



Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 10:05 PM JST

PDB ID : 8ZOC / pdb_00008zoc
EMDB ID : EMD-60288
Title : Structure of the canthaxanthin mutant PSI-9VCPI supercomplex in Nan-
nochloropsis oceanica
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 2.85 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:

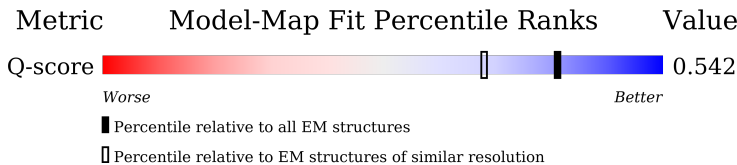
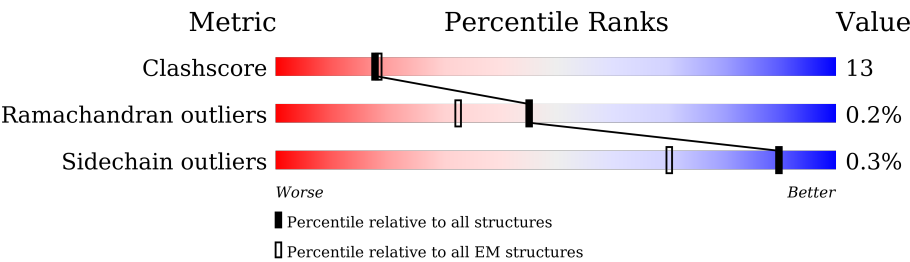
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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

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

The reported resolution of this entry is 2.85 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	11965 (2.35 - 3.35)

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	
2	9	232	
3	8	200	
4	4	202	

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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	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	4	317	X	-	-	-
23	CLA	5	305	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	5	313	X	-	-	-
23	CLA	5	314	X	-	-	-
23	CLA	5	315	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	6	317	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	9	314	X	-	-	-
23	CLA	9	315	X	-	-	-
23	CLA	9	316	X	-	-	-
23	CLA	9	318	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	a	839	X	-	-	-
23	CLA	a	840	X	-	-	-
23	CLA	a	841	X	-	-	-
23	CLA	a	842	X	-	-	-
23	CLA	a	844	X	-	-	-
23	CLA	a	854	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	b	837	X	-	-	-
23	CLA	b	838	X	-	-	-
23	CLA	b	839	X	-	-	-
23	CLA	b	840	X	-	-	-
23	CLA	f	802	X	-	-	-
23	CLA	f	803	X	-	-	-
23	CLA	h	204	X	-	-	-
23	CLA	j	102	X	-	-	-
23	CLA	j	103	X	-	-	-
23	CLA	l	202	X	-	-	-
23	CLA	l	203	X	-	-	-
23	CLA	l	204	X	-	-	-
32	SF4	c	102	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 43772 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			

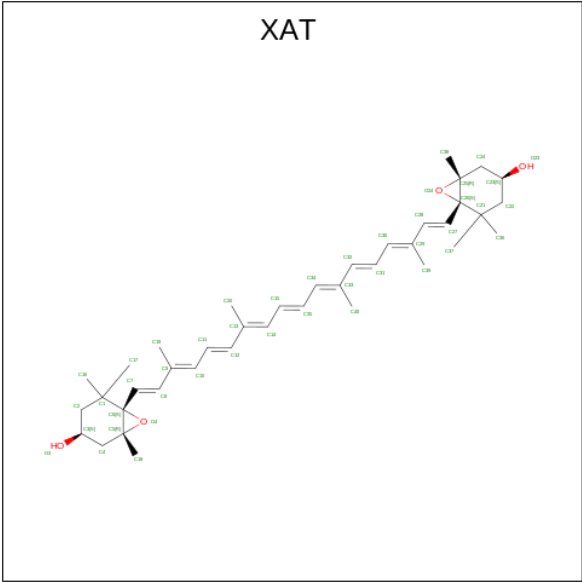
- Molecule 19 is a protein called PsaS.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	55	Total	C	N	O		0	0
			275	165	55	55			

- 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	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	
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	

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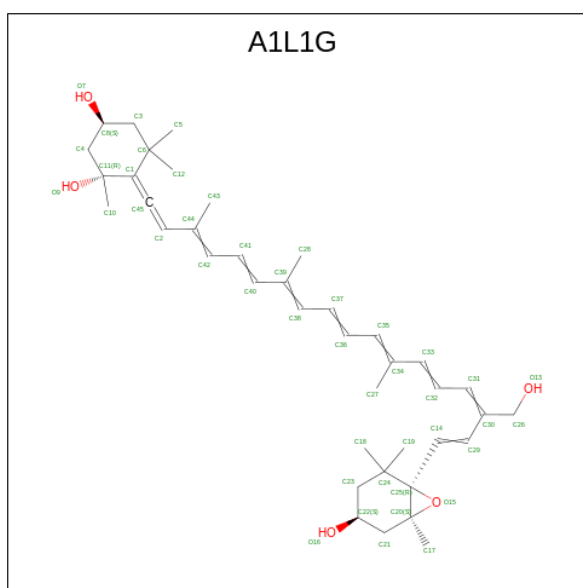
Mol	Chain	Residues	Atoms			AltConf
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	4	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	3	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			44	40	4	
21	6	1	Total	C	O	0
			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	
21	1	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	a	1	Total	C	O	0
			44	40	4	
21	j	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-oxabicyclo[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).



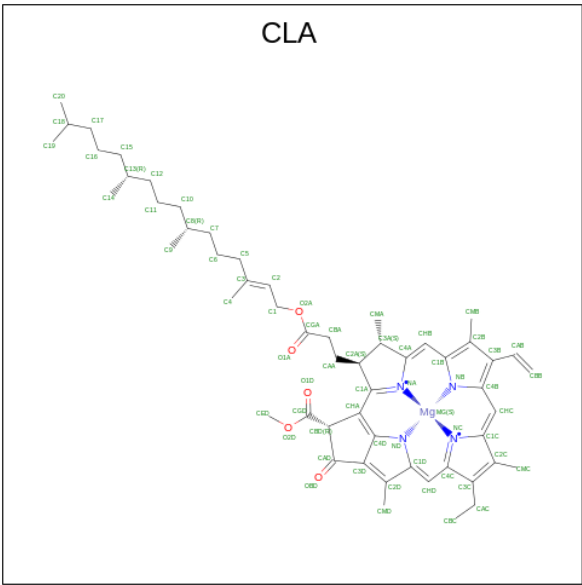
Mol	Chain	Residues	Atoms			AltConf
22	5	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	9	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	
22	3	1	Total	C	O	0
			45	40	5	
22	7	1	Total	C	O	0
			45	40	5	

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Mol	Chain	Residues	Atoms			AltConf
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	
23	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
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
			65	55	1	4	5	
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	6	1	Total	C	Mg	N	O	0
			65	55	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	

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Mol	Chain	Residues	Atoms					AltConf
23	2	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
			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	

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Mol	Chain	Residues	Atoms					AltConf
23	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
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	

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Mol	Chain	Residues	Atoms					AltConf
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
			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	

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

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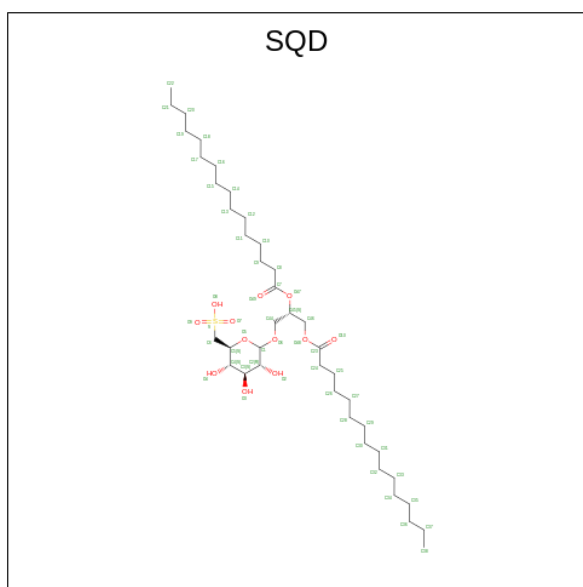
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			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
			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	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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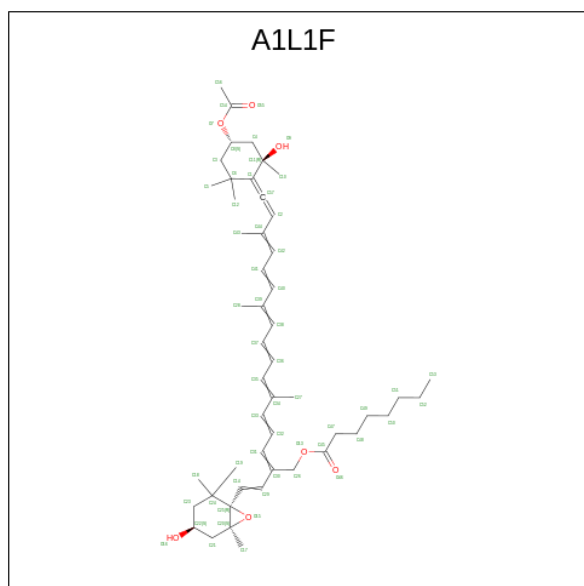
Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	j	1	Total	C	Mg	N	O	0
			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).



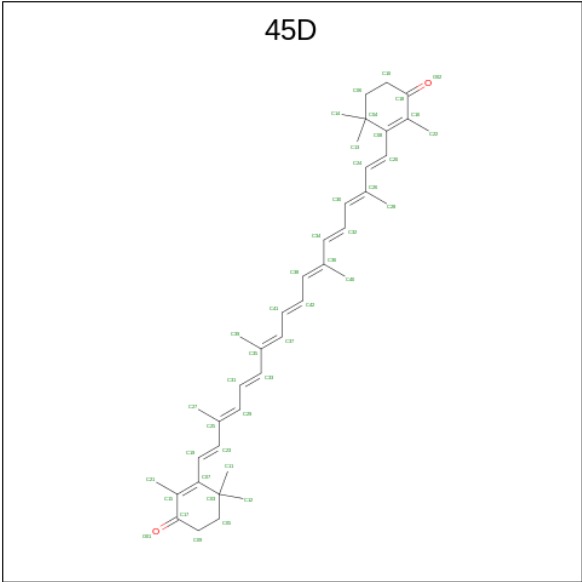
Mol	Chain	Residues	Atoms				AltConf
24	5	1	Total	C	O	S	0
			35	22	12	1	
24	1	1	Total	C	O	S	0
			45	32	12	1	

- 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).



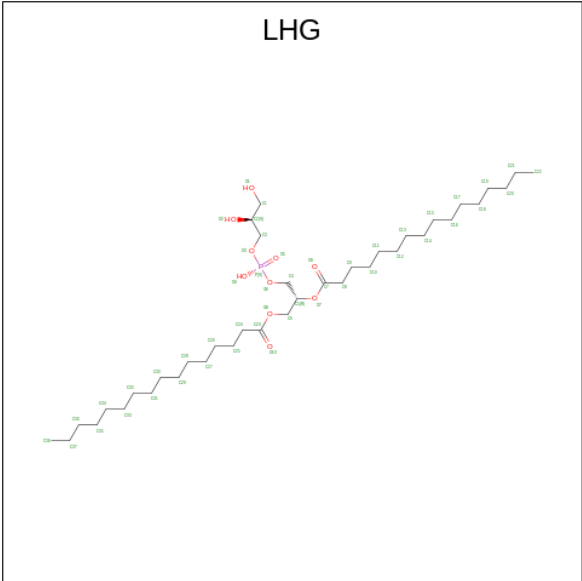
Mol	Chain	Residues	Atoms				AltConf
25	9	1	Total	C	O		0
			57	50	7		
25	8	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			57	50	7		
25	6	1	Total	C	O		0
			53	46	7		
25	1	1	Total	C	O		0
			57	50	7		
25	h	1	Total	C	O		0
			57	50	7		

- Molecule 26 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	9	1	Total	C	O	0
			42	40	2	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



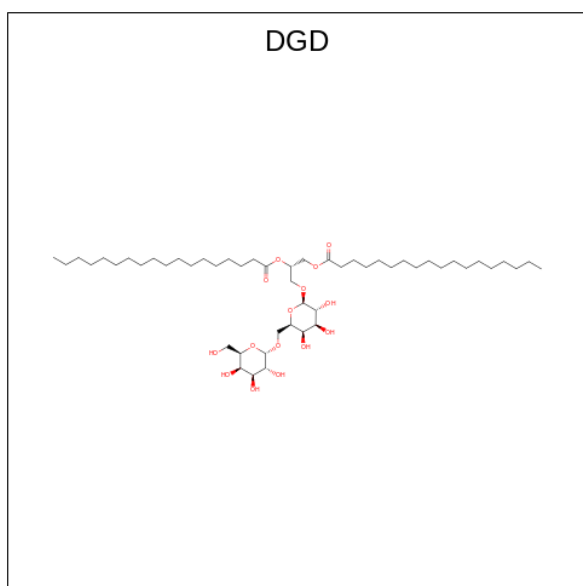
Mol	Chain	Residues	Atoms				AltConf
27	9	1	Total	C	O	P	0
			36	25	10	1	
27	9	1	Total	C	O	P	0
			46	35	10	1	

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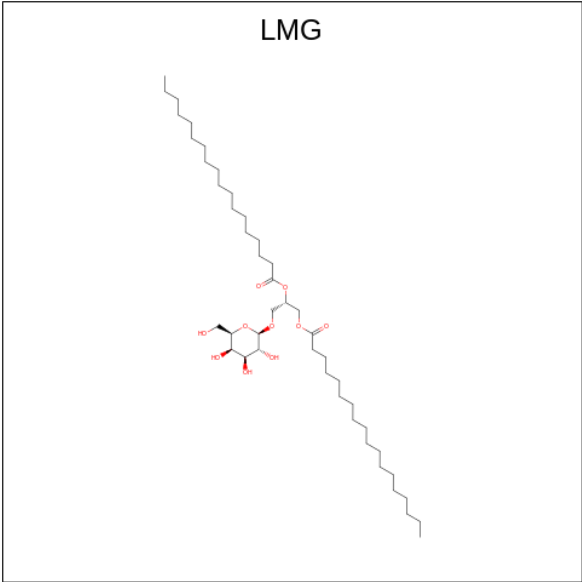
Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	C	O	P	0
			48	37	10	1	
27	a	1	Total	C	O	P	0
			27	16	10	1	
27	b	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



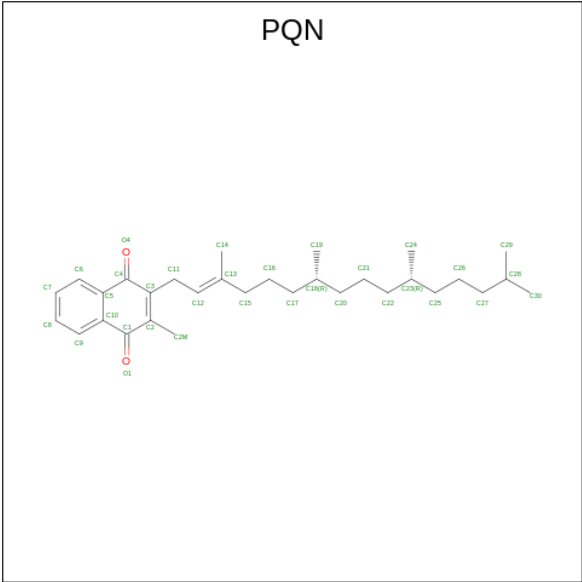
Mol	Chain	Residues	Atoms			AltConf
28	8	1	Total	C	O	0
			40	25	15	
28	4	1	Total	C	O	0
			40	25	15	
28	b	1	Total	C	O	0
			57	42	15	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



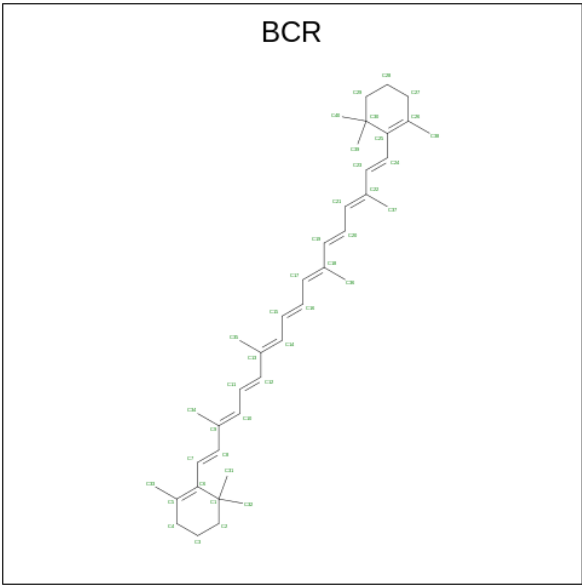
Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			35	25	10	
29	a	1	Total	C	O	0
			34	24	10	
29	j	1	Total	C	O	0
			32	22	10	

- Molecule 30 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



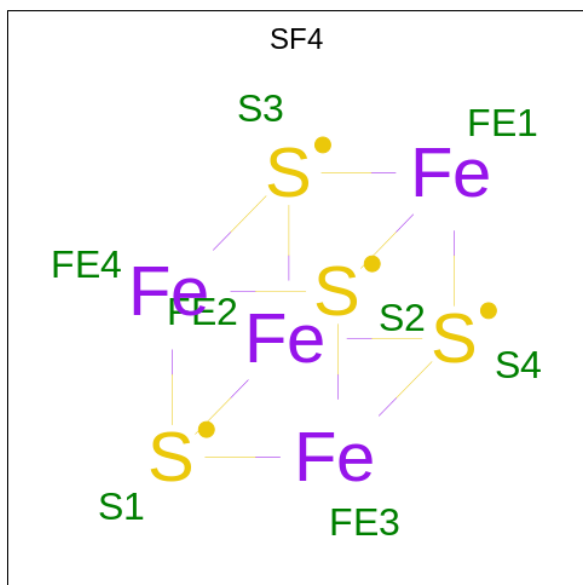
Mol	Chain	Residues	Atoms		AltConf
31	a	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
31	b	1	Total C 40 40	0
31	f	1	Total C 40 40	0
31	f	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	i	1	Total C 40 40	0
31	j	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	l	1	Total C 40 40	0
31	m	1	Total C 40 40	0

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

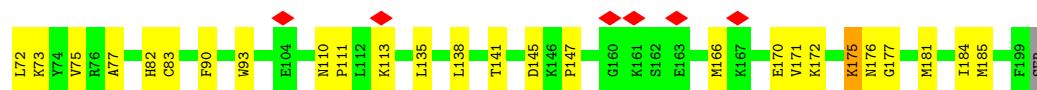


Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total Fe S 8 4 4	0

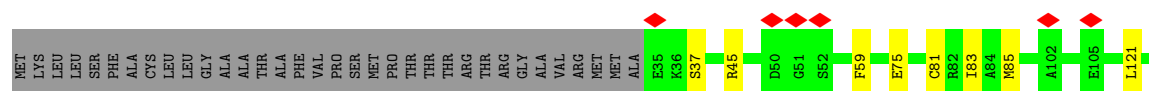
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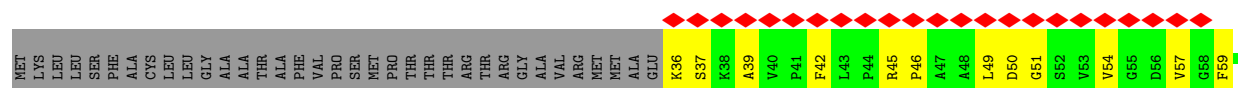
Mol	Chain	Residues	Atoms			AltConf
32	c	1	Total	Fe	S	0
			8	4	4	
32	c	1	Total	Fe	S	0
			8	4	4	



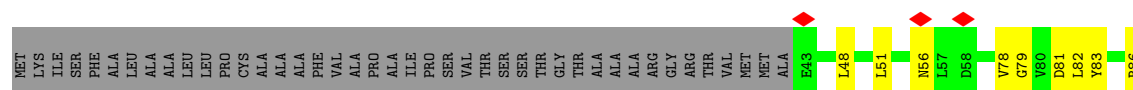
• Molecule 4: VCPI-4/7



• Molecule 4: VCPI-4/7



• Molecule 5: VCPI-3

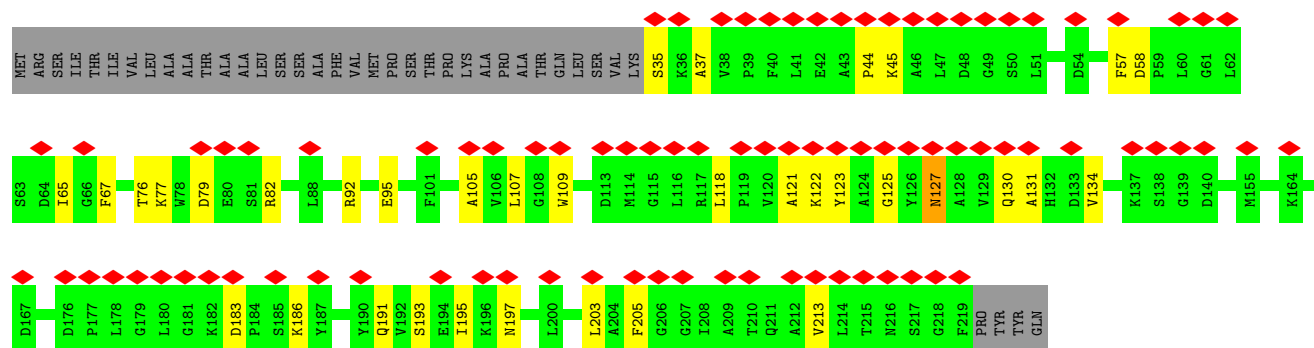
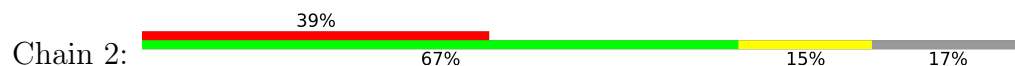


• Molecule 6: VCPI-6

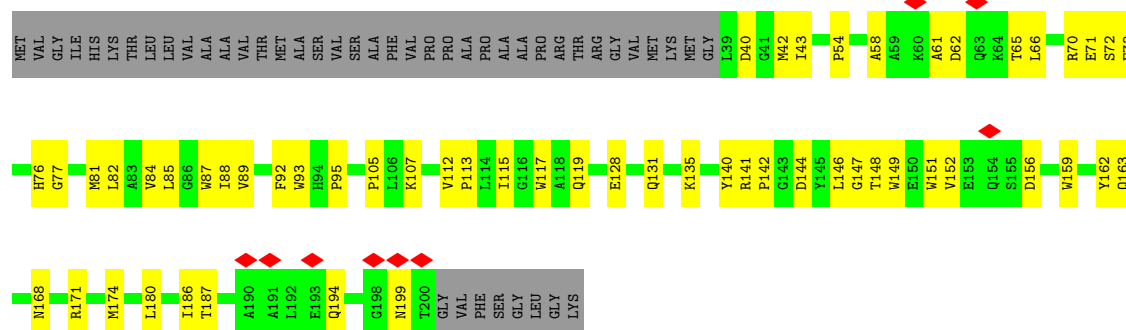




- Molecule 7: VCPI-2

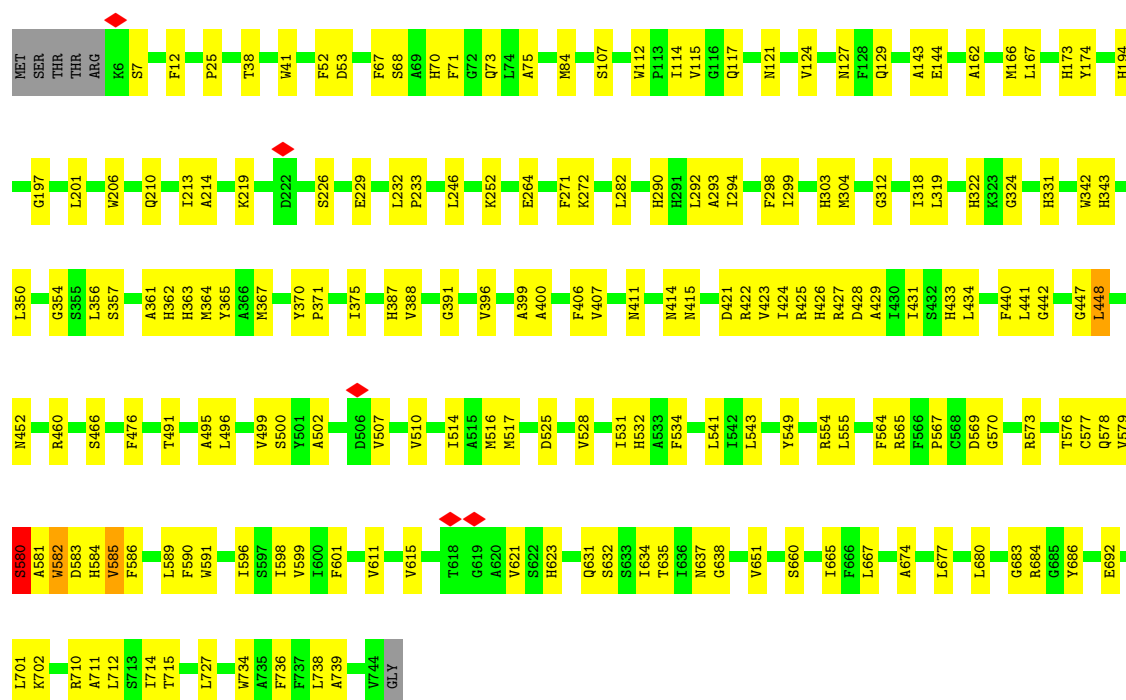


- Molecule 8: VCPI-1



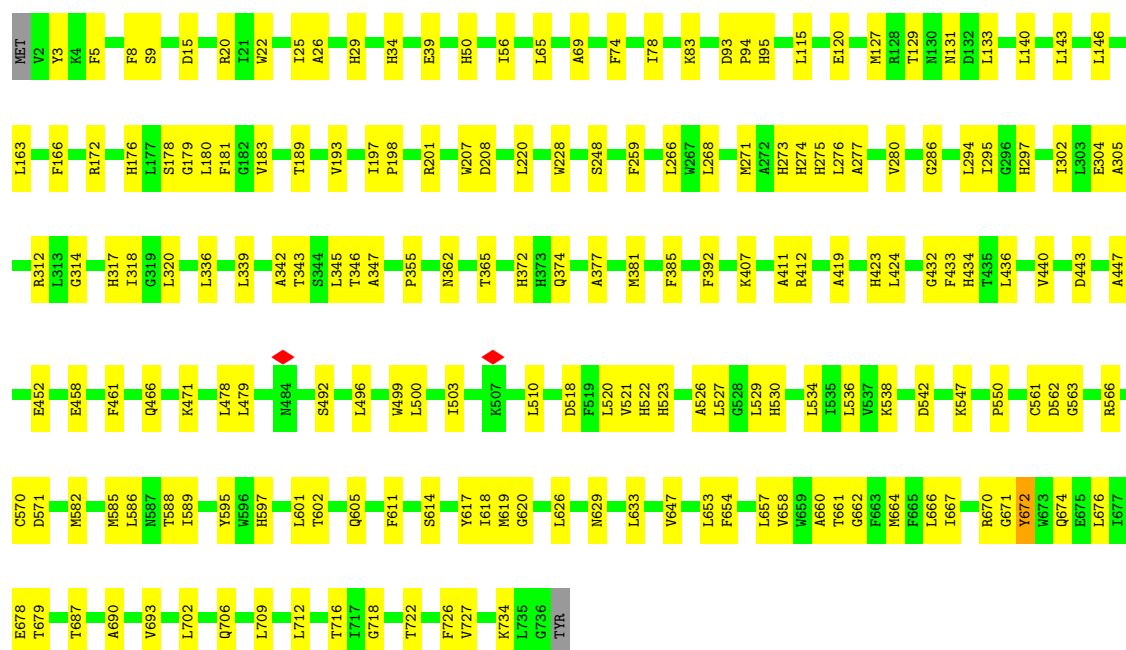
- Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1





• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 75% 25%

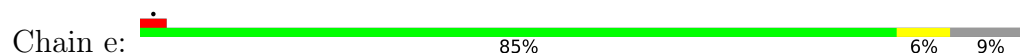


• Molecule 11: Photosystem I reaction center subunit II

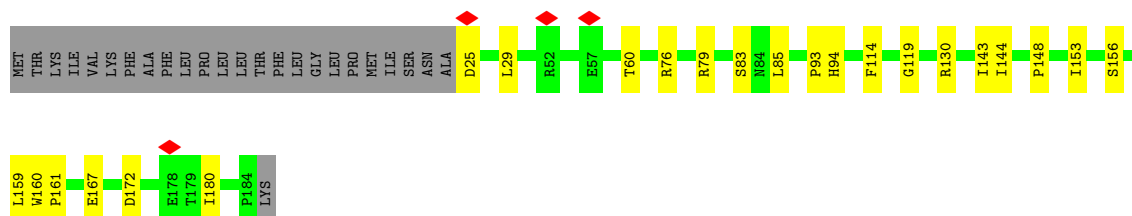
Chain d: 77% 18%



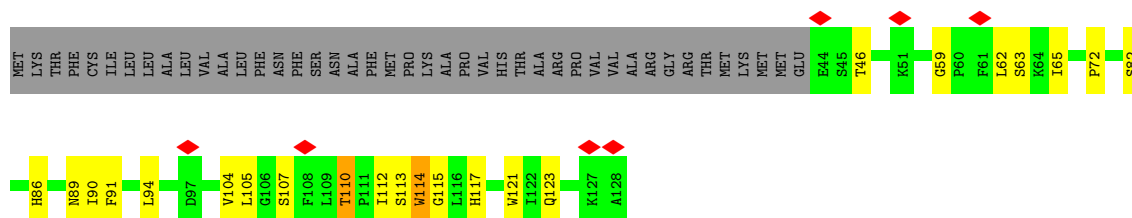
• Molecule 12: Photosystem I reaction center subunit IV



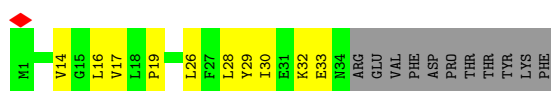
• Molecule 13: Photosystem I reaction center subunit III



• Molecule 14: Psar



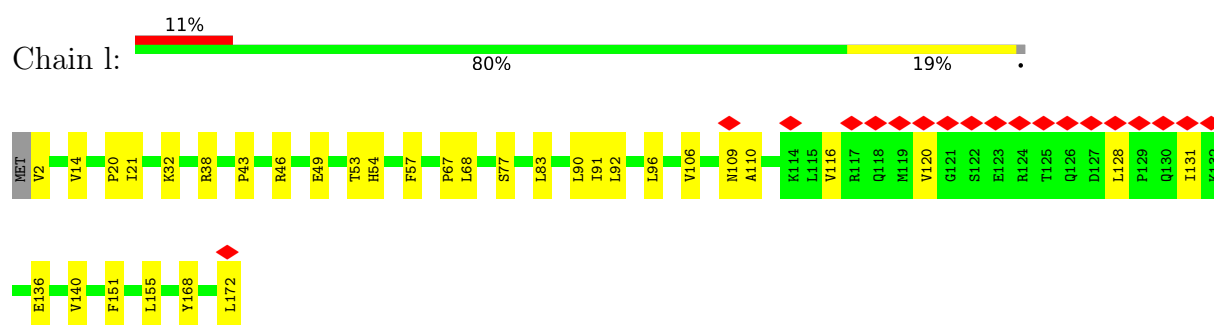
• Molecule 15: Photosystem I reaction center subunit VIII



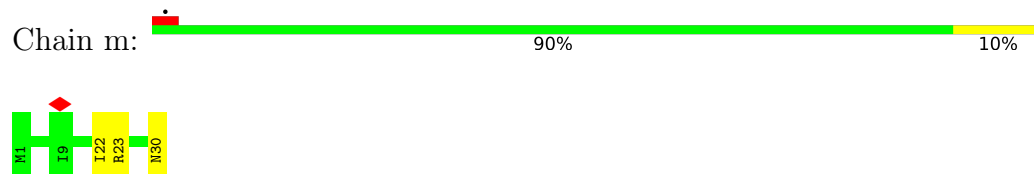
• Molecule 16: Photosystem I reaction center subunit IX



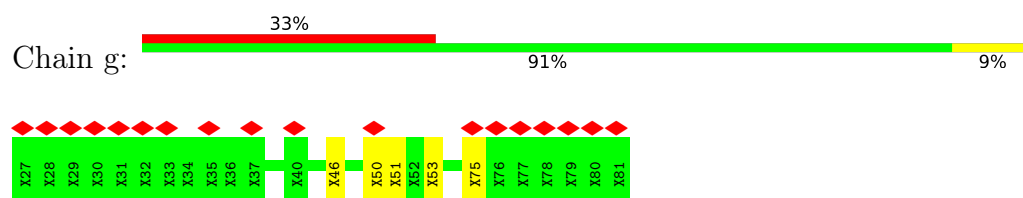
• Molecule 17: PSI subunit V



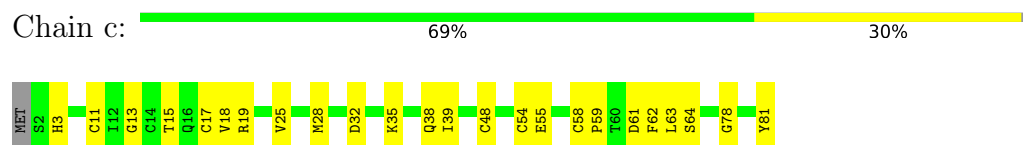
- Molecule 18: PsaM



- 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	64350	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 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.811	Depositor
Minimum map value	-0.420	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.287	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: A1L1F, SF4, BCR, XAT, LMG, CLA, LHG, A1L1G, SQD, 45D, DGD, PQN

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	0.33	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	0.18	0/1248	0.37	0/1700
5	3	0.12	0/1350	0.27	0/1821
6	6	0.17	0/1390	0.31	0/1883
7	2	0.14	0/1405	0.36	0/1904
8	1	0.13	0/1293	0.33	0/1759
9	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
10	b	0.20	0/6080	0.32	1/8302 (0.0%)
11	d	0.12	0/1040	0.32	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	0.14	0/278	0.33	0/378
16	j	0.15	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	0.23	5/30489 (0.0%)	0.33	8/41469 (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	-7.04	1.43	1.52
3	8	44	LEU	C-O	-6.11	1.15	1.23
9	a	581	ALA	CA-C	-5.46	1.45	1.52
14	h	114	TRP	C-O	-5.26	1.18	1.24
9	a	582	TRP	CA-C	-5.03	1.45	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	581	ALA	N-CA-C	-8.62	102.51	113.72
9	a	448	LEU	N-CA-C	-6.08	104.22	111.69
3	8	39	LYS	N-CA-C	-6.06	105.72	113.23
9	a	584	HIS	N-CA-C	-5.82	106.53	113.97
10	b	672	TYR	N-CA-C	-5.56	106.33	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	-5.06	105.47	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	39	0
2	9	1466	0	1470	52	0
3	8	1258	0	1280	32	0
4	4	1268	0	1288	23	0
4	7	1220	0	1209	43	0
5	3	1324	0	1340	23	0
6	6	1352	0	1334	30	0
7	2	1372	0	1347	23	0
8	1	1262	0	1237	42	0
9	a	5827	0	5697	141	0
10	b	5865	0	5710	151	0
11	d	1014	0	1015	19	0
12	e	494	0	495	4	0
13	f	1266	0	1262	21	0
14	h	646	0	649	19	0
15	i	271	0	292	12	0
16	j	339	0	342	21	0
17	l	1283	0	1278	26	0
18	m	210	0	226	3	0
19	g	275	0	62	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	c	596	0	583	20	0
21	1	88	0	112	5	0
21	2	220	0	280	23	0
21	3	176	0	224	19	0
21	4	220	0	280	26	0
21	5	132	0	168	18	0
21	6	176	0	224	20	0
21	7	176	0	224	29	0
21	8	132	0	168	16	0
21	9	88	0	112	14	0
21	a	44	0	56	4	0
21	j	44	0	56	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	14	0
23	2	544	0	452	12	0
23	3	458	0	378	8	0
23	4	613	0	522	33	0
23	5	563	0	472	23	0
23	6	564	0	485	15	0
23	7	576	0	444	22	0
23	8	507	0	429	23	0
23	9	519	0	452	37	0
23	a	2579	0	2562	144	0
23	b	2410	0	2464	136	0
23	f	117	0	115	2	0
23	h	55	0	49	3	0
23	j	100	0	86	10	0
23	l	148	0	123	3	0
24	1	45	0	54	2	0
24	5	35	0	34	1	0
25	1	57	0	0	2	0
25	6	110	0	0	6	0
25	8	57	0	0	2	0
25	9	57	0	0	2	0
25	h	57	0	0	4	0
26	9	42	0	52	8	0
27	9	82	0	110	5	0
27	a	75	0	93	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	b	31	0	32	1	0
28	4	40	0	38	11	0
28	8	40	0	38	2	0
28	b	57	0	72	6	0
29	2	35	0	40	3	0
29	a	34	0	38	10	0
29	j	32	0	34	6	0
30	a	33	0	46	5	0
30	b	33	0	46	3	0
31	a	160	0	224	15	0
31	b	240	0	336	26	0
31	f	80	0	112	15	0
31	h	80	0	112	8	0
31	i	40	0	56	2	0
31	j	40	0	56	9	0
31	l	80	0	112	14	0
31	m	40	0	56	1	0
32	a	8	0	0	0	0
32	c	16	0	0	3	0
All	All	43772	0	42670	1138	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 13.

All (1138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:193:ALA:HB1	28:4:318:DGD:HE62	1.13	1.13
4:4:193:ALA:HB1	28:4:318:DGD:C6E	1.85	1.05
28:4:318:DGD:O4E	28:4:318:DGD:O5E	1.61	1.02
21:2:303:XAT:H32	23:2:308:CLA:HAB	1.52	0.90
21:5:302:XAT:H12	23:5:307:CLA:HAB	1.53	0.90
9:a:531:ILE:HD12	23:a:801:CLA:H172	1.63	0.80
23:a:806:CLA:O1A	23:a:814:CLA:HBA1	1.81	0.80
21:8:303:XAT:H12	23:8:312:CLA:HAB	1.67	0.77
4:4:193:ALA:CB	28:4:318:DGD:HE62	2.07	0.75
23:b:825:CLA:HMA1	31:b:845:BCR:H17C	1.66	0.75
21:4:303:XAT:H12	23:4:308:CLA:HAB	1.67	0.75
23:1:312:CLA:HHC	23:1:312:CLA:HBB1	1.69	0.75
21:2:303:XAT:H181	23:2:314:CLA:HBB1	1.70	0.73
2:9:179:LEU:HD22	26:9:305:45D:H113	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:167:GLU:HG3	13:f:172:ASP:HB3	1.73	0.71
23:4:317:CLA:H2A	28:4:318:DGD:HE62	1.73	0.70
16:j:22:THR:HA	16:j:25:PHE:CE1	2.28	0.69
8:1:43:ILE:O	8:1:70:ARG:NH2	2.25	0.69
23:b:833:CLA:H72	31:b:845:BCR:H391	1.72	0.69
23:b:807:CLA:H151	23:b:828:CLA:HBB2	1.74	0.69
1:5:179:LEU:HD12	13:f:159:LEU:HD11	1.75	0.69
31:a:847:BCR:H362	31:a:848:BCR:H21C	1.73	0.69
9:a:363:HIS:ND1	23:a:819:CLA:OBD	2.26	0.68
9:a:569:ASP:OD2	9:a:573:ARG:NH2	2.27	0.68
21:4:302:XAT:H14	23:4:310:CLA:H12	1.76	0.67
8:1:194:GLN:HG3	8:1:199:ASN:HB3	1.77	0.67
10:b:273:HIS:HD1	23:b:817:CLA:HAB	1.58	0.67
8:1:146:LEU:HD13	23:a:844:CLA:H91	1.77	0.66
23:a:804:CLA:HED1	16:j:15:LEU:HD22	1.76	0.66
23:4:317:CLA:HAA2	28:4:318:DGD:HE5	1.77	0.66
10:b:9:SER:HB2	28:b:848:DGD:HE62	1.78	0.66
1:5:113:ARG:NH1	1:5:116:GLU:OE1	2.29	0.65
23:a:834:CLA:H142	31:b:846:BCR:H15C	1.79	0.65
15:i:29:TYR:HA	15:i:32:LYS:HE2	1.78	0.65
16:j:31:ARG:HD3	21:j:101:XAT:H222	1.77	0.65
9:a:112:TRP:HB3	21:j:101:XAT:H373	1.77	0.65
10:b:304:GLU:HG2	10:b:318:ILE:HG13	1.79	0.65
21:4:303:XAT:H193	23:4:308:CLA:H142	1.78	0.65
21:6:303:XAT:H30	23:6:308:CLA:HAB	1.77	0.65
8:1:70:ARG:NH1	8:1:73:GLU:OE1	2.28	0.65
10:b:295:ILE:HG13	23:b:820:CLA:HED1	1.77	0.65
14:h:114:TRP:HA	14:h:117:HIS:NE2	2.11	0.65
10:b:336:LEU:HD21	23:b:829:CLA:HAB	1.78	0.65
9:a:356:LEU:HD11	23:a:820:CLA:H71	1.78	0.64
6:6:236:ALA:HB1	6:6:247:VAL:HG21	1.77	0.64
2:9:191:ALA:O	2:9:195:ASN:ND2	2.30	0.64
13:f:79:ARG:NH1	16:j:35:ASP:O	2.30	0.64
13:f:25:ASP:N	13:f:29:LEU:O	2.30	0.64
6:6:162:LEU:HG	23:h:204:CLA:HBC2	1.80	0.64
23:b:813:CLA:H121	23:b:818:CLA:H72	1.79	0.64
9:a:197:GLY:O	9:a:201:LEU:HB2	1.97	0.64
23:b:823:CLA:HBB1	23:b:837:CLA:H151	1.79	0.64
6:6:246:SER:HB2	23:6:315:CLA:CAA	2.28	0.63
23:a:808:CLA:HMB2	31:j:104:BCR:HC8	1.79	0.63
21:4:305:XAT:H363	21:3:301:XAT:H10	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:362:HIS:HA	9:a:365:TYR:CE1	2.33	0.63
21:4:304:XAT:H32	23:4:313:CLA:HAB	1.80	0.63
4:7:120:ALA:HB1	23:7:311:CLA:HMD1	1.78	0.63
9:a:684:ARG:H	10:b:570:CYS:HB2	1.63	0.63
16:j:21:PHE:HA	23:j:103:CLA:HBB2	1.80	0.63
1:5:120:GLY:O	1:5:124:MET:HG3	1.98	0.63
9:a:114:ILE:HB	21:j:101:XAT:H372	1.81	0.63
9:a:589:LEU:HD21	23:a:831:CLA:HBC1	1.81	0.63
21:3:305:XAT:H32	23:3:313:CLA:HAB	1.80	0.63
16:j:26:VAL:HG11	31:j:104:BCR:H24C	1.81	0.63
10:b:424:LEU:HD13	10:b:534:LEU:HA	1.81	0.63
4:7:136:VAL:HG11	23:b:820:CLA:HBA1	1.81	0.62
10:b:129:THR:HG22	10:b:131:ASN:H	1.63	0.62
1:5:130:PHE:CE1	21:5:302:XAT:O24	2.52	0.62
4:7:136:VAL:HG22	23:7:312:CLA:HMA1	1.80	0.62
9:a:298:PHE:HE1	23:a:822:CLA:HAB	1.64	0.62
10:b:115:LEU:HA	10:b:365:THR:HG22	1.80	0.62
9:a:298:PHE:CE1	23:a:822:CLA:HAB	2.35	0.62
23:8:305:CLA:CGA	28:8:315:DGD:HE5	2.29	0.62
21:7:303:XAT:H362	23:7:308:CLA:H51	1.81	0.62
11:d:86:ARG:HB2	11:d:96:LEU:HD11	1.82	0.62
25:h:203:A1L1F:C4	25:h:203:A1L1F:C12	2.78	0.62
9:a:162:ALA:O	9:a:166:MET:HG2	2.00	0.62
10:b:561:CYS:SG	10:b:563:GLY:N	2.71	0.62
23:b:830:CLA:HAB	23:b:837:CLA:HBB2	1.82	0.62
24:5:316:SQD:H2	21:4:301:XAT:H373	1.82	0.62
7:2:76:THR:O	7:2:82:ARG:NH1	2.33	0.62
11:d:12:LYS:HB2	11:d:51:LYS:HB3	1.82	0.61
1:5:225:ILE:HG22	23:5:314:CLA:HAB	1.82	0.61
9:a:167:LEU:HD11	23:a:810:CLA:H193	1.83	0.61
23:a:818:CLA:C3D	29:a:853:LMG:HC91	2.30	0.61
10:b:660:ALA:HB3	23:b:804:CLA:HBB2	1.83	0.61
4:7:144:GLU:HB2	10:b:294:LEU:HD11	1.82	0.61
21:5:302:XAT:H162	23:5:307:CLA:H2	1.82	0.61
1:5:190:ARG:NH1	1:5:191:GLU:O	2.34	0.61
2:9:182:ALA:HB3	2:9:190:GLU:HG2	1.82	0.61
23:4:317:CLA:H2A	28:4:318:DGD:C6E	2.30	0.61
5:3:199:ALA:O	5:3:203:MET:HG3	2.01	0.61
8:1:186:ILE:HG13	8:1:187:THR:HG23	1.83	0.61
25:1:304:A1L1F:C2	23:a:844:CLA:H11	2.31	0.61
9:a:121:ASN:HB3	9:a:129:GLN:HB3	1.83	0.61

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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	0.61
11:d:88:TYR:HB2	11:d:92:ASP:HB2	1.81	0.60
6:6:109:GLY:O	10:b:312:ARG:NH1	2.34	0.60
5:3:92:HIS:HB3	5:3:197:MET:SD	2.42	0.60
10:b:412:ARG:NH2	23:b:830:CLA:O1D	2.35	0.60
4:4:170:MET:HE1	23:4:313:CLA:H43	1.84	0.60
5:3:83:TYR:OH	5:3:163:ARG:NH1	2.35	0.60
21:2:303:XAT:H363	23:2:308:CLA:H2	1.84	0.60
8:1:72:SER:O	8:1:76:HIS:ND1	2.28	0.59
9:a:507:VAL:HG22	9:a:517:MET:HG3	1.85	0.59
23:b:831:CLA:HBC3	31:f:804:BCR:H362	1.82	0.59
4:4:185:PHE:CZ	21:4:303:XAT:H30	2.37	0.59
10:b:29:HIS:ND1	23:b:807:CLA:O1A	2.28	0.59
23:8:305:CLA:HAA2	28:8:315:DGD:HE5	1.82	0.59
7:2:44:PRO:HG3	7:2:58:ASP:HB3	1.83	0.59
4:7:50:ASP:OD1	4:7:51:GLY:N	2.32	0.59
9:a:429:ALA:O	9:a:433:HIS:ND1	2.31	0.59
23:a:820:CLA:H92	23:a:830:CLA:H91	1.84	0.59
3:8:185:MET:HE2	23:8:308:CLA:HBB2	1.83	0.59
9:a:53:ASP:OD2	9:a:343:HIS:NE2	2.35	0.59
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.59
21:8:302:XAT:H32	23:8:307:CLA:HAB	1.85	0.59
2:9:185:PRO:HA	23:9:313:CLA:HBA2	1.85	0.58
23:a:804:CLA:ND	16:j:12:PRO:HG3	2.17	0.58
23:a:833:CLA:HBC2	23:a:840:CLA:HMC2	1.83	0.58
4:7:88:THR:HG21	21:7:304:XAT:H12	1.85	0.58
9:a:70:HIS:ND1	23:a:814:CLA:OBD	2.31	0.58
17:l:38:ARG:O	17:l:46:ARG:NH2	2.35	0.58
23:a:818:CLA:C1D	29:a:853:LMG:H291	2.34	0.58
22:1:301:A1L1G:C18	23:1:306:CLA:HAC2	2.32	0.58
10:b:69:ALA:HB2	10:b:133:LEU:HB2	1.86	0.58
10:b:74:PHE:O	10:b:78:ILE:HG12	2.04	0.58
31:b:842:BCR:H23C	31:h:202:BCR:H323	1.86	0.58
9:a:107:SER:HB2	9:a:124:VAL:HG11	1.85	0.58
10:b:178:SER:HB3	10:b:286:GLY:HA3	1.86	0.58
11:d:97:HIS:HB3	11:d:98:PRO:HD3	1.86	0.58
21:5:301:XAT:H14	23:5:309:CLA:H12	1.86	0.58
21:6:305:XAT:H373	27:b:847:LHG:HC61	1.86	0.58
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.57
1:5:155:VAL:HG21	23:5:309:CLA:HAA2	1.86	0.57
2:9:62:PHE:HZ	26:9:305:45D:H062	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:6:317:CLA:HAA1	14:h:121:TRP:CD1	2.39	0.57
31:f:801:BCR:HC32	23:j:102:CLA:H43	1.86	0.57
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.57
9:a:517:MET:HE1	9:a:623:HIS:NE2	2.19	0.57
9:a:324:GLY:HA3	27:a:846:LHG:HC32	1.87	0.57
9:a:598:ILE:HG13	23:a:801:CLA:H192	1.86	0.57
3:8:60:PHE:HE1	23:8:305:CLA:HBC3	1.70	0.57
5:3:86:ARG:NH1	5:3:89:GLU:OE1	2.38	0.57
21:2:303:XAT:C36	23:2:308:CLA:H2	2.35	0.57
9:a:292:LEU:HD21	23:a:818:CLA:CAB	2.34	0.57
23:b:804:CLA:CGA	23:b:804:CLA:H3A	2.34	0.57
2:9:107:LEU:HD11	2:9:140:ILE:HD11	1.87	0.57
9:a:734:TRP:NE1	23:a:829:CLA:O1A	2.36	0.57
4:4:136:VAL:HG22	23:4:312:CLA:HMA1	1.87	0.57
1:5:111:TRP:NE1	23:5:308:CLA:O1A	2.32	0.56
23:6:317:CLA:C2	23:b:840:CLA:HBB2	2.34	0.56
9:a:651:VAL:HG22	9:a:739:ALA:HB3	1.87	0.56
23:b:806:CLA:HBA1	23:b:813:CLA:HBA1	1.87	0.56
1:5:112:LEU:HD22	23:5:307:CLA:H12	1.86	0.56
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.56
6:6:248:PRO:HG2	23:6:315:CLA:HBC2	1.87	0.56
10:b:693:VAL:HG11	23:b:801:CLA:HAB	1.87	0.56
21:9:303:XAT:H363	3:8:135:LEU:HD12	1.86	0.56
5:3:48:LEU:HD13	5:3:51:LEU:HD12	1.87	0.56
4:7:185:PHE:CD2	21:7:303:XAT:H12	2.39	0.56
10:b:39:GLU:HB3	10:b:163:LEU:HD11	1.87	0.56
2:9:222:ASP:HB2	2:9:230:LEU:HD13	1.86	0.56
23:a:802:CLA:CGA	23:a:802:CLA:H3A	2.35	0.56
23:a:818:CLA:CHD	29:a:853:LMG:H291	2.36	0.56
11:d:105:GLU:HG2	20:c:19:ARG:HB3	1.88	0.56
17:l:54:HIS:HA	17:l:57:PHE:CE2	2.41	0.56
23:3:312:CLA:H42	31:a:848:BCR:H272	1.85	0.56
9:a:114:ILE:HG13	9:a:115:VAL:HG13	1.86	0.56
29:a:853:LMG:H112	29:a:853:LMG:C9	2.35	0.56
29:a:853:LMG:H112	29:a:853:LMG:O8	2.05	0.56
23:b:821:CLA:HHB	23:b:822:CLA:H2	1.88	0.56
23:a:826:CLA:HBA1	23:a:830:CLA:H193	1.86	0.56
15:i:26:LEU:HD13	31:l:205:BCR:HC8	1.86	0.56
5:3:182:PHE:HZ	23:3:313:CLA:HED3	1.70	0.56
23:a:854:CLA:H112	16:j:14:LEU:HD22	1.88	0.56
17:l:92:LEU:HB3	31:l:205:BCR:H401	1.88	0.56

