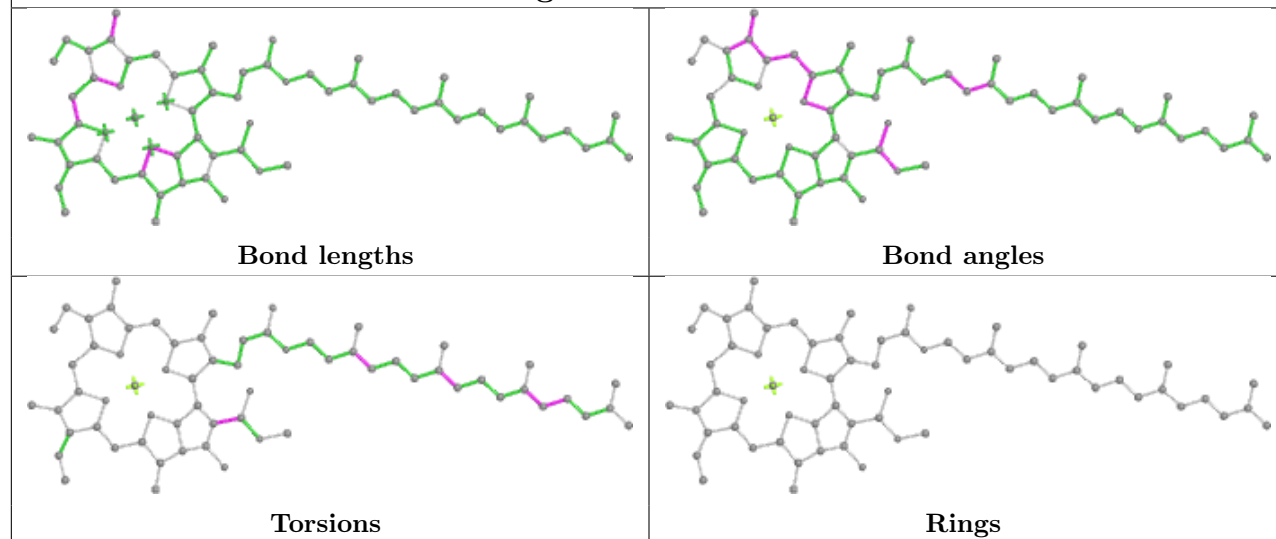


Torsions

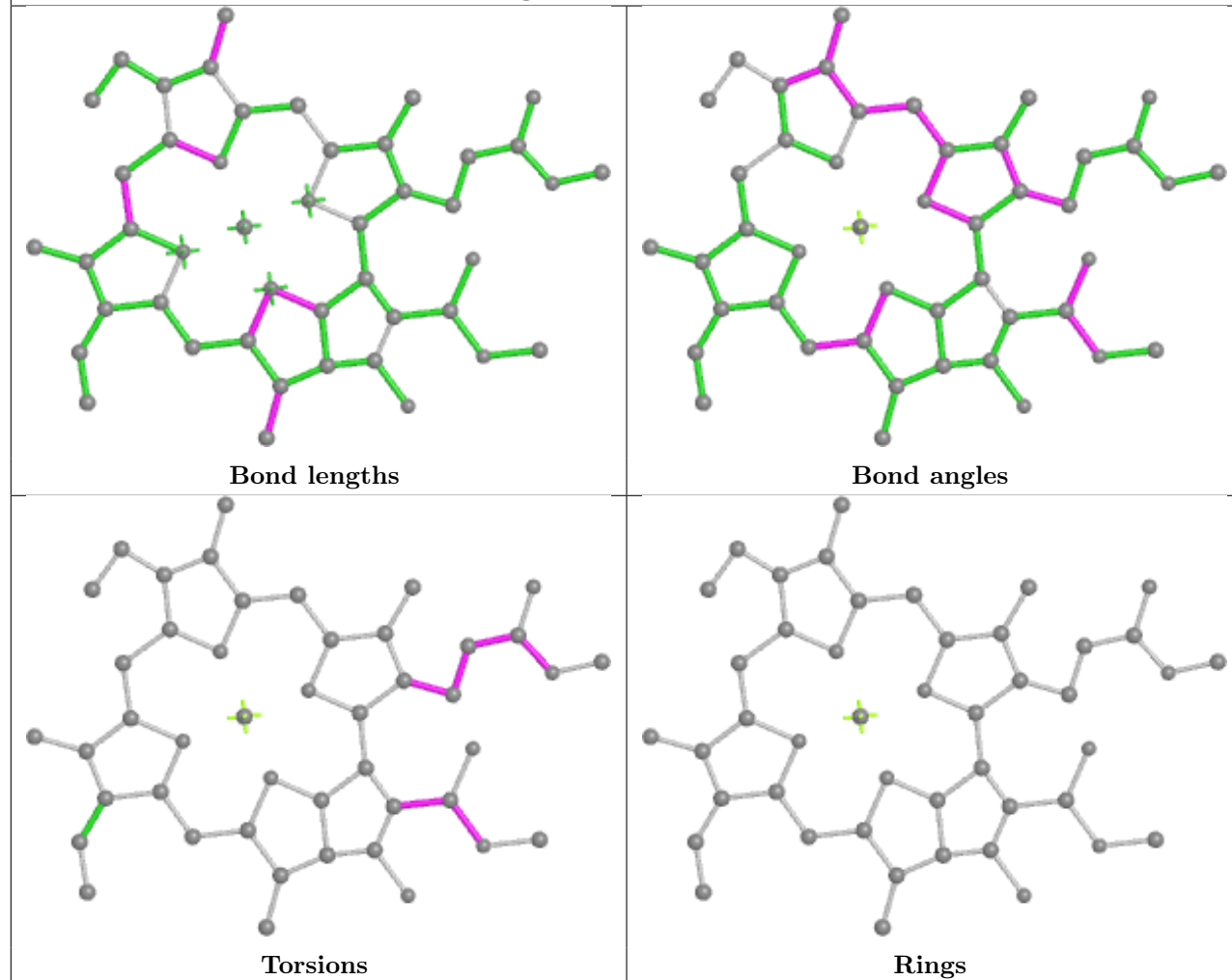


Rings

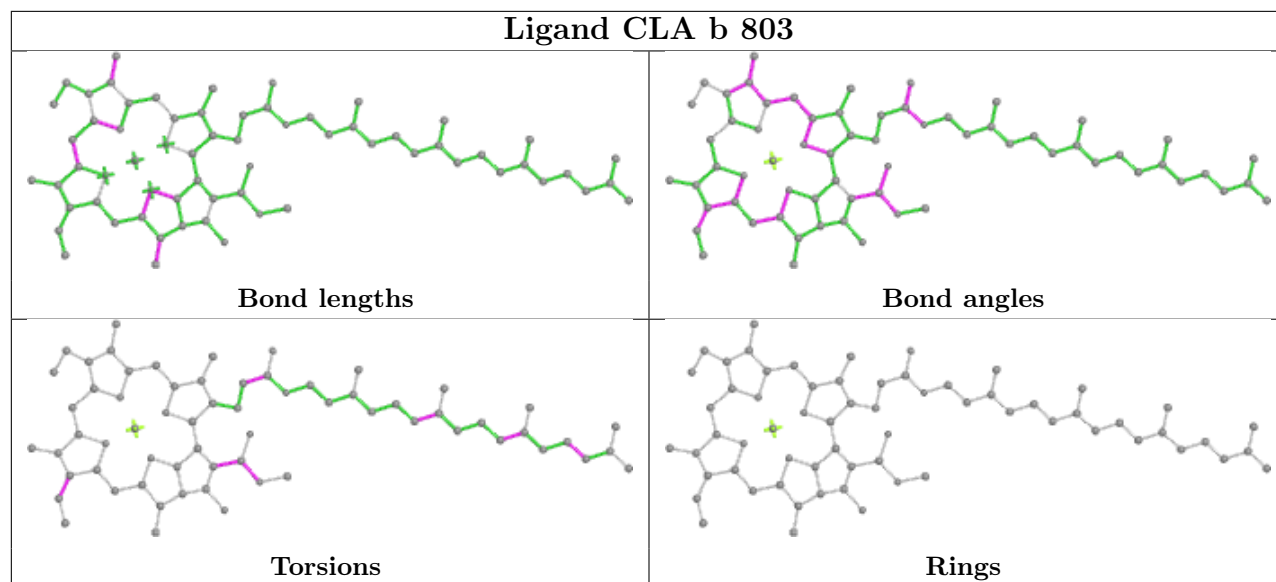
Ligand CLA a 840



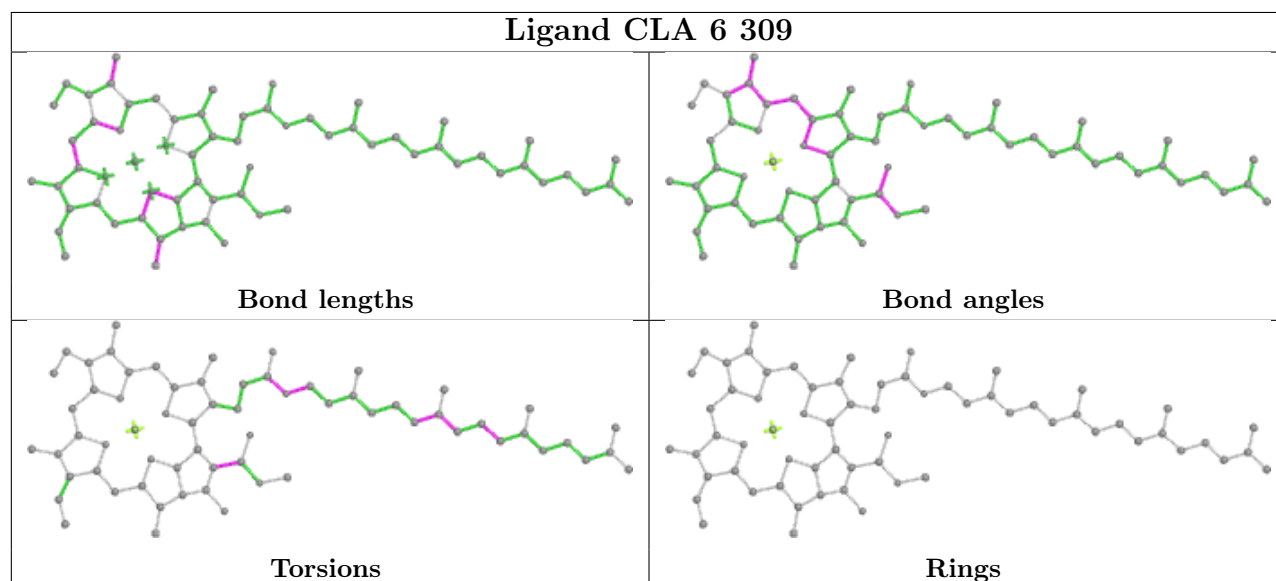
Ligand CLA 9 312



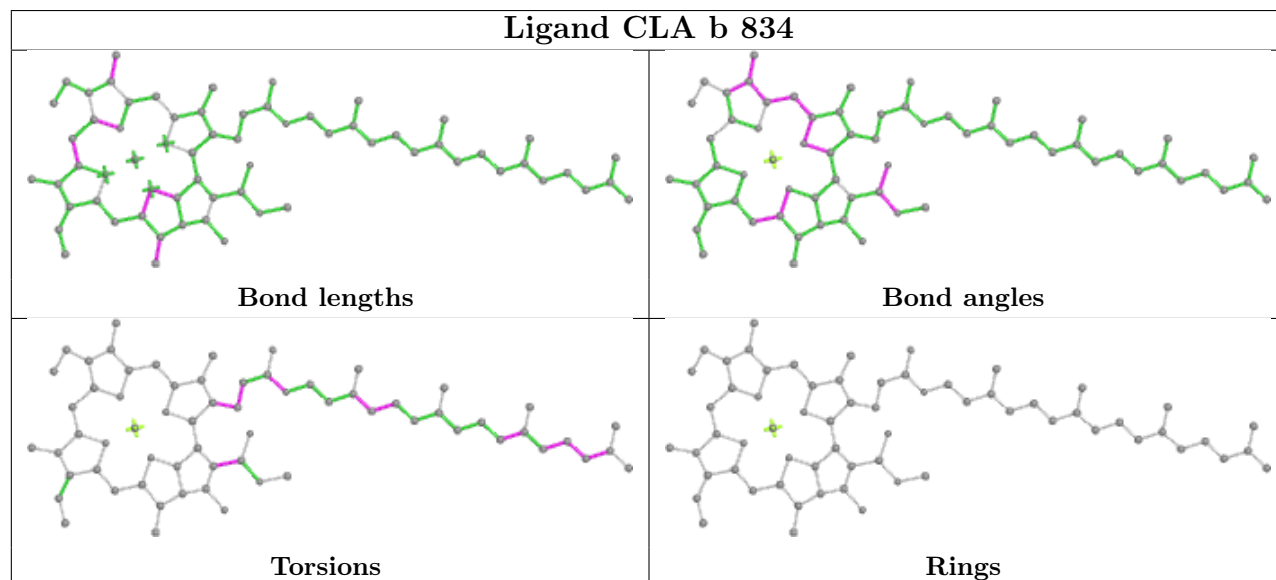
Ligand CLA b 803

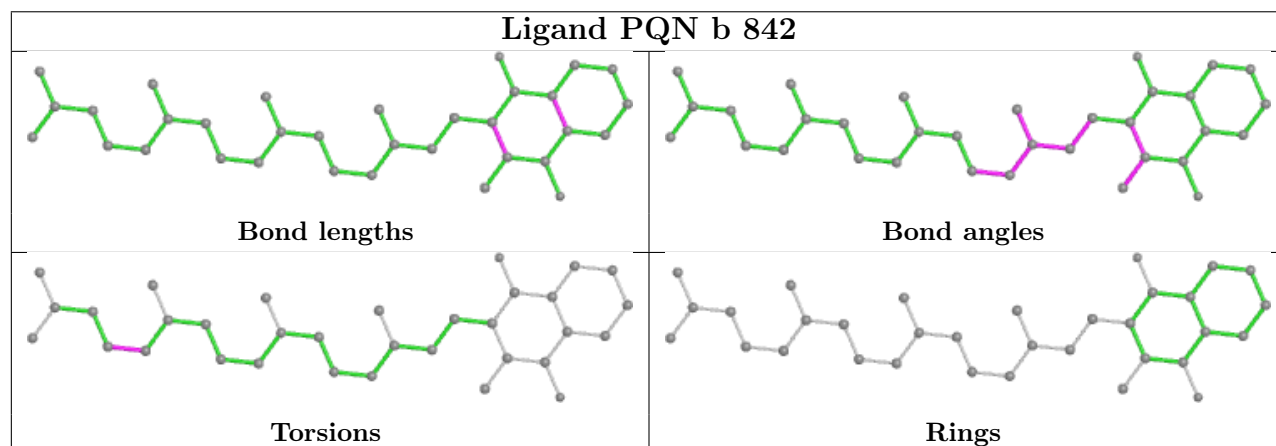
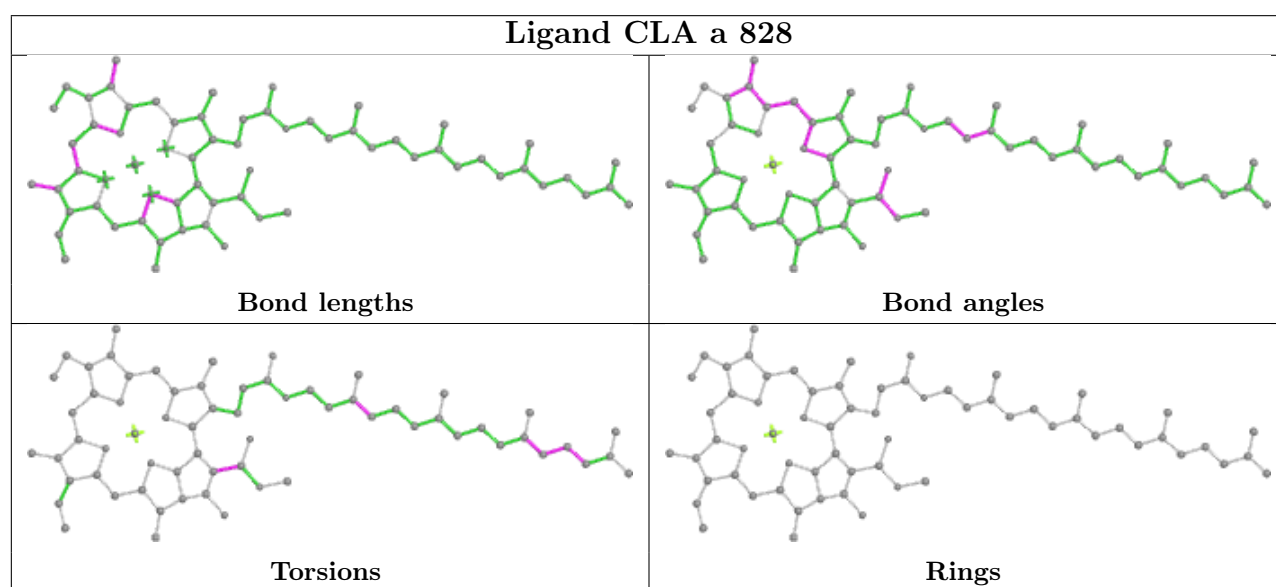
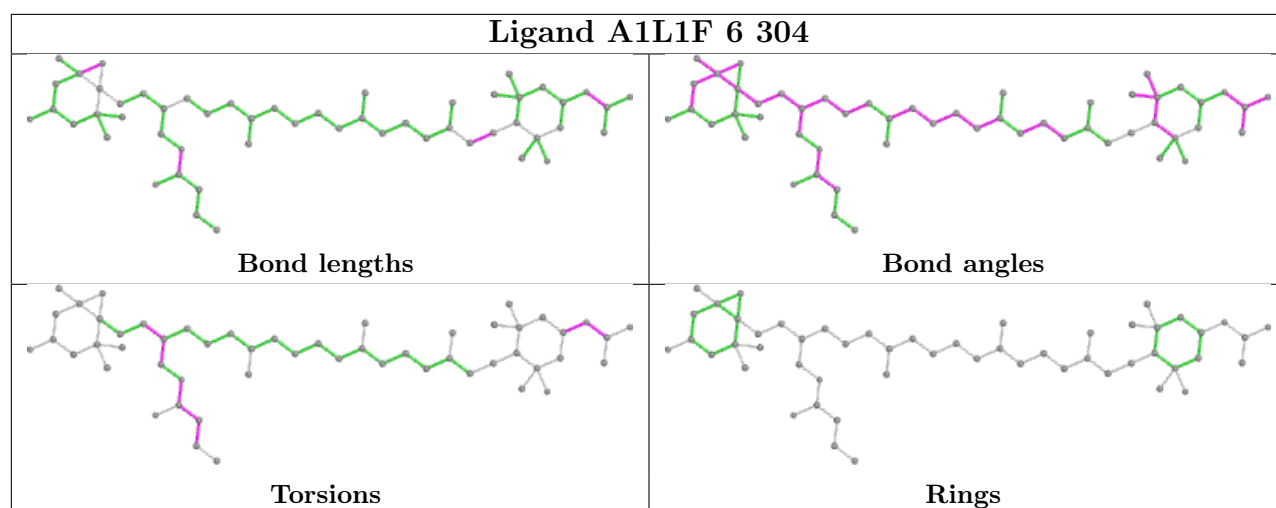


Ligand CLA 6 309

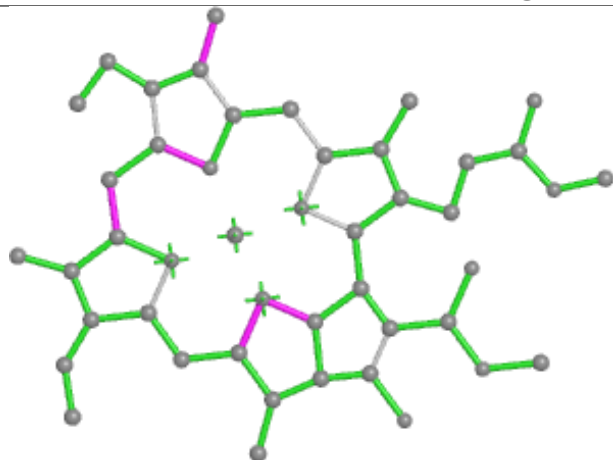


Ligand CLA b 834

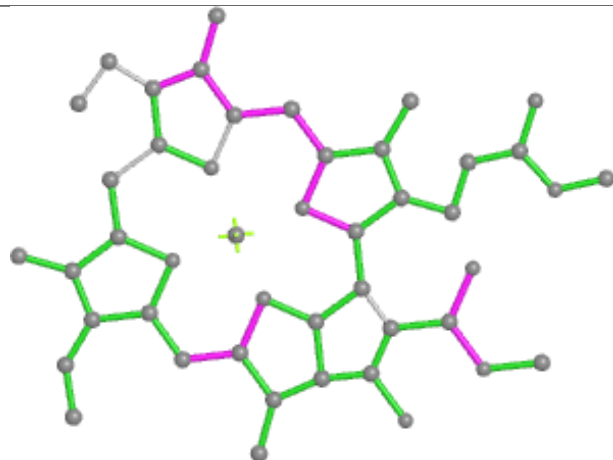




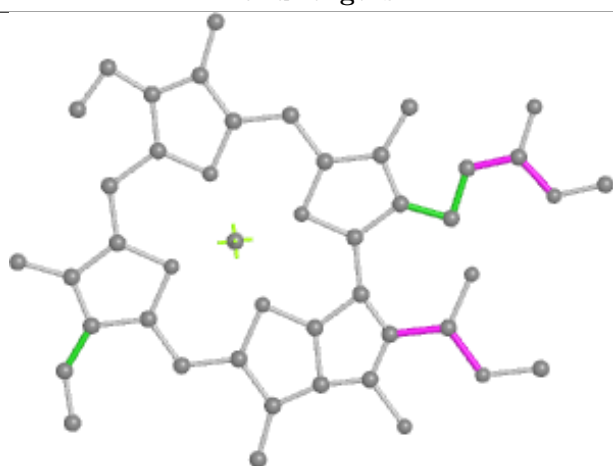
Ligand CLA 1 309



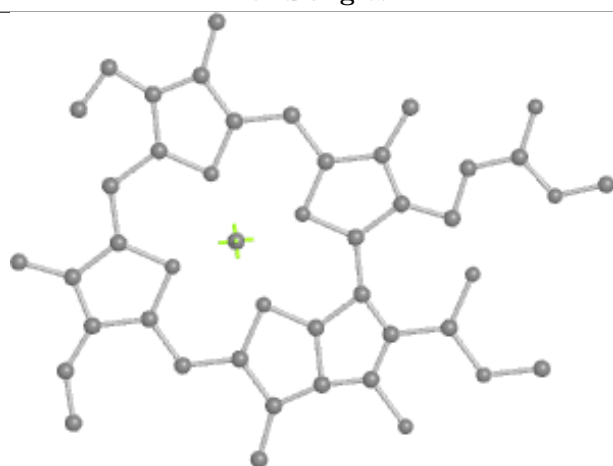
Bond lengths



Bond angles

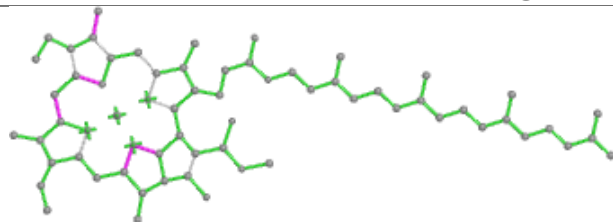


Torsions

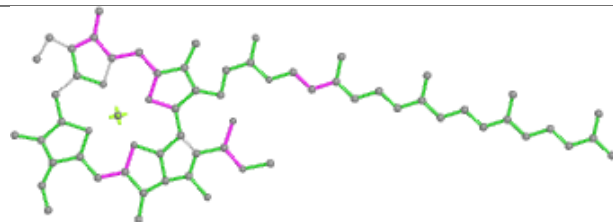


Rings

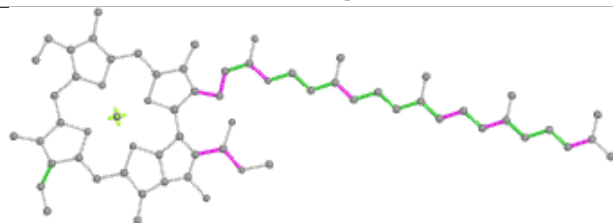
Ligand CLA b 810



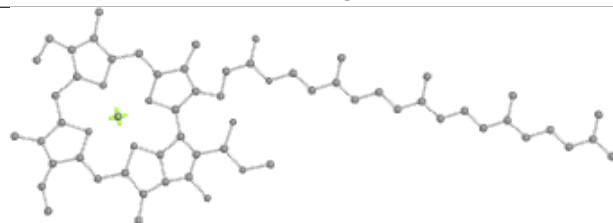
Bond lengths



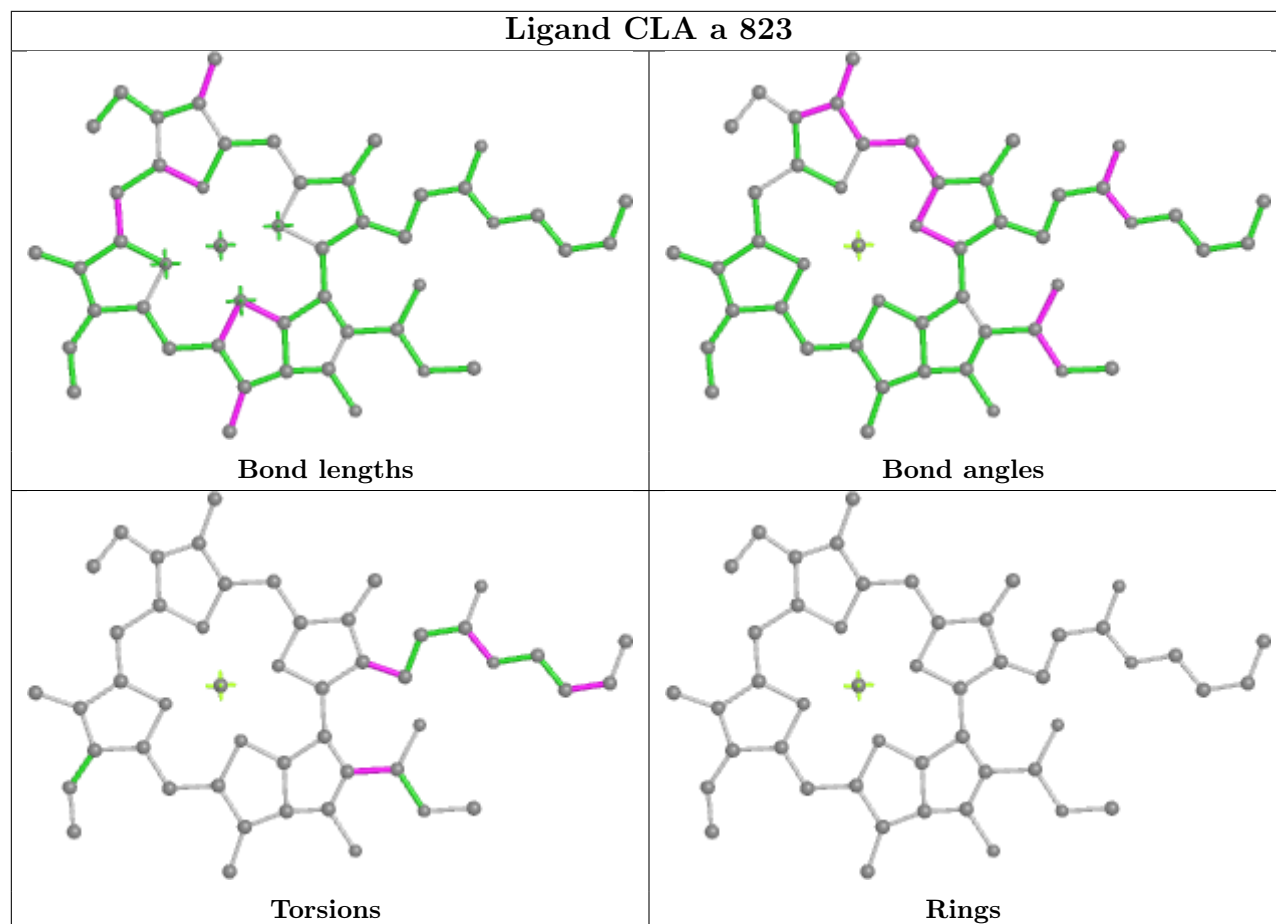
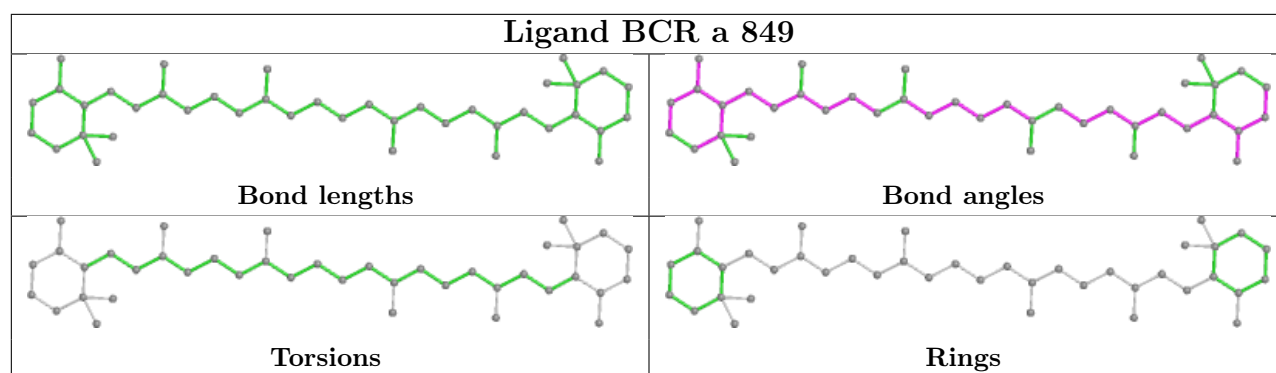
Bond angles



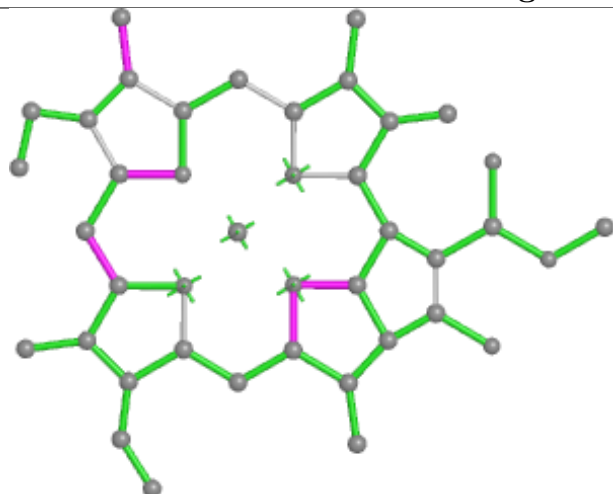
Torsions



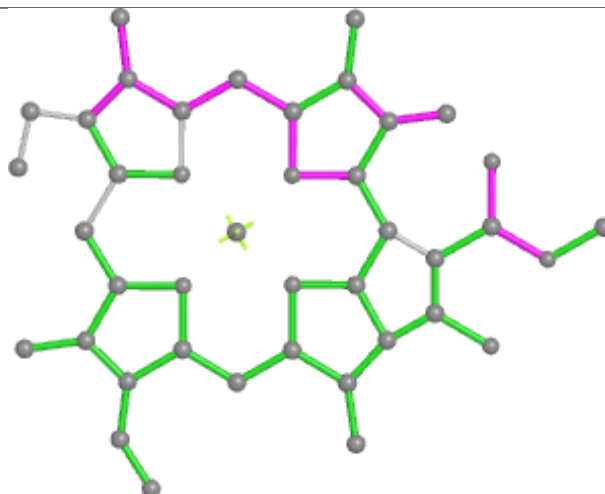
Rings



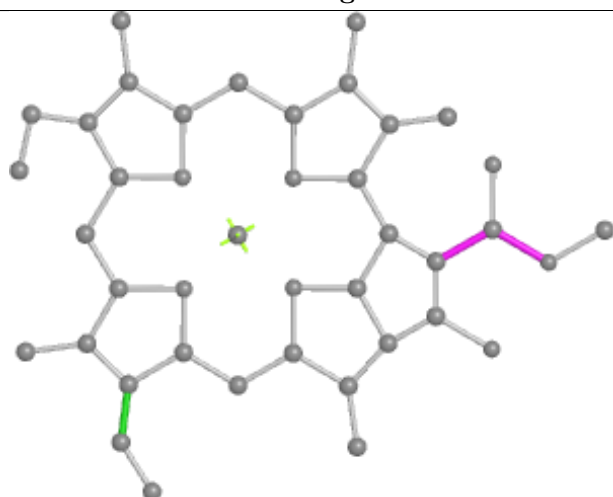
Ligand CLA 8 314



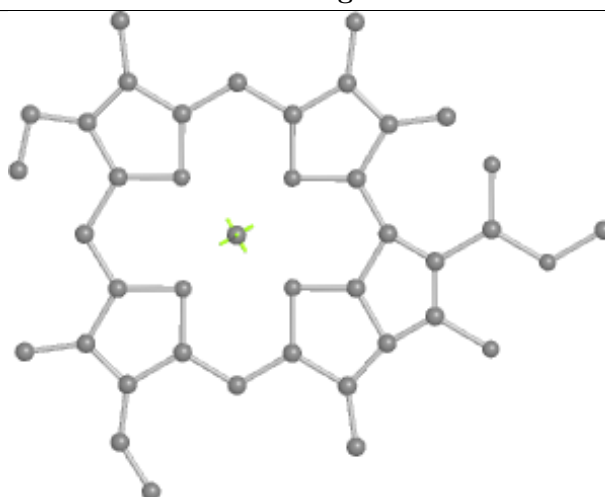
Bond lengths



Bond angles

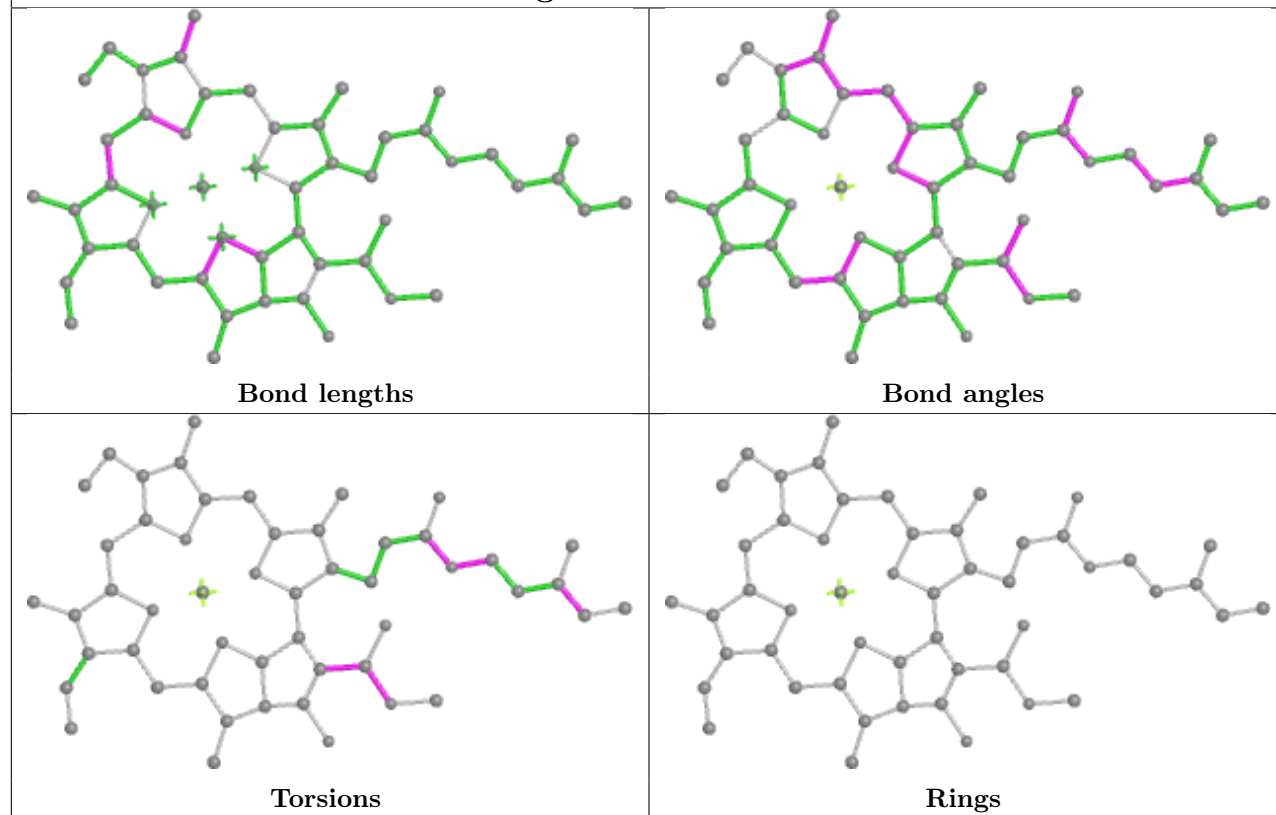


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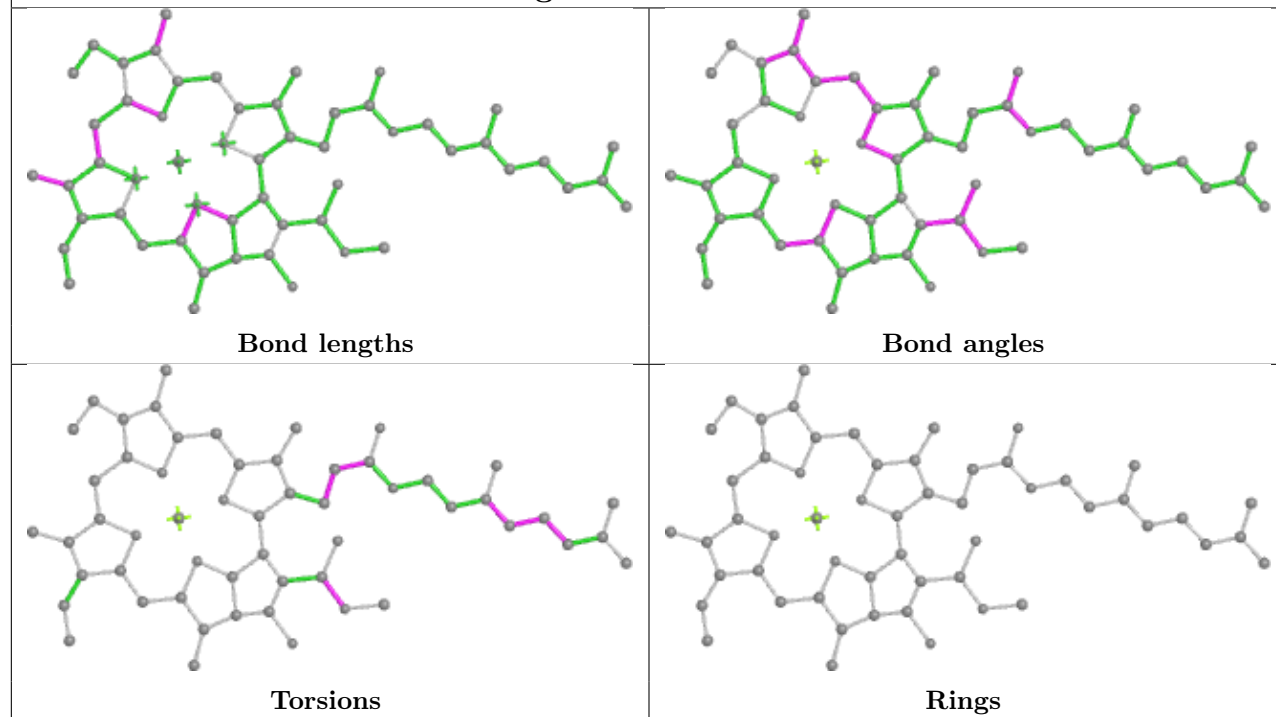


Rings

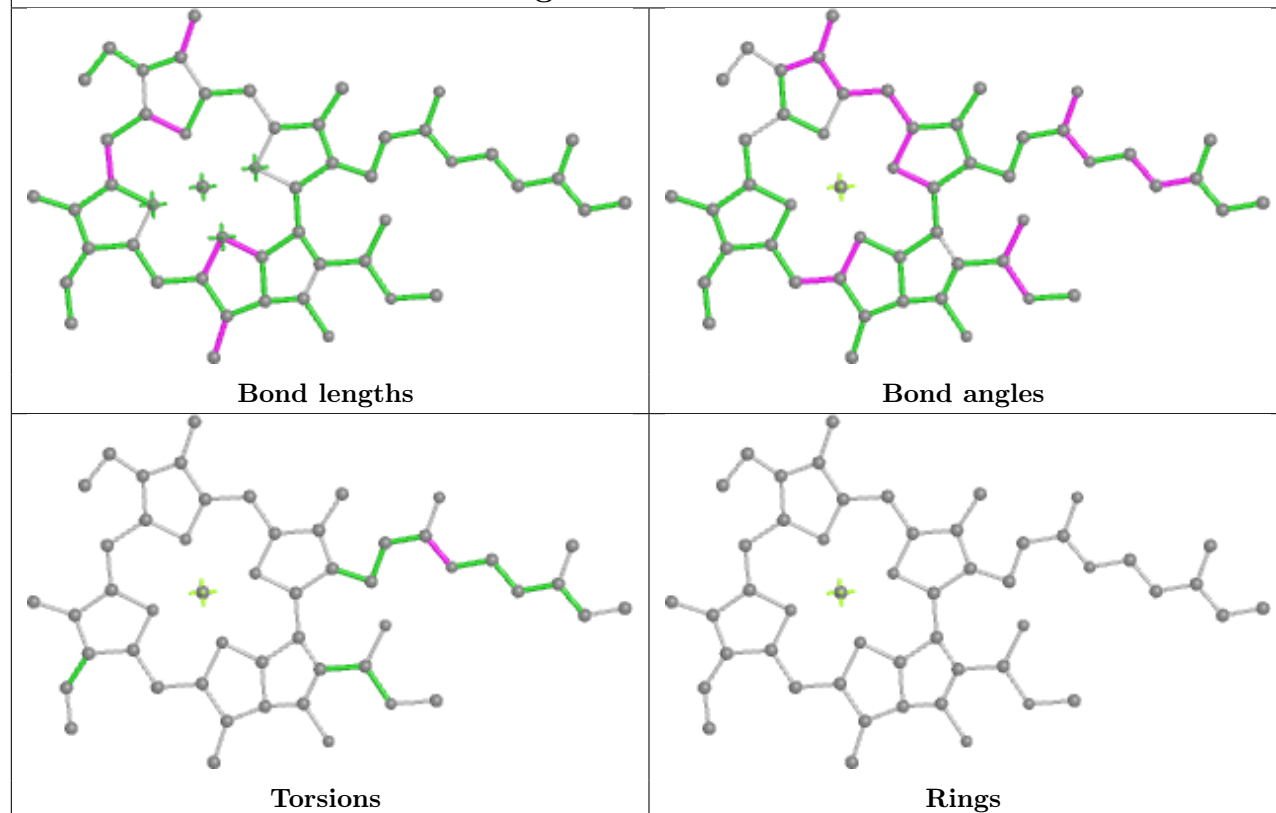
Ligand CLA 5 312



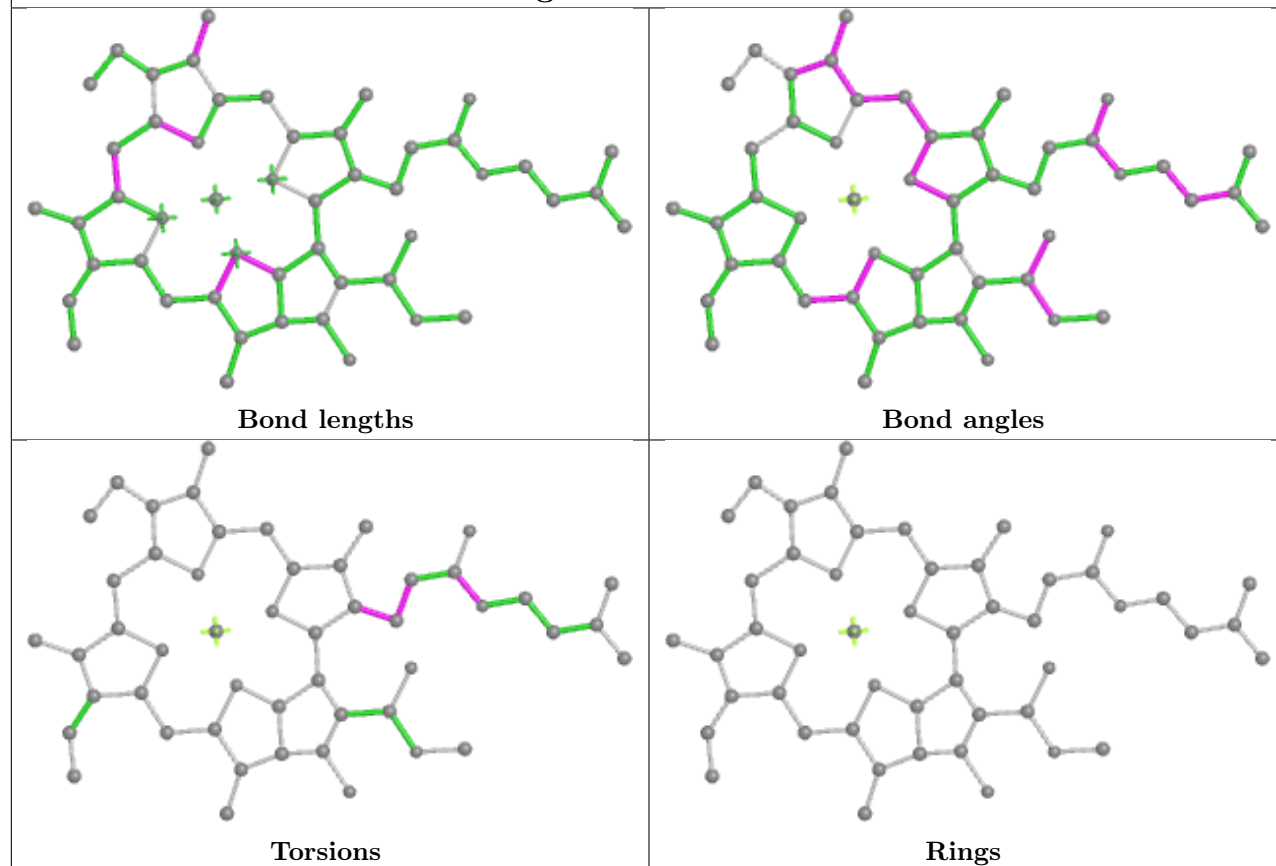
Ligand CLA h 203

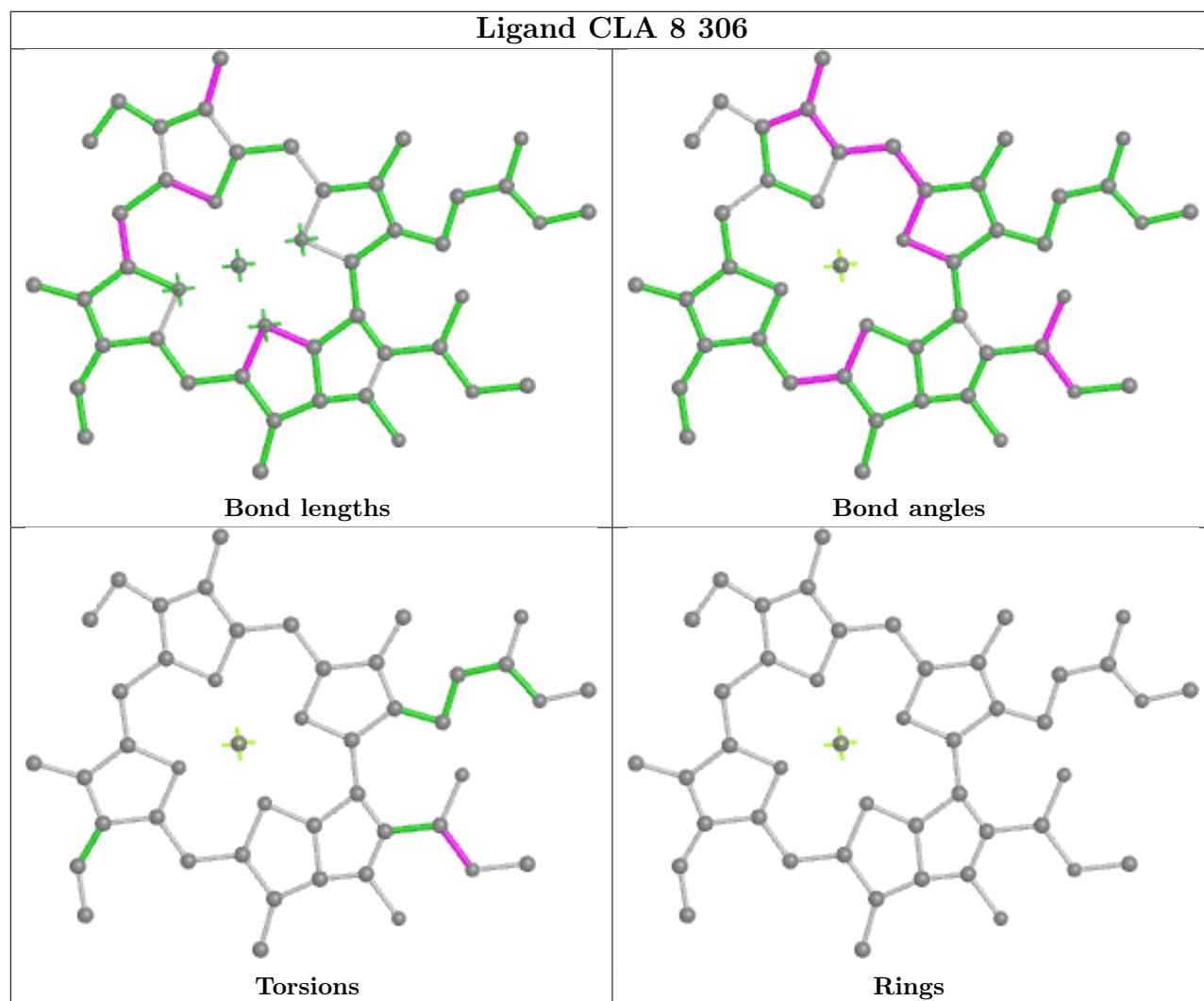
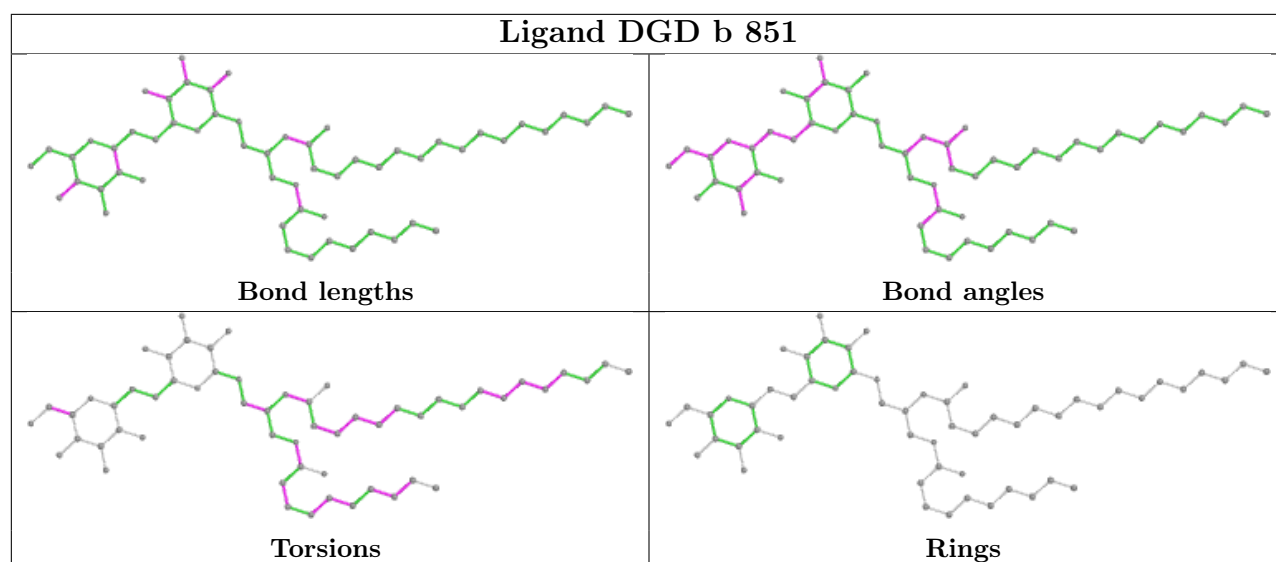