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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
9:a:441:LEU:HB3	9:a:534:PHE:HB2	1.88	0.55
8:1:88:ILE:HG22	8:1:92:PHE:HE1	1.71	0.55
9:a:660:SER:HB2	10:b:447:ALA:HB1	1.88	0.55
10:b:582:MET:HG3	10:b:712:LEU:HD21	1.87	0.55
23:b:805:CLA:H18	15:i:14:VAL:HG22	1.87	0.55
2:9:85:GLY:O	2:9:89:MET:HG3	2.07	0.55
2:9:93:ILE:HG13	21:9:304:XAT:H8	1.89	0.55
9:a:651:VAL:HG21	9:a:736:PHE:HA	1.88	0.55
23:a:822:CLA:HBC3	23:a:828:CLA:H172	1.87	0.55
10:b:521:VAL:HG21	10:b:595:TYR:HB2	1.89	0.55
2:9:117:TRP:O	2:9:120:TRP:CD1	2.60	0.55
10:b:93:ASP:OD1	10:b:95:HIS:ND1	2.33	0.55
23:a:841:CLA:H72	31:f:801:BCR:H17C	1.88	0.55
23:a:841:CLA:H92	31:f:801:BCR:H15C	1.88	0.55
3:8:75:VAL:HG23	23:8:307:CLA:HMA2	1.89	0.55
23:a:825:CLA:H12	31:a:849:BCR:H14C	1.88	0.55
2:9:153:PHE:HA	17:l:151:PHE:HE2	1.71	0.55
10:b:5:PHE:HB2	15:i:30:ILE:HA	1.89	0.55
6:6:248:PRO:HD2	25:6:304:A1L1F:C56	2.36	0.55
2:9:162:LYS:NZ	23:9:312:CLA:O1A	2.40	0.55
4:4:185:PHE:CE2	21:4:303:XAT:H30	2.42	0.55
7:2:35:SER:OG	7:2:37:ALA:O	2.22	0.55
10:b:633:LEU:HD22	10:b:726:PHE:HA	1.89	0.55
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.54
9:a:388:VAL:HG12	9:a:596:ILE:HG23	1.89	0.54
16:j:14:LEU:HD21	29:j:105:LMG:H141	1.89	0.54
22:5:303:A1L1G:C41	23:5:312:CLA:HMC1	2.38	0.54
25:8:304:A1L1F:C2	18:m:23:ARG:HD3	2.38	0.54
9:a:213:ILE:HG23	9:a:233:PRO:HB3	1.87	0.54
9:a:591:TRP:HE1	23:b:804:CLA:C1D	2.21	0.54
10:b:355:PRO:HG3	23:b:818:CLA:HBA1	1.90	0.54
6:6:154:PHE:HB2	21:6:303:XAT:H22	1.89	0.54
9:a:210:GLN:HA	9:a:214:ALA:HB3	1.89	0.54
23:a:829:CLA:H101	31:j:104:BCR:H341	1.89	0.54
20:c:15:THR:HG22	20:c:28:MET:HG3	1.89	0.54
2:9:149:ALA:O	2:9:153:PHE:HD1	1.90	0.54
4:4:140:SER:OG	16:j:1:MET:SD	2.57	0.54
9:a:219:LYS:HD3	9:a:246:LEU:HB3	1.90	0.54
4:4:121:LEU:HD23	4:4:124:ILE:HD12	1.90	0.54
10:b:443:ASP:OD1	10:b:617:TYR:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:32:VAL:HG11	20:c:35:LYS:HD3	1.89	0.54
8:1:115:ILE:O	8:1:119:GLN:NE2	2.40	0.54
9:a:667:LEU:HD11	10:b:619:MET:HB2	1.89	0.54
4:4:83:ILE:HD11	21:4:302:XAT:H362	1.90	0.53
9:a:290:HIS:HB2	23:a:819:CLA:C1B	2.37	0.53
10:b:22:TRP:CG	10:b:706:GLN:HE22	2.26	0.53
23:9:312:CLA:HBA1	23:9:312:CLA:HBD	1.89	0.53
4:7:200:PRO:O	21:7:304:XAT:O3	2.26	0.53
10:b:709:LEU:HD11	28:b:848:DGD:HB41	1.90	0.53
23:b:823:CLA:HBB2	23:b:840:CLA:H52	1.90	0.53
23:8:305:CLA:HBC2	4:7:134:ILE:HG13	1.91	0.53
9:a:702:LYS:HB3	13:f:130:ARG:HD3	1.89	0.53
3:8:175:LYS:HB3	23:8:306:CLA:HMD2	1.90	0.53
3:8:177:GLY:O	3:8:181:MET:HG3	2.09	0.53
23:a:835:CLA:O2D	23:a:835:CLA:H2A	2.09	0.53
23:a:831:CLA:H42	27:a:845:LHG:H251	1.90	0.53
10:b:317:HIS:HB3	10:b:320:LEU:HD12	1.89	0.53
23:a:825:CLA:HMA3	23:a:844:CLA:HAB	1.91	0.53
11:d:63:ARG:NH2	11:d:65:GLU:OE1	2.41	0.53
4:7:128:THR:HG23	22:7:302:A1L1G:C17	2.39	0.53
23:b:816:CLA:H91	14:h:105:LEU:HG	1.91	0.53
3:8:36:ALA:N	3:8:44:LEU:O	2.42	0.53
23:4:317:CLA:O2D	28:4:318:DGD:HE61	2.09	0.53
4:7:46:PRO:HG2	4:7:49:LEU:HD12	1.90	0.53
9:a:197:GLY:HA3	23:a:814:CLA:HBB1	1.89	0.53
10:b:661:THR:O	10:b:664:MET:HB3	2.08	0.53
21:5:302:XAT:C16	23:5:307:CLA:H2	2.39	0.53
9:a:573:ARG:HG3	20:c:78:GLY:HA3	1.90	0.53
9:a:422:ARG:O	9:a:426:HIS:ND1	2.41	0.52
10:b:140:LEU:HG	31:b:844:BCR:H382	1.90	0.52
2:9:107:LEU:HG	2:9:136:ALA:HB1	1.91	0.52
9:a:396:VAL:HG11	9:a:589:LEU:HG	1.91	0.52
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.92	0.52
4:4:81:CYS:HB3	4:4:178:GLY:HA3	1.91	0.52
6:6:184:TYR:CZ	6:6:186:GLY:HA3	2.44	0.52
8:1:61:ALA:HB1	8:1:65:THR:HB	1.90	0.52
23:b:829:CLA:H42	28:b:848:DGD:HB42	1.91	0.52
11:d:95:LEU:HD22	19:g:75:UNK:HA	1.91	0.52
19:g:51:UNK:O	19:g:53:UNK:N	2.42	0.52
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.52
23:a:809:CLA:CHC	23:a:810:CLA:HMD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:419:ALA:O	10:b:423:HIS:ND1	2.39	0.52
23:a:834:CLA:H151	30:b:841:PQN:H202	1.91	0.52
23:b:801:CLA:H101	23:b:801:CLA:HBB1	1.91	0.52
4:4:193:ALA:O	28:4:318:DGD:O6E	2.28	0.52
9:a:686:TYR:OH	23:a:802:CLA:OBD	2.21	0.52
10:b:189:THR:HG21	10:b:276:LEU:HB2	1.91	0.52
10:b:718:GLY:O	10:b:722:THR:HG22	2.09	0.52
6:6:124:HIS:HB3	6:6:231:MET:HE2	1.92	0.52
4:7:121:LEU:HD13	23:7:316:CLA:HBC3	1.92	0.52
23:a:810:CLA:HAB	23:j:102:CLA:HMD2	1.91	0.52
23:a:820:CLA:HAB	23:a:820:CLA:H8	1.90	0.52
13:f:85:LEU:HD13	13:f:93:PRO:HB3	1.92	0.52
2:9:192:GLU:HB2	23:9:312:CLA:C1B	2.39	0.52
5:3:79:GLY:O	5:3:158:ARG:NH1	2.43	0.52
10:b:662:GLY:O	10:b:666:LEU:HG	2.10	0.52
23:b:836:CLA:HBC3	31:f:804:BCR:H401	1.91	0.52
3:8:70:ALA:H	23:b:811:CLA:HED1	1.75	0.52
11:d:33:ILE:HG22	11:d:58:VAL:HG22	1.92	0.52
13:f:143:ILE:HG13	13:f:144:ILE:HG13	1.92	0.52
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.51
8:1:77:GLY:O	8:1:81:MET:HG3	2.09	0.51
8:1:85:LEU:HB3	23:1:308:CLA:HMC2	1.92	0.51
10:b:208:ASP:OD1	10:b:208:ASP:N	2.43	0.51
23:b:836:CLA:HBC3	31:f:804:BCR:H292	1.91	0.51
5:3:93:CYS:HB3	5:3:193:GLY:HA3	1.92	0.51
4:7:45:ARG:NH1	4:7:49:LEU:O	2.42	0.51
6:6:153:ASP:OD1	6:6:155:THR:OG1	2.26	0.51
6:6:232:ILE:HD13	25:6:301:A1L1F:C31	2.39	0.51
9:a:460:ARG:NH2	23:a:835:CLA:O1D	2.44	0.51
9:a:431:ILE:HG13	9:a:549:TYR:HE1	1.74	0.51
9:a:577:CYS:O	10:b:671:GLY:HA3	2.11	0.51
10:b:602:THR:HG21	10:b:611:PHE:HB2	1.93	0.51
20:c:11:CYS:SG	20:c:39:ILE:HG13	2.50	0.51
20:c:58:CYS:SG	20:c:63:LEU:HA	2.51	0.51
6:6:131:ALA:HB2	21:6:303:XAT:H10	1.92	0.51
10:b:179:GLY:O	10:b:183:VAL:HB	2.10	0.51
10:b:342:ALA:O	10:b:346:THR:HG23	2.11	0.51
3:8:172:LYS:O	3:8:176:ASN:ND2	2.39	0.51
7:2:121:ALA:O	7:2:122:LYS:HG2	2.10	0.51
23:b:823:CLA:HAB	23:b:830:CLA:HMD1	1.93	0.51
23:6:317:CLA:HBA1	23:6:317:CLA:HBD	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:301:A1L1G:C44	23:9:315:CLA:HBC3	2.41	0.51
6:6:249:LEU:HB2	25:6:304:A1L1F:O55	2.10	0.51
25:1:304:A1L1F:C56	27:a:846:LHG:H241	2.41	0.51
23:b:807:CLA:H52	28:b:848:DGD:HB72	1.93	0.51
25:h:203:A1L1F:O46	23:h:204:CLA:H52	2.11	0.51
2:9:179:LEU:HD22	26:9:305:45D:C11	2.40	0.50
23:a:827:CLA:H93	23:a:840:CLA:H52	1.92	0.50
10:b:478:LEU:HG	10:b:479:LEU:HG	1.93	0.50
3:8:50:LEU:HD11	3:8:61:ASP:HB2	1.93	0.50
29:a:853:LMG:H131	29:a:853:LMG:H292	1.93	0.50
10:b:26:ALA:HA	23:b:829:CLA:H43	1.93	0.50
23:b:811:CLA:H72	23:b:812:CLA:HBC3	1.93	0.50
13:f:160:TRP:CD1	13:f:161:PRO:HD3	2.46	0.50
20:c:13:GLY:O	20:c:38:GLN:NE2	2.44	0.50
2:9:179:LEU:HA	23:9:308:CLA:HMD1	1.93	0.50
23:3:308:CLA:HED2	23:3:308:CLA:H2A	1.94	0.50
6:6:112:PRO:HB3	6:6:116:TRP:CD1	2.47	0.50
23:a:818:CLA:O1A	29:a:853:LMG:O10	2.30	0.50
2:9:218:LEU:HG	23:9:314:CLA:HMA2	1.92	0.50
9:a:252:LYS:NZ	9:a:264:GLU:OE1	2.41	0.50
10:b:434:HIS:CD2	31:b:849:BCR:H333	2.46	0.50
2:9:137:ARG:NH1	23:9:318:CLA:OBD	2.41	0.50
2:9:191:ALA:HB1	23:9:313:CLA:HAA1	1.93	0.50
23:a:818:CLA:HHC	23:a:818:CLA:HBB1	1.93	0.50
10:b:274:HIS:HB2	23:b:817:CLA:C1B	2.41	0.50
10:b:305:ALA:HB2	14:h:46:THR:HB	1.93	0.50
17:l:38:ARG:NH1	17:l:49:GLU:OE1	2.40	0.50
1:5:130:PHE:HE1	21:5:302:XAT:O24	1.94	0.50
21:4:303:XAT:C16	23:4:308:CLA:H2	2.41	0.50
9:a:425:ARG:NH2	11:d:15:GLY:O	2.44	0.50
31:b:849:BCR:H23C	16:j:33:TYR:CD2	2.47	0.50
17:l:109:ASN:OD1	17:l:110:ALA:N	2.35	0.50
23:5:312:CLA:CGA	23:5:312:CLA:H3A	2.41	0.50
2:9:117:TRP:O	2:9:120:TRP:NE1	2.45	0.50
21:7:301:XAT:H10	23:7:315:CLA:HMD1	1.93	0.50
2:9:32:THR:H	2:9:33:PRO:HD2	1.77	0.50
9:a:440:PHE:HE2	23:a:839:CLA:HAB	1.76	0.50
21:5:301:XAT:H193	23:5:310:CLA:HBA2	1.94	0.49
5:3:87:GLU:OE2	5:3:163:ARG:NH2	2.31	0.49
7:2:77:LYS:O	7:2:79:ASP:N	2.43	0.49
7:2:107:LEU:HB3	23:2:310:CLA:HMC2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:411:ASN:ND2	9:a:414:ASN:OD1	2.37	0.49
9:a:565:ARG:HG2	9:a:715:THR:HG21	1.93	0.49
10:b:50:HIS:ND1	23:b:813:CLA:OBD	2.38	0.49
10:b:492:SER:HA	10:b:496:LEU:HD12	1.94	0.49
23:b:832:CLA:HBB2	31:f:801:BCR:HC41	1.94	0.49
8:1:112:VAL:HB	8:1:117:TRP:NE1	2.27	0.49
25:6:304:A1L1F:C33	23:6:313:CLA:HAB	2.43	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
10:b:722:THR:HG23	23:b:803:CLA:O1D	2.11	0.49
20:c:17:CYS:HB3	32:c:102:SF4:S4	2.52	0.49
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.49
10:b:25:ILE:HG12	31:l:205:BCR:H312	1.94	0.49
4:4:159:ASN:C	4:4:161:ALA:H	2.21	0.49
23:a:818:CLA:CHD	23:a:819:CLA:HBB2	2.43	0.49
3:8:60:PHE:CE1	23:8:305:CLA:HBC3	2.48	0.49
7:2:183:ASP:O	7:2:186:LYS:N	2.44	0.49
10:b:3:TYR:HB2	15:i:33:GLU:HA	1.95	0.49
17:l:106:VAL:H	17:l:140:VAL:HG23	1.77	0.49
20:c:17:CYS:SG	20:c:18:VAL:N	2.85	0.49
4:7:42:PHE:HE2	23:7:306:CLA:HAB	1.77	0.49
4:7:185:PHE:O	4:7:189:VAL:HG22	2.13	0.49
9:a:615:VAL:HG22	9:a:621:VAL:HG22	1.95	0.49
10:b:266:LEU:HD22	23:b:817:CLA:HBA1	1.95	0.49
17:l:43:PRO:HD3	17:l:136:GLU:CD	2.38	0.49
19:g:46:UNK:O	19:g:50:UNK:N	2.45	0.49
6:6:104:GLU:OE2	6:6:105:ARG:NH1	2.45	0.49
9:a:423:VAL:HA	9:a:426:HIS:CE1	2.47	0.49
9:a:554:ARG:HB2	10:b:678:GLU:OE1	2.13	0.49
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.49
23:4:309:CLA:HAC1	23:4:316:CLA:HAB	1.95	0.49
9:a:292:LEU:HD12	23:a:816:CLA:HMC3	1.95	0.49
23:a:803:CLA:H2	10:b:657:LEU:HD22	1.95	0.49
10:b:407:LYS:HB3	10:b:411:ALA:HB3	1.95	0.49
5:3:145:ILE:O	5:3:149:ILE:HG12	2.13	0.49
23:a:802:CLA:H41	10:b:436:LEU:HD22	1.95	0.49
10:b:166:PHE:O	10:b:172:ARG:NH2	2.46	0.49
1:5:171:GLU:HG3	23:5:311:CLA:NB	2.28	0.48
10:b:273:HIS:ND1	23:b:817:CLA:HAB	2.25	0.48
23:b:824:CLA:H141	23:b:824:CLA:H193	1.95	0.48
23:b:839:CLA:H13	31:i:101:BCR:H19C	1.95	0.48

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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	0.48
5:3:81:ASP:N	5:3:81:ASP:OD1	2.46	0.48
4:7:54:VAL:HG21	4:7:74:GLN:HE21	1.77	0.48
21:5:304:XAT:C10	23:5:315:CLA:HBC3	2.44	0.48
25:8:304:A1L1F:C36	23:8:311:CLA:H51	2.43	0.48
4:7:81:CYS:O	4:7:85:MET:HG3	2.13	0.48
9:a:712:LEU:N	30:a:843:PQN:O4	2.45	0.48
10:b:277:ALA:HA	23:b:816:CLA:HMC2	1.95	0.48
10:b:597:HIS:CE1	10:b:601:LEU:HD11	2.48	0.48
2:9:91:GLY:HA3	21:9:303:XAT:H173	1.94	0.48
10:b:8:PHE:HB2	10:b:34:HIS:CG	2.49	0.48
10:b:562:ASP:OD2	10:b:566:ARG:NH2	2.38	0.48
11:d:95:LEU:HD11	11:d:98:PRO:HD2	1.95	0.48
2:9:88:ALA:HA	21:9:303:XAT:H8	1.95	0.48
23:9:311:CLA:H2A	23:9:311:CLA:O2D	2.14	0.48
3:8:36:ALA:HB3	3:8:45:LYS:HZ2	1.78	0.48
7:2:92:ARG:NH1	7:2:95:GLU:OE1	2.47	0.48
4:7:124:ILE:HA	23:7:311:CLA:HBC3	1.95	0.48
9:a:712:LEU:HD21	30:a:843:PQN:H151	1.95	0.48
23:a:825:CLA:H71	23:a:840:CLA:H62	1.96	0.48
23:a:839:CLA:H62	23:a:839:CLA:H41	1.54	0.48
29:a:853:LMG:C11	29:a:853:LMG:HC92	2.41	0.48
23:a:818:CLA:H3A	23:a:818:CLA:HBA2	1.57	0.48
14:h:114:TRP:HA	14:h:117:HIS:CD2	2.49	0.48
15:i:26:LEU:HD22	31:l:205:BCR:H323	1.94	0.48
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.48
23:9:316:CLA:H202	17:l:90:LEU:HD22	1.96	0.48
9:a:290:HIS:HB2	23:a:819:CLA:CHB	2.44	0.48
9:a:637:ASN:HB2	10:b:653:LEU:HD11	1.95	0.48
10:b:595:TYR:CZ	23:b:835:CLA:HBC3	2.49	0.48
14:h:72:PRO:HG3	25:h:203:A1L1F:C56	2.43	0.48
5:3:78:VAL:HG12	5:3:78:VAL:O	2.13	0.48
6:6:131:ALA:CB	21:6:303:XAT:H10	2.44	0.48
23:b:802:CLA:H93	23:b:802:CLA:H112	1.70	0.48
23:b:821:CLA:CHB	23:b:822:CLA:H2	2.44	0.48
8:1:42:MET:HE1	8:1:66:LEU:HD22	1.96	0.48
10:b:176:HIS:O	10:b:180:LEU:HB3	2.14	0.48
5:3:203:MET:HE2	21:3:305:XAT:O4	2.13	0.48
9:a:674:ALA:HB3	23:a:802:CLA:HBB2	1.94	0.48
10:b:526:ALA:O	10:b:530:HIS:ND1	2.37	0.48
23:b:838:CLA:HAB	30:b:841:PQN:H172	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:184:ALA:HA	23:4:315:CLA:HBB1	1.96	0.47
10:b:586:LEU:HD21	10:b:716:THR:HG23	1.96	0.47
15:i:26:LEU:HB3	31:l:205:BCR:H323	1.96	0.47
16:j:2:LYS:O	29:j:105:LMG:HC61	2.13	0.47
7:2:191:GLN:O	7:2:195:ILE:HD12	2.15	0.47
23:2:316:CLA:C2C	29:2:317:LMG:H111	2.44	0.47
8:1:144:ASP:OD2	8:1:148:THR:OG1	2.23	0.47
9:a:127:ASN:HD21	13:f:60:THR:HG21	1.79	0.47
24:1:315:SQD:H161	24:1:315:SQD:H132	1.72	0.47
23:a:832:CLA:HAB	23:a:840:CLA:HBB2	1.96	0.47
23:a:841:CLA:H61	23:b:832:CLA:H42	1.95	0.47
10:b:181:PHE:HE2	23:b:819:CLA:HAB	1.78	0.47
10:b:432:GLY:HA2	10:b:527:LEU:HD22	1.96	0.47
10:b:443:ASP:OD1	10:b:618:ILE:N	2.46	0.47
23:b:822:CLA:H43	14:h:115:GLY:C	2.40	0.47
14:h:107:SER:O	14:h:110:THR:OG1	2.32	0.47
4:7:37:SER:HB2	4:7:45:ARG:HA	1.97	0.47
21:7:301:XAT:H35	21:7:301:XAT:H401	1.71	0.47
8:1:84:VAL:O	8:1:88:ILE:HG12	2.14	0.47
9:a:375:ILE:HG21	9:a:510:VAL:HB	1.96	0.47
9:a:514:ILE:HD11	9:a:621:VAL:HG13	1.96	0.47
10:b:271:MET:O	10:b:275:HIS:ND1	2.47	0.47
10:b:297:HIS:HB3	10:b:302:ILE:HD11	1.97	0.47
3:8:58:PHE:HZ	3:8:175:LYS:HZ1	1.62	0.47
3:8:73:LYS:HD3	3:8:145:ASP:HA	1.96	0.47
21:2:305:XAT:H15	21:2:305:XAT:H201	1.78	0.47
21:7:303:XAT:H15	21:7:303:XAT:H201	1.78	0.47
8:1:88:ILE:HG22	8:1:92:PHE:CE1	2.49	0.47
23:a:820:CLA:H203	23:a:828:CLA:H3A	1.96	0.47
10:b:433:PHE:HZ	31:f:801:BCR:H372	1.80	0.47
23:b:830:CLA:HAB	23:b:837:CLA:CBB	2.44	0.47
23:4:317:CLA:CGD	28:4:318:DGD:HE61	2.45	0.47
23:6:308:CLA:CGA	23:6:308:CLA:H3A	2.45	0.47
9:a:114:ILE:HG23	9:a:115:VAL:HG22	1.96	0.47
9:a:144:GLU:HG2	9:a:206:TRP:HH2	1.80	0.47
9:a:400:ALA:HB2	9:a:585:VAL:HG11	1.95	0.47
10:b:385:PHE:HB3	10:b:536:LEU:HB3	1.97	0.47
23:b:808:CLA:H93	23:b:808:CLA:H61	1.71	0.47
12:e:51:ASN:CG	20:c:61:ASP:HB2	2.39	0.47
14:h:82:SER:O	14:h:86:HIS:ND1	2.27	0.47
23:9:314:CLA:CED	23:9:314:CLA:H2A	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:171:VAL:HG13	3:8:175:LYS:HE3	1.97	0.47
23:8:311:CLA:HBB1	23:8:311:CLA:HMB3	1.97	0.47
6:6:118:GLN:O	6:6:121:GLU:HB2	2.14	0.47
10:b:412:ARG:HH21	23:b:830:CLA:CGD	2.27	0.47
23:b:840:CLA:H161	23:b:840:CLA:H141	1.74	0.47
11:d:20:TRP:CZ2	17:l:14:VAL:HG12	2.50	0.47
27:9:307:LHG:H341	17:l:91:ILE:HD11	1.96	0.47
3:8:141:THR:HA	3:8:147:PRO:HB3	1.97	0.47
21:8:303:XAT:H34	23:8:313:CLA:HBB1	1.96	0.47
9:a:476:PHE:HB3	23:a:838:CLA:H11	1.96	0.47
23:a:834:CLA:CAD	31:l:201:BCR:H10C	2.45	0.47
10:b:65:LEU:HD11	31:b:844:BCR:H281	1.95	0.47
10:b:538:LYS:O	10:b:542:ASP:HB2	2.15	0.47
31:b:849:BCR:H23C	16:j:33:TYR:HD2	1.78	0.47
3:8:83:CYS:HB3	3:8:177:GLY:HA3	1.97	0.47
23:3:308:CLA:H2A	23:3:308:CLA:CED	2.44	0.47
7:2:65:ILE:HG22	7:2:67:PHE:H	1.80	0.47
8:1:73:GLU:HB2	23:1:306:CLA:C1B	2.45	0.47
9:a:354:GLY:HA2	9:a:391:GLY:HA2	1.97	0.47
9:a:677:LEU:HB2	23:a:802:CLA:HMC2	1.97	0.47
23:j:102:CLA:NB	31:j:104:BCR:H281	2.30	0.47
1:5:96:VAL:HG12	23:5:307:CLA:OBD	2.15	0.47
23:9:316:CLA:H71	17:l:83:LEU:HG	1.97	0.47
6:6:194:ASP:OD1	6:6:194:ASP:N	2.48	0.47
10:b:670:ARG:C	10:b:672:TYR:H	2.22	0.47
23:b:823:CLA:H2A	23:b:823:CLA:HED3	1.95	0.47
3:8:110:ASN:HB3	3:8:113:LYS:HB2	1.96	0.46
23:7:308:CLA:H91	23:7:308:CLA:H112	1.67	0.46
9:a:38:THR:HB	9:a:710:ARG:HG3	1.97	0.46
23:a:829:CLA:HBB1	23:a:829:CLA:HMB1	1.97	0.46
11:d:83:LYS:HG2	11:d:98:PRO:HG2	1.97	0.46
21:6:302:XAT:H201	21:6:302:XAT:H15	1.71	0.46
21:7:304:XAT:H191	23:7:314:CLA:HAB	1.97	0.46
9:a:114:ILE:O	9:a:117:GLN:HG2	2.16	0.46
10:b:372:HIS:HB2	23:b:827:CLA:C1B	2.45	0.46
23:h:204:CLA:H2A	23:h:204:CLA:HED3	1.97	0.46
21:3:301:XAT:H15	21:3:301:XAT:H201	1.79	0.46
4:7:185:PHE:HE1	21:7:303:XAT:H162	1.79	0.46
29:a:853:LMG:H112	29:a:853:LMG:HC92	1.98	0.46
10:b:127:MET:HE1	31:b:844:BCR:H282	1.97	0.46
23:b:822:CLA:H42	14:h:62:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:844:BCR:HC8	31:b:844:BCR:H311	1.97	0.46
4:4:185:PHE:CZ	21:4:303:XAT:H28	2.50	0.46
21:2:303:XAT:H35	21:2:303:XAT:H401	1.71	0.46
9:a:68:SER:OG	9:a:174:TYR:HB2	2.14	0.46
23:a:854:CLA:H143	29:j:105:LMG:H142	1.97	0.46
10:b:120:GLU:OE2	10:b:362:ASN:ND2	2.39	0.46
6:6:118:GLN:HB3	6:6:197:VAL:HG11	1.96	0.46
4:7:160:PHE:HE2	21:7:304:XAT:H373	1.81	0.46
21:7:303:XAT:H32	23:7:308:CLA:HAB	1.97	0.46
9:a:342:TRP:CD1	23:a:826:CLA:H192	2.51	0.46
10:b:143:LEU:HD23	10:b:146:LEU:HD12	1.97	0.46
10:b:268:LEU:HD23	10:b:271:MET:HE3	1.98	0.46
1:5:232:HIS:HE1	21:5:304:XAT:H14	1.81	0.46
2:9:49:MET:HA	2:9:52:LYS:HD3	1.97	0.46
2:9:126:THR:OG1	2:9:129:GLU:OE2	2.34	0.46
23:1:306:CLA:H91	23:1:306:CLA:H112	1.69	0.46
23:a:801:CLA:H61	23:a:803:CLA:O1D	2.15	0.46
16:j:30:ASN:ND2	23:j:102:CLA:O1A	2.47	0.46
17:l:68:LEU:O	17:l:77:SER:OG	2.24	0.46
17:l:168:TYR:O	17:l:172:LEU:HB2	2.16	0.46
23:9:308:CLA:H93	23:9:308:CLA:H111	1.70	0.46
3:8:93:TRP:CE2	3:8:111:PRO:HG2	2.51	0.46
21:8:301:XAT:H11	21:8:301:XAT:H191	1.84	0.46
21:8:302:XAT:H15	21:8:302:XAT:H201	1.73	0.46
23:4:310:CLA:H141	23:4:310:CLA:H162	1.69	0.46
5:3:179:PRO:C	5:3:181:LYS:H	2.24	0.46
6:6:94:TRP:CZ3	21:6:303:XAT:H383	2.50	0.46
4:7:120:ALA:O	4:7:124:ILE:HG13	2.16	0.46
9:a:502:ALA:HB2	9:a:516:MET:HE2	1.97	0.46
23:a:834:CLA:H162	23:a:834:CLA:H202	1.79	0.46
23:b:820:CLA:H3A	23:b:820:CLA:HBA2	1.33	0.46
23:b:823:CLA:HHB	23:b:840:CLA:O1D	2.16	0.46
15:i:28:LEU:O	15:i:32:LYS:HG3	2.16	0.46
16:j:5:LEU:HB3	29:j:105:LMG:HC72	1.96	0.46
2:9:201:LEU:HD21	21:9:304:XAT:H371	1.96	0.46
23:9:316:CLA:HBA2	17:l:67:PRO:HG3	1.97	0.46
21:4:301:XAT:H31	21:4:301:XAT:H391	1.73	0.46
8:1:40:ASP:HB2	8:1:42:MET:HG3	1.97	0.46
9:a:282:LEU:HD21	9:a:367:MET:HB3	1.98	0.46
23:a:831:CLA:H92	23:a:831:CLA:H61	1.70	0.46
23:b:817:CLA:H41	23:b:833:CLA:HAA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:j:102:CLA:H61	23:j:102:CLA:H41	1.64	0.46
22:9:306:A1L1G:C31	23:9:310:CLA:HBD	2.46	0.46
4:4:193:ALA:HB1	28:4:318:DGD:O5E	2.16	0.46
8:1:89:VAL:O	8:1:93:TRP:N	2.49	0.46
23:a:818:CLA:NC	29:a:853:LMG:H302	2.31	0.46
29:j:105:LMG:H292	29:j:105:LMG:H111	1.98	0.46
23:9:316:CLA:HBC3	23:a:803:CLA:H151	1.97	0.45
3:8:166:MET:O	3:8:170:GLU:HG3	2.16	0.45
21:6:302:XAT:H191	21:6:302:XAT:H11	1.65	0.45
10:b:687:THR:HG23	10:b:690:ALA:HB3	1.97	0.45
23:b:822:CLA:HHC	23:b:840:CLA:HED1	1.98	0.45
14:h:112:ILE:O	14:h:115:GLY:N	2.49	0.45
20:c:3:HIS:HB2	20:c:48:CYS:SG	2.56	0.45
21:3:301:XAT:H31	21:3:301:XAT:H391	1.83	0.45
21:2:305:XAT:H31	21:2:305:XAT:H391	1.71	0.45
23:a:806:CLA:H72	31:a:848:BCR:HC8	1.98	0.45
23:a:822:CLA:H12	23:a:825:CLA:HBA2	1.98	0.45
23:a:835:CLA:H61	31:l:201:BCR:H363	1.99	0.45
10:b:339:LEU:O	10:b:343:THR:HG22	2.16	0.45
15:i:14:VAL:O	15:i:19:PRO:HD2	2.17	0.45
7:2:131:ALA:HA	7:2:134:VAL:HG12	1.98	0.45
21:7:304:XAT:H32	23:7:313:CLA:HAB	1.98	0.45
10:b:50:HIS:HE1	23:b:806:CLA:H171	1.81	0.45
23:b:805:CLA:H2	23:b:805:CLA:H61	1.62	0.45
13:f:119:GLY:HA3	13:f:160:TRP:CE2	2.51	0.45
13:f:143:ILE:O	16:j:11:ALA:N	2.48	0.45
14:h:65:ILE:O	14:h:123:GLN:NE2	2.49	0.45
14:h:112:ILE:O	14:h:113:SER:C	2.60	0.45
16:j:26:VAL:CG1	31:j:104:BCR:H403	2.47	0.45
23:9:318:CLA:H111	23:9:318:CLA:H142	1.61	0.45
9:a:570:GLY:O	9:a:576:THR:OG1	2.32	0.45
23:a:804:CLA:H41	23:a:841:CLA:HMC1	1.98	0.45
10:b:392:PHE:CE2	31:b:845:BCR:HC42	2.51	0.45
23:b:823:CLA:HBA1	31:h:201:BCR:H16C	1.98	0.45
23:b:838:CLA:H12	31:l:205:BCR:H15C	1.98	0.45
2:9:55:PHE:CZ	26:9:305:45D:C27	3.00	0.45
2:9:80:ALA:O	2:9:84:ASN:ND2	2.49	0.45
21:4:302:XAT:H30	23:4:310:CLA:H151	1.98	0.45
23:4:311:CLA:H2A	23:4:311:CLA:O2D	2.17	0.45
23:b:818:CLA:H3A	23:b:818:CLA:HBA2	1.37	0.45
23:b:832:CLA:H18	31:f:804:BCR:H17C	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:302:XAT:H35	21:5:302:XAT:H401	1.87	0.45
3:8:82:HIS:HB3	3:8:181:MET:SD	2.56	0.45
3:8:138:LEU:HB2	23:8:311:CLA:HMA1	1.99	0.45
6:6:124:HIS:CB	6:6:231:MET:HE2	2.47	0.45
21:2:301:XAT:H31	21:2:301:XAT:H391	1.72	0.45
21:7:304:XAT:H191	21:7:304:XAT:H11	1.77	0.45
9:a:226:SER:HG	9:a:229:GLU:HG2	1.82	0.45
9:a:491:THR:OG1	23:a:836:CLA:OBD	2.32	0.45
23:b:811:CLA:H51	23:b:812:CLA:H43	1.97	0.45
23:b:825:CLA:HAA2	23:b:826:CLA:OBD	2.16	0.45
1:5:124:MET:HE3	23:5:312:CLA:HMC2	1.98	0.45
2:9:93:ILE:CG1	21:9:304:XAT:H8	2.47	0.45
22:9:301:A1L1G:O13	21:9:304:XAT:H28	2.16	0.45
27:9:307:LHG:H352	15:i:16:LEU:HD22	1.99	0.45
6:6:85:PHE:HB3	6:6:93:PRO:HA	1.99	0.45
23:6:314:CLA:H2A	23:6:314:CLA:O1A	2.15	0.45
4:7:79:LYS:HE3	4:7:79:LYS:HB2	1.79	0.45
8:1:105:PRO:C	8:1:107:LYS:H	2.24	0.45
21:1:302:XAT:H35	21:1:302:XAT:H401	1.72	0.45
23:1:312:CLA:HMA2	24:1:315:SQD:H141	1.99	0.45
9:a:312:GLY:HA2	23:a:823:CLA:HMD2	1.99	0.45
23:a:839:CLA:H161	23:a:839:CLA:H141	1.68	0.45
1:5:116:GLU:HB2	23:5:307:CLA:C1B	2.46	0.45
1:5:164:PHE:HE1	23:f:802:CLA:H121	1.81	0.45
21:5:304:XAT:H15	21:5:304:XAT:H201	1.76	0.45
2:9:153:PHE:CG	17:l:151:PHE:HE2	2.34	0.45
8:1:140:TYR:OH	8:1:142:PRO:O	2.25	0.45
21:1:303:XAT:H15	21:1:303:XAT:H201	1.85	0.45
9:a:686:TYR:CE1	10:b:538:LYS:HD2	2.52	0.45
10:b:678:GLU:HG2	20:c:81:TYR:HE1	1.81	0.45
13:f:160:TRP:CG	13:f:161:PRO:HD3	2.52	0.45
21:8:301:XAT:H382	23:8:312:CLA:HAC2	1.99	0.45
4:4:170:MET:CE	23:4:313:CLA:H12	2.47	0.45
23:2:316:CLA:C1C	29:2:317:LMG:H111	2.46	0.45
21:7:304:XAT:H171	23:7:315:CLA:HBB1	1.99	0.45
9:a:370:TYR:OH	23:a:830:CLA:OBD	2.28	0.45
9:a:665:ILE:HG23	23:a:809:CLA:H171	1.99	0.45
23:a:813:CLA:H62	23:a:813:CLA:H41	1.85	0.45
23:a:819:CLA:HBA2	23:a:819:CLA:H3A	1.53	0.45
23:a:825:CLA:H62	23:a:825:CLA:H41	1.84	0.45
23:b:817:CLA:HBA2	23:b:817:CLA:H3A	1.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:i:101:BCR:H15C	31:i:101:BCR:H351	1.85	0.45
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.45
21:9:304:XAT:H11	21:9:304:XAT:H191	1.87	0.45
4:4:37:SER:HB3	4:4:45:ARG:HA	1.98	0.45
7:2:105:ALA:HB1	21:2:303:XAT:H161	1.98	0.45
9:a:25:PRO:HB2	9:a:41:TRP:HH2	1.81	0.45
9:a:407:VAL:HG11	9:a:564:PHE:N	2.32	0.45
23:a:834:CLA:H201	31:l:205:BCR:H343	1.98	0.45
10:b:201:ARG:HG2	10:b:248:SER:HB2	1.99	0.45
10:b:228:TRP:HZ3	31:h:202:BCR:H363	1.82	0.45
10:b:605:GLN:HE21	10:b:734:LYS:HB3	1.82	0.45
21:4:305:XAT:H35	21:4:305:XAT:H401	1.77	0.44
21:3:304:XAT:H35	21:3:304:XAT:H401	1.68	0.44
8:1:141:ARG:HD3	8:1:149:TRP:HB3	1.99	0.44
21:1:303:XAT:H183	23:1:308:CLA:C2B	2.47	0.44
9:a:71:PHE:HD1	9:a:166:MET:HE3	1.82	0.44
23:a:801:CLA:CED	23:a:801:CLA:HAA2	2.46	0.44
23:9:316:CLA:H112	23:9:318:CLA:HAB	1.99	0.44
21:4:305:XAT:H391	21:4:305:XAT:H31	1.62	0.44
6:6:121:GLU:OE2	23:6:308:CLA:C1B	2.65	0.44
21:6:305:XAT:H401	21:6:305:XAT:H35	1.64	0.44
4:7:77:GLU:HB2	23:7:308:CLA:CHB	2.48	0.44
9:a:367:MET:HG2	9:a:500:SER:HB2	1.99	0.44
10:b:466:GLN:NE2	23:b:835:CLA:OBD	2.34	0.44
10:b:518:ASP:OD2	10:b:595:TYR:OH	2.23	0.44
10:b:654:PHE:O	10:b:658:VAL:HG23	2.17	0.44
11:d:20:TRP:HB2	11:d:24:ALA:HB3	1.99	0.44
2:9:207:VAL:HG21	23:9:308:CLA:H191	1.99	0.44
23:9:308:CLA:H92	23:9:308:CLA:H61	1.76	0.44
9:a:73:GLN:HG2	23:a:806:CLA:H3A	2.00	0.44
9:a:194:HIS:ND1	23:a:826:CLA:OBD	2.48	0.44
23:a:827:CLA:H3A	23:a:827:CLA:HBA2	1.79	0.44
23:b:813:CLA:H161	23:b:813:CLA:H192	1.76	0.44
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.44
1:5:106:PHE:HB2	13:f:148:PRO:HG3	1.99	0.44
21:5:301:XAT:H35	21:5:301:XAT:H401	1.77	0.44
21:5:302:XAT:H383	23:5:309:CLA:C2B	2.48	0.44
2:9:153:PHE:HA	17:l:151:PHE:CE2	2.51	0.44
23:9:316:CLA:H141	23:9:316:CLA:H162	1.75	0.44
21:8:302:XAT:H35	21:8:302:XAT:H401	1.76	0.44
4:7:78:ILE:HG12	4:7:175:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:415:ASN:O	9:a:421:ASP:HB2	2.18	0.44
9:a:532:HIS:CE1	9:a:599:VAL:HA	2.53	0.44
10:b:280:VAL:HG21	23:b:816:CLA:HAB	1.98	0.44
25:9:302:A1L1F:C42	23:9:311:CLA:O1A	2.66	0.44
4:7:36:LYS:HB2	4:7:45:ARG:H	1.83	0.44
4:7:112:HIS:O	4:7:116:VAL:HG13	2.18	0.44
31:a:849:BCR:H11C	31:a:849:BCR:H341	1.84	0.44
10:b:26:ALA:HB1	28:b:848:DGD:O1B	2.17	0.44
31:b:843:BCR:H11C	31:b:843:BCR:H341	1.76	0.44
13:f:79:ARG:O	13:f:83:SER:HB2	2.17	0.44
14:h:59:GLY:O	14:h:63:SER:OG	2.23	0.44
17:l:116:VAL:HG11	17:l:128:LEU:C	2.42	0.44
8:1:156:ASP:OD2	17:l:2:VAL:N	2.51	0.44
23:b:839:CLA:HBA1	23:b:839:CLA:H3A	1.59	0.44
10:b:458:GLU:OE1	13:f:94:HIS:ND1	2.46	0.44
23:b:827:CLA:H61	23:b:827:CLA:H102	1.85	0.44
31:f:804:BCR:H341	31:f:804:BCR:H11C	1.73	0.44
31:l:205:BCR:H11C	31:l:205:BCR:H341	1.84	0.44
20:c:54:CYS:SG	20:c:55:GLU:N	2.91	0.44
2:9:153:PHE:CE2	17:l:155:LEU:HD22	2.53	0.44
5:3:121:GLN:HA	5:3:124:VAL:HG12	1.99	0.44
6:6:132:PHE:O	6:6:136:ILE:HG12	2.17	0.44
21:6:303:XAT:H31	21:6:303:XAT:H391	1.87	0.44
23:2:310:CLA:H141	23:2:310:CLA:H162	1.74	0.44
23:2:310:CLA:H162	23:2:310:CLA:H192	1.71	0.44
23:7:316:CLA:HBA1	23:7:316:CLA:H3A	1.59	0.44
8:1:171:ARG:HA	8:1:174:MET:HE3	2.00	0.44
9:a:304:MET:HG3	23:a:823:CLA:C3C	2.47	0.44
23:a:833:CLA:H72	23:l:203:CLA:H12	2.00	0.44
23:a:844:CLA:C1C	27:a:846:LHG:HC31	2.48	0.44
10:b:526:ALA:HB2	23:b:836:CLA:HMA1	2.00	0.44
23:b:839:CLA:H92	23:b:839:CLA:H61	1.73	0.44
31:b:845:BCR:H20C	31:b:845:BCR:H361	1.86	0.44
23:9:314:CLA:H2A	23:9:314:CLA:O2D	2.18	0.44
7:2:118:LEU:N	23:2:310:CLA:OBD	2.47	0.44
9:a:517:MET:HE2	9:a:611:VAL:HA	2.00	0.44
10:b:259:PHE:CZ	10:b:510:LEU:HD12	2.52	0.44
10:b:343:THR:HG23	10:b:377:ALA:HB2	2.00	0.44
10:b:676:LEU:O	10:b:679:THR:OG1	2.33	0.44
20:c:59:PRO:HD2	32:c:102:SF4:S2	2.58	0.44
2:9:120:TRP:CD1	2:9:121:VAL:HG13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:172:LYS:HB3	2:9:172:LYS:HE2	1.45	0.43
21:8:302:XAT:H191	21:8:302:XAT:H11	1.71	0.43
23:a:807:CLA:H43	27:a:845:LHG:H252	2.00	0.43
23:a:826:CLA:HMB3	23:a:826:CLA:HBB1	1.99	0.43
23:a:832:CLA:HBA1	23:a:832:CLA:H3A	1.80	0.43
23:a:854:CLA:H142	23:a:854:CLA:H111	1.80	0.43
10:b:140:LEU:HD23	10:b:140:LEU:HA	1.87	0.43
23:b:838:CLA:H192	23:b:838:CLA:H162	1.73	0.43
14:h:72:PRO:CG	25:h:203:A1L1F:C56	2.95	0.43
21:8:301:XAT:H31	21:8:301:XAT:H391	1.92	0.43
4:7:142:MET:C	4:7:144:GLU:H	2.26	0.43
4:7:170:MET:HE2	23:7:313:CLA:H12	1.99	0.43
8:1:152:VAL:HG11	8:1:159:TRP:CD1	2.53	0.43
9:a:442:GLY:HA3	23:b:804:CLA:O1A	2.18	0.43
9:a:683:GLY:HA3	10:b:571:ASP:HB2	1.99	0.43
31:a:847:BCR:H20C	31:a:847:BCR:H361	1.80	0.43
23:5:309:CLA:H92	23:5:309:CLA:H61	1.77	0.43
2:9:144:HIS:CD2	23:9:314:CLA:HBC3	2.53	0.43
4:4:183:LEU:HD11	23:4:308:CLA:HAC1	2.00	0.43
23:4:310:CLA:C1A	23:4:310:CLA:CGA	2.96	0.43
23:4:310:CLA:H142	23:4:310:CLA:H112	1.78	0.43
5:3:189:GLU:HB2	23:3:313:CLA:C1B	2.47	0.43
4:7:85:MET:HE3	4:7:177:ASN:HB3	1.99	0.43
8:1:62:ASP:OD1	8:1:62:ASP:N	2.49	0.43
9:a:52:PHE:CD2	23:a:806:CLA:HMC2	2.53	0.43
9:a:194:HIS:HE1	23:a:826:CLA:H72	1.83	0.43
9:a:447:GLY:HA3	23:a:835:CLA:HAB	1.99	0.43
9:a:567:PRO:HB3	9:a:714:ILE:HB	2.01	0.43
23:a:827:CLA:H13	23:a:827:CLA:H172	1.77	0.43
10:b:529:LEU:HD23	10:b:588:THR:HG21	2.00	0.43
23:b:814:CLA:H2	23:b:814:CLA:H61	1.77	0.43
23:b:835:CLA:H12	23:b:836:CLA:O1A	2.18	0.43
20:c:25:VAL:HG21	20:c:48:CYS:HA	1.99	0.43
21:7:304:XAT:H31	21:7:304:XAT:H391	1.87	0.43
9:a:143:ALA:HB2	9:a:371:PRO:HD2	2.00	0.43
23:a:807:CLA:H92	23:a:807:CLA:H61	1.69	0.43
23:a:810:CLA:HBB1	31:j:104:BCR:H23C	2.00	0.43
23:a:829:CLA:H91	23:a:831:CLA:H192	2.00	0.43
10:b:172:ARG:HD2	23:b:824:CLA:OBD	2.18	0.43
21:j:101:XAT:H11	21:j:101:XAT:H191	1.91	0.43
23:j:103:CLA:O1D	23:j:103:CLA:H2A	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:l:96:LEU:HG	31:l:205:BCR:H24C	2.01	0.43
23:9:316:CLA:HBB1	23:9:316:CLA:HMB3	1.99	0.43
27:9:317:LHG:H302	27:9:317:LHG:H272	1.86	0.43
4:4:59:PHE:HE1	23:4:306:CLA:HBC3	1.83	0.43
23:4:308:CLA:H192	23:4:308:CLA:H161	1.77	0.43
6:6:242:PHE:HZ	21:6:305:XAT:H183	1.84	0.43
7:2:118:LEU:HB2	7:2:123:TYR:HD2	1.83	0.43
7:2:127:ASN:OD1	7:2:130:GLN:N	2.46	0.43
8:1:95:PRO:HD2	23:1:308:CLA:HMD3	1.99	0.43
9:a:84:MET:SD	23:a:829:CLA:HED1	2.58	0.43
9:a:580:SER:HB2	9:a:582:TRP:H	1.82	0.43
31:a:848:BCR:H11C	31:a:848:BCR:H341	1.86	0.43
23:b:812:CLA:HBA2	23:b:812:CLA:H3A	1.61	0.43
11:d:81:ASN:H	11:d:81:ASN:ND2	2.16	0.43
21:5:304:XAT:H35	21:5:304:XAT:H401	1.80	0.43
23:9:318:CLA:HMC2	15:i:17:VAL:HG21	2.01	0.43
3:8:47:PRO:HG2	3:8:50:LEU:HG	2.00	0.43
5:3:205:LEU:HD12	5:3:205:LEU:HA	1.86	0.43
21:2:305:XAT:H35	21:2:305:XAT:H401	1.74	0.43
8:1:128:GLU:HG3	21:1:302:XAT:H372	2.01	0.43
23:1:314:CLA:HBA1	23:1:314:CLA:H3A	1.69	0.43
9:a:75:ALA:HB2	9:a:166:MET:HB2	2.01	0.43
23:a:803:CLA:O1A	23:a:803:CLA:H3A	2.19	0.43
10:b:140:LEU:HD23	10:b:143:LEU:HD12	2.01	0.43
10:b:274:HIS:HB2	23:b:817:CLA:CHB	2.49	0.43
23:b:802:CLA:H162	23:b:802:CLA:H122	1.60	0.43
23:b:813:CLA:H143	23:b:824:CLA:H51	1.99	0.43
12:e:16:TYR:CD2	12:e:44:ASN:HA	2.54	0.43
2:9:198:VAL:HG12	21:9:304:XAT:H34	2.01	0.43
3:8:72:LEU:HD13	23:8:307:CLA:HED1	1.99	0.43
23:4:308:CLA:H112	23:4:308:CLA:H143	1.66	0.43
5:3:133:PRO:HB2	21:3:301:XAT:H23	2.00	0.43
21:7:305:XAT:H35	21:7:305:XAT:H401	1.87	0.43
9:a:578:GLN:HA	9:a:583:ASP:OD2	2.18	0.43
10:b:172:ARG:HB2	23:b:813:CLA:HBC2	2.00	0.43
10:b:220:LEU:HD21	31:b:842:BCR:H391	2.01	0.43
5:3:103:ILE:HD11	21:3:304:XAT:H363	2.01	0.43
21:3:301:XAT:H35	21:3:301:XAT:H401	1.81	0.43
25:6:301:A1L1F:C42	23:6:315:CLA:O1D	2.67	0.43
21:6:306:XAT:H11	21:6:306:XAT:H191	1.89	0.43
21:7:303:XAT:H362	23:7:308:CLA:H2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:171:ARG:HA	8:1:174:MET:CE	2.49	0.43
10:b:440:VAL:HG12	23:j:102:CLA:HAC1	2.01	0.43
23:b:801:CLA:H141	23:b:801:CLA:H161	1.63	0.43
23:b:809:CLA:H142	23:b:809:CLA:H111	1.70	0.43
23:b:816:CLA:CHD	23:b:817:CLA:HBB2	2.49	0.43
16:j:12:PRO:HB2	21:j:101:XAT:H21	2.01	0.43
2:9:91:GLY:HA3	21:9:303:XAT:O4	2.19	0.43
26:9:305:45D:H421	26:9:305:45D:H401	1.90	0.43
21:3:304:XAT:H12	23:3:309:CLA:HAB	2.01	0.43
21:6:302:XAT:H35	21:6:302:XAT:H401	1.74	0.43
21:6:306:XAT:H15	21:6:306:XAT:H201	1.78	0.43
21:2:305:XAT:H11	21:2:305:XAT:H191	1.90	0.43
21:7:304:XAT:H15	21:7:304:XAT:H201	1.73	0.43
8:1:168:ASN:HA	8:1:171:ARG:HD2	2.01	0.43
9:a:701:LEU:HD12	23:a:841:CLA:HMA2	2.00	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
21:a:852:XAT:H173	21:a:852:XAT:H3	1.83	0.43
10:b:302:ILE:HD13	23:b:822:CLA:HMD2	1.99	0.43
10:b:424:LEU:HG	23:b:837:CLA:CBB	2.48	0.43
23:b:813:CLA:H161	23:b:813:CLA:H141	1.77	0.43
23:b:838:CLA:H62	23:b:838:CLA:H41	1.71	0.43
31:b:849:BCR:H11C	31:b:849:BCR:H341	1.73	0.43
31:b:849:BCR:H15C	31:b:849:BCR:H351	1.91	0.43
31:j:104:BCR:H341	31:j:104:BCR:H11C	1.72	0.43
21:8:303:XAT:C34	23:8:313:CLA:HBB1	2.49	0.43
8:1:58:ALA:HB1	8:1:66:LEU:HD21	2.00	0.43
9:a:271:PHE:HE2	9:a:495:ALA:HB2	1.84	0.43
10:b:345:LEU:CD1	23:b:826:CLA:HAA1	2.49	0.43
23:b:828:CLA:H41	23:b:828:CLA:H61	1.75	0.43
21:4:302:XAT:H11	21:4:302:XAT:H191	1.89	0.42
7:2:125:GLY:O	7:2:127:ASN:N	2.44	0.42
4:7:81:CYS:SG	4:7:175:LEU:HD23	2.59	0.42
4:7:185:PHE:CE1	21:7:303:XAT:H162	2.53	0.42
9:a:565:ARG:HD2	27:a:845:LHG:HC61	2.00	0.42
27:a:845:LHG:H311	27:a:845:LHG:H282	1.94	0.42
23:b:835:CLA:H51	23:b:835:CLA:H11	1.73	0.42
23:b:838:CLA:H161	17:l:92:LEU:HD21	1.99	0.42
21:j:101:XAT:H35	21:j:101:XAT:H401	1.80	0.42
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.42
2:9:138:ALA:O	2:9:142:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:75:GLU:OE1	4:4:148:ARG:NH2	2.47	0.42
6:6:189:TRP:CZ3	21:6:305:XAT:H363	2.53	0.42
21:6:306:XAT:H401	21:6:306:XAT:H35	1.71	0.42
21:7:303:XAT:C36	23:7:308:CLA:H2	2.49	0.42
9:a:364:MET:HE1	23:a:830:CLA:CAD	2.49	0.42
23:a:801:CLA:HBD	23:a:801:CLA:HED2	1.48	0.42
23:a:828:CLA:H162	23:a:828:CLA:H122	1.66	0.42
23:a:840:CLA:H72	31:a:850:BCR:H373	2.00	0.42
23:b:801:CLA:H52	23:b:801:CLA:H12	1.85	0.42
23:b:825:CLA:HBA2	23:b:825:CLA:H3A	1.73	0.42
23:j:102:CLA:HBA1	23:j:102:CLA:H3A	1.91	0.42
2:9:222:ASP:OD1	2:9:227:GLY:HA2	2.19	0.42
3:8:184:ILE:HG21	21:8:302:XAT:H12	2.01	0.42
21:4:304:XAT:H11	21:4:304:XAT:H191	1.90	0.42
5:3:172:PRO:HD2	21:3:305:XAT:H242	2.00	0.42
21:3:303:XAT:H11	21:3:303:XAT:H191	1.89	0.42
21:3:303:XAT:H15	21:3:303:XAT:H201	1.79	0.42
7:2:193:SER:O	7:2:197:ASN:ND2	2.35	0.42
23:2:307:CLA:H3A	23:2:307:CLA:HBA2	1.76	0.42
4:7:174:GLU:HB2	23:7:313:CLA:C1B	2.50	0.42
22:7:302:A1L1G:O9	23:7:311:CLA:O1A	2.37	0.42
23:1:306:CLA:H162	23:1:306:CLA:H202	1.69	0.42
10:b:626:LEU:HD22	23:b:803:CLA:HMD3	2.01	0.42
11:d:32:ILE:HG21	11:d:70:LEU:HD23	2.00	0.42
13:f:114:PHE:HB2	31:f:801:BCR:C32	2.49	0.42
2:9:120:TRP:HB3	10:b:94:PRO:HA	2.02	0.42
21:9:304:XAT:H173	21:9:304:XAT:H3	1.90	0.42
26:9:305:45D:H411	26:9:305:45D:H393	1.81	0.42
21:4:305:XAT:H363	21:3:301:XAT:C10	2.49	0.42
9:a:361:ALA:HB2	9:a:387:HIS:HB2	2.01	0.42
9:a:555:LEU:HD11	10:b:674:GLN:HB3	2.01	0.42
9:a:692:GLU:CD	10:b:547:LYS:HB2	2.44	0.42
10:b:347:ALA:HB3	10:b:374:GLN:HE21	1.85	0.42
23:b:807:CLA:H102	23:b:807:CLA:H161	2.01	0.42
23:b:814:CLA:CHA	23:b:814:CLA:HBA1	2.49	0.42
23:b:837:CLA:H101	23:b:837:CLA:H13	1.78	0.42
23:b:839:CLA:H141	23:b:839:CLA:H161	1.91	0.42
21:9:303:XAT:H7	23:9:309:CLA:HAB	2.01	0.42
5:3:51:LEU:HD23	5:3:51:LEU:HA	1.87	0.42
6:6:115:LYS:HE2	6:6:188:PHE:CE1	2.55	0.42
8:1:82:LEU:HD11	23:1:311:CLA:HBC1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:684:ARG:NH1	9:a:711:ALA:O	2.52	0.42
23:a:806:CLA:H162	23:a:806:CLA:H141	1.59	0.42
10:b:597:HIS:CE1	10:b:727:VAL:HG23	2.54	0.42
10:b:702:LEU:HD22	10:b:706:GLN:NE2	2.35	0.42
30:b:841:PQN:H243	30:b:841:PQN:H262	1.84	0.42
31:h:202:BCR:H20C	31:h:202:BCR:H361	1.88	0.42
3:8:172:LYS:HD3	23:8:313:CLA:HAA2	2.01	0.42
23:4:307:CLA:HBD	23:4:314:CLA:OBD	2.20	0.42
7:2:205:PHE:CD2	21:2:303:XAT:H12	2.54	0.42
21:7:303:XAT:H11	21:7:303:XAT:H191	1.70	0.42
9:a:466:SER:HG	9:a:631:GLN:HE22	1.63	0.42
9:a:680:LEU:HB3	10:b:667:ILE:HG12	2.02	0.42
23:a:807:CLA:H102	23:a:807:CLA:H161	2.00	0.42
23:a:816:CLA:C4B	21:a:852:XAT:H242	2.50	0.42
10:b:207:TRP:HE1	23:b:814:CLA:H11	1.84	0.42
23:b:828:CLA:H3A	23:b:828:CLA:HBA2	1.76	0.42
17:l:53:THR:HG22	23:l:202:CLA:C1B	2.49	0.42
1:5:98:PHE:HE1	23:5:305:CLA:HBC3	1.84	0.42
2:9:217:ILE:HG21	23:9:314:CLA:HHB	2.01	0.42
3:8:42:PRO:HB2	4:7:154:LYS:HB2	2.02	0.42
23:a:806:CLA:H72	31:a:848:BCR:C8	2.50	0.42
10:b:381:MET:HE1	31:b:845:BCR:H352	2.02	0.42
10:b:647:VAL:HG21	23:b:809:CLA:HAC1	2.00	0.42
23:b:833:CLA:H122	23:b:833:CLA:H8	1.92	0.42
13:f:153:ILE:O	13:f:156:SER:OG	2.31	0.42
2:9:204:VAL:HG22	23:9:308:CLA:H203	2.01	0.42
2:9:218:LEU:HD23	2:9:218:LEU:HA	1.84	0.42
4:4:85:MET:HE3	4:4:177:ASN:HB3	2.00	0.42
23:4:306:CLA:CHA	23:4:306:CLA:HBA1	2.48	0.42
23:4:309:CLA:H3A	23:4:309:CLA:HBA1	1.77	0.42
23:6:317:CLA:H162	23:6:317:CLA:H141	1.78	0.42
7:2:109:TRP:CE3	21:2:303:XAT:H22	2.54	0.42
8:1:151:TRP:CH2	17:l:20:PRO:HA	2.54	0.42
9:a:525:ASP:HA	9:a:528:VAL:HG12	2.01	0.42
23:a:804:CLA:C4D	16:j:12:PRO:HG3	2.50	0.42
23:a:831:CLA:H93	23:a:842:CLA:HED3	2.01	0.42
10:b:56:ILE:HD11	31:m:101:BCR:HC7	2.02	0.42
23:b:802:CLA:HMA1	23:b:803:CLA:H161	2.02	0.42
23:b:805:CLA:H162	23:b:805:CLA:H141	1.67	0.42
23:b:816:CLA:CBB	31:h:202:BCR:H14C	2.50	0.42
13:f:85:LEU:HD23	13:f:85:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:l:32:LYS:HD2	17:l:32:LYS:HA	1.86	0.42
21:5:302:XAT:H31	21:5:302:XAT:H391	1.94	0.42
21:4:303:XAT:H163	23:4:308:CLA:H2	2.02	0.42
7:2:203:LEU:HD13	21:2:301:XAT:C10	2.50	0.42
21:2:302:XAT:H31	21:2:302:XAT:H391	1.84	0.42
29:2:317:LMG:H292	29:2:317:LMG:H321	1.35	0.42
21:5:301:XAT:H11	21:5:301:XAT:H191	1.86	0.42
2:9:217:ILE:HB	23:9:314:CLA:H3A	2.02	0.42
21:4:303:XAT:H15	21:4:303:XAT:H201	1.82	0.42
21:4:304:XAT:H30	23:4:313:CLA:H71	2.02	0.42
21:3:305:XAT:H35	21:3:305:XAT:H401	1.77	0.42
21:2:303:XAT:H11	21:2:303:XAT:H191	1.66	0.42
9:a:356:LEU:HB2	23:a:828:CLA:H41	2.02	0.42
23:a:823:CLA:CHD	21:a:852:XAT:H183	2.49	0.42
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.41
6:6:135:VAL:HG13	21:6:303:XAT:H163	2.02	0.41
4:7:71:SER:HB3	4:7:142:MET:CE	2.49	0.41
8:1:71:GLU:HG2	8:1:142:PRO:O	2.20	0.41
9:a:399:ALA:HB1	9:a:543:LEU:HB3	2.02	0.41
23:a:834:CLA:H142	31:b:846:BCR:H17C	2.01	0.41
31:a:850:BCR:H15C	31:a:850:BCR:H351	1.77	0.41
10:b:197:ILE:HB	10:b:198:PRO:HD3	2.02	0.41
10:b:452:GLU:OE2	13:f:76:ARG:NE	2.42	0.41
10:b:500:LEU:HA	10:b:503:ILE:HG22	2.02	0.41
31:b:842:BCR:H351	31:b:842:BCR:H15C	1.73	0.41
31:b:849:BCR:H361	31:b:849:BCR:H20C	1.76	0.41
11:d:107:VAL:HG21	20:c:38:GLN:HB3	2.01	0.41
2:9:173:ASP:O	2:9:174:GLU:C	2.63	0.41
27:9:317:LHG:H291	27:9:317:LHG:H321	1.66	0.41
23:8:307:CLA:H122	23:8:307:CLA:H161	1.87	0.41
6:6:237:PHE:CE1	6:6:250:LEU:HD11	2.55	0.41
21:2:304:XAT:H31	21:2:304:XAT:H391	1.85	0.41
9:a:67:PHE:HE2	9:a:173:HIS:CG	2.38	0.41
9:a:727:LEU:HD22	23:a:842:CLA:HMA3	2.01	0.41
23:a:812:CLA:H112	23:a:812:CLA:H142	1.85	0.41
31:f:804:BCR:H371	31:f:804:BCR:H24C	1.83	0.41
16:j:14:LEU:CD2	29:j:105:LMG:H141	2.49	0.41
31:l:205:BCR:H15C	31:l:205:BCR:H351	1.74	0.41
3:8:47:PRO:HG3	3:8:61:ASP:HB3	2.01	0.41
21:8:303:XAT:H35	21:8:303:XAT:H401	1.93	0.41
21:7:301:XAT:H11	21:7:301:XAT:H191	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:304:XAT:H30	23:7:313:CLA:H71	2.01	0.41
23:1:311:CLA:H72	17:l:21:ILE:HG12	2.02	0.41
9:a:290:HIS:O	9:a:294:ILE:HG12	2.20	0.41
9:a:357:SER:HB2	23:a:830:CLA:HMC2	2.01	0.41
10:b:193:VAL:O	10:b:198:PRO:HD3	2.20	0.41
10:b:518:ASP:O	10:b:522:HIS:ND1	2.38	0.41
31:h:202:BCR:H24C	31:h:202:BCR:H371	1.92	0.41
31:l:201:BCR:H352	23:l:203:CLA:HAB	2.02	0.41
2:9:91:GLY:CA	21:9:303:XAT:H173	2.51	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
4:7:87:ALA:HB1	21:7:303:XAT:H161	2.01	0.41
21:7:303:XAT:H35	21:7:303:XAT:H401	1.77	0.41
21:7:305:XAT:H11	21:7:305:XAT:H191	1.84	0.41
9:a:427:ARG:NH2	11:d:46:THR:O	2.53	0.41
23:a:806:CLA:H202	23:a:806:CLA:H161	1.70	0.41
11:d:88:TYR:HB3	11:d:89:PRO:HD2	2.01	0.41
6:6:121:GLU:OE2	23:6:308:CLA:C2B	2.68	0.41
8:1:147:GLY:HA2	8:1:149:TRP:CZ3	2.55	0.41
9:a:293:ALA:HB1	23:a:818:CLA:HBC2	2.02	0.41
9:a:406:PHE:HE2	9:a:424:ILE:HD11	1.86	0.41
9:a:586:PHE:CE1	9:a:590:PHE:HE2	2.39	0.41
9:a:601:PHE:CZ	23:a:801:CLA:HED3	2.55	0.41
10:b:342:ALA:HB2	23:b:824:CLA:H43	2.02	0.41
23:b:824:CLA:H62	23:b:824:CLA:H41	1.79	0.41
31:b:846:BCR:H15C	31:b:846:BCR:H351	1.85	0.41
11:d:70:LEU:O	11:d:74:LEU:HG	2.19	0.41
21:5:302:XAT:H11	21:5:302:XAT:H191	1.65	0.41
25:9:302:A1L1F:C28	23:9:310:CLA:HMC1	2.51	0.41
23:9:314:CLA:H51	23:9:314:CLA:C1C	2.50	0.41
23:8:307:CLA:H203	23:8:307:CLA:H162	1.74	0.41
21:6:305:XAT:H11	21:6:305:XAT:H191	1.84	0.41
21:2:304:XAT:H15	21:2:304:XAT:H201	1.91	0.41
9:a:632:SER:O	9:a:638:GLY:HA3	2.21	0.41
23:a:818:CLA:OBD	23:a:837:CLA:HED2	2.21	0.41
21:a:852:XAT:H15	21:a:852:XAT:H201	1.67	0.41
10:b:471:LYS:HB2	10:b:471:LYS:HE2	1.89	0.41
10:b:520:LEU:HD23	10:b:520:LEU:HA	1.88	0.41
1:5:115:ALA:O	1:5:119:ASN:ND2	2.42	0.41
27:9:317:LHG:H312	18:m:22:ILE:HD12	2.02	0.41
4:7:160:PHE:CE2	21:7:304:XAT:H373	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:162:TYR:CE2	23:a:844:CLA:HBD	2.56	0.41
9:a:232:LEU:HD23	9:a:232:LEU:HA	1.92	0.41
9:a:272:LYS:HG2	9:a:496:LEU:HD12	2.02	0.41
9:a:299:ILE:O	9:a:303:HIS:ND1	2.53	0.41
10:b:273:HIS:HB3	23:b:817:CLA:HMB1	2.03	0.41
10:b:629:ASN:HA	10:b:734:LYS:HE2	2.02	0.41
23:b:812:CLA:H41	23:b:812:CLA:H62	1.62	0.41
23:b:826:CLA:H161	23:b:826:CLA:H141	1.82	0.41
31:f:801:BCR:H11C	31:f:801:BCR:H341	1.95	0.41
31:l:201:BCR:H20C	31:l:201:BCR:H361	1.96	0.41
2:9:120:TRP:CH2	23:9:318:CLA:H43	2.56	0.41
21:4:303:XAT:H383	23:4:310:CLA:C2B	2.51	0.41
5:3:56:ASN:HB3	5:3:82:LEU:HD22	2.01	0.41
25:6:304:A1L1F:C33	23:6:313:CLA:HHC	2.51	0.41
21:2:303:XAT:H391	21:2:303:XAT:H31	1.70	0.41
8:1:87:TRP:CG	8:1:180:LEU:HD13	2.56	0.41
9:a:350:LEU:HD23	9:a:350:LEU:HA	1.95	0.41
9:a:434:LEU:HG	9:a:541:LEU:HB2	2.03	0.41
9:a:452:ASN:HD22	9:a:634:ILE:HB	1.85	0.41
23:a:841:CLA:HED3	23:a:841:CLA:H2A	2.01	0.41
31:a:849:BCR:H15C	31:a:849:BCR:H351	1.79	0.41
10:b:314:GLY:HA3	10:b:412:ARG:HD2	2.02	0.41
10:b:585:MET:O	10:b:589:ILE:HG12	2.20	0.41
23:b:809:CLA:H93	23:b:809:CLA:H62	1.80	0.41
23:b:826:CLA:HMB2	23:b:833:CLA:HBA1	2.03	0.41
31:b:842:BCR:H341	31:b:842:BCR:H11C	1.74	0.41
14:h:94:LEU:HD12	14:h:94:LEU:HA	1.94	0.41
16:j:14:LEU:HD23	16:j:14:LEU:HA	1.84	0.41
1:5:83:LEU:HD23	1:5:83:LEU:HA	1.93	0.41
1:5:98:PHE:CD2	23:5:305:CLA:HMD2	2.56	0.41
1:5:149:VAL:HG22	21:5:304:XAT:H182	2.02	0.41
23:5:307:CLA:HBC1	21:4:301:XAT:H383	2.01	0.41
2:9:72:LEU:HD23	2:9:72:LEU:HA	1.94	0.41
21:9:304:XAT:H35	21:9:304:XAT:H401	1.86	0.41
3:8:44:LEU:HD22	4:7:137:ILE:HG22	2.03	0.41
21:4:303:XAT:H11	21:4:303:XAT:H191	1.74	0.41
21:2:301:XAT:H15	21:2:301:XAT:H201	1.77	0.41
4:7:59:PHE:HE1	23:7:306:CLA:HBC3	1.85	0.41
23:7:307:CLA:CAD	23:7:314:CLA:HMA3	2.51	0.41
8:1:131:GLN:O	8:1:135:LYS:HG3	2.21	0.41
23:1:306:CLA:H3A	23:1:306:CLA:O2A	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:319:LEU:O	9:a:331:HIS:HB2	2.21	0.41
9:a:440:PHE:CE2	23:a:839:CLA:HAB	2.55	0.41
10:b:346:THR:HG21	23:b:828:CLA:HHD	2.03	0.41
10:b:614:SER:O	10:b:620:GLY:HA3	2.21	0.41
23:b:801:CLA:H51	23:b:838:CLA:H102	2.01	0.41
23:b:804:CLA:HBC2	23:b:804:CLA:HHD	2.03	0.41
23:b:826:CLA:HED1	31:b:845:BCR:H21C	2.02	0.41
15:i:29:TYR:HE1	18:m:30:ASN:HD21	1.67	0.41
23:5:308:CLA:CBB	23:5:315:CLA:HAB	2.51	0.41
2:9:201:LEU:HD13	23:9:308:CLA:HBC1	2.03	0.41
21:4:304:XAT:H31	21:4:304:XAT:H391	1.92	0.41
23:4:317:CLA:H62	23:4:317:CLA:H92	1.83	0.41
7:2:92:ARG:NH2	23:2:308:CLA:HED3	2.36	0.41
23:1:310:CLA:H111	23:1:310:CLA:H71	1.89	0.41
9:a:318:ILE:O	9:a:322:HIS:ND1	2.54	0.41
23:a:805:CLA:HBA1	23:a:805:CLA:H3A	1.89	0.41
23:a:807:CLA:H161	23:a:807:CLA:H192	1.83	0.41
23:a:829:CLA:O1D	23:a:830:CLA:HMA1	2.21	0.41
23:a:835:CLA:H141	23:a:835:CLA:H161	1.84	0.41
23:b:809:CLA:C4A	23:b:809:CLA:HBA2	2.50	0.41
23:b:816:CLA:C9	14:h:105:LEU:HG	2.49	0.41
12:e:51:ASN:ND2	20:c:61:ASP:HB2	2.35	0.41
21:j:101:XAT:H15	21:j:101:XAT:H201	1.82	0.41
20:c:32:ASP:OD1	20:c:32:ASP:N	2.53	0.41
4:7:39:ALA:HB2	4:7:57:VAL:HG23	2.03	0.40
8:1:54:PRO:HD2	21:1:303:XAT:H242	2.02	0.40
9:a:114:ILE:HD12	9:a:114:ILE:HA	1.93	0.40
9:a:342:TRP:HB3	23:a:806:CLA:HAC1	2.02	0.40
23:a:828:CLA:H152	23:a:840:CLA:H191	2.03	0.40
30:a:843:PQN:H252	30:a:843:PQN:H211	1.82	0.40
10:b:83:LYS:HE3	10:b:83:LYS:HB3	1.85	0.40
10:b:461:PHE:HB2	23:b:836:CLA:CAD	2.52	0.40
23:b:807:CLA:H161	23:b:807:CLA:H192	1.73	0.40
23:b:836:CLA:H91	23:b:836:CLA:H111	1.93	0.40
23:b:839:CLA:H152	23:b:839:CLA:H111	1.87	0.40
31:b:844:BCR:H351	31:b:844:BCR:H15C	1.78	0.40
31:h:201:BCR:H371	31:h:201:BCR:H24C	1.87	0.40
8:1:186:ILE:HG13	8:1:187:THR:N	2.36	0.40
9:a:738:LEU:HD23	9:a:738:LEU:HA	1.80	0.40
23:a:826:CLA:H141	23:a:826:CLA:H161	1.81	0.40
23:a:828:CLA:H61	23:a:828:CLA:H2	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:842:CLA:H12	30:a:843:PQN:H301	2.02	0.40
10:b:433:PHE:CZ	31:f:801:BCR:H372	2.56	0.40
10:b:499:TRP:CD1	23:b:833:CLA:HED2	2.57	0.40
10:b:523:HIS:CE1	31:b:849:BCR:H322	2.56	0.40
10:b:550:PRO:HD2	20:c:62:PHE:CE1	2.57	0.40
23:b:827:CLA:H143	23:b:827:CLA:H161	1.78	0.40
14:h:104:VAL:HG22	31:h:202:BCR:H383	2.02	0.40
20:c:64:SER:HB2	32:c:102:SF4:S3	2.62	0.40
23:5:305:CLA:HAB	4:4:153:PHE:O	2.21	0.40
26:9:305:45D:H403	23:9:308:CLA:HBB1	2.03	0.40
23:9:311:CLA:HBA1	23:9:311:CLA:H3A	1.77	0.40
3:8:90:PHE:CE1	21:8:303:XAT:H30	2.57	0.40
21:8:302:XAT:H403	23:8:307:CLA:H202	2.02	0.40
21:8:303:XAT:H383	23:8:314:CLA:C3B	2.52	0.40
21:8:303:XAT:C11	23:8:312:CLA:HMC1	2.52	0.40
7:2:205:PHE:HE1	21:2:303:XAT:H162	1.84	0.40
23:a:804:CLA:H11	30:a:843:PQN:H201	2.04	0.40
23:a:806:CLA:H52	31:a:848:BCR:HC8	2.03	0.40
31:a:847:BCR:H15C	31:a:847:BCR:H351	1.84	0.40
10:b:547:LYS:HE2	13:f:180:ILE:HD11	2.03	0.40
23:b:827:CLA:H13	23:b:829:CLA:H141	2.02	0.40
23:b:833:CLA:H141	23:b:833:CLA:H161	1.85	0.40
13:f:114:PHE:HB2	31:f:801:BCR:H321	2.02	0.40
31:j:104:BCR:H20C	31:j:104:BCR:H361	1.91	0.40
1:5:221:ARG:HA	1:5:224:MET:HE3	2.04	0.40
23:4:309:CLA:HED2	23:4:309:CLA:HBD	1.83	0.40
23:4:317:CLA:HMB3	21:3:301:XAT:H392	2.03	0.40
21:3:301:XAT:H23	21:3:301:XAT:H373	1.95	0.40
21:6:303:XAT:H35	21:6:303:XAT:H401	1.83	0.40
21:2:304:XAT:H11	21:2:304:XAT:H191	1.89	0.40
9:a:452:ASN:HB3	9:a:635:THR:HG22	2.04	0.40
23:a:842:CLA:H62	23:a:842:CLA:H101	1.90	0.40
31:a:848:BCR:H15C	31:a:848:BCR:H351	1.78	0.40
23:b:807:CLA:H201	23:b:827:CLA:H143	2.03	0.40
23:b:835:CLA:HMB1	23:b:835:CLA:HBB1	2.02	0.40
31:j:104:BCR:H24C	31:j:104:BCR:H371	1.85	0.40
1:5:117:LEU:HD23	1:5:117:LEU:HA	1.92	0.40
2:9:83:TRP:O	2:9:87:HIS:ND1	2.51	0.40
26:9:305:45D:H321	26:9:305:45D:H281	1.82	0.40
3:8:55:ALA:HB1	3:8:171:VAL:HG23	2.03	0.40
3:8:77:ALA:HB2	3:8:147:PRO:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:304:XAT:H15	21:4:304:XAT:H201	1.87	0.40
5:3:106:VAL:HG11	23:3:311:CLA:HED1	2.04	0.40
21:3:303:XAT:H31	21:3:303:XAT:H391	1.95	0.40
21:6:303:XAT:H15	21:6:303:XAT:H201	1.64	0.40
23:6:309:CLA:H112	23:6:309:CLA:H152	1.83	0.40
4:7:113:ASP:HA	4:7:116:VAL:HG22	2.04	0.40
21:7:303:XAT:H31	21:7:303:XAT:H391	1.73	0.40
8:1:43:ILE:HG21	8:1:163:GLN:HB2	2.04	0.40
8:1:113:PRO:C	8:1:115:ILE:H	2.30	0.40
9:a:499:VAL:HG12	23:a:819:CLA:H11	2.03	0.40
23:a:829:CLA:H112	23:a:829:CLA:H143	1.90	0.40
23:a:829:CLA:H93	23:a:829:CLA:H111	1.89	0.40
23:a:841:CLA:HAA2	23:b:831:CLA:HMB1	2.02	0.40
31:a:849:BCR:H371	31:a:849:BCR:H24C	1.86	0.40
10:b:709:LEU:CD1	28:b:848:DGD:HB41	2.51	0.40
23:b:810:CLA:H142	23:b:810:CLA:H111	1.83	0.40
23:f:802:CLA:H11	23:j:102:CLA:H122	2.03	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	43
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	22	40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	8	18
8	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
9	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	69
10	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
11	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
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%)	76 (92%)	6 (7%)	1 (1%)	11	23
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	23
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%)	3551 (94%)	238 (6%)	9 (0%)	45	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	9	32	THR
7	2	45	LYS
17	1	120	VAL
7	2	127	ASN
7	2	213	VAL
9	a	580	SER
17	l	131	ILE
4	4	146	SER
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	82
3	8	132/160 (82%)	131 (99%)	1 (1%)	79	90
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	122/159 (77%)	121 (99%)	1 (1%)	79	90
5	3	136/164 (83%)	136 (100%)	0	100	100
6	6	135/201 (67%)	134 (99%)	1 (1%)	81	91
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	91
10	b	599/602 (100%)	599 (100%)	0	100	100
11	d	107/113 (95%)	107 (100%)	0	100	100
12	e	56/62 (90%)	56 (100%)	0	100	100
13	f	138/162 (85%)	138 (100%)	0	100	100
14	h	71/107 (66%)	70 (99%)	1 (1%)	62	82
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%)	3048 (100%)	10 (0%)	90	96