Ligand CLA b 821

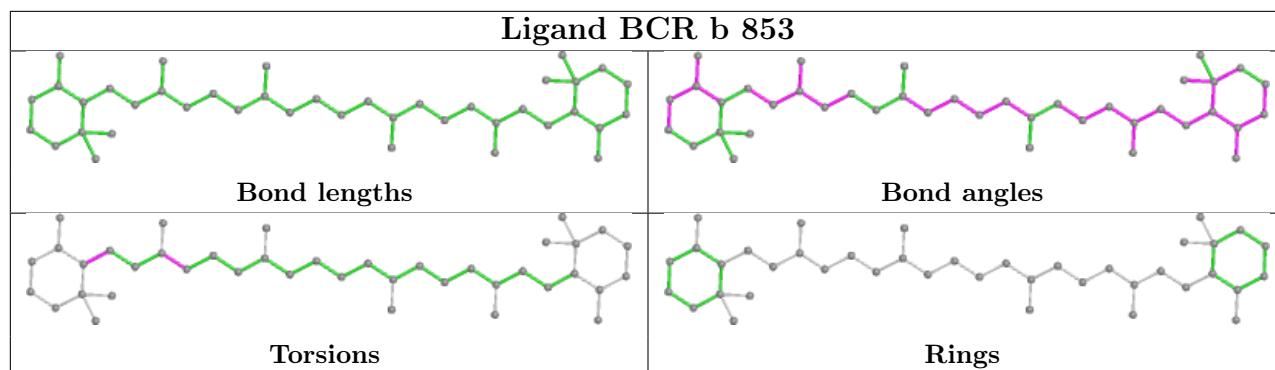


Ligand CLA 3 311

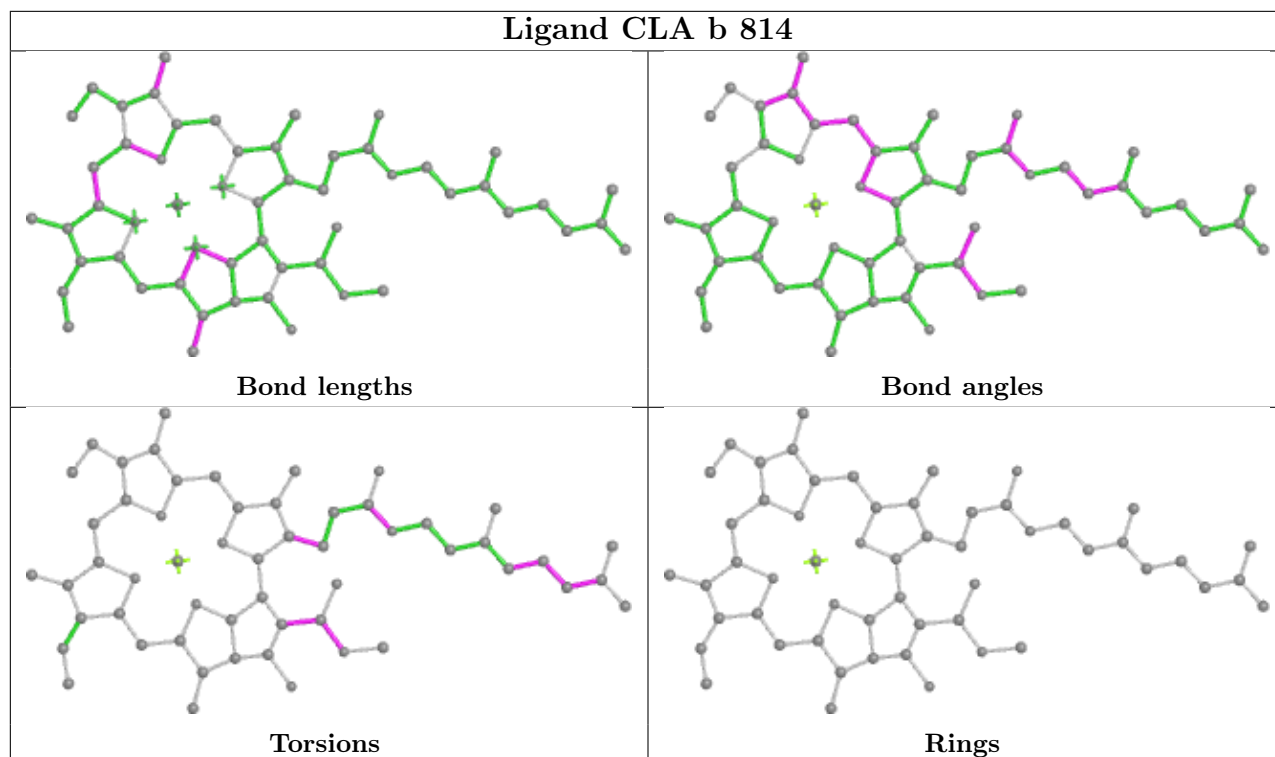




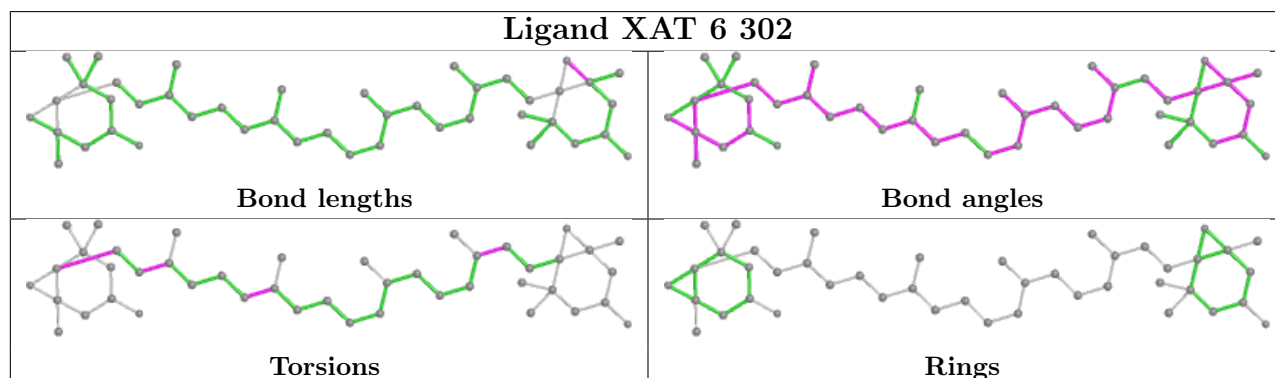
Ligand BCR b 853



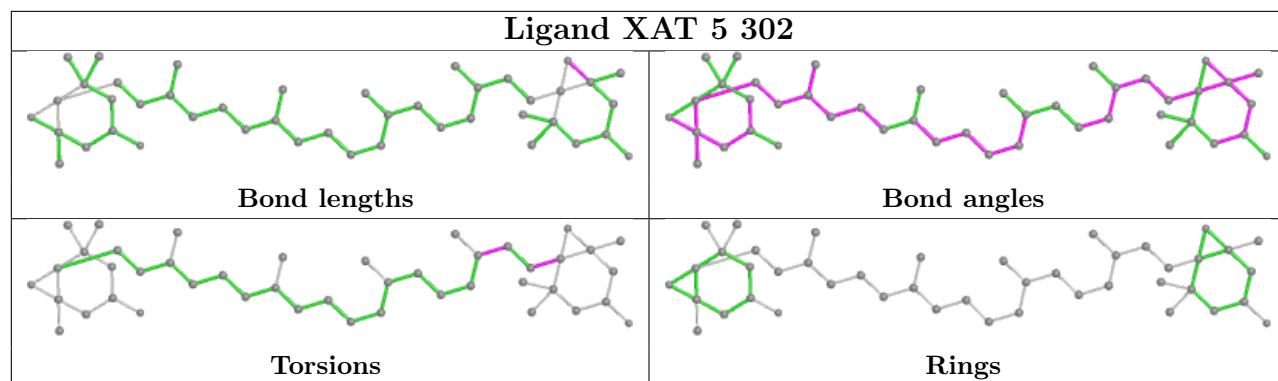
Ligand CLA b 814



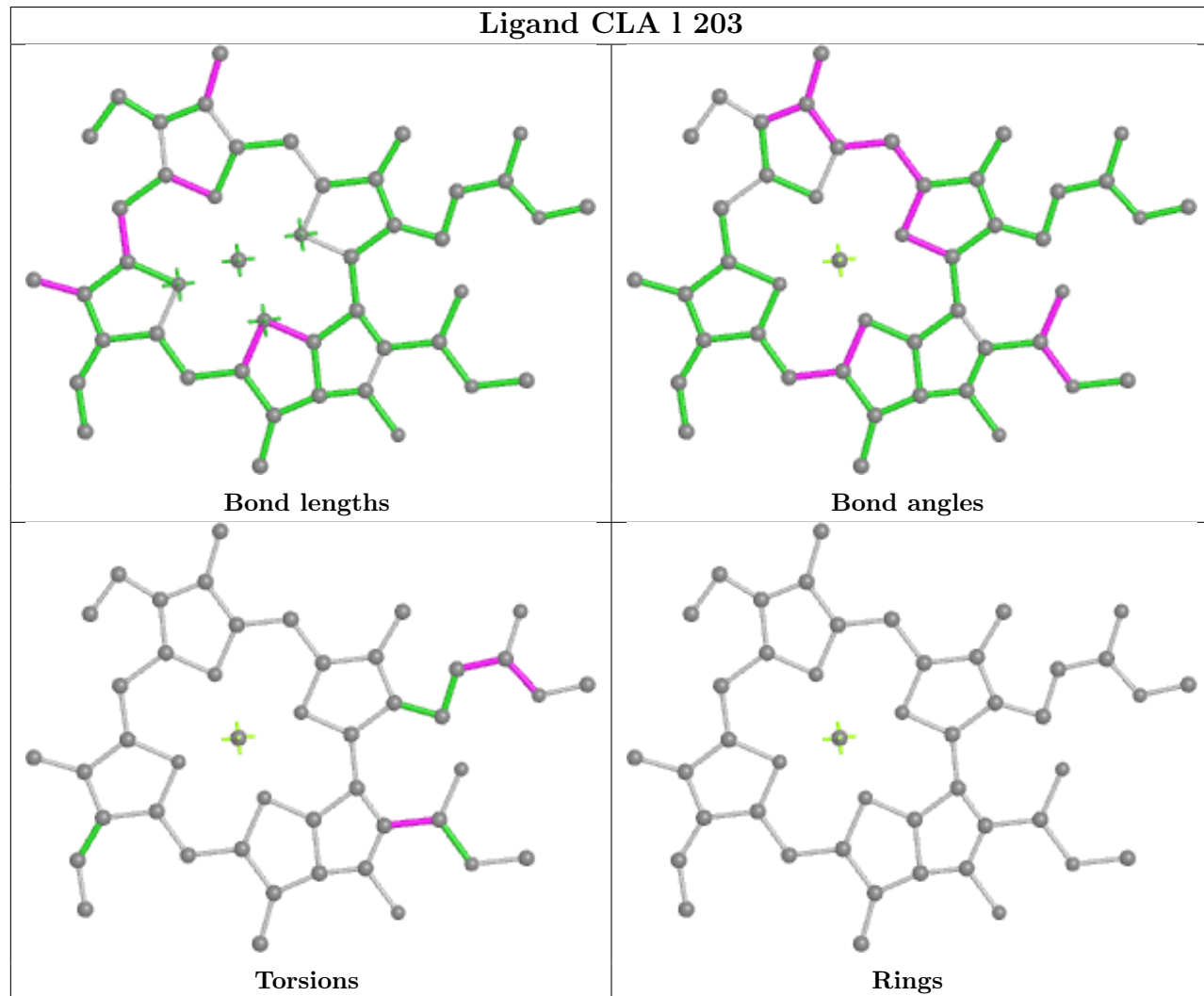
Ligand XAT 6 302



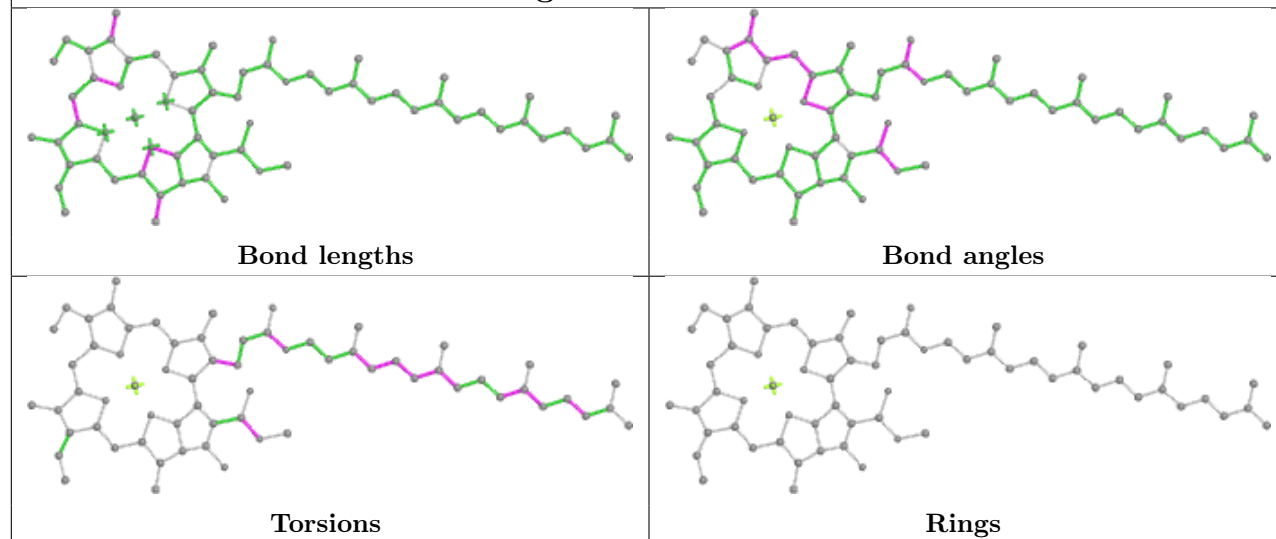
Ligand XAT 5 302



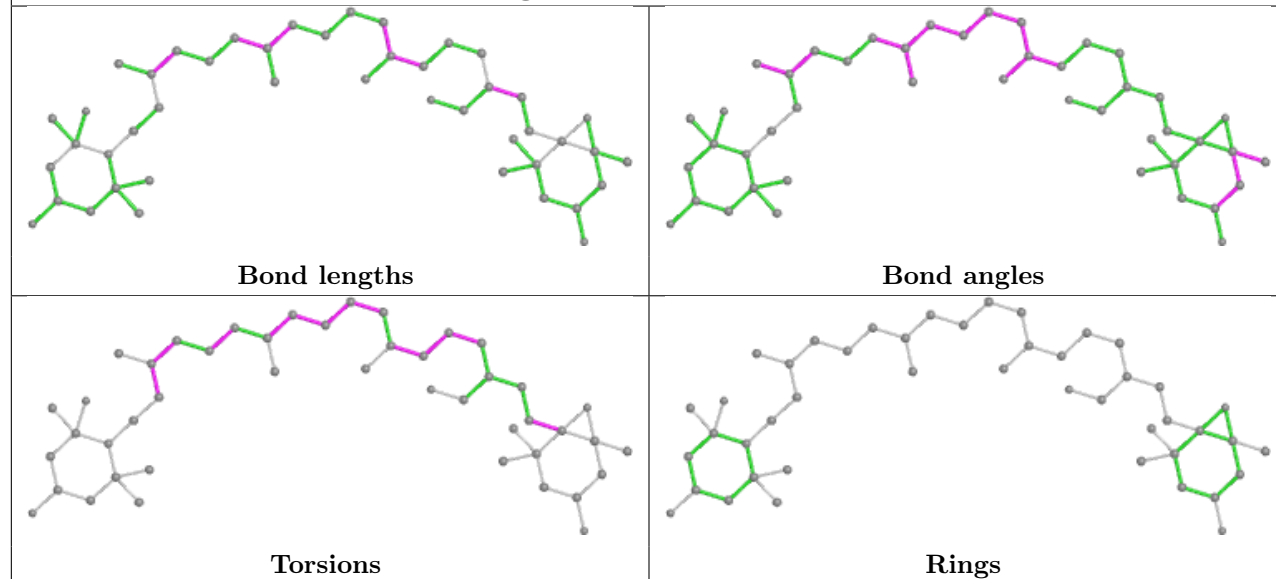
Ligand CLA 1 203



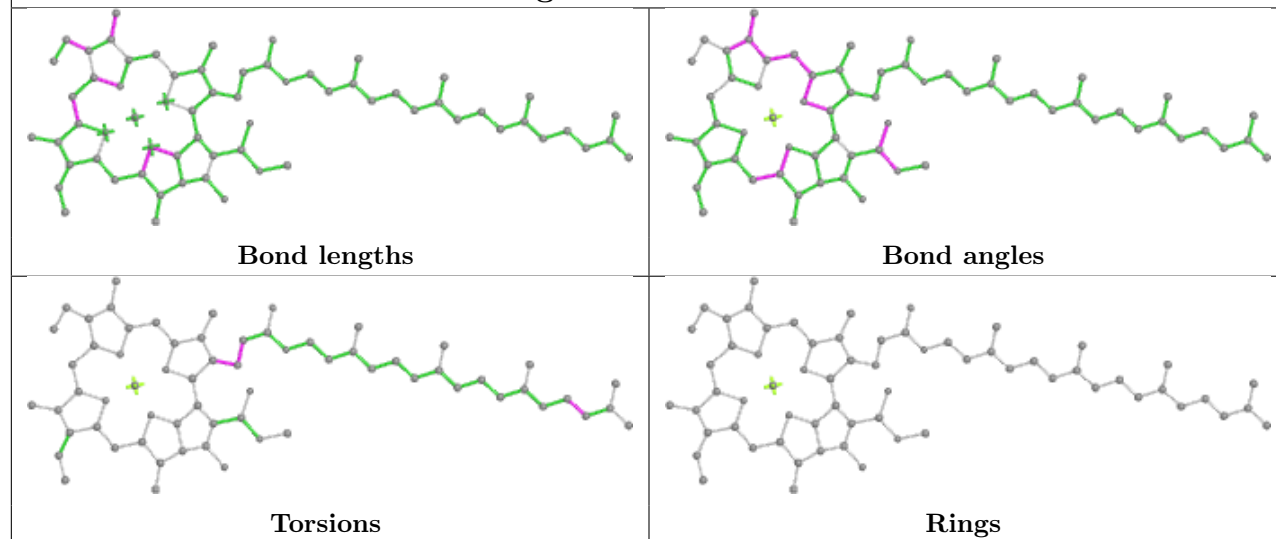
Ligand CLA a 807



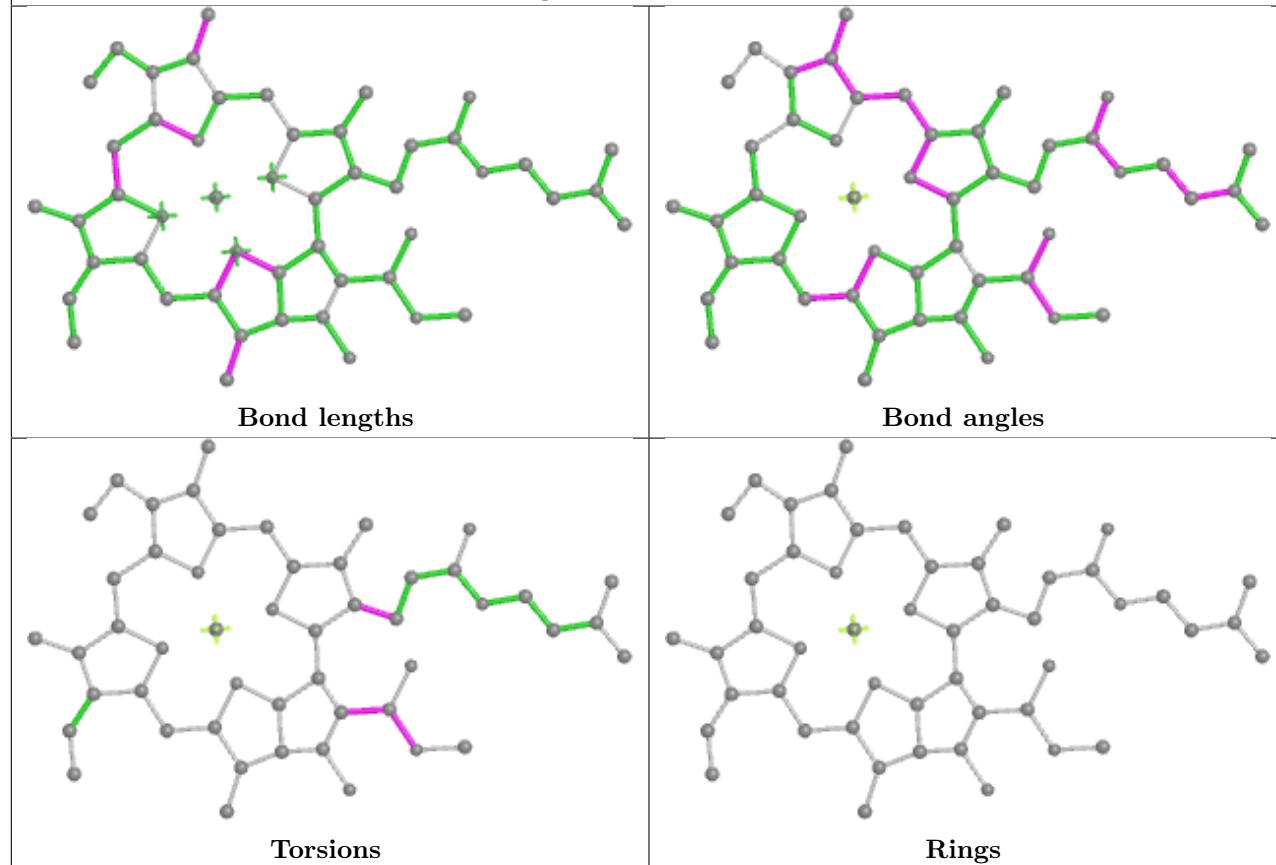
Ligand A1L1G 7 302



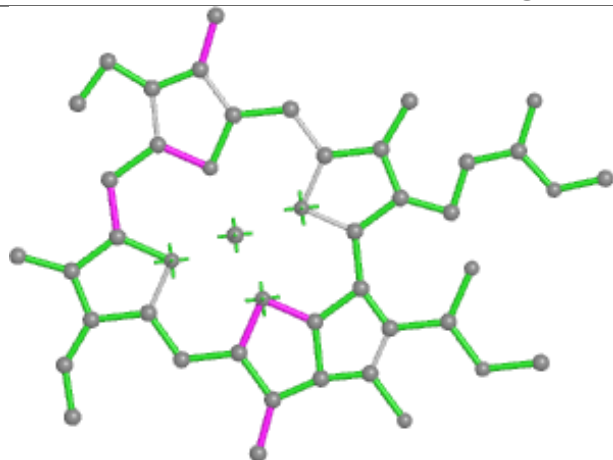
Ligand CLA a 803



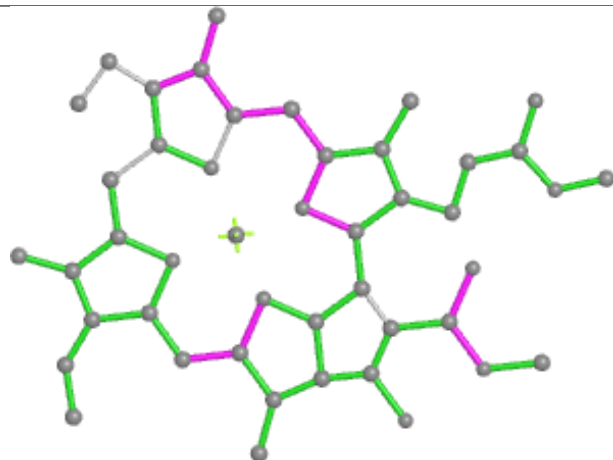
Ligand CLA a 832



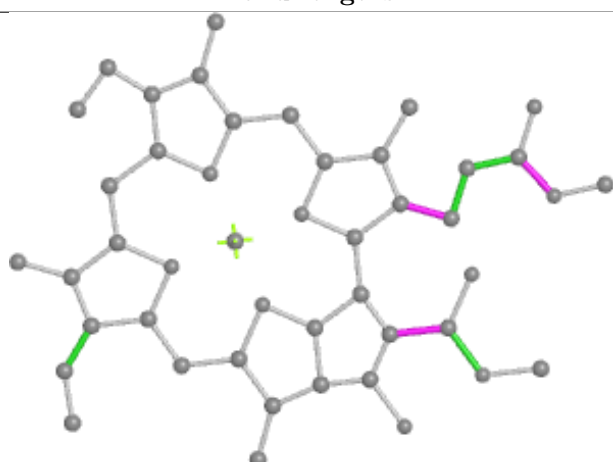
Ligand CLA a 824



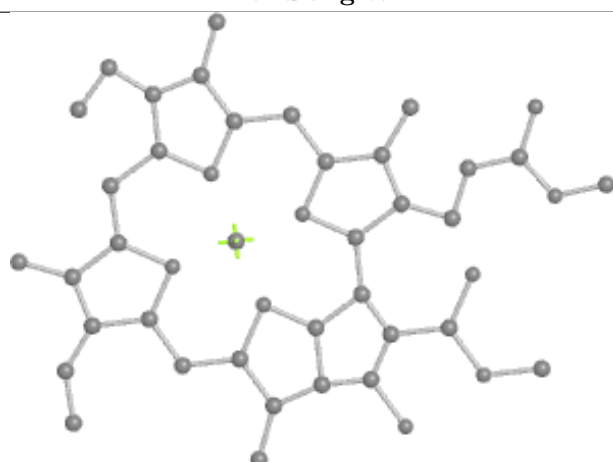
Bond lengths



Bond angles

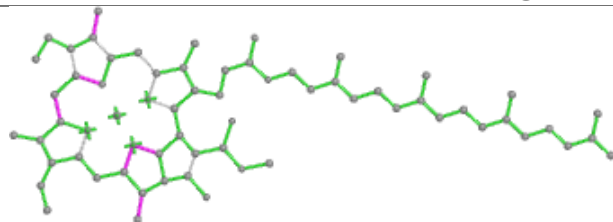


Torsions

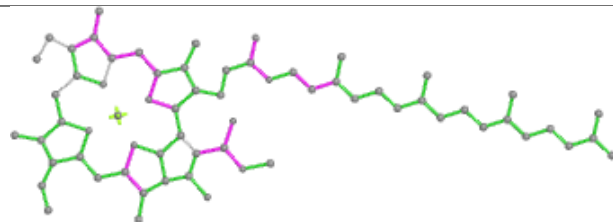


Rings

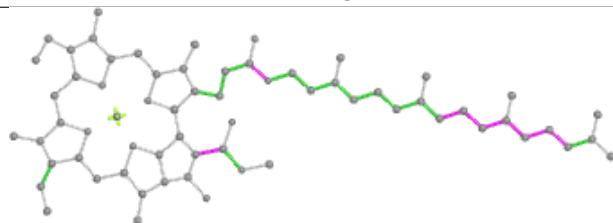
Ligand CLA b 829



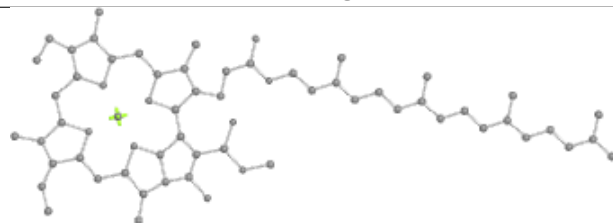
Bond lengths



Bond angles

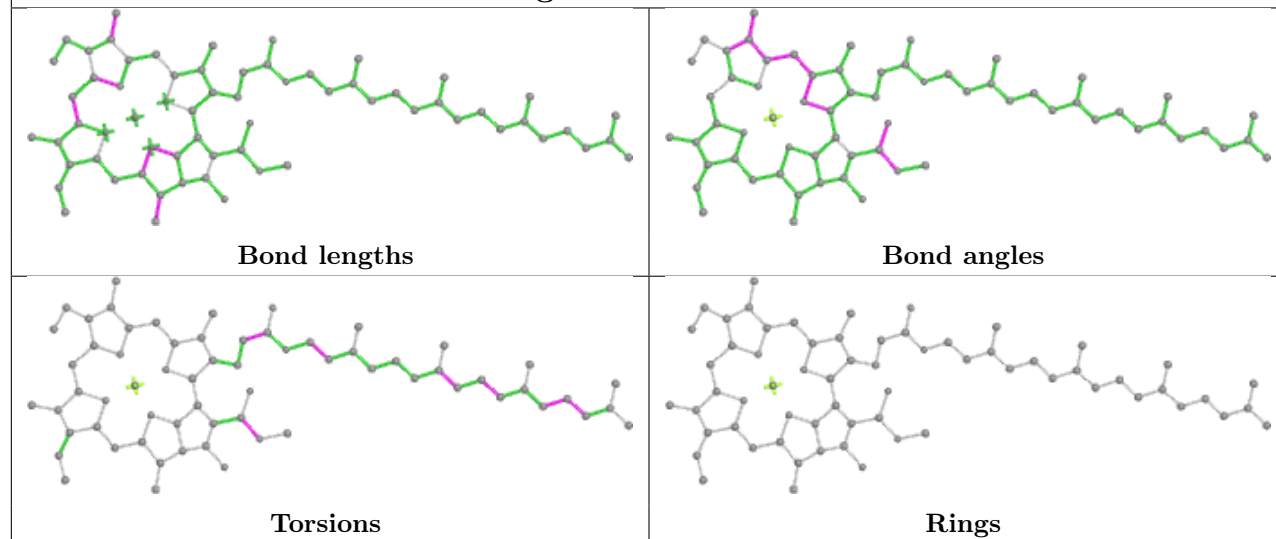


Torsions

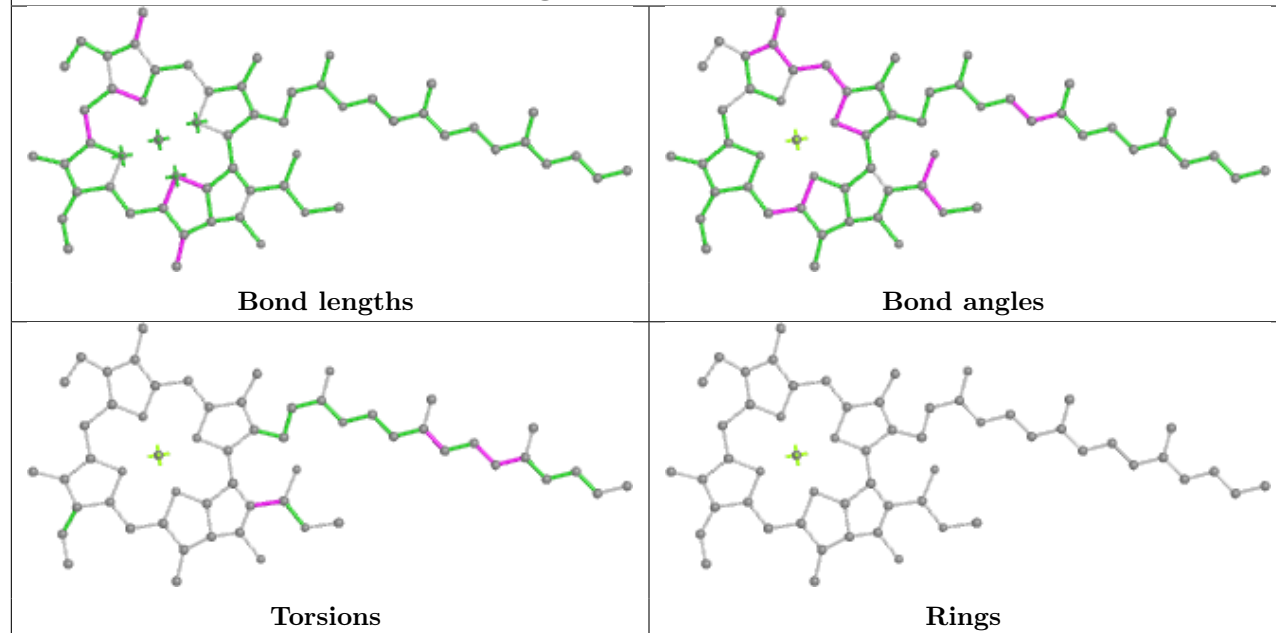


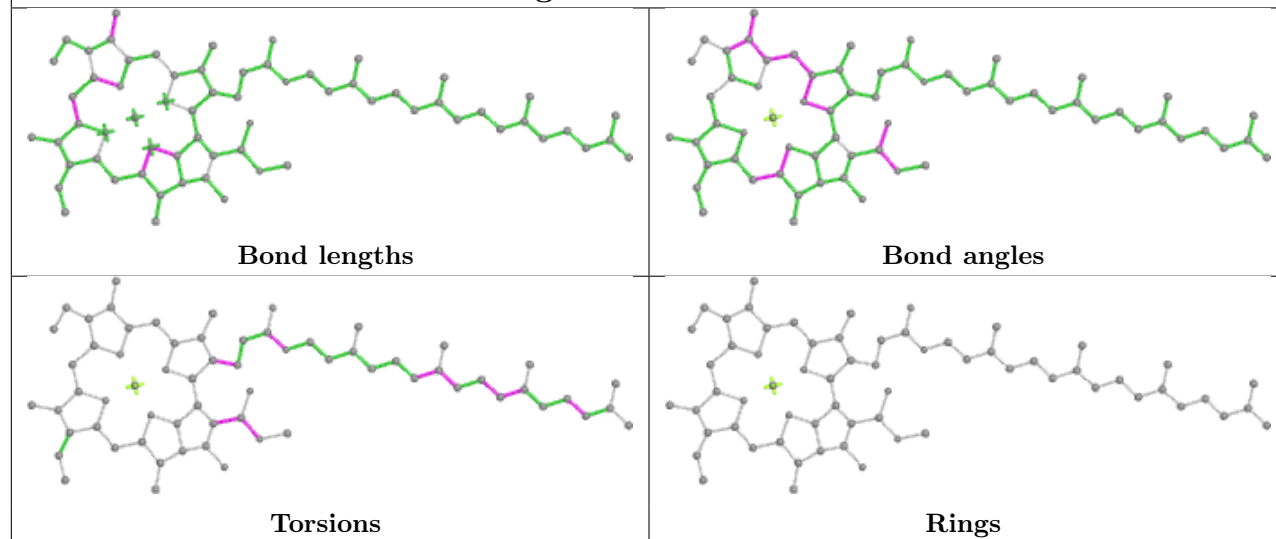
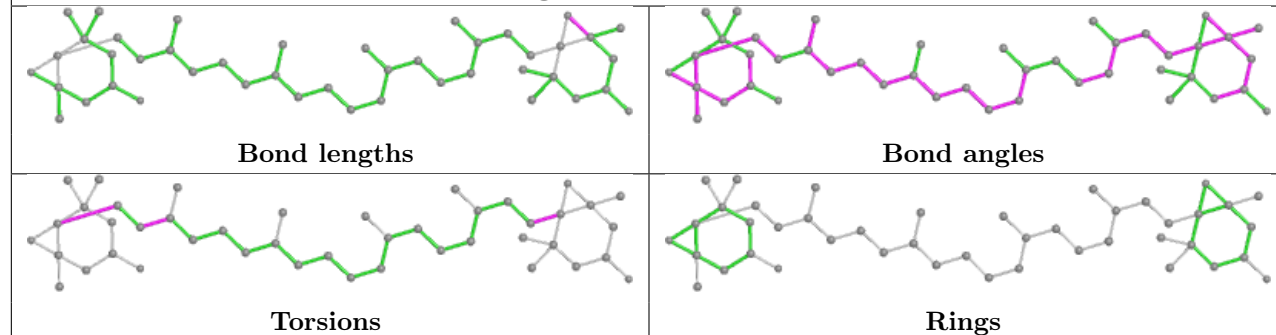
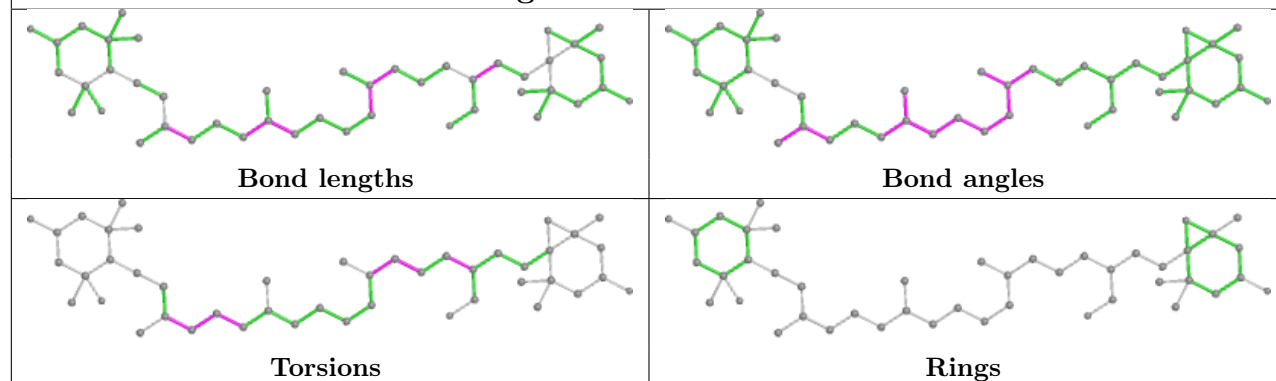
Rings