All (10) 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
14	h	110	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	133	GLN
2	9	104	HIS
3	8	156	ASN
5	3	156	GLN
5	3	169	ASN
8	1	63	GLN
8	1	119	GLN
8	1	132	ASN
8	1	194	GLN
9	a	127	ASN
9	a	186	ASN
10	b	80	ASN
10	b	112	ASN
10	b	326	ASN
10	b	605	GLN
10	b	629	ASN
11	d	7	GLN
13	f	166	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	4	310	-	65,73,73	1.49	5 (7%)	76,113,113	1.42	8 (10%)
23	CLA	b	820	-	50,58,73	1.70	6 (12%)	58,95,113	1.60	10 (17%)
22	A1L1G	7	302	-	38,47,47	1.44	6 (15%)	49,71,71	1.50	9 (18%)
23	CLA	a	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
21	XAT	3	301	-	39,47,47	0.90	1 (2%)	54,74,74	2.55	18 (33%)
23	CLA	7	311	-	46,54,73	1.79	6 (13%)	53,90,113	1.57	7 (13%)
23	CLA	7	313	-	54,62,73	1.66	5 (9%)	62,99,113	1.50	9 (14%)
31	BCR	1	205	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
23	CLA	3	308	-	47,55,73	1.76	5 (10%)	54,91,113	1.57	8 (14%)
23	CLA	5	312	-	52,60,73	1.66	5 (9%)	60,97,113	1.56	9 (15%)
22	A1L1G	9	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.57	10 (20%)
23	CLA	f	802	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	a	804	-	55,63,73	1.62	6 (10%)	64,101,113	1.55	9 (14%)
21	XAT	5	301	-	39,47,47	0.94	1 (2%)	54,74,74	2.57	19 (35%)
23	CLA	a	825	-	55,63,73	1.61	5 (9%)	64,101,113	1.45	8 (12%)
23	CLA	j	102	-	58,66,73	1.59	6 (10%)	67,104,113	1.42	8 (11%)
21	XAT	7	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.63	20 (37%)
28	DGD	b	848	-	58,58,67	1.15	7 (12%)	72,72,81	1.53	10 (13%)
31	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.05	16 (28%)
21	XAT	6	302	-	39,47,47	0.91	0	54,74,74	2.81	20 (37%)
21	XAT	7	304	-	39,47,47	0.91	1 (2%)	54,74,74	2.67	21 (38%)
23	CLA	1	309	8	46,54,73	1.78	6 (13%)	53,90,113	1.50	7 (13%)
31	BCR	b	844	-	41,41,41	0.68	0	56,56,56	2.10	16 (28%)
23	CLA	7	308	-	60,68,73	1.53	5 (8%)	70,107,113	1.44	7 (10%)
25	A1L1F	6	301	-	50,59,59	1.30	5 (10%)	62,85,85	2.50	20 (32%)
23	CLA	3	314	5	47,55,73	1.74	5 (10%)	54,91,113	1.54	6 (11%)
31	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
25	A1L1F	6	304	-	46,55,59	1.32	4 (8%)	58,81,85	2.56	20 (34%)
23	CLA	8	307	3	65,73,73	1.47	5 (7%)	76,113,113	1.38	8 (10%)
23	CLA	2	307	-	47,55,73	1.73	5 (10%)	54,91,113	1.64	7 (12%)
23	CLA	a	840	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	8 (10%)
21	XAT	8	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.66	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	XAT	8	301	-	39,47,47	0.91	1 (2%)	54,74,74	2.53	19 (35%)
23	CLA	b	802	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
23	CLA	6	312	6	51,59,73	1.68	6 (11%)	59,96,113	1.52	6 (10%)
23	CLA	b	832	-	65,73,73	1.46	5 (7%)	76,113,113	1.39	7 (9%)
31	BCR	b	842	-	41,41,41	0.71	0	56,56,56	2.29	20 (35%)
23	CLA	a	821	-	45,53,73	1.77	6 (13%)	52,89,113	1.64	6 (11%)
23	CLA	b	826	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	6 (7%)
23	CLA	a	820	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	9 (11%)
21	XAT	9	303	-	39,47,47	0.94	1 (2%)	54,74,74	2.61	19 (35%)
23	CLA	8	312	3	52,60,73	1.65	5 (9%)	60,97,113	1.52	8 (13%)
23	CLA	1	313	-	41,49,73	1.85	6 (14%)	47,84,113	1.64	7 (14%)
23	CLA	a	841	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	9 (11%)
23	CLA	2	306	-	41,50,73	1.86	6 (14%)	46,85,113	1.56	6 (13%)
23	CLA	a	801	-	65,73,73	1.50	8 (12%)	76,113,113	1.38	7 (9%)
21	XAT	4	301	-	39,47,47	0.94	2 (5%)	54,74,74	2.63	19 (35%)
23	CLA	a	822	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
23	CLA	a	817	-	45,53,73	1.80	5 (11%)	52,89,113	1.58	6 (11%)
23	CLA	4	308	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	9 (11%)
23	CLA	1	310	8	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
23	CLA	b	812	-	53,61,73	1.64	5 (9%)	61,98,113	1.49	8 (13%)
31	BCR	f	801	-	41,41,41	0.68	0	56,56,56	2.14	16 (28%)
23	CLA	4	316	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
23	CLA	b	806	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	7 (9%)
23	CLA	3	309	5	56,64,73	1.60	6 (10%)	65,102,113	1.46	7 (10%)
30	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.09	3 (7%)
23	CLA	1	203	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	7 (10%)
23	CLA	6	310	-	52,60,73	1.66	5 (9%)	60,97,113	1.53	8 (13%)
23	CLA	a	816	-	50,58,73	1.68	6 (12%)	58,95,113	1.58	8 (13%)
23	CLA	5	311	-	51,59,73	1.65	5 (9%)	59,96,113	1.53	9 (15%)
21	XAT	4	302	-	39,47,47	0.91	0	54,74,74	2.57	20 (37%)
21	XAT	6	305	-	39,47,47	0.90	1 (2%)	54,74,74	2.73	19 (35%)
23	CLA	2	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.56	7 (13%)
23	CLA	7	310	-	46,54,73	1.76	5 (10%)	53,90,113	1.56	6 (11%)
23	CLA	5	314	-	52,60,73	1.66	6 (11%)	60,97,113	1.54	8 (13%)
23	CLA	a	831	-	65,73,73	1.50	5 (7%)	76,113,113	1.47	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	4	313	-	53,61,73	1.65	5 (9%)	61,98,113	1.49	8 (13%)
23	CLA	a	836	-	50,58,73	1.69	5 (10%)	58,95,113	1.51	9 (15%)
23	CLA	b	824	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	7 (9%)
25	A1L1F	9	302	-	50,59,59	1.37	5 (10%)	62,85,85	2.71	19 (30%)
25	A1L1F	8	304	-	50,59,59	1.30	4 (8%)	62,85,85	2.79	23 (37%)
29	LMG	a	853	-	34,34,55	1.13	2 (5%)	42,42,63	1.16	3 (7%)
31	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.13	14 (25%)
31	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
23	CLA	b	805	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	a	803	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	6 (7%)
21	XAT	8	303	-	39,47,47	0.88	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	b	816	-	55,63,73	1.62	5 (9%)	64,101,113	1.48	9 (14%)
29	LMG	j	105	-	32,32,55	1.12	2 (6%)	40,40,63	1.14	3 (7%)
23	CLA	4	312	-	46,54,73	1.78	5 (10%)	53,90,113	1.52	7 (13%)
23	CLA	b	813	-	65,73,73	1.48	5 (7%)	76,113,113	1.38	8 (10%)
23	CLA	8	311	-	56,64,73	1.58	5 (8%)	65,102,113	1.51	8 (12%)
23	CLA	4	306	4	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
23	CLA	a	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	9 (11%)
23	CLA	b	829	-	65,73,73	1.51	6 (9%)	76,113,113	1.44	10 (13%)
23	CLA	a	818	-	56,64,73	1.62	5 (8%)	65,102,113	1.43	8 (12%)
23	CLA	b	835	-	58,66,73	1.56	5 (8%)	67,104,113	1.53	8 (11%)
23	CLA	7	307	-	45,53,73	1.79	5 (11%)	52,89,113	1.57	7 (13%)
30	PQN	b	841	-	34,34,34	1.55	2 (5%)	42,45,45	1.20	4 (9%)
23	CLA	a	819	-	54,62,73	1.63	5 (9%)	62,99,113	1.45	7 (11%)
23	CLA	a	802	-	58,66,73	1.55	5 (8%)	67,104,113	1.49	7 (10%)
23	CLA	b	819	-	55,63,73	1.63	6 (10%)	64,101,113	1.44	8 (12%)
23	CLA	b	801	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	9	316	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
23	CLA	h	204	-	55,63,73	1.62	6 (10%)	64,101,113	1.48	9 (14%)
23	CLA	3	312	5	59,67,73	1.57	6 (10%)	68,105,113	1.43	7 (10%)
31	BCR	l	201	-	41,41,41	0.71	0	56,56,56	1.96	17 (30%)
23	CLA	2	315	-	42,50,73	1.86	5 (11%)	48,85,113	1.56	7 (14%)
23	CLA	a	823	-	49,57,73	1.68	5 (10%)	55,93,113	1.60	7 (12%)
23	CLA	b	814	-	55,63,73	1.61	6 (10%)	64,101,113	1.55	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	7	314	-	45,53,73	1.80	6 (13%)	52,89,113	1.65	7 (13%)
31	BCR	b	849	-	41,41,41	0.73	0	56,56,56	2.06	15 (26%)
23	CLA	8	314	-	41,49,73	1.87	5 (12%)	47,84,113	1.65	7 (14%)
23	CLA	2	314	-	56,64,73	1.61	6 (10%)	65,102,113	1.44	7 (10%)
23	CLA	4	317	-	55,63,73	1.63	5 (9%)	64,101,113	1.47	7 (10%)
23	CLA	b	823	-	53,61,73	1.63	6 (11%)	61,98,113	1.47	8 (13%)
27	LHG	b	847	23	30,30,48	1.33	6 (20%)	33,36,54	1.15	2 (6%)
23	CLA	a	807	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
23	CLA	a	808	-	51,59,73	1.71	6 (11%)	59,96,113	1.50	8 (13%)
23	CLA	a	832	-	50,58,73	1.70	6 (12%)	58,95,113	1.54	8 (13%)
31	BCR	b	846	-	41,41,41	0.75	0	56,56,56	1.78	15 (26%)
23	CLA	a	811	-	56,64,73	1.59	5 (8%)	65,102,113	1.48	8 (12%)
23	CLA	l	202	-	42,50,73	1.83	6 (14%)	48,85,113	1.64	7 (14%)
31	BCR	m	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	6 (10%)
23	CLA	a	813	-	54,62,73	1.63	5 (9%)	62,99,113	1.44	7 (11%)
23	CLA	b	838	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	6	309	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	6 (7%)
23	CLA	1	308	8	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
23	CLA	a	835	-	65,73,73	1.47	5 (7%)	76,113,113	1.43	8 (10%)
21	XAT	4	303	-	39,47,47	0.89	0	54,74,74	2.57	18 (33%)
23	CLA	6	316	6	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
23	CLA	l	204	-	46,54,73	1.75	6 (13%)	53,90,113	1.56	7 (13%)
23	CLA	6	308	-	58,66,73	1.60	6 (10%)	67,104,113	1.42	6 (8%)
29	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.31	4 (9%)
22	A1L1G	5	303	-	38,47,47	1.41	6 (15%)	49,71,71	1.46	7 (14%)
24	SQD	5	316	23	34,35,54	1.47	4 (11%)	43,46,65	1.34	7 (16%)
22	A1L1G	9	306	-	38,47,47	1.41	6 (15%)	49,71,71	1.53	8 (16%)
23	CLA	9	311	-	46,54,73	1.75	5 (10%)	53,90,113	1.61	8 (15%)
25	A1L1F	h	203	-	50,59,59	1.38	5 (10%)	62,85,85	2.60	22 (35%)
23	CLA	9	314	-	55,63,73	1.61	6 (10%)	64,101,113	1.50	8 (12%)
23	CLA	1	305	-	61,69,73	1.55	5 (8%)	71,108,113	1.39	7 (9%)
28	DGD	8	315	23	41,41,67	1.05	2 (4%)	55,55,81	1.11	5 (9%)
23	CLA	2	316	7	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
23	CLA	6	315	6	41,49,73	1.86	5 (12%)	47,84,113	1.63	6 (12%)
21	XAT	7	303	-	39,47,47	0.97	1 (2%)	54,74,74	2.59	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	806	-	65,73,73	1.49	11 (16%)	76,113,113	1.67	13 (17%)
21	XAT	j	101	-	39,47,47	0.89	0	54,74,74	2.72	18 (33%)
23	CLA	3	313	-	52,60,73	1.66	5 (9%)	60,97,113	1.52	9 (15%)
23	CLA	4	311	-	46,54,73	1.78	6 (13%)	53,90,113	1.55	7 (13%)
23	CLA	2	313	7	41,49,73	1.84	5 (12%)	47,84,113	1.68	8 (17%)
23	CLA	7	309	-	46,55,73	1.76	5 (10%)	52,91,113	1.53	7 (13%)
23	CLA	4	314	4	45,53,73	1.81	5 (11%)	52,89,113	1.56	7 (13%)
23	CLA	7	312	-	48,56,73	1.71	6 (12%)	55,92,113	1.55	8 (14%)
32	SF4	c	102	-	0,12,12	-	-	-	-	-
23	CLA	a	833	-	55,63,73	1.58	5 (9%)	64,101,113	1.54	7 (10%)
23	CLA	1	306	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	10 (13%)
23	CLA	b	809	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	8 (10%)
23	CLA	b	810	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	7 (9%)
21	XAT	4	304	-	39,47,47	0.89	1 (2%)	54,74,74	2.56	16 (29%)
23	CLA	2	308	7	54,62,73	1.65	5 (9%)	62,99,113	1.45	8 (12%)
23	CLA	a	826	-	65,73,73	1.47	6 (9%)	76,113,113	1.45	6 (7%)
23	CLA	b	839	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	8 (10%)
24	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	5 (9%)
32	SF4	c	101	-	0,12,12	-	-	-	-	-
23	CLA	a	838	-	51,59,73	1.66	6 (11%)	59,96,113	1.56	9 (15%)
23	CLA	1	312	8	52,60,73	1.70	5 (9%)	60,97,113	1.48	8 (13%)
21	XAT	2	301	-	39,47,47	0.93	1 (2%)	54,74,74	2.71	19 (35%)
23	CLA	a	828	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
23	CLA	5	310	-	46,54,73	1.76	5 (10%)	53,90,113	1.54	7 (13%)
23	CLA	9	312	-	46,54,73	1.74	6 (13%)	53,90,113	1.68	8 (15%)
23	CLA	b	834	-	53,61,73	1.68	6 (11%)	61,98,113	1.51	8 (13%)
23	CLA	b	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	7 (9%)
23	CLA	a	837	9	45,53,73	1.79	6 (13%)	52,89,113	1.58	7 (13%)
31	BCR	b	845	-	41,41,41	0.76	0	56,56,56	2.19	22 (39%)
21	XAT	2	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.50	18 (33%)
23	CLA	b	808	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	9 (11%)
23	CLA	a	814	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	5	315	-	46,54,73	1.75	5 (10%)	53,90,113	1.56	7 (13%)
23	CLA	7	315	4	41,49,73	1.86	5 (12%)	47,84,113	1.65	7 (14%)
21	XAT	6	303	-	39,47,47	0.89	1 (2%)	54,74,74	2.65	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	7	316	-	51,59,73	1.64	6 (11%)	59,96,113	1.60	8 (13%)
23	CLA	7	317	-	45,53,73	1.80	5 (11%)	52,89,113	1.59	6 (11%)
21	XAT	3	304	-	39,47,47	0.90	1 (2%)	54,74,74	2.62	19 (35%)
32	SF4	a	851	-	0,12,12	-	-	-	-	-
23	CLA	8	310	-	46,54,73	1.77	6 (13%)	53,90,113	1.55	7 (13%)
23	CLA	2	310	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
23	CLA	a	842	-	65,73,73	1.51	6 (9%)	76,113,113	1.38	7 (9%)
31	BCR	h	202	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
23	CLA	b	825	-	64,72,73	1.48	6 (9%)	74,111,113	1.45	8 (10%)
23	CLA	1	307	-	54,62,73	1.62	5 (9%)	62,99,113	1.51	8 (12%)
21	XAT	3	303	-	39,47,47	0.90	1 (2%)	54,74,74	2.59	21 (38%)
23	CLA	9	318	-	62,70,73	1.55	6 (9%)	72,109,113	1.38	8 (11%)
23	CLA	6	307	-	46,54,73	1.77	5 (10%)	53,90,113	1.54	7 (13%)
23	CLA	1	311	-	53,61,73	1.63	5 (9%)	61,98,113	1.51	9 (14%)
23	CLA	6	317	-	65,73,73	1.50	5 (7%)	76,113,113	1.45	7 (9%)
23	CLA	a	844	27	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)
23	CLA	5	309	1	65,73,73	1.49	5 (7%)	76,113,113	1.37	7 (9%)
23	CLA	9	315	2	42,50,73	1.82	5 (11%)	48,85,113	1.60	7 (14%)
23	CLA	a	824	-	46,54,73	1.77	6 (13%)	53,90,113	1.50	7 (13%)
23	CLA	5	308	-	55,63,73	1.63	6 (10%)	64,101,113	1.47	7 (10%)
23	CLA	9	310	-	46,54,73	1.74	5 (10%)	53,90,113	1.65	6 (11%)
21	XAT	a	852	-	39,47,47	0.95	2 (5%)	54,74,74	2.69	20 (37%)
23	CLA	4	307	-	56,64,73	1.62	5 (8%)	65,102,113	1.44	7 (10%)
23	CLA	a	812	23	62,70,73	1.51	6 (9%)	72,109,113	1.44	8 (11%)
23	CLA	6	313	-	52,60,73	1.65	5 (9%)	60,97,113	1.50	7 (11%)
31	BCR	a	849	-	41,41,41	0.72	0	56,56,56	2.17	20 (35%)
31	BCR	j	104	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
23	CLA	3	311	-	50,58,73	1.70	5 (10%)	58,95,113	1.55	9 (15%)
23	CLA	b	828	-	65,73,73	1.51	6 (9%)	76,113,113	1.32	7 (9%)
23	CLA	2	311	-	58,66,73	1.59	5 (8%)	67,104,113	1.42	7 (10%)
27	LHG	9	317	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
23	CLA	5	313	1	45,53,73	1.81	5 (11%)	52,89,113	1.57	6 (11%)
23	CLA	b	831	-	49,57,73	1.70	5 (10%)	55,93,113	1.56	8 (14%)
23	CLA	5	305	1	46,54,73	1.77	6 (13%)	53,90,113	1.54	8 (15%)
28	DGD	4	318	-	41,41,67	1.07	2 (4%)	55,55,81	1.82	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	8	309	-	57,65,73	1.59	5 (8%)	66,103,113	1.45	9 (13%)
21	XAT	7	305	-	39,47,47	0.86	0	54,74,74	2.65	20 (37%)
21	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	15 (27%)
21	XAT	2	304	-	39,47,47	0.88	0	54,74,74	2.54	20 (37%)
21	XAT	2	305	-	39,47,47	0.91	1 (2%)	54,74,74	2.43	18 (33%)
22	A1L1G	3	302	-	38,47,47	1.47	6 (15%)	49,71,71	1.39	7 (14%)
25	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
23	CLA	j	103	16	42,50,73	1.82	5 (11%)	48,85,113	1.65	6 (12%)
22	A1L1G	3	306	-	38,47,47	1.43	6 (15%)	49,71,71	1.50	9 (18%)
21	XAT	1	303	-	39,47,47	0.90	0	54,74,74	2.52	19 (35%)
23	CLA	5	306	24	45,53,73	1.79	5 (11%)	52,89,113	1.57	6 (11%)
23	CLA	b	811	-	54,62,73	1.67	7 (12%)	67,100,113	1.49	9 (13%)
23	CLA	8	313	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	6 (11%)
23	CLA	b	822	-	60,68,73	1.54	6 (10%)	70,107,113	1.38	8 (11%)
23	CLA	b	840	27	65,73,73	1.52	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	7	306	4	48,56,73	1.73	6 (12%)	55,92,113	1.52	7 (12%)
23	CLA	3	310	-	56,64,73	1.59	5 (8%)	65,102,113	1.45	7 (10%)
26	45D	9	305	-	43,43,43	1.10	4 (9%)	54,60,60	2.17	18 (33%)
27	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
23	CLA	b	830	-	41,49,73	1.83	6 (14%)	47,84,113	1.64	8 (17%)
23	CLA	a	810	9	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	f	803	13	52,60,73	1.67	5 (9%)	60,97,113	1.50	8 (13%)
23	CLA	b	833	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
23	CLA	a	854	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
23	CLA	8	308	-	55,63,73	1.62	5 (9%)	64,101,113	1.50	9 (14%)
23	CLA	a	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.59	7 (13%)
23	CLA	b	817	-	59,67,73	1.56	6 (10%)	68,105,113	1.51	9 (13%)
23	CLA	b	821	-	51,59,73	1.64	5 (9%)	59,96,113	1.56	9 (15%)
23	CLA	4	315	4	41,49,73	1.87	5 (12%)	47,84,113	1.65	8 (17%)
23	CLA	3	307	5	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
23	CLA	2	312	-	47,55,73	1.75	5 (10%)	54,91,113	1.57	7 (12%)
22	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.58	11 (22%)
23	CLA	8	305	3	43,51,73	1.78	5 (11%)	49,86,113	1.64	7 (14%)
23	CLA	b	818	-	60,68,73	1.57	5 (8%)	70,107,113	1.41	7 (10%)
23	CLA	b	807	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	a	846	23	26,26,48	1.28	5 (19%)	29,32,54	1.21	2 (6%)
31	BCR	a	850	-	41,41,41	0.73	0	56,56,56	2.16	14 (25%)
23	CLA	a	809	9	65,73,73	1.44	5 (7%)	76,113,113	1.43	9 (11%)
23	CLA	9	309	2	46,54,73	1.76	6 (13%)	53,90,113	1.54	7 (13%)
23	CLA	b	804	-	65,73,73	1.45	6 (9%)	76,113,113	1.55	12 (15%)
23	CLA	1	314	-	45,53,73	1.80	5 (11%)	52,89,113	1.55	6 (11%)
21	XAT	2	303	-	39,47,47	0.97	1 (2%)	54,74,74	2.63	20 (37%)
21	XAT	4	305	-	39,47,47	0.91	1 (2%)	54,74,74	2.75	19 (35%)
23	CLA	9	308	2	65,73,73	1.50	7 (10%)	76,113,113	1.42	9 (11%)
23	CLA	3	315	5	46,54,73	1.79	6 (13%)	53,90,113	1.52	7 (13%)
23	CLA	b	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
23	CLA	6	311	6	42,50,73	1.84	5 (11%)	48,85,113	1.57	7 (14%)
23	CLA	6	314	-	46,54,73	1.73	5 (10%)	53,90,113	1.62	6 (11%)
23	CLA	b	837	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	8 (10%)
23	CLA	b	836	-	65,73,73	1.47	5 (7%)	76,113,113	1.41	9 (11%)
27	LHG	9	307	-	35,35,48	1.22	6 (17%)	38,41,54	0.97	2 (5%)
23	CLA	a	829	-	62,70,73	1.52	5 (8%)	72,109,113	1.41	8 (11%)
23	CLA	b	815	-	45,53,73	1.77	5 (11%)	52,89,113	1.60	7 (13%)
23	CLA	8	306	28	46,54,73	1.76	5 (10%)	53,90,113	1.54	7 (13%)
23	CLA	5	307	1	60,68,73	1.53	5 (8%)	70,107,113	1.42	8 (11%)
23	CLA	4	309	-	50,58,73	1.69	5 (10%)	58,95,113	1.56	8 (13%)
21	XAT	6	306	-	39,47,47	0.94	2 (5%)	54,74,74	2.60	19 (35%)
21	XAT	5	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.58	20 (37%)
23	CLA	a	830	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	8 (10%)
31	BCR	b	843	-	41,41,41	0.71	0	56,56,56	1.92	16 (28%)
23	CLA	9	313	2	46,54,73	1.76	5 (10%)	53,90,113	1.62	7 (13%)
21	XAT	3	305	-	39,47,47	0.88	1 (2%)	54,74,74	2.57	16 (29%)
23	CLA	a	834	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	9 (11%)
23	CLA	a	805	23	55,63,73	1.61	5 (9%)	64,101,113	1.51	8 (12%)
31	BCR	h	201	-	41,41,41	0.71	0	56,56,56	1.97	21 (37%)
21	XAT	5	304	-	39,47,47	0.89	0	54,74,74	2.86	22 (40%)

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	4	310	-	1/1/15/20	16/37/115/115	-
23	CLA	b	820	-	1/1/12/20	7/19/97/115	-
22	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
23	CLA	a	839	-	1/1/15/20	15/37/115/115	-
23	CLA	7	313	-	1/1/12/20	7/24/102/115	-
23	CLA	7	311	-	1/1/11/20	5/15/93/115	-
21	XAT	3	301	-	-	3/31/93/93	0/4/4/4
31	BCR	1	205	-	-	8/29/63/63	0/2/2/2
23	CLA	3	308	-	1/1/11/20	5/16/94/115	-
23	CLA	5	312	-	1/1/12/20	0/22/100/115	-
22	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
23	CLA	f	802	-	1/1/15/20	13/37/115/115	-
23	CLA	a	804	-	1/1/13/20	10/25/103/115	-
23	CLA	j	102	-	1/1/13/20	16/29/107/115	-
23	CLA	a	825	-	1/1/13/20	8/25/103/115	-
21	XAT	5	301	-	-	3/31/93/93	0/4/4/4
21	XAT	7	301	-	-	6/31/93/93	0/4/4/4
28	DGD	b	848	-	-	20/46/86/95	0/2/2/2
31	BCR	f	804	-	-	4/29/63/63	0/2/2/2
21	XAT	6	302	-	-	7/31/93/93	0/4/4/4
21	XAT	7	304	-	-	6/31/93/93	0/4/4/4
23	CLA	1	309	8	1/1/11/20	6/15/93/115	-
31	BCR	b	844	-	-	6/29/63/63	0/2/2/2
23	CLA	7	308	-	1/1/14/20	14/31/109/115	-
25	A1L1F	6	301	-	-	11/43/99/99	0/3/3/3
23	CLA	3	314	5	1/1/11/20	7/16/94/115	-
31	BCR	a	847	-	-	0/29/63/63	0/2/2/2
25	A1L1F	6	304	-	-	12/39/95/99	0/3/3/3
23	CLA	8	307	3	1/1/15/20	13/37/115/115	-
23	CLA	2	307	-	1/1/11/20	6/16/94/115	-
23	CLA	a	840	-	1/1/15/20	8/37/115/115	-
21	XAT	8	302	-	-	4/31/93/93	0/4/4/4
23	CLA	b	802	-	1/1/15/20	17/37/115/115	-
21	XAT	8	301	-	-	3/31/93/93	0/4/4/4
23	CLA	6	312	6	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	832	-	1/1/15/20	13/37/115/115	-
31	BCR	b	842	-	-	2/29/63/63	0/2/2/2
23	CLA	a	821	-	1/1/11/20	2/13/91/115	-
23	CLA	b	826	-	1/1/15/20	5/37/115/115	-
23	CLA	a	820	-	1/1/15/20	15/37/115/115	-
21	XAT	9	303	-	-	4/31/93/93	0/4/4/4
23	CLA	8	312	3	1/1/12/20	2/22/100/115	-
23	CLA	1	313	-	1/1/10/20	3/8/86/115	-
23	CLA	a	841	-	1/1/15/20	15/37/115/115	-
23	CLA	2	306	-	1/1/10/20	2/9/87/115	-
23	CLA	a	801	-	1/1/15/20	22/37/115/115	-
21	XAT	4	301	-	-	4/31/93/93	0/4/4/4
23	CLA	a	822	-	1/1/15/20	5/37/115/115	-
23	CLA	a	817	-	1/1/11/20	6/13/91/115	-
23	CLA	4	308	-	1/1/15/20	14/37/115/115	-
23	CLA	1	310	8	1/1/15/20	18/37/115/115	-
23	CLA	b	812	-	1/1/12/20	6/23/101/115	-
31	BCR	f	801	-	-	3/29/63/63	0/2/2/2
23	CLA	4	316	-	1/1/11/20	7/15/93/115	-
23	CLA	b	806	-	1/1/15/20	16/37/115/115	-
23	CLA	3	309	5	1/1/13/20	5/27/105/115	-
30	PQN	a	843	-	-	5/23/43/43	0/2/2/2
23	CLA	1	203	-	1/1/14/20	6/31/109/115	-
23	CLA	6	310	-	1/1/12/20	7/22/100/115	-
23	CLA	a	816	-	1/1/12/20	5/19/97/115	-
23	CLA	5	311	-	1/1/12/20	8/21/99/115	-
23	CLA	2	309	-	1/1/11/20	4/15/93/115	-
23	CLA	a	836	-	1/1/12/20	6/19/97/115	-
21	XAT	4	302	-	-	0/31/93/93	0/4/4/4
23	CLA	7	310	-	1/1/11/20	6/15/93/115	-
23	CLA	5	314	-	1/1/12/20	4/22/100/115	-
23	CLA	a	831	-	1/1/15/20	11/37/115/115	-
23	CLA	4	313	-	1/1/12/20	6/23/101/115	-
23	CLA	b	824	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	XAT	6	305	-	-	4/31/93/93	0/4/4/4
25	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
25	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
29	LMG	a	853	-	-	13/29/49/70	0/1/1/1
31	BCR	i	101	-	-	3/29/63/63	0/2/2/2
31	BCR	a	848	-	-	0/29/63/63	0/2/2/2
23	CLA	b	805	-	1/1/15/20	12/37/115/115	-
23	CLA	a	803	-	1/1/15/20	3/37/115/115	-
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	b	816	-	1/1/13/20	4/25/103/115	-
29	LMG	j	105	-	-	11/27/47/70	0/1/1/1
23	CLA	4	312	-	1/1/11/20	4/15/93/115	-
23	CLA	b	813	-	1/1/15/20	14/37/115/115	-
23	CLA	8	311	-	1/1/13/20	8/27/105/115	-
23	CLA	4	306	4	1/1/11/20	7/13/91/115	-
23	CLA	a	827	-	1/1/15/20	8/37/115/115	-
23	CLA	b	829	-	1/1/15/20	10/37/115/115	-
23	CLA	a	818	-	1/1/13/20	11/27/105/115	-
23	CLA	b	835	-	1/1/13/20	11/29/107/115	-
23	CLA	7	307	-	1/1/11/20	5/13/91/115	-
30	PQN	b	841	-	-	1/23/43/43	0/2/2/2
23	CLA	a	819	-	1/1/12/20	4/24/102/115	-
23	CLA	a	802	-	1/1/13/20	7/29/107/115	-
23	CLA	b	819	-	1/1/13/20	3/25/103/115	-
23	CLA	b	801	-	1/1/15/20	20/37/115/115	-
23	CLA	9	316	-	1/1/15/20	17/37/115/115	-
23	CLA	h	204	-	1/1/13/20	9/25/103/115	-
23	CLA	3	312	5	1/1/13/20	9/30/108/115	-
31	BCR	l	201	-	-	4/29/63/63	0/2/2/2
23	CLA	2	315	-	1/1/10/20	1/10/88/115	-
23	CLA	a	823	-	1/1/11/20	7/18/96/115	-
23	CLA	b	814	-	1/1/13/20	13/25/103/115	-
23	CLA	7	314	-	1/1/11/20	4/13/91/115	-
31	BCR	b	849	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	8	314	-	1/1/10/20	5/8/86/115	-
23	CLA	2	314	-	1/1/13/20	13/27/105/115	-
23	CLA	4	317	-	1/1/13/20	7/25/103/115	-
23	CLA	b	823	-	1/1/12/20	8/23/101/115	-
27	LHG	b	847	23	-	20/35/35/53	-
23	CLA	a	807	-	1/1/15/20	18/37/115/115	-
23	CLA	a	808	-	1/1/12/20	3/21/99/115	-
23	CLA	a	832	-	1/1/12/20	5/19/97/115	-
31	BCR	b	846	-	-	2/29/63/63	0/2/2/2
23	CLA	a	811	-	1/1/13/20	8/27/105/115	-
23	CLA	l	202	-	1/1/10/20	2/10/88/115	-
31	BCR	m	101	-	-	9/29/63/63	0/2/2/2
23	CLA	a	813	-	1/1/12/20	9/24/102/115	-
23	CLA	b	838	-	1/1/15/20	13/37/115/115	-
23	CLA	6	309	-	1/1/15/20	10/37/115/115	-
23	CLA	1	308	8	1/1/15/20	13/37/115/115	-
23	CLA	a	835	-	1/1/15/20	12/37/115/115	-
23	CLA	6	316	6	1/1/11/20	7/15/93/115	-
23	CLA	1	204	-	1/1/11/20	4/15/93/115	-
21	XAT	4	303	-	-	3/31/93/93	0/4/4/4
23	CLA	6	308	-	1/1/13/20	4/29/107/115	-
29	LMG	2	317	-	-	11/30/50/70	0/1/1/1
22	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
24	SQD	5	316	23	-	11/30/50/69	0/1/1/1
23	CLA	9	311	-	1/1/11/20	7/15/93/115	-
22	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
25	A1L1F	h	203	-	-	11/43/99/99	1/3/3/3
23	CLA	9	314	-	1/1/13/20	9/25/103/115	-
23	CLA	1	305	-	1/1/14/20	10/33/111/115	-
28	DGD	8	315	23	-	11/29/69/95	0/2/2/2
23	CLA	2	316	7	1/1/11/20	5/15/93/115	-
23	CLA	6	315	6	1/1/10/20	3/8/86/115	-
23	CLA	a	806	-	1/1/15/20	12/37/115/115	-
21	XAT	7	303	-	-	8/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	XAT	j	101	-	-	5/31/93/93	0/4/4/4
23	CLA	3	313	-	1/1/12/20	1/22/100/115	-
23	CLA	4	311	-	1/1/11/20	8/15/93/115	-
23	CLA	2	313	7	1/1/10/20	4/8/86/115	-
23	CLA	7	309	-	1/1/11/20	5/15/93/115	-
23	CLA	4	314	4	1/1/11/20	3/13/91/115	-
23	CLA	7	312	-	1/1/11/20	3/17/95/115	-
32	SF4	c	102	-	-	-	0/6/5/5
23	CLA	a	833	-	1/1/13/20	2/25/103/115	-
23	CLA	1	306	-	1/1/15/20	15/37/115/115	-
23	CLA	b	809	-	1/1/15/20	11/37/115/115	-
23	CLA	b	810	-	1/1/15/20	16/37/115/115	-
21	XAT	4	304	-	-	0/31/93/93	0/4/4/4
23	CLA	2	308	7	1/1/12/20	5/24/102/115	-
23	CLA	a	826	-	1/1/15/20	9/37/115/115	-
23	CLA	b	839	-	1/1/15/20	17/37/115/115	-
24	SQD	1	315	-	-	19/40/60/69	0/1/1/1
32	SF4	c	101	-	-	-	0/6/5/5
23	CLA	a	838	-	1/1/12/20	6/21/99/115	-
23	CLA	1	312	8	1/1/12/20	3/22/100/115	-
21	XAT	2	301	-	-	3/31/93/93	0/4/4/4
23	CLA	a	828	-	1/1/15/20	9/37/115/115	-
23	CLA	5	310	-	1/1/11/20	6/15/93/115	-
23	CLA	9	312	-	1/1/11/20	9/15/93/115	-
23	CLA	b	834	-	1/1/12/20	8/23/101/115	-
23	CLA	b	803	-	1/1/15/20	18/37/115/115	-
23	CLA	a	837	9	1/1/11/20	4/13/91/115	-
31	BCR	b	845	-	-	1/29/63/63	0/2/2/2
23	CLA	b	808	-	1/1/15/20	12/37/115/115	-
21	XAT	2	302	-	-	0/31/93/93	0/4/4/4
23	CLA	a	814	-	1/1/15/20	20/37/115/115	-
23	CLA	5	315	-	1/1/11/20	5/15/93/115	-
23	CLA	7	315	4	1/1/10/20	4/8/86/115	-
23	CLA	7	317	-	1/1/11/20	5/13/91/115	-
23	CLA	7	316	-	1/1/12/20	11/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	XAT	6	303	-	-	5/31/93/93	0/4/4/4
21	XAT	3	304	-	-	3/31/93/93	0/4/4/4
32	SF4	a	851	-	-	-	0/6/5/5
23	CLA	8	310	-	1/1/11/20	5/15/93/115	-
23	CLA	2	310	-	1/1/15/20	14/37/115/115	-
23	CLA	a	842	-	1/1/15/20	9/37/115/115	-
31	BCR	h	202	-	-	2/29/63/63	0/2/2/2
23	CLA	b	825	-	1/1/14/20	6/36/114/115	-
23	CLA	1	307	-	1/1/12/20	6/24/102/115	-
21	XAT	3	303	-	-	3/31/93/93	0/4/4/4
23	CLA	9	318	-	1/1/14/20	9/34/112/115	-
23	CLA	6	307	-	1/1/11/20	1/15/93/115	-
23	CLA	1	311	-	1/1/12/20	6/23/101/115	-
23	CLA	6	317	-	1/1/15/20	9/37/115/115	-
23	CLA	a	844	27	1/1/15/20	16/37/115/115	-
23	CLA	5	309	1	1/1/15/20	14/37/115/115	-
23	CLA	9	315	2	1/1/10/20	6/10/88/115	-
23	CLA	a	824	-	1/1/11/20	4/15/93/115	-
23	CLA	5	308	-	1/1/13/20	4/25/103/115	-
23	CLA	9	310	-	1/1/11/20	6/15/93/115	-
23	CLA	4	307	-	1/1/13/20	7/27/105/115	-
23	CLA	a	812	23	1/1/14/20	9/34/112/115	-
21	XAT	a	852	-	-	7/31/93/93	0/4/4/4
23	CLA	6	313	-	1/1/12/20	2/22/100/115	-
31	BCR	a	849	-	-	0/29/63/63	0/2/2/2
31	BCR	j	104	-	-	4/29/63/63	0/2/2/2
23	CLA	3	311	-	1/1/12/20	4/19/97/115	-
23	CLA	b	828	-	1/1/15/20	11/37/115/115	-
23	CLA	2	311	-	1/1/13/20	5/29/107/115	-
27	LHG	9	317	-	-	28/50/50/53	-
23	CLA	5	313	1	1/1/11/20	4/13/91/115	-
23	CLA	b	831	-	1/1/11/20	6/18/96/115	-
23	CLA	5	305	1	1/1/11/20	4/15/93/115	-
28	DGD	4	318	-	-	10/29/69/95	0/2/2/2
23	CLA	8	309	-	1/1/13/20	8/28/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	XAT	7	305	-	-	2/31/93/93	0/4/4/4
21	XAT	1	302	-	-	0/31/93/93	0/4/4/4
21	XAT	2	304	-	-	3/31/93/93	0/4/4/4
21	XAT	2	305	-	-	2/31/93/93	0/4/4/4
22	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
25	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
23	CLA	j	103	16	1/1/10/20	5/10/88/115	-
22	A1L1G	3	306	-	-	18/29/85/85	0/3/3/3
21	XAT	1	303	-	-	0/31/93/93	0/4/4/4
23	CLA	5	306	24	1/1/11/20	7/13/91/115	-
23	CLA	b	811	-	1/1/13/20	5/25/101/115	-
23	CLA	8	313	-	1/1/11/20	3/15/93/115	-
23	CLA	b	822	-	1/1/14/20	7/31/109/115	-
23	CLA	b	840	27	1/1/15/20	9/37/115/115	-
23	CLA	7	306	4	1/1/11/20	10/17/95/115	-
23	CLA	3	310	-	1/1/13/20	4/27/105/115	-
26	45D	9	305	-	-	9/29/69/69	0/2/2/2
27	LHG	a	845	-	-	27/52/52/53	-
23	CLA	b	830	-	1/1/10/20	1/8/86/115	-
23	CLA	a	810	9	1/1/15/20	13/37/115/115	-
23	CLA	f	803	13	1/1/12/20	2/22/100/115	-
23	CLA	b	833	-	1/1/15/20	14/37/115/115	-
23	CLA	a	854	-	1/1/15/20	13/37/115/115	-
23	CLA	8	308	-	1/1/13/20	7/25/103/115	-
23	CLA	a	815	-	1/1/11/20	2/13/91/115	-
23	CLA	b	817	-	1/1/13/20	10/30/108/115	-
23	CLA	b	821	-	1/1/12/20	2/21/99/115	-
23	CLA	4	315	4	1/1/10/20	5/8/86/115	-
23	CLA	3	307	5	1/1/11/20	1/13/91/115	-
23	CLA	2	312	-	1/1/11/20	4/16/94/115	-
23	CLA	b	818	-	1/1/14/20	14/31/109/115	-
23	CLA	8	305	3	1/1/10/20	2/11/89/115	-
22	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
23	CLA	b	807	-	1/1/15/20	19/37/115/115	-
27	LHG	a	846	23	-	16/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	a	850	-	-	4/29/63/63	0/2/2/2
23	CLA	a	809	9	1/1/15/20	15/37/115/115	-
23	CLA	9	309	2	1/1/11/20	3/15/93/115	-
23	CLA	b	804	-	1/1/15/20	10/37/115/115	-
23	CLA	1	314	-	1/1/11/20	5/13/91/115	-
23	CLA	3	315	5	1/1/11/20	8/15/93/115	-
21	XAT	4	305	-	-	4/31/93/93	0/4/4/4
23	CLA	9	308	2	1/1/15/20	15/37/115/115	-
21	XAT	2	303	-	-	6/31/93/93	0/4/4/4
23	CLA	b	827	-	1/1/15/20	14/37/115/115	-
23	CLA	6	311	6	1/1/10/20	2/10/88/115	-
23	CLA	6	314	-	1/1/11/20	6/15/93/115	-
23	CLA	b	837	-	1/1/15/20	8/37/115/115	-
23	CLA	b	836	-	1/1/15/20	8/37/115/115	-
27	LHG	9	307	-	-	21/40/40/53	-
23	CLA	a	829	-	1/1/14/20	15/34/112/115	-
23	CLA	b	815	-	1/1/11/20	3/13/91/115	-
23	CLA	8	306	28	1/1/11/20	2/15/93/115	-
23	CLA	5	307	1	1/1/14/20	7/31/109/115	-
23	CLA	4	309	-	1/1/12/20	7/19/97/115	-
23	CLA	a	830	-	1/1/15/20	15/37/115/115	-
21	XAT	5	302	-	-	3/31/93/93	0/4/4/4
21	XAT	6	306	-	-	4/31/93/93	0/4/4/4
31	BCR	b	843	-	-	2/29/63/63	0/2/2/2
23	CLA	9	313	2	1/1/11/20	9/15/93/115	-
21	XAT	3	305	-	-	0/31/93/93	0/4/4/4
23	CLA	a	834	-	1/1/15/20	7/37/115/115	-
23	CLA	a	805	23	1/1/13/20	6/25/103/115	-
31	BCR	h	201	-	-	0/29/63/63	0/2/2/2
21	XAT	5	304	-	-	1/31/93/93	0/4/4/4