Ligand CLA a 826

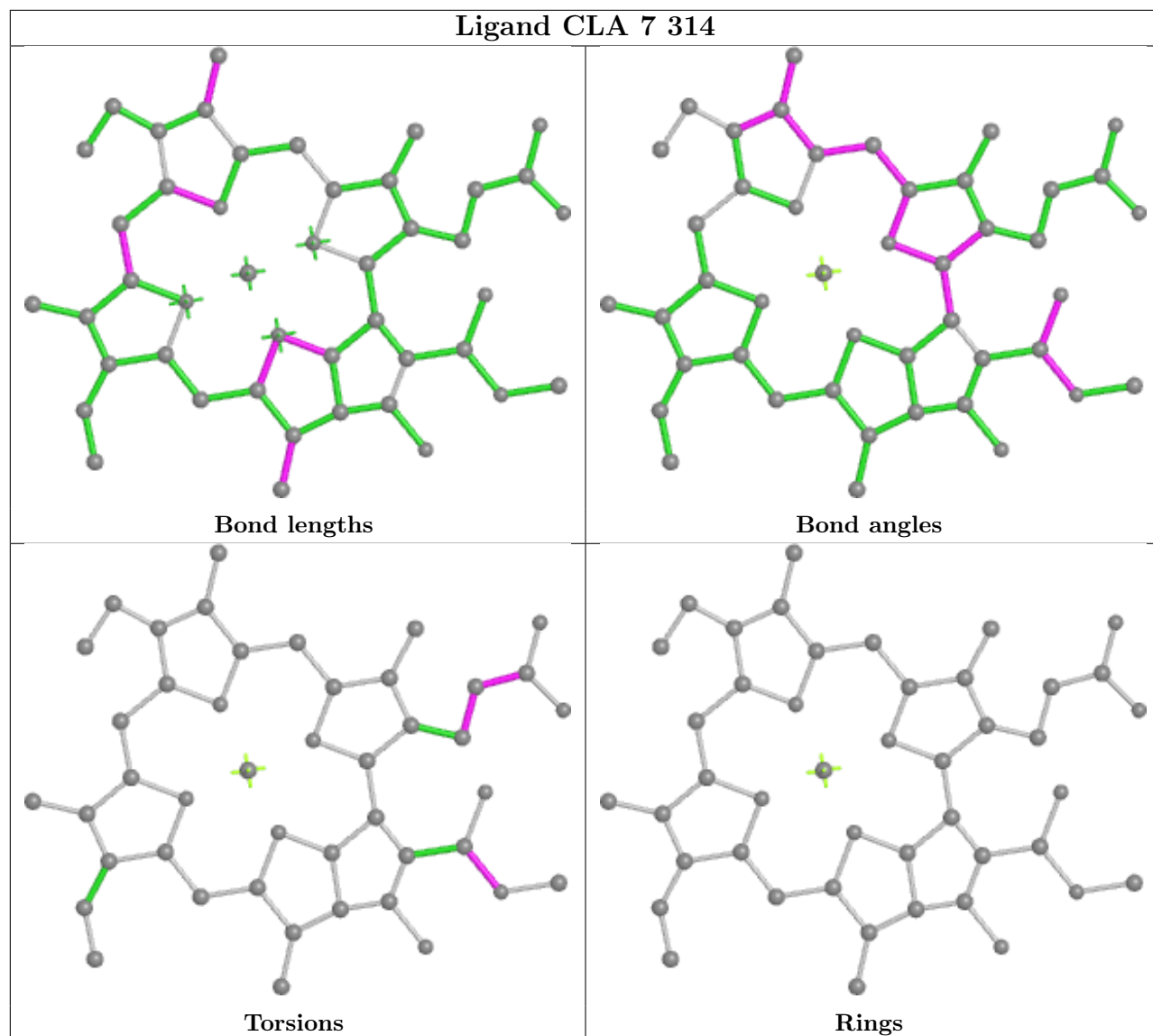


Ligand CLA a 802

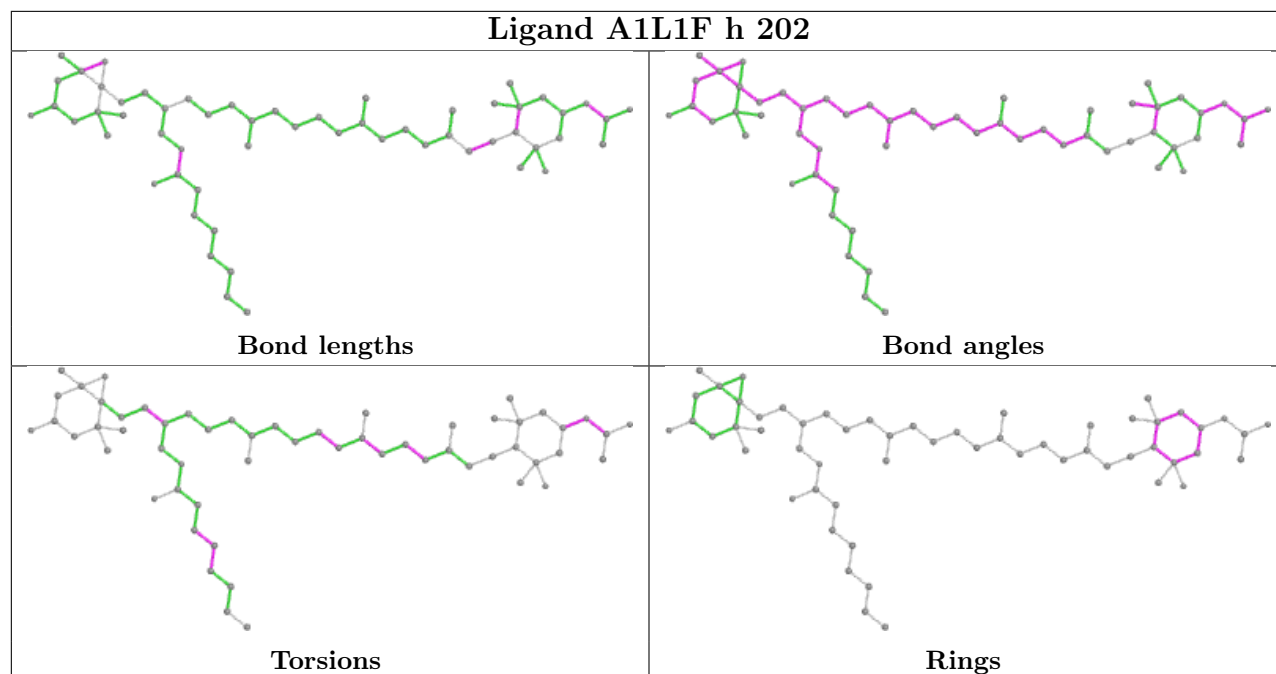


Ligand CLA b 805**Ligand XAT 4 304****Ligand A1L1G 5 304**

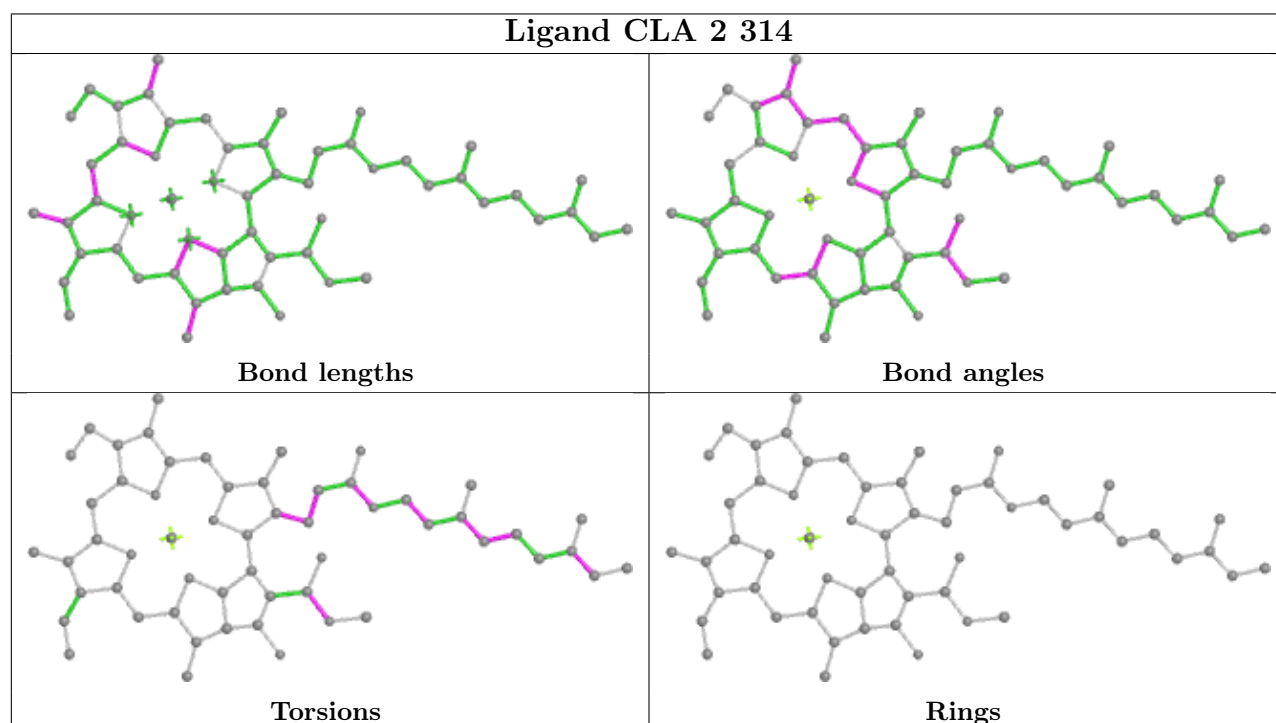
Ligand CLA 7 314



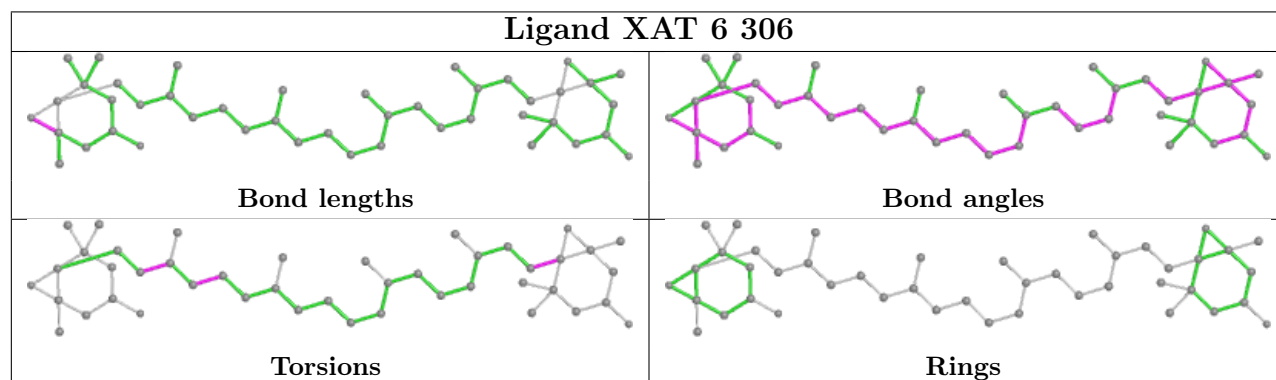
Ligand A1L1F h 202

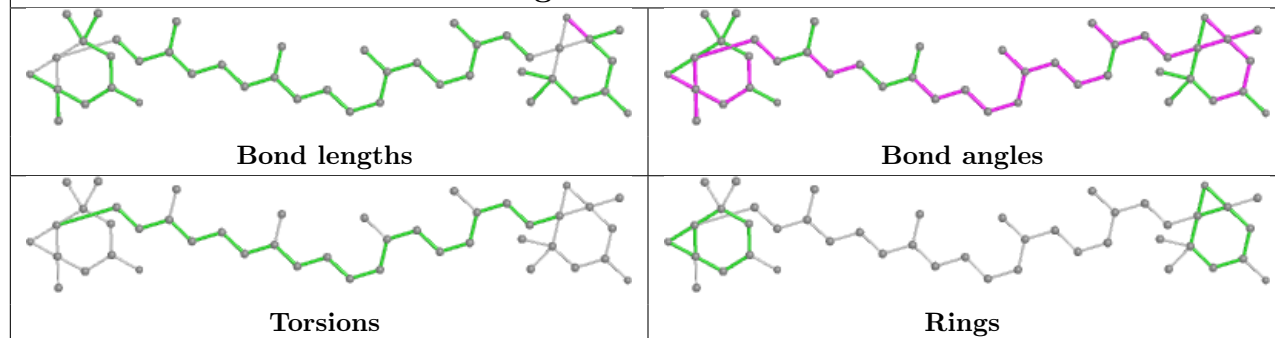
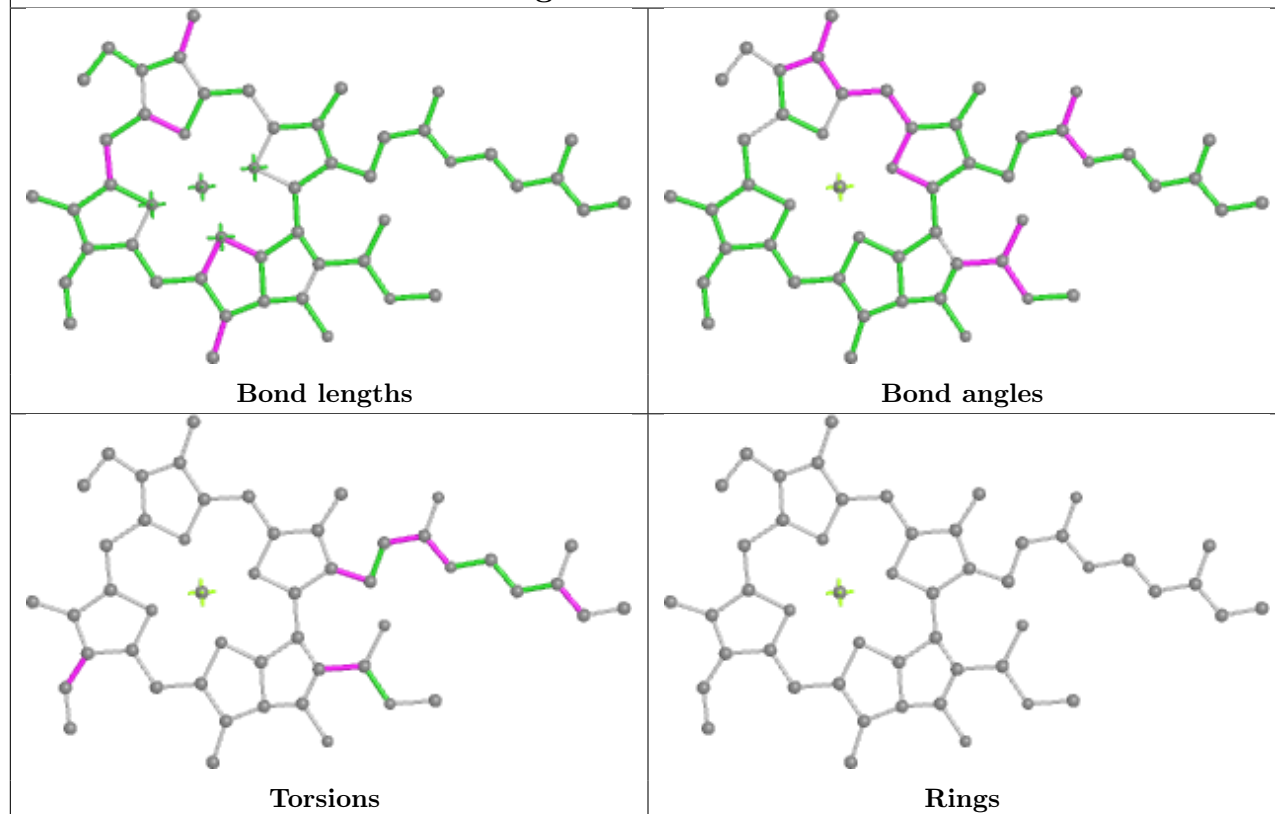
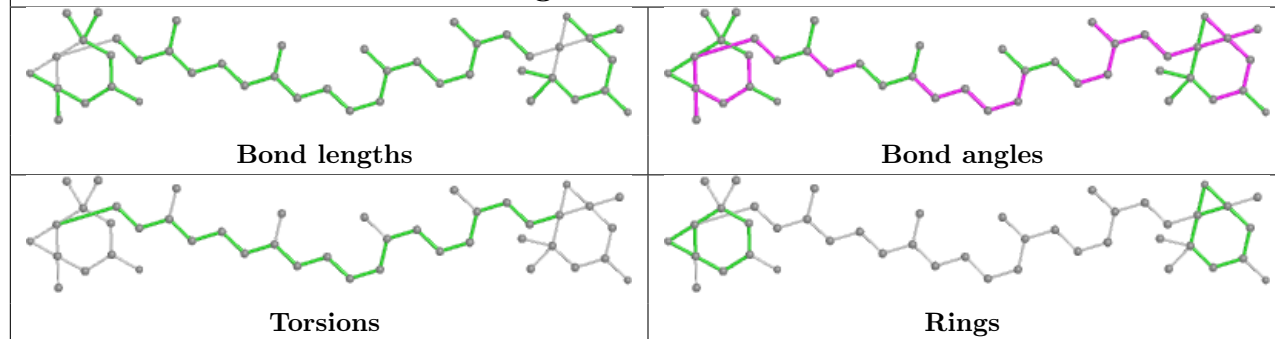


Ligand CLA 2 314

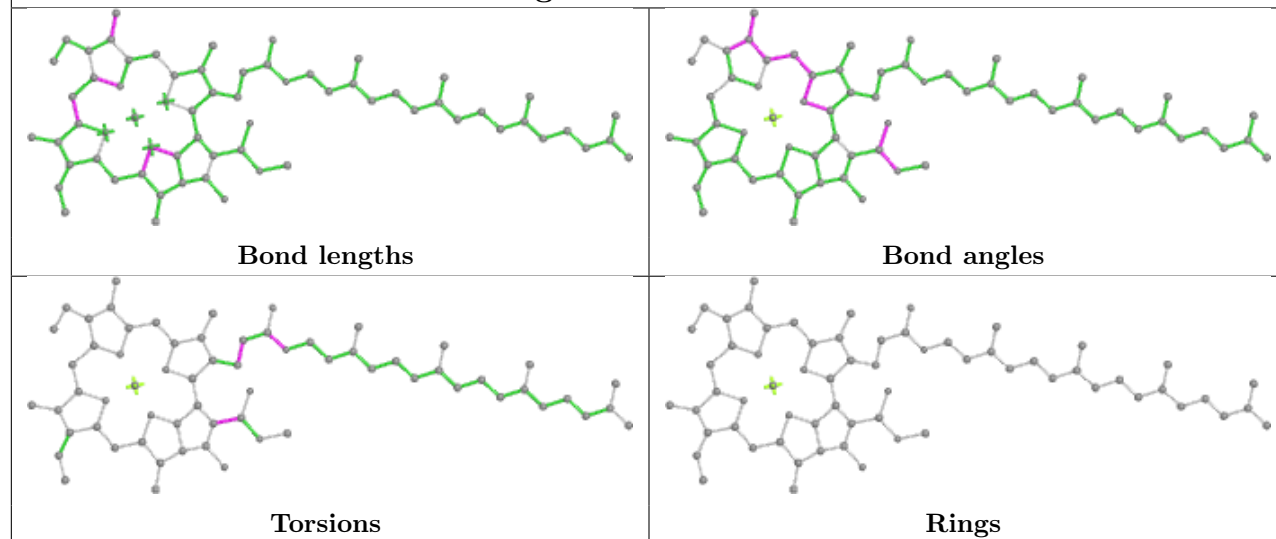


Ligand XAT 6 306

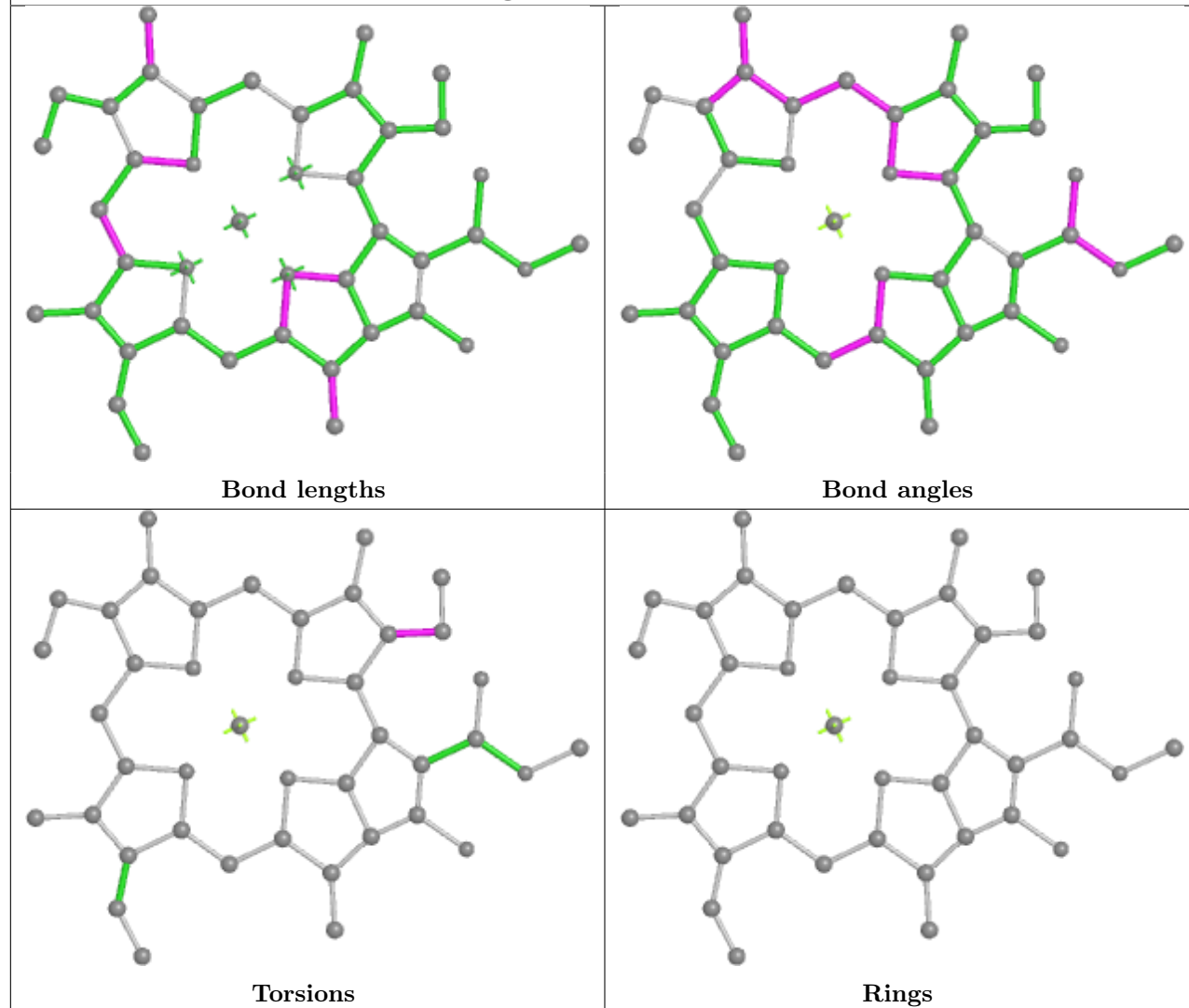


Ligand XAT 3 305**Ligand CLA 7 316****Ligand XAT 4 303**

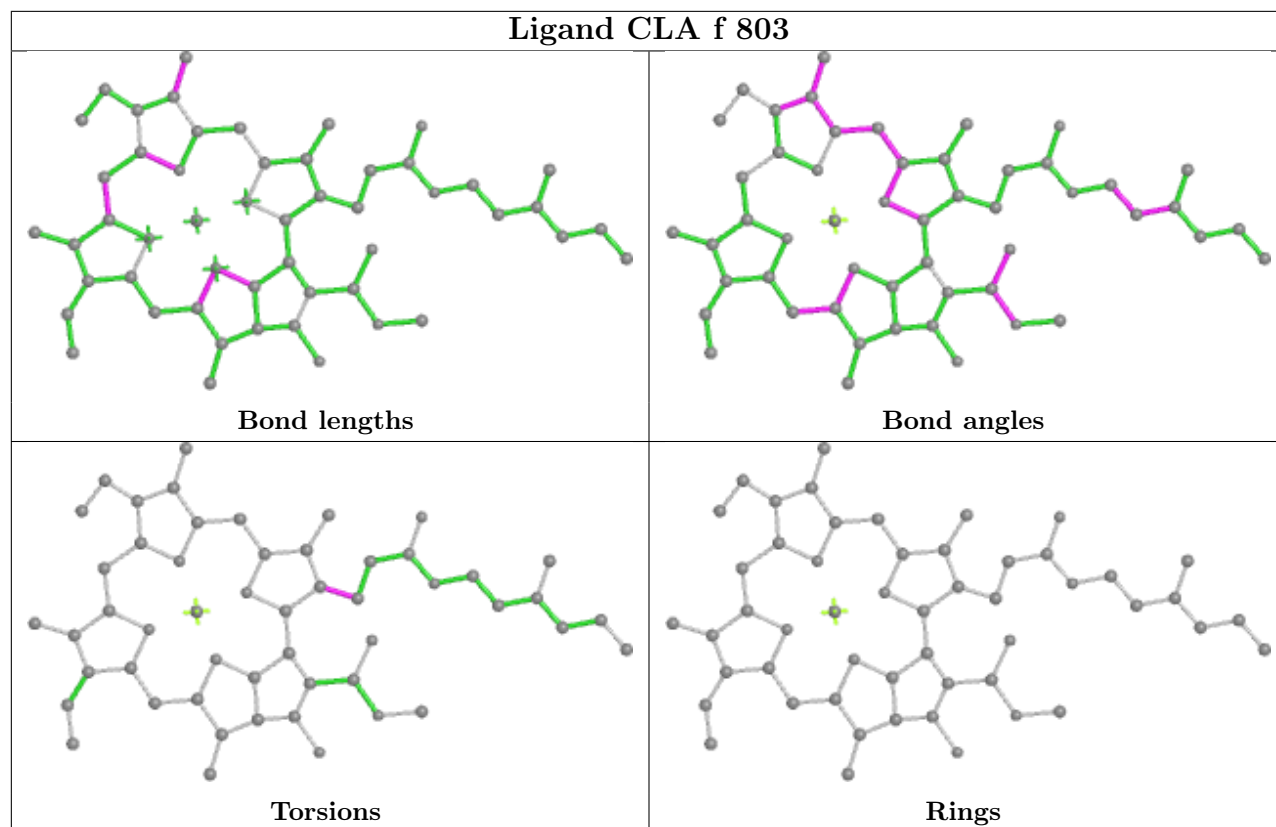
Ligand CLA b 826



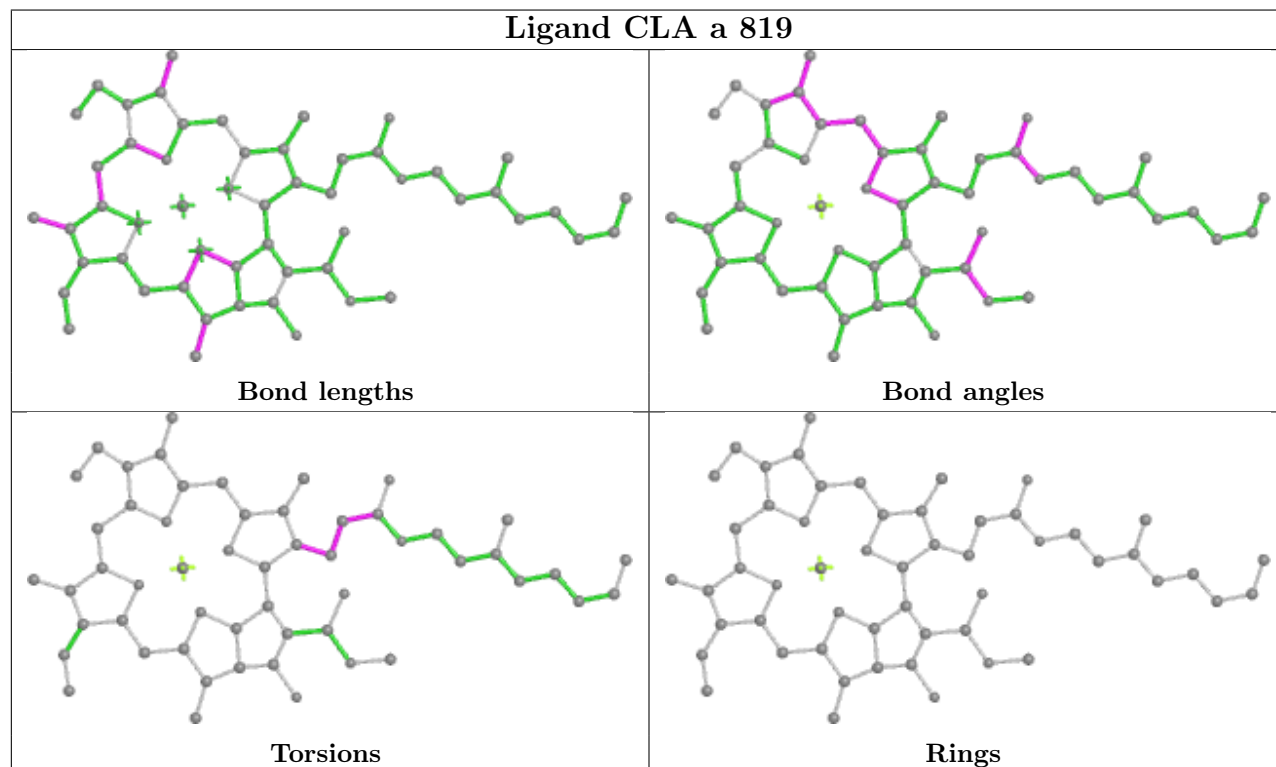
Ligand CLA 2 315



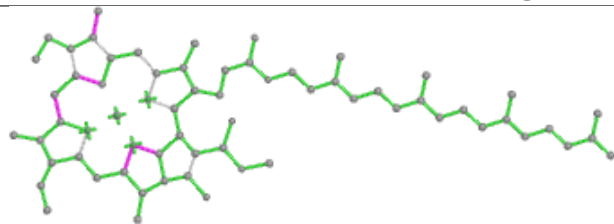
Ligand CLA f 803



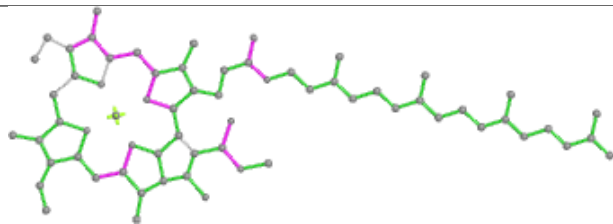
Ligand CLA a 819



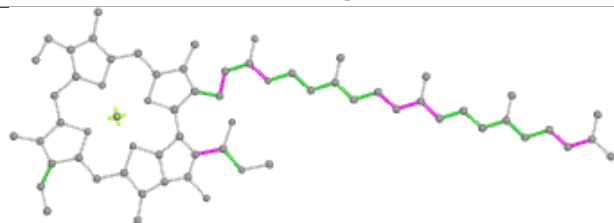
Ligand CLA 8 307



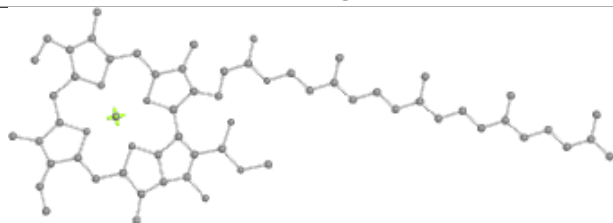
Bond lengths



Bond angles

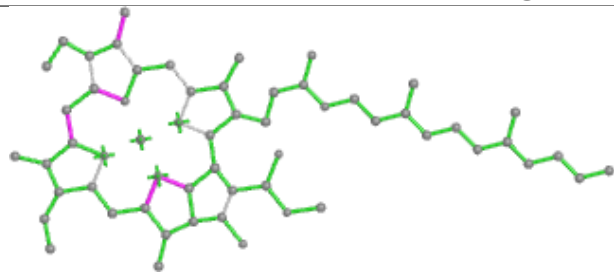


Torsions

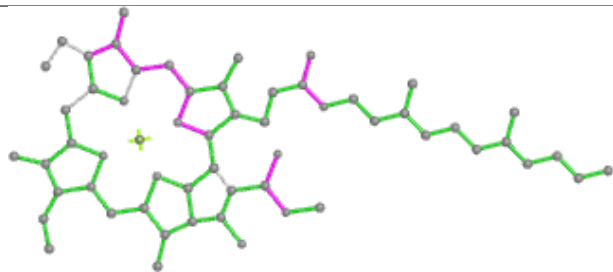


Rings

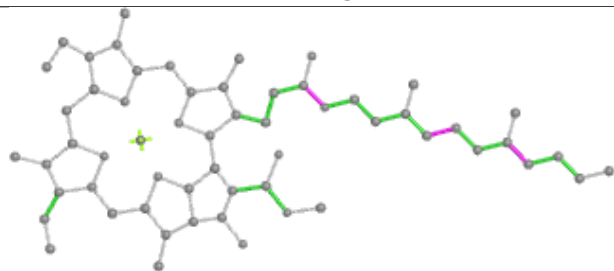
Ligand CLA 2 311



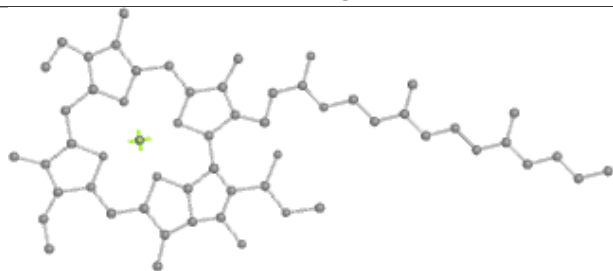
Bond lengths



Bond angles

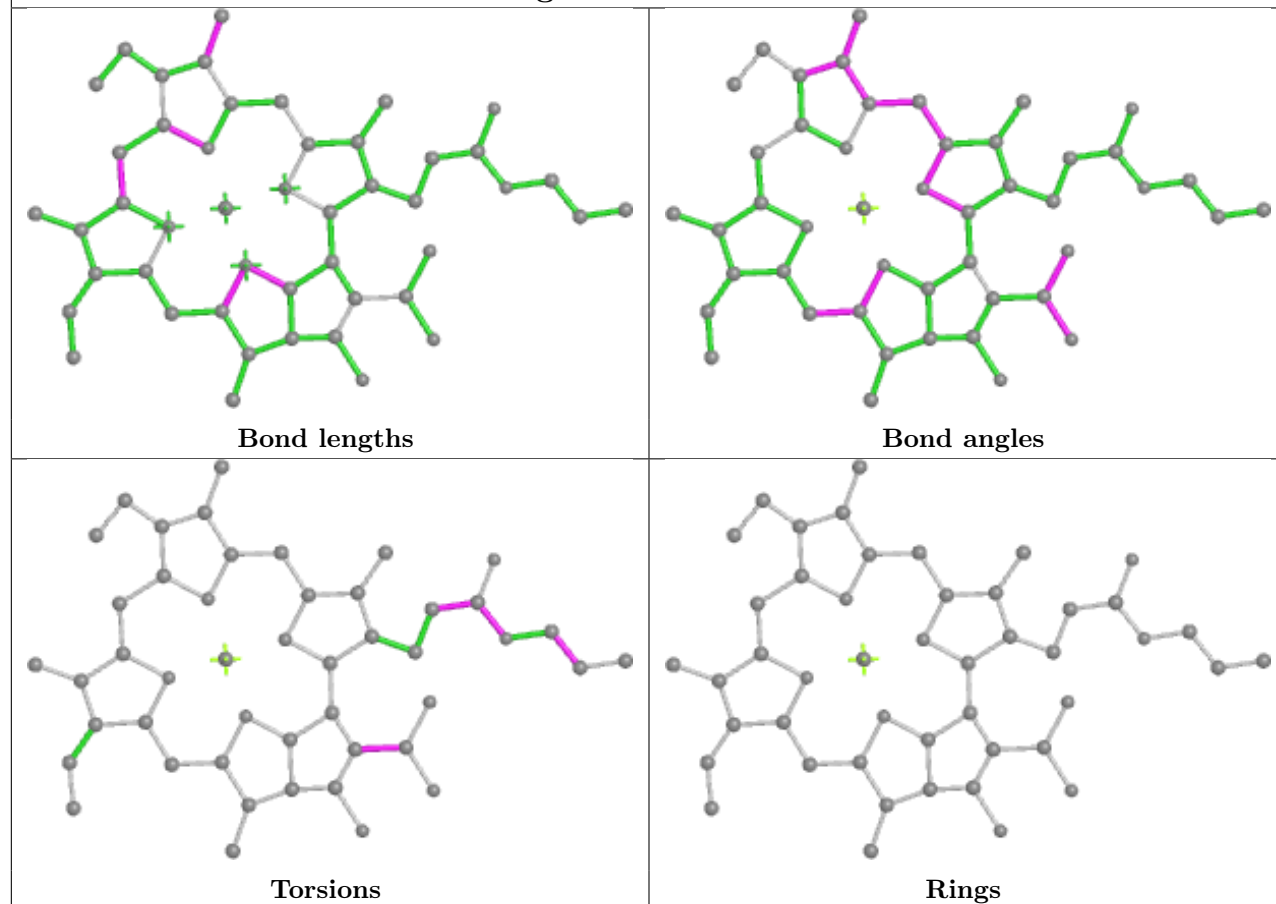


Torsions

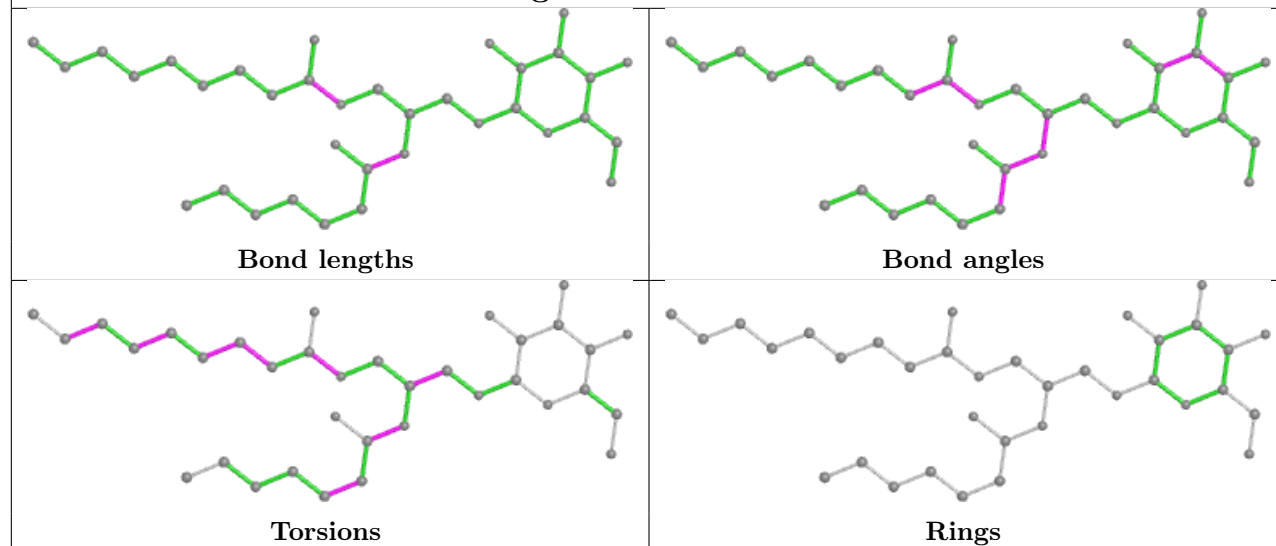


Rings

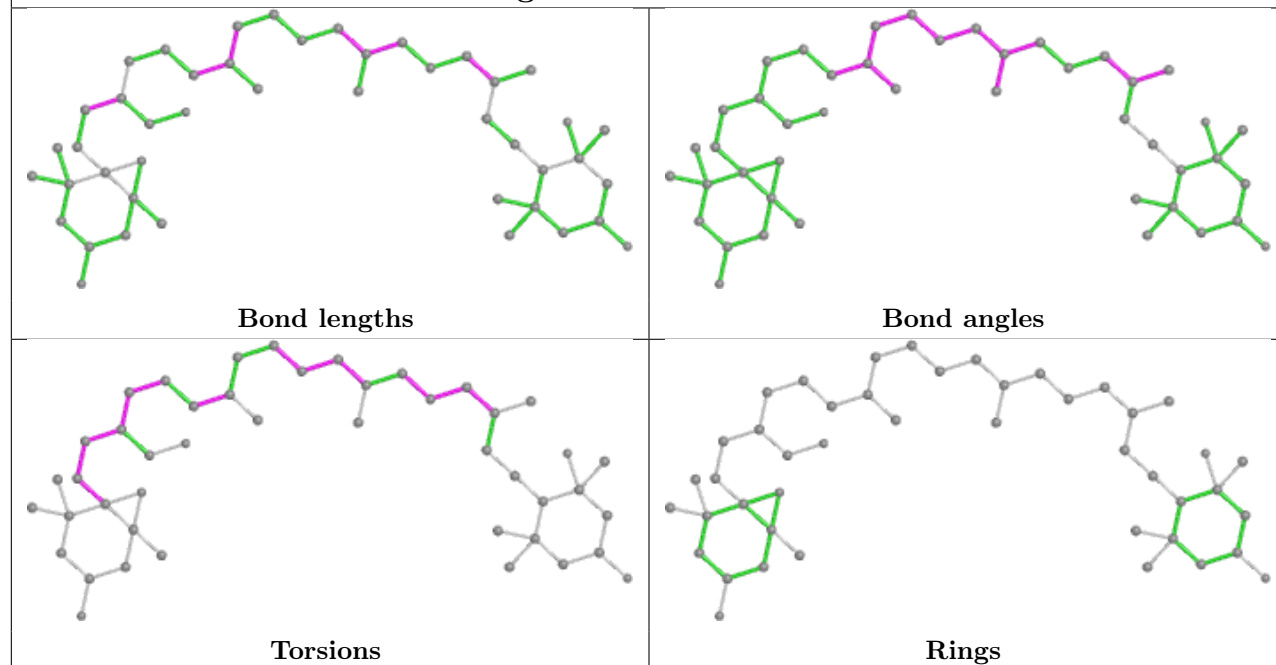
Ligand CLA 7 309



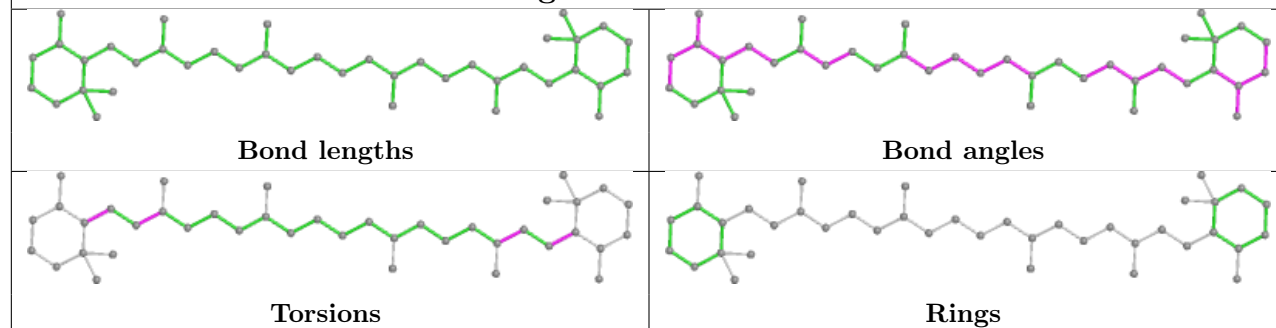
Ligand LMG 2 317



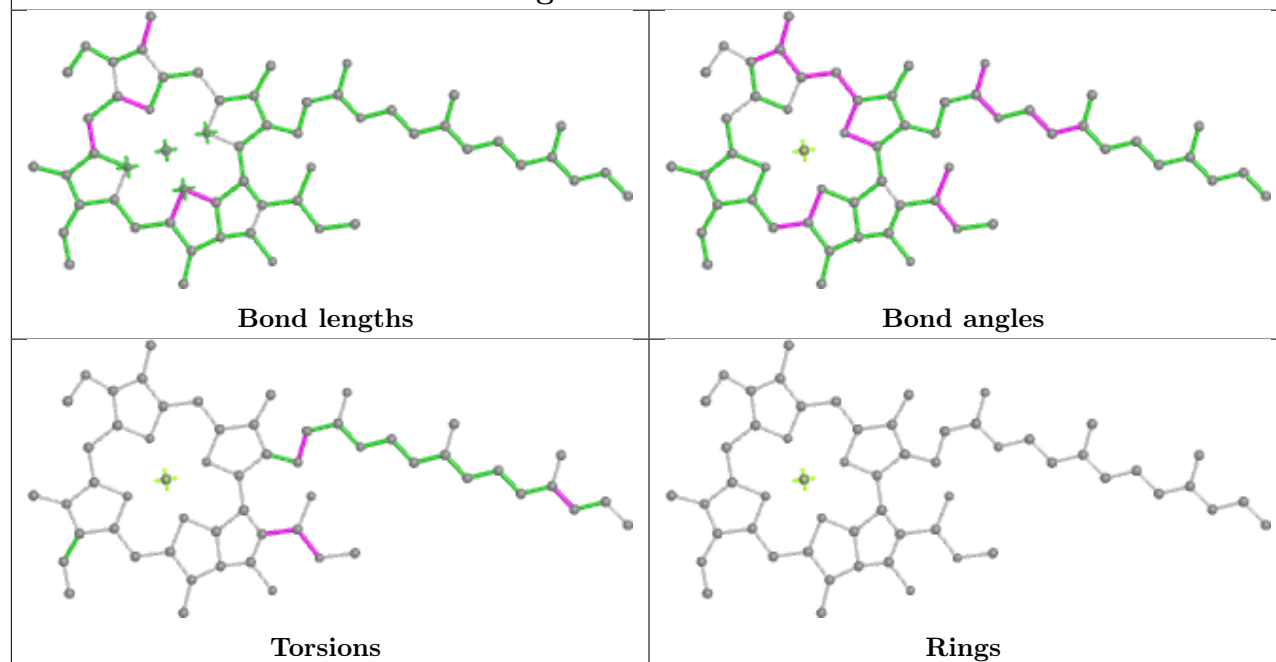
Ligand A1L1G 3 302

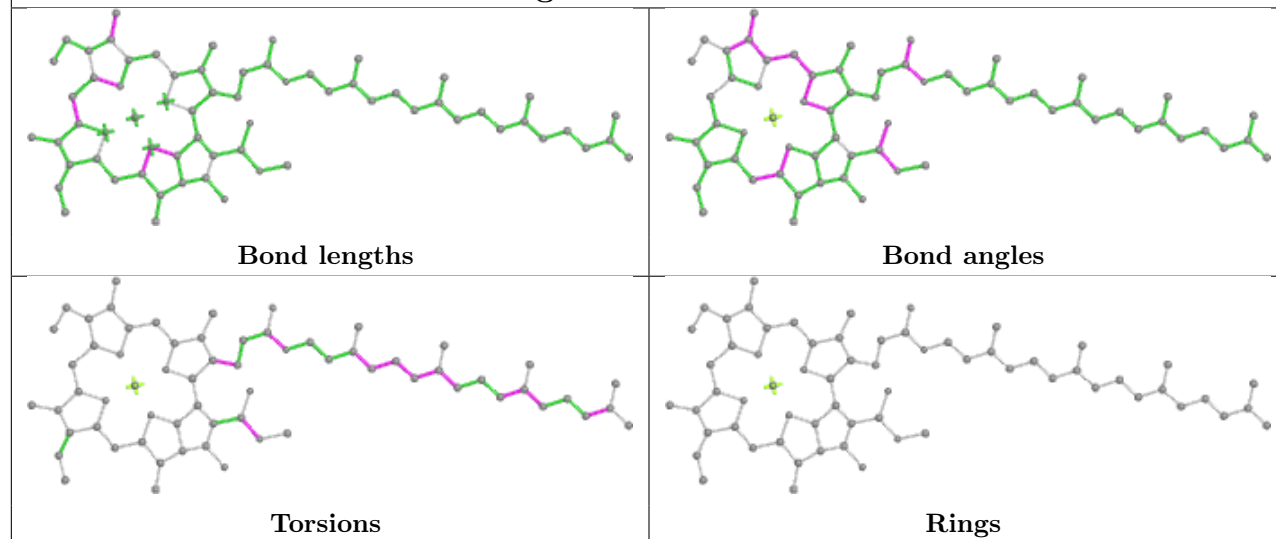
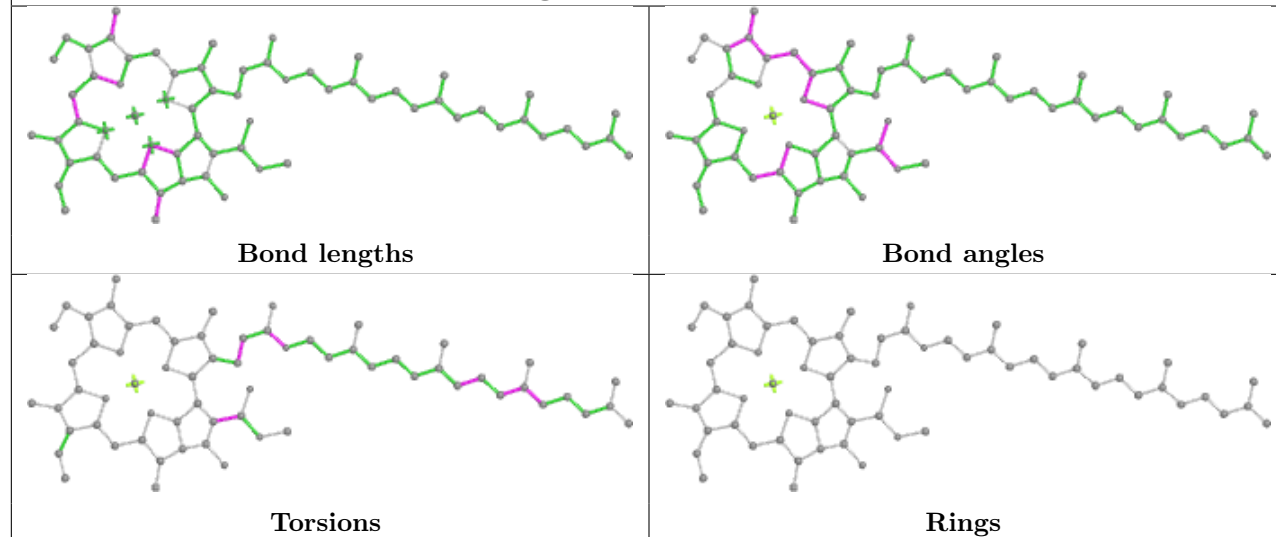