All (1196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	312	CLA	C4B-NB	7.88	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	3	315	CLA	C4B-NB	7.76	1.42	1.35
23	a	818	CLA	C4B-NB	7.74	1.42	1.35
23	a	842	CLA	C4B-NB	7.72	1.42	1.35
23	2	315	CLA	C4B-NB	7.72	1.42	1.35
23	4	315	CLA	C4B-NB	7.67	1.42	1.35
23	b	837	CLA	C4B-NB	7.67	1.42	1.35
23	b	820	CLA	C4B-NB	7.66	1.42	1.35
23	a	808	CLA	C4B-NB	7.66	1.42	1.35
23	b	834	CLA	C4B-NB	7.65	1.42	1.35
23	6	308	CLA	C4B-NB	7.64	1.42	1.35
23	5	313	CLA	C4B-NB	7.64	1.42	1.35
23	4	311	CLA	C4B-NB	7.64	1.42	1.35
23	2	312	CLA	C4B-NB	7.64	1.42	1.35
23	8	313	CLA	C4B-NB	7.63	1.42	1.35
23	1	309	CLA	C4B-NB	7.62	1.42	1.35
23	7	311	CLA	C4B-NB	7.62	1.42	1.35
23	6	317	CLA	C4B-NB	7.61	1.42	1.35
23	4	314	CLA	C4B-NB	7.61	1.42	1.35
23	2	311	CLA	C4B-NB	7.61	1.42	1.35
23	9	318	CLA	C4B-NB	7.60	1.42	1.35
23	2	308	CLA	C4B-NB	7.60	1.42	1.35
23	j	102	CLA	C4B-NB	7.60	1.42	1.35
23	1	305	CLA	C4B-NB	7.59	1.42	1.35
23	7	313	CLA	C4B-NB	7.59	1.42	1.35
23	4	307	CLA	C4B-NB	7.58	1.42	1.35
23	b	829	CLA	C4B-NB	7.58	1.42	1.35
23	4	312	CLA	C4B-NB	7.58	1.42	1.35
23	a	817	CLA	C4B-NB	7.58	1.42	1.35
23	3	308	CLA	C4B-NB	7.57	1.42	1.35
23	4	306	CLA	C4B-NB	7.57	1.42	1.35
23	b	828	CLA	C4B-NB	7.57	1.42	1.35
23	6	311	CLA	C4B-NB	7.57	1.42	1.35
23	2	306	CLA	C4B-NB	7.56	1.42	1.35
23	b	818	CLA	C4B-NB	7.56	1.42	1.35
30	a	843	PQN	C3-C2	7.56	1.49	1.35
23	3	311	CLA	C4B-NB	7.56	1.42	1.35
23	5	305	CLA	C4B-NB	7.56	1.42	1.35
23	8	314	CLA	C4B-NB	7.56	1.41	1.35
23	f	803	CLA	C4B-NB	7.55	1.41	1.35
23	7	315	CLA	C4B-NB	7.55	1.41	1.35
23	b	826	CLA	C4B-NB	7.55	1.41	1.35
23	a	824	CLA	C4B-NB	7.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	314	CLA	C4B-NB	7.53	1.41	1.35
23	1	314	CLA	C4B-NB	7.53	1.41	1.35
23	6	307	CLA	C4B-NB	7.53	1.41	1.35
23	a	831	CLA	C4B-NB	7.53	1.41	1.35
23	1	313	CLA	C4B-NB	7.53	1.41	1.35
23	5	310	CLA	C4B-NB	7.53	1.41	1.35
23	1	310	CLA	C4B-NB	7.52	1.41	1.35
23	a	804	CLA	C4B-NB	7.52	1.41	1.35
23	4	317	CLA	C4B-NB	7.52	1.41	1.35
23	b	840	CLA	C4B-NB	7.52	1.41	1.35
23	b	839	CLA	C4B-NB	7.51	1.41	1.35
23	b	801	CLA	C4B-NB	7.51	1.41	1.35
23	2	314	CLA	C4B-NB	7.51	1.41	1.35
23	9	309	CLA	C4B-NB	7.50	1.41	1.35
23	4	309	CLA	C4B-NB	7.50	1.41	1.35
23	j	103	CLA	C4B-NB	7.50	1.41	1.35
23	4	316	CLA	C4B-NB	7.50	1.41	1.35
23	l	202	CLA	C4B-NB	7.49	1.41	1.35
23	2	310	CLA	C4B-NB	7.49	1.41	1.35
23	a	822	CLA	C4B-NB	7.49	1.41	1.35
23	a	837	CLA	C4B-NB	7.49	1.41	1.35
23	b	814	CLA	C4B-NB	7.48	1.41	1.35
23	a	813	CLA	C4B-NB	7.48	1.41	1.35
23	2	309	CLA	C4B-NB	7.48	1.41	1.35
23	7	317	CLA	C4B-NB	7.48	1.41	1.35
23	2	316	CLA	C4B-NB	7.48	1.41	1.35
23	8	309	CLA	C4B-NB	7.48	1.41	1.35
23	7	307	CLA	C4B-NB	7.47	1.41	1.35
23	5	306	CLA	C4B-NB	7.47	1.41	1.35
23	7	310	CLA	C4B-NB	7.47	1.41	1.35
23	b	805	CLA	C4B-NB	7.47	1.41	1.35
23	a	810	CLA	C4B-NB	7.46	1.41	1.35
23	8	306	CLA	C4B-NB	7.46	1.41	1.35
23	6	310	CLA	C4B-NB	7.46	1.41	1.35
23	7	309	CLA	C4B-NB	7.46	1.41	1.35
23	b	802	CLA	C4B-NB	7.46	1.41	1.35
23	8	310	CLA	C4B-NB	7.46	1.41	1.35
23	a	820	CLA	C4B-NB	7.46	1.41	1.35
23	a	805	CLA	C4B-NB	7.46	1.41	1.35
23	4	313	CLA	C4B-NB	7.45	1.41	1.35
23	a	854	CLA	C4B-NB	7.45	1.41	1.35
23	a	825	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	831	CLA	C4B-NB	7.45	1.41	1.35
23	6	316	CLA	C4B-NB	7.45	1.41	1.35
23	9	308	CLA	C4B-NB	7.45	1.41	1.35
23	6	312	CLA	C4B-NB	7.45	1.41	1.35
23	7	306	CLA	C4B-NB	7.45	1.41	1.35
23	8	308	CLA	C4B-NB	7.45	1.41	1.35
23	b	827	CLA	C4B-NB	7.45	1.41	1.35
23	9	315	CLA	C4B-NB	7.44	1.41	1.35
23	8	312	CLA	C4B-NB	7.44	1.41	1.35
23	3	307	CLA	C4B-NB	7.44	1.41	1.35
23	5	309	CLA	C4B-NB	7.44	1.41	1.35
23	4	310	CLA	C4B-NB	7.44	1.41	1.35
23	6	309	CLA	C4B-NB	7.43	1.41	1.35
23	7	314	CLA	C4B-NB	7.43	1.41	1.35
23	6	314	CLA	C4B-NB	7.43	1.41	1.35
23	3	310	CLA	C4B-NB	7.42	1.41	1.35
23	2	313	CLA	C4B-NB	7.42	1.41	1.35
23	1	307	CLA	C4B-NB	7.42	1.41	1.35
23	1	308	CLA	C4B-NB	7.42	1.41	1.35
23	b	824	CLA	C4B-NB	7.42	1.41	1.35
23	b	822	CLA	C4B-NB	7.41	1.41	1.35
23	b	816	CLA	C4B-NB	7.41	1.41	1.35
23	a	841	CLA	C4B-NB	7.41	1.41	1.35
23	b	838	CLA	C4B-NB	7.41	1.41	1.35
23	a	829	CLA	C4B-NB	7.41	1.41	1.35
23	a	832	CLA	C4B-NB	7.40	1.41	1.35
23	3	309	CLA	C4B-NB	7.40	1.41	1.35
23	b	811	CLA	C4B-NB	7.40	1.41	1.35
23	b	833	CLA	C4B-NB	7.39	1.41	1.35
23	3	313	CLA	C4B-NB	7.39	1.41	1.35
23	a	821	CLA	C4B-NB	7.39	1.41	1.35
23	3	312	CLA	C4B-NB	7.39	1.41	1.35
23	b	803	CLA	C4B-NB	7.38	1.41	1.35
23	3	314	CLA	C4B-NB	7.38	1.41	1.35
23	a	812	CLA	C4B-NB	7.38	1.41	1.35
23	a	836	CLA	C4B-NB	7.38	1.41	1.35
23	5	315	CLA	C4B-NB	7.38	1.41	1.35
30	b	841	PQN	C3-C2	7.36	1.48	1.35
23	9	310	CLA	C4B-NB	7.36	1.41	1.35
23	b	804	CLA	C4B-NB	7.36	1.41	1.35
23	h	204	CLA	C4B-NB	7.36	1.41	1.35
23	7	312	CLA	C4B-NB	7.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	823	CLA	C4B-NB	7.36	1.41	1.35
23	a	816	CLA	C4B-NB	7.36	1.41	1.35
23	a	839	CLA	C4B-NB	7.36	1.41	1.35
23	b	819	CLA	C4B-NB	7.35	1.41	1.35
23	l	203	CLA	C4B-NB	7.35	1.41	1.35
23	a	830	CLA	C4B-NB	7.35	1.41	1.35
23	5	307	CLA	C4B-NB	7.35	1.41	1.35
23	a	826	CLA	C4B-NB	7.35	1.41	1.35
23	b	836	CLA	C4B-NB	7.34	1.41	1.35
23	5	312	CLA	C4B-NB	7.34	1.41	1.35
23	b	808	CLA	C4B-NB	7.34	1.41	1.35
23	a	833	CLA	C4B-NB	7.34	1.41	1.35
23	9	313	CLA	C4B-NB	7.34	1.41	1.35
23	a	835	CLA	C4B-NB	7.34	1.41	1.35
23	5	314	CLA	C4B-NB	7.34	1.41	1.35
23	5	308	CLA	C4B-NB	7.34	1.41	1.35
23	7	308	CLA	C4B-NB	7.34	1.41	1.35
23	8	311	CLA	C4B-NB	7.33	1.41	1.35
23	b	809	CLA	C4B-NB	7.33	1.41	1.35
23	b	810	CLA	C4B-NB	7.33	1.41	1.35
23	a	834	CLA	C4B-NB	7.33	1.41	1.35
23	a	815	CLA	C4B-NB	7.32	1.41	1.35
23	a	811	CLA	C4B-NB	7.32	1.41	1.35
23	9	311	CLA	C4B-NB	7.32	1.41	1.35
23	6	315	CLA	C4B-NB	7.32	1.41	1.35
23	b	806	CLA	C4B-NB	7.31	1.41	1.35
23	b	815	CLA	C4B-NB	7.31	1.41	1.35
23	a	827	CLA	C4B-NB	7.31	1.41	1.35
23	9	316	CLA	C4B-NB	7.31	1.41	1.35
23	a	819	CLA	C4B-NB	7.30	1.41	1.35
23	a	803	CLA	C4B-NB	7.29	1.41	1.35
23	6	313	CLA	C4B-NB	7.29	1.41	1.35
23	l	204	CLA	C4B-NB	7.29	1.41	1.35
23	f	802	CLA	C4B-NB	7.29	1.41	1.35
23	b	832	CLA	C4B-NB	7.29	1.41	1.35
23	a	814	CLA	C4B-NB	7.29	1.41	1.35
23	9	312	CLA	C4B-NB	7.29	1.41	1.35
23	1	306	CLA	C4B-NB	7.28	1.41	1.35
23	8	305	CLA	C4B-NB	7.28	1.41	1.35
23	b	835	CLA	C4B-NB	7.28	1.41	1.35
23	1	311	CLA	C4B-NB	7.27	1.41	1.35
23	a	802	CLA	C4B-NB	7.25	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	844	CLA	C4B-NB	7.25	1.41	1.35
23	b	812	CLA	C4B-NB	7.25	1.41	1.35
23	b	817	CLA	C4B-NB	7.24	1.41	1.35
23	a	807	CLA	C4B-NB	7.23	1.41	1.35
23	b	825	CLA	C4B-NB	7.23	1.41	1.35
23	a	838	CLA	C4B-NB	7.23	1.41	1.35
23	b	813	CLA	C4B-NB	7.23	1.41	1.35
23	2	307	CLA	C4B-NB	7.22	1.41	1.35
23	b	830	CLA	C4B-NB	7.22	1.41	1.35
23	b	823	CLA	C4B-NB	7.22	1.41	1.35
23	5	311	CLA	C4B-NB	7.21	1.41	1.35
23	8	307	CLA	C4B-NB	7.20	1.41	1.35
23	4	308	CLA	C4B-NB	7.19	1.41	1.35
23	7	316	CLA	C4B-NB	7.19	1.41	1.35
23	a	801	CLA	C4B-NB	7.19	1.41	1.35
23	b	821	CLA	C4B-NB	7.17	1.41	1.35
23	b	807	CLA	C4B-NB	7.15	1.41	1.35
23	a	828	CLA	C4B-NB	7.05	1.41	1.35
23	a	809	CLA	C4B-NB	7.03	1.41	1.35
23	a	806	CLA	C4B-NB	6.11	1.40	1.35
30	a	843	PQN	C10-C5	4.84	1.48	1.40
30	b	841	PQN	C10-C5	4.84	1.48	1.40
24	5	316	SQD	O8-S	4.61	1.63	1.47
25	9	302	A1L1F	O7-C54	4.60	1.45	1.35
25	h	203	A1L1F	O7-C54	4.59	1.45	1.35
24	1	315	SQD	O8-S	4.58	1.63	1.47
25	8	304	A1L1F	O7-C54	4.55	1.45	1.35
25	1	304	A1L1F	O7-C54	4.52	1.45	1.35
25	6	304	A1L1F	O7-C54	4.50	1.45	1.35
25	6	301	A1L1F	O7-C54	4.40	1.45	1.35
28	8	315	DGD	O1G-C1A	4.29	1.45	1.33
24	1	315	SQD	O48-C23	4.29	1.45	1.33
29	a	853	LMG	O8-C28	4.22	1.45	1.33
24	5	316	SQD	O48-C23	4.22	1.45	1.33
25	1	304	A1L1F	O13-C45	4.21	1.45	1.33
24	1	315	SQD	O47-C7	4.20	1.46	1.34
25	h	203	A1L1F	O13-C45	4.17	1.45	1.33
29	a	853	LMG	O7-C10	4.15	1.46	1.34
24	5	316	SQD	O47-C7	4.09	1.45	1.34
25	6	304	A1L1F	O13-C45	4.09	1.45	1.33
25	6	301	A1L1F	O13-C45	4.09	1.45	1.33
25	8	304	A1L1F	O13-C45	4.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	j	105	LMG	O8-C28	4.08	1.45	1.33
28	4	318	DGD	O1G-C1A	4.06	1.45	1.33
29	2	317	LMG	O8-C28	4.04	1.45	1.33
23	a	806	CLA	C4D-ND	-4.04	1.32	1.37
23	6	315	CLA	C1D-ND	3.99	1.42	1.37
28	b	848	DGD	O2G-C1B	3.98	1.45	1.34
23	6	308	CLA	C1D-ND	3.96	1.42	1.37
23	3	308	CLA	C1D-ND	3.96	1.42	1.37
23	6	317	CLA	C1D-ND	3.96	1.42	1.37
29	2	317	LMG	O7-C10	3.96	1.45	1.34
23	2	313	CLA	C1D-ND	3.95	1.42	1.37
28	b	848	DGD	O1G-C1A	3.95	1.44	1.33
25	9	302	A1L1F	O13-C45	3.95	1.44	1.33
23	9	313	CLA	C1D-ND	3.95	1.42	1.37
23	b	840	CLA	C1D-ND	3.94	1.42	1.37
23	9	312	CLA	C1D-ND	3.94	1.42	1.37
23	7	307	CLA	C1D-ND	3.94	1.42	1.37
23	7	306	CLA	C1D-ND	3.93	1.42	1.37
23	b	826	CLA	C1D-ND	3.92	1.42	1.37
23	9	310	CLA	C1D-ND	3.92	1.42	1.37
23	7	315	CLA	C1D-ND	3.92	1.42	1.37
23	2	315	CLA	C1D-ND	3.92	1.42	1.37
23	a	804	CLA	C1D-ND	3.92	1.42	1.37
23	8	308	CLA	C1D-ND	3.91	1.42	1.37
23	a	840	CLA	C1D-ND	3.91	1.42	1.37
23	8	314	CLA	C1D-ND	3.90	1.42	1.37
23	b	824	CLA	C1D-ND	3.90	1.42	1.37
23	6	307	CLA	C1D-ND	3.90	1.42	1.37
23	3	314	CLA	C1D-ND	3.90	1.42	1.37
23	8	310	CLA	C1D-ND	3.90	1.42	1.37
23	4	314	CLA	C1D-ND	3.90	1.42	1.37
23	a	811	CLA	C1D-ND	3.90	1.42	1.37
23	8	305	CLA	C1D-ND	3.89	1.42	1.37
23	6	313	CLA	C1D-ND	3.89	1.42	1.37
23	1	310	CLA	C1D-ND	3.89	1.42	1.37
23	9	314	CLA	C1D-ND	3.89	1.42	1.37
23	f	802	CLA	C1D-ND	3.89	1.42	1.37
25	8	304	A1L1F	C57-C2	-3.89	1.25	1.32
23	8	313	CLA	C1D-ND	3.88	1.42	1.37
23	5	305	CLA	C1D-ND	3.88	1.42	1.37
23	3	315	CLA	C1D-ND	3.88	1.42	1.37
23	1	312	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	308	CLA	C1D-ND	3.88	1.42	1.37
23	5	311	CLA	C1D-ND	3.87	1.42	1.37
23	2	306	CLA	C1D-ND	3.87	1.42	1.37
29	j	105	LMG	O7-C10	3.87	1.45	1.34
23	8	309	CLA	C1D-ND	3.87	1.42	1.37
23	6	309	CLA	C1D-ND	3.87	1.42	1.37
23	a	828	CLA	C1D-ND	3.87	1.42	1.37
23	7	313	CLA	C1D-ND	3.87	1.42	1.37
23	b	807	CLA	C1D-ND	3.87	1.42	1.37
23	2	307	CLA	C1D-ND	3.87	1.42	1.37
23	b	812	CLA	C1D-ND	3.86	1.42	1.37
22	1	301	A1L1G	C38-C39	3.86	1.40	1.35
23	5	310	CLA	C1D-ND	3.86	1.42	1.37
23	a	837	CLA	C1D-ND	3.86	1.42	1.37
23	3	312	CLA	C1D-ND	3.85	1.42	1.37
23	7	317	CLA	C1D-ND	3.85	1.42	1.37
23	8	307	CLA	C1D-ND	3.85	1.42	1.37
23	4	307	CLA	C1D-ND	3.85	1.42	1.37
23	a	814	CLA	C1D-ND	3.85	1.42	1.37
23	5	313	CLA	C1D-ND	3.85	1.42	1.37
28	4	318	DGD	O2G-C1B	3.85	1.45	1.34
23	j	103	CLA	C1D-ND	3.85	1.42	1.37
25	h	203	A1L1F	C57-C2	-3.84	1.25	1.32
23	b	818	CLA	C1D-ND	3.84	1.42	1.37
23	6	316	CLA	C1D-ND	3.84	1.42	1.37
23	7	311	CLA	C1D-ND	3.84	1.42	1.37
23	5	306	CLA	C1D-ND	3.84	1.42	1.37
23	7	310	CLA	C1D-ND	3.84	1.42	1.37
23	a	839	CLA	C1D-ND	3.83	1.42	1.37
23	5	314	CLA	C1D-ND	3.83	1.42	1.37
23	6	310	CLA	C1D-ND	3.83	1.42	1.37
23	b	817	CLA	C1D-ND	3.82	1.42	1.37
23	b	831	CLA	C1D-ND	3.82	1.42	1.37
23	4	317	CLA	C1D-ND	3.82	1.42	1.37
23	a	838	CLA	C1D-ND	3.82	1.42	1.37
23	b	834	CLA	C1D-ND	3.82	1.42	1.37
23	5	309	CLA	C1D-ND	3.82	1.42	1.37
23	2	308	CLA	C1D-ND	3.82	1.42	1.37
23	b	833	CLA	C1D-ND	3.82	1.42	1.37
23	1	314	CLA	C1D-ND	3.82	1.42	1.37
23	7	314	CLA	C1D-ND	3.82	1.42	1.37
23	a	829	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	315	CLA	C1D-ND	3.81	1.42	1.37
23	4	316	CLA	C1D-ND	3.81	1.42	1.37
23	b	828	CLA	C1D-ND	3.81	1.42	1.37
23	7	308	CLA	C1D-ND	3.81	1.42	1.37
23	3	313	CLA	C1D-ND	3.81	1.42	1.37
23	3	311	CLA	C1D-ND	3.81	1.42	1.37
23	a	822	CLA	C1D-ND	3.81	1.42	1.37
23	a	842	CLA	C1D-ND	3.80	1.42	1.37
23	2	312	CLA	C1D-ND	3.80	1.42	1.37
23	a	835	CLA	C1D-ND	3.80	1.42	1.37
23	b	816	CLA	C1D-ND	3.80	1.42	1.37
23	l	202	CLA	C1D-ND	3.80	1.42	1.37
23	2	314	CLA	C1D-ND	3.80	1.42	1.37
23	b	820	CLA	C1D-ND	3.80	1.42	1.37
23	b	839	CLA	C1D-ND	3.80	1.42	1.37
23	a	821	CLA	C1D-ND	3.80	1.42	1.37
23	b	835	CLA	C1D-ND	3.80	1.42	1.37
23	a	807	CLA	C1D-ND	3.80	1.42	1.37
23	a	809	CLA	C1D-ND	3.80	1.42	1.37
23	2	311	CLA	C1D-ND	3.80	1.42	1.37
23	b	821	CLA	C1D-ND	3.80	1.42	1.37
23	1	309	CLA	C1D-ND	3.79	1.42	1.37
23	l	204	CLA	C1D-ND	3.79	1.42	1.37
22	1	301	A1L1G	C35-C34	3.79	1.40	1.35
25	9	302	A1L1F	C57-C2	-3.79	1.25	1.32
23	1	311	CLA	C1D-ND	3.79	1.42	1.37
23	4	312	CLA	C1D-ND	3.79	1.42	1.37
23	a	826	CLA	C1D-ND	3.79	1.42	1.37
23	2	309	CLA	C1D-ND	3.79	1.42	1.37
23	7	316	CLA	C1D-ND	3.79	1.42	1.37
23	a	844	CLA	C1D-ND	3.79	1.42	1.37
23	a	819	CLA	C1D-ND	3.79	1.42	1.37
23	a	817	CLA	C1D-ND	3.78	1.42	1.37
23	9	315	CLA	C1D-ND	3.78	1.42	1.37
23	6	311	CLA	C1D-ND	3.78	1.42	1.37
23	b	805	CLA	C1D-ND	3.78	1.42	1.37
23	b	815	CLA	C1D-ND	3.78	1.42	1.37
23	a	816	CLA	C1D-ND	3.78	1.42	1.37
23	4	306	CLA	C1D-ND	3.78	1.42	1.37
23	a	836	CLA	C1D-ND	3.78	1.42	1.37
23	4	310	CLA	C1D-ND	3.77	1.42	1.37
23	1	306	CLA	C1D-ND	3.77	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	834	CLA	C1D-ND	3.77	1.42	1.37
23	b	801	CLA	C1D-ND	3.77	1.42	1.37
23	a	854	CLA	C1D-ND	3.77	1.42	1.37
23	a	825	CLA	C1D-ND	3.77	1.42	1.37
23	5	312	CLA	C1D-ND	3.77	1.42	1.37
23	b	813	CLA	C1D-ND	3.77	1.42	1.37
23	j	102	CLA	C1D-ND	3.77	1.42	1.37
23	6	314	CLA	C1D-ND	3.76	1.42	1.37
23	a	841	CLA	C1D-ND	3.76	1.42	1.37
23	h	204	CLA	C1D-ND	3.76	1.42	1.37
23	f	803	CLA	C1D-ND	3.76	1.42	1.37
23	9	318	CLA	C1D-ND	3.76	1.42	1.37
23	9	308	CLA	C1D-ND	3.76	1.42	1.37
23	a	813	CLA	C1D-ND	3.75	1.42	1.37
23	3	309	CLA	C1D-ND	3.75	1.42	1.37
23	6	312	CLA	C1D-ND	3.75	1.42	1.37
23	a	815	CLA	C1D-ND	3.75	1.42	1.37
23	a	820	CLA	C1D-ND	3.75	1.42	1.37
23	5	315	CLA	C1D-ND	3.75	1.42	1.37
22	7	302	A1L1G	C38-C39	3.75	1.40	1.35
23	3	310	CLA	C1D-ND	3.75	1.42	1.37
23	1	308	CLA	C1D-ND	3.75	1.42	1.37
23	b	814	CLA	C1D-ND	3.75	1.42	1.37
23	1	307	CLA	C1D-ND	3.75	1.42	1.37
23	a	823	CLA	C1D-ND	3.75	1.42	1.37
23	b	827	CLA	C1D-ND	3.74	1.42	1.37
28	8	315	DGD	O2G-C1B	3.74	1.44	1.34
23	7	309	CLA	C1D-ND	3.74	1.42	1.37
23	7	312	CLA	C1D-ND	3.74	1.42	1.37
23	b	819	CLA	C1D-ND	3.74	1.42	1.37
23	1	305	CLA	C1D-ND	3.74	1.42	1.37
23	a	808	CLA	C1D-ND	3.74	1.42	1.37
23	b	837	CLA	C1D-ND	3.73	1.42	1.37
23	b	808	CLA	C1D-ND	3.73	1.42	1.37
23	b	838	CLA	C1D-ND	3.73	1.42	1.37
23	a	818	CLA	C1D-ND	3.73	1.42	1.37
23	b	836	CLA	C1D-ND	3.73	1.42	1.37
23	9	316	CLA	C1D-ND	3.73	1.42	1.37
23	8	306	CLA	C1D-ND	3.72	1.42	1.37
23	4	308	CLA	C1D-ND	3.72	1.42	1.37
23	4	313	CLA	C1D-ND	3.72	1.42	1.37
23	a	832	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	822	CLA	C1D-ND	3.72	1.42	1.37
23	b	829	CLA	C1D-ND	3.71	1.42	1.37
25	6	304	A1L1F	C57-C2	-3.71	1.25	1.32
23	a	805	CLA	C1D-ND	3.71	1.42	1.37
23	a	831	CLA	C1D-ND	3.71	1.42	1.37
23	3	307	CLA	C1D-ND	3.70	1.42	1.37
23	4	309	CLA	C1D-ND	3.70	1.42	1.37
23	1	313	CLA	C1D-ND	3.70	1.42	1.37
23	b	825	CLA	C1D-ND	3.70	1.42	1.37
23	9	311	CLA	C1D-ND	3.70	1.42	1.37
23	b	809	CLA	C1D-ND	3.70	1.42	1.37
22	3	302	A1L1G	C35-C34	3.70	1.40	1.35
23	8	311	CLA	C1D-ND	3.69	1.42	1.37
23	a	810	CLA	C1D-ND	3.69	1.42	1.37
23	a	827	CLA	C1D-ND	3.69	1.42	1.37
31	m	101	BCR	C1-C6	-3.69	1.48	1.53
23	4	311	CLA	C1D-ND	3.69	1.42	1.37
22	9	301	A1L1G	C38-C39	3.69	1.40	1.35
23	b	810	CLA	C1D-ND	3.69	1.42	1.37
23	2	316	CLA	C1D-ND	3.68	1.42	1.37
22	9	301	A1L1G	C35-C34	3.67	1.40	1.35
23	5	307	CLA	C1D-ND	3.67	1.42	1.37
23	1	203	CLA	C1D-ND	3.67	1.42	1.37
22	9	306	A1L1G	C35-C34	3.67	1.40	1.35
25	6	301	A1L1F	C57-C2	-3.67	1.25	1.32
23	b	823	CLA	C1D-ND	3.66	1.42	1.37
23	a	812	CLA	C1D-ND	3.66	1.42	1.37
23	a	824	CLA	C1D-ND	3.66	1.42	1.37
23	8	312	CLA	C1D-ND	3.65	1.42	1.37
23	a	830	CLA	C1D-ND	3.64	1.42	1.37
23	b	806	CLA	C1D-ND	3.64	1.42	1.37
23	2	310	CLA	C1D-ND	3.64	1.42	1.37
23	a	803	CLA	C1D-ND	3.64	1.42	1.37
22	3	306	A1L1G	C38-C39	3.64	1.40	1.35
23	b	832	CLA	C1D-ND	3.64	1.42	1.37
22	3	302	A1L1G	C38-C39	3.62	1.40	1.35
23	b	802	CLA	C1D-ND	3.62	1.42	1.37
23	b	803	CLA	C1D-ND	3.61	1.42	1.37
23	b	811	CLA	C1D-ND	3.60	1.42	1.37
23	a	802	CLA	C1D-ND	3.59	1.42	1.37
25	1	304	A1L1F	C57-C2	-3.58	1.26	1.32
23	9	309	CLA	C1D-ND	3.58	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	303	A1L1G	C38-C39	3.52	1.40	1.35
23	a	801	CLA	C1D-ND	3.52	1.42	1.37
23	b	830	CLA	C1D-ND	3.52	1.42	1.37
22	7	302	A1L1G	C35-C34	3.51	1.40	1.35
23	b	811	CLA	CAB-C3B	-3.50	1.44	1.51
22	9	306	A1L1G	C38-C39	3.47	1.40	1.35
23	a	833	CLA	C1D-ND	3.47	1.42	1.37
22	3	302	A1L1G	C42-C44	3.46	1.40	1.35
22	5	303	A1L1G	C35-C34	3.45	1.40	1.35
22	3	306	A1L1G	C35-C34	3.37	1.40	1.35
23	4	313	CLA	CHC-C1C	3.32	1.43	1.35
23	b	804	CLA	C1D-ND	3.27	1.41	1.37
23	4	312	CLA	CHC-C1C	3.26	1.43	1.35
23	a	802	CLA	CHC-C1C	3.26	1.43	1.35
23	7	313	CLA	CHC-C1C	3.26	1.43	1.35
23	a	822	CLA	CHC-C1C	3.25	1.43	1.35
23	a	818	CLA	CHC-C1C	3.24	1.43	1.35
23	b	838	CLA	CHC-C1C	3.24	1.43	1.35
23	8	311	CLA	CHC-C1C	3.24	1.43	1.35
23	a	819	CLA	CHC-C1C	3.23	1.43	1.35
23	b	811	CLA	CHC-C1C	3.23	1.43	1.35
23	7	311	CLA	CHC-C1C	3.23	1.43	1.35
23	2	308	CLA	CHC-C1C	3.22	1.43	1.35
23	b	816	CLA	CHC-C1C	3.22	1.43	1.35
23	9	318	CLA	CHC-C1C	3.22	1.43	1.35
23	a	828	CLA	C4D-ND	-3.22	1.33	1.37
23	9	308	CLA	CHC-C1C	3.22	1.43	1.35
23	2	315	CLA	CHC-C1C	3.22	1.43	1.35
23	3	315	CLA	CHC-C1C	3.22	1.43	1.35
23	a	829	CLA	CHC-C1C	3.22	1.43	1.35
23	b	815	CLA	CHC-C1C	3.21	1.43	1.35
23	6	311	CLA	CHC-C1C	3.21	1.43	1.35
23	a	820	CLA	CHC-C1C	3.21	1.43	1.35
23	a	854	CLA	CHC-C1C	3.21	1.43	1.35
23	6	308	CLA	CHC-C1C	3.21	1.43	1.35
23	b	814	CLA	CHC-C1C	3.21	1.43	1.35
23	1	310	CLA	CHC-C1C	3.21	1.43	1.35
23	b	835	CLA	CHC-C1C	3.20	1.43	1.35
23	b	836	CLA	CHC-C1C	3.20	1.43	1.35
23	a	832	CLA	CHC-C1C	3.20	1.43	1.35
23	a	841	CLA	CHC-C1C	3.20	1.43	1.35
23	8	312	CLA	CHC-C1C	3.20	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	h	204	CLA	CHC-C1C	3.20	1.43	1.35
23	9	311	CLA	CHC-C1C	3.20	1.43	1.35
23	5	312	CLA	CHC-C1C	3.20	1.43	1.35
23	2	309	CLA	CHC-C1C	3.19	1.43	1.35
23	1	312	CLA	CHC-C1C	3.19	1.43	1.35
23	8	314	CLA	CHC-C1C	3.19	1.43	1.35
23	5	314	CLA	CHC-C1C	3.19	1.43	1.35
23	8	313	CLA	CHC-C1C	3.19	1.43	1.35
23	6	313	CLA	CHC-C1C	3.19	1.43	1.35
23	b	833	CLA	CHC-C1C	3.19	1.43	1.35
23	b	806	CLA	CHC-C1C	3.19	1.43	1.35
23	b	802	CLA	CHC-C1C	3.19	1.43	1.35
23	8	309	CLA	CHC-C1C	3.19	1.43	1.35
23	5	306	CLA	CHC-C1C	3.19	1.43	1.35
23	1	308	CLA	CHC-C1C	3.18	1.43	1.35
23	a	826	CLA	CHC-C1C	3.18	1.43	1.35
23	a	844	CLA	CHC-C1C	3.18	1.43	1.35
23	1	314	CLA	CHC-C1C	3.18	1.43	1.35
23	a	827	CLA	CHC-C1C	3.18	1.43	1.35
23	b	831	CLA	CHC-C1C	3.18	1.43	1.35
23	5	309	CLA	CHC-C1C	3.18	1.43	1.35
23	5	311	CLA	CHC-C1C	3.18	1.43	1.35
23	3	311	CLA	CHC-C1C	3.18	1.43	1.35
23	7	314	CLA	CHC-C1C	3.18	1.43	1.35
23	5	315	CLA	CHC-C1C	3.18	1.43	1.35
23	2	311	CLA	CHC-C1C	3.18	1.43	1.35
23	b	813	CLA	CHC-C1C	3.18	1.43	1.35
23	8	306	CLA	CHC-C1C	3.18	1.43	1.35
23	a	824	CLA	CHC-C1C	3.18	1.43	1.35
23	1	204	CLA	CHC-C1C	3.18	1.43	1.35
23	7	306	CLA	CHC-C1C	3.18	1.43	1.35
23	4	314	CLA	CHC-C1C	3.17	1.43	1.35
23	a	804	CLA	CHC-C1C	3.17	1.43	1.35
23	a	813	CLA	CHC-C1C	3.17	1.43	1.35
23	3	309	CLA	CHC-C1C	3.17	1.43	1.35
23	2	313	CLA	CHC-C1C	3.17	1.43	1.35
23	b	825	CLA	CHC-C1C	3.17	1.43	1.35
23	4	317	CLA	CHC-C1C	3.17	1.43	1.35
23	7	312	CLA	CHC-C1C	3.17	1.43	1.35
23	b	828	CLA	CHC-C1C	3.17	1.43	1.35
23	2	314	CLA	CHC-C1C	3.17	1.43	1.35
23	a	833	CLA	CHC-C1C	3.17	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	809	CLA	CHC-C1C	3.17	1.43	1.35
23	b	834	CLA	CHC-C1C	3.17	1.43	1.35
23	a	808	CLA	CHC-C1C	3.17	1.43	1.35
23	3	307	CLA	CHC-C1C	3.17	1.43	1.35
23	7	308	CLA	CHC-C1C	3.17	1.43	1.35
23	3	313	CLA	CHC-C1C	3.17	1.43	1.35
23	b	805	CLA	CHC-C1C	3.17	1.43	1.35
23	2	312	CLA	CHC-C1C	3.16	1.43	1.35
23	f	803	CLA	CHC-C1C	3.16	1.43	1.35
23	l	203	CLA	CHC-C1C	3.16	1.43	1.35
23	b	832	CLA	CHC-C1C	3.16	1.43	1.35
23	a	828	CLA	CHC-C1C	3.16	1.43	1.35
23	a	836	CLA	CHC-C1C	3.16	1.43	1.35
23	a	837	CLA	CHC-C1C	3.16	1.43	1.35
23	5	307	CLA	CHC-C1C	3.16	1.43	1.35
23	2	310	CLA	CHC-C1C	3.16	1.43	1.35
23	a	816	CLA	CHC-C1C	3.16	1.43	1.35
23	b	812	CLA	CHC-C1C	3.16	1.43	1.35
23	5	313	CLA	CHC-C1C	3.15	1.43	1.35
23	b	837	CLA	CHC-C1C	3.15	1.43	1.35
23	4	309	CLA	CHC-C1C	3.15	1.43	1.35
23	8	305	CLA	CHC-C1C	3.15	1.43	1.35
23	a	842	CLA	CHC-C1C	3.15	1.43	1.35
23	a	839	CLA	CHC-C1C	3.15	1.43	1.35
23	4	307	CLA	CHC-C1C	3.15	1.43	1.35
23	1	307	CLA	CHC-C1C	3.15	1.43	1.35
23	9	313	CLA	CHC-C1C	3.15	1.43	1.35
23	b	823	CLA	CHC-C1C	3.15	1.43	1.35
23	1	309	CLA	CHC-C1C	3.15	1.43	1.35
23	l	202	CLA	CHC-C1C	3.15	1.43	1.35
23	1	311	CLA	CHC-C1C	3.15	1.43	1.35
23	b	809	CLA	CHC-C1C	3.15	1.43	1.35
23	a	812	CLA	CHC-C1C	3.15	1.43	1.35
23	b	827	CLA	CHC-C1C	3.15	1.43	1.35
23	6	316	CLA	CHC-C1C	3.15	1.43	1.35
23	9	312	CLA	CHC-C1C	3.15	1.43	1.35
23	f	802	CLA	CHC-C1C	3.15	1.43	1.35
23	a	814	CLA	CHC-C1C	3.15	1.43	1.35
23	b	830	CLA	CHC-C1C	3.15	1.43	1.35
23	2	316	CLA	CHC-C1C	3.14	1.43	1.35
23	b	817	CLA	CHC-C1C	3.14	1.43	1.35
23	9	309	CLA	CHC-C1C	3.14	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	815	CLA	CHC-C1C	3.14	1.43	1.35
23	4	315	CLA	CHC-C1C	3.14	1.43	1.35
23	9	314	CLA	CHC-C1C	3.14	1.43	1.35
23	a	805	CLA	CHC-C1C	3.14	1.43	1.35
23	6	309	CLA	CHC-C1C	3.14	1.43	1.35
23	5	310	CLA	CHC-C1C	3.14	1.43	1.35
23	4	310	CLA	CHC-C1C	3.14	1.43	1.35
23	3	312	CLA	CHC-C1C	3.14	1.43	1.35
23	6	314	CLA	CHC-C1C	3.14	1.43	1.35
23	b	807	CLA	CHC-C1C	3.14	1.43	1.35
23	8	310	CLA	CHC-C1C	3.14	1.43	1.35
23	a	830	CLA	CHC-C1C	3.13	1.43	1.35
23	7	307	CLA	CHC-C1C	3.13	1.43	1.35
23	a	834	CLA	CHC-C1C	3.13	1.43	1.35
23	b	824	CLA	CHC-C1C	3.13	1.43	1.35
23	9	310	CLA	CHC-C1C	3.13	1.43	1.35
23	7	310	CLA	CHC-C1C	3.13	1.43	1.35
23	6	307	CLA	CHC-C1C	3.13	1.43	1.35
23	a	803	CLA	CHC-C1C	3.13	1.43	1.35
23	a	823	CLA	CHC-C1C	3.13	1.43	1.35
23	a	817	CLA	CHC-C1C	3.13	1.43	1.35
31	m	101	BCR	C30-C25	-3.13	1.49	1.53
23	b	840	CLA	CHC-C1C	3.13	1.43	1.35
23	b	804	CLA	CHC-C1C	3.13	1.43	1.35
23	1	313	CLA	CHC-C1C	3.13	1.43	1.35
23	b	819	CLA	CHC-C1C	3.13	1.43	1.35
23	a	838	CLA	CHC-C1C	3.13	1.43	1.35
23	3	310	CLA	CHC-C1C	3.12	1.43	1.35
23	4	306	CLA	CHC-C1C	3.12	1.43	1.35
23	j	102	CLA	CHC-C1C	3.12	1.43	1.35
23	4	308	CLA	CHC-C1C	3.12	1.43	1.35
23	b	822	CLA	CHC-C1C	3.12	1.43	1.35
23	7	309	CLA	CHC-C1C	3.12	1.43	1.35
23	3	314	CLA	CHC-C1C	3.12	1.43	1.35
23	7	315	CLA	CHC-C1C	3.12	1.43	1.35
23	a	803	CLA	C4D-ND	-3.12	1.33	1.37
23	h	204	CLA	C4D-ND	-3.12	1.33	1.37
23	4	311	CLA	CHC-C1C	3.12	1.43	1.35
23	b	817	CLA	C4D-ND	-3.12	1.33	1.37
23	3	308	CLA	CHC-C1C	3.11	1.42	1.35
23	5	308	CLA	CHC-C1C	3.11	1.42	1.35
23	6	310	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	827	CLA	C4D-ND	-3.11	1.33	1.37
23	1	305	CLA	CHC-C1C	3.11	1.42	1.35
23	a	825	CLA	CHC-C1C	3.11	1.42	1.35
23	9	316	CLA	CHC-C1C	3.11	1.42	1.35
23	9	315	CLA	CHC-C1C	3.11	1.42	1.35
23	7	317	CLA	CHC-C1C	3.11	1.42	1.35
23	4	308	CLA	C4D-ND	-3.10	1.33	1.37
22	9	301	A1L1G	C42-C44	3.10	1.39	1.35
23	b	820	CLA	CHC-C1C	3.10	1.42	1.35
23	a	811	CLA	CHC-C1C	3.10	1.42	1.35
23	a	835	CLA	CHC-C1C	3.10	1.42	1.35
23	5	305	CLA	CHC-C1C	3.10	1.42	1.35
23	a	810	CLA	CHC-C1C	3.10	1.42	1.35
23	b	801	CLA	CHC-C1C	3.10	1.42	1.35
23	b	803	CLA	CHC-C1C	3.10	1.42	1.35
23	4	316	CLA	CHC-C1C	3.10	1.42	1.35
23	6	315	CLA	CHC-C1C	3.10	1.42	1.35
22	7	302	A1L1G	C42-C44	3.09	1.39	1.35
23	1	306	CLA	CHC-C1C	3.09	1.42	1.35
23	a	821	CLA	CHC-C1C	3.09	1.42	1.35
23	b	821	CLA	CHC-C1C	3.09	1.42	1.35
23	8	308	CLA	CHC-C1C	3.09	1.42	1.35
23	2	307	CLA	CHC-C1C	3.09	1.42	1.35
23	9	308	CLA	C4D-ND	-3.09	1.33	1.37
23	8	307	CLA	CHC-C1C	3.09	1.42	1.35
23	6	317	CLA	CHC-C1C	3.09	1.42	1.35
23	b	808	CLA	CHC-C1C	3.08	1.42	1.35
23	b	840	CLA	C4D-ND	-3.08	1.33	1.37
23	5	312	CLA	C4D-ND	-3.08	1.33	1.37
23	b	826	CLA	C4D-ND	-3.08	1.33	1.37
23	a	807	CLA	CHC-C1C	3.08	1.42	1.35
23	a	840	CLA	CHC-C1C	3.08	1.42	1.35
23	b	826	CLA	CHC-C1C	3.08	1.42	1.35
23	l	203	CLA	C4D-ND	-3.07	1.33	1.37
23	b	830	CLA	C4D-ND	-3.07	1.33	1.37
23	b	832	CLA	C4D-ND	-3.07	1.33	1.37
23	2	306	CLA	CHC-C1C	3.07	1.42	1.35
23	j	103	CLA	CHC-C1C	3.07	1.42	1.35
23	9	316	CLA	C4D-ND	-3.06	1.33	1.37
23	8	307	CLA	C4D-ND	-3.06	1.33	1.37
23	b	818	CLA	CHC-C1C	3.06	1.42	1.35
23	a	829	CLA	C4D-ND	-3.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	316	CLA	CHC-C1C	3.06	1.42	1.35
23	a	854	CLA	C4D-ND	-3.06	1.33	1.37
23	3	309	CLA	C4D-ND	-3.05	1.33	1.37
23	b	829	CLA	CMB-C2B	-3.05	1.45	1.51
23	a	801	CLA	CHC-C1C	3.05	1.42	1.35
23	7	309	CLA	C4D-ND	-3.05	1.33	1.37
23	a	830	CLA	C4D-ND	-3.05	1.33	1.37
23	6	312	CLA	CHC-C1C	3.04	1.42	1.35
23	5	307	CLA	C4D-ND	-3.04	1.33	1.37
23	6	313	CLA	C4D-ND	-3.04	1.33	1.37
23	b	819	CLA	C4D-ND	-3.04	1.33	1.37
23	a	808	CLA	C4D-ND	-3.04	1.33	1.37
23	b	810	CLA	CHC-C1C	3.03	1.42	1.35
23	b	816	CLA	C4D-ND	-3.03	1.33	1.37
23	4	309	CLA	C4D-ND	-3.02	1.33	1.37
23	b	835	CLA	C4D-ND	-3.02	1.33	1.37
23	a	831	CLA	CMB-C2B	-3.02	1.45	1.51
23	a	814	CLA	C4D-ND	-3.02	1.33	1.37
23	b	822	CLA	C4D-ND	-3.02	1.33	1.37
23	5	308	CLA	C4D-ND	-3.01	1.33	1.37
23	7	313	CLA	C4D-ND	-3.01	1.33	1.37
23	3	313	CLA	C4D-ND	-3.01	1.33	1.37
23	1	305	CLA	C4D-ND	-3.01	1.33	1.37
23	b	825	CLA	C4D-ND	-3.01	1.33	1.37
23	1	311	CLA	C4D-ND	-3.01	1.33	1.37
23	a	842	CLA	C4D-ND	-3.00	1.33	1.37
23	a	831	CLA	CHC-C1C	3.00	1.42	1.35
23	a	807	CLA	C4D-ND	-2.99	1.33	1.37
23	b	828	CLA	C4D-ND	-2.99	1.33	1.37
23	b	813	CLA	C4D-ND	-2.99	1.33	1.37
23	b	836	CLA	C4D-ND	-2.99	1.33	1.37
23	8	312	CLA	C4D-ND	-2.99	1.33	1.37
23	b	807	CLA	C4D-ND	-2.99	1.33	1.37
23	f	802	CLA	C4D-ND	-2.99	1.33	1.37
23	j	102	CLA	C4D-ND	-2.99	1.33	1.37
23	a	824	CLA	C4D-ND	-2.98	1.33	1.37
23	a	833	CLA	C4D-ND	-2.98	1.33	1.37
23	2	308	CLA	C4D-ND	-2.98	1.33	1.37
23	b	838	CLA	C4D-ND	-2.98	1.33	1.37
23	2	309	CLA	C4D-ND	-2.98	1.33	1.37
23	5	313	CLA	C4D-ND	-2.98	1.33	1.37
23	1	202	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	308	CLA	C4D-ND	-2.97	1.33	1.37
23	9	318	CLA	C4D-ND	-2.97	1.33	1.37
23	a	838	CLA	C4D-ND	-2.97	1.33	1.37
23	3	310	CLA	C4D-ND	-2.97	1.33	1.37
23	4	313	CLA	C4D-ND	-2.97	1.33	1.37
23	b	808	CLA	C4D-ND	-2.97	1.33	1.37
23	5	311	CLA	C4D-ND	-2.96	1.33	1.37
23	6	310	CLA	C4D-ND	-2.96	1.33	1.37
23	a	832	CLA	C4D-ND	-2.96	1.33	1.37
23	5	309	CLA	C4D-ND	-2.96	1.33	1.37
23	7	310	CLA	C4D-ND	-2.96	1.33	1.37
23	b	806	CLA	C4D-ND	-2.96	1.33	1.37
23	5	315	CLA	C4D-ND	-2.95	1.33	1.37
23	a	806	CLA	CHC-C1C	2.95	1.42	1.35
23	4	312	CLA	C4D-ND	-2.95	1.33	1.37
23	b	823	CLA	C4D-ND	-2.95	1.33	1.37
23	l	204	CLA	C4D-ND	-2.95	1.33	1.37
23	a	831	CLA	C4D-ND	-2.95	1.33	1.37
23	b	815	CLA	C4D-ND	-2.95	1.33	1.37
23	b	829	CLA	CHC-C1C	2.95	1.42	1.35
23	8	310	CLA	C4D-ND	-2.95	1.33	1.37
23	a	817	CLA	C4D-ND	-2.95	1.33	1.37
23	a	816	CLA	C4D-ND	-2.94	1.33	1.37
23	b	812	CLA	C4D-ND	-2.94	1.33	1.37
23	a	819	CLA	C4D-ND	-2.94	1.33	1.37
23	a	822	CLA	C4D-ND	-2.94	1.33	1.37
23	3	311	CLA	C4D-ND	-2.94	1.33	1.37
23	8	311	CLA	C4D-ND	-2.94	1.33	1.37
23	b	834	CLA	C4D-ND	-2.94	1.33	1.37
23	9	310	CLA	C4D-ND	-2.93	1.33	1.37
23	7	311	CLA	C4D-ND	-2.93	1.33	1.37
23	7	306	CLA	C4D-ND	-2.93	1.33	1.37
23	a	815	CLA	C4D-ND	-2.93	1.33	1.37
23	7	308	CLA	C4D-ND	-2.93	1.33	1.37
23	9	313	CLA	C4D-ND	-2.93	1.33	1.37
23	5	306	CLA	C4D-ND	-2.93	1.33	1.37
23	b	837	CLA	C4D-ND	-2.93	1.33	1.37
23	1	310	CLA	C4D-ND	-2.92	1.33	1.37
23	b	811	CLA	C4D-ND	-2.92	1.33	1.37
23	a	844	CLA	C4D-ND	-2.92	1.33	1.37
23	9	309	CLA	C4D-ND	-2.92	1.33	1.37
23	4	310	CLA	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	316	SQD	C6-S	-2.92	1.66	1.77
23	1	309	CLA	C4D-ND	-2.92	1.33	1.37
23	a	834	CLA	C4D-ND	-2.92	1.33	1.37
23	a	811	CLA	C4D-ND	-2.92	1.33	1.37
23	8	313	CLA	C4D-ND	-2.91	1.33	1.37
23	9	312	CLA	C4D-ND	-2.91	1.33	1.37
23	4	316	CLA	C4D-ND	-2.91	1.33	1.37
23	b	820	CLA	C4D-ND	-2.91	1.33	1.37
23	b	833	CLA	C4D-ND	-2.91	1.33	1.37
23	9	315	CLA	C4D-ND	-2.91	1.33	1.37
23	8	306	CLA	C4D-ND	-2.91	1.33	1.37
25	9	302	A1L1F	C6-C1	-2.91	1.49	1.54
23	a	825	CLA	C4D-ND	-2.90	1.33	1.37
23	9	311	CLA	C4D-ND	-2.90	1.33	1.37
23	4	317	CLA	C4D-ND	-2.90	1.33	1.37
23	a	801	CLA	C4D-ND	-2.90	1.33	1.37
23	b	805	CLA	C4D-ND	-2.90	1.33	1.37
23	b	839	CLA	CHC-C1C	2.90	1.42	1.35
23	2	315	CLA	C4D-ND	-2.90	1.33	1.37
23	a	812	CLA	C4D-ND	-2.90	1.33	1.37
24	1	315	SQD	C6-S	-2.90	1.66	1.77
23	b	801	CLA	C4D-ND	-2.89	1.33	1.37
23	1	313	CLA	C4D-ND	-2.89	1.33	1.37
23	b	802	CLA	C4D-ND	-2.89	1.33	1.37
23	a	813	CLA	C4D-ND	-2.89	1.33	1.37
23	3	314	CLA	C4D-ND	-2.89	1.33	1.37
23	2	316	CLA	C4D-ND	-2.89	1.33	1.37
23	7	315	CLA	C4D-ND	-2.89	1.33	1.37
23	a	810	CLA	C4D-ND	-2.89	1.33	1.37
23	b	824	CLA	C4D-ND	-2.89	1.33	1.37
23	7	312	CLA	C4D-ND	-2.89	1.33	1.37
23	6	312	CLA	C4D-ND	-2.88	1.33	1.37
23	a	823	CLA	C4D-ND	-2.88	1.33	1.37
23	1	307	CLA	C4D-ND	-2.88	1.33	1.37
23	f	803	CLA	C4D-ND	-2.88	1.33	1.37
23	8	309	CLA	C4D-ND	-2.87	1.33	1.37
23	a	839	CLA	C4D-ND	-2.87	1.33	1.37
23	b	839	CLA	C4D-ND	-2.87	1.33	1.37
23	4	306	CLA	C4D-ND	-2.87	1.33	1.37
23	1	306	CLA	C4D-ND	-2.87	1.33	1.37
23	a	809	CLA	C4D-ND	-2.87	1.33	1.37
23	7	317	CLA	C4D-ND	-2.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	805	CLA	C4D-ND	-2.87	1.33	1.37
23	b	827	CLA	C4D-ND	-2.86	1.33	1.37
23	6	307	CLA	C4D-ND	-2.86	1.33	1.37
23	b	818	CLA	C4D-ND	-2.86	1.33	1.37
23	b	810	CLA	C4D-ND	-2.86	1.33	1.37
23	a	804	CLA	C4D-ND	-2.86	1.33	1.37
27	a	845	LHG	C26-C25	-2.86	1.35	1.51
23	b	831	CLA	C4D-ND	-2.86	1.33	1.37
23	3	312	CLA	C4D-ND	-2.86	1.33	1.37
23	a	820	CLA	C4D-ND	-2.86	1.33	1.37
23	a	826	CLA	C4D-ND	-2.86	1.33	1.37
23	a	837	CLA	C4D-ND	-2.85	1.33	1.37
23	b	821	CLA	C4D-ND	-2.85	1.33	1.37
23	1	312	CLA	C4D-ND	-2.85	1.33	1.37
23	8	305	CLA	C4D-ND	-2.85	1.33	1.37
23	a	840	CLA	C4D-ND	-2.85	1.33	1.37
23	5	314	CLA	C4D-ND	-2.85	1.33	1.37
23	7	307	CLA	C4D-ND	-2.85	1.33	1.37
23	4	314	CLA	C4D-ND	-2.85	1.33	1.37
23	3	315	CLA	C4D-ND	-2.85	1.33	1.37
23	6	311	CLA	C4D-ND	-2.84	1.33	1.37
23	a	836	CLA	C4D-ND	-2.84	1.33	1.37
22	1	301	A1L1G	C42-C44	2.84	1.39	1.35
23	2	314	CLA	C4D-ND	-2.83	1.33	1.37
23	4	307	CLA	C4D-ND	-2.83	1.33	1.37
23	6	315	CLA	C4D-ND	-2.83	1.33	1.37
23	a	835	CLA	C4D-ND	-2.83	1.33	1.37
23	a	802	CLA	C4D-ND	-2.83	1.33	1.37
23	a	806	CLA	CMB-C2B	-2.83	1.45	1.51
23	5	310	CLA	C4D-ND	-2.83	1.33	1.37
23	3	307	CLA	C4D-ND	-2.83	1.33	1.37
23	b	803	CLA	C4D-ND	-2.83	1.33	1.37
26	9	305	45D	C04-C08	-2.83	1.49	1.53
23	8	314	CLA	C4D-ND	-2.83	1.33	1.37
23	8	308	CLA	C4D-ND	-2.83	1.33	1.37
23	6	316	CLA	C4D-ND	-2.82	1.33	1.37
27	9	317	LHG	C26-C25	-2.82	1.35	1.51
23	a	818	CLA	C4D-ND	-2.82	1.33	1.37
23	4	315	CLA	C4D-ND	-2.82	1.33	1.37
23	6	309	CLA	C4D-ND	-2.82	1.33	1.37
23	2	310	CLA	C4D-ND	-2.82	1.33	1.37
23	2	311	CLA	C4D-ND	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	312	CLA	C4D-ND	-2.81	1.33	1.37
23	j	103	CLA	C4D-ND	-2.81	1.33	1.37
23	b	809	CLA	C4D-ND	-2.80	1.33	1.37
23	6	314	CLA	C4D-ND	-2.80	1.33	1.37
23	2	313	CLA	C4D-ND	-2.80	1.33	1.37
27	b	847	LHG	C26-C25	-2.80	1.35	1.51
23	2	306	CLA	C4D-ND	-2.80	1.33	1.37
27	9	307	LHG	C26-C25	-2.80	1.35	1.51
23	6	308	CLA	C4D-ND	-2.79	1.33	1.37
23	7	314	CLA	C4D-ND	-2.78	1.33	1.37
23	a	841	CLA	C4D-ND	-2.78	1.33	1.37
23	b	814	CLA	C4D-ND	-2.78	1.33	1.37
23	5	305	CLA	C4D-ND	-2.78	1.33	1.37
22	9	301	A1L1G	C33-C34	-2.78	1.40	1.45
23	3	308	CLA	C4D-ND	-2.76	1.33	1.37
23	2	307	CLA	C4D-ND	-2.76	1.33	1.37
23	a	821	CLA	C4D-ND	-2.76	1.33	1.37
23	9	314	CLA	C4D-ND	-2.75	1.33	1.37
23	7	316	CLA	C4D-ND	-2.75	1.33	1.37
23	a	801	CLA	CMB-C2B	-2.74	1.45	1.51
23	1	314	CLA	C4D-ND	-2.74	1.33	1.37
23	6	317	CLA	C4D-ND	-2.73	1.33	1.37
23	b	829	CLA	C4D-ND	-2.73	1.33	1.37
23	4	311	CLA	C4D-ND	-2.73	1.33	1.37
23	b	819	CLA	CMB-C2B	-2.70	1.46	1.51
23	b	801	CLA	CMB-C2B	-2.67	1.46	1.51
23	2	307	CLA	CMB-C2B	-2.66	1.46	1.51
23	b	810	CLA	CMB-C2B	-2.64	1.46	1.51
22	5	303	A1L1G	C33-C34	-2.62	1.40	1.45
25	h	203	A1L1F	C6-C1	-2.62	1.50	1.54
25	h	203	A1L1F	O15-C20	-2.62	1.42	1.46
22	5	303	A1L1G	C42-C44	2.62	1.39	1.35
23	b	839	CLA	CMB-C2B	-2.62	1.46	1.51
22	3	306	A1L1G	C40-C39	-2.62	1.40	1.45
23	8	310	CLA	CMB-C2B	-2.61	1.46	1.51
23	a	832	CLA	CMB-C2B	-2.61	1.46	1.51
23	b	804	CLA	C4D-ND	-2.61	1.34	1.37
22	3	306	A1L1G	C33-C34	-2.59	1.40	1.45
23	4	311	CLA	CMB-C2B	-2.59	1.46	1.51
23	2	310	CLA	CMB-C2B	-2.58	1.46	1.51
22	3	306	A1L1G	C42-C44	2.57	1.39	1.35
23	a	836	CLA	CMB-C2B	-2.57	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	301	A1L1F	O15-C20	-2.57	1.42	1.46
23	a	820	CLA	CMB-C2B	-2.55	1.46	1.51
22	9	306	A1L1G	C33-C34	-2.55	1.40	1.45
22	3	302	A1L1G	C33-C34	-2.55	1.40	1.45
22	7	302	A1L1G	C33-C34	-2.55	1.40	1.45
22	9	306	A1L1G	C42-C44	2.55	1.39	1.35
23	9	309	CLA	CMB-C2B	-2.54	1.46	1.51
23	a	806	CLA	C1D-ND	2.54	1.40	1.37
23	b	817	CLA	CMB-C2B	-2.53	1.46	1.51
23	b	834	CLA	CMB-C2B	-2.53	1.46	1.51
23	b	830	CLA	CMB-C2B	-2.53	1.46	1.51
23	7	311	CLA	CMB-C2B	-2.53	1.46	1.51
23	b	818	CLA	CMB-C2B	-2.52	1.46	1.51
22	5	303	A1L1G	C40-C39	-2.52	1.40	1.45
23	a	802	CLA	CMB-C2B	-2.52	1.46	1.51
23	4	317	CLA	CMB-C2B	-2.51	1.46	1.51
23	3	307	CLA	CMB-C2B	-2.51	1.46	1.51
23	a	824	CLA	CMB-C2B	-2.51	1.46	1.51
23	a	803	CLA	CMB-C2B	-2.51	1.46	1.51
23	a	822	CLA	CMB-C2B	-2.50	1.46	1.51
23	a	808	CLA	CMB-C2B	-2.50	1.46	1.51
23	b	828	CLA	CMB-C2B	-2.50	1.46	1.51
22	3	302	A1L1G	C40-C39	-2.49	1.40	1.45
23	5	312	CLA	CMB-C2B	-2.48	1.46	1.51
23	a	837	CLA	CMB-C2B	-2.48	1.46	1.51
23	b	829	CLA	CMD-C2D	-2.48	1.45	1.50
21	9	303	XAT	O4-C5	-2.48	1.42	1.46
22	1	301	A1L1G	C33-C34	-2.48	1.40	1.45
23	1	202	CLA	CMB-C2B	-2.47	1.46	1.51
23	1	203	CLA	CMB-C2B	-2.47	1.46	1.51
23	a	817	CLA	CMB-C2B	-2.47	1.46	1.51
23	6	312	CLA	CMB-C2B	-2.47	1.46	1.51
23	a	810	CLA	CMB-C2B	-2.47	1.46	1.51
23	8	313	CLA	CMB-C2B	-2.46	1.46	1.51
23	4	313	CLA	CMB-C2B	-2.46	1.46	1.51
23	j	103	CLA	CMB-C2B	-2.46	1.46	1.51
23	7	315	CLA	CMB-C2B	-2.46	1.46	1.51
23	b	809	CLA	CMB-C2B	-2.46	1.46	1.51
23	6	313	CLA	CMB-C2B	-2.45	1.46	1.51
23	a	806	CLA	CMD-C2D	-2.45	1.45	1.50
23	a	818	CLA	CMB-C2B	-2.45	1.46	1.51
23	b	838	CLA	CMB-C2B	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	309	CLA	CMB-C2B	-2.45	1.46	1.51
23	3	311	CLA	CMB-C2B	-2.45	1.46	1.51
22	9	306	A1L1G	C40-C39	-2.45	1.40	1.45
23	1	314	CLA	CMB-C2B	-2.44	1.46	1.51
23	4	314	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	811	CLA	CMB-C2B	-2.44	1.46	1.51
22	7	302	A1L1G	C40-C39	-2.44	1.40	1.45
23	b	824	CLA	CMB-C2B	-2.44	1.46	1.51
23	1	307	CLA	CMB-C2B	-2.44	1.46	1.51
23	a	854	CLA	CMB-C2B	-2.43	1.46	1.51
23	a	842	CLA	CMB-C2B	-2.43	1.46	1.51
23	b	812	CLA	CMB-C2B	-2.43	1.46	1.51
23	1	310	CLA	CMB-C2B	-2.43	1.46	1.51
23	a	835	CLA	CMB-C2B	-2.43	1.46	1.51
23	2	306	CLA	CMB-C2B	-2.42	1.46	1.51
23	l	204	CLA	CMB-C2B	-2.42	1.46	1.51
23	1	312	CLA	CMB-C2B	-2.42	1.46	1.51
23	5	309	CLA	CMB-C2B	-2.42	1.46	1.51
23	5	306	CLA	CMB-C2B	-2.42	1.46	1.51
23	7	314	CLA	CMB-C2B	-2.42	1.46	1.51
23	6	316	CLA	CMB-C2B	-2.42	1.46	1.51
23	b	825	CLA	CMB-C2B	-2.42	1.46	1.51
23	7	307	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	840	CLA	CMB-C2B	-2.41	1.46	1.51
23	4	312	CLA	CMB-C2B	-2.41	1.46	1.51
22	3	302	A1L1G	C29-C30	-2.41	1.40	1.45
23	9	308	CLA	CMB-C2B	-2.41	1.46	1.51
23	1	313	CLA	CMB-C2B	-2.41	1.46	1.51
23	8	312	CLA	CMB-C2B	-2.41	1.46	1.51
23	b	840	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	815	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	819	CLA	CMB-C2B	-2.41	1.46	1.51
23	a	801	CLA	CMD-C2D	-2.41	1.45	1.50
23	5	310	CLA	CMB-C2B	-2.41	1.46	1.51
23	b	827	CLA	CMB-C2B	-2.41	1.46	1.51
23	9	318	CLA	CMB-C2B	-2.41	1.46	1.51
23	1	311	CLA	CMB-C2B	-2.41	1.46	1.51
23	9	311	CLA	CMB-C2B	-2.41	1.46	1.51
23	2	314	CLA	CMB-C2B	-2.40	1.46	1.51
23	a	827	CLA	CMB-C2B	-2.40	1.46	1.51
23	8	308	CLA	CMB-C2B	-2.40	1.46	1.51
23	b	813	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	305	CLA	CMB-C2B	-2.40	1.46	1.51
23	8	314	CLA	CMB-C2B	-2.40	1.46	1.51
23	6	315	CLA	CMB-C2B	-2.40	1.46	1.51
23	j	102	CLA	CMB-C2B	-2.40	1.46	1.51
23	2	315	CLA	CMB-C2B	-2.39	1.46	1.51
23	4	306	CLA	CMB-C2B	-2.39	1.46	1.51
23	7	309	CLA	CMB-C2B	-2.39	1.46	1.51
23	3	312	CLA	CMB-C2B	-2.39	1.46	1.51
23	a	821	CLA	CMB-C2B	-2.39	1.46	1.51
23	4	315	CLA	CMB-C2B	-2.39	1.46	1.51
23	2	309	CLA	CMB-C2B	-2.39	1.46	1.51
23	2	311	CLA	CMB-C2B	-2.39	1.46	1.51
23	5	315	CLA	CMB-C2B	-2.39	1.46	1.51
23	a	834	CLA	CMB-C2B	-2.39	1.46	1.51
23	b	815	CLA	CMB-C2B	-2.39	1.46	1.51
23	4	316	CLA	CMB-C2B	-2.39	1.46	1.51
23	a	806	CLA	CMC-C2C	-2.39	1.45	1.50
23	7	317	CLA	CMB-C2B	-2.39	1.46	1.51
23	6	309	CLA	CMB-C2B	-2.39	1.46	1.51
23	a	841	CLA	CMB-C2B	-2.39	1.46	1.51
23	3	314	CLA	CMB-C2B	-2.39	1.46	1.51
23	3	308	CLA	CMB-C2B	-2.39	1.46	1.51
23	a	830	CLA	CMC-C2C	-2.39	1.45	1.50
23	6	311	CLA	CMB-C2B	-2.39	1.46	1.51
23	5	313	CLA	CMB-C2B	-2.38	1.46	1.51
23	h	204	CLA	CMB-C2B	-2.38	1.46	1.51
23	5	314	CLA	CMB-C2B	-2.38	1.46	1.51
23	a	825	CLA	CMB-C2B	-2.38	1.46	1.51
23	a	813	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	836	CLA	CMB-C2B	-2.38	1.46	1.51
23	6	317	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	833	CLA	CMB-C2B	-2.38	1.46	1.51
23	3	309	CLA	CMB-C2B	-2.37	1.46	1.51
27	b	847	LHG	O8-C6	-2.37	1.39	1.45
23	3	315	CLA	CMB-C2B	-2.37	1.46	1.51
23	1	306	CLA	CMB-C2B	-2.37	1.46	1.51
23	b	802	CLA	CMB-C2B	-2.37	1.46	1.51
23	3	313	CLA	CMB-C2B	-2.37	1.46	1.51
23	a	838	CLA	CMB-C2B	-2.37	1.46	1.51
23	a	806	CLA	C3B-CAB	-2.37	1.43	1.47
23	2	308	CLA	CMB-C2B	-2.36	1.46	1.51
23	7	312	CLA	CMB-C2B	-2.36	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	837	CLA	CMB-C2B	-2.36	1.46	1.51
22	9	301	A1L1G	C29-C30	-2.36	1.40	1.45
23	4	310	CLA	CMB-C2B	-2.36	1.46	1.51
23	6	307	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	820	CLA	CMB-C2B	-2.36	1.46	1.51
23	f	803	CLA	CMB-C2B	-2.36	1.46	1.51
23	4	307	CLA	CMB-C2B	-2.36	1.46	1.51
23	5	308	CLA	CMB-C2B	-2.36	1.46	1.51
27	a	846	LHG	O8-C6	-2.36	1.39	1.45
23	8	309	CLA	CMB-C2B	-2.36	1.46	1.51
23	2	316	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	822	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	806	CLA	CMB-C2B	-2.36	1.46	1.51
23	a	804	CLA	CMB-C2B	-2.36	1.46	1.51
23	8	306	CLA	CMB-C2B	-2.36	1.46	1.51
23	7	310	CLA	CMB-C2B	-2.36	1.46	1.51
23	a	811	CLA	CMB-C2B	-2.36	1.46	1.51
23	9	314	CLA	CMB-C2B	-2.36	1.46	1.51
23	a	839	CLA	CMB-C2B	-2.36	1.46	1.51
23	5	307	CLA	CMB-C2B	-2.35	1.46	1.51
23	9	315	CLA	CMB-C2B	-2.35	1.46	1.51
23	a	826	CLA	CMB-C2B	-2.35	1.46	1.51
23	a	828	CLA	CMB-C2B	-2.35	1.46	1.51
27	9	317	LHG	O8-C23	2.35	1.40	1.33
23	a	812	CLA	CMB-C2B	-2.35	1.46	1.51
23	8	307	CLA	CMB-C2B	-2.35	1.46	1.51
23	5	305	CLA	CMB-C2B	-2.35	1.46	1.51
23	a	814	CLA	CMB-C2B	-2.35	1.46	1.51
23	a	829	CLA	CMB-C2B	-2.35	1.46	1.51
23	b	832	CLA	CMB-C2B	-2.35	1.46	1.51
25	9	302	A1L1F	O15-C20	-2.35	1.42	1.46
23	b	831	CLA	CMB-C2B	-2.35	1.46	1.51
27	9	307	LHG	O7-C7	2.35	1.40	1.34
23	b	826	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	808	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	807	CLA	CMB-C2B	-2.34	1.46	1.51
23	3	310	CLA	CMB-C2B	-2.34	1.46	1.51
23	6	308	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	823	CLA	CMB-C2B	-2.34	1.46	1.51
27	b	847	LHG	O8-C23	2.34	1.40	1.33
23	b	835	CLA	CMB-C2B	-2.34	1.46	1.51
27	a	845	LHG	O8-C6	-2.34	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	313	CLA	CMB-C2B	-2.34	1.46	1.51
23	9	313	CLA	CMB-C2B	-2.34	1.46	1.51
23	4	308	CLA	CMB-C2B	-2.34	1.46	1.51
23	9	312	CLA	CMB-C2B	-2.34	1.46	1.51
23	a	830	CLA	CMB-C2B	-2.33	1.46	1.51
23	7	316	CLA	CMB-C2B	-2.33	1.46	1.51
23	2	312	CLA	CMB-C2B	-2.33	1.46	1.51
23	2	313	CLA	CMB-C2B	-2.33	1.46	1.51
23	7	306	CLA	CMB-C2B	-2.33	1.46	1.51
27	9	317	LHG	O8-C6	-2.33	1.39	1.45
23	b	821	CLA	CMB-C2B	-2.33	1.46	1.51
23	b	803	CLA	CMB-C2B	-2.33	1.46	1.51
23	1	308	CLA	CMB-C2B	-2.33	1.46	1.51
23	b	805	CLA	CMB-C2B	-2.33	1.46	1.51
23	9	310	CLA	CMB-C2B	-2.33	1.46	1.51
23	f	802	CLA	CMB-C2B	-2.33	1.46	1.51
23	a	809	CLA	CMB-C2B	-2.33	1.46	1.51
23	a	833	CLA	CMB-C2B	-2.33	1.46	1.51
22	1	301	A1L1G	C40-C39	-2.32	1.41	1.45
23	4	309	CLA	CMB-C2B	-2.32	1.46	1.51
23	6	310	CLA	CMB-C2B	-2.32	1.46	1.51
26	9	305	45D	C08-C16	-2.32	1.32	1.35
23	4	311	CLA	CMD-C2D	-2.32	1.45	1.50
23	8	311	CLA	CMB-C2B	-2.32	1.46	1.51
23	a	805	CLA	CMB-C2B	-2.32	1.46	1.51
23	b	814	CLA	CMB-C2B	-2.31	1.46	1.51
23	a	816	CLA	CMB-C2B	-2.31	1.46	1.51
23	8	305	CLA	CMB-C2B	-2.31	1.46	1.51
23	a	807	CLA	CMB-C2B	-2.31	1.46	1.51
27	9	307	LHG	O8-C6	-2.31	1.39	1.45
23	a	844	CLA	CMB-C2B	-2.31	1.46	1.51
23	a	823	CLA	CMB-C2B	-2.31	1.46	1.51
23	b	816	CLA	CMB-C2B	-2.31	1.46	1.51
23	9	316	CLA	CMB-C2B	-2.30	1.46	1.51
27	a	845	LHG	O7-C7	2.30	1.40	1.34
23	9	308	CLA	CMC-C2C	-2.30	1.45	1.50
25	1	304	A1L1F	O15-C20	-2.29	1.42	1.46
23	a	806	CLA	C3B-C2B	-2.29	1.37	1.40
23	6	314	CLA	CMB-C2B	-2.29	1.46	1.51
27	9	307	LHG	O8-C23	2.29	1.40	1.33
27	9	317	LHG	O7-C7	2.29	1.40	1.34
27	a	845	LHG	O8-C23	2.28	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	846	LHG	O8-C23	2.28	1.40	1.33
25	1	304	A1L1F	C6-C1	-2.28	1.50	1.54
23	7	308	CLA	CMB-C2B	-2.27	1.46	1.51
27	a	846	LHG	O7-C5	-2.27	1.40	1.46
27	a	846	LHG	O7-C7	2.26	1.40	1.34
23	5	311	CLA	CMB-C2B	-2.26	1.46	1.51
22	3	306	A1L1G	C29-C30	-2.25	1.40	1.45
22	9	301	A1L1G	C40-C39	-2.25	1.41	1.45
27	b	847	LHG	O7-C7	2.24	1.40	1.34
27	b	847	LHG	O7-C5	-2.24	1.41	1.46
22	1	301	A1L1G	C29-C30	-2.24	1.40	1.45
23	b	822	CLA	CMD-C2D	-2.23	1.46	1.50
27	a	845	LHG	O7-C5	-2.22	1.41	1.46
23	b	809	CLA	CMD-C2D	-2.22	1.46	1.50
27	9	317	LHG	O7-C5	-2.21	1.41	1.46
23	a	824	CLA	CMD-C2D	-2.20	1.46	1.50
22	5	303	A1L1G	C29-C30	-2.20	1.40	1.45
21	3	305	XAT	O4-C5	-2.20	1.43	1.46
23	a	810	CLA	CMD-C2D	-2.20	1.46	1.50
23	b	804	CLA	CMB-C2B	-2.20	1.47	1.51
23	b	830	CLA	CMD-C2D	-2.19	1.46	1.50
25	6	301	A1L1F	C6-C1	-2.18	1.50	1.54
23	a	801	CLA	C3B-CAB	-2.18	1.43	1.47
23	a	830	CLA	CMD-C2D	-2.18	1.46	1.50
23	b	823	CLA	CMD-C2D	-2.17	1.46	1.50
26	9	305	45D	C07-C15	-2.16	1.32	1.35
23	a	801	CLA	CMC-C2C	-2.16	1.46	1.50
23	a	828	CLA	CMC-C2C	-2.16	1.46	1.50
22	9	306	A1L1G	C29-C30	-2.16	1.40	1.45
23	a	806	CLA	CAA-C2A	-2.16	1.50	1.54
23	3	307	CLA	CMD-C2D	-2.15	1.46	1.50
26	9	305	45D	C03-C07	-2.15	1.50	1.53
21	1	302	XAT	O4-C5	-2.15	1.43	1.46
27	9	307	LHG	O7-C5	-2.15	1.41	1.46
23	a	804	CLA	CMC-C2C	-2.15	1.46	1.50
23	7	314	CLA	CMD-C2D	-2.14	1.46	1.50
23	7	316	CLA	CMD-C2D	-2.14	1.46	1.50
23	5	305	CLA	CMD-C2D	-2.13	1.46	1.50
28	b	848	DGD	O3D-C3D	-2.13	1.38	1.43
23	9	309	CLA	CMD-C2D	-2.13	1.46	1.50
23	b	828	CLA	CMD-C2D	-2.13	1.46	1.50
28	b	848	DGD	O4D-C4D	-2.13	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	806	CLA	MG-ND	-2.12	2.01	2.05
21	4	301	XAT	O24-C25	-2.12	1.43	1.46
28	b	848	DGD	C1E-C2E	2.11	1.58	1.52
23	b	803	CLA	CMD-C2D	-2.11	1.46	1.50
25	8	304	A1L1F	O15-C20	-2.11	1.43	1.46
21	5	302	XAT	O4-C5	-2.11	1.43	1.46
21	4	304	XAT	O24-C25	-2.11	1.43	1.46
23	6	312	CLA	CMD-C2D	-2.10	1.46	1.50
23	b	811	CLA	CMD-C2D	-2.10	1.46	1.50
23	2	310	CLA	CMD-C2D	-2.10	1.46	1.50
21	a	852	XAT	O4-C5	-2.10	1.43	1.46
21	5	301	XAT	O4-C5	-2.10	1.43	1.46
23	a	821	CLA	CMD-C2D	-2.10	1.46	1.50
21	7	301	XAT	O24-C25	-2.09	1.43	1.46
23	b	809	CLA	CMC-C2C	-2.09	1.46	1.50
23	b	814	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	837	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	801	CLA	CMD-C2D	-2.09	1.46	1.50
21	3	301	XAT	O24-C25	-2.08	1.43	1.46
21	2	303	XAT	O4-C5	-2.08	1.43	1.46
23	b	838	CLA	CMD-C2D	-2.08	1.46	1.50
23	a	832	CLA	CMD-C2D	-2.07	1.46	1.50
27	9	317	LHG	P-O6	2.07	1.67	1.59
23	b	833	CLA	CMD-C2D	-2.07	1.46	1.50
23	5	308	CLA	CMD-C2D	-2.07	1.46	1.50
23	a	842	CLA	CMD-C2D	-2.07	1.46	1.50
23	a	803	CLA	C3B-CAB	-2.07	1.43	1.47
23	2	316	CLA	CMD-C2D	-2.06	1.46	1.50
23	b	803	CLA	CMC-C2C	-2.06	1.46	1.50
27	b	847	LHG	P-O6	2.06	1.67	1.59
21	3	303	XAT	O4-C5	-2.06	1.43	1.46
21	8	303	XAT	O4-C5	-2.06	1.43	1.46
23	a	812	CLA	CMD-C2D	-2.06	1.46	1.50
27	9	307	LHG	P-O6	2.05	1.67	1.59
23	b	834	CLA	CMD-C2D	-2.05	1.46	1.50
21	2	302	XAT	O4-C5	-2.05	1.43	1.46
23	b	820	CLA	CMD-C2D	-2.05	1.46	1.50
21	8	302	XAT	O4-C5	-2.05	1.43	1.46
27	a	845	LHG	P-O6	2.05	1.67	1.59
23	j	102	CLA	CMD-C2D	-2.05	1.46	1.50
23	a	826	CLA	CMD-C2D	-2.05	1.46	1.50
23	b	825	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	302	A1L1G	C29-C30	-2.05	1.40	1.45
25	6	304	A1L1F	O15-C20	-2.05	1.43	1.46
23	a	834	CLA	CMD-C2D	-2.04	1.46	1.50
21	2	301	XAT	O4-C5	-2.04	1.43	1.46
23	9	318	CLA	CMD-C2D	-2.04	1.46	1.50
23	3	309	CLA	CMD-C2D	-2.04	1.46	1.50
23	2	306	CLA	CMD-C2D	-2.04	1.46	1.50
23	9	312	CLA	CMD-C2D	-2.04	1.46	1.50
23	8	310	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	816	CLA	CMD-C2D	-2.03	1.46	1.50
21	4	305	XAT	O4-C5	-2.03	1.43	1.46
23	b	819	CLA	CMD-C2D	-2.03	1.46	1.50
23	7	312	CLA	CMD-C2D	-2.03	1.46	1.50
23	4	308	CLA	CMD-C2D	-2.03	1.46	1.50
23	1	202	CLA	CMD-C2D	-2.03	1.46	1.50
23	a	827	CLA	CMD-C2D	-2.03	1.46	1.50
21	9	304	XAT	O4-C5	-2.03	1.43	1.46
21	3	304	XAT	O24-C25	-2.03	1.43	1.46
28	b	848	DGD	O2D-C2D	-2.03	1.38	1.43
21	7	303	XAT	O4-C5	-2.03	1.43	1.46
21	7	304	XAT	O24-C25	-2.03	1.43	1.46
23	3	315	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	817	CLA	CMD-C2D	-2.02	1.46	1.50
23	6	308	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	840	CLA	C3B-C2B	-2.02	1.37	1.40
23	1	309	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	839	CLA	CMD-C2D	-2.02	1.46	1.50
23	1	203	CLA	CMC-C2C	-2.02	1.46	1.50
21	a	852	XAT	O24-C25	-2.02	1.43	1.46
23	3	312	CLA	CMD-C2D	-2.02	1.46	1.50
23	7	311	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	803	CLA	CMD-C2D	-2.02	1.46	1.50
23	1	204	CLA	CMC-C2C	-2.02	1.46	1.50
23	b	802	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	804	CLA	CMD-C2D	-2.02	1.46	1.50
23	a	838	CLA	CMD-C2D	-2.02	1.46	1.50
23	2	314	CLA	CMC-C2C	-2.02	1.46	1.50
23	9	314	CLA	CMD-C2D	-2.01	1.46	1.50
21	6	306	XAT	O24-C25	-2.01	1.43	1.46
23	2	309	CLA	CMD-C2D	-2.01	1.46	1.50
21	4	301	XAT	O4-C5	-2.01	1.43	1.46
21	6	305	XAT	O4-C5	-2.01	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	808	CLA	CMD-C2D	-2.01	1.46	1.50
23	h	204	CLA	CMC-C2C	-2.01	1.46	1.50
21	6	303	XAT	O4-C5	-2.01	1.43	1.46
21	2	305	XAT	O4-C5	-2.01	1.43	1.46
23	1	313	CLA	CMD-C2D	-2.01	1.46	1.50
27	a	846	LHG	P-O6	2.01	1.67	1.59
23	9	308	CLA	CMD-C2D	-2.01	1.46	1.50
21	6	306	XAT	O4-C5	-2.01	1.43	1.46
28	b	848	DGD	O4E-C4E	-2.01	1.38	1.43
23	7	306	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	807	CLA	CMD-C2D	-2.01	1.46	1.50
23	a	807	CLA	CMD-C2D	-2.00	1.46	1.50
23	a	837	CLA	CMD-C2D	-2.00	1.46	1.50
23	b	827	CLA	CMD-C2D	-2.00	1.46	1.50
23	a	808	CLA	CMD-C2D	-2.00	1.46	1.50
23	5	314	CLA	CMD-C2D	-2.00	1.46	1.50
21	8	301	XAT	O4-C5	-2.00	1.43	1.46
23	8	313	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	13.19	123.29	113.38
28	4	318	DGD	C6E-C5E-C4E	-9.41	90.97	113.00
25	6	301	A1L1F	O15-C20-C21	8.71	119.92	113.38
25	6	304	A1L1F	O15-C20-C21	8.65	119.88	113.38
25	8	304	A1L1F	O15-C20-C21	8.49	119.76	113.38