Ligand BCR i 102

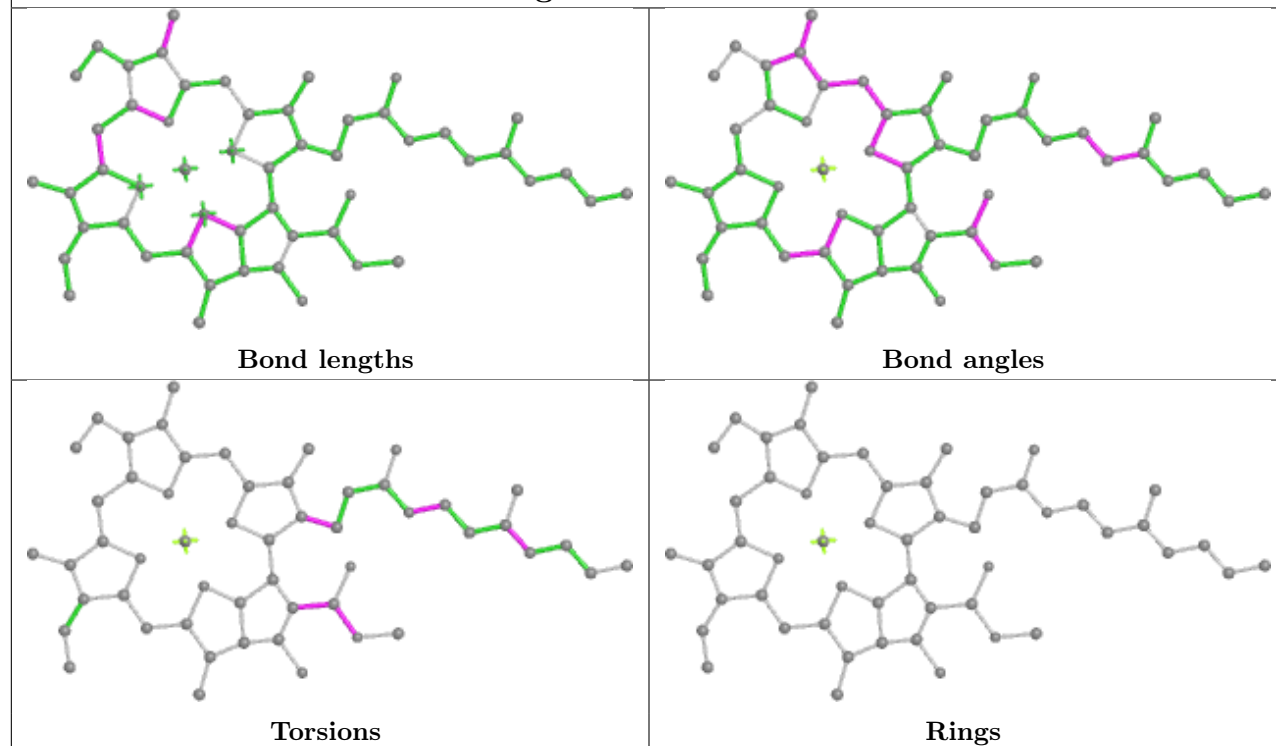


Ligand CLA 8 309

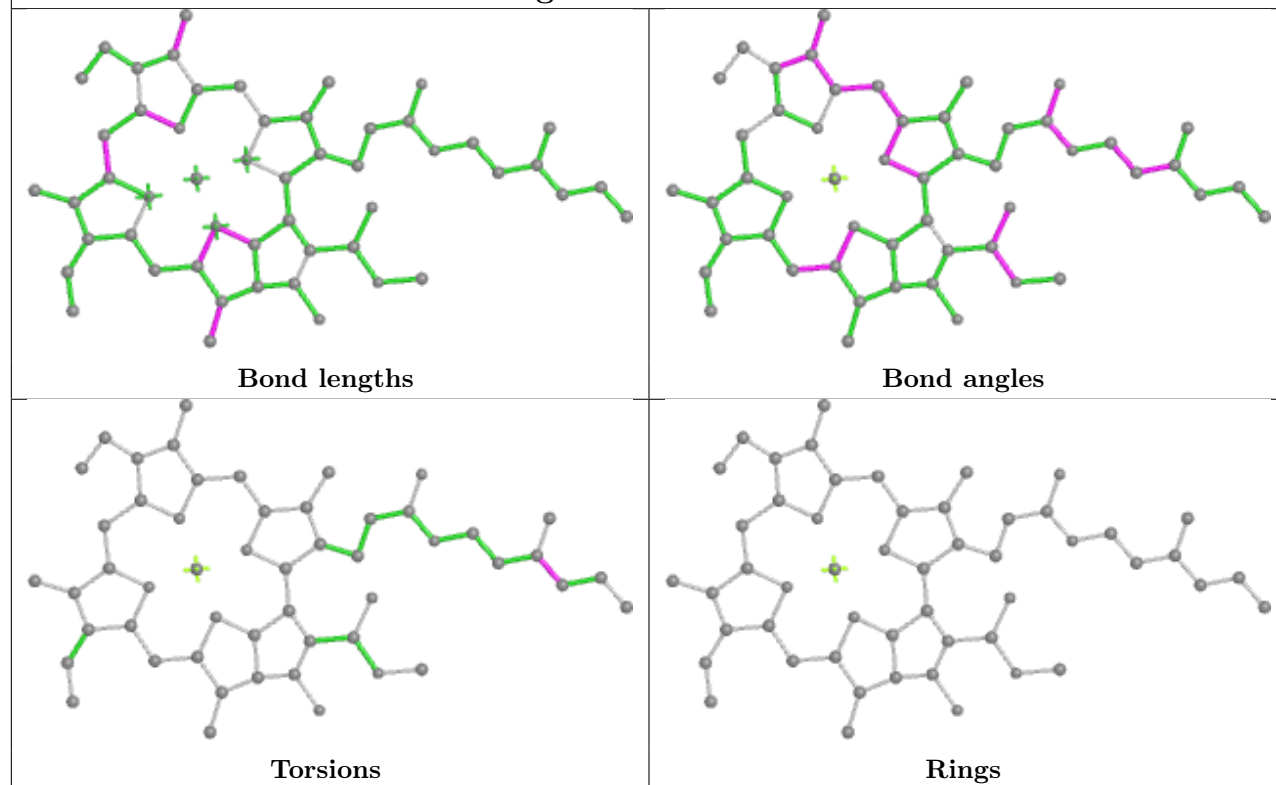


Ligand CLA 1 310**Ligand CLA a 842**

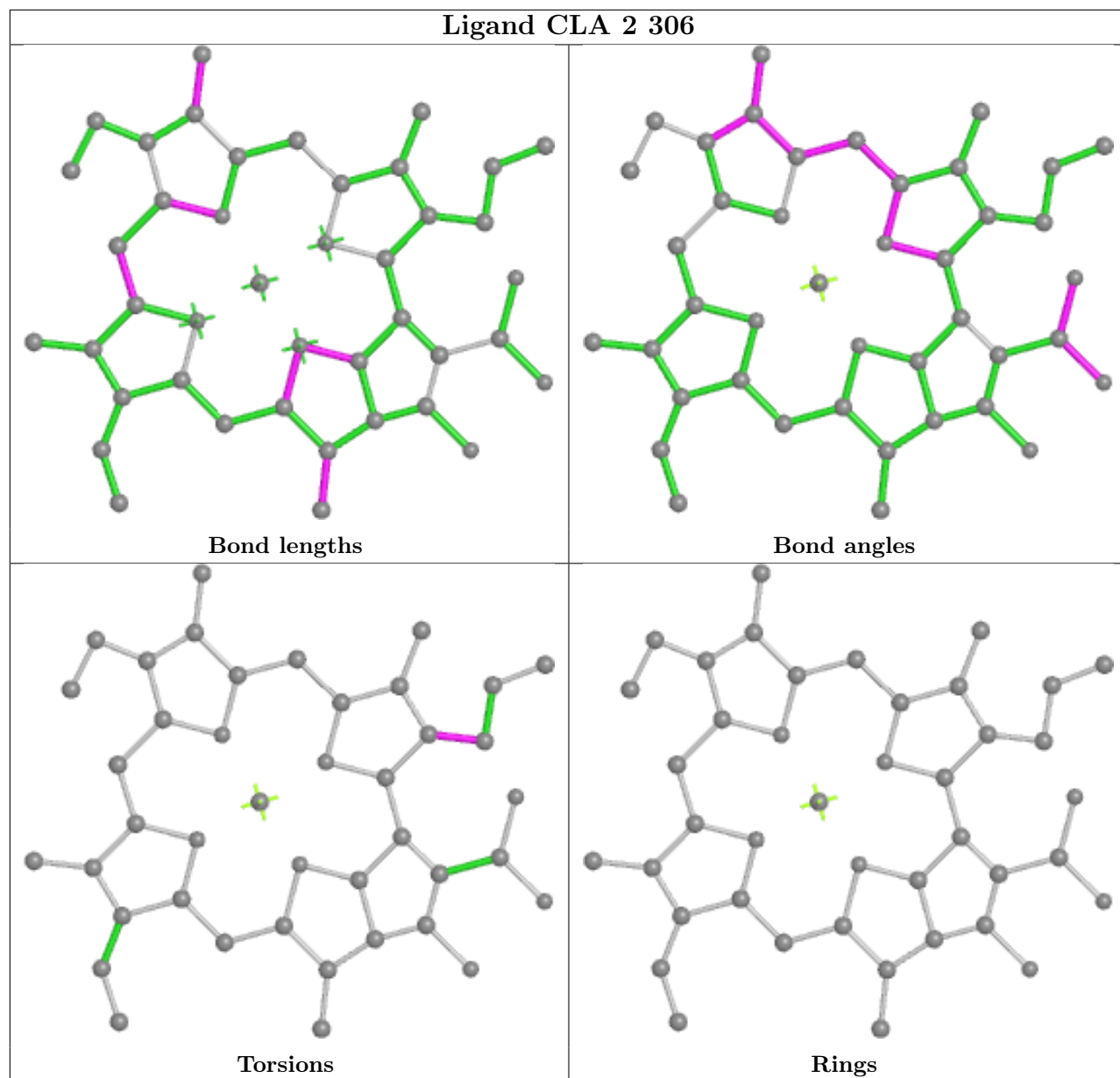
Ligand CLA b 835

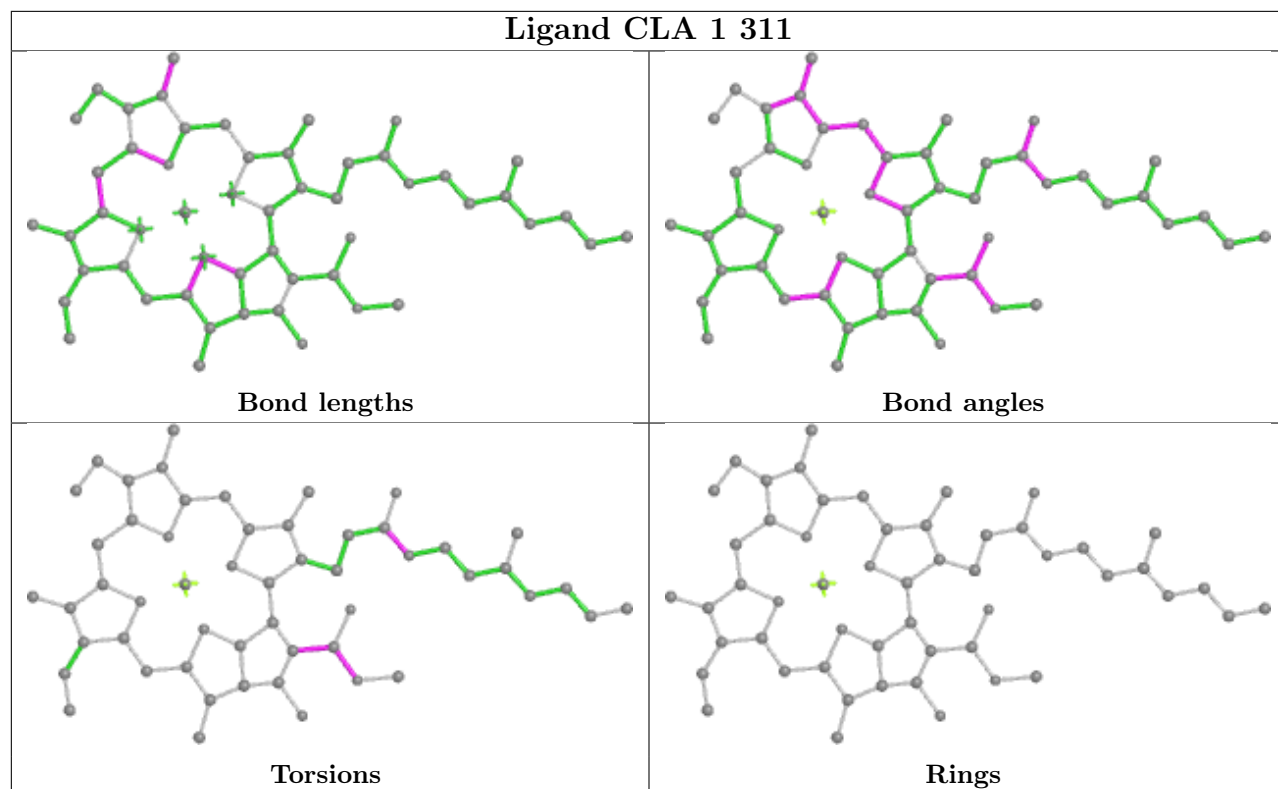


Ligand CLA 3 313

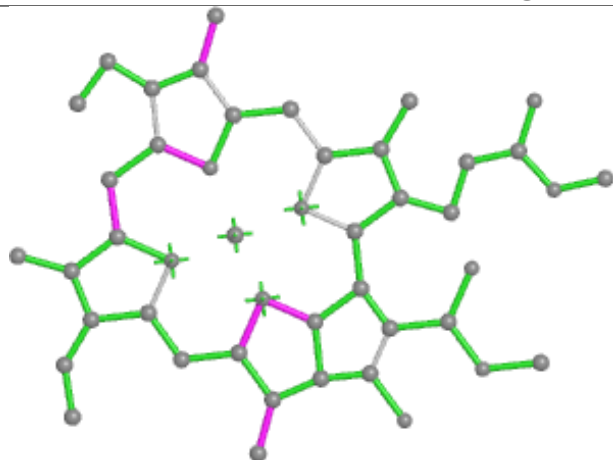


Ligand CLA 2 306

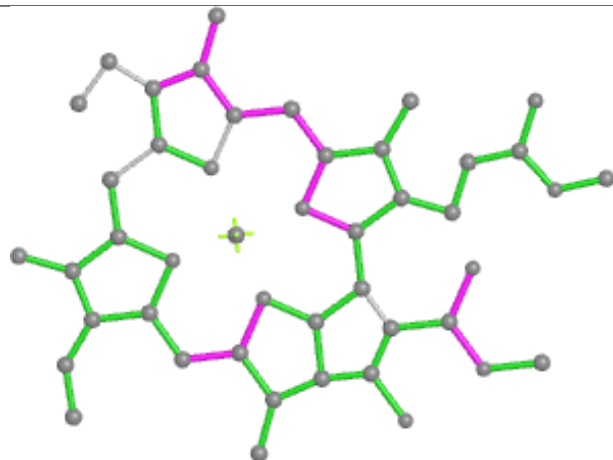




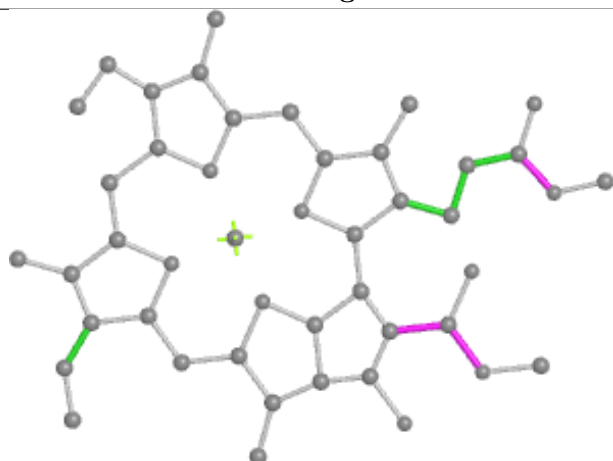
Ligand CLA 8 310



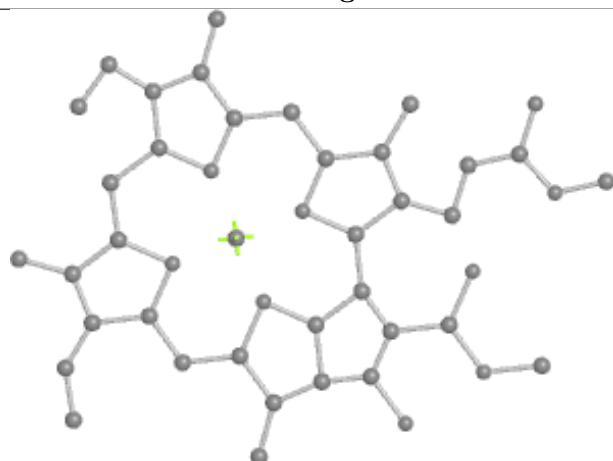
Bond lengths



Bond angles

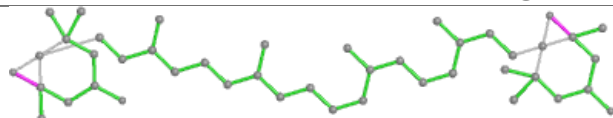


Torsions

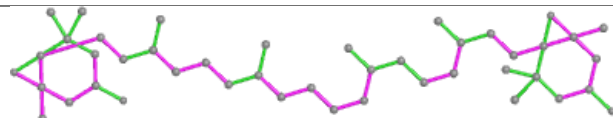


Rings

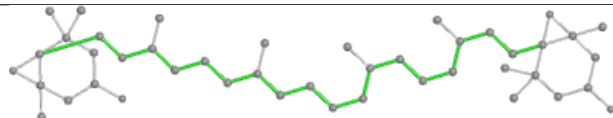
Ligand XAT 1 302



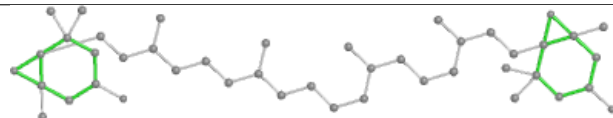
Bond lengths



Bond angles

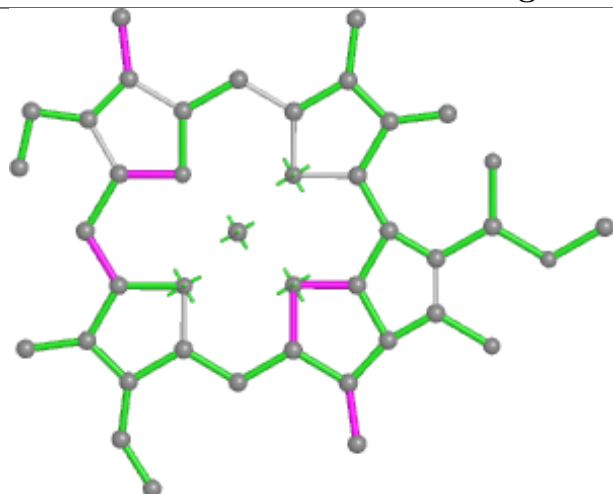


Torsions

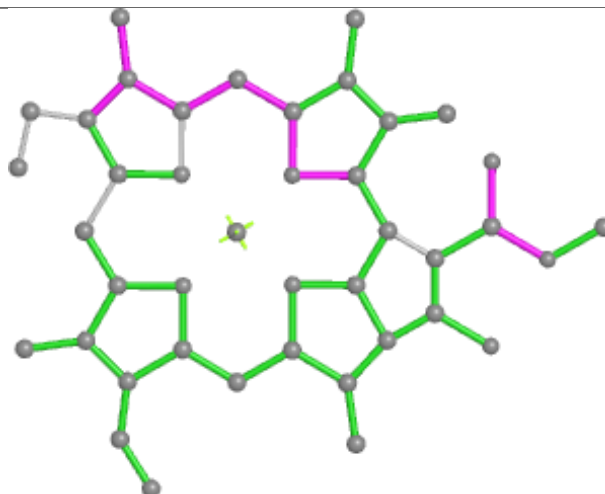


Rings

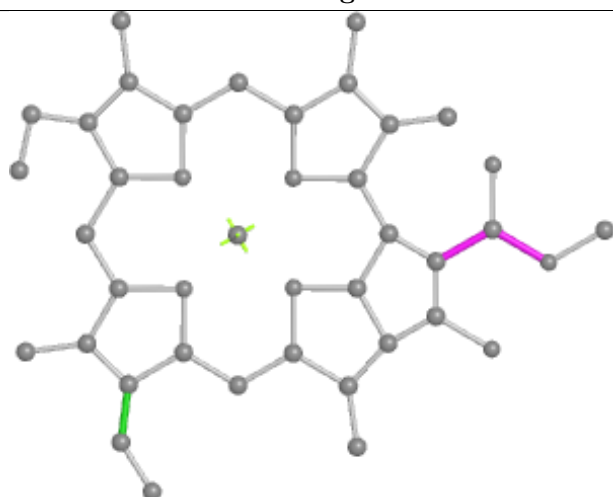
Ligand CLA 6 315



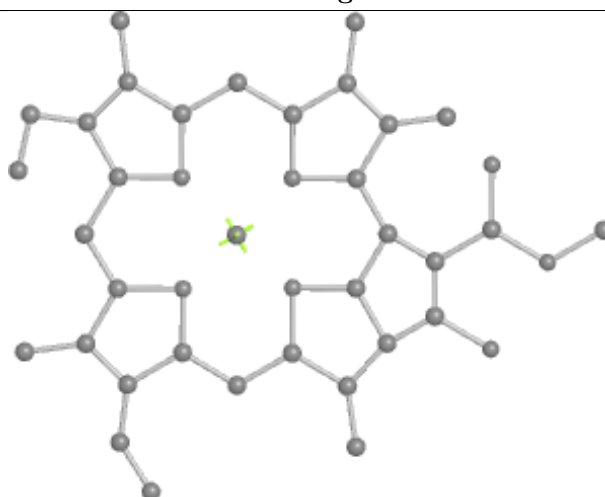
Bond lengths



Bond angles

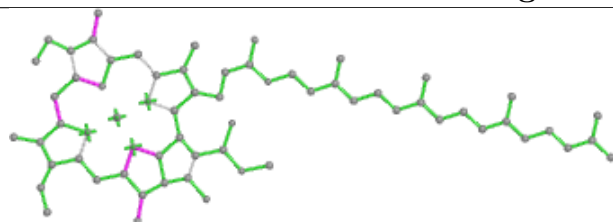


Torsions

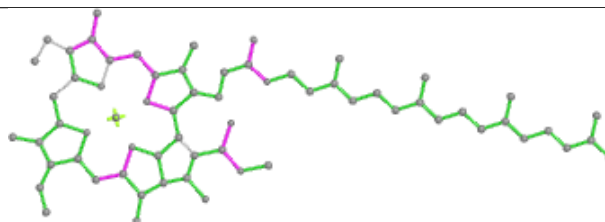


Rings

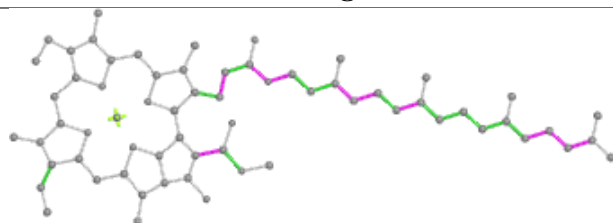
Ligand CLA a 839



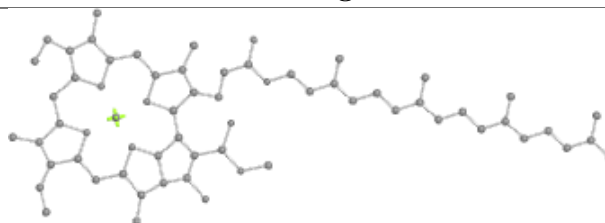
Bond lengths



Bond angles

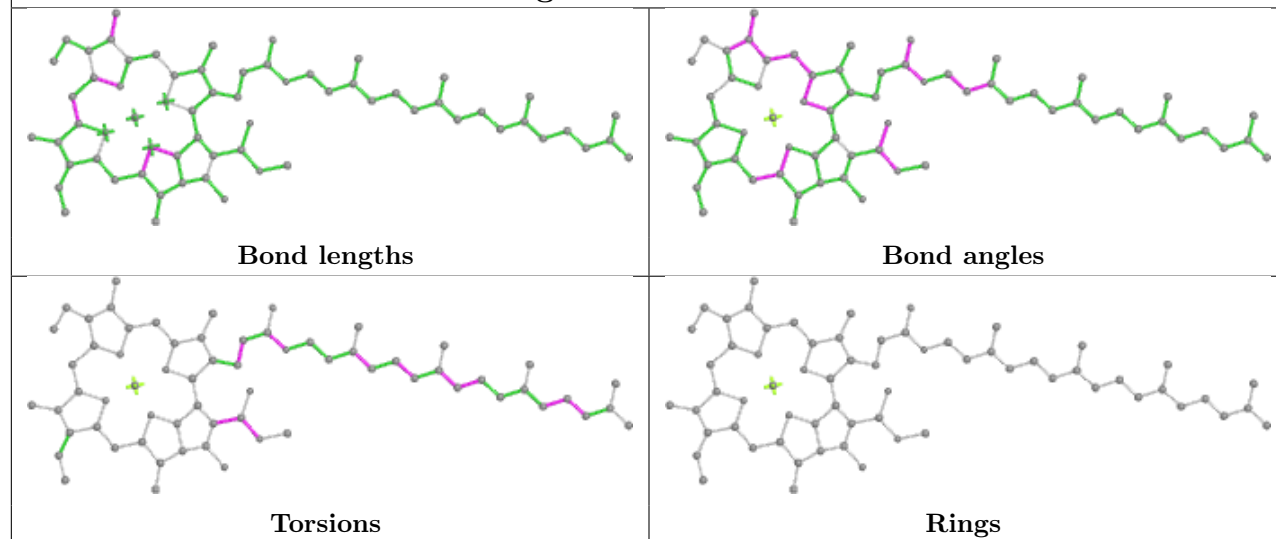


Torsions

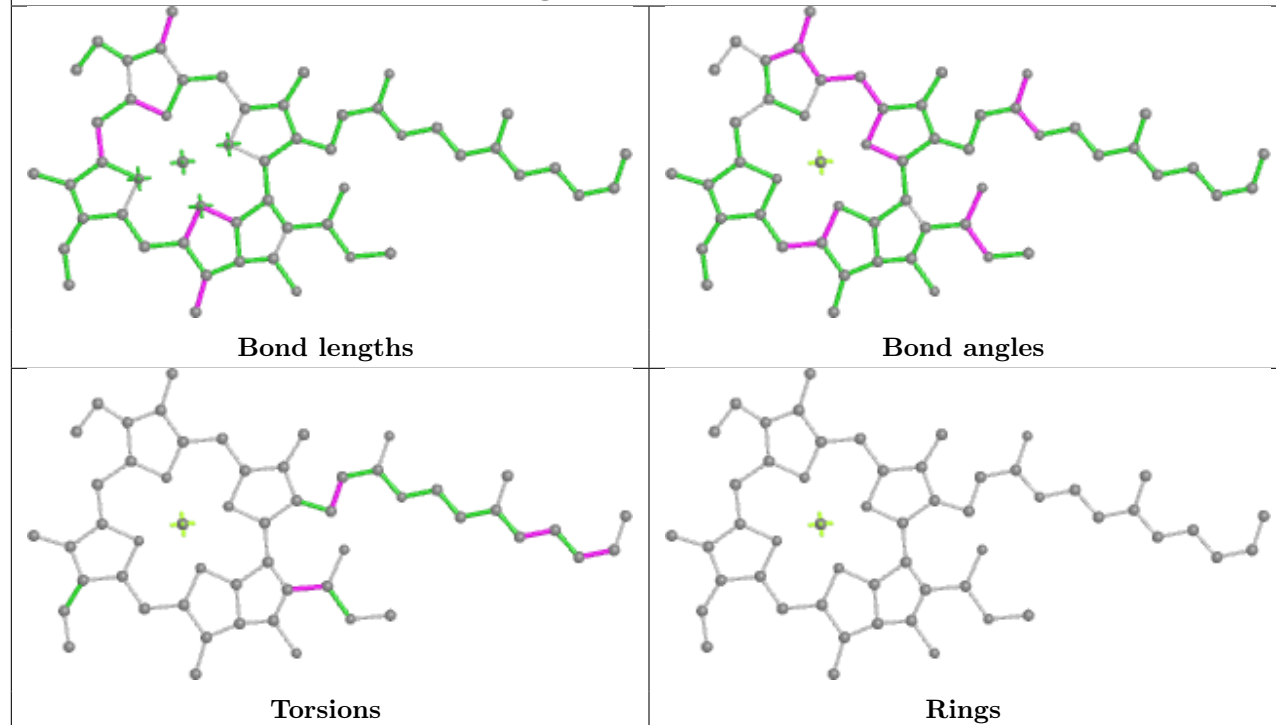


Rings

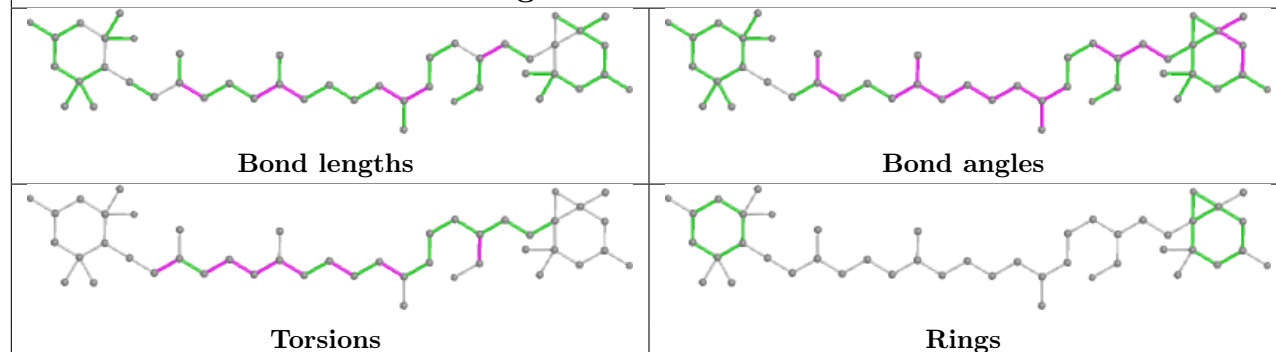
Ligand CLA a 841

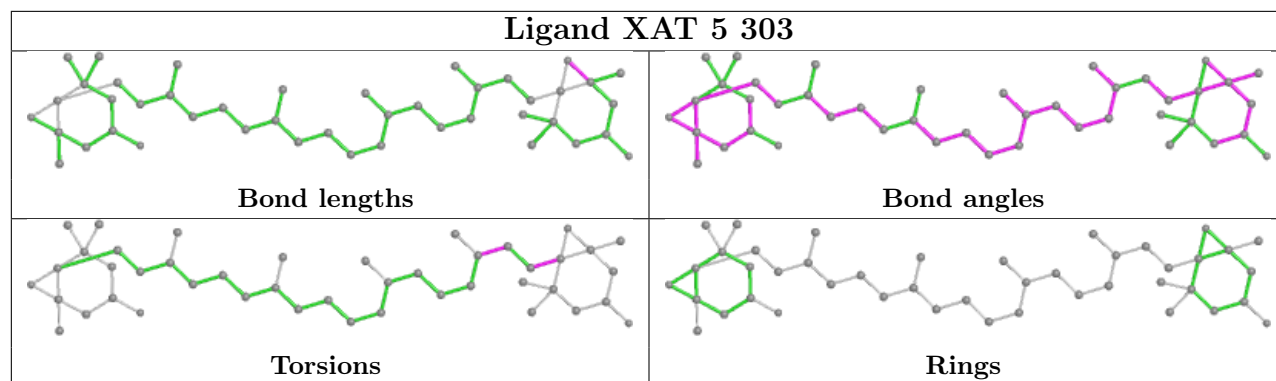
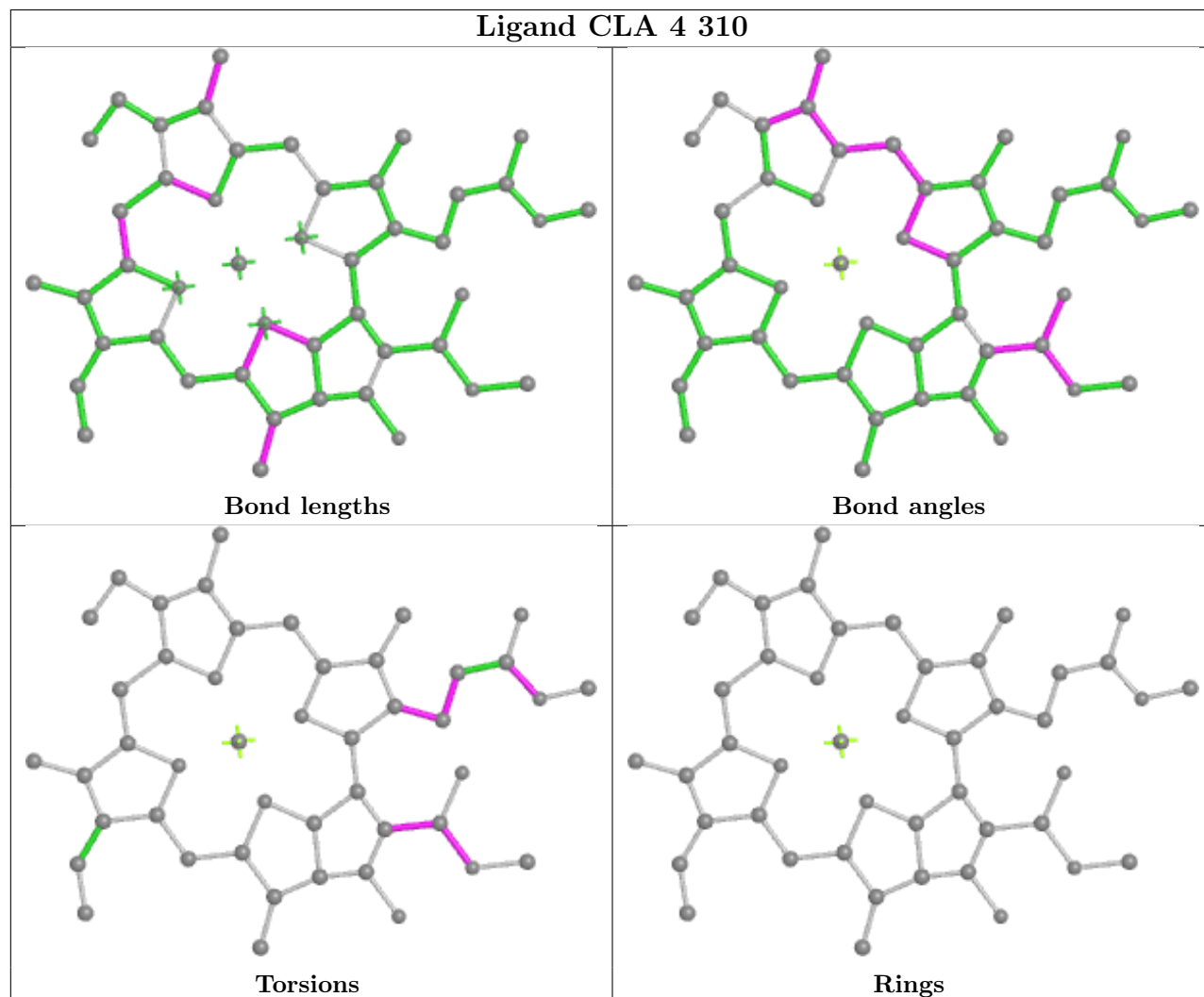


Ligand CLA 2 308

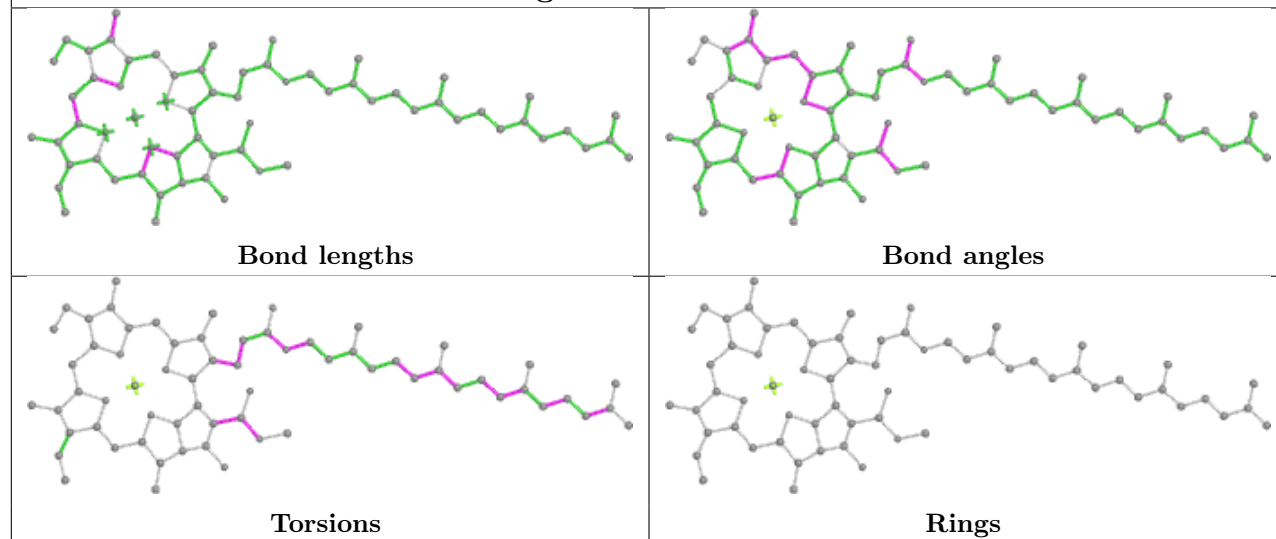


Ligand A1L1G 1 301

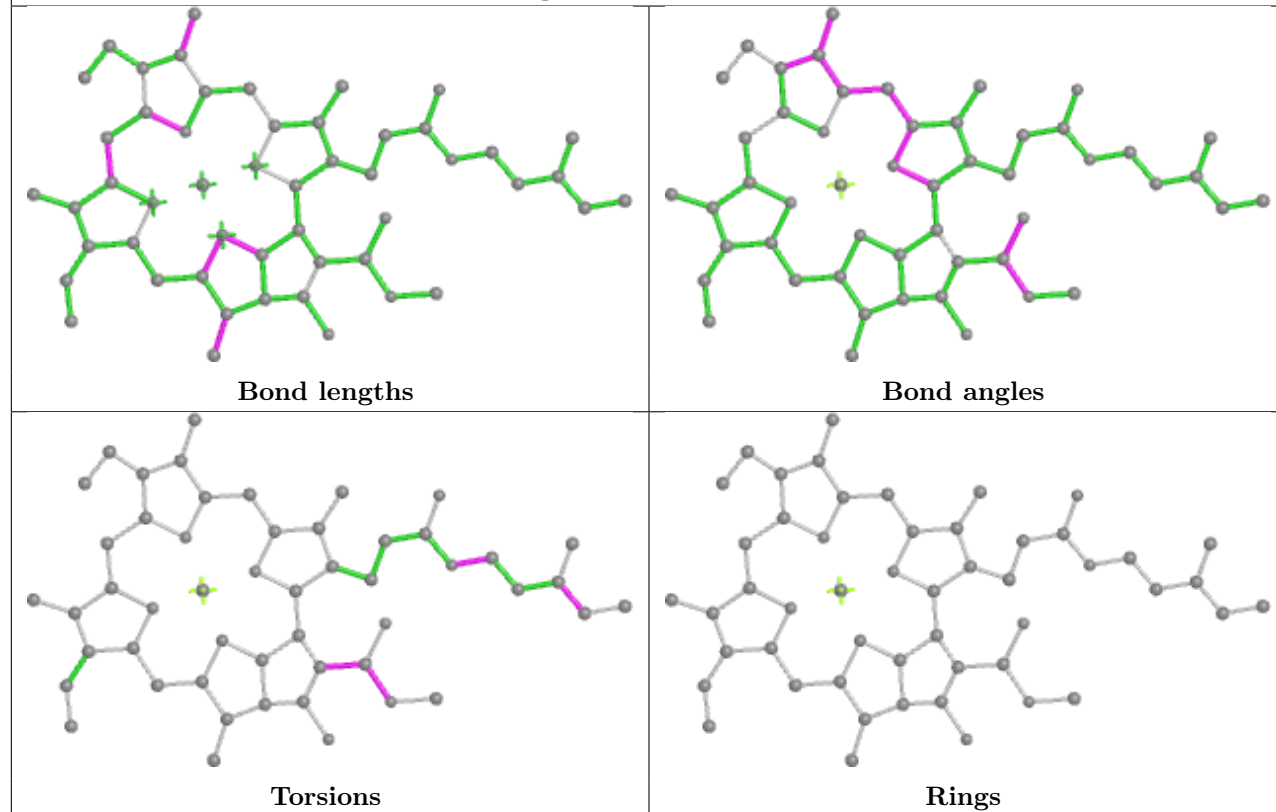


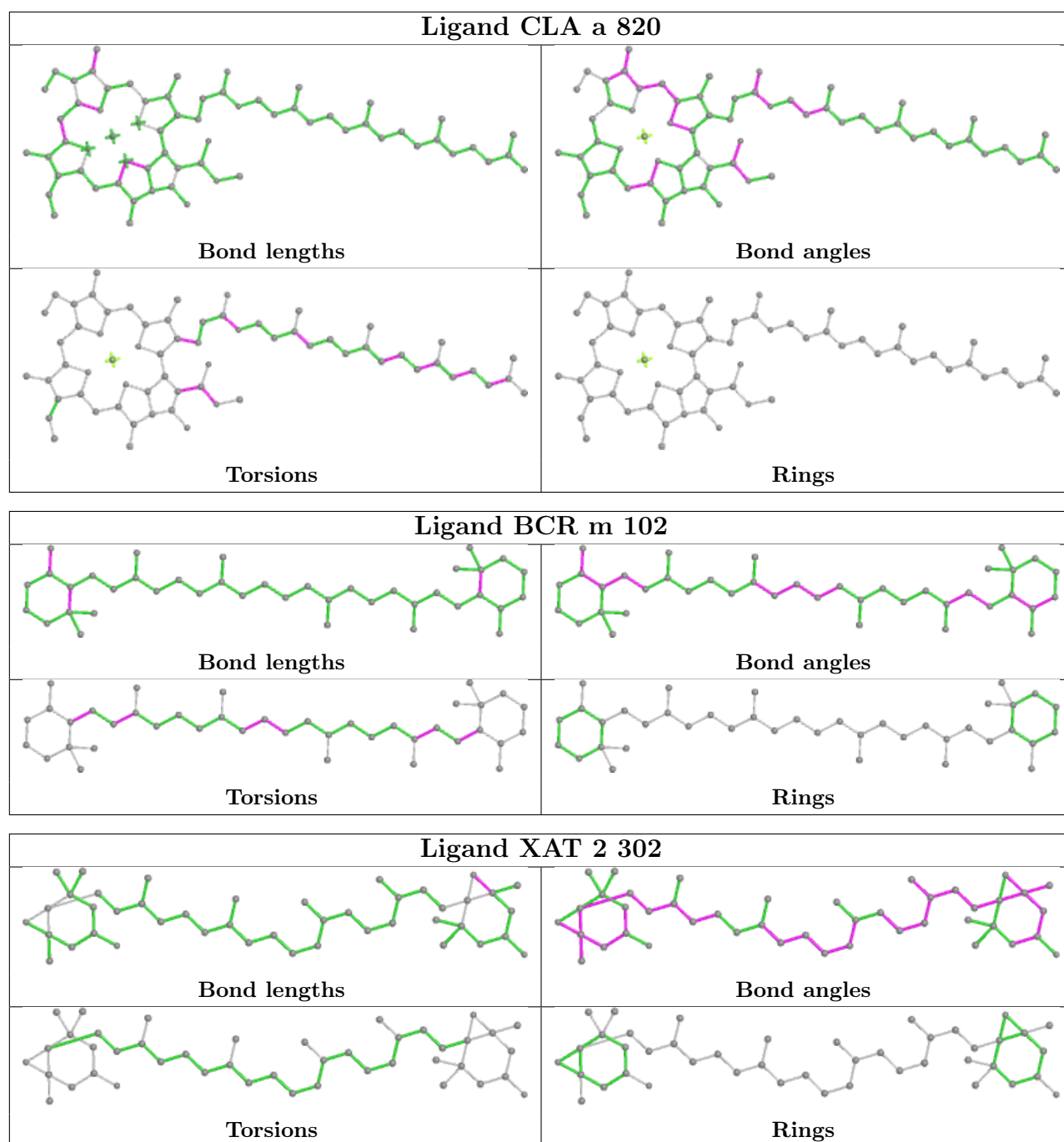
Ligand XAT 5 303**Ligand CLA 4 310**

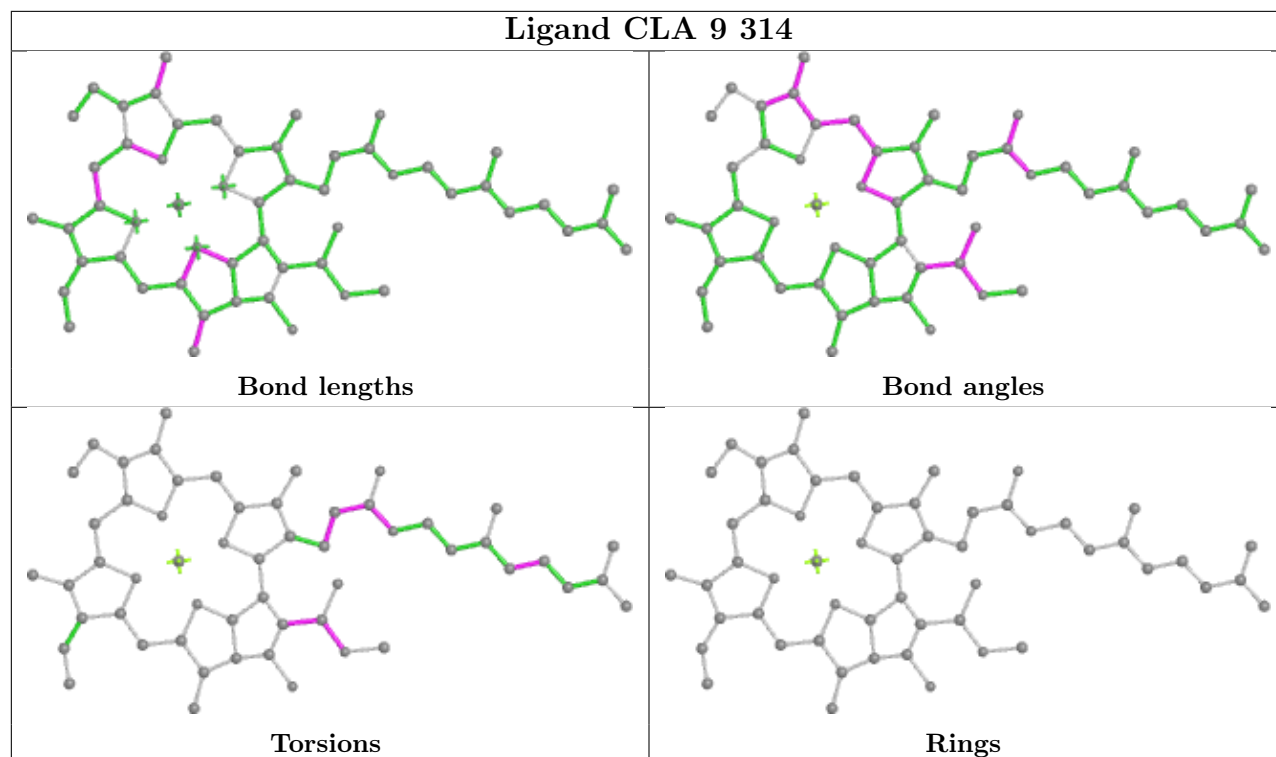
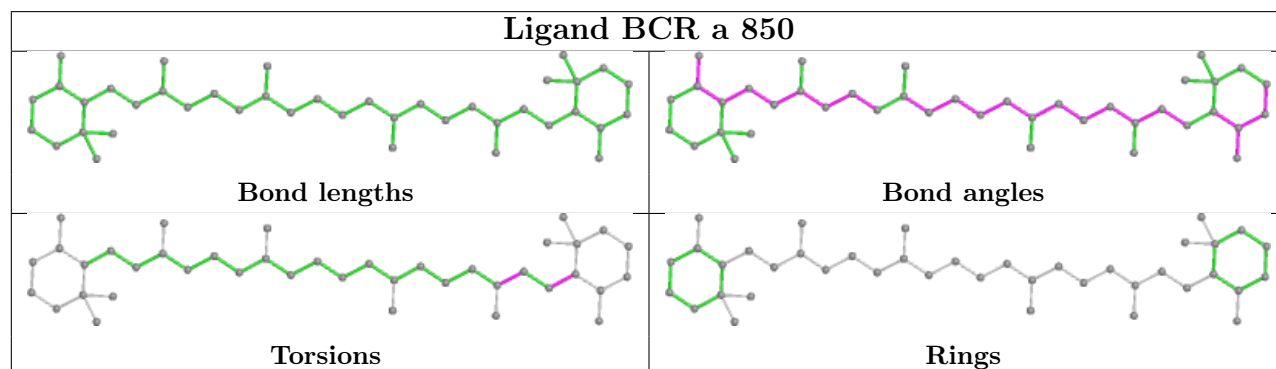
Ligand CLA a 814