25	9	302	A1L1F	C17-C20-C25	-8.48	108.05	122.26
25	6	301	A1L1F	C17-C20-C25	-8.44	108.11	122.26
25	h	203	A1L1F	O15-C20-C21	8.39	119.69	113.38
25	h	203	A1L1F	C17-C20-C25	-8.36	108.25	122.26
25	6	304	A1L1F	C17-C20-C25	-8.27	108.40	122.26
25	8	304	A1L1F	C17-C20-C25	-8.21	108.50	122.26
25	1	304	A1L1F	C17-C20-C25	-8.09	108.70	122.26
25	8	304	A1L1F	C37-C38-C39	-7.85	116.11	127.31
21	6	305	XAT	C18-C5-C4	7.68	122.92	114.28
23	7	314	CLA	C4A-NA-C1A	7.43	110.05	106.71
21	6	303	XAT	C38-C25-C26	-7.41	109.85	122.26
23	9	310	CLA	C4A-NA-C1A	7.32	110.00	106.71
23	a	806	CLA	C4A-NA-C1A	7.31	109.99	106.71
23	9	313	CLA	C4A-NA-C1A	7.31	109.99	106.71
25	1	304	A1L1F	O15-C20-C21	7.30	118.87	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	303	XAT	C38-C25-C24	7.28	122.47	114.28
23	b	839	CLA	C4A-NA-C1A	7.27	109.97	106.71
21	3	305	XAT	C38-C25-C24	7.21	122.39	114.28
23	4	310	CLA	C4A-NA-C1A	7.20	109.94	106.71
21	5	304	XAT	C38-C25-C24	7.19	122.36	114.28
23	l	203	CLA	C4A-NA-C1A	7.19	109.94	106.71
21	1	303	XAT	C38-C25-C24	7.18	122.36	114.28
21	4	305	XAT	C38-C25-C24	7.17	122.35	114.28
23	b	803	CLA	C4A-NA-C1A	7.14	109.92	106.71
21	7	304	XAT	C38-C25-C24	7.13	122.31	114.28
21	7	305	XAT	C38-C25-C24	7.11	122.28	114.28
23	a	833	CLA	C4A-NA-C1A	7.11	109.90	106.71
23	a	810	CLA	C4A-NA-C1A	7.10	109.90	106.71
23	a	821	CLA	C4A-NA-C1A	7.10	109.90	106.71
23	b	809	CLA	C4A-NA-C1A	7.09	109.89	106.71
21	a	852	XAT	C15-C14-C13	-7.09	117.19	127.31
21	9	304	XAT	C38-C25-C24	7.06	122.22	114.28
23	a	835	CLA	C4A-NA-C1A	7.06	109.88	106.71
21	j	101	XAT	C38-C25-C24	7.04	122.20	114.28
23	b	820	CLA	C4A-NA-C1A	7.04	109.87	106.71
23	a	826	CLA	C4A-NA-C1A	7.03	109.87	106.71
23	j	103	CLA	C4A-NA-C1A	7.03	109.87	106.71
31	f	801	BCR	C24-C23-C22	-7.02	115.63	126.23
21	4	304	XAT	C38-C25-C24	7.01	122.17	114.28
23	6	312	CLA	C4A-NA-C1A	7.01	109.86	106.71
23	a	823	CLA	C4A-NA-C1A	7.00	109.85	106.71
23	9	308	CLA	C4A-NA-C1A	6.99	109.85	106.71
21	5	304	XAT	C18-C5-C4	6.97	122.12	114.28
21	3	304	XAT	C38-C25-C24	6.97	122.12	114.28
21	6	305	XAT	C38-C25-C24	6.96	122.11	114.28
23	7	317	CLA	C4A-NA-C1A	6.93	109.82	106.71
23	b	805	CLA	C4A-NA-C1A	6.89	109.81	106.71
23	4	317	CLA	C4A-NA-C1A	6.88	109.80	106.71
21	8	301	XAT	C38-C25-C24	6.87	122.01	114.28
23	a	828	CLA	C4A-NA-C1A	6.87	109.80	106.71
21	2	301	XAT	C18-C5-C6	-6.86	110.77	122.26
23	a	801	CLA	C4A-NA-C1A	6.86	109.79	106.71
21	1	302	XAT	C38-C25-C24	6.85	121.99	114.28
21	5	304	XAT	C6-C7-C8	-6.85	111.51	125.99
23	b	827	CLA	C4A-NA-C1A	6.85	109.78	106.71
21	6	302	XAT	C38-C25-C24	6.85	121.98	114.28
23	b	821	CLA	C4A-NA-C1A	6.84	109.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	301	XAT	C38-C25-C26	-6.84	110.80	122.26
21	4	303	XAT	C38-C25-C24	6.83	121.97	114.28
23	6	310	CLA	C4A-NA-C1A	6.83	109.78	106.71
23	f	802	CLA	C4A-NA-C1A	6.83	109.78	106.71
21	2	304	XAT	C38-C25-C24	6.82	121.95	114.28
23	4	316	CLA	C4A-NA-C1A	6.82	109.77	106.71
21	4	305	XAT	C38-C25-C26	-6.81	110.84	122.26
23	b	806	CLA	C4A-NA-C1A	6.80	109.77	106.71
23	1	306	CLA	C4A-NA-C1A	6.80	109.76	106.71
21	8	303	XAT	C38-C25-C24	6.80	121.93	114.28
21	a	852	XAT	C38-C25-C24	6.80	121.93	114.28
21	8	301	XAT	C38-C25-C26	-6.79	110.88	122.26
21	9	303	XAT	C38-C25-C26	-6.79	110.88	122.26
23	b	824	CLA	C4A-NA-C1A	6.79	109.76	106.71
23	3	308	CLA	C4A-NA-C1A	6.78	109.75	106.71
21	3	304	XAT	C38-C25-C26	-6.78	110.90	122.26
23	b	810	CLA	C4A-NA-C1A	6.78	109.75	106.71
23	7	316	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	b	814	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	b	801	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	b	812	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	a	807	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	5	306	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	9	316	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	6	314	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	8	312	CLA	C4A-NA-C1A	6.74	109.74	106.71
21	6	303	XAT	C38-C25-C24	6.74	121.86	114.28
23	2	312	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	6	316	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	2	316	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	a	842	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	a	817	CLA	C4A-NA-C1A	6.72	109.73	106.71
23	6	317	CLA	C4A-NA-C1A	6.71	109.72	106.71
23	a	839	CLA	C4A-NA-C1A	6.71	109.72	106.71
23	a	809	CLA	C4A-NA-C1A	6.71	109.72	106.71
21	8	303	XAT	C18-C5-C6	-6.71	111.02	122.26
21	8	302	XAT	C38-C25-C24	6.71	121.83	114.28
23	a	825	CLA	C4A-NA-C1A	6.71	109.72	106.71
21	9	304	XAT	C38-C25-C26	-6.70	111.03	122.26
23	a	841	CLA	C4A-NA-C1A	6.70	109.72	106.71
21	4	302	XAT	C38-C25-C24	6.69	121.81	114.28
21	2	304	XAT	C18-C5-C4	6.69	121.81	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	311	CLA	C4A-NA-C1A	6.69	109.71	106.71
23	a	805	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	4	311	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	1	308	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	b	836	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	a	854	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	l	202	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	5	310	CLA	C4A-NA-C1A	6.67	109.71	106.71
23	4	307	CLA	C4A-NA-C1A	6.67	109.71	106.71
23	5	314	CLA	C4A-NA-C1A	6.67	109.70	106.71
21	6	302	XAT	C11-C10-C9	-6.67	117.79	127.31
23	3	312	CLA	C4A-NA-C1A	6.67	109.70	106.71
23	2	311	CLA	C4A-NA-C1A	6.67	109.70	106.71
23	b	832	CLA	C4A-NA-C1A	6.67	109.70	106.71
23	6	309	CLA	C4A-NA-C1A	6.67	109.70	106.71
23	a	834	CLA	C4A-NA-C1A	6.67	109.70	106.71
23	a	838	CLA	C4A-NA-C1A	6.67	109.70	106.71
21	5	304	XAT	C18-C5-C6	-6.66	111.09	122.26
21	7	304	XAT	C18-C5-C6	-6.66	111.10	122.26
23	a	831	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	8	311	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	3	313	CLA	C4A-NA-C1A	6.66	109.70	106.71
21	7	301	XAT	C18-C5-C6	-6.65	111.11	122.26
23	b	807	CLA	C4A-NA-C1A	6.65	109.70	106.71
21	2	301	XAT	C18-C5-C4	6.65	121.76	114.28
21	3	301	XAT	C18-C5-C4	6.65	121.76	114.28
23	a	840	CLA	C4A-NA-C1A	6.65	109.69	106.71
21	7	301	XAT	C18-C5-C4	6.65	121.76	114.28
21	3	304	XAT	C18-C5-C6	-6.65	111.12	122.26
21	3	303	XAT	C38-C25-C24	6.64	121.75	114.28
23	a	804	CLA	C4A-NA-C1A	6.64	109.69	106.71
23	a	812	CLA	C4A-NA-C1A	6.63	109.69	106.71
23	f	803	CLA	C4A-NA-C1A	6.63	109.69	106.71
23	4	315	CLA	C4A-NA-C1A	6.63	109.69	106.71
23	a	811	CLA	C4A-NA-C1A	6.62	109.68	106.71
23	5	312	CLA	C4A-NA-C1A	6.62	109.68	106.71
23	3	311	CLA	C4A-NA-C1A	6.62	109.68	106.71
23	9	314	CLA	C4A-NA-C1A	6.62	109.68	106.71
21	6	302	XAT	C38-C25-C26	-6.62	111.17	122.26
21	j	101	XAT	C38-C25-C26	-6.61	111.17	122.26
21	7	303	XAT	C38-C25-C26	-6.61	111.18	122.26
23	8	314	CLA	C4A-NA-C1A	6.61	109.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	l	204	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	b	808	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	7	315	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	b	815	CLA	C4A-NA-C1A	6.60	109.67	106.71
31	i	101	BCR	C24-C23-C22	-6.60	116.26	126.23
23	1	305	CLA	C4A-NA-C1A	6.60	109.67	106.71
21	8	302	XAT	C38-C25-C26	-6.60	111.20	122.26
23	a	829	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	5	313	CLA	C4A-NA-C1A	6.59	109.67	106.71
23	3	314	CLA	C4A-NA-C1A	6.58	109.67	106.71
23	a	827	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	6	315	CLA	C4A-NA-C1A	6.57	109.66	106.71
21	5	302	XAT	C18-C5-C6	-6.57	111.25	122.26
21	7	304	XAT	C38-C25-C26	-6.57	111.25	122.26
23	8	313	CLA	C4A-NA-C1A	6.57	109.66	106.71
21	5	301	XAT	C38-C25-C24	6.57	121.67	114.28
21	4	301	XAT	C18-C5-C4	6.57	121.67	114.28
23	3	309	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	2	309	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	a	837	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	b	818	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	3	315	CLA	C4A-NA-C1A	6.56	109.66	106.71
21	6	305	XAT	C38-C25-C26	-6.56	111.27	122.26
21	8	302	XAT	C18-C5-C6	-6.56	111.27	122.26
23	j	102	CLA	C4A-NA-C1A	6.56	109.65	106.71
23	a	832	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	a	844	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	7	307	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	7	312	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	1	307	CLA	C4A-NA-C1A	6.55	109.65	106.71
23	8	305	CLA	C4A-NA-C1A	6.54	109.65	106.71
21	4	301	XAT	C31-C30-C29	-6.54	117.97	127.31
21	2	303	XAT	C18-C5-C6	-6.54	111.30	122.26
21	7	305	XAT	C38-C25-C26	-6.54	111.30	122.26
23	5	308	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	8	309	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	7	303	XAT	C38-C25-C24	6.53	121.63	114.28
23	2	307	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	a	830	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	4	303	XAT	C18-C5-C6	-6.53	111.31	122.26
21	3	305	XAT	C38-C25-C26	-6.53	111.31	122.26
23	7	310	CLA	C4A-NA-C1A	6.53	109.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	304	XAT	C38-C25-C26	-6.53	111.32	122.26
23	b	822	CLA	C4A-NA-C1A	6.53	109.64	106.71
31	a	850	BCR	C24-C23-C22	-6.53	116.38	126.23
23	a	808	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	4	306	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	b	838	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	4	314	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	6	308	CLA	C4A-NA-C1A	6.51	109.63	106.71
21	4	301	XAT	C18-C5-C6	-6.51	111.35	122.26
21	2	305	XAT	C18-C5-C6	-6.51	111.35	122.26
23	b	835	CLA	C4A-NA-C1A	6.50	109.63	106.71
21	7	303	XAT	C18-C5-C6	-6.50	111.37	122.26
23	6	311	CLA	C4A-NA-C1A	6.49	109.62	106.71
21	4	303	XAT	C38-C25-C26	-6.49	111.38	122.26
21	4	302	XAT	C18-C5-C4	6.49	121.58	114.28
23	b	826	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	8	307	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	b	833	CLA	C4A-NA-C1A	6.48	109.62	106.71
21	2	303	XAT	C38-C25-C26	-6.48	111.40	122.26
23	9	312	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	2	315	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	b	823	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	6	307	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	h	204	CLA	C4A-NA-C1A	6.47	109.62	106.71
23	a	822	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	9	318	CLA	C4A-NA-C1A	6.46	109.61	106.71
21	6	306	XAT	C18-C5-C6	-6.46	111.43	122.26
21	2	304	XAT	C38-C25-C26	-6.46	111.43	122.26
21	6	303	XAT	C18-C5-C6	-6.46	111.44	122.26
21	6	303	XAT	C18-C5-C4	6.46	121.55	114.28
21	3	303	XAT	C18-C5-C6	-6.46	111.44	122.26
23	7	308	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	2	314	CLA	C4A-NA-C1A	6.45	109.61	106.71
23	a	836	CLA	C4A-NA-C1A	6.45	109.61	106.71
23	b	831	CLA	C4A-NA-C1A	6.45	109.61	106.71
21	8	303	XAT	C18-C5-C4	6.45	121.54	114.28
23	b	813	CLA	C4A-NA-C1A	6.45	109.61	106.71
21	2	304	XAT	C18-C5-C6	-6.45	111.46	122.26
23	2	313	CLA	C4A-NA-C1A	6.44	109.60	106.71
23	a	816	CLA	C4A-NA-C1A	6.44	109.60	106.71
23	a	818	CLA	C4A-NA-C1A	6.44	109.60	106.71
23	8	306	CLA	C4A-NA-C1A	6.43	109.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	309	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	a	824	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	1	312	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	a	814	CLA	C4A-NA-C1A	6.41	109.59	106.71
21	5	302	XAT	C26-C27-C28	-6.40	112.46	125.99
23	1	313	CLA	C4A-NA-C1A	6.40	109.58	106.71
21	j	101	XAT	C18-C5-C6	-6.40	111.54	122.26
21	1	302	XAT	C38-C25-C26	-6.40	111.54	122.26
23	1	311	CLA	C4A-NA-C1A	6.39	109.58	106.71
21	3	301	XAT	C18-C5-C6	-6.39	111.54	122.26
23	3	307	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	4	309	CLA	C4A-NA-C1A	6.39	109.58	106.71
21	6	302	XAT	C18-C5-C6	-6.39	111.55	122.26
23	3	310	CLA	C4A-NA-C1A	6.39	109.58	106.71
21	3	303	XAT	C38-C25-C26	-6.39	111.56	122.26
23	5	315	CLA	C4A-NA-C1A	6.38	109.58	106.71
23	7	309	CLA	C4A-NA-C1A	6.38	109.58	106.71
23	b	834	CLA	C4A-NA-C1A	6.38	109.58	106.71
23	2	306	CLA	C4A-NA-C1A	6.38	109.57	106.71
21	7	305	XAT	C18-C5-C6	-6.38	111.57	122.26
23	9	311	CLA	C4A-NA-C1A	6.37	109.57	106.71
23	7	306	CLA	C4A-NA-C1A	6.37	109.57	106.71
23	7	313	CLA	C4A-NA-C1A	6.37	109.57	106.71
23	b	819	CLA	C4A-NA-C1A	6.37	109.57	106.71
21	7	305	XAT	C18-C5-C4	6.37	121.44	114.28
23	4	308	CLA	C4A-NA-C1A	6.35	109.56	106.71
23	4	312	CLA	C4A-NA-C1A	6.35	109.56	106.71
21	2	302	XAT	C38-C25-C24	6.35	121.43	114.28
21	2	303	XAT	C38-C25-C24	6.35	121.43	114.28
21	j	101	XAT	C18-C5-C4	6.35	121.42	114.28
21	4	302	XAT	C18-C5-C6	-6.35	111.62	122.26
23	b	825	CLA	C4A-NA-C1A	6.35	109.56	106.71
21	9	303	XAT	C18-C5-C6	-6.34	111.63	122.26
23	a	819	CLA	C4A-NA-C1A	6.34	109.56	106.71
21	3	303	XAT	C18-C5-C4	6.34	121.41	114.28
23	a	813	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	7	311	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	8	308	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	a	815	CLA	C4A-NA-C1A	6.32	109.55	106.71
23	1	310	CLA	C4A-NA-C1A	6.31	109.54	106.71
21	3	305	XAT	C18-C5-C4	6.30	121.37	114.28
21	4	305	XAT	C31-C30-C29	-6.30	118.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	302	XAT	C18-C5-C6	-6.30	111.70	122.26
21	4	304	XAT	C18-C5-C6	-6.30	111.70	122.26
21	1	302	XAT	C18-C5-C4	6.30	121.37	114.28
23	1	314	CLA	C4A-NA-C1A	6.30	109.54	106.71
21	4	305	XAT	C18-C5-C6	-6.29	111.71	122.26
21	8	302	XAT	C11-C10-C9	-6.28	118.34	127.31
21	3	301	XAT	C38-C25-C26	-6.28	111.73	122.26
23	5	305	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	a	802	CLA	C4A-NA-C1A	6.28	109.53	106.71
21	4	303	XAT	C18-C5-C4	6.28	121.34	114.28
31	i	101	BCR	C20-C21-C22	-6.28	118.35	127.31
21	1	303	XAT	C18-C5-C6	-6.27	111.75	122.26
23	5	307	CLA	C4A-NA-C1A	6.27	109.53	106.71
21	3	305	XAT	C18-C5-C6	-6.27	111.75	122.26
21	3	304	XAT	C18-C5-C4	6.27	121.33	114.28
21	4	302	XAT	C38-C25-C26	-6.27	111.76	122.26
21	2	302	XAT	C18-C5-C6	-6.26	111.76	122.26
21	6	306	XAT	C38-C25-C26	-6.26	111.77	122.26
23	b	829	CLA	C4A-NA-C1A	6.26	109.52	106.71
21	8	301	XAT	C18-C5-C6	-6.26	111.77	122.26
21	a	852	XAT	C38-C25-C26	-6.26	111.77	122.26
21	8	303	XAT	C38-C25-C26	-6.25	111.78	122.26
21	4	304	XAT	C38-C25-C26	-6.25	111.79	122.26
21	2	301	XAT	C38-C25-C24	6.25	121.31	114.28
21	1	303	XAT	C38-C25-C26	-6.23	111.81	122.26
23	2	310	CLA	C4A-NA-C1A	6.23	109.51	106.71
23	1	309	CLA	C4A-NA-C1A	6.23	109.51	106.71
21	6	306	XAT	C18-C5-C4	6.22	121.28	114.28
23	a	820	CLA	C4A-NA-C1A	6.22	109.50	106.71
21	4	304	XAT	C18-C5-C4	6.21	121.27	114.28
21	5	301	XAT	C18-C5-C6	-6.21	111.85	122.26
21	3	301	XAT	C38-C25-C24	6.19	121.25	114.28
23	b	811	CLA	C4A-NA-C1A	6.19	109.49	106.71
23	9	315	CLA	C4A-NA-C1A	6.18	109.48	106.71
21	1	303	XAT	C18-C5-C4	6.18	121.23	114.28
23	b	816	CLA	C4A-NA-C1A	6.17	109.48	106.71
23	b	840	CLA	C4A-NA-C1A	6.17	109.48	106.71
21	2	302	XAT	C38-C25-C26	-6.17	111.92	122.26
21	6	306	XAT	C38-C25-C24	6.17	121.22	114.28
21	6	302	XAT	C18-C5-C4	6.15	121.20	114.28
21	5	302	XAT	C38-C25-C24	6.15	121.20	114.28
23	9	309	CLA	C4A-NA-C1A	6.15	109.47	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	305	XAT	C35-C34-C33	-6.14	118.55	127.31
23	b	804	CLA	C4A-NA-C1A	6.14	109.47	106.71
26	9	305	45D	C31-C29-C25	-6.13	118.57	127.31
21	a	852	XAT	C26-C27-C28	-6.10	113.09	125.99
23	6	313	CLA	C4A-NA-C1A	6.09	109.44	106.71
23	b	817	CLA	C4A-NA-C1A	6.09	109.44	106.71
21	2	301	XAT	C31-C30-C29	-6.07	118.64	127.31
21	2	301	XAT	C38-C25-C26	-6.07	112.08	122.26
23	4	313	CLA	C4A-NA-C1A	6.07	109.44	106.71
23	b	837	CLA	C4A-NA-C1A	6.07	109.44	106.71
21	7	304	XAT	C18-C5-C4	6.07	121.10	114.28
23	b	828	CLA	C4A-NA-C1A	6.05	109.43	106.71
21	6	303	XAT	C15-C14-C13	-6.05	118.67	127.31
21	2	305	XAT	C18-C5-C4	6.05	121.08	114.28
21	4	305	XAT	C18-C5-C4	6.03	121.06	114.28
23	8	310	CLA	C4A-NA-C1A	6.01	109.41	106.71
23	2	308	CLA	C4A-NA-C1A	5.99	109.40	106.71
21	2	302	XAT	C18-C5-C4	5.98	121.01	114.28
23	b	802	CLA	C4A-NA-C1A	5.98	109.39	106.71
21	5	304	XAT	C26-C27-C28	-5.94	113.44	125.99
31	b	842	BCR	C7-C8-C9	-5.92	117.28	126.23
21	8	301	XAT	C18-C5-C4	5.91	120.93	114.28
23	b	830	CLA	C4A-NA-C1A	5.91	109.36	106.71
21	7	303	XAT	C18-C5-C4	5.90	120.92	114.28
21	5	302	XAT	C18-C5-C4	5.90	120.92	114.28
21	7	301	XAT	C38-C25-C24	5.90	120.92	114.28
25	8	304	A1L1F	O15-C20-C17	5.89	122.11	115.06
21	8	302	XAT	C18-C5-C4	5.88	120.89	114.28
21	j	101	XAT	C6-C7-C8	-5.86	113.60	125.99
25	h	203	A1L1F	C37-C38-C39	-5.85	118.96	127.31
21	5	301	XAT	C18-C5-C4	5.84	120.85	114.28
31	b	849	BCR	C16-C17-C18	-5.83	118.99	127.31
21	7	301	XAT	C31-C30-C29	-5.82	119.01	127.31
21	7	301	XAT	C38-C25-C26	-5.80	112.55	122.26
21	9	303	XAT	C18-C5-C4	5.79	120.79	114.28
21	2	303	XAT	C18-C5-C4	5.78	120.78	114.28
21	5	302	XAT	C38-C25-C26	-5.77	112.58	122.26
31	a	850	BCR	C20-C21-C22	-5.74	119.12	127.31
21	4	301	XAT	C35-C34-C33	-5.69	119.19	127.31
21	4	301	XAT	C38-C25-C24	5.69	120.68	114.28
21	5	302	XAT	C11-C10-C9	-5.69	119.19	127.31
21	9	304	XAT	C26-C27-C28	-5.64	114.06	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	304	A1L1F	O15-C20-C17	5.64	121.81	115.06
31	b	842	BCR	C11-C10-C9	-5.64	119.27	127.31
31	f	801	BCR	C16-C17-C18	-5.63	119.27	127.31
31	b	844	BCR	C24-C23-C22	-5.62	117.74	126.23
21	6	305	XAT	C18-C5-C6	-5.57	112.92	122.26
21	6	305	XAT	C31-C30-C29	-5.54	119.40	127.31
31	b	844	BCR	C7-C8-C9	-5.53	117.88	126.23
21	7	305	XAT	C15-C14-C13	-5.51	119.44	127.31
21	8	303	XAT	C26-C27-C28	-5.48	114.41	125.99
25	6	301	A1L1F	O15-C20-C17	5.47	121.61	115.06
25	h	203	A1L1F	O15-C20-C17	5.47	121.61	115.06
31	j	104	BCR	C28-C27-C26	-5.47	104.30	114.08
31	b	845	BCR	C16-C17-C18	-5.46	119.51	127.31
21	9	303	XAT	C15-C14-C13	-5.44	119.54	127.31
21	3	301	XAT	C6-C7-C8	-5.43	114.50	125.99
23	a	803	CLA	C4A-NA-C1A	5.43	109.15	106.71
31	f	804	BCR	C15-C14-C13	-5.40	119.60	127.31
21	3	304	XAT	C35-C34-C33	-5.40	119.61	127.31
21	6	306	XAT	C31-C30-C29	-5.39	119.61	127.31
31	f	801	BCR	C20-C21-C22	-5.39	119.61	127.31
21	2	303	XAT	C35-C34-C33	-5.37	119.65	127.31
21	6	302	XAT	C15-C14-C13	-5.36	119.66	127.31
21	2	303	XAT	C31-C30-C29	-5.34	119.70	127.31
21	4	301	XAT	C38-C25-C26	-5.33	113.33	122.26
31	b	844	BCR	C33-C5-C6	-5.33	118.55	124.53
28	b	848	DGD	O2G-C1B-C2B	5.31	122.96	111.50
25	6	301	A1L1F	C36-C37-C38	-5.31	112.60	123.47
21	a	852	XAT	C18-C5-C6	-5.30	113.37	122.26
31	a	849	BCR	C3-C4-C5	-5.30	104.62	114.08
21	4	303	XAT	C26-C27-C28	-5.29	114.80	125.99
31	b	842	BCR	C3-C4-C5	-5.29	104.64	114.08
21	4	305	XAT	C15-C14-C13	-5.28	119.78	127.31
21	2	305	XAT	C31-C30-C29	-5.28	119.78	127.31
31	b	842	BCR	C15-C14-C13	-5.27	119.78	127.31
21	4	304	XAT	C26-C27-C28	-5.26	114.87	125.99
21	2	302	XAT	C35-C34-C33	-5.26	119.80	127.31
21	7	301	XAT	C35-C34-C33	-5.24	119.83	127.31
21	a	852	XAT	C6-C7-C8	-5.24	114.91	125.99
25	8	304	A1L1F	C41-C42-C44	-5.24	119.83	127.31
21	6	302	XAT	C31-C30-C29	-5.22	119.86	127.31
21	a	852	XAT	C18-C5-C4	5.21	120.15	114.28
21	6	306	XAT	C35-C34-C33	-5.21	119.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	l	201	BCR	C7-C8-C9	-5.21	118.36	126.23
21	7	304	XAT	C11-C10-C9	-5.21	119.88	127.31
21	2	301	XAT	C35-C34-C33	-5.21	119.88	127.31
21	2	303	XAT	C11-C10-C9	-5.21	119.88	127.31
21	2	304	XAT	C6-C7-C8	-5.20	114.99	125.99
21	9	303	XAT	C26-C27-C28	-5.20	114.99	125.99
21	j	101	XAT	C26-C27-C28	-5.17	115.06	125.99
25	8	304	A1L1F	O7-C54-C56	5.16	120.58	111.09
31	l	205	BCR	C24-C23-C22	-5.15	118.46	126.23
31	h	201	BCR	C3-C4-C5	-5.14	104.90	114.08
21	8	303	XAT	C15-C14-C13	-5.11	120.02	127.31
21	2	305	XAT	C35-C34-C33	-5.09	120.05	127.31
25	6	304	A1L1F	O15-C20-C17	5.08	121.14	115.06
21	1	302	XAT	C35-C34-C33	-5.07	120.07	127.31
21	8	303	XAT	C6-C7-C8	-5.05	115.32	125.99
21	7	305	XAT	C26-C27-C28	-5.05	115.33	125.99
21	3	305	XAT	C26-C27-C28	-5.04	115.33	125.99
31	a	847	BCR	C16-C17-C18	-5.01	120.15	127.31
31	b	849	BCR	C11-C10-C9	-5.00	120.17	127.31
21	6	302	XAT	C35-C34-C33	-4.99	120.19	127.31
21	5	301	XAT	C26-C27-C28	-4.99	115.45	125.99
21	4	304	XAT	C6-C7-C8	-4.98	115.47	125.99
21	1	302	XAT	C26-C27-C28	-4.96	115.50	125.99
26	9	305	45D	C20-C24-C26	-4.96	118.73	126.23
21	3	305	XAT	C6-C7-C8	-4.94	115.54	125.99
31	a	850	BCR	C16-C17-C18	-4.94	120.26	127.31
31	b	849	BCR	C20-C21-C22	-4.94	120.27	127.31
31	f	804	BCR	C11-C10-C9	-4.93	120.28	127.31
21	1	303	XAT	C6-C7-C8	-4.90	115.62	125.99
21	7	304	XAT	C26-C27-C28	-4.89	115.66	125.99
21	2	301	XAT	C15-C14-C13	-4.89	120.33	127.31
31	a	849	BCR	C16-C17-C18	-4.87	120.35	127.31
21	2	305	XAT	C6-C7-C8	-4.86	115.71	125.99
21	4	303	XAT	C11-C10-C9	-4.86	120.37	127.31
21	2	301	XAT	C6-C7-C8	-4.86	115.71	125.99
21	j	101	XAT	C11-C10-C9	-4.84	120.41	127.31
31	j	104	BCR	C11-C10-C9	-4.84	120.41	127.31
31	l	205	BCR	C15-C14-C13	-4.83	120.41	127.31
21	7	303	XAT	C31-C30-C29	-4.83	120.42	127.31
21	5	302	XAT	C15-C14-C13	-4.81	120.44	127.31
31	b	849	BCR	C38-C26-C25	-4.80	119.13	124.53
21	1	302	XAT	C6-C7-C8	-4.79	115.86	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	304	XAT	C15-C14-C13	-4.79	120.48	127.31
31	i	101	BCR	C16-C17-C18	-4.78	120.49	127.31
23	a	831	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
21	7	301	XAT	C6-C7-C8	-4.76	115.94	125.99
21	4	302	XAT	C26-C27-C28	-4.75	115.95	125.99
31	h	202	BCR	C16-C17-C18	-4.74	120.54	127.31
21	7	304	XAT	C35-C34-C33	-4.74	120.55	127.31
21	8	301	XAT	C26-C27-C28	-4.71	116.04	125.99
23	b	829	CLA	CMB-C2B-C1B	-4.70	121.23	128.46
21	4	302	XAT	C6-C7-C8	-4.69	116.08	125.99
21	7	305	XAT	C6-C7-C8	-4.69	116.08	125.99
21	9	304	XAT	C15-C14-C13	-4.68	120.64	127.31
23	b	817	CLA	CMB-C2B-C1B	-4.67	121.28	128.46
31	b	849	BCR	C7-C8-C9	-4.67	119.18	126.23
21	3	303	XAT	C26-C27-C28	-4.66	116.13	125.99
21	7	304	XAT	C15-C14-C13	-4.66	120.66	127.31
21	3	304	XAT	C6-C7-C8	-4.61	116.26	125.99
21	4	302	XAT	C35-C34-C33	-4.59	120.75	127.31
31	b	843	BCR	C11-C10-C9	-4.59	120.76	127.31
21	7	303	XAT	C11-C10-C9	-4.58	120.77	127.31
21	8	302	XAT	C15-C14-C13	-4.58	120.77	127.31
31	b	846	BCR	C16-C17-C18	-4.57	120.79	127.31
21	7	301	XAT	C27-C28-C29	-4.56	118.45	125.53
21	5	301	XAT	C35-C34-C33	-4.56	120.81	127.31
21	8	302	XAT	C26-C27-C28	-4.56	116.36	125.99
21	2	305	XAT	C15-C14-C13	-4.55	120.81	127.31
25	9	302	A1L1F	O7-C54-C56	4.54	119.45	111.09
25	6	304	A1L1F	O7-C54-C56	4.54	119.44	111.09
21	4	305	XAT	C26-C27-C28	-4.54	116.40	125.99
21	6	306	XAT	C6-C7-C8	-4.52	116.44	125.99
31	b	843	BCR	C7-C8-C9	-4.50	119.43	126.23
21	7	303	XAT	C35-C34-C33	-4.50	120.89	127.31
21	2	302	XAT	C6-C7-C8	-4.50	116.48	125.99
21	3	303	XAT	C6-C7-C8	-4.49	116.49	125.99
21	2	304	XAT	C26-C27-C28	-4.49	116.50	125.99
21	8	302	XAT	C35-C34-C33	-4.49	120.91	127.31
25	h	203	A1L1F	O7-C54-C56	4.48	119.33	111.09
21	3	305	XAT	C35-C34-C33	-4.48	120.92	127.31
21	7	303	XAT	C26-C27-C28	-4.46	116.55	125.99
25	6	301	A1L1F	O7-C54-C56	4.45	119.27	111.09
25	9	302	A1L1F	C36-C35-C34	-4.43	120.98	127.31
23	a	802	CLA	CMB-C2B-C1B	-4.43	121.66	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	848	BCR	C16-C17-C18	-4.42	121.00	127.31
31	a	848	BCR	C15-C14-C13	-4.42	121.00	127.31
28	b	848	DGD	O5D-C6D-C5D	-4.40	100.90	109.05
31	j	104	BCR	C15-C14-C13	-4.39	121.05	127.31
31	a	849	BCR	C15-C14-C13	-4.38	121.06	127.31
31	a	850	BCR	C15-C14-C13	-4.38	121.06	127.31
31	b	844	BCR	C16-C17-C18	-4.37	121.07	127.31
29	2	317	LMG	O7-C10-C11	4.37	120.92	111.50
21	3	303	XAT	C15-C14-C13	-4.37	121.08	127.31
31	b	842	BCR	C16-C17-C18	-4.36	121.08	127.31
28	4	318	DGD	O6E-C5E-C6E	4.36	117.28	106.44
25	h	203	A1L1F	C25-C14-C29	-4.35	116.79	125.99
21	3	303	XAT	C35-C34-C33	-4.33	121.13	127.31
23	b	835	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
21	j	101	XAT	C35-C34-C33	-4.32	121.14	127.31
31	b	846	BCR	C33-C5-C6	-4.32	119.67	124.53
25	6	304	A1L1F	C26-C30-C31	-4.31	119.29	124.93
21	8	301	XAT	C35-C34-C33	-4.31	121.16	127.31
31	j	104	BCR	C16-C17-C18	-4.31	121.16	127.31
21	5	304	XAT	C35-C34-C33	-4.31	121.16	127.31
23	2	307	CLA	CMB-C2B-C1B	-4.31	121.85	128.46
23	6	314	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
21	4	301	XAT	C6-C7-C8	-4.29	116.92	125.99
21	6	302	XAT	C6-C7-C8	-4.29	116.93	125.99
21	6	306	XAT	C15-C14-C13	-4.27	121.21	127.31
26	9	305	45D	C42-C38-C36	-4.27	121.22	127.31
23	a	844	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
21	3	301	XAT	C15-C14-C13	-4.26	121.24	127.31
21	3	304	XAT	C31-C30-C29	-4.25	121.24	127.31
23	4	313	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
23	a	826	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
23	a	833	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
23	b	825	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
30	b	841	PQN	C11-C12-C13	-4.24	119.74	126.79
28	4	318	DGD	O2G-C1B-C2B	4.23	120.63	111.50
25	9	302	A1L1F	C14-C29-C30	-4.23	118.01	125.47
21	9	304	XAT	C18-C5-C4	4.23	119.04	114.28
22	9	301	A1L1G	C37-C36-C35	4.22	132.12	123.47
31	f	804	BCR	C24-C23-C22	-4.22	119.86	126.23
25	h	203	A1L1F	C41-C42-C44	-4.21	121.30	127.31
31	b	843	BCR	C15-C14-C13	-4.21	121.30	127.31
21	4	305	XAT	C35-C34-C33	-4.21	121.30	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	308	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
21	4	304	XAT	C35-C34-C33	-4.21	121.31	127.31
27	a	845	LHG	O7-C7-C8	4.20	120.56	111.50
21	2	305	XAT	C38-C25-C24	4.19	118.99	114.28
23	a	809	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
23	8	305	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
23	8	311	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
23	a	829	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
31	h	202	BCR	C33-C5-C6	-4.19	119.83	124.53
31	b	844	BCR	C15-C14-C13	-4.19	121.34	127.31
21	7	303	XAT	C15-C14-C13	-4.18	121.34	127.31
31	b	845	BCR	C24-C23-C22	-4.18	119.92	126.23
31	h	201	BCR	C16-C17-C18	-4.18	121.34	127.31
21	6	305	XAT	C27-C28-C29	-4.18	119.04	125.53
25	1	304	A1L1F	C37-C38-C39	-4.18	121.34	127.31
23	3	310	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
31	l	201	BCR	C15-C14-C13	-4.18	121.35	127.31
31	j	104	BCR	C7-C8-C9	-4.18	119.93	126.23
25	1	304	A1L1F	O7-C54-C56	4.17	118.77	111.09
31	a	850	BCR	C38-C26-C25	-4.17	119.84	124.53
23	a	820	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
23	6	309	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
23	a	823	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
31	l	205	BCR	C20-C21-C22	-4.16	121.37	127.31
23	6	313	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
31	b	845	BCR	C20-C21-C22	-4.16	121.38	127.31
23	a	806	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
31	l	201	BCR	C33-C5-C6	-4.14	119.88	124.53
21	3	304	XAT	C15-C14-C13	-4.14	121.41	127.31
25	8	304	A1L1F	C41-C40-C39	-4.13	114.81	126.42
23	b	814	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
23	a	816	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
21	7	305	XAT	C11-C10-C9	-4.12	121.44	127.31
25	1	304	A1L1F	C17-C20-C21	4.11	118.91	114.28
23	8	308	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
29	a	853	LMG	O7-C10-C11	4.10	120.35	111.50
25	8	304	A1L1F	C32-C31-C30	-4.10	121.42	127.26
23	b	832	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
31	f	804	BCR	C7-C8-C9	-4.10	120.04	126.23
27	b	847	LHG	O7-C7-C8	4.10	120.34	111.50
23	7	316	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
23	1	307	CLA	CMB-C2B-C1B	-4.09	122.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	801	BCR	C3-C4-C5	-4.08	106.79	114.08
31	a	848	BCR	C11-C10-C9	-4.08	121.49	127.31
31	a	847	BCR	C38-C26-C25	-4.08	119.95	124.53
31	b	845	BCR	C7-C8-C9	-4.08	120.08	126.23
23	a	804	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
21	5	301	XAT	C11-C10-C9	-4.07	121.50	127.31
23	a	803	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
31	b	845	BCR	C16-C15-C14	-4.06	115.15	123.47
31	b	842	BCR	C28-C27-C26	-4.06	106.82	114.08
23	2	308	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
23	5	307	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
23	9	309	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
23	9	316	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
21	4	301	XAT	C15-C14-C13	-4.04	121.55	127.31
23	a	805	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
31	l	205	BCR	C38-C26-C25	-4.02	120.01	124.53
23	b	810	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
21	4	305	XAT	C6-C7-C8	-4.01	117.52	125.99
23	5	311	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
23	7	311	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
23	a	839	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
21	7	303	XAT	C6-C7-C8	-4.00	117.53	125.99
23	b	821	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
23	b	826	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
23	b	807	CLA	CMB-C2B-C1B	-3.99	122.32	128.46
23	b	806	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
31	b	845	BCR	C15-C14-C13	-3.98	121.64	127.31
25	8	304	A1L1F	C37-C36-C35	-3.98	115.33	123.47
25	6	301	A1L1F	C37-C38-C39	-3.97	121.64	127.31
21	3	301	XAT	C35-C34-C33	-3.97	121.64	127.31
26	9	305	45D	C32-C30-C26	-3.97	121.64	127.31
27	a	846	LHG	O7-C7-C8	3.97	120.06	111.50
23	8	310	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
23	4	308	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
23	8	307	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
31	b	845	BCR	C28-C27-C26	-3.97	106.99	114.08
31	f	804	BCR	C33-C5-C6	-3.97	120.07	124.53
21	4	305	XAT	C11-C10-C9	-3.96	121.66	127.31
25	6	301	A1L1F	C8-O7-C54	-3.96	110.52	117.90
27	9	317	LHG	O7-C7-C8	3.96	120.03	111.50
29	j	105	LMG	O7-C10-C11	3.95	120.02	111.50
23	a	838	CLA	CMB-C2B-C1B	-3.95	122.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	303	XAT	C26-C27-C28	-3.95	117.64	125.99
21	a	852	XAT	C31-C30-C29	-3.95	121.68	127.31
25	6	304	A1L1F	C36-C35-C34	-3.94	121.68	127.31
23	1	308	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
23	9	312	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
21	9	304	XAT	C18-C5-C6	-3.94	115.66	122.26
23	b	831	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
23	b	816	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
21	2	302	XAT	C31-C30-C29	-3.93	121.70	127.31
23	8	312	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
21	1	303	XAT	C26-C27-C28	-3.93	117.69	125.99
31	l	201	BCR	C11-C10-C9	-3.93	121.71	127.31
31	f	804	BCR	C38-C26-C25	-3.92	120.12	124.53
25	6	304	A1L1F	C37-C38-C39	-3.92	121.71	127.31
21	4	303	XAT	C15-C14-C13	-3.92	121.72	127.31
23	b	802	CLA	CMB-C2B-C1B	-3.92	122.45	128.46
23	4	309	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	a	822	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	7	313	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	b	804	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
23	3	309	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
21	2	305	XAT	C27-C28-C29	-3.90	119.47	125.53
31	i	101	BCR	C7-C8-C9	-3.90	120.34	126.23
23	2	310	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	f	802	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	b	813	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
21	2	302	XAT	C15-C14-C13	-3.90	121.75	127.31
23	9	314	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
23	5	312	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
21	2	303	XAT	C15-C14-C13	-3.88	121.77	127.31
23	a	815	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
23	l	202	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
21	2	302	XAT	C26-C27-C28	-3.86	117.83	125.99
21	j	101	XAT	C15-C14-C13	-3.86	121.81	127.31
25	6	304	A1L1F	C17-C20-C21	3.85	118.61	114.28
31	a	847	BCR	C20-C21-C22	-3.85	121.82	127.31
23	a	827	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
23	2	312	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
23	b	815	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
28	8	315	DGD	O2G-C1B-C2B	3.84	119.79	111.50
22	3	306	A1L1G	C36-C37-C38	3.84	131.35	123.47
31	f	804	BCR	C20-C21-C22	-3.84	121.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	817	CLA	CMB-C2B-C3B	3.84	131.86	124.68
21	7	301	XAT	C15-C14-C13	-3.83	121.84	127.31
31	l	201	BCR	C16-C17-C18	-3.83	121.84	127.31
23	6	317	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
23	a	811	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
23	b	805	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
23	5	314	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
23	l	203	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
22	1	301	A1L1G	C37-C36-C35	3.82	131.30	123.47
23	1	306	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
31	l	205	BCR	C33-C5-C6	-3.81	120.25	124.53
31	b	846	BCR	C15-C14-C13	-3.81	121.87	127.31
31	l	205	BCR	C16-C17-C18	-3.81	121.88	127.31
23	2	313	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
23	b	824	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
31	a	849	BCR	C28-C27-C26	-3.80	107.30	114.08
23	7	310	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
31	f	804	BCR	C16-C17-C18	-3.79	121.90	127.31
25	h	203	A1L1F	C36-C35-C34	-3.79	121.91	127.31
21	6	306	XAT	C27-C28-C29	-3.79	119.66	125.53
26	9	305	45D	C41-C37-C35	-3.78	121.91	127.31
23	7	312	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
23	b	827	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
23	a	814	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
31	f	801	BCR	C16-C15-C14	-3.77	115.76	123.47
21	5	301	XAT	C15-C14-C13	-3.76	121.94	127.31
23	9	315	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
24	1	315	SQD	O47-C7-C8	3.76	119.60	111.50
23	a	812	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
31	j	104	BCR	C20-C21-C22	-3.75	121.95	127.31
23	5	315	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
23	1	310	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
22	5	303	A1L1G	C36-C37-C38	3.75	131.16	123.47
23	a	806	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
25	9	302	A1L1F	O15-C20-C17	3.74	119.54	115.06
23	2	309	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
23	b	830	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
21	8	301	XAT	C15-C14-C13	-3.73	121.98	127.31
23	9	310	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
23	9	308	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
21	2	303	XAT	C26-C27-C28	-3.73	118.11	125.99
21	1	303	XAT	C35-C34-C33	-3.73	121.99	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	850	BCR	C33-C5-C6	-3.73	120.34	124.53
23	1	311	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
23	a	837	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
23	a	803	CLA	CMB-C2B-C3B	3.72	131.64	124.68
23	7	306	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
31	h	201	BCR	C15-C14-C13	-3.71	122.01	127.31
23	3	313	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
23	3	311	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
23	a	830	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
31	b	843	BCR	C3-C4-C5	-3.70	107.47	114.08
22	9	306	A1L1G	C37-C36-C35	3.69	131.04	123.47
23	7	309	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
23	b	804	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
21	a	852	XAT	C35-C34-C33	-3.69	122.04	127.31
23	a	826	CLA	CMB-C2B-C3B	3.69	131.58	124.68
21	3	301	XAT	C31-C30-C29	-3.69	122.04	127.31
21	3	301	XAT	C26-C27-C28	-3.69	118.19	125.99
23	b	834	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
23	h	204	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
31	a	849	BCR	C20-C21-C22	-3.68	122.06	127.31
23	a	828	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
21	2	301	XAT	C27-C28-C29	-3.67	119.83	125.53
23	b	820	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	6	301	A1L1F	C42-C41-C40	-3.67	111.77	123.22
21	7	304	XAT	C6-C7-C8	-3.67	118.24	125.99
21	2	303	XAT	C6-C7-C8	-3.66	118.26	125.99
22	7	302	A1L1G	C37-C36-C35	3.65	130.95	123.47
23	b	835	CLA	CMB-C2B-C3B	3.65	131.51	124.68
21	8	301	XAT	C11-C10-C9	-3.65	122.11	127.31
23	a	821	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
23	b	838	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
31	b	845	BCR	C3-C4-C5	-3.64	107.57	114.08
21	6	302	XAT	C26-C27-C28	-3.64	118.29	125.99
23	a	802	CLA	CMB-C2B-C3B	3.64	131.49	124.68
23	5	309	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
25	9	302	A1L1F	C32-C31-C30	-3.63	122.09	127.26
31	a	847	BCR	C33-C5-C6	-3.63	120.45	124.53
23	6	308	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
23	b	828	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
23	a	829	CLA	CMB-C2B-C3B	3.62	131.44	124.68
21	4	302	XAT	C35-C15-C14	-3.61	116.07	123.47
23	b	836	CLA	CMB-C2B-C1B	-3.61	122.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	310	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
21	8	301	XAT	C6-C7-C8	-3.60	118.37	125.99
31	h	202	BCR	C7-C8-C9	-3.59	120.81	126.23
23	b	811	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	8	309	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
23	b	812	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
23	b	822	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
23	2	307	CLA	CMB-C2B-C3B	3.58	131.38	124.68
21	1	302	XAT	C11-C10-C9	-3.58	122.20	127.31
23	a	809	CLA	CMB-C2B-C3B	3.57	131.37	124.68
23	4	310	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
23	b	811	CLA	CAB-C3B-C4B	-3.57	122.97	128.46
23	6	314	CLA	CMB-C2B-C3B	3.57	131.36	124.68
31	a	849	BCR	C11-C10-C9	-3.57	122.22	127.31
31	l	205	BCR	C3-C4-C5	-3.57	107.70	114.08
23	a	808	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
23	l	204	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
25	6	304	A1L1F	C32-C31-C30	-3.56	122.18	127.26
23	8	306	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
22	9	301	A1L1G	C27-C34-C35	-3.56	117.94	122.92
23	b	808	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
21	6	305	XAT	C15-C14-C13	-3.55	122.24	127.31
23	a	844	CLA	CMB-C2B-C3B	3.55	131.33	124.68
21	8	303	XAT	C15-C35-C34	-3.55	116.20	123.47
23	b	833	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
23	7	308	CLA	CMB-C2B-C3B	3.55	131.32	124.68
31	b	843	BCR	C33-C5-C6	-3.55	120.55	124.53
21	6	305	XAT	C11-C10-C9	-3.55	122.25	127.31
23	a	833	CLA	CMB-C2B-C3B	3.54	131.31	124.68
31	i	101	BCR	C33-C5-C6	-3.54	120.55	124.53
23	a	835	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
31	a	847	BCR	C7-C8-C9	-3.54	120.89	126.23
23	b	832	CLA	CMB-C2B-C3B	3.53	131.29	124.68
26	9	305	45D	C05-C09-C17	-3.53	106.53	112.85
31	l	205	BCR	C11-C10-C9	-3.53	122.27	127.31
23	b	804	CLA	CHB-C4A-NA	3.53	129.39	124.51
23	8	305	CLA	CMB-C2B-C3B	3.53	131.28	124.68
23	8	311	CLA	CMB-C2B-C3B	3.53	131.28	124.68
23	b	818	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
21	9	303	XAT	C11-C10-C9	-3.52	122.28	127.31
22	9	301	A1L1G	C36-C37-C38	3.52	130.69	123.47
23	a	832	CLA	CMB-C2B-C1B	-3.52	123.05	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	303	XAT	C35-C34-C33	-3.52	122.29	127.31
23	a	813	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
23	b	825	CLA	CMB-C2B-C3B	3.52	131.26	124.68
23	4	313	CLA	CMB-C2B-C3B	3.52	131.26	124.68
22	9	306	A1L1G	C36-C37-C38	3.52	130.68	123.47
23	a	806	CLA	CAA-CBA-CGA	-3.52	102.98	113.25
23	a	842	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
31	h	202	BCR	C38-C26-C25	-3.51	120.58	124.53
31	a	847	BCR	C15-C14-C13	-3.51	122.30	127.31
23	9	316	CLA	CMB-C2B-C3B	3.51	131.24	124.68
31	h	201	BCR	C24-C23-C22	-3.51	120.94	126.23
24	5	316	SQD	O47-C7-C8	3.51	119.06	111.50
31	a	849	BCR	C4-C5-C6	-3.50	117.64	122.73
23	1	305	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	5	303	A1L1G	C28-C39-C38	-3.50	118.02	122.92
23	4	314	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
23	1	312	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
21	4	302	XAT	C11-C10-C9	-3.50	122.32	127.31
23	a	823	CLA	CMB-C2B-C3B	3.50	131.22	124.68
21	6	303	XAT	C7-C8-C9	-3.50	120.11	125.53
21	8	302	XAT	C31-C30-C29	-3.49	122.32	127.31
23	b	814	CLA	CMB-C2B-C3B	3.49	131.21	124.68
21	6	303	XAT	C35-C34-C33	-3.49	122.33	127.31
23	3	310	CLA	CMB-C2B-C3B	3.49	131.20	124.68
31	a	848	BCR	C24-C23-C22	-3.49	120.97	126.23
23	5	305	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	b	802	CLA	CMB-C2B-C3B	3.48	131.20	124.68
23	5	313	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	7	302	A1L1G	C36-C37-C38	3.48	130.60	123.47
23	b	809	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
21	1	303	XAT	C15-C14-C13	-3.47	122.35	127.31
21	9	303	XAT	C35-C34-C33	-3.47	122.35	127.31
23	9	313	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
22	7	302	A1L1G	C27-C34-C35	-3.47	118.07	122.92
22	3	302	A1L1G	C36-C37-C38	3.47	130.58	123.47
23	3	314	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
23	2	308	CLA	CMB-C2B-C3B	3.46	131.16	124.68
23	6	309	CLA	CMB-C2B-C3B	3.46	131.16	124.68
23	4	317	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	3	307	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	a	831	CLA	CMB-C2B-C3B	3.46	131.16	124.68
31	i	101	BCR	C28-C27-C26	-3.46	107.89	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	306	A1L1G	C28-C39-C38	-3.46	118.07	122.92
23	4	315	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
31	a	849	BCR	C7-C8-C9	-3.46	121.01	126.23
23	5	306	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
21	6	303	XAT	C31-C30-C29	-3.45	122.39	127.31
21	7	304	XAT	C31-C30-C29	-3.45	122.39	127.31
23	7	316	CLA	CMB-C2B-C3B	3.45	131.13	124.68
23	a	806	CLA	CMB-C2B-C3B	3.45	131.13	124.68
23	a	807	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
23	9	314	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
23	a	818	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
23	8	308	CLA	CMB-C2B-C3B	3.44	131.12	124.68
22	1	301	A1L1G	C28-C39-C38	-3.44	118.10	122.92
23	9	318	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
22	9	306	A1L1G	C27-C34-C35	-3.44	118.10	122.92
23	5	308	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
23	a	805	CLA	CMB-C2B-C3B	3.44	131.12	124.68
21	3	303	XAT	C11-C10-C9	-3.44	122.40	127.31
31	a	848	BCR	C20-C21-C22	-3.44	122.40	127.31
23	b	819	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	3	302	A1L1G	C37-C36-C35	3.44	130.52	123.47
23	4	306	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
21	2	304	XAT	C31-C30-C29	-3.44	122.41	127.31
23	4	316	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
23	6	307	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
23	a	816	CLA	CMB-C2B-C3B	3.44	131.10	124.68
23	2	314	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
27	a	846	LHG	O8-C23-C24	3.43	120.39	111.38
23	b	826	CLA	CMB-C2B-C3B	3.43	131.10	124.68
22	9	301	A1L1G	C28-C39-C38	-3.43	118.12	122.92
23	3	308	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	6	313	CLA	CMB-C2B-C3B	3.43	131.09	124.68
23	a	817	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	a	819	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	a	841	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
23	b	823	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
22	3	302	A1L1G	C28-C39-C38	-3.43	118.12	122.92
23	b	837	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
21	2	305	XAT	C24-C23-C22	-3.42	104.16	110.77
22	1	301	A1L1G	C27-C34-C35	-3.42	118.13	122.92
23	8	313	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
23	9	312	CLA	CAA-C2A-C3A	-3.42	103.42	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	102	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
21	2	304	XAT	C11-C10-C9	-3.42	122.43	127.31
23	2	306	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
31	a	847	BCR	C24-C23-C22	-3.42	121.07	126.23
23	1	313	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
23	1	309	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
31	a	847	BCR	C11-C10-C9	-3.41	122.44	127.31
23	8	314	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
22	7	302	A1L1G	C28-C39-C38	-3.41	118.14	122.92
23	7	317	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
21	3	305	XAT	C15-C14-C13	-3.41	122.44	127.31
23	f	803	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
21	5	302	XAT	C6-C7-C8	-3.41	118.79	125.99
23	a	820	CLA	CMB-C2B-C3B	3.40	131.05	124.68
23	3	315	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
23	6	312	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
23	9	312	CLA	CMB-C2B-C3B	3.40	131.04	124.68
21	9	304	XAT	C35-C34-C33	-3.40	122.46	127.31
23	6	311	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
22	3	306	A1L1G	C27-C34-C35	-3.40	118.17	122.92
23	2	311	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	1	307	CLA	CMB-C2B-C3B	3.39	131.03	124.68
23	4	307	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	a	804	CLA	CMB-C2B-C3B	3.39	131.02	124.68
23	a	825	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
23	a	810	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
23	a	840	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
25	9	302	A1L1F	C37-C38-C39	-3.39	122.48	127.31
23	b	807	CLA	CMB-C2B-C3B	3.38	131.01	124.68
25	1	304	A1L1F	C8-O7-C54	-3.38	111.59	117.90
21	5	301	XAT	C7-C8-C9	-3.38	120.28	125.53
23	4	308	CLA	CMB-C2B-C3B	3.38	131.01	124.68
23	a	854	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
23	1	314	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
23	4	312	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	3	302	A1L1G	C27-C34-C35	-3.38	118.19	122.92
23	6	316	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
23	b	831	CLA	CMB-C2B-C3B	3.37	130.99	124.68
22	9	301	A1L1G	C33-C34-C35	3.37	124.12	118.94
23	b	806	CLA	CMB-C2B-C3B	3.37	130.98	124.68
23	7	314	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
27	9	307	LHG	O7-C7-C8	3.36	120.18	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	307	CLA	CMB-C2B-C3B	3.36	130.97	124.68
31	a	849	BCR	C24-C23-C22	-3.36	121.15	126.23
23	2	315	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
23	7	315	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
23	b	821	CLA	CMB-C2B-C3B	3.36	130.97	124.68
22	5	303	A1L1G	C37-C36-C35	3.36	130.36	123.47
23	j	103	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
31	h	202	BCR	C11-C10-C9	-3.36	122.51	127.31
23	7	307	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
21	8	303	XAT	C30-C31-C32	-3.36	112.74	123.22
23	5	311	CLA	CMB-C2B-C3B	3.36	130.96	124.68
23	b	829	CLA	CMB-C2B-C3B	3.35	130.95	124.68
23	b	804	CLA	CMB-C2B-C3B	3.35	130.95	124.68
21	j	101	XAT	C10-C11-C12	-3.35	112.77	123.22
23	2	316	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
21	5	301	XAT	C6-C7-C8	-3.35	118.92	125.99
21	1	303	XAT	C24-C23-C22	-3.35	104.31	110.77
23	8	307	CLA	CMB-C2B-C3B	3.35	130.94	124.68
22	3	306	A1L1G	C28-C39-C38	-3.34	118.24	122.92
23	9	311	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
31	a	847	BCR	C3-C4-C5	-3.34	108.11	114.08
31	b	845	BCR	C10-C11-C12	-3.34	112.80	123.22
23	a	824	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	8	304	A1L1F	C31-C32-C33	-3.34	112.80	123.22
23	a	838	CLA	CMB-C2B-C3B	3.33	130.92	124.68
22	5	303	A1L1G	C27-C34-C35	-3.33	118.26	122.92
23	a	839	CLA	CMB-C2B-C3B	3.32	130.89	124.68
23	4	311	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
23	b	813	CLA	CMB-C2B-C3B	3.32	130.89	124.68
23	a	834	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
31	i	101	BCR	C15-C14-C13	-3.32	122.58	127.31
25	6	304	A1L1F	C14-C29-C30	-3.32	119.62	125.47
23	3	309	CLA	CMB-C2B-C3B	3.32	130.88	124.68
23	6	315	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
23	7	313	CLA	CMB-C2B-C3B	3.32	130.88	124.68
21	1	303	XAT	C31-C30-C29	-3.31	122.58	127.31
21	4	303	XAT	C6-C7-C8	-3.31	119.00	125.99
23	a	827	CLA	CMB-C2B-C3B	3.31	130.87	124.68
23	f	802	CLA	CMB-C2B-C3B	3.31	130.87	124.68
23	b	801	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
21	4	301	XAT	C11-C10-C9	-3.31	122.59	127.31
21	6	303	XAT	C11-C10-C9	-3.31	122.59	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	308	CLA	CMB-C2B-C3B	3.31	130.86	124.68
23	5	310	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	9	302	A1L1F	C25-C14-C29	-3.30	119.01	125.99
23	5	312	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
23	9	311	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
30	a	843	PQN	C14-C13-C15	3.30	120.82	115.27
23	4	309	CLA	CMB-C2B-C3B	3.30	130.84	124.68
22	1	301	A1L1G	C36-C37-C38	3.30	130.22	123.47
25	8	304	A1L1F	C14-C29-C30	-3.29	119.66	125.47
23	b	840	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
23	9	309	CLA	CMB-C2B-C3B	3.29	130.84	124.68
23	3	312	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
28	b	848	DGD	C2G-O2G-C1B	-3.29	109.70	117.79
23	b	816	CLA	CMB-C2B-C3B	3.29	130.83	124.68
21	6	305	XAT	C7-C8-C9	-3.28	120.43	125.53
22	1	301	A1L1G	C43-C44-C42	-3.27	118.34	122.92
31	j	104	BCR	C24-C23-C22	-3.27	121.30	126.23
23	6	317	CLA	CMB-C2B-C3B	3.26	130.79	124.68
21	5	304	XAT	C24-C23-C22	-3.26	104.47	110.77
23	8	312	CLA	CMB-C2B-C3B	3.26	130.78	124.68
23	5	314	CLA	CMB-C2B-C3B	3.26	130.78	124.68
25	h	203	A1L1F	C17-C20-C21	3.26	117.95	114.28
23	7	311	CLA	CMB-C2B-C3B	3.26	130.77	124.68
23	9	314	CLA	CMB-C2B-C3B	3.25	130.76	124.68
23	j	103	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
25	6	301	A1L1F	C25-C14-C29	-3.24	119.14	125.99
21	5	304	XAT	C4-C3-C2	-3.24	104.52	110.77
25	h	203	A1L1F	C31-C32-C33	-3.24	113.11	123.22
31	i	101	BCR	C11-C10-C9	-3.24	122.69	127.31
21	4	304	XAT	C15-C14-C13	-3.23	122.69	127.31
21	5	301	XAT	C24-C23-C22	-3.23	104.53	110.77
25	8	304	A1L1F	C26-C30-C31	-3.23	120.70	124.93
22	9	306	A1L1G	C33-C34-C35	3.23	123.90	118.94
23	2	312	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	a	815	CLA	CMB-C2B-C3B	3.23	130.71	124.68
21	3	304	XAT	C26-C27-C28	-3.22	119.17	125.99
22	5	303	A1L1G	C40-C39-C38	3.22	123.89	118.94
31	a	850	BCR	C7-C8-C9	-3.22	121.37	126.23
31	l	201	BCR	C38-C26-C25	-3.22	120.91	124.53
23	a	822	CLA	CMB-C2B-C3B	3.22	130.70	124.68
21	a	852	XAT	C10-C11-C12	-3.21	113.18	123.22
21	9	304	XAT	C11-C10-C9	-3.21	122.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	852	XAT	C11-C10-C9	-3.21	122.73	127.31
25	1	304	A1L1F	C14-C29-C30	-3.21	119.81	125.47
31	h	201	BCR	C20-C21-C22	-3.21	122.73	127.31
23	b	805	CLA	CMB-C2B-C3B	3.21	130.68	124.68
23	b	809	CLA	O2A-CGA-O1A	-3.21	115.49	123.59
23	b	820	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	5	312	CLA	CMB-C2B-C3B	3.21	130.68	124.68
22	1	301	A1L1G	C33-C34-C35	3.21	123.86	118.94
23	b	827	CLA	CMB-C2B-C3B	3.20	130.67	124.68
23	b	824	CLA	CMB-C2B-C3B	3.20	130.67	124.68
23	a	836	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
23	b	815	CLA	CMB-C2B-C3B	3.20	130.66	124.68
21	1	302	XAT	C15-C14-C13	-3.20	122.74	127.31
23	8	310	CLA	CMB-C2B-C3B	3.20	130.66	124.68
25	h	203	A1L1F	C37-C36-C35	-3.20	116.93	123.47
23	a	814	CLA	CMB-C2B-C3B	3.20	130.66	124.68
21	6	303	XAT	C24-C23-C22	-3.19	104.60	110.77
23	2	313	CLA	CMB-C2B-C3B	3.19	130.65	124.68
23	9	315	CLA	CMB-C2B-C3B	3.19	130.65	124.68
31	a	848	BCR	C33-C5-C6	-3.19	120.94	124.53
23	a	828	CLA	CMB-C2B-C3B	3.19	130.64	124.68
31	b	849	BCR	C24-C23-C22	-3.19	121.42	126.23
23	1	306	CLA	CMB-C2B-C3B	3.18	130.64	124.68
23	b	810	CLA	CMB-C2B-C3B	3.18	130.63	124.68
21	2	301	XAT	C11-C10-C9	-3.18	122.77	127.31
25	6	301	A1L1F	C26-C30-C31	-3.18	120.77	124.93
23	a	835	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
23	5	315	CLA	CMB-C2B-C3B	3.17	130.61	124.68
23	a	812	CLA	CMB-C2B-C3B	3.17	130.61	124.68
31	a	848	BCR	C3-C4-C5	-3.17	108.42	114.08
26	9	305	45D	C09-C05-C03	-3.17	108.09	113.18
22	1	301	A1L1G	C40-C39-C38	3.17	123.80	118.94
23	1	202	CLA	CMB-C2B-C3B	3.17	130.60	124.68
31	a	850	BCR	C11-C10-C9	-3.17	122.79	127.31
26	9	305	45D	C22-C16-C18	3.16	120.18	115.48
31	1	201	BCR	C24-C23-C22	-3.16	121.45	126.23
22	3	306	A1L1G	C37-C36-C35	3.16	129.96	123.47
23	a	811	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	1	313	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	a	804	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
23	2	309	CLA	CMB-C2B-C3B	3.15	130.57	124.68
31	b	843	BCR	C16-C17-C18	-3.15	122.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	839	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
21	9	303	XAT	C6-C7-C8	-3.15	119.33	125.99
31	a	848	BCR	C38-C26-C25	-3.15	120.99	124.53
23	9	308	CLA	CMB-C2B-C3B	3.15	130.56	124.68
23	1	310	CLA	CMB-C2B-C3B	3.15	130.56	124.68
21	3	303	XAT	C24-C23-C22	-3.15	104.70	110.77
21	9	303	XAT	C24-C23-C22	-3.14	104.70	110.77
31	b	846	BCR	C10-C11-C12	-3.14	113.41	123.22
22	3	302	A1L1G	C33-C34-C35	3.14	123.76	118.94
21	4	303	XAT	C24-C23-C22	-3.14	104.71	110.77
21	7	305	XAT	C35-C34-C33	-3.14	122.83	127.31
23	1	311	CLA	CMB-C2B-C3B	3.14	130.55	124.68
21	9	304	XAT	C24-C23-C22	-3.14	104.71	110.77
23	7	316	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
23	a	830	CLA	CMB-C2B-C3B	3.14	130.55	124.68
31	a	849	BCR	C38-C26-C25	-3.14	121.01	124.53
23	9	310	CLA	CMB-C2B-C3B	3.14	130.55	124.68
23	7	310	CLA	CMB-C2B-C3B	3.13	130.54	124.68
22	9	306	A1L1G	C40-C39-C38	3.13	123.75	118.94
21	4	304	XAT	C24-C23-C22	-3.13	104.72	110.77
21	6	303	XAT	C6-C7-C8	-3.13	119.38	125.99
23	5	309	CLA	CMB-C2B-C3B	3.12	130.52	124.68
23	a	803	CLA	C1B-CHB-C4A	-3.12	123.93	130.12
21	3	304	XAT	C11-C10-C9	-3.12	122.86	127.31
23	a	818	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
21	2	301	XAT	C26-C27-C28	-3.12	119.40	125.99
31	b	849	BCR	C33-C5-C6	-3.12	121.03	124.53
23	7	312	CLA	CMB-C2B-C3B	3.12	130.51	124.68
21	8	301	XAT	C24-C23-C22	-3.11	104.76	110.77
31	a	849	BCR	C33-C5-C4	3.11	119.59	113.62
31	h	201	BCR	C33-C5-C4	3.11	119.59	113.62
28	4	318	DGD	O1G-C1A-C2A	3.11	121.66	111.91
23	b	832	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
23	h	204	CLA	CMB-C2B-C3B	3.10	130.49	124.68
23	7	306	CLA	CMB-C2B-C3B	3.10	130.47	124.68
23	a	837	CLA	CMB-C2B-C3B	3.09	130.47	124.68
22	7	302	A1L1G	C40-C39-C38	3.09	123.69	118.94
23	b	820	CLA	CMB-C2B-C3B	3.09	130.46	124.68
25	8	304	A1L1F	C36-C35-C34	-3.09	122.90	127.31
31	h	201	BCR	C38-C26-C25	-3.09	121.06	124.53
23	3	313	CLA	CMB-C2B-C3B	3.09	130.45	124.68
22	9	301	A1L1G	C40-C39-C38	3.09	123.67	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	316	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
23	1	203	CLA	CMB-C2B-C3B	3.08	130.44	124.68
22	3	306	A1L1G	C40-C39-C38	3.08	123.66	118.94
21	5	301	XAT	C31-C30-C29	-3.07	122.92	127.31
23	a	821	CLA	CMB-C2B-C3B	3.07	130.43	124.68
23	3	311	CLA	CMB-C2B-C3B	3.07	130.43	124.68
21	4	304	XAT	C35-C15-C14	-3.07	117.18	123.47
23	2	310	CLA	CMB-C2B-C3B	3.07	130.43	124.68
22	9	306	A1L1G	C43-C44-C42	-3.07	118.62	122.92
21	7	304	XAT	C24-C23-C22	-3.07	104.85	110.77
23	b	802	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
22	7	302	A1L1G	C33-C34-C35	3.07	123.64	118.94
23	4	311	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	b	830	CLA	CMB-C2B-C3B	3.06	130.41	124.68
21	a	852	XAT	C35-C15-C14	-3.06	117.20	123.47
31	b	842	BCR	C20-C21-C22	-3.06	122.94	127.31
21	2	303	XAT	C19-C9-C10	-3.06	118.64	122.92
23	3	308	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
31	b	845	BCR	C11-C10-C9	-3.06	122.95	127.31
23	b	809	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	9	302	A1L1F	C42-C41-C40	-3.06	113.68	123.22
23	b	812	CLA	CMB-C2B-C3B	3.05	130.39	124.68
23	7	309	CLA	CMB-C2B-C3B	3.05	130.39	124.68
25	8	304	A1L1F	C25-C14-C29	-3.05	119.54	125.99
23	a	801	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
21	1	302	XAT	C31-C30-C29	-3.05	122.96	127.31
31	1	205	BCR	C8-C7-C6	-3.05	118.64	127.20
28	8	315	DGD	O1G-C1A-C2A	3.05	121.47	111.91
21	a	852	XAT	C31-C32-C33	-3.04	117.87	126.42
22	7	302	A1L1G	C43-C44-C42	-3.04	118.66	122.92
25	h	203	A1L1F	C12-C6-C1	-3.04	107.75	110.47
23	8	308	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
23	7	314	CLA	CHB-C4A-NA	3.04	128.71	124.51
23	a	809	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
31	a	848	BCR	C8-C7-C6	-3.03	118.68	127.20
21	6	306	XAT	C26-C27-C28	-3.03	119.58	125.99
21	6	306	XAT	C11-C10-C9	-3.03	122.98	127.31
23	4	307	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	6	308	CLA	CMB-C2B-C3B	3.03	130.34	124.68
21	3	304	XAT	C4-C3-C2	-3.02	104.93	110.77
23	a	835	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	3	306	A1L1G	C43-C44-C42	-3.02	118.69	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	801	BCR	C8-C7-C6	-3.02	118.72	127.20
23	b	836	CLA	CMB-C2B-C3B	3.02	130.33	124.68
23	b	808	CLA	CMB-C2B-C3B	3.02	130.32	124.68
23	b	834	CLA	CMB-C2B-C3B	3.02	130.32	124.68
23	a	831	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
23	b	822	CLA	CMB-C2B-C3B	3.01	130.31	124.68
23	b	838	CLA	CMB-C2B-C3B	3.01	130.31	124.68
23	b	816	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
21	8	302	XAT	C24-C23-C22	-3.01	104.97	110.77
21	4	305	XAT	C24-C23-C22	-3.01	104.97	110.77
23	9	313	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
21	6	305	XAT	C35-C15-C14	-3.01	117.32	123.47
23	4	309	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
22	5	303	A1L1G	C33-C34-C35	3.00	123.55	118.94
31	h	202	BCR	C16-C15-C14	-3.00	117.33	123.47
23	b	808	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
31	h	202	BCR	C15-C14-C13	-3.00	123.03	127.31
23	b	833	CLA	CMB-C2B-C3B	3.00	130.28	124.68
23	l	204	CLA	CMB-C2B-C3B	2.99	130.28	124.68
23	8	309	CLA	CMB-C2B-C3B	2.99	130.28	124.68
23	6	310	CLA	CMB-C2B-C3B	2.99	130.28	124.68
28	b	848	DGD	O3E-C3E-C2E	-2.99	103.43	110.35
23	9	310	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
21	3	305	XAT	C4-C3-C2	-2.99	105.00	110.77
21	8	303	XAT	C24-C23-C22	-2.99	105.00	110.77
23	b	836	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
21	6	305	XAT	C24-C23-C22	-2.99	105.01	110.77
22	3	302	A1L1G	C40-C39-C38	2.98	123.52	118.94
23	b	811	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
23	a	807	CLA	CMB-C2B-C3B	2.98	130.26	124.68
21	7	305	XAT	C4-C3-C2	-2.98	105.01	110.77
23	a	830	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	1	314	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	b	814	CLA	CHB-C4A-NA	2.98	128.63	124.51
22	3	306	A1L1G	C33-C34-C35	2.98	123.51	118.94
21	8	302	XAT	C6-C7-C8	-2.98	119.70	125.99
23	b	803	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
31	b	843	BCR	C38-C26-C25	-2.97	121.20	124.53
25	6	301	A1L1F	C17-C20-C21	2.96	117.61	114.28
23	b	839	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	a	839	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
31	b	846	BCR	C8-C7-C6	-2.96	118.90	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	850	BCR	C28-C27-C26	-2.96	108.80	114.08
23	6	307	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	b	829	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
23	b	834	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
23	4	310	CLA	CMB-C2B-C3B	2.95	130.20	124.68
25	9	302	A1L1F	C26-C30-C31	-2.95	121.07	124.93
23	6	309	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
21	6	302	XAT	C24-C23-C22	-2.95	105.08	110.77
23	a	808	CLA	CMB-C2B-C3B	2.95	130.20	124.68
23	5	308	CLA	CMB-C2B-C3B	2.95	130.19	124.68
23	3	309	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	7	313	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	b	824	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	b	814	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
23	2	313	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	6	317	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	a	812	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
21	4	301	XAT	C31-C32-C33	-2.94	118.15	126.42
21	3	305	XAT	C31-C30-C29	-2.94	123.11	127.31
23	3	307	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	h	201	BCR	C8-C7-C6	-2.94	118.94	127.20
23	b	818	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
21	6	302	XAT	C11-C12-C13	-2.94	118.16	126.42
21	1	302	XAT	C35-C15-C14	-2.94	117.46	123.47
23	8	306	CLA	CMB-C2B-C3B	2.94	130.17	124.68
23	1	311	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
23	9	314	CLA	O2D-CGD-CBD	2.93	116.48	111.27
21	4	304	XAT	C4-C3-C2	-2.93	105.11	110.77
23	9	313	CLA	CMB-C2B-C3B	2.93	130.17	124.68
21	7	305	XAT	C24-C23-C22	-2.93	105.11	110.77
23	b	818	CLA	CMB-C2B-C3B	2.93	130.16	124.68
31	b	849	BCR	C16-C15-C14	-2.93	117.47	123.47
21	8	303	XAT	C4-C3-C2	-2.93	105.12	110.77
21	3	305	XAT	C24-C23-C22	-2.93	105.12	110.77
23	a	832	CLA	CMB-C2B-C3B	2.93	130.16	124.68
23	2	309	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
21	7	303	XAT	C19-C9-C10	-2.93	118.83	122.92
23	7	308	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
23	a	840	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
21	3	301	XAT	C4-C3-C2	-2.92	105.13	110.77
21	5	304	XAT	C5-C4-C3	-2.92	106.97	112.75
23	3	314	CLA	CMB-C2B-C3B	2.92	130.14	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	304	A1L1F	C11-C1-C6	2.92	122.59	119.70
23	7	314	CLA	CMB-C2B-C3B	2.92	130.14	124.68
23	b	840	CLA	CMB-C2B-C3B	2.92	130.14	124.68
23	4	308	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	5	303	A1L1G	C43-C44-C42	-2.92	118.84	122.92
23	4	314	CLA	CMB-C2B-C3B	2.91	130.13	124.68
23	1	313	CLA	CMB-C2B-C3B	2.91	130.13	124.68
21	5	302	XAT	C24-C23-C22	-2.91	105.15	110.77
31	b	845	BCR	C33-C5-C6	-2.91	121.26	124.53
23	b	817	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	6	313	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	4	303	XAT	C30-C31-C32	-2.91	114.14	123.22
21	6	305	XAT	C31-C32-C33	-2.90	118.26	126.42
31	f	801	BCR	C33-C5-C6	-2.90	121.27	124.53
23	j	102	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
21	2	303	XAT	C4-C3-C2	-2.90	105.17	110.77
21	7	301	XAT	C4-C3-C2	-2.90	105.17	110.77
23	b	809	CLA	CMB-C2B-C3B	2.90	130.10	124.68
23	6	316	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	b	826	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	9	301	A1L1G	C43-C44-C42	-2.90	118.87	122.92
23	b	806	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
23	2	316	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
31	f	801	BCR	C20-C19-C18	-2.89	118.28	126.42
31	b	844	BCR	C38-C26-C25	-2.89	121.28	124.53
23	a	817	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	b	805	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	a	810	CLA	CMB-C2B-C3B	2.89	130.09	124.68
21	1	302	XAT	C4-C3-C2	-2.89	105.19	110.77
21	2	304	XAT	C24-C23-C22	-2.89	105.19	110.77
23	4	317	CLA	CMB-C2B-C3B	2.89	130.08	124.68
23	2	310	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	b	837	CLA	CMB-C2B-C3B	2.88	130.07	124.68
23	a	813	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	7	312	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	8	306	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	l	202	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	a	820	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	h	202	BCR	C23-C24-C25	-2.88	119.12	127.20
24	5	316	SQD	C44-O6-C1	-2.88	108.12	113.74
23	5	315	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	4	312	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	823	CLA	CMB-C2B-C3B	2.87	130.05	124.68
23	2	314	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	6	316	CLA	CMB-C2B-C3B	2.87	130.05	124.68
23	b	828	CLA	CMB-C2B-C3B	2.87	130.05	124.68
23	9	312	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	a	837	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
21	4	302	XAT	C24-C23-C22	-2.87	105.24	110.77
31	a	848	BCR	C7-C8-C9	-2.86	121.91	126.23
23	3	308	CLA	CMB-C2B-C3B	2.86	130.04	124.68
23	1	312	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	b	837	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	6	311	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	7	315	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	a	825	CLA	CMB-C2B-C3B	2.86	130.03	124.68
23	5	307	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
21	9	304	XAT	C15-C35-C34	-2.86	117.62	123.47
23	1	307	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	6	308	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
21	4	302	XAT	C4-C3-C2	-2.85	105.26	110.77
23	1	305	CLA	CMB-C2B-C3B	2.85	130.02	124.68
23	a	819	CLA	CMB-C2B-C3B	2.85	130.02	124.68
23	8	311	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
21	4	301	XAT	C4-C3-C2	-2.85	105.26	110.77
31	b	846	BCR	C15-C16-C17	-2.85	117.63	123.47
23	2	307	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	8	310	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	3	307	CLA	CMB-C2B-C3B	2.85	130.01	124.68
21	1	302	XAT	C24-C23-C22	-2.85	105.27	110.77
21	a	852	XAT	C24-C23-C22	-2.85	105.27	110.77
23	a	823	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	b	804	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
23	5	309	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
23	a	811	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	a	825	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	a	813	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	2	307	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	4	315	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	6	315	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	5	312	CLA	O2D-CGD-CBD	2.84	116.32	111.27
31	h	201	BCR	C4-C5-C6	-2.84	118.61	122.73
23	3	311	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
21	5	304	XAT	C19-C9-C8	2.84	122.55	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	309	CLA	CMB-C2B-C3B	2.84	129.99	124.68
23	a	841	CLA	CMB-C2B-C3B	2.84	129.99	124.68
21	5	302	XAT	C35-C34-C33	-2.84	123.26	127.31
21	6	305	XAT	O4-C5-C4	2.84	115.51	113.38
23	b	838	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	6	314	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
23	9	315	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	a	827	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	3	303	XAT	C4-C3-C2	-2.83	105.30	110.77
23	a	817	CLA	CMB-C2B-C3B	2.83	129.97	124.68
23	5	310	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	2	304	XAT	C4-C3-C2	-2.83	105.31	110.77
23	8	313	CLA	CMB-C2B-C3B	2.83	129.97	124.68
23	8	314	CLA	CMB-C2B-C3B	2.83	129.97	124.68
21	j	101	XAT	C4-C3-C2	-2.83	105.31	110.77
25	8	304	A1L1F	C17-C20-C21	2.82	117.46	114.28
23	a	815	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	1	314	CLA	CMB-C2B-C3B	2.82	129.96	124.68
23	j	103	CLA	CMB-C2B-C3B	2.82	129.96	124.68
23	a	826	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	5	305	CLA	CMB-C2B-C3B	2.82	129.96	124.68
23	a	841	CLA	CHB-C4A-NA	2.82	128.41	124.51
28	4	318	DGD	O5E-C6E-C5E	-2.82	101.61	111.29
21	2	305	XAT	C11-C10-C9	-2.82	123.28	127.31
31	b	844	BCR	C20-C21-C22	-2.82	123.28	127.31
23	a	833	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	3	302	A1L1G	C43-C44-C42	-2.82	118.97	122.92
23	j	102	CLA	CMB-C2B-C3B	2.82	129.95	124.68
23	a	816	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	7	306	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	8	307	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
21	8	303	XAT	C11-C10-C9	-2.81	123.29	127.31
21	3	304	XAT	C24-C23-C22	-2.81	105.34	110.77
21	1	303	XAT	C4-C3-C2	-2.81	105.34	110.77
23	7	315	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	9	314	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
23	9	311	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	8	312	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	a	832	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	8	305	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	3	313	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	a	842	CLA	CMB-C2B-C3B	2.81	129.93	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	9	318	CLA	CMB-C2B-C3B	2.81	129.93	124.68
23	f	803	CLA	CMB-C2B-C3B	2.81	129.93	124.68
23	a	805	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	b	827	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	7	307	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	6	310	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	1	310	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
21	9	304	XAT	C4-C3-C2	-2.81	105.36	110.77
21	7	305	XAT	C15-C35-C34	-2.80	117.73	123.47
31	b	846	BCR	C21-C20-C19	-2.80	114.47	123.22
23	b	831	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	8	313	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
21	6	305	XAT	C26-C27-C28	-2.80	120.07	125.99
23	b	828	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	5	306	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	7	310	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	1	305	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	a	840	CLA	CMB-C2B-C3B	2.80	129.91	124.68
23	7	317	CLA	CMB-C2B-C3B	2.80	129.91	124.68
25	1	304	A1L1F	C36-C35-C34	-2.80	123.32	127.31
31	b	844	BCR	C34-C9-C10	-2.80	119.01	122.92
23	h	204	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	2	311	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	9	311	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	5	308	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
21	2	301	XAT	C4-C3-C2	-2.79	105.38	110.77
23	5	313	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	9	310	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	3	312	CLA	CHB-C4A-NA	2.79	128.37	124.51
21	9	304	XAT	C30-C31-C32	-2.79	114.51	123.22
23	b	821	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	1	301	A1L1G	C20-C21-C22	-2.79	107.23	112.75
23	4	306	CLA	CMB-C2B-C3B	2.79	129.89	124.68
23	9	308	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	a	836	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
21	9	303	XAT	C15-C35-C34	-2.78	117.77	123.47
23	6	312	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	a	821	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	2	308	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	4	312	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	1	304	A1L1F	C20-C21-C22	-2.78	107.24	112.75
21	4	304	XAT	C11-C10-C9	-2.78	123.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	l	203	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	8	309	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	j	104	BCR	C38-C26-C27	2.78	118.96	113.62
23	5	313	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	4	313	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	b	842	BCR	C33-C5-C4	2.78	118.96	113.62
23	2	306	CLA	CMB-C2B-C3B	2.78	129.88	124.68
23	a	802	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	1	306	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	b	844	BCR	C37-C22-C21	-2.78	119.03	122.92
23	b	840	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	3	314	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	2	315	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	b	815	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	b	819	CLA	CMB-C2B-C3B	2.78	129.87	124.68
23	1	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
28	b	848	DGD	C6D-O5D-C1E	2.77	119.16	113.74
23	3	312	CLA	CMB-C2B-C3B	2.77	129.86	124.68
23	2	314	CLA	CMB-C2B-C3B	2.77	129.86	124.68
23	a	834	CLA	CMB-C2B-C3B	2.77	129.86	124.68
21	4	302	XAT	C31-C30-C29	-2.77	123.36	127.31
28	b	848	DGD	O1G-C1A-C2A	2.77	120.60	111.91
23	b	823	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	b	841	PQN	C16-C15-C13	-2.77	106.19	113.45
23	b	801	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	a	828	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	a	803	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
29	2	317	LMG	O8-C28-C29	2.77	120.59	111.91
23	9	312	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
21	2	305	XAT	C38-C25-C26	-2.77	117.63	122.26
23	5	314	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	9	316	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	7	317	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
25	h	203	A1L1F	C26-C30-C31	-2.76	121.32	124.93
31	b	843	BCR	C21-C20-C19	-2.76	114.60	123.22
23	4	316	CLA	CMB-C2B-C3B	2.76	129.84	124.68
21	7	301	XAT	C11-C10-C9	-2.76	123.37	127.31
23	b	811	CLA	CMB-C2B-C3B	2.76	130.09	124.69
31	a	849	BCR	C2-C1-C6	2.76	114.73	110.48
23	4	307	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	6	307	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	2	315	CLA	CMB-C2B-C3B	2.76	129.84	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	6	311	CLA	CMB-C2B-C3B	2.76	129.84	124.68
21	4	305	XAT	C4-C3-C2	-2.75	105.45	110.77
31	a	850	BCR	C38-C26-C27	2.75	118.91	113.62
21	4	301	XAT	C26-C27-C28	-2.75	120.17	125.99
23	a	841	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
31	b	842	BCR	C4-C5-C6	-2.75	118.74	122.73
21	6	303	XAT	C15-C35-C34	-2.75	117.84	123.47
23	a	844	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	a	854	CLA	CMB-C2B-C3B	2.75	129.82	124.68
23	a	819	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	b	830	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	7	307	CLA	CMB-C2B-C3B	2.75	129.81	124.68
23	4	306	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	3	315	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
23	a	838	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
23	2	316	CLA	CMB-C2B-C3B	2.74	129.81	124.68
21	3	301	XAT	C10-C11-C12	-2.74	114.66	123.22
21	8	303	XAT	C39-C29-C28	2.74	122.40	118.08
21	2	301	XAT	C24-C23-C22	-2.74	105.48	110.77
23	3	315	CLA	CMB-C2B-C3B	2.74	129.80	124.68
21	2	305	XAT	C4-C3-C2	-2.73	105.49	110.77
21	2	302	XAT	C35-C15-C14	-2.73	117.87	123.47
31	b	842	BCR	C38-C26-C25	-2.73	121.46	124.53
23	a	824	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
23	f	802	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
23	b	812	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	7	315	CLA	CAA-C2A-C3A	-2.73	109.72	116.10
21	3	303	XAT	C31-C30-C29	-2.73	123.41	127.31
23	5	305	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	a	805	CLA	CHB-C4A-NA	2.73	128.29	124.51
29	a	853	LMG	O8-C28-C29	2.73	120.47	111.91
23	f	803	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	b	822	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
25	8	304	A1L1F	O13-C45-C47	2.73	120.47	111.91
25	8	304	A1L1F	O7-C54-O55	-2.73	117.55	122.96
23	b	819	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
25	1	304	A1L1F	C26-O13-C45	2.73	121.74	115.68
23	b	825	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	b	835	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	a	807	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	a	820	CLA	C1-C2-C3	-2.72	121.33	126.04
31	i	101	BCR	C20-C19-C18	-2.72	118.77	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	304	XAT	C7-C8-C9	-2.72	121.31	125.53
23	8	314	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
21	3	305	XAT	C35-C15-C14	-2.72	117.91	123.47
23	l	204	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
23	b	810	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
21	1	303	XAT	C10-C11-C12	-2.71	114.75	123.22
31	j	104	BCR	C23-C24-C25	-2.71	119.58	127.20
23	7	311	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
26	9	305	45D	C24-C20-C08	-2.71	119.59	127.20
21	j	101	XAT	C24-C23-C22	-2.71	105.54	110.77
31	b	842	BCR	C24-C23-C22	-2.71	122.14	126.23
23	5	310	CLA	CMB-C2B-C3B	2.71	129.74	124.68
31	h	202	BCR	C24-C23-C22	-2.71	122.14	126.23
25	h	203	A1L1F	O13-C45-C47	2.71	120.40	111.91
21	2	301	XAT	C31-C32-C33	-2.71	118.81	126.42
23	a	826	CLA	CHB-C4A-NA	2.71	128.25	124.51
31	b	849	BCR	C20-C19-C18	-2.70	118.82	126.42
21	4	301	XAT	C39-C29-C30	-2.70	119.14	122.92
23	l	203	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	9	305	45D	C23-C19-C07	-2.70	119.61	127.20
24	1	315	SQD	O48-C23-C24	2.70	120.39	111.91
23	a	808	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	9	309	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	9	302	A1L1F	O13-C45-C47	2.70	120.38	111.91
23	a	814	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	4	314	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
31	h	202	BCR	C20-C21-C22	-2.70	123.46	127.31
21	j	101	XAT	C15-C35-C34	-2.70	117.95	123.47
23	7	317	CLA	CHB-C4A-NA	2.70	128.24	124.51
21	2	302	XAT	C24-C23-C22	-2.69	105.57	110.77
21	j	101	XAT	C31-C30-C29	-2.69	123.47	127.31
23	b	811	CLA	CAB-C3B-C2B	2.69	129.96	124.69
31	b	842	BCR	C23-C24-C25	-2.69	119.64	127.20
23	a	821	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	a	835	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	4	315	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
21	3	301	XAT	C19-C9-C8	2.69	122.31	118.08
21	8	301	XAT	C7-C8-C9	-2.69	121.36	125.53
23	a	829	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
31	h	201	BCR	C7-C8-C9	-2.68	122.18	126.23
23	2	312	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
23	6	317	CLA	C1-C2-C3	-2.68	121.40	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	301	XAT	C27-C28-C29	-2.68	121.37	125.53
21	8	303	XAT	C35-C34-C33	-2.68	123.49	127.31
23	6	312	CLA	CMB-C2B-C3B	2.68	129.69	124.68
21	4	302	XAT	C15-C14-C13	-2.68	123.49	127.31
25	h	203	A1L1F	C8-O7-C54	-2.67	112.91	117.90
23	5	314	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	b	807	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	3	312	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
21	6	306	XAT	C4-C3-C2	-2.67	105.61	110.77
31	i	101	BCR	C29-C30-C25	2.67	114.59	110.48
31	h	201	BCR	C10-C11-C12	-2.67	114.89	123.22
23	4	315	CLA	CHB-C4A-NA	2.67	128.20	124.51
21	5	302	XAT	C4-C3-C2	-2.67	105.62	110.77
21	j	101	XAT	C31-C32-C33	-2.67	118.92	126.42
27	9	317	LHG	O8-C23-C24	2.67	120.28	111.91
23	4	313	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
31	b	844	BCR	C11-C10-C9	-2.67	123.51	127.31
24	5	316	SQD	O48-C23-C24	2.66	120.27	111.91
21	4	305	XAT	C31-C32-C33	-2.66	118.94	126.42
23	a	804	CLA	C1-C2-C3	-2.66	121.44	126.04
23	2	313	CLA	CAA-C2A-C3A	-2.66	109.89	116.10
31	b	845	BCR	C35-C13-C12	2.66	122.27	118.08
21	2	304	XAT	C15-C14-C13	-2.66	123.51	127.31
30	b	841	PQN	C2M-C2-C3	-2.66	120.06	124.40
21	6	305	XAT	C6-C7-C8	-2.66	120.38	125.99
21	5	304	XAT	C10-C11-C12	-2.65	114.93	123.22
23	b	824	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	4	310	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
21	4	303	XAT	C4-C3-C2	-2.65	105.65	110.77
23	a	834	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
23	a	822	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
21	4	305	XAT	C7-C8-C9	-2.65	121.42	125.53
25	6	301	A1L1F	O13-C45-C47	2.65	120.22	111.91
31	b	842	BCR	C2-C1-C6	2.65	114.56	110.48
23	9	316	CLA	CHB-C4A-NA	2.65	128.17	124.51
21	6	303	XAT	C4-C3-C2	-2.65	105.66	110.77
23	b	806	CLA	CHB-C4A-NA	2.65	128.17	124.51
23	a	810	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
28	b	848	DGD	C1E-O6E-C5E	2.65	118.88	113.69
21	8	302	XAT	C4-C3-C2	-2.65	105.66	110.77
23	b	818	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
21	5	304	XAT	C31-C30-C29	-2.64	123.54	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	801	BCR	C33-C5-C4	2.64	118.68	113.62
23	1	312	CLA	CMB-C2B-C3B	2.64	129.61	124.68
31	m	101	BCR	C33-C5-C6	-2.64	121.57	124.53
23	a	833	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	3	301	XAT	C24-C23-C22	-2.63	105.69	110.77
21	7	303	XAT	C24-C23-C22	-2.63	105.69	110.77
31	a	847	BCR	C16-C15-C14	-2.63	118.08	123.47
23	4	317	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	7	304	XAT	C4-C3-C2	-2.63	105.69	110.77
23	b	819	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
31	f	801	BCR	C10-C11-C12	-2.63	115.01	123.22
23	4	308	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
23	a	829	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
21	4	305	XAT	C39-C29-C30	-2.63	119.24	122.92
21	5	301	XAT	C35-C15-C14	-2.63	118.09	123.47
23	b	826	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
26	9	305	45D	C41-C42-C38	-2.63	118.10	123.47
23	a	807	CLA	CHB-C4A-NA	2.62	128.14	124.51
21	4	303	XAT	C39-C29-C28	2.62	122.21	118.08
21	6	302	XAT	C4-C3-C2	-2.62	105.71	110.77
23	a	842	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
21	4	304	XAT	C31-C30-C29	-2.62	123.57	127.31
21	2	305	XAT	C31-C32-C33	-2.62	119.06	126.42
23	6	315	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	6	317	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	4	317	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	b	840	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
23	b	809	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	a	814	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	b	801	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	j	103	CLA	CHB-C4A-NA	2.61	128.12	124.51
21	4	301	XAT	C27-C28-C29	-2.61	121.48	125.53
31	h	202	BCR	C21-C20-C19	-2.61	115.07	123.22
21	5	304	XAT	C8-C9-C10	-2.61	114.94	118.94
23	7	309	CLA	O2D-CGD-O1D	-2.61	118.17	124.09
25	h	203	A1L1F	C20-C21-C22	-2.61	107.59	112.75
23	a	832	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	a	824	CLA	CMB-C2B-C3B	2.61	129.55	124.68
23	2	311	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
23	9	311	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
23	4	315	CLA	CAA-C2A-C3A	-2.60	110.02	116.10
21	2	304	XAT	C35-C15-C14	-2.60	118.14	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	303	XAT	C30-C31-C32	-2.60	115.09	123.22
23	9	318	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	b	816	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
23	a	802	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
23	a	809	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	4	310	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	5	306	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	2	311	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	8	311	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
23	7	316	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	8	311	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	a	819	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	b	830	CLA	CAA-C2A-C3A	-2.60	110.04	116.10
31	l	205	BCR	C28-C27-C26	-2.60	109.44	114.08
27	b	847	LHG	O8-C23-C24	2.59	120.05	111.91
25	h	203	A1L1F	C29-C30-C31	-2.59	115.00	118.93
23	b	833	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	j	105	LMG	O8-C28-C29	2.59	120.04	111.91
23	a	818	CLA	CMB-C2B-C3B	2.59	129.53	124.68
23	1	314	CLA	CHB-C4A-NA	2.59	128.10	124.51
31	a	849	BCR	C16-C15-C14	-2.59	118.17	123.47
23	b	802	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
23	b	817	CLA	CHB-C4A-NA	2.59	128.09	124.51
21	8	301	XAT	C4-C3-C2	-2.59	105.77	110.77
31	h	201	BCR	C2-C1-C6	2.59	114.47	110.48
23	3	315	CLA	CHB-C4A-NA	2.59	128.09	124.51
27	9	307	LHG	O8-C23-C24	2.59	120.03	111.91
25	1	304	A1L1F	C26-C30-C31	-2.59	121.55	124.93
23	b	809	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
23	5	311	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
31	m	101	BCR	C15-C16-C17	-2.59	118.18	123.47
23	9	309	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
23	b	801	CLA	CMB-C2B-C3B	2.58	129.51	124.68
23	b	820	CLA	C1-C2-C3	-2.58	122.57	126.75
26	9	305	45D	C27-C25-C29	-2.58	119.30	122.92
23	5	313	CLA	CHB-C4A-NA	2.58	128.09	124.51
31	h	202	BCR	C28-C27-C26	-2.58	109.46	114.08
23	1	306	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	a	804	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	5	311	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
23	b	817	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
23	5	312	CLA	CHB-C4A-NA	2.58	128.08	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	303	XAT	C4-C3-C2	-2.58	105.79	110.77
23	1	309	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	4	311	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	7	303	XAT	C4-C3-C2	-2.58	105.80	110.77
23	b	825	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
23	5	306	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	7	313	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
23	a	854	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
31	l	201	BCR	C20-C21-C22	-2.57	123.64	127.31
23	9	313	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	b	813	CLA	CHB-C4A-NA	2.57	128.06	124.51
31	m	101	BCR	C27-C26-C25	2.57	126.46	122.73
23	2	308	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
23	6	316	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	3	310	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
23	4	306	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	a	810	CLA	CHB-C4A-NA	2.56	128.06	124.51
23	a	825	CLA	CHB-C4A-NA	2.56	128.06	124.51
23	f	802	CLA	CHB-C4A-NA	2.56	128.06	124.51
21	6	302	XAT	C27-C28-C29	-2.56	121.56	125.53
31	b	846	BCR	C24-C23-C22	-2.56	122.36	126.23
25	1	304	A1L1F	O13-C45-C47	2.56	119.94	111.91
23	1	308	CLA	C1-C2-C3	-2.56	121.61	126.04
23	5	308	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	b	812	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	1	312	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	b	835	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	8	301	XAT	C31-C30-C29	-2.56	123.66	127.31
31	j	104	BCR	C33-C5-C6	-2.56	121.66	124.53
23	b	820	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	6	306	XAT	C24-C23-C22	-2.56	105.84	110.77
27	a	845	LHG	O8-C23-C24	2.56	119.93	111.91
31	b	845	BCR	C8-C7-C6	-2.56	120.03	127.20
31	a	849	BCR	C23-C24-C25	-2.55	120.03	127.20
23	3	308	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	b	813	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
23	b	834	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	a	806	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	a	827	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	a	832	CLA	C1-C2-C3	-2.55	122.63	126.75
23	a	806	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	6	314	CLA	CHB-C4A-NA	2.54	128.03	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	302	XAT	C4-C3-C2	-2.54	105.86	110.77
21	2	302	XAT	C11-C10-C9	-2.54	123.68	127.31
23	2	306	CLA	O2D-CGD-O1D	-2.54	118.32	124.09
31	b	846	BCR	C34-C9-C8	2.54	122.08	118.08
23	2	307	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
23	a	827	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
21	5	304	XAT	C15-C35-C34	-2.54	118.27	123.47
23	a	838	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	3	314	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	f	803	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	b	803	CLA	CMB-C2B-C3B	2.54	129.43	124.68
23	8	308	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	b	837	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
23	1	308	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	9	308	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
21	8	302	XAT	C11-C12-C13	-2.53	119.30	126.42
23	a	802	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	b	836	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	4	311	CLA	CMB-C2B-C3B	2.53	129.42	124.68
23	8	312	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	a	822	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	1	315	SQD	O8-S-C6	2.53	109.77	105.74
23	b	803	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	b	805	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	4	307	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	1	309	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
23	5	312	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
23	3	313	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	l	204	CLA	CHB-C4A-NA	2.52	128.00	124.51
31	b	845	BCR	C38-C26-C25	-2.52	121.69	124.53
31	b	849	BCR	C15-C14-C13	-2.52	123.71	127.31
23	b	833	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	a	853	LMG	C8-O7-C10	-2.52	111.58	117.79
23	a	836	CLA	CHB-C4A-NA	2.52	128.00	124.51
21	9	303	XAT	C7-C8-C9	-2.52	121.62	125.53
23	a	801	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
23	b	831	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	5	316	SQD	O7-S-C6	2.52	109.93	106.94
23	6	311	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	b	829	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
31	b	845	BCR	C33-C5-C4	2.52	118.45	113.62
23	3	312	CLA	C1B-CHB-C4A	-2.52	125.13	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	302	XAT	C19-C9-C10	-2.52	119.40	122.92
25	8	304	A1L1F	C12-C6-C1	-2.52	108.22	110.47
21	1	303	XAT	C35-C15-C14	-2.51	118.33	123.47
23	a	808	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	8	314	CLA	CAA-C2A-C3A	-2.51	110.23	116.10
23	3	309	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
23	l	203	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
31	l	201	BCR	C28-C27-C26	-2.51	109.59	114.08
23	a	831	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
23	4	314	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	6	312	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	2	312	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	b	833	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
23	8	309	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	6	304	A1L1F	O13-C45-C47	2.51	119.78	111.91
23	a	822	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
31	l	205	BCR	C38-C26-C27	2.51	118.43	113.62
23	1	307	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	a	840	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	h	203	A1L1F	C27-C34-C33	2.51	122.03	118.08
23	2	313	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	a	852	XAT	O4-C5-C4	2.51	115.26	113.38
21	8	301	XAT	C35-C15-C14	-2.51	118.34	123.47
21	6	302	XAT	C31-C32-C33	-2.50	119.38	126.42
31	b	843	BCR	C24-C23-C22	-2.50	122.45	126.23
31	f	804	BCR	C15-C16-C17	-2.50	118.34	123.47
23	8	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
21	6	302	XAT	C19-C9-C10	-2.50	119.42	122.92
21	7	304	XAT	C19-C9-C10	-2.50	119.42	122.92
23	a	814	CLA	CHD-C1D-ND	-2.50	122.16	124.45
23	8	314	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	a	836	CLA	CMB-C2B-C3B	2.50	129.36	124.68
23	a	817	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	7	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	h	204	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	b	807	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	b	829	CLA	C2D-C1D-ND	-2.50	108.26	110.10
31	l	205	BCR	C15-C16-C17	-2.50	118.36	123.47
31	b	846	BCR	C20-C21-C22	-2.50	123.75	127.31
23	8	313	CLA	CHB-C4A-NA	2.50	127.96	124.51
23	a	816	CLA	CHB-C4A-NA	2.50	127.96	124.51
31	l	201	BCR	C34-C9-C10	-2.49	119.43	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	820	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
31	f	801	BCR	C2-C1-C6	2.49	114.32	110.48
23	a	815	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	5	305	CLA	CHB-C4A-NA	2.49	127.96	124.51
28	b	848	DGD	O2G-C1B-O1B	-2.49	117.68	123.70
23	b	839	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	5	310	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	7	313	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	6	315	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	b	822	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
23	6	310	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	l	202	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	b	819	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	3	307	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	4	316	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	6	301	A1L1F	C31-C32-C33	-2.49	115.46	123.22
23	2	314	CLA	CHB-C4A-NA	2.48	127.95	124.51
23	a	811	CLA	CHB-C4A-NA	2.48	127.95	124.51
23	a	812	CLA	CHB-C4A-NA	2.48	127.95	124.51
23	a	841	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
23	7	315	CLA	CHB-C4A-NA	2.48	127.95	124.51
21	5	304	XAT	C39-C29-C28	2.48	121.99	118.08
23	b	804	CLA	CHD-C1D-ND	-2.48	122.17	124.45
22	9	301	A1L1G	C20-C21-C22	-2.48	107.84	112.75
23	a	835	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
23	a	818	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	1	310	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	6	317	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
21	5	302	XAT	C19-C9-C10	-2.48	119.46	122.92
23	2	309	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	a	802	CLA	C1-C2-C3	-2.47	121.77	126.04
23	b	834	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	a	805	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