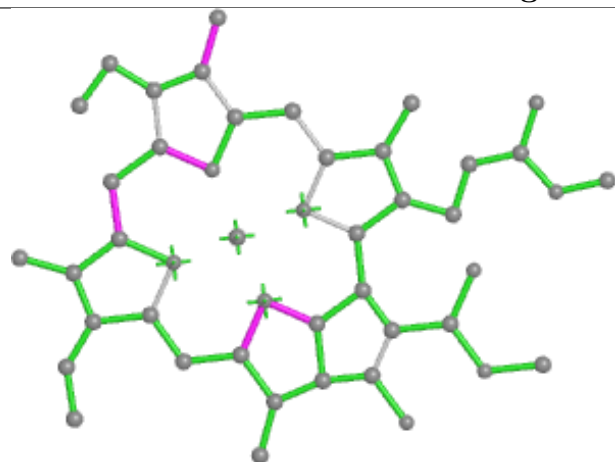
Ligand CLA 6 312



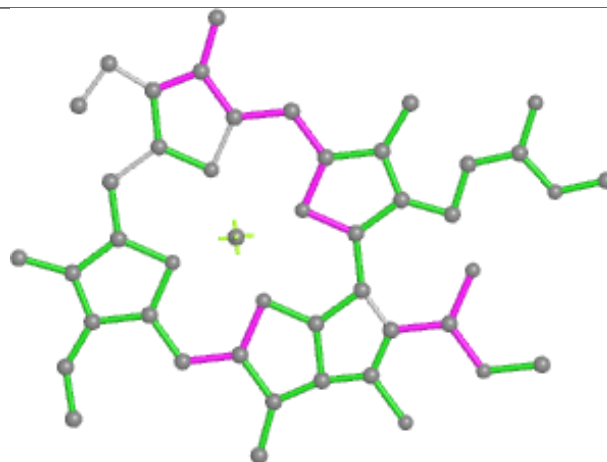


Ligand CLA 9 314**Ligand BCR a 850**

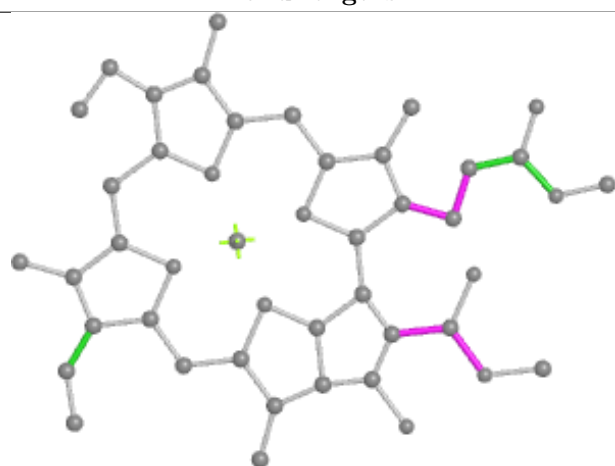
Ligand CLA 9 311



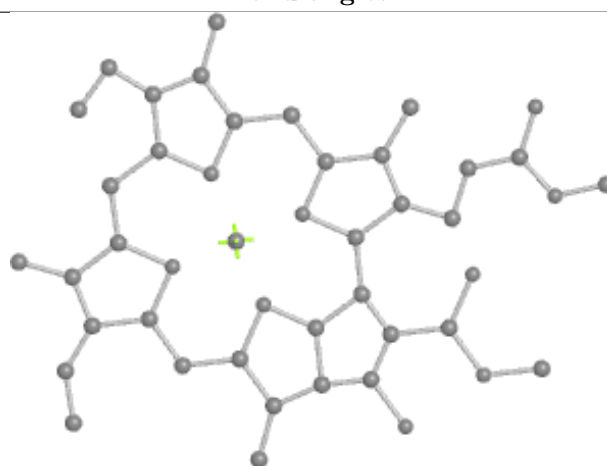
Bond lengths



Bond angles

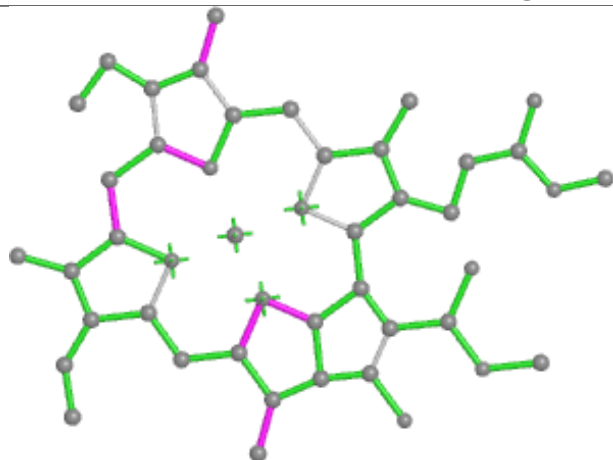


Torsions

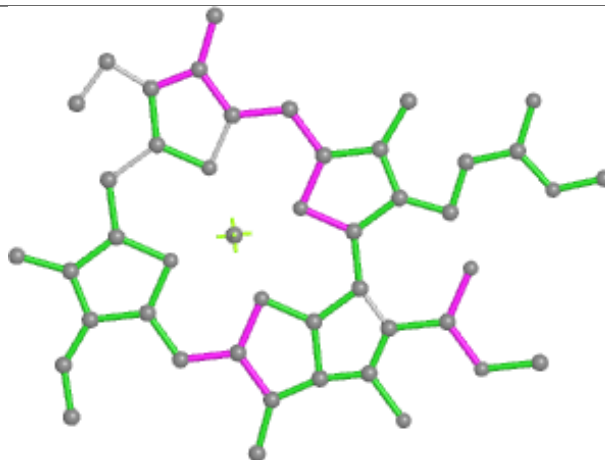


Rings

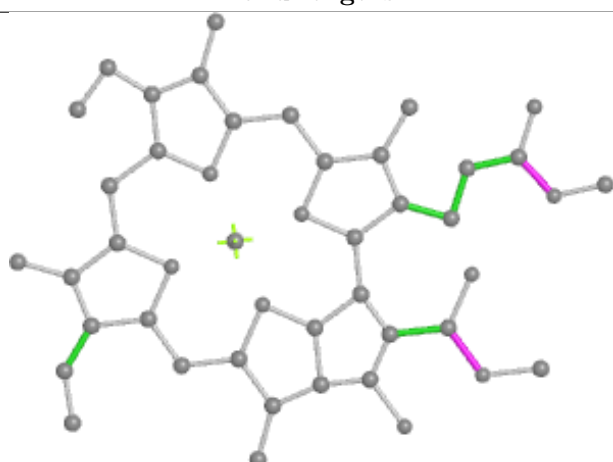
Ligand CLA 5 306



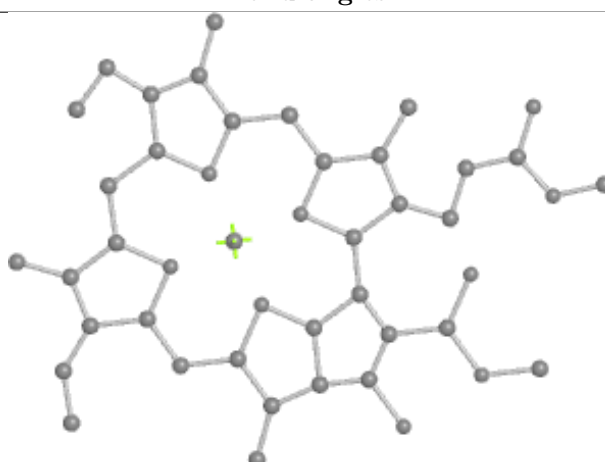
Bond lengths



Bond angles

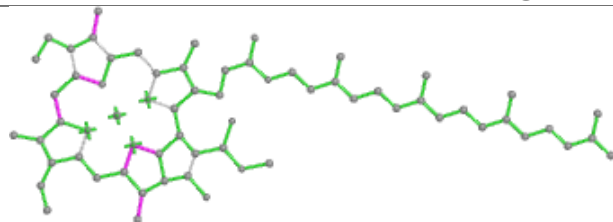


Torsions

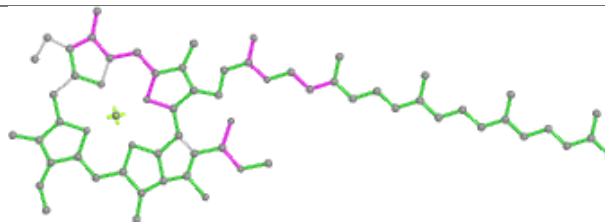


Rings

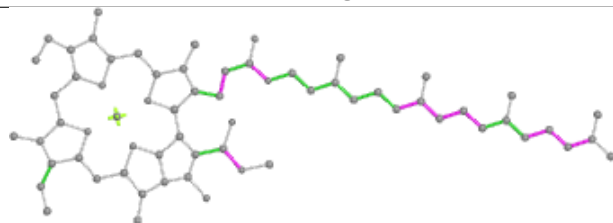
Ligand CLA b 827



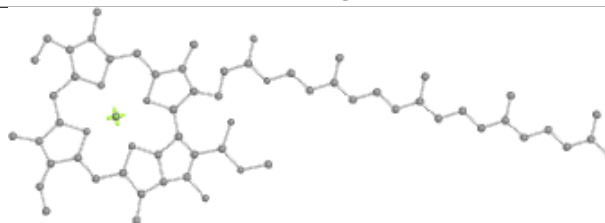
Bond lengths



Bond angles

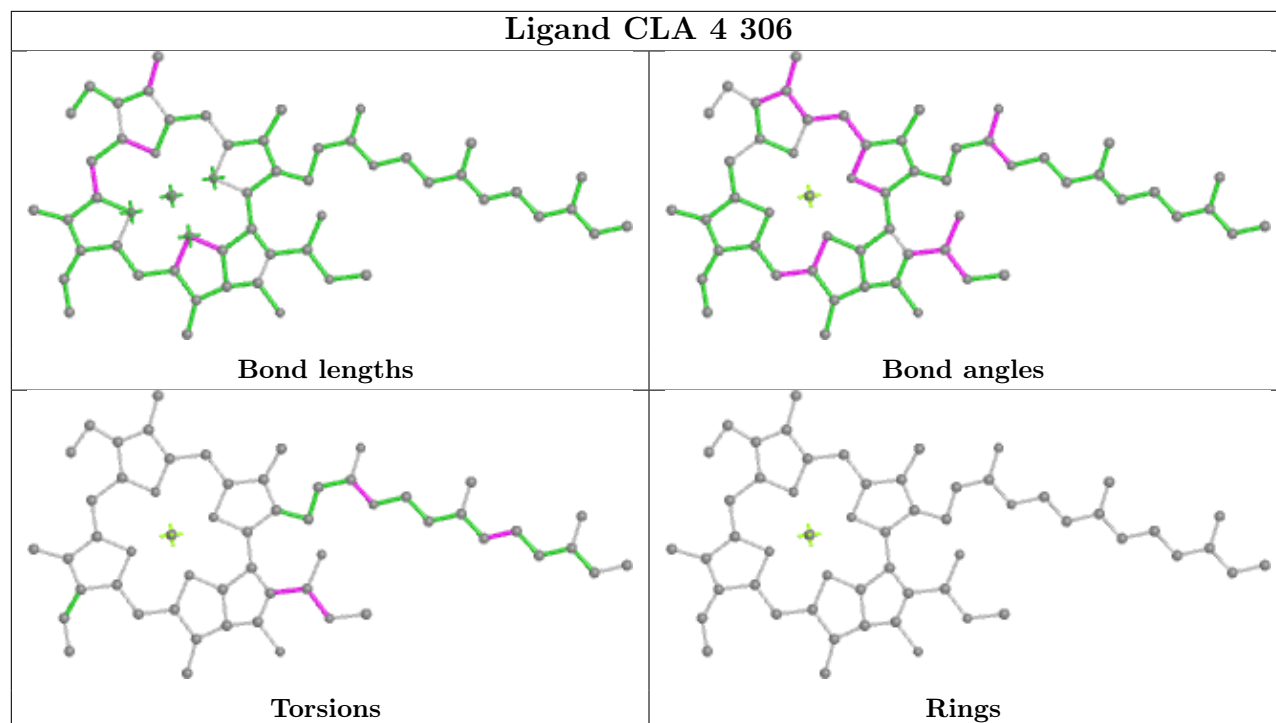


Torsions

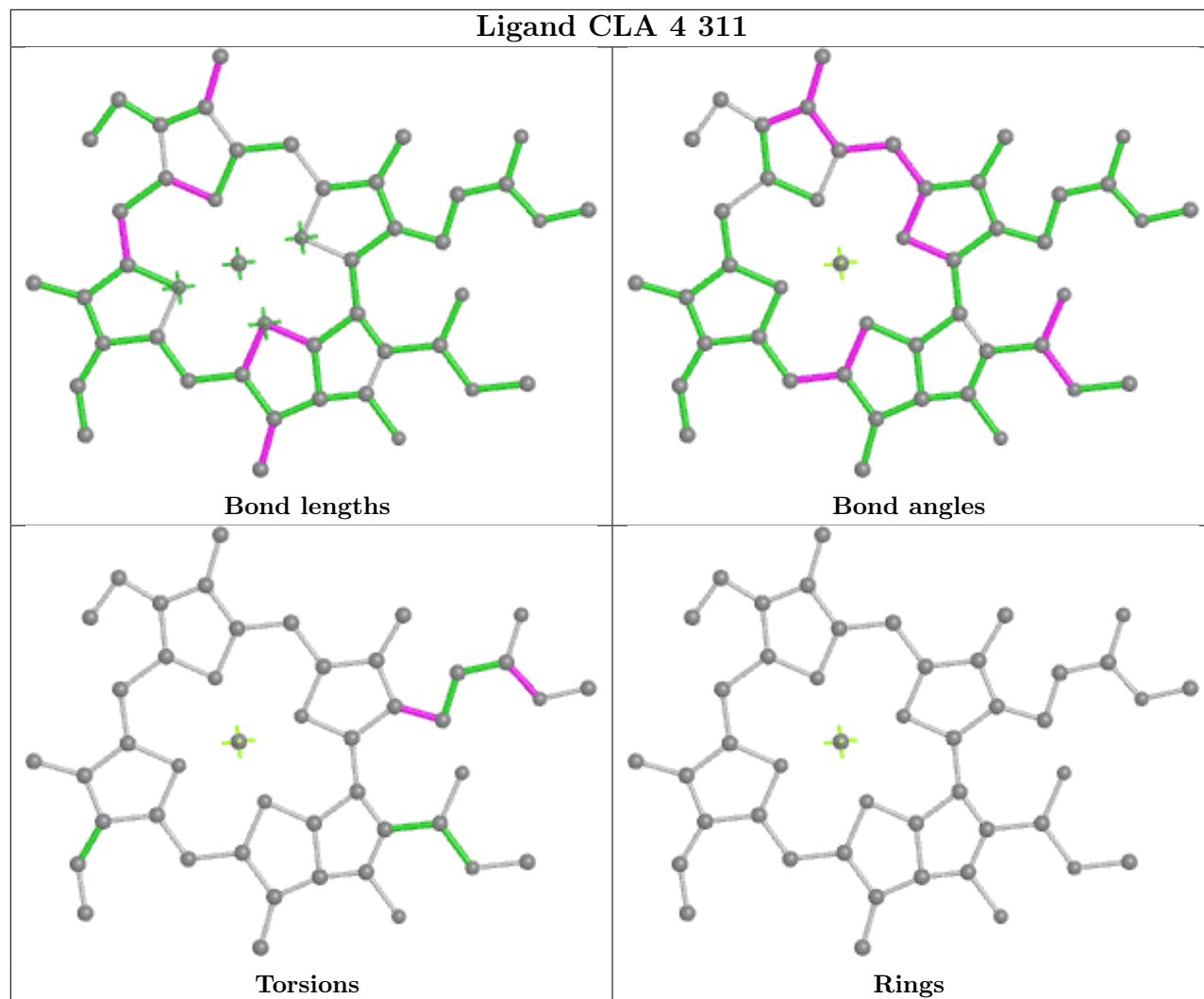


Rings

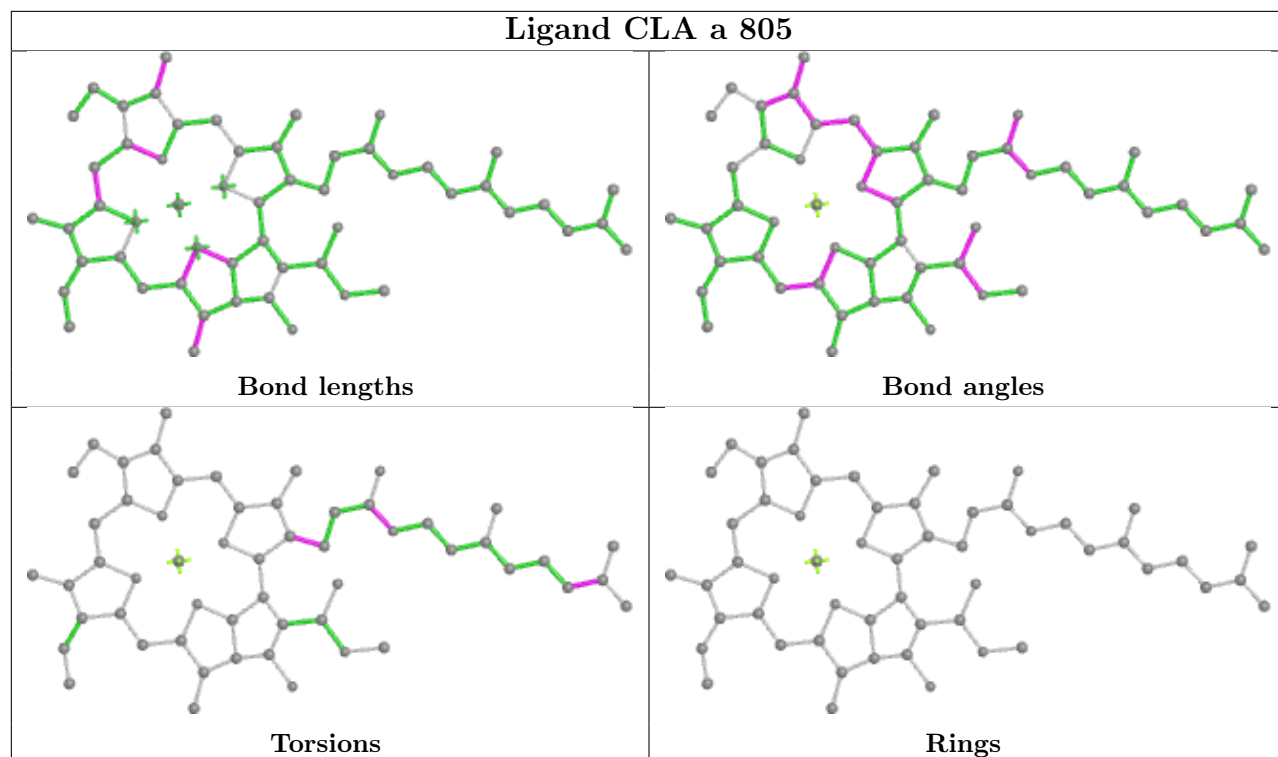
Ligand CLA 4 306



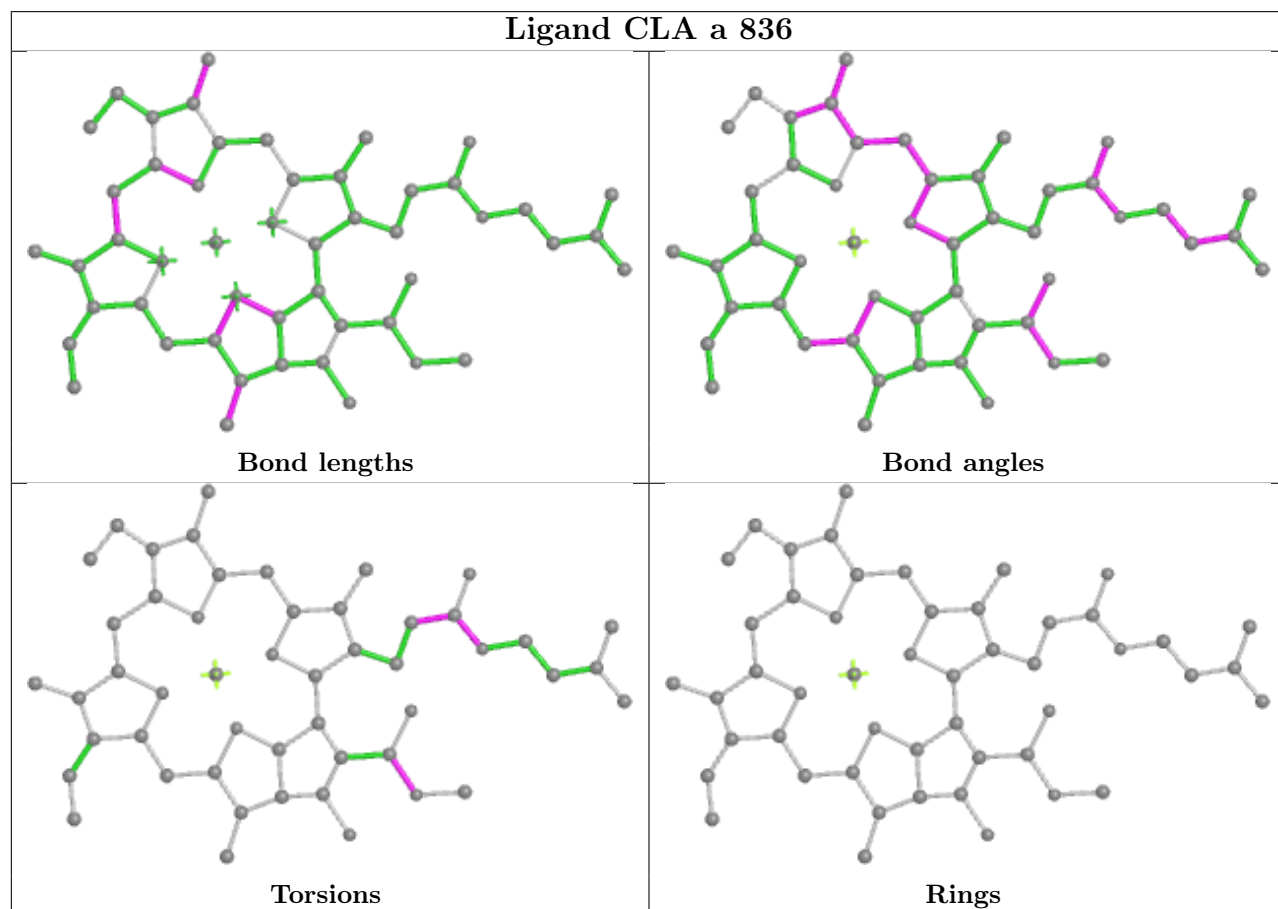
Ligand CLA 4 311

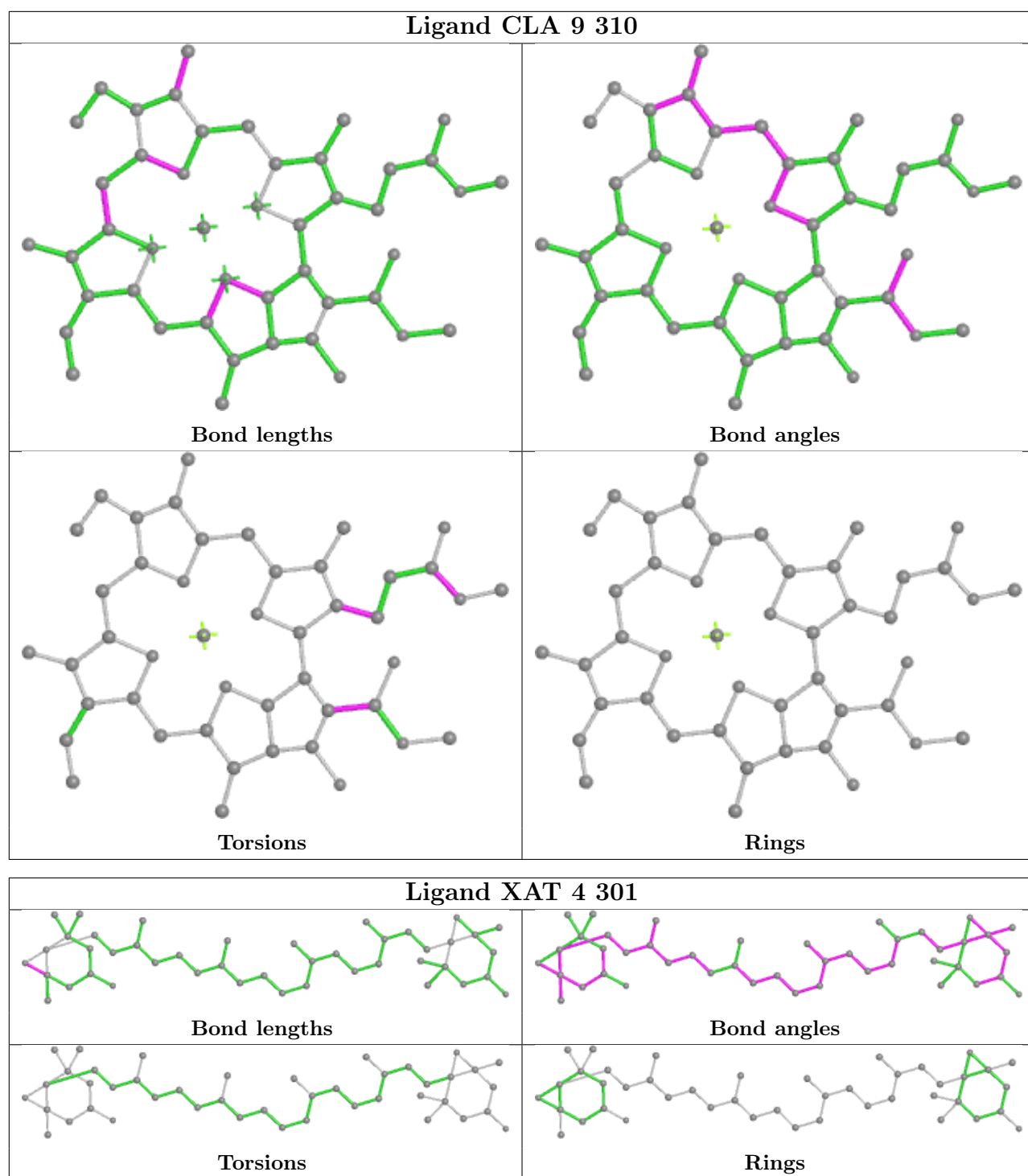


Ligand CLA a 805



Ligand CLA a 836





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

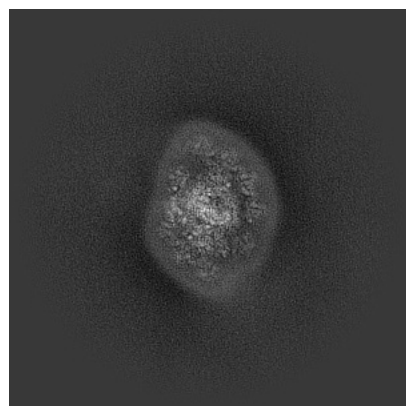
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60292. These allow visual inspection of the internal detail of the map and identification of artifacts.

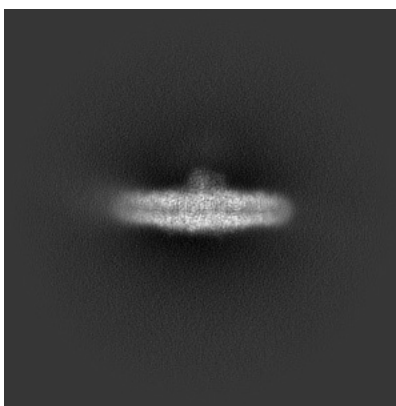
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

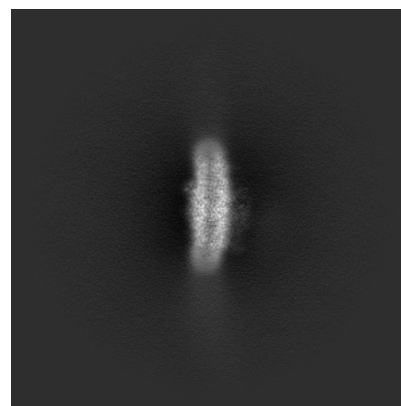
6.1.1 Primary map



X

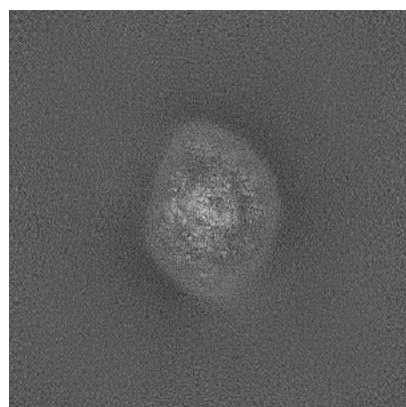


Y



Z

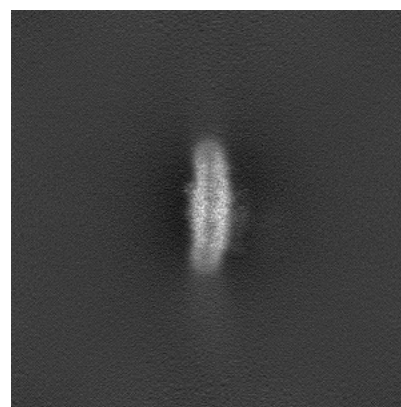
6.1.2 Raw map



X



Y

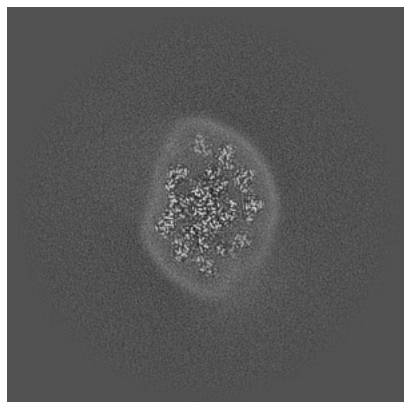


Z

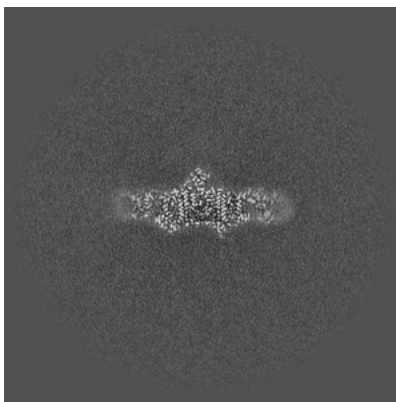
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

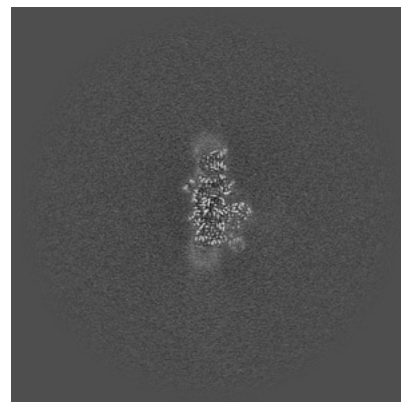
6.2.1 Primary map



X Index: 256

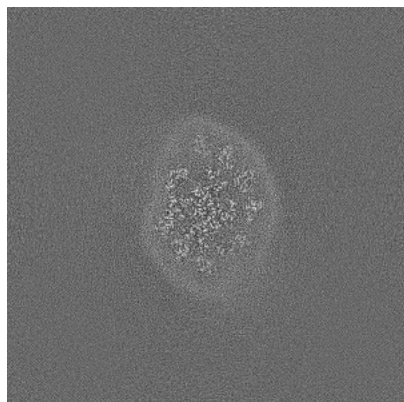


Y Index: 256

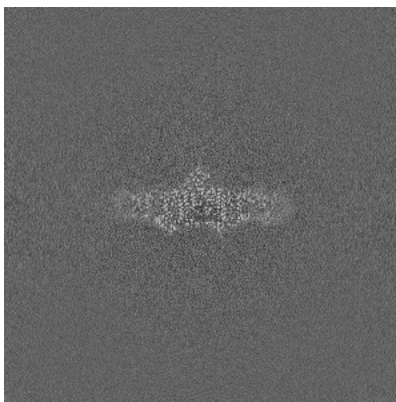


Z Index: 256

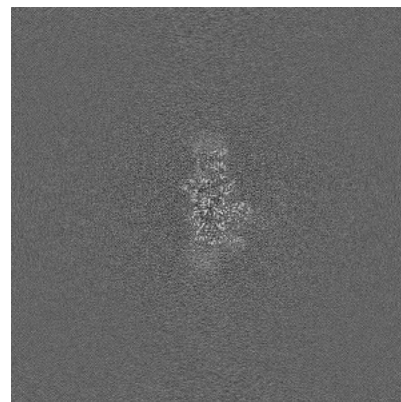
6.2.2 Raw map



X Index: 256



Y Index: 256

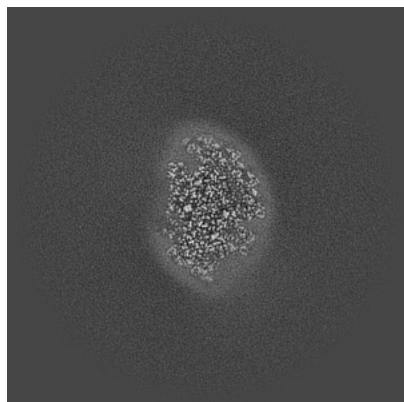


Z Index: 256

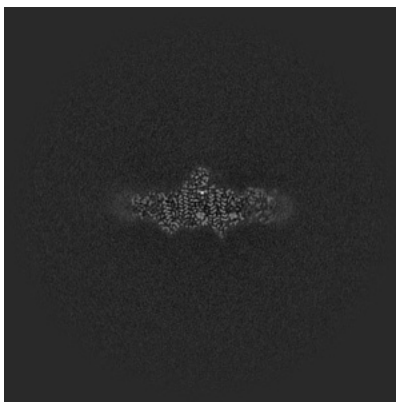
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

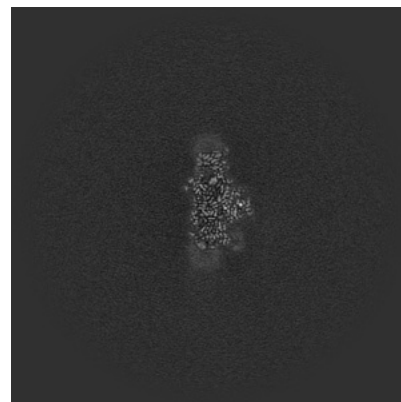
6.3.1 Primary map



X Index: 267

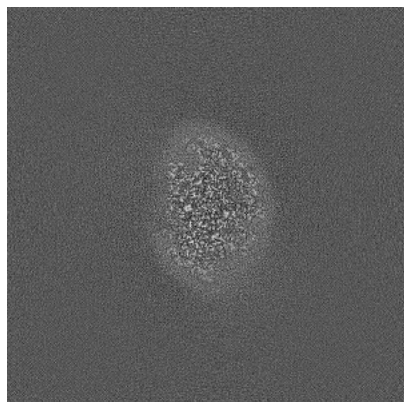


Y Index: 254

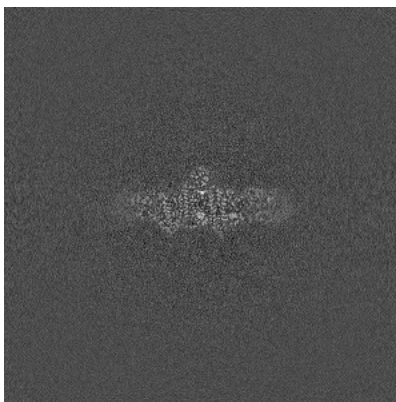


Z Index: 252

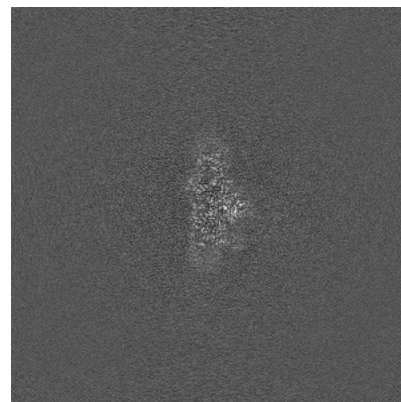
6.3.2 Raw map



X Index: 267



Y Index: 254

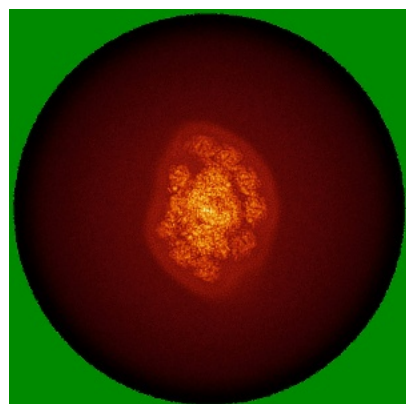


Z Index: 253

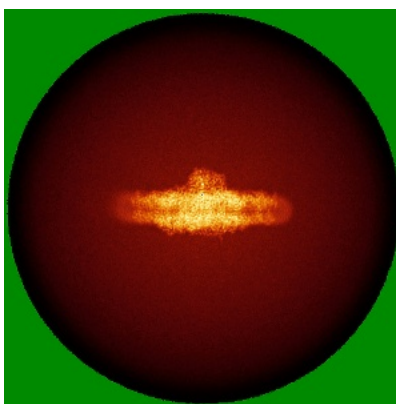
The images above show the largest variance slices of the map in three orthogonal directions.

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

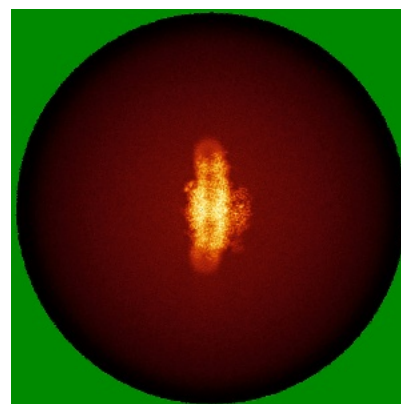
6.4.1 Primary map



X

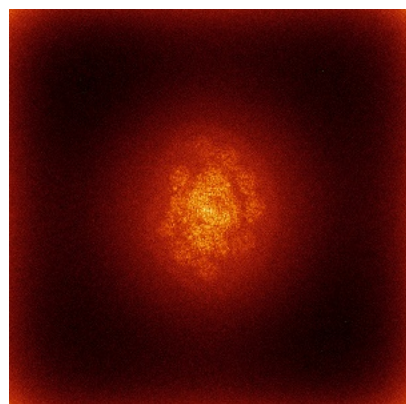


Y

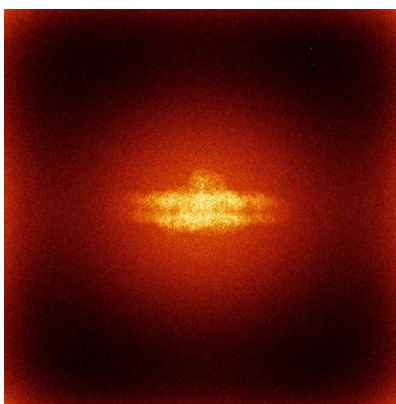


Z

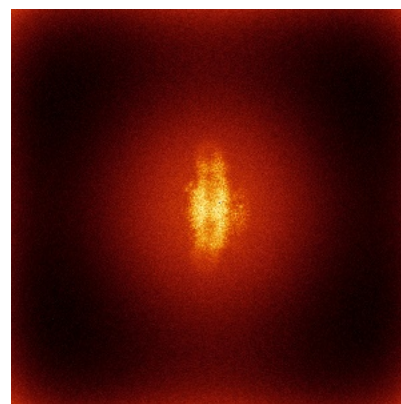
6.4.2 Raw map



X



Y

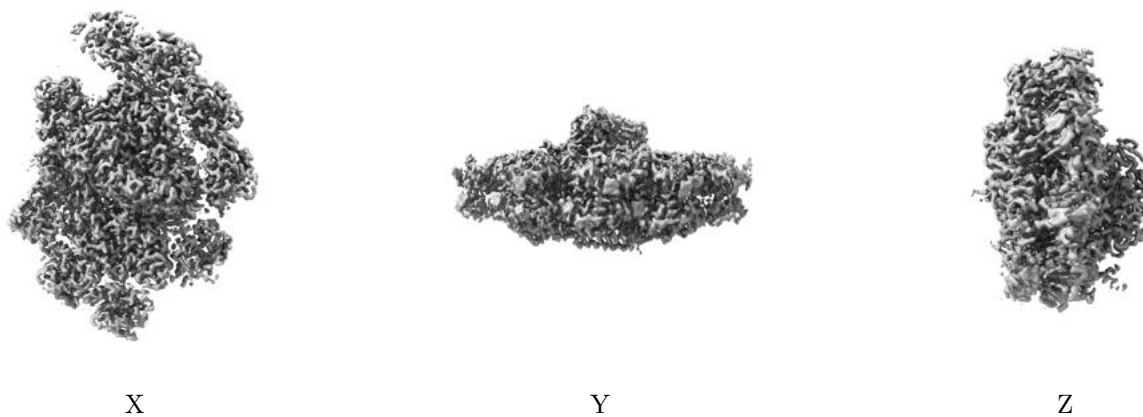


Z

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.

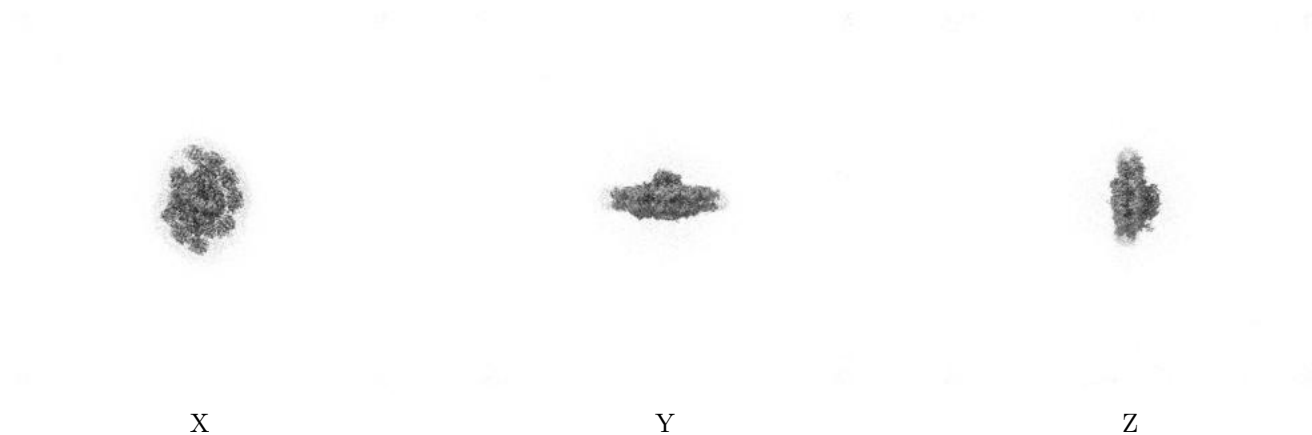
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.293. 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.

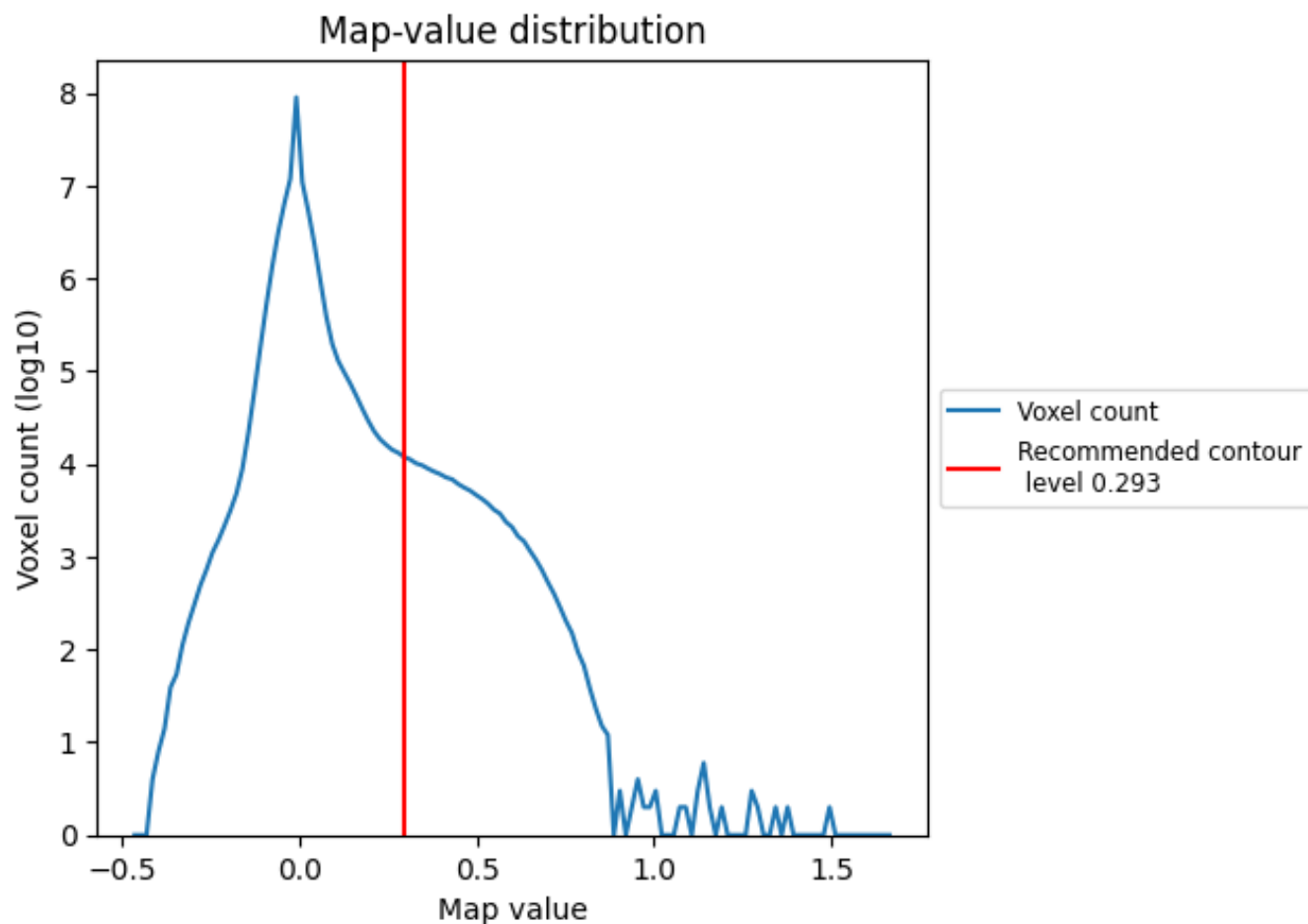
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

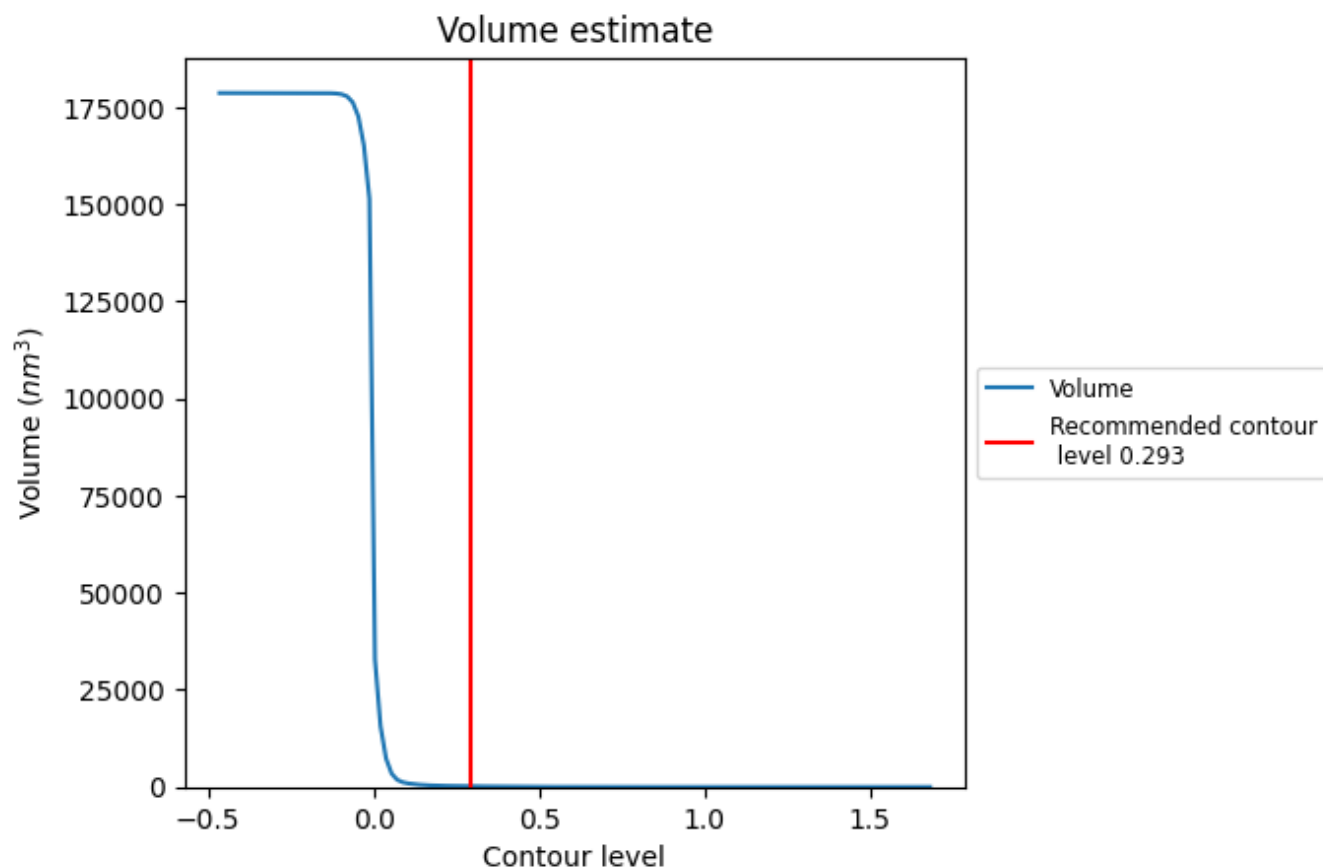
This section contains the results of statistical analysis of the map.

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.

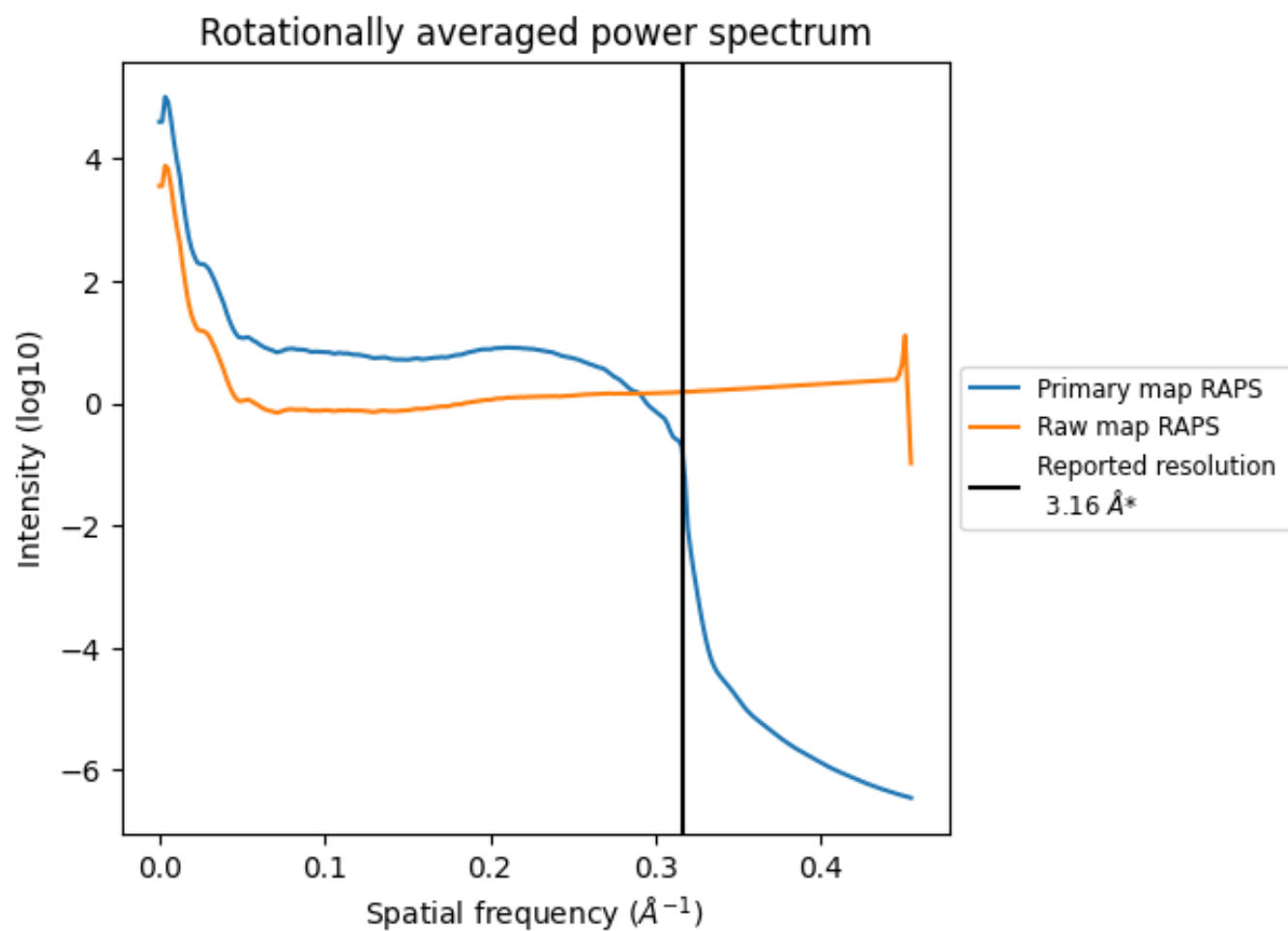
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm^3 ; this corresponds to an approximate mass of 159 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 [i](#)

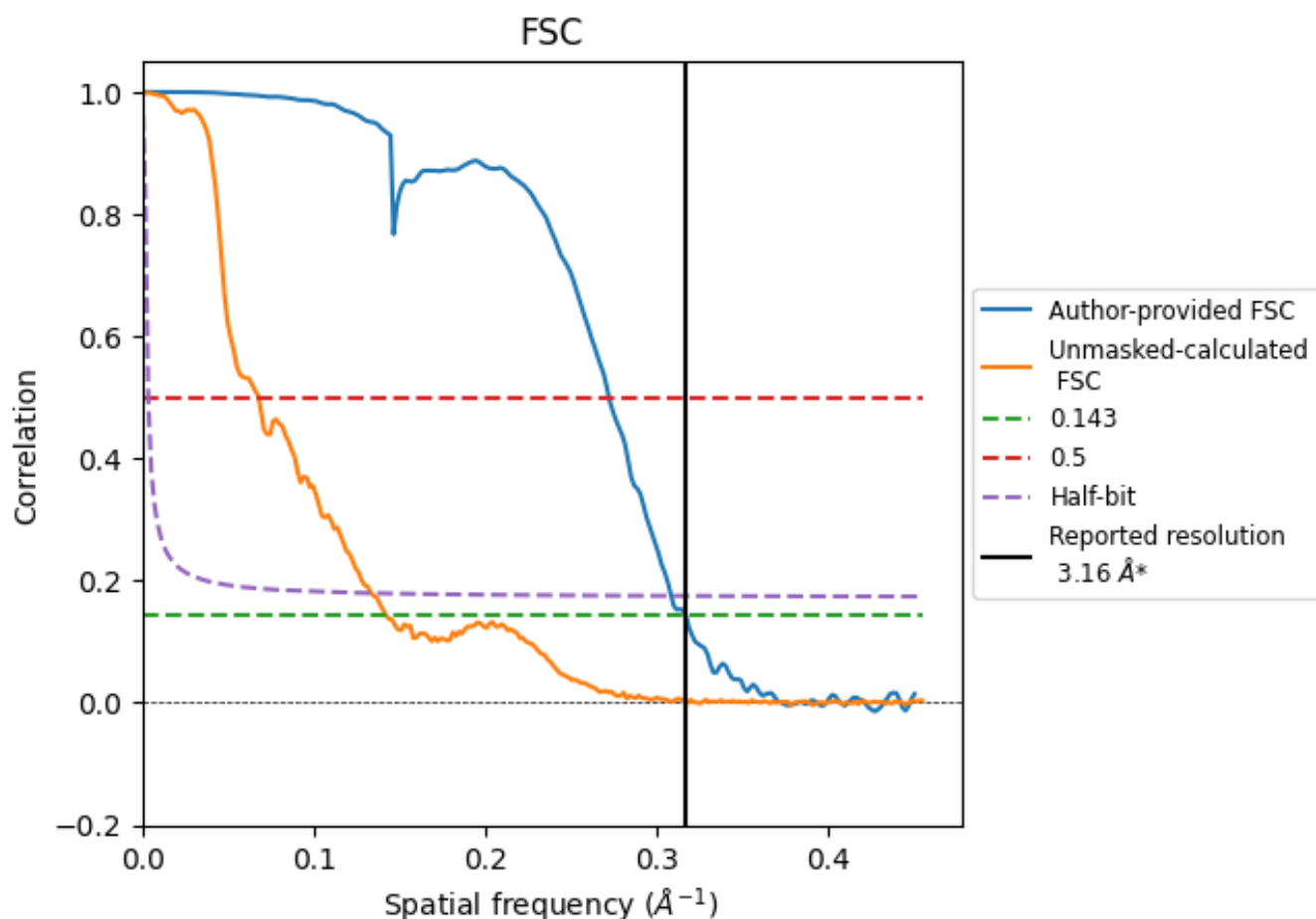


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 \AA^{-1}

8.2 Resolution estimates [i](#)

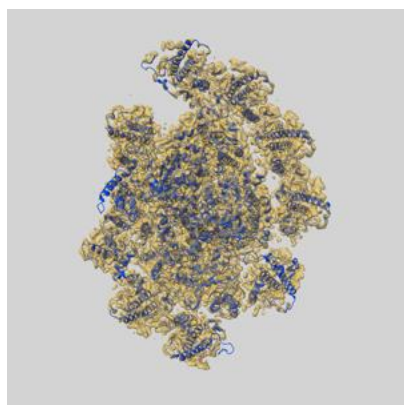
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.68	3.24
Unmasked-calculated*	7.04	14.77	7.49

*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 7.04 differs from the reported value 3.16 by more than 10 %

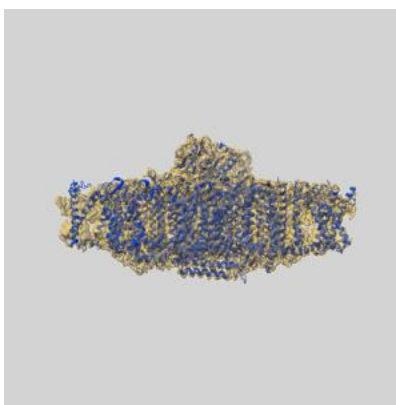
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60292 and PDB model 8ZOG. Per-residue inclusion information can be found in section 3 on page 31.

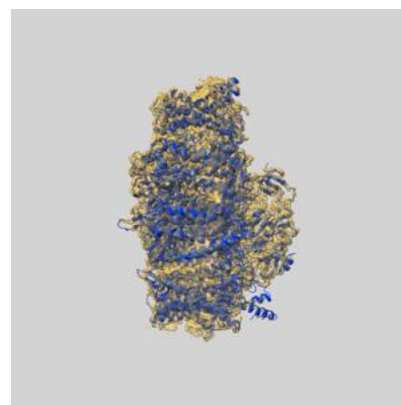
9.1 Map-model overlay [i](#)



X



Y



Z

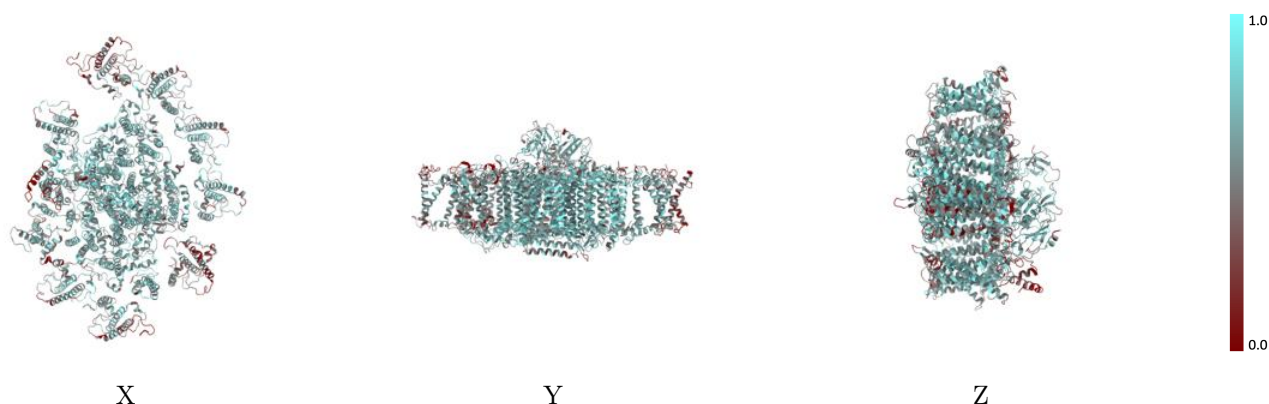
The images above show the 3D surface view of the map at the recommended contour level 0.293 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



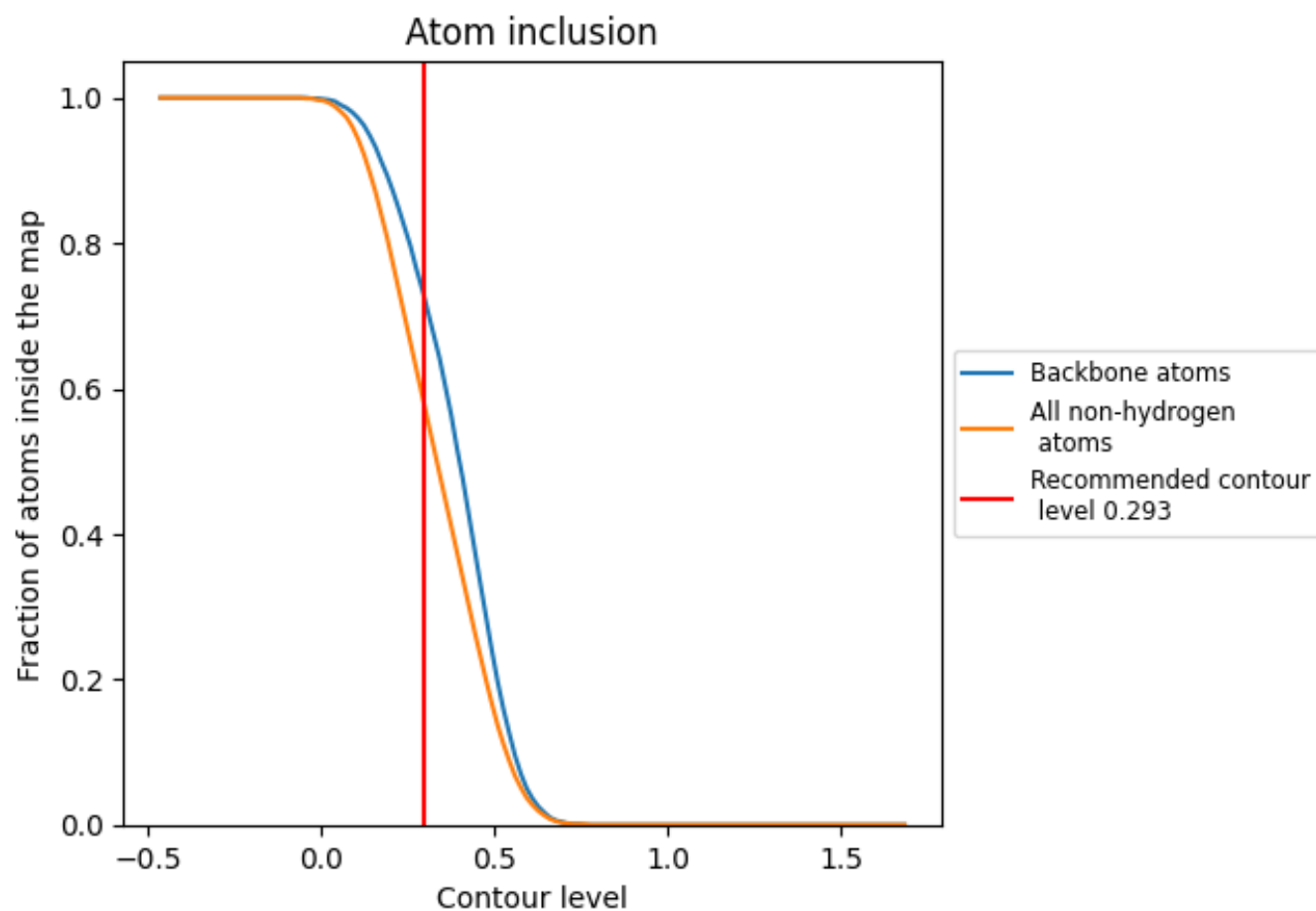
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.293).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 58% 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 (0.293) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5850	 0.4720
1	 0.5640	 0.4770
2	 0.3310	 0.3980
3	 0.5440	 0.4740
4	 0.5870	 0.4750
5	 0.5840	 0.4770
6	 0.3990	 0.4320
7	 0.4560	 0.4360
8	 0.5790	 0.4770
9	 0.5250	 0.4670
a	 0.6600	 0.4850
b	 0.6580	 0.4860
c	 0.7320	 0.5180
d	 0.6210	 0.5030
e	 0.6050	 0.5020
f	 0.5980	 0.4580
g	 0.3840	 0.4000
h	 0.5930	 0.4870
i	 0.6260	 0.5090
j	 0.6150	 0.5000
l	 0.6110	 0.4600
m	 0.5600	 0.4880