21	5	304	XAT	C30-C31-C32	-2.47	115.51	123.22
23	7	311	CLA	CHB-C4A-NA	2.47	127.93	124.51
21	5	301	XAT	C4-C3-C2	-2.47	106.00	110.77
23	a	812	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
23	7	308	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	9	316	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
23	a	837	CLA	CHB-C4A-NA	2.47	127.93	124.51
30	b	841	PQN	C14-C13-C15	2.47	119.42	115.27
23	6	307	CLA	CHB-C4A-NA	2.47	127.92	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	839	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	b	821	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	a	841	CLA	C1-C2-C3	-2.47	121.78	126.04
23	b	815	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	b	808	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	1	310	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	6	309	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	a	837	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	8	305	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	b	838	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	5	315	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	4	301	XAT	C35-C15-C14	-2.46	118.44	123.47
22	3	306	A1L1G	C17-C20-C21	2.46	117.05	114.28
23	a	823	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	b	820	CLA	O2D-CGD-CBD	2.46	115.64	111.27
25	6	304	A1L1F	C25-C14-C29	-2.46	120.80	125.99
31	j	104	BCR	C27-C26-C25	-2.46	119.16	122.73
23	7	306	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	h	201	BCR	C21-C20-C19	-2.46	115.55	123.22
21	7	304	XAT	C11-C12-C13	-2.46	119.52	126.42
23	9	308	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	l	205	BCR	C33-C5-C4	2.45	118.33	113.62
21	7	301	XAT	C35-C15-C14	-2.45	118.45	123.47
23	a	809	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	9	309	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	4	309	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	2	315	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	b	828	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	l	204	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	2	316	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	1	304	A1L1F	C27-C34-C33	2.45	121.94	118.08
31	b	843	BCR	C15-C16-C17	-2.45	118.45	123.47
23	4	309	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	2	306	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	9	302	A1L1F	C36-C37-C38	-2.45	118.45	123.47
23	a	832	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
21	8	303	XAT	C28-C29-C30	-2.45	115.18	118.94
23	5	308	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	a	806	CLA	O1D-CGD-CBD	2.45	129.49	124.48
31	j	104	BCR	C15-C16-C17	-2.45	118.46	123.47
23	2	311	CLA	CHB-C4A-NA	2.45	127.89	124.51
23	7	310	CLA	CHB-C4A-NA	2.45	127.89	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	854	CLA	CHB-C4A-NA	2.45	127.89	124.51
31	f	804	BCR	C28-C27-C26	-2.45	109.71	114.08
21	5	302	XAT	C31-C30-C29	-2.44	123.82	127.31
23	a	854	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	3	311	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	a	828	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	9	304	XAT	C39-C29-C28	2.44	121.92	118.08
23	8	310	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	b	808	CLA	CHB-C4A-NA	2.44	127.88	124.51
31	h	202	BCR	C33-C5-C4	2.44	118.30	113.62
23	b	831	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
31	h	201	BCR	C33-C5-C6	-2.44	121.79	124.53
31	b	842	BCR	C15-C16-C17	-2.44	118.48	123.47
23	a	812	CLA	CHD-C1D-ND	-2.44	122.22	124.45
23	4	312	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
25	6	304	A1L1F	C42-C41-C40	-2.43	115.62	123.22
23	8	308	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
25	h	203	A1L1F	C41-C40-C39	-2.43	119.58	126.42
23	b	830	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	b	827	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	b	813	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	b	806	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	a	804	CLA	O2D-CGD-CBD	2.43	115.58	111.27
23	3	310	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	b	827	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	b	832	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	h	204	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
31	l	201	BCR	C21-C20-C19	-2.43	115.64	123.22
31	b	845	BCR	C39-C30-C25	-2.43	106.36	110.30
23	5	311	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	4	313	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	8	304	A1L1F	C28-C39-C38	-2.43	119.53	122.92
23	a	814	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
31	b	846	BCR	C38-C26-C25	-2.42	121.81	124.53
23	a	820	CLA	CHB-C4A-NA	2.42	127.86	124.51
21	7	305	XAT	C31-C30-C29	-2.42	123.85	127.31
23	a	807	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	a	818	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	a	810	CLA	C1-C2-C3	-2.42	121.86	126.04
21	2	303	XAT	C8-C9-C10	2.42	122.65	118.94
31	a	848	BCR	C33-C5-C4	2.42	118.26	113.62
23	a	825	CLA	C1B-CHB-C4A	-2.42	125.33	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	7	312	CLA	CHB-C4A-NA	2.42	127.85	124.51
25	h	203	A1L1F	C23-C22-C21	-2.42	106.11	110.77
23	b	816	CLA	CHB-C4A-NA	2.42	127.85	124.51
23	4	312	CLA	CHB-C4A-NA	2.42	127.85	124.51
21	7	303	XAT	C8-C9-C10	2.41	122.65	118.94
23	3	309	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	a	840	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	b	825	CLA	CHB-C4A-NA	2.41	127.85	124.51
26	9	305	45D	C21-C15-C17	2.41	119.07	115.48
23	1	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	9	315	CLA	CHB-C4A-NA	2.41	127.85	124.51
21	4	302	XAT	C10-C11-C12	-2.41	115.69	123.22
23	a	830	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	9	318	CLA	CHB-C4A-NA	2.41	127.84	124.51
26	9	305	45D	C10-C06-C04	-2.41	109.31	113.18
23	9	314	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	a	808	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	a	836	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	b	816	CLA	CHD-C1D-ND	-2.41	122.24	124.45
23	1	313	CLA	CHB-C4A-NA	2.40	127.83	124.51
31	j	104	BCR	C38-C26-C25	-2.40	121.83	124.53
23	b	803	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	j	102	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	5	314	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
31	a	850	BCR	C8-C7-C6	-2.40	120.47	127.20
25	6	304	A1L1F	C11-C1-C6	2.40	122.08	119.70
23	b	822	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	7	308	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	a	833	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	7	314	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
23	a	842	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	5	307	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	8	307	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
21	3	304	XAT	C31-C32-C33	-2.39	119.69	126.42
31	b	842	BCR	C29-C30-C25	2.39	114.16	110.48
21	6	303	XAT	C11-C12-C13	-2.39	119.70	126.42
23	1	313	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	b	818	CLA	CHB-C4A-NA	2.39	127.82	124.51
31	b	842	BCR	C21-C20-C19	-2.39	115.76	123.22
23	6	313	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	a	835	CLA	O2D-CGD-CBD	2.39	115.51	111.27
31	b	844	BCR	C28-C27-C26	-2.39	109.81	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	310	CLA	CHB-C4A-NA	2.39	127.81	124.51
21	3	305	XAT	C10-C11-C12	-2.39	115.77	123.22
25	6	304	A1L1F	C31-C32-C33	-2.39	115.77	123.22
23	8	306	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	1	203	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	5	315	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
23	9	318	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
23	3	311	CLA	C1-C2-C3	-2.38	122.89	126.75
23	9	312	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
23	9	311	CLA	O2D-CGD-CBD	2.38	115.50	111.27
23	7	312	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	5	309	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	8	310	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	j	102	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	6	313	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	a	804	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	b	811	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	a	834	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	a	839	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
31	a	850	BCR	C10-C11-C12	-2.38	115.80	123.22
23	b	833	CLA	CHD-C1D-ND	-2.38	122.27	124.45
23	b	836	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	4	308	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	7	309	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	8	302	XAT	C7-C8-C9	-2.37	121.84	125.53
23	a	813	CLA	CHB-C4A-NA	2.37	127.80	124.51
23	1	308	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	a	824	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	f	802	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	7	314	CLA	C2A-C1A-CHA	2.37	128.01	123.86
23	b	832	CLA	CHD-C1D-ND	-2.37	122.27	124.45
29	j	105	LMG	C8-O7-C10	-2.37	111.95	117.79
23	b	810	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	1	313	CLA	CAA-C2A-C3A	-2.37	110.56	116.10
23	1	311	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
31	h	202	BCR	C8-C7-C6	-2.37	120.55	127.20
23	a	803	CLA	CHD-C1D-ND	-2.37	122.28	124.45
23	a	801	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
31	h	202	BCR	C10-C11-C12	-2.37	115.83	123.22
25	h	203	A1L1F	O7-C54-O55	-2.37	118.26	122.96
23	b	811	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
31	a	850	BCR	C16-C15-C14	-2.37	118.63	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	823	CLA	CHB-C4A-NA	2.37	127.78	124.51
23	l	202	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
25	8	304	A1L1F	C23-C22-C21	-2.36	106.21	110.77
31	a	848	BCR	C15-C16-C17	-2.36	118.63	123.47
23	a	806	CLA	C5-C3-C2	-2.36	116.33	121.12
23	6	309	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	b	815	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	9	310	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	9	315	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	8	312	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	b	820	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
31	b	843	BCR	C28-C27-C26	-2.36	109.86	114.08
23	1	305	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	3	313	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	7	309	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	7	311	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
31	b	849	BCR	C36-C18-C17	-2.36	119.62	122.92
21	5	304	XAT	C25-C24-C23	-2.36	108.08	112.75
21	4	302	XAT	C30-C31-C32	-2.36	115.85	123.22
21	2	303	XAT	C24-C23-C22	-2.36	106.22	110.77
23	b	824	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	a	826	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	b	812	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	b	830	CLA	CHB-C4A-NA	2.36	127.77	124.51
23	b	838	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	a	834	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
25	6	304	A1L1F	O7-C54-O55	-2.36	118.28	122.96
23	a	816	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
31	h	201	BCR	C16-C15-C14	-2.35	118.65	123.47
23	2	315	CLA	CHB-C4A-NA	2.35	127.77	124.51
23	a	801	CLA	CMB-C2B-C3B	2.35	129.08	124.68
21	3	303	XAT	C30-C31-C32	-2.35	115.88	123.22
23	7	314	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	b	810	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	a	831	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	7	310	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	a	827	CLA	CHD-C1D-ND	-2.35	122.30	124.45
23	a	815	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
23	3	308	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
23	6	308	CLA	CHB-C4A-NA	2.35	127.75	124.51
23	b	825	CLA	CHD-C1D-ND	-2.34	122.30	124.45
23	6	310	CLA	C1B-CHB-C4A	-2.34	125.47	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	301	XAT	C40-C33-C34	-2.34	119.64	122.92
31	a	847	BCR	C23-C24-C25	-2.34	120.62	127.20
23	9	313	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
23	4	315	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
31	a	847	BCR	C33-C5-C4	2.34	118.11	113.62
28	8	315	DGD	C2G-O2G-C1B	-2.34	112.03	117.79
21	9	304	XAT	O4-C5-C4	2.34	115.14	113.38
23	a	844	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
22	7	302	A1L1G	C17-C20-C21	2.34	116.91	114.28
23	b	804	CLA	C3C-C4C-NC	-2.34	107.95	110.57
25	9	302	A1L1F	O7-C54-O55	-2.33	118.32	122.96
25	6	304	A1L1F	C5-C6-C1	-2.33	108.38	110.47
21	7	301	XAT	C31-C32-C33	-2.33	119.86	126.42
23	b	805	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	a	810	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	7	313	CLA	CHD-C1D-ND	-2.33	122.31	124.45
23	b	836	CLA	CHD-C1D-ND	-2.33	122.31	124.45
23	a	841	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
23	b	807	CLA	C1-C2-C3	-2.33	122.01	126.04
23	4	312	CLA	CHD-C1D-ND	-2.33	122.31	124.45
23	b	840	CLA	CHB-C4A-NA	2.33	127.73	124.51
31	b	843	BCR	C23-C24-C25	-2.33	120.66	127.20
31	l	201	BCR	C15-C16-C17	-2.33	118.70	123.47
23	2	314	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
23	a	844	CLA	CHB-C4A-NA	2.33	127.73	124.51
23	8	309	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
23	f	803	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
23	5	307	CLA	CHB-C4A-NA	2.33	127.73	124.51
23	a	828	CLA	C1-C2-C3	-2.33	122.02	126.04
23	7	309	CLA	CHD-C1D-ND	-2.33	122.32	124.45
23	4	311	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
31	b	843	BCR	C33-C5-C4	2.33	118.08	113.62
31	i	101	BCR	C37-C22-C21	-2.32	119.67	122.92
23	1	309	CLA	CHB-C4A-NA	2.32	127.73	124.51
25	1	304	A1L1F	C31-C32-C33	-2.32	115.96	123.22
23	5	309	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
23	6	312	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
21	2	301	XAT	C10-C11-C12	-2.32	115.97	123.22
26	9	305	45D	C19-C23-C25	-2.32	122.73	126.23
23	a	819	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	a	806	CLA	C6-C5-C3	-2.32	107.37	113.45
31	b	842	BCR	C11-C12-C13	-2.32	119.89	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	317	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	b	835	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
21	8	303	XAT	C40-C33-C32	2.32	121.73	118.08
23	a	811	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
21	9	303	XAT	C39-C29-C28	2.32	121.73	118.08
23	a	828	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
25	6	301	A1L1F	C36-C35-C34	-2.32	124.00	127.31
23	a	836	CLA	C1-C2-C3	-2.32	123.00	126.75
21	2	304	XAT	C35-C34-C33	-2.32	124.00	127.31
23	3	314	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	8	314	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
23	4	314	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
31	a	848	BCR	C10-C11-C12	-2.31	116.00	123.22
23	8	313	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	6	306	XAT	C31-C32-C33	-2.31	119.92	126.42
23	9	311	CLA	CHD-C1D-ND	-2.31	122.33	124.45
23	4	313	CLA	CHD-C1D-ND	-2.31	122.33	124.45
21	7	304	XAT	O4-C5-C4	2.31	115.12	113.38
23	3	315	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	1	312	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	b	814	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
31	b	842	BCR	C38-C26-C27	2.31	118.05	113.62
31	m	101	BCR	C8-C7-C6	-2.31	120.72	127.20
30	a	843	PQN	C11-C12-C13	-2.31	122.95	126.79
31	i	101	BCR	C16-C15-C14	-2.31	118.75	123.47
23	b	807	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
21	j	101	XAT	C39-C29-C28	2.31	121.71	118.08
23	5	310	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	2	313	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	2	310	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
23	5	306	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
31	b	849	BCR	C23-C24-C25	-2.30	120.73	127.20
31	f	804	BCR	C3-C4-C5	-2.30	109.96	114.08
31	f	804	BCR	C11-C12-C13	-2.30	119.94	126.42
21	6	303	XAT	O24-C25-C38	2.30	117.82	115.06
21	7	303	XAT	O4-C5-C4	2.30	115.11	113.38
23	1	311	CLA	CHD-C1D-ND	-2.30	122.34	124.45
21	5	301	XAT	O4-C5-C4	2.30	115.11	113.38
25	6	301	A1L1F	O7-C54-O55	-2.30	118.39	122.96
23	a	841	CLA	CHD-C1D-ND	-2.30	122.34	124.45
23	6	307	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	a	830	CLA	C1-C2-C3	-2.30	122.07	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	313	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
23	1	307	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
23	j	103	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	2	303	XAT	O4-C5-C4	2.30	115.11	113.38
23	7	316	CLA	O2D-CGD-CBD	2.30	115.35	111.27
23	3	311	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	8	302	XAT	O4-C5-C4	2.29	115.11	113.38
23	5	310	CLA	CHD-C1D-ND	-2.29	122.35	124.45
31	j	104	BCR	C34-C9-C10	-2.29	119.71	122.92
23	b	832	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	3	301	XAT	C15-C35-C34	-2.29	118.78	123.47
23	a	805	CLA	CHD-C1D-ND	-2.29	122.35	124.45
23	b	801	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	8	306	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	6	315	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	b	837	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	a	810	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	6	301	A1L1F	C14-C29-C30	-2.29	121.44	125.47
25	1	304	A1L1F	C37-C36-C35	-2.29	118.79	123.47
21	2	302	XAT	C10-C11-C12	-2.29	116.08	123.22
23	1	314	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	a	821	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	a	842	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	8	308	CLA	O2A-CGA-O1A	-2.29	117.83	123.59
23	4	306	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
23	a	838	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
21	a	852	XAT	C19-C9-C8	2.28	121.67	118.08
23	5	314	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
21	3	304	XAT	C27-C28-C29	-2.28	121.99	125.53
23	3	307	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	b	834	CLA	CHD-C1D-ND	-2.28	122.36	124.45
21	3	304	XAT	C40-C33-C34	-2.28	119.73	122.92
31	b	845	BCR	C21-C20-C19	-2.28	116.11	123.22
23	a	817	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	7	311	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	a	816	CLA	C1-C2-C3	-2.28	123.07	126.75
23	1	305	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	2	310	CLA	CHB-C4A-NA	2.28	127.66	124.51
31	a	848	BCR	C16-C15-C14	-2.27	118.81	123.47
26	9	305	45D	C23-C25-C29	2.27	122.43	118.94
31	l	201	BCR	C23-C24-C25	-2.27	120.81	127.20
23	8	309	CLA	C1-C2-C3	-2.27	122.11	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	310	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
21	4	303	XAT	O4-C5-C4	2.27	115.09	113.38
31	b	845	BCR	C34-C9-C8	2.27	121.66	118.08
23	a	805	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	2	312	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	7	306	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	a	820	CLA	CHD-C1D-ND	-2.27	122.37	124.45
21	1	303	XAT	C27-C28-C29	-2.27	122.00	125.53
23	a	824	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	7	316	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
31	a	849	BCR	C38-C26-C27	2.27	117.98	113.62
23	b	839	CLA	CMB-C2B-C3B	2.27	128.92	124.68
25	1	304	A1L1F	O7-C54-O55	-2.27	118.46	122.96
23	6	311	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	1	301	A1L1G	C17-C20-C21	2.27	116.83	114.28
23	8	305	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
23	2	306	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
21	9	303	XAT	O4-C5-C4	2.26	115.08	113.38
23	a	823	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
23	b	823	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
21	7	301	XAT	C26-C27-C28	-2.26	121.21	125.99
23	7	313	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	7	317	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	5	302	XAT	C15-C35-C34	-2.26	118.85	123.47
31	f	801	BCR	C28-C27-C26	-2.26	110.04	114.08
23	4	310	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
31	m	101	BCR	C24-C23-C22	-2.26	122.83	126.23
23	1	306	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
23	1	305	CLA	CHD-C1D-ND	-2.26	122.38	124.45
23	b	829	CLA	CHB-C4A-NA	2.26	127.63	124.51
23	a	827	CLA	CAA-C2A-C1A	-2.25	104.59	111.97
23	a	836	CLA	CHD-C1D-ND	-2.25	122.38	124.45
21	5	302	XAT	O4-C5-C4	2.25	115.07	113.38
23	6	316	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	2	309	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	4	307	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	b	821	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	5	312	CLA	CHD-C1D-ND	-2.25	122.39	124.45
22	9	301	A1L1G	C29-C30-C31	2.25	122.34	118.93
23	5	305	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	b	803	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	b	840	CLA	CHD-C1D-ND	-2.25	122.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	9	303	XAT	O24-C25-C38	2.25	117.75	115.06
31	a	848	BCR	C21-C20-C19	-2.25	116.21	123.22
24	1	315	SQD	O9-S-C6	2.24	109.61	106.94
31	b	849	BCR	C38-C26-C27	2.24	117.92	113.62
23	a	813	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
25	6	301	A1L1F	C23-C22-C21	-2.24	106.44	110.77
23	6	308	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
21	4	305	XAT	C15-C35-C34	-2.24	118.89	123.47
31	b	845	BCR	C38-C26-C27	2.24	117.92	113.62
25	9	302	A1L1F	C20-C21-C22	-2.24	108.32	112.75
23	7	307	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	b	818	CLA	CHD-C1D-ND	-2.24	122.40	124.45
23	6	314	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	8	308	CLA	C1-C2-C3	-2.24	122.17	126.04
21	2	304	XAT	C20-C13-C12	2.23	121.60	118.08
23	4	309	CLA	CHD-C1D-ND	-2.23	122.40	124.45
21	7	304	XAT	O24-C25-C38	2.23	117.73	115.06
22	1	301	A1L1G	C14-C29-C30	-2.23	121.53	125.47
21	5	302	XAT	C11-C12-C13	-2.23	120.14	126.42
23	h	204	CLA	CHD-C1D-ND	-2.23	122.40	124.45
23	b	810	CLA	C1-C2-C3	-2.23	122.18	126.04
23	2	316	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
21	5	301	XAT	O24-C25-C38	2.23	117.73	115.06
21	8	301	XAT	C30-C31-C32	-2.23	116.26	123.22
23	8	309	CLA	CHD-C1D-ND	-2.23	122.41	124.45
23	a	818	CLA	O2D-CGD-CBD	2.23	115.23	111.27
31	h	202	BCR	C37-C22-C23	2.23	121.58	118.08
23	a	806	CLA	CHD-C1D-ND	-2.23	122.41	124.45
24	5	316	SQD	C45-O47-C7	-2.23	112.31	117.79
23	7	315	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
23	3	313	CLA	CHD-C1D-ND	-2.23	122.41	124.45
22	9	301	A1L1G	C14-C29-C30	-2.23	121.55	125.47
31	b	846	BCR	C35-C13-C12	2.22	121.58	118.08
23	a	822	CLA	CHD-C1D-ND	-2.22	122.41	124.45
21	8	302	XAT	C8-C9-C10	2.22	122.35	118.94
21	6	303	XAT	C20-C13-C14	-2.22	119.81	122.92
23	1	309	CLA	CHD-C1D-ND	-2.22	122.41	124.45
23	2	311	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
23	b	826	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	b	806	CLA	CHD-C1D-ND	-2.22	122.41	124.45
23	b	831	CLA	CHD-C1D-ND	-2.22	122.41	124.45
23	b	804	CLA	O2A-CGA-O1A	-2.22	117.99	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	809	CLA	O2D-CGD-CBD	2.22	115.21	111.27
25	6	301	A1L1F	C32-C31-C30	-2.22	124.10	127.26
23	4	316	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	b	821	CLA	C1-C2-C3	-2.22	122.21	126.04
23	5	307	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
21	5	301	XAT	C30-C31-C32	-2.22	116.30	123.22
31	h	201	BCR	C11-C10-C9	-2.21	124.15	127.31
31	a	850	BCR	C20-C19-C18	-2.21	120.19	126.42
23	b	836	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
31	a	849	BCR	C21-C20-C19	-2.21	116.31	123.22
21	7	305	XAT	C39-C29-C28	2.21	121.56	118.08
21	4	305	XAT	O24-C25-C38	2.21	117.71	115.06
23	a	806	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
26	9	305	45D	C06-C10-C18	-2.21	108.89	112.85
23	a	829	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	b	835	CLA	CAC-C3C-C4C	2.21	127.68	124.81
25	9	302	A1L1F	C26-O13-C45	2.21	120.60	115.68
21	6	306	XAT	C35-C15-C14	-2.21	118.95	123.47
21	2	302	XAT	O4-C5-C4	2.21	115.04	113.38
21	2	303	XAT	C39-C29-C30	-2.21	119.83	122.92
23	8	310	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	4	308	CLA	CHD-C1D-ND	-2.21	122.42	124.45
31	l	201	BCR	C29-C30-C25	2.21	113.88	110.48
21	6	306	XAT	O4-C5-C4	2.21	115.04	113.38
22	7	302	A1L1G	C20-C21-C22	-2.21	108.39	112.75
31	b	845	BCR	C23-C24-C25	-2.21	121.01	127.20
21	7	301	XAT	C39-C29-C30	-2.21	119.83	122.92
31	f	801	BCR	C15-C14-C13	-2.20	124.17	127.31
21	3	303	XAT	C15-C35-C34	-2.20	118.96	123.47
21	7	301	XAT	C24-C23-C22	-2.20	106.52	110.77
23	a	819	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
21	6	302	XAT	C20-C13-C14	-2.20	119.84	122.92
23	b	802	CLA	CHD-C1D-ND	-2.20	122.43	124.45
31	b	844	BCR	C33-C5-C4	2.20	117.84	113.62
31	f	801	BCR	C35-C13-C12	2.20	121.54	118.08
21	2	305	XAT	O4-C5-C4	2.20	115.03	113.38
31	f	801	BCR	C34-C9-C8	2.20	121.54	118.08
21	2	305	XAT	C19-C9-C8	2.20	121.54	118.08
23	l	202	CLA	CHD-C1D-ND	-2.20	122.44	124.45
25	6	304	A1L1F	C36-C37-C38	-2.19	118.98	123.47
23	b	828	CLA	CHB-C4A-NA	2.19	127.55	124.51
22	3	306	A1L1G	C20-C21-C22	-2.19	108.41	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	8	311	CLA	CHD-C1D-ND	-2.19	122.44	124.45
21	2	303	XAT	C40-C33-C34	-2.19	119.85	122.92
23	5	309	CLA	CHD-C1D-ND	-2.19	122.44	124.45
23	a	801	CLA	CHB-C4A-NA	2.19	127.54	124.51
21	1	303	XAT	C19-C9-C8	2.19	121.53	118.08
21	2	305	XAT	C15-C35-C34	-2.19	118.99	123.47
21	8	303	XAT	O4-C5-C18	2.19	117.68	115.06
23	2	308	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	b	838	CLA	CHD-C1D-ND	-2.19	122.44	124.45
31	b	844	BCR	C7-C6-C5	-2.19	116.16	121.46
21	3	303	XAT	O24-C25-C38	2.19	117.68	115.06
21	7	305	XAT	C30-C31-C32	-2.19	116.40	123.22
25	9	302	A1L1F	C31-C32-C33	-2.18	116.40	123.22
23	a	833	CLA	C1-C2-C3	-2.18	122.27	126.04
23	7	312	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	8	301	XAT	O4-C5-C4	2.18	115.02	113.38
23	b	805	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
21	2	303	XAT	C31-C32-C33	-2.18	120.30	126.42
23	b	804	CLA	O1D-CGD-CBD	2.18	128.94	124.48
23	a	829	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	1	312	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
21	4	305	XAT	O4-C5-C4	2.18	115.02	113.38
21	3	301	XAT	C8-C9-C10	-2.18	115.60	118.94
23	b	839	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
21	3	305	XAT	C19-C9-C8	2.17	121.50	118.08
23	1	310	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	2	301	XAT	O4-C5-C4	2.17	115.02	113.38
31	a	849	BCR	C8-C7-C6	-2.17	121.10	127.20
31	l	201	BCR	C39-C30-C25	-2.17	106.77	110.30
21	j	101	XAT	O4-C5-C4	2.17	115.01	113.38
21	3	303	XAT	C35-C15-C14	-2.17	119.02	123.47
21	8	302	XAT	C20-C13-C14	-2.17	119.88	122.92
23	a	825	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	a	820	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	b	813	CLA	C1-C2-C3	-2.17	122.29	126.04
21	8	301	XAT	O24-C25-C38	2.17	117.66	115.06
31	h	202	BCR	C35-C13-C12	2.17	121.50	118.08
21	1	303	XAT	O4-C5-C4	2.17	115.01	113.38
31	h	201	BCR	C34-C9-C8	2.17	121.49	118.08
21	a	852	XAT	C40-C33-C32	2.16	121.49	118.08
23	a	834	CLA	C1-C2-C3	-2.16	122.30	126.04
23	1	312	CLA	CHD-C1D-ND	-2.16	122.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	839	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	6	302	XAT	O24-C25-C38	2.16	117.65	115.06
23	a	804	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
23	4	310	CLA	CHD-C1D-ND	-2.16	122.47	124.45
31	b	843	BCR	C36-C18-C19	2.16	121.48	118.08
23	b	821	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	a	830	CLA	CHB-C4A-NA	2.16	127.50	124.51
21	4	303	XAT	C7-C8-C9	-2.16	122.18	125.53
24	5	316	SQD	O9-S-C6	2.16	109.50	106.94
30	a	843	PQN	C2M-C2-C3	-2.16	120.88	124.40
23	a	816	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	3	311	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	a	831	CLA	O2D-CGD-CBD	2.16	115.10	111.27
31	a	848	BCR	C23-C24-C25	-2.16	121.14	127.20
23	6	307	CLA	CHD-C1D-ND	-2.16	122.47	124.45
21	8	302	XAT	O24-C25-C38	2.16	117.64	115.06
23	8	312	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	a	834	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	3	312	CLA	CHD-C1D-ND	-2.15	122.47	124.45
23	a	813	CLA	CHD-C1D-ND	-2.15	122.47	124.45
23	b	812	CLA	CHD-C1D-ND	-2.15	122.47	124.45
23	b	835	CLA	C1-C2-C3	-2.15	122.32	126.04
23	f	803	CLA	CHD-C1D-ND	-2.15	122.47	124.45
21	4	303	XAT	O24-C25-C38	2.15	117.64	115.06
25	9	302	A1L1F	C23-C22-C21	-2.15	106.61	110.77
23	6	310	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
21	6	305	XAT	C10-C11-C12	-2.15	116.50	123.22
21	3	304	XAT	O4-C5-C18	2.15	117.63	115.06
31	b	843	BCR	C11-C12-C13	-2.15	120.37	126.42
23	a	809	CLA	CHD-C1D-ND	-2.15	122.48	124.45
25	6	304	A1L1F	C20-C21-C22	-2.15	108.50	112.75
23	8	307	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	5	312	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
31	b	843	BCR	C37-C22-C23	2.15	121.46	118.08
23	5	311	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
31	i	101	BCR	C23-C22-C21	2.14	122.23	118.94
23	1	308	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
28	b	848	DGD	O3D-C3D-C4D	-2.14	105.40	110.35
23	a	815	CLA	CHD-C1D-ND	-2.14	122.49	124.45
31	l	201	BCR	C3-C4-C5	-2.14	110.26	114.08
21	5	304	XAT	O24-C25-C38	2.14	117.62	115.06
23	8	308	CLA	O2D-CGD-CBD	2.14	115.07	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	201	BCR	C23-C24-C25	-2.14	121.19	127.20
21	6	305	XAT	C40-C33-C34	-2.14	119.93	122.92
23	a	812	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
23	a	854	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	b	821	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	j	102	CLA	CHD-C1D-ND	-2.14	122.49	124.45
31	a	847	BCR	C8-C7-C6	-2.14	121.20	127.20
23	b	837	CLA	C1-C2-C3	-2.14	122.35	126.04
21	5	302	XAT	C20-C13-C14	-2.14	119.93	122.92
23	a	844	CLA	CHD-C1D-ND	-2.13	122.49	124.45
23	a	831	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
23	f	802	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
21	6	302	XAT	O4-C5-C4	2.13	114.98	113.38
23	a	806	CLA	C6-C7-C8	-2.13	109.02	115.92
29	2	317	LMG	C8-O7-C10	-2.13	112.54	117.79
22	1	301	A1L1G	C29-C30-C31	2.13	122.16	118.93
21	7	304	XAT	C25-C24-C23	-2.13	108.53	112.75
23	b	823	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	a	811	CLA	CHD-C1D-ND	-2.13	122.50	124.45
31	b	845	BCR	C29-C30-C25	2.13	113.76	110.48
21	j	101	XAT	O24-C25-C38	2.13	117.61	115.06
23	5	311	CLA	CHD-C1D-ND	-2.13	122.50	124.45
21	4	302	XAT	C20-C13-C12	2.13	121.43	118.08
21	4	301	XAT	O4-C5-C4	2.13	114.98	113.38
31	a	849	BCR	C10-C11-C12	-2.13	116.58	123.22
31	i	101	BCR	C10-C11-C12	-2.13	116.58	123.22
21	2	303	XAT	O4-C5-C18	2.12	117.60	115.06
31	m	101	BCR	C15-C14-C13	-2.12	124.28	127.31
23	a	839	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
21	5	302	XAT	O4-C5-C18	2.12	117.60	115.06
31	a	847	BCR	C38-C26-C27	2.12	117.69	113.62
23	4	306	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	7	308	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	a	838	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
21	4	302	XAT	C39-C29-C28	2.12	121.42	118.08
23	5	307	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	a	808	CLA	CHD-C1D-ND	-2.12	122.50	124.45
21	3	303	XAT	C39-C29-C28	2.12	121.42	118.08
23	9	314	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	7	316	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
21	9	304	XAT	C10-C11-C12	-2.12	116.60	123.22
21	5	302	XAT	O24-C25-C26	-2.12	57.20	58.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	201	BCR	C15-C16-C17	-2.12	119.13	123.47
21	2	304	XAT	C10-C11-C12	-2.12	116.61	123.22
23	4	309	CLA	C1-C2-C3	-2.12	123.33	126.75
23	b	815	CLA	CHD-C1D-ND	-2.12	122.51	124.45
21	7	303	XAT	O24-C25-C38	2.12	117.59	115.06
23	3	313	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	b	808	CLA	CHD-C1D-ND	-2.12	122.51	124.45
21	6	303	XAT	O4-C5-C4	2.12	114.97	113.38
23	9	318	CLA	CHD-C1D-ND	-2.11	122.51	124.45
31	j	104	BCR	C16-C15-C14	-2.11	119.14	123.47
21	7	305	XAT	O24-C25-C38	2.11	117.59	115.06
21	2	301	XAT	C39-C29-C30	-2.11	119.96	122.92
23	8	305	CLA	CHD-C1D-ND	-2.11	122.51	124.45
21	9	304	XAT	O24-C25-C38	2.11	117.59	115.06
21	7	301	XAT	C10-C11-C12	-2.11	116.62	123.22
21	5	304	XAT	C35-C15-C14	-2.11	119.15	123.47
23	2	308	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
21	7	305	XAT	O4-C5-C18	2.11	117.59	115.06
23	2	309	CLA	CHD-C1D-ND	-2.11	122.51	124.45
23	4	308	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	8	309	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
21	4	301	XAT	C28-C29-C30	2.11	122.18	118.94
25	6	301	A1L1F	C12-C6-C1	-2.11	108.58	110.47
23	b	822	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	b	829	CLA	C1-C2-C3	-2.11	122.40	126.04
23	2	308	CLA	CHD-C1D-ND	-2.11	122.52	124.45
21	2	301	XAT	O24-C25-C38	2.11	117.58	115.06
21	3	303	XAT	C10-C11-C12	-2.11	116.65	123.22
23	a	829	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
31	a	848	BCR	C34-C9-C8	2.11	121.39	118.08
23	9	312	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	b	811	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	b	839	CLA	C1-C2-C3	-2.10	122.41	126.04
23	b	802	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
23	5	315	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	4	311	CLA	O2D-CGD-CBD	2.10	115.00	111.27
31	a	847	BCR	C28-C27-C26	-2.10	110.32	114.08
31	j	104	BCR	C3-C4-C5	-2.10	110.32	114.08
25	h	203	A1L1F	C26-O13-C45	2.10	120.36	115.68
23	b	823	CLA	C1-C2-C3	-2.10	122.41	126.04
23	a	837	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	b	838	CLA	O2A-CGA-O1A	-2.10	118.29	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	306	XAT	O24-C25-C38	2.10	117.57	115.06
21	4	303	XAT	C35-C15-C14	-2.10	119.17	123.47
21	5	304	XAT	O4-C5-C18	2.10	117.57	115.06
21	2	304	XAT	O24-C25-C38	2.10	117.57	115.06
23	a	807	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
23	7	312	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
31	l	201	BCR	C37-C22-C23	2.10	121.38	118.08
23	9	318	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	b	820	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	b	807	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	b	801	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
31	a	849	BCR	C15-C16-C17	-2.10	119.18	123.47
21	9	303	XAT	C11-C12-C13	-2.10	120.53	126.42
23	b	828	CLA	CHD-C1D-ND	-2.10	122.53	124.45
23	4	307	CLA	O2D-CGD-CBD	2.10	114.99	111.27
31	b	846	BCR	C23-C24-C25	-2.10	121.32	127.20
21	4	304	XAT	O4-C5-C18	2.09	117.57	115.06
29	2	317	LMG	C4-C3-C2	-2.09	107.17	110.82
21	2	302	XAT	O24-C25-C38	2.09	117.56	115.06
23	9	316	CLA	CHD-C1D-ND	-2.09	122.53	124.45
21	6	305	XAT	O24-C25-C38	2.09	117.56	115.06
23	7	307	CLA	CHD-C1D-ND	-2.09	122.53	124.45
21	7	304	XAT	C20-C13-C14	-2.09	120.00	122.92
23	b	829	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
21	3	303	XAT	O4-C5-C4	2.09	114.95	113.38
21	7	303	XAT	C15-C35-C34	-2.09	119.20	123.47
21	3	303	XAT	O4-C5-C18	2.09	117.56	115.06
21	2	305	XAT	O4-C5-C18	2.09	117.56	115.06
23	4	308	CLA	O2D-CGD-CBD	2.09	114.97	111.27
28	8	315	DGD	O2G-C1B-O1B	-2.09	118.66	123.70
21	5	302	XAT	C30-C31-C32	-2.09	116.71	123.22
23	9	308	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
31	b	849	BCR	C32-C1-C6	-2.08	106.92	110.30
31	b	842	BCR	C37-C22-C23	2.08	121.36	118.08
21	1	303	XAT	C11-C10-C9	-2.08	124.34	127.31
21	3	301	XAT	O4-C5-C18	2.08	117.55	115.06
31	b	846	BCR	C37-C22-C23	2.08	121.36	118.08
23	7	313	CLA	C1-C2-C3	-2.08	122.44	126.04
23	1	306	CLA	C1-C2-C3	-2.08	122.44	126.04
21	8	301	XAT	O4-C5-C18	2.08	117.55	115.06
21	3	304	XAT	C35-C15-C14	-2.08	119.21	123.47
23	a	844	CLA	C1-C2-C3	-2.08	122.44	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	852	XAT	O24-C25-C38	2.08	117.55	115.06
25	6	301	A1L1F	C5-C6-C1	-2.08	108.61	110.47
21	4	305	XAT	O4-C5-C18	2.08	117.55	115.06
21	6	303	XAT	O4-C5-C18	2.08	117.55	115.06
21	9	304	XAT	C40-C33-C32	2.08	121.35	118.08
23	6	311	CLA	CHD-C1D-ND	-2.08	122.55	124.45
23	b	813	CLA	CHD-C1D-ND	-2.08	122.55	124.45
21	6	303	XAT	C27-C28-C29	-2.07	122.31	125.53
23	a	824	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	b	819	CLA	CHD-C1D-ND	-2.07	122.55	124.45
21	2	302	XAT	C27-C28-C29	-2.07	122.31	125.53
23	4	313	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	b	812	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
31	f	804	BCR	C35-C13-C14	-2.07	120.02	122.92
23	1	310	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	3	309	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	b	834	CLA	C1-C2-C3	-2.07	122.46	126.04
21	7	305	XAT	C7-C8-C9	-2.07	122.31	125.53
21	5	301	XAT	O4-C5-C18	2.07	117.54	115.06
23	b	808	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	5	305	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	9	308	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	a	836	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	b	831	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	a	840	CLA	CHD-C1D-ND	-2.07	122.55	124.45
21	4	302	XAT	O24-C25-C38	2.07	117.53	115.06
23	b	819	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
21	a	852	XAT	C39-C29-C28	2.07	121.33	118.08
25	8	304	A1L1F	C20-C21-C22	-2.06	108.66	112.75
21	1	302	XAT	O24-C25-C38	2.06	117.53	115.06
23	8	311	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
23	b	839	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
25	9	302	A1L1F	C17-C20-C21	2.06	116.60	114.28
23	a	844	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
23	b	824	CLA	CHD-C1D-ND	-2.06	122.56	124.45
21	a	852	XAT	C20-C13-C14	-2.06	120.03	122.92
31	b	844	BCR	C8-C9-C10	2.06	122.11	118.94
23	a	825	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	f	803	CLA	C1-C2-C3	-2.06	122.48	126.04
23	4	317	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	b	801	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	b	817	CLA	CHD-C1D-ND	-2.06	122.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	302	XAT	O4-C5-C4	2.06	114.93	113.38
23	a	834	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	b	830	CLA	CMA-C3A-C2A	-2.06	111.30	116.10
23	a	854	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	9	309	CLA	CHD-C1D-ND	-2.06	122.56	124.45
25	8	304	A1L1F	C27-C34-C33	2.06	121.31	118.08
23	b	827	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
21	1	302	XAT	O4-C5-C18	2.05	117.52	115.06
21	8	303	XAT	O24-C25-C38	2.05	117.52	115.06
23	9	308	CLA	C1-C2-C3	-2.05	122.49	126.04
23	2	312	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
23	1	306	CLA	CAC-C3C-C4C	2.05	127.47	124.81
21	9	304	XAT	C31-C30-C29	-2.05	124.38	127.31
31	a	849	BCR	C37-C22-C23	2.05	121.31	118.08
23	4	315	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	2	307	CLA	C2A-C1A-CHA	2.05	127.45	123.86
23	b	816	CLA	C1-C2-C3	-2.05	122.50	126.04
23	j	102	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	b	814	CLA	C1-C2-C3	-2.05	122.50	126.04
21	7	304	XAT	C8-C9-C10	2.05	122.09	118.94
23	b	840	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	5	308	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
31	b	844	BCR	C16-C15-C14	-2.05	119.28	123.47
21	2	303	XAT	O24-C25-C38	2.05	117.51	115.06
21	2	304	XAT	C15-C35-C34	-2.05	119.28	123.47
23	a	827	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	6	310	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	b	820	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	h	204	CLA	O2D-CGD-CBD	2.05	114.91	111.27
21	3	305	XAT	O4-C5-C18	2.05	117.51	115.06
21	3	305	XAT	O24-C25-C38	2.05	117.51	115.06
23	b	837	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
31	f	804	BCR	C33-C5-C4	2.05	117.55	113.62
28	b	848	DGD	O5E-C6E-C5E	-2.05	104.27	111.29
23	b	829	CLA	O2D-CGD-CBD	2.05	114.91	111.27
23	b	805	CLA	CHD-C1D-ND	-2.05	122.57	124.45
31	f	801	BCR	C36-C18-C17	-2.05	120.06	122.92
23	a	809	CLA	O2D-CGD-CBD	2.05	114.90	111.27
23	3	313	CLA	C1-C2-C3	-2.04	122.51	126.04
21	2	304	XAT	C40-C33-C32	2.04	121.30	118.08
23	f	802	CLA	C1-C2-C3	-2.04	122.51	126.04
21	3	304	XAT	O24-C25-C38	2.04	117.50	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	801	CLA	O1D-CGD-CBD	2.04	128.66	124.48
31	h	201	BCR	C35-C13-C12	2.04	121.30	118.08
23	a	808	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	9	305	45D	C31-C33-C35	-2.04	120.68	126.42
23	5	314	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	3	315	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	4	302	XAT	O4-C5-C18	2.04	117.50	115.06
21	7	301	XAT	O4-C5-C4	2.04	114.91	113.38
21	7	304	XAT	C31-C32-C33	-2.04	120.69	126.42
31	b	849	BCR	C34-C9-C10	-2.04	120.07	122.92
23	4	314	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	2	315	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	1	307	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	3	301	XAT	O24-C25-C38	2.04	117.50	115.06
23	8	312	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	a	818	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	b	817	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
31	h	201	BCR	C28-C27-C26	-2.04	110.44	114.08
21	8	302	XAT	O4-C5-C18	2.03	117.49	115.06
23	1	311	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
21	4	301	XAT	O4-C5-C18	2.03	117.49	115.06
23	a	822	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	9	306	A1L1G	C20-C21-C22	2.03	116.77	112.75
24	1	315	SQD	O7-S-C6	2.03	109.36	106.94
23	1	204	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	5	311	CLA	C1-C2-C3	-2.03	122.53	126.04
23	2	310	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	a	832	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
21	5	301	XAT	C39-C29-C28	2.03	121.28	118.08
23	b	803	CLA	O2D-CGD-CBD	2.03	114.88	111.27
31	a	848	BCR	C28-C27-C26	-2.03	110.45	114.08
23	9	315	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	h	204	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	9	316	CLA	C1-C2-C3	-2.03	122.53	126.04
23	a	840	CLA	C1-C2-C3	-2.03	122.53	126.04
31	f	804	BCR	C21-C20-C19	-2.03	116.89	123.22
23	1	306	CLA	CHD-C1D-ND	-2.03	122.59	124.45
31	a	847	BCR	C20-C19-C18	-2.03	120.72	126.42
21	4	304	XAT	C19-C9-C8	2.03	121.27	118.08
21	2	302	XAT	C19-C9-C8	2.03	121.27	118.08
21	6	306	XAT	C10-C11-C12	-2.03	116.89	123.22
23	b	804	CLA	O2D-CGD-CBD	2.03	114.87	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	306	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
21	9	303	XAT	C19-C9-C8	2.02	121.27	118.08
21	1	303	XAT	O24-C25-C38	2.02	117.48	115.06
23	b	808	CLA	O2D-CGD-CBD	2.02	114.86	111.27
21	2	304	XAT	C30-C31-C32	-2.02	116.90	123.22
21	6	302	XAT	C39-C29-C30	-2.02	120.09	122.92
23	1	307	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
21	7	304	XAT	O4-C5-C18	2.02	117.48	115.06
21	2	301	XAT	C19-C9-C8	2.02	121.26	118.08
21	7	301	XAT	C19-C9-C8	2.02	121.26	118.08
31	j	104	BCR	C29-C30-C25	2.02	113.59	110.48
23	b	817	CLA	C1-C2-C3	-2.02	122.55	126.04
25	6	304	A1L1F	C12-C6-C1	-2.02	108.66	110.47
23	8	307	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
28	8	315	DGD	C4D-C3D-C2D	-2.02	107.30	110.82
23	4	316	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	2	314	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	a	823	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
21	6	306	XAT	O4-C5-C18	2.02	117.47	115.06
21	7	301	XAT	O4-C5-C18	2.02	117.47	115.06
21	1	303	XAT	C20-C13-C12	2.02	121.26	118.08
21	7	305	XAT	C11-C12-C13	-2.02	120.75	126.42
23	3	311	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	a	811	CLA	C1-C2-C3	-2.02	122.55	126.04
31	b	846	BCR	C33-C5-C4	2.02	117.49	113.62
23	a	814	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
24	5	316	SQD	O8-S-C6	2.02	108.95	105.74
21	3	304	XAT	O4-C5-C4	2.02	114.90	113.38
23	7	306	CLA	CHD-C1D-ND	-2.02	122.60	124.45
21	2	305	XAT	C10-C11-C12	-2.01	116.93	123.22
23	1	311	CLA	O2D-CGD-CBD	2.01	114.85	111.27
23	a	835	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
21	4	304	XAT	O24-C25-C38	2.01	117.47	115.06
21	2	304	XAT	O4-C5-C18	2.01	117.47	115.06
31	b	844	BCR	C1-C6-C7	2.01	121.47	115.78
23	3	308	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
23	2	313	CLA	CHD-C1D-ND	-2.01	122.61	124.45
31	f	804	BCR	C8-C7-C6	-2.01	121.55	127.20
23	a	830	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
21	4	303	XAT	O4-C5-C18	2.01	117.47	115.06
23	9	313	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	8	306	CLA	CHD-C1D-ND	-2.01	122.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	310	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	3	308	CLA	O2D-CGD-CBD	2.01	114.84	111.27
21	7	305	XAT	O4-C5-C4	2.01	114.89	113.38
23	b	804	CLA	CAC-C3C-C4C	2.01	127.42	124.81
23	a	809	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	b	816	CLA	O2D-CGD-CBD	2.01	114.84	111.27
23	b	825	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
21	7	303	XAT	O4-C5-C18	2.01	117.46	115.06
23	b	807	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	6	313	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	a	842	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	1	304	A1L1F	C25-C14-C29	-2.01	121.75	125.99
28	4	318	DGD	C4D-C3D-C2D	-2.01	107.32	110.82
23	a	838	CLA	CHD-C1D-ND	-2.01	122.61	124.45
31	b	845	BCR	C2-C1-C6	2.00	113.57	110.48
23	6	316	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	5	305	CLA	C2D-C1D-ND	-2.00	108.63	110.10
31	j	104	BCR	C21-C20-C19	-2.00	116.96	123.22
23	a	838	CLA	C1-C2-C3	-2.00	122.58	126.04
21	7	303	XAT	C31-C32-C33	-2.00	120.79	126.42
21	3	303	XAT	C19-C9-C8	2.00	121.23	118.08
21	8	301	XAT	C39-C29-C28	2.00	121.23	118.08
23	b	814	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	b	836	CLA	O2D-CGD-CBD	2.00	114.83	111.27
23	b	822	CLA	CHD-C1D-ND	-2.00	122.61	124.45
31	b	842	BCR	C33-C5-C6	-2.00	122.28	124.53

All (188) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	5	305	CLA	ND
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	9	308	CLA	ND

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Mol	Chain	Res	Type	Atom
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	9	318	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	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
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	4	317	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

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Mol	Chain	Res	Type	Atom
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	6	317	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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
23	a	844	CLA	ND
23	a	854	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
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

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Mol	Chain	Res	Type	Atom
23	f	802	CLA	ND
23	f	803	CLA	ND
23	h	204	CLA	ND
23	j	102	CLA	ND
23	j	103	CLA	ND
23	l	202	CLA	ND
23	l	203	CLA	ND
23	l	204	CLA	ND

All (2081) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	5	302	XAT	O4-C6-C7-C8
21	5	302	XAT	C7-C8-C9-C10
21	5	302	XAT	C7-C8-C9-C19
21	9	303	XAT	O4-C6-C7-C8
21	9	304	XAT	O24-C26-C27-C28
21	8	301	XAT	C7-C8-C9-C19
21	8	302	XAT	O4-C6-C7-C8
21	8	302	XAT	C7-C8-C9-C10
21	8	302	XAT	C7-C8-C9-C19
21	4	301	XAT	C27-C28-C29-C30
21	4	301	XAT	C27-C28-C29-C39
21	4	303	XAT	O4-C6-C7-C8
21	4	303	XAT	C7-C8-C9-C10
21	4	303	XAT	C7-C8-C9-C19
21	4	305	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

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Mol	Chain	Res	Type	Atoms
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	852	XAT	C7-C8-C9-C10
21	a	852	XAT	C7-C8-C9-C19
21	a	852	XAT	C11-C12-C13-C14
21	a	852	XAT	C11-C12-C13-C20
21	a	852	XAT	C27-C28-C29-C30
21	a	852	XAT	C27-C28-C29-C39
21	j	101	XAT	O4-C6-C7-C8
21	j	101	XAT	C7-C8-C9-C10
21	j	101	XAT	C7-C8-C9-C19
21	j	101	XAT	O24-C26-C27-C28
22	5	303	A1L1G	C26-C30-C31-C32
22	5	303	A1L1G	C31-C32-C33-C34
22	5	303	A1L1G	C32-C33-C34-C27
22	5	303	A1L1G	C32-C33-C34-C35
22	5	303	A1L1G	C41-C42-C44-C2
22	5	303	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

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Mol	Chain	Res	Type	Atoms
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
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	307	CLA	CHA-CBD-CGD-O1D
23	5	307	CLA	CHA-CBD-CGD-O2D
23	5	308	CLA	CBD-CGD-O2D-CED
23	5	309	CLA	CHA-CBD-CGD-O1D
23	5	309	CLA	CHA-CBD-CGD-O2D
23	5	309	CLA	CAD-CBD-CGD-O1D
23	5	309	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	5	310	CLA	CBD-CGD-O2D-CED
23	5	314	CLA	C1A-C2A-CAA-CBA
23	5	314	CLA	C3A-C2A-CAA-CBA
23	5	315	CLA	CBD-CGD-O2D-CED
23	5	315	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	9	316	CLA	C1A-C2A-CAA-CBA
23	9	316	CLA	CHA-CBD-CGD-O1D
23	9	316	CLA	CHA-CBD-CGD-O2D
23	9	316	CLA	CAD-CBD-CGD-O1D
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
23	4	306	CLA	C1A-C2A-CAA-CBA
23	4	307	CLA	CHA-CBD-CGD-O2D
23	4	309	CLA	CHA-CBD-CGD-O1D
23	4	309	CLA	CHA-CBD-CGD-O2D
23	4	309	CLA	CBD-CGD-O2D-CED
23	4	310	CLA	C1A-C2A-CAA-CBA
23	4	311	CLA	CBA-CGA-O2A-C1
23	4	311	CLA	CBD-CGD-O2D-CED
23	4	312	CLA	C1A-C2A-CAA-CBA
23	4	312	CLA	C3A-C2A-CAA-CBA
23	4	313	CLA	CHA-CBD-CGD-O1D
23	4	313	CLA	CHA-CBD-CGD-O2D
23	4	315	CLA	CHA-CBD-CGD-O1D
23	4	315	CLA	CHA-CBD-CGD-O2D
23	4	316	CLA	C2A-CAA-CBA-CGA
23	4	316	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	4	317	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	6	317	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
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	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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
23	a	844	CLA	CHA-CBD-CGD-O2D
23	a	854	CLA	C1A-C2A-CAA-CBA
23	b	803	CLA	CHA-CBD-CGD-O1D
23	b	803	CLA	CHA-CBD-CGD-O2D
23	b	803	CLA	CBD-CGD-O2D-CED
23	b	804	CLA	CBD-CGD-O2D-CED
23	b	805	CLA	C2A-CAA-CBA-CGA
23	b	806	CLA	C1A-C2A-CAA-CBA
23	b	806	CLA	C3A-C2A-CAA-CBA
23	b	806	CLA	CHA-CBD-CGD-O1D
23	b	806	CLA	CHA-CBD-CGD-O2D
23	b	806	CLA	CAD-CBD-CGD-O1D
23	b	810	CLA	C1A-C2A-CAA-CBA
23	b	810	CLA	C2A-CAA-CBA-CGA
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
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	C3A-C2A-CAA-CBA
23	b	833	CLA	C11-C12-C13-C14
23	b	834	CLA	CBD-CGD-O2D-CED
23	b	836	CLA	CHA-CBD-CGD-O1D
23	b	836	CLA	CHA-CBD-CGD-O2D
23	b	839	CLA	C1A-C2A-CAA-CBA
23	b	839	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	b	839	CLA	CHA-CBD-CGD-O1D
23	b	839	CLA	CHA-CBD-CGD-O2D
23	b	839	CLA	CAD-CBD-CGD-O1D
23	b	839	CLA	CBD-CGD-O2D-CED
23	j	102	CLA	C1A-C2A-CAA-CBA
23	j	102	CLA	C2-C3-C5-C6
23	j	102	CLA	C4-C3-C5-C6
23	j	103	CLA	CAD-CBD-CGD-O1D
23	j	103	CLA	CAD-CBD-CGD-O2D
23	j	103	CLA	CBD-CGD-O2D-CED
23	l	202	CLA	CHA-CBD-CGD-O1D
23	l	202	CLA	CHA-CBD-CGD-O2D
23	l	203	CLA	CHA-CBD-CGD-O1D
23	l	203	CLA	CHA-CBD-CGD-O2D
23	l	203	CLA	C6-C7-C8-C9
24	5	316	SQD	O49-C7-O47-C45
24	5	316	SQD	C8-C7-O47-C45
24	5	316	SQD	C5-C6-S-O7
24	5	316	SQD	C5-C6-S-O8
24	5	316	SQD	C5-C6-S-O9
24	1	315	SQD	O5-C5-C6-S
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	C29-C14-C25-C24
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	203	A1L1F	C56-C54-O7-C8
25	h	203	A1L1F	O55-C54-O7-C8
26	9	305	45D	C04-C08-C20-C24
27	9	307	LHG	C3-O3-P-O4
27	9	307	LHG	C3-O3-P-O5
27	9	307	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
27	9	307	LHG	O9-C7-O7-C5
27	9	307	LHG	C8-C7-O7-C5
27	9	317	LHG	C1-C2-C3-O3
27	9	317	LHG	C3-O3-P-O4
27	9	317	LHG	O9-C7-O7-C5
27	9	317	LHG	C8-C7-O7-C5
27	a	845	LHG	O1-C1-C2-C3
27	a	845	LHG	C3-O3-P-O4
27	a	845	LHG	C4-O6-P-O3
27	a	845	LHG	C4-O6-P-O5
27	a	845	LHG	O6-C4-C5-O7
27	a	845	LHG	O7-C5-C6-O8
27	a	846	LHG	O1-C1-C2-C3
27	a	846	LHG	O6-C4-C5-O7
27	b	847	LHG	O1-C1-C2-C3
27	b	847	LHG	C1-C2-C3-O3
27	b	847	LHG	O2-C2-C3-O3
27	b	847	LHG	C3-O3-P-O5
27	b	847	LHG	C4-O6-P-O3
27	b	847	LHG	C4-O6-P-O4
27	b	847	LHG	C4-O6-P-O5
28	8	315	DGD	C2B-C1B-O2G-C2G
28	8	315	DGD	C2E-C1E-O5D-C6D
28	8	315	DGD	O6E-C1E-O5D-C6D
28	4	318	DGD	C2B-C1B-O2G-C2G
28	4	318	DGD	O1B-C1B-O2G-C2G
28	4	318	DGD	C2E-C1E-O5D-C6D
28	4	318	DGD	O6E-C1E-O5D-C6D
29	2	317	LMG	O1-C7-C8-O7
29	a	853	LMG	C11-C10-O7-C8
29	j	105	LMG	O9-C10-O7-C8
29	j	105	LMG	C11-C10-O7-C8
31	a	850	BCR	C23-C24-C25-C26
31	b	842	BCR	C7-C8-C9-C10
31	b	842	BCR	C7-C8-C9-C34
31	b	844	BCR	C1-C6-C7-C8
31	b	844	BCR	C5-C6-C7-C8
31	i	101	BCR	C21-C22-C23-C24
31	i	101	BCR	C37-C22-C23-C24
31	j	104	BCR	C7-C8-C9-C10
31	j	104	BCR	C7-C8-C9-C34
31	m	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	m	101	BCR	C7-C8-C9-C34
31	m	101	BCR	C21-C22-C23-C24
31	m	101	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	310	CLA	O1D-CGD-O2D-CED
23	9	315	CLA	O1D-CGD-O2D-CED
23	4	309	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	803	CLA	O1D-CGD-O2D-CED
23	b	834	CLA	O1D-CGD-O2D-CED
23	5	313	CLA	CBD-CGD-O2D-CED
23	9	318	CLA	CBD-CGD-O2D-CED
23	8	306	CLA	CBD-CGD-O2D-CED
23	4	306	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	1	307	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
27	9	317	LHG	O10-C23-O8-C6
29	2	317	LMG	O10-C28-O8-C9
23	7	310	CLA	O1A-CGA-O2A-C1
23	4	316	CLA	O1D-CGD-O2D-CED
23	7	315	CLA	O1D-CGD-O2D-CED
23	b	804	CLA	O1D-CGD-O2D-CED
23	5	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	4	317	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	839	CLA	O1D-CGD-O2D-CED
23	j	103	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
27	9	317	LHG	C24-C23-O8-C6
23	5	305	CLA	CBD-CGD-O2D-CED
23	5	306	CLA	CBD-CGD-O2D-CED
23	5	309	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
23	2	316	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	806	CLA	CBD-CGD-O2D-CED
23	b	819	CLA	CBD-CGD-O2D-CED
23	b	835	CLA	CBD-CGD-O2D-CED
23	h	204	CLA	CBD-CGD-O2D-CED
23	4	310	CLA	O1A-CGA-O2A-C1
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
27	b	847	LHG	O10-C23-O8-C6
28	8	315	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
29	a	853	LMG	O10-C28-O8-C9
23	4	311	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	311	CLA	O1D-CGD-O2D-CED
23	6	314	CLA	O1D-CGD-O2D-CED
23	4	307	CLA	CBD-CGD-O2D-CED
23	6	312	CLA	CBD-CGD-O2D-CED
23	7	308	CLA	CBD-CGD-O2D-CED
23	a	818	CLA	CBD-CGD-O2D-CED
23	a	837	CLA	CBD-CGD-O2D-CED
28	8	315	DGD	O1B-C1B-O2G-C2G
29	a	853	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	204	CLA	O1A-CGA-O2A-C1
23	1	309	CLA	O1D-CGD-O2D-CED
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
23	a	810	CLA	C3-C5-C6-C7
23	b	802	CLA	C3-C5-C6-C7
23	b	805	CLA	C3-C5-C6-C7
23	b	807	CLA	C3-C5-C6-C7
23	b	809	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
29	2	317	LMG	C29-C28-O8-C9
29	a	853	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
25	1	304	A1L1F	O55-C54-O7-C8
23	9	316	CLA	CBD-CGD-O2D-CED
23	3	309	CLA	CBD-CGD-O2D-CED
23	3	315	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	1	204	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	a	841	CLA	CBD-CGD-O2D-CED
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	833	CLA	C2A-CAA-CBA-CGA
23	b	838	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
23	1	310	CLA	C3-C5-C6-C7
23	b	818	CLA	C3-C5-C6-C7
23	9	316	CLA	CBA-CGA-O2A-C1
23	4	310	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	806	CLA	CBA-CGA-O2A-C1
23	b	818	CLA	CBA-CGA-O2A-C1
27	9	307	LHG	C24-C23-O8-C6
27	b	847	LHG	C24-C23-O8-C6
28	8	315	DGD	C2A-C1A-O1G-C1G
29	j	105	LMG	C29-C28-O8-C9
29	j	105	LMG	C12-C13-C14-C15
23	6	313	CLA	O1D-CGD-O2D-CED
23	7	317	CLA	CBD-CGD-O2D-CED
29	j	105	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
23	5	311	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	806	CLA	O1A-CGA-O2A-C1
23	b	818	CLA	O1A-CGA-O2A-C1
29	j	105	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	308	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	840	CLA	CBD-CGD-O2D-CED
23	9	318	CLA	O1D-CGD-O2D-CED
23	8	306	CLA	O1D-CGD-O2D-CED
27	9	307	LHG	O2-C2-C3-O3
27	9	317	LHG	O2-C2-C3-O3
27	a	845	LHG	O2-C2-C3-O3
23	7	306	CLA	CBA-CGA-O2A-C1
23	a	812	CLA	CBA-CGA-O2A-C1
23	b	839	CLA	CBA-CGA-O2A-C1
23	a	836	CLA	O1A-CGA-O2A-C1
23	b	823	CLA	O1A-CGA-O2A-C1
27	9	307	LHG	O10-C23-O8-C6
23	4	306	CLA	O1D-CGD-O2D-CED
23	9	312	CLA	CBA-CGA-O2A-C1
23	6	314	CLA	CBA-CGA-O2A-C1
23	5	311	CLA	CBD-CGD-O2D-CED
23	b	822	CLA	CBD-CGD-O2D-CED
23	b	839	CLA	O1A-CGA-O2A-C1
25	9	302	A1L1F	C47-C48-C49-C50
27	a	845	LHG	C12-C13-C14-C15
29	2	317	LMG	C29-C30-C31-C32
28	b	848	DGD	O6E-C5E-C6E-O5E
23	5	309	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	a	807	CLA	C3-C5-C6-C7
23	a	835	CLA	C3-C5-C6-C7
23	5	311	CLA	CBA-CGA-O2A-C1
23	6	309	CLA	CBA-CGA-O2A-C1
23	a	820	CLA	CBA-CGA-O2A-C1
27	a	845	LHG	C28-C29-C30-C31
23	9	316	CLA	O1A-CGA-O2A-C1
23	a	807	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	310	CLA	C2A-CAA-CBA-CGA
23	4	311	CLA	C2A-CAA-CBA-CGA
23	b	801	CLA	C2A-CAA-CBA-CGA
23	b	826	CLA	C2A-CAA-CBA-CGA
23	5	313	CLA	O1D-CGD-O2D-CED
29	a	853	LMG	O6-C5-C6-O5
29	j	105	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
27	a	845	LHG	C23-C24-C25-C26
23	a	804	CLA	O1D-CGD-O2D-CED
23	b	806	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
23	b	807	CLA	CBD-CGD-O2D-CED
23	b	835	CLA	O1D-CGD-O2D-CED
27	9	307	LHG	C1-C2-C3-O3
27	a	845	LHG	C1-C2-C3-O3
23	h	204	CLA	O1D-CGD-O2D-CED
23	5	308	CLA	CBA-CGA-O2A-C1
23	8	311	CLA	CBA-CGA-O2A-C1
23	3	311	CLA	CBA-CGA-O2A-C1
23	6	317	CLA	CBA-CGA-O2A-C1
23	a	809	CLA	CBA-CGA-O2A-C1
23	a	839	CLA	CBA-CGA-O2A-C1
23	a	854	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	b	820	CLA	CBA-CGA-O2A-C1
23	b	826	CLA	CBA-CGA-O2A-C1
23	b	833	CLA	CBA-CGA-O2A-C1
23	4	315	CLA	CBD-CGD-O2D-CED
23	6	317	CLA	CBD-CGD-O2D-CED
29	a	853	LMG	C4-C5-C6-O5
23	5	305	CLA	O1D-CGD-O2D-CED
22	5	303	A1L1G	C40-C41-C42-C44
25	8	304	A1L1F	C40-C41-C42-C44
23	a	810	CLA	C13-C15-C16-C17
23	9	318	CLA	C8-C10-C11-C12
23	8	307	CLA	C5-C6-C7-C8
23	a	807	CLA	C5-C6-C7-C8
23	b	809	CLA	C5-C6-C7-C8
27	a	846	LHG	O2-C2-C3-O3
29	a	853	LMG	C28-C29-C30-C31
23	8	311	CLA	O1A-CGA-O2A-C1
23	a	809	CLA	O1A-CGA-O2A-C1
23	a	854	CLA	O1A-CGA-O2A-C1
23	a	813	CLA	C2-C3-C5-C6
23	9	318	CLA	C11-C10-C8-C9
23	9	318	CLA	C11-C12-C13-C14
23	8	307	CLA	C11-C10-C8-C9
23	8	311	CLA	C6-C7-C8-C9
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	805	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	838	CLA	C6-C7-C8-C9
23	f	802	CLA	C11-C12-C13-C14
23	2	316	CLA	O1D-CGD-O2D-CED
23	a	814	CLA	O1D-CGD-O2D-CED
23	b	807	CLA	C15-C16-C17-C18
23	2	310	CLA	C2A-CAA-CBA-CGA
23	7	310	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	h	204	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
31	b	849	BCR	C7-C8-C9-C34
31	l	205	BCR	C7-C8-C9-C34
31	l	205	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
31	b	849	BCR	C7-C8-C9-C10
31	l	205	BCR	C7-C8-C9-C10
31	l	205	BCR	C21-C22-C23-C24
28	b	848	DGD	C1A-C2A-C3A-C4A
23	3	311	CLA	O1A-CGA-O2A-C1
23	6	317	CLA	O1A-CGA-O2A-C1
23	b	820	CLA	O1A-CGA-O2A-C1
23	a	834	CLA	C15-C16-C17-C18
23	b	801	CLA	C15-C16-C17-C18
25	6	301	A1L1F	O55-C54-O7-C8
25	1	304	A1L1F	C49-C50-C51-C52
23	9	313	CLA	CBA-CGA-O2A-C1
23	4	316	CLA	CBA-CGA-O2A-C1
23	2	312	CLA	CBA-CGA-O2A-C1
23	b	838	CLA	CBA-CGA-O2A-C1
23	2	310	CLA	C15-C16-C17-C18
23	a	809	CLA	C5-C6-C7-C8
23	b	832	CLA	C13-C15-C16-C17
23	b	833	CLA	C13-C15-C16-C17
23	5	309	CLA	O1D-CGD-O2D-CED
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	309	CLA	C13-C15-C16-C17
23	9	308	CLA	C5-C6-C7-C8
23	9	318	CLA	C10-C11-C12-C13
23	4	308	CLA	C10-C11-C12-C13
23	1	306	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
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	809	CLA	C8-C10-C11-C12
23	b	840	CLA	C13-C15-C16-C17
23	l	203	CLA	C10-C11-C12-C13
23	5	308	CLA	O1A-CGA-O2A-C1
27	a	846	LHG	C7-C8-C9-C10
27	b	847	LHG	C7-C8-C9-C10
29	a	853	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	836	CLA	C5-C6-C7-C8
25	1	304	A1L1F	C45-C47-C48-C49
23	b	802	CLA	CBD-CGD-O2D-CED
23	7	306	CLA	O2A-C1-C2-C3
23	7	309	CLA	O2A-C1-C2-C3
23	7	308	CLA	C4-C3-C5-C6
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	808	CLA	C12-C13-C15-C16
23	a	801	CLA	C3-C5-C6-C7
23	a	839	CLA	O1A-CGA-O2A-C1
23	b	833	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

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Mol	Chain	Res	Type	Atoms
23	5	306	CLA	O1D-CGD-O2D-CED
23	6	312	CLA	O1D-CGD-O2D-CED
23	7	308	CLA	O1D-CGD-O2D-CED
23	a	837	CLA	O1D-CGD-O2D-CED
23	9	308	CLA	C8-C10-C11-C12
23	1	306	CLA	C15-C16-C17-C18
23	b	840	CLA	C10-C11-C12-C13
23	5	305	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	303	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	4	307	CLA	O1D-CGD-O2D-CED
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	f	802	CLA	C13-C15-C16-C17
23	h	204	CLA	C5-C6-C7-C8
23	2	312	CLA	O1A-CGA-O2A-C1
23	7	316	CLA	O1A-CGA-O2A-C1
23	7	308	CLA	C10-C11-C12-C13
23	b	836	CLA	C8-C10-C11-C12
30	b	841	PQN	C23-C25-C26-C27
23	3	315	CLA	O1D-CGD-O2D-CED
23	a	839	CLA	C13-C15-C16-C17
23	b	801	CLA	C13-C15-C16-C17
23	b	802	CLA	C8-C10-C11-C12
23	b	827	CLA	C13-C15-C16-C17
23	f	802	CLA	C5-C6-C7-C8
23	l	203	CLA	C8-C10-C11-C12
27	a	845	LHG	C3-O3-P-O6
27	b	847	LHG	C3-O3-P-O6
23	7	313	CLA	C3-C5-C6-C7
28	b	848	DGD	C4E-C5E-C6E-O5E
23	4	317	CLA	CBA-CGA-O2A-C1
23	a	816	CLA	CBA-CGA-O2A-C1
23	b	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	b	831	CLA	CBA-CGA-O2A-C1
23	6	314	CLA	O1A-CGA-O2A-C1
23	b	801	CLA	C8-C10-C11-C12
23	9	316	CLA	O1D-CGD-O2D-CED
23	1	308	CLA	C4-C3-C5-C6
23	8	313	CLA	O1A-CGA-O2A-C1
23	7	316	CLA	C2C-C3C-CAC-CBC
23	5	306	CLA	C2A-CAA-CBA-CGA
23	1	314	CLA	C2A-CAA-CBA-CGA
23	b	828	CLA	C2A-CAA-CBA-CGA
23	9	316	CLA	C16-C17-C18-C20
23	a	801	CLA	C16-C17-C18-C20
23	4	313	CLA	C3-C5-C6-C7
23	a	814	CLA	CBA-CGA-O2A-C1
23	a	838	CLA	CBA-CGA-O2A-C1
23	b	824	CLA	C5-C6-C7-C8
22	9	306	A1L1G	C40-C41-C42-C44
27	a	845	LHG	C11-C10-C9-C8
28	4	318	DGD	C3B-C4B-C5B-C6B
23	a	836	CLA	CBD-CGD-O2D-CED
24	1	315	SQD	C8-C7-O47-C45
23	9	310	CLA	CBA-CGA-O2A-C1
23	a	824	CLA	CBA-CGA-O2A-C1
23	b	829	CLA	C10-C11-C12-C13
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
27	9	307	LHG	C34-C35-C36-C37
28	b	848	DGD	C9B-CAB-CBB-CCB
23	3	309	CLA	O1D-CGD-O2D-CED
23	a	841	CLA	O1D-CGD-O2D-CED
23	b	823	CLA	O1D-CGD-O2D-CED
23	b	833	CLA	C16-C17-C18-C19
23	b	840	CLA	C16-C17-C18-C20
23	a	833	CLA	CBA-CGA-O2A-C1
23	a	844	CLA	CBA-CGA-O2A-C1
27	9	307	LHG	C31-C32-C33-C34
24	1	315	SQD	O49-C7-O47-C45
23	a	854	CLA	C5-C6-C7-C8
23	b	839	CLA	C5-C6-C7-C8
27	a	845	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	a	835	CLA	O1D-CGD-O2D-CED
23	b	838	CLA	O1A-CGA-O2A-C1
27	9	307	LHG	C27-C28-C29-C30
27	9	307	LHG	C28-C29-C30-C31
27	a	845	LHG	C13-C14-C15-C16
23	7	317	CLA	O1D-CGD-O2D-CED
23	b	827	CLA	O1D-CGD-O2D-CED
22	5	303	A1L1G	C29-C30-C31-C32
22	9	301	A1L1G	C29-C30-C31-C32
22	9	306	A1L1G	C29-C30-C31-C32
25	9	302	A1L1F	C45-C47-C48-C49
23	a	834	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
27	9	317	LHG	C9-C10-C11-C12
23	4	317	CLA	O1A-CGA-O2A-C1
23	a	816	CLA	O1A-CGA-O2A-C1
23	b	802	CLA	O1A-CGA-O2A-C1
23	4	308	CLA	C16-C17-C18-C20
23	b	811	CLA	C6-C7-C8-C9
23	4	310	CLA	C4-C3-C5-C6
23	b	839	CLA	C4-C3-C5-C6
28	4	318	DGD	C2B-C3B-C4B-C5B
23	1	308	CLA	C2-C3-C5-C6
23	b	807	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
29	2	317	LMG	C28-C29-C30-C31
23	5	315	CLA	C2C-C3C-CAC-CBC
27	9	317	LHG	C11-C12-C13-C14
28	b	848	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

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Mol	Chain	Res	Type	Atoms
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
31	a	850	BCR	C37-C22-C23-C24
31	f	801	BCR	C37-C22-C23-C24
28	b	848	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
31	a	850	BCR	C21-C22-C23-C24
31	f	801	BCR	C21-C22-C23-C24
23	b	827	CLA	C8-C10-C11-C12
30	a	843	PQN	C25-C26-C27-C28
25	8	304	A1L1F	C45-C47-C48-C49
23	b	840	CLA	O1D-CGD-O2D-CED
27	9	317	LHG	C28-C29-C30-C31
23	a	814	CLA	O1A-CGA-O2A-C1
23	9	316	CLA	C16-C17-C18-C19
23	f	802	CLA	C16-C17-C18-C19
23	f	802	CLA	C16-C17-C18-C20
23	6	317	CLA	C10-C11-C12-C13
23	a	827	CLA	C8-C10-C11-C12
23	a	841	CLA	C8-C10-C11-C12
23	b	806	CLA	C15-C16-C17-C18
23	b	835	CLA	C5-C6-C7-C8
23	6	316	CLA	CBD-CGD-O2D-CED
24	1	315	SQD	C11-C10-C9-C8
27	9	317	LHG	C14-C15-C16-C17
23	a	814	CLA	C5-C6-C7-C8
23	b	809	CLA	C10-C11-C12-C13
25	9	302	A1L1F	C48-C49-C50-C51
25	1	304	A1L1F	C47-C48-C49-C50
25	h	203	A1L1F	C47-C48-C49-C50
23	4	308	CLA	O1D-CGD-O2D-CED
23	a	810	CLA	O1D-CGD-O2D-CED
23	9	310	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	9	313	CLA	C3A-C2A-CAA-CBA
23	4	310	CLA	C3A-C2A-CAA-CBA
23	3	312	CLA	C3A-C2A-CAA-CBA
23	3	314	CLA	C3A-C2A-CAA-CBA
23	6	317	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	854	CLA	C3A-C2A-CAA-CBA
23	b	810	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	a	807	CLA	O1D-CGD-O2D-CED
23	b	831	CLA	O1A-CGA-O2A-C1
23	b	801	CLA	C16-C17-C18-C20
23	b	811	CLA	C6-C7-C8-C10
28	b	848	DGD	C4B-C5B-C6B-C7B
23	3	314	CLA	CBD-CGD-O2D-CED
28	b	848	DGD	C2B-C3B-C4B-C5B
22	9	301	A1L1G	C35-C36-C37-C38
22	3	306	A1L1G	C35-C36-C37-C38
31	m	101	BCR	C14-C15-C16-C17
23	b	816	CLA	CBA-CGA-O2A-C1
23	4	310	CLA	C2-C3-C5-C6
23	a	828	CLA	C2-C3-C5-C6
23	b	839	CLA	C2-C3-C5-C6
23	j	102	CLA	CBD-CGD-O2D-CED
27	a	845	LHG	O1-C1-C2-O2
27	a	846	LHG	O1-C1-C2-O2
27	b	847	LHG	O1-C1-C2-O2
23	b	833	CLA	C16-C17-C18-C20
23	b	808	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	808	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	9	305	45D	C16-C08-C20-C24
31	a	850	BCR	C23-C24-C25-C30
31	b	843	BCR	C1-C6-C7-C8
31	b	843	BCR	C5-C6-C7-C8
31	l	201	BCR	C1-C6-C7-C8
31	l	205	BCR	C23-C24-C25-C26
31	l	205	BCR	C23-C24-C25-C30
31	m	101	BCR	C5-C6-C7-C8
27	9	307	LHG	C30-C31-C32-C33
23	a	823	CLA	CBA-CGA-O2A-C1
23	b	807	CLA	CBA-CGA-O2A-C1
23	b	835	CLA	CBA-CGA-O2A-C1
23	a	809	CLA	C13-C15-C16-C17
23	b	829	CLA	C15-C16-C17-C18
23	b	838	CLA	C15-C16-C17-C18
27	a	845	LHG	C26-C27-C28-C29
23	2	314	CLA	C11-C10-C8-C9
23	4	316	CLA	O1A-CGA-O2A-C1
23	a	840	CLA	C13-C15-C16-C17
23	b	805	CLA	C13-C15-C16-C17
23	j	102	CLA	C8-C10-C11-C12
23	l	310	CLA	C4-C3-C5-C6
23	a	807	CLA	C4-C3-C5-C6
23	a	828	CLA	C4-C3-C5-C6
23	9	316	CLA	C2-C3-C5-C6
23	3	312	CLA	C6-C7-C8-C10
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	b	802	CLA	C11-C12-C13-C15
23	b	807	CLA	C11-C12-C13-C15
23	b	810	CLA	C11-C10-C8-C7
23	b	837	CLA	C11-C12-C13-C15
23	9	308	CLA	O1A-CGA-O2A-C1
23	b	804	CLA	C2C-C3C-CAC-CBC
23	b	810	CLA	C5-C6-C7-C8
25	6	304	A1L1F	C4-C8-O7-C54
23	a	825	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	b	824	CLA	CBA-CGA-O2A-C1
23	4	308	CLA	C15-C16-C17-C18
23	b	832	CLA	C15-C16-C17-C18
28	b	848	DGD	CAB-CBB-CCB-CDB
23	a	811	CLA	C11-C10-C8-C7
24	1	315	SQD	C7-C8-C9-C10
29	2	317	LMG	C10-C11-C12-C13
23	a	806	CLA	C13-C15-C16-C17
28	b	848	DGD	C6A-C7A-C8A-C9A
23	4	307	CLA	C3-C5-C6-C7
28	8	315	DGD	C2B-C3B-C4B-C5B
23	b	816	CLA	O1A-CGA-O2A-C1
28	4	318	DGD	O6D-C1D-O3G-C3G
23	8	307	CLA	C15-C16-C17-C18
27	a	846	LHG	C8-C7-O7-C5
28	b	848	DGD	C2B-C1B-O2G-C2G
27	b	847	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
27	a	846	LHG	O9-C7-O7-C5
23	2	308	CLA	C3-C5-C6-C7
23	5	311	CLA	O1D-CGD-O2D-CED
28	4	318	DGD	O1G-C1G-C2G-O2G
23	b	840	CLA	C16-C17-C18-C19
23	4	308	CLA	C13-C15-C16-C17
23	b	809	CLA	C15-C16-C17-C18
23	9	316	CLA	C4-C3-C5-C6
23	b	807	CLA	C4-C3-C5-C6
23	b	834	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	803	CLA	C2-C3-C5-C6
23	4	308	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	807	CLA	C14-C13-C15-C16
23	a	814	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	a	826	CLA	C11-C10-C8-C9
23	a	831	CLA	C11-C10-C8-C9
23	b	802	CLA	C11-C12-C13-C14
23	b	807	CLA	C11-C12-C13-C14
23	b	807	CLA	C14-C13-C15-C16
23	b	810	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	837	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
21	5	301	XAT	C7-C8-C9-C19
21	7	304	XAT	C7-C8-C9-C19
22	9	306	A1L1G	C32-C33-C34-C27
25	h	203	A1L1F	C28-C39-C40-C41
26	9	305	45D	C19-C23-C25-C27
23	b	810	CLA	C10-C11-C12-C13
23	7	316	CLA	C4C-C3C-CAC-CBC
26	9	305	45D	C19-C23-C25-C29
23	a	823	CLA	O1A-CGA-O2A-C1
23	b	807	CLA	O1A-CGA-O2A-C1
23	b	835	CLA	O1A-CGA-O2A-C1
23	5	306	CLA	C1A-C2A-CAA-CBA
23	9	310	CLA	C1A-C2A-CAA-CBA
23	9	313	CLA	C1A-C2A-CAA-CBA
23	4	313	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

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Mol	Chain	Res	Type	Atoms
23	b	837	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
23	7	313	CLA	C5-C6-C7-C8
25	h	203	A1L1F	C40-C41-C42-C44
23	5	305	CLA	O1A-CGA-O2A-C1
23	1	305	CLA	C8-C10-C11-C12
23	a	844	CLA	C10-C11-C12-C13
27	9	317	LHG	C3-O3-P-O6
25	9	302	A1L1F	C49-C50-C51-C52
27	9	317	LHG	C29-C30-C31-C32
23	b	813	CLA	C3-C5-C6-C7
23	b	807	CLA	O1D-CGD-O2D-CED
23	b	822	CLA	O1D-CGD-O2D-CED
28	b	848	DGD	CBB-CCB-CDB-CEB
23	b	829	CLA	C13-C15-C16-C17
27	a	845	LHG	O6-C4-C5-C6
23	5	315	CLA	C4C-C3C-CAC-CBC
23	a	812	CLA	C10-C11-C12-C13
23	a	806	CLA	C16-C17-C18-C19
23	4	315	CLA	O1D-CGD-O2D-CED
27	9	317	LHG	C12-C13-C14-C15
23	b	835	CLA	C2C-C3C-CAC-CBC
23	6	317	CLA	O1D-CGD-O2D-CED
25	h	203	A1L1F	C4-C8-O7-C54
23	b	824	CLA	O1A-CGA-O2A-C1
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	a	839	CLA	C3-C5-C6-C7
23	b	801	CLA	C3-C5-C6-C7
27	a	845	LHG	C4-C5-C6-O8
27	b	847	LHG	C4-C5-C6-O8
28	4	318	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
28	b	848	DGD	C3A-C4A-C5A-C6A
29	j	105	LMG	C13-C14-C15-C16
23	8	310	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	6	301	A1L1F	C50-C51-C52-C53
27	9	317	LHG	C11-C10-C9-C8
23	5	310	CLA	CAA-CBA-CGA-O2A
25	6	304	A1L1F	C45-C47-C48-C49
27	b	847	LHG	C8-C7-O7-C5
23	a	854	CLA	C10-C11-C12-C13
23	a	804	CLA	C4-C3-C5-C6
23	a	820	CLA	C4-C3-C5-C6
23	b	803	CLA	C4-C3-C5-C6
23	a	844	CLA	C16-C17-C18-C19
23	8	307	CLA	CBA-CGA-O2A-C1
25	h	203	A1L1F	C48-C49-C50-C51
23	1	311	CLA	CBD-CGD-O2D-CED
23	1	308	CLA	C13-C15-C16-C17
23	b	839	CLA	C13-C15-C16-C17
30	a	843	PQN	C23-C25-C26-C27
29	a	853	LMG	C14-C15-C16-C17
23	b	802	CLA	O1D-CGD-O2D-CED
23	f	802	CLA	O1D-CGD-O2D-CED
23	9	314	CLA	C3-C5-C6-C7
28	b	848	DGD	CCB-CDB-CEB-CFB
23	a	829	CLA	C8-C10-C11-C12
23	a	835	CLA	CBA-CGA-O2A-C1
23	a	825	CLA	O1A-CGA-O2A-C1
23	3	315	CLA	CAA-CBA-CGA-O2A
23	b	818	CLA	C11-C12-C13-C14
23	1	310	CLA	C5-C6-C7-C8
23	a	810	CLA	C5-C6-C7-C8
23	b	836	CLA	C2C-C3C-CAC-CBC
23	8	314	CLA	CBD-CGD-O2D-CED
27	a	845	LHG	C7-C8-C9-C10
23	a	826	CLA	C15-C16-C17-C18
28	4	318	DGD	C2D-C1D-O3G-C3G
25	6	301	A1L1F	C47-C48-C49-C50
23	b	804	CLA	C15-C16-C17-C18
23	b	814	CLA	C6-C7-C8-C9
23	a	801	CLA	C4-C3-C5-C6
23	b	813	CLA	C4-C3-C5-C6
23	b	838	CLA	C4-C3-C5-C6
23	1	308	CLA	C15-C16-C17-C18
23	9	316	CLA	C11-C12-C13-C15
23	4	308	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
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	803	CLA	C12-C13-C15-C16
23	b	807	CLA	C11-C10-C8-C7
23	b	807	CLA	C12-C13-C15-C16
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	833	CLA	C11-C12-C13-C15
23	b	838	CLA	C6-C7-C8-C10
23	f	802	CLA	C11-C12-C13-C15
23	4	317	CLA	C3-C5-C6-C7
23	9	316	CLA	C11-C12-C13-C14
23	7	308	CLA	C11-C10-C8-C9
23	a	801	CLA	C11-C12-C13-C14
23	a	807	CLA	C11-C12-C13-C14
23	a	809	CLA	C14-C13-C15-C16
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	803	CLA	C6-C7-C8-C9
23	b	803	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	808	CLA	C11-C10-C8-C9
23	b	828	CLA	C11-C12-C13-C14
23	b	836	CLA	C14-C13-C15-C16
23	j	102	CLA	C6-C7-C8-C9
25	h	203	A1L1F	C3-C8-O7-C54
27	9	307	LHG	C25-C26-C27-C28
23	4	307	CLA	CBA-CGA-O2A-C1
23	a	841	CLA	CBA-CGA-O2A-C1
23	a	812	CLA	C8-C10-C11-C12
23	a	819	CLA	C2A-CAA-CBA-CGA
23	8	307	CLA	O1A-CGA-O2A-C1
21	7	303	XAT	C7-C8-C9-C19
22	3	306	A1L1G	C32-C33-C34-C27
23	a	844	CLA	C16-C17-C18-C20
21	4	305	XAT	C27-C28-C29-C30
27	b	847	LHG	C9-C10-C11-C12
23	h	204	CLA	C3-C5-C6-C7
23	a	826	CLA	O1D-CGD-O2D-CED
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
28	b	848	DGD	C2A-C1A-O1G-C1G
23	b	805	CLA	C16-C17-C18-C20
27	b	847	LHG	O6-C4-C5-C6
23	b	833	CLA	C3-C5-C6-C7
23	a	844	CLA	C15-C16-C17-C18
23	b	802	CLA	C4-C3-C5-C6
23	a	801	CLA	C2-C3-C5-C6
23	a	807	CLA	C2-C3-C5-C6
23	b	807	CLA	C10-C11-C12-C13
23	j	102	CLA	C5-C6-C7-C8
28	b	848	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	809	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
27	9	317	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
23	4	311	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	j	102	CLA	C3A-C2A-CAA-CBA
23	b	812	CLA	C5-C6-C7-C8
27	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
27	a	846	LHG	C4-C5-C6-O8
29	2	317	LMG	O1-C7-C8-C9
28	b	848	DGD	C7A-C8A-C9A-CAA
23	b	835	CLA	C3-C5-C6-C7
25	6	301	A1L1F	C48-C49-C50-C51
27	9	307	LHG	C33-C34-C35-C36
23	a	840	CLA	C4-C3-C5-C6
23	b	818	CLA	C11-C12-C13-C15
23	a	806	CLA	CBD-CGD-O2D-CED
23	3	314	CLA	O1D-CGD-O2D-CED
23	6	316	CLA	O1D-CGD-O2D-CED
23	a	827	CLA	C3-C5-C6-C7
23	7	314	CLA	C2A-CAA-CBA-CGA
23	a	803	CLA	C15-C16-C17-C18
29	j	105	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	317	CLA	C5-C6-C7-C8
23	4	307	CLA	O1A-CGA-O2A-C1
23	4	308	CLA	C16-C17-C18-C19
23	a	806	CLA	C16-C17-C18-C20
23	b	822	CLA	C10-C11-C12-C13
22	9	301	A1L1G	O13-C26-C30-C31
27	b	847	LHG	O9-C7-O7-C5
23	7	308	CLA	C2-C1-O2A-CGA
25	1	304	A1L1F	C14-C29-C30-C31
23	b	803	CLA	C13-C15-C16-C17
23	b	806	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	9	308	CLA	C11-C10-C8-C9
23	4	310	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	b	802	CLA	C6-C7-C8-C9
23	b	802	CLA	C11-C10-C8-C9
23	b	804	CLA	C6-C7-C8-C9
23	b	806	CLA	C6-C7-C8-C9
23	b	810	CLA	C6-C7-C8-C9
23	b	824	CLA	C11-C12-C13-C14
23	b	837	CLA	C14-C13-C15-C16
23	b	838	CLA	C11-C12-C13-C14
23	5	309	CLA	C5-C6-C7-C8
23	1	310	CLA	C16-C17-C18-C20
23	b	827	CLA	C16-C17-C18-C20
31	b	846	BCR	C5-C6-C7-C8
31	b	849	BCR	C23-C24-C25-C26
31	b	849	BCR	C23-C24-C25-C30
31	f	804	BCR	C23-C24-C25-C26
31	l	201	BCR	C5-C6-C7-C8
31	l	205	BCR	C1-C6-C7-C8
31	l	205	BCR	C5-C6-C7-C8
23	a	854	CLA	C8-C10-C11-C12
23	b	810	CLA	CAA-CBA-CGA-O2A
21	4	305	XAT	C27-C28-C29-C39
26	9	305	45D	C31-C33-C35-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	103	CLA	C1A-C2A-CAA-CBA
23	4	310	CLA	C15-C16-C17-C18
23	1	306	CLA	C16-C17-C18-C20
23	9	313	CLA	O1D-CGD-O2D-CED
23	b	807	CLA	C5-C6-C7-C8
23	b	828	CLA	C5-C6-C7-C8
29	a	853	LMG	C12-C13-C14-C15
27	9	317	LHG	O6-C4-C5-C6
27	a	846	LHG	O6-C4-C5-C6
27	9	307	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	9	308	CLA	C11-C12-C13-C15
23	9	318	CLA	C11-C10-C8-C7
23	8	307	CLA	C11-C10-C8-C7
23	8	309	CLA	C11-C10-C8-C7
23	4	310	CLA	C11-C10-C8-C7
23	6	309	CLA	C6-C7-C8-C10
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	803	CLA	C6-C7-C8-C10
23	b	803	CLA	C11-C10-C8-C7
23	b	808	CLA	C11-C10-C8-C7
23	b	810	CLA	C6-C7-C8-C10
23	b	813	CLA	C11-C10-C8-C7
23	b	824	CLA	C6-C7-C8-C10
23	b	828	CLA	C12-C13-C15-C16
23	b	836	CLA	C12-C13-C15-C16
23	b	837	CLA	C12-C13-C15-C16
23	b	838	CLA	C12-C13-C15-C16
23	j	102	CLA	C6-C7-C8-C10
24	1	315	SQD	C9-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	9	308	CLA	C16-C17-C18-C20
23	b	805	CLA	C16-C17-C18-C19
23	a	842	CLA	C8-C10-C11-C12
23	a	841	CLA	O1A-CGA-O2A-C1
23	6	310	CLA	C2A-CAA-CBA-CGA
29	2	317	LMG	C31-C32-C33-C34
23	a	827	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	9	308	CLA	C16-C17-C18-C19
23	4	313	CLA	CBA-CGA-O2A-C1
22	7	302	A1L1G	C45-C2-C44-C43
23	5	314	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	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	854	CLA	CAD-CBD-CGD-O2D
23	b	802	CLA	CAD-CBD-CGD-O2D
23	b	806	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	833	CLA	CAD-CBD-CGD-O2D
23	b	838	CLA	CAD-CBD-CGD-O2D
23	b	839	CLA	CAD-CBD-CGD-O2D
25	8	304	A1L1F	C57-C2-C44-C43
29	a	853	LMG	C9-C8-O7-C10
23	a	841	CLA	C13-C15-C16-C17
23	a	808	CLA	O1D-CGD-O2D-CED
23	b	838	CLA	C13-C15-C16-C17
27	a	845	LHG	C9-C10-C11-C12
29	2	317	LMG	C33-C34-C35-C36
28	8	315	DGD	C1G-C2G-C3G-O3G
23	b	811	CLA	O1A-CGA-O2A-C1
23	2	307	CLA	C2A-CAA-CBA-CGA
23	2	314	CLA	C2A-CAA-CBA-CGA
23	7	313	CLA	CBD-CGD-O2D-CED
23	2	310	CLA	C16-C17-C18-C19
23	b	810	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

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Mol	Chain	Res	Type	Atoms
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	307	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	804	CLA	CHA-CBD-CGD-O1D
23	b	804	CLA	CHA-CBD-CGD-O2D
23	b	809	CLA	CHA-CBD-CGD-O1D
23	b	809	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	834	CLA	CHA-CBD-CGD-O1D
23	b	834	CLA	CHA-CBD-CGD-O2D
23	b	835	CLA	CHA-CBD-CGD-O1D
23	3	314	CLA	O1A-CGA-O2A-C1
23	7	312	CLA	O2A-C1-C2-C3
28	8	315	DGD	O2G-C2G-C3G-O3G
23	9	318	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

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Mol	Chain	Res	Type	Atoms
23	b	828	CLA	O1A-CGA-O2A-C1
28	b	848	DGD	O1A-C1A-O1G-C1G
23	j	102	CLA	O1D-CGD-O2D-CED
23	b	817	CLA	C10-C11-C12-C13
29	a	853	LMG	C31-C32-C33-C34
23	9	314	CLA	O1A-CGA-O2A-C1
23	1	310	CLA	C2-C3-C5-C6
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	313	CLA	O1A-CGA-O2A-C1
23	b	802	CLA	C2A-CAA-CBA-CGA
23	b	808	CLA	C2A-CAA-CBA-CGA
21	6	302	XAT	C7-C8-C9-C19
21	5	301	XAT	C7-C8-C9-C10
21	6	302	XAT	C7-C8-C9-C10
25	h	203	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	310	CLA	C16-C17-C18-C19
23	1	308	CLA	CBD-CGD-O2D-CED
21	2	304	XAT	C33-C34-C35-C15
23	8	314	CLA	O1D-CGD-O2D-CED
23	a	806	CLA	O1D-CGD-O2D-CED
23	1	307	CLA	C5-C6-C7-C8
23	2	314	CLA	C4-C3-C5-C6
23	8	311	CLA	C3-C5-C6-C7
27	9	307	LHG	C2-C3-O3-P
23	b	834	CLA	C2-C3-C5-C6
27	9	317	LHG	C3-O3-P-O5
27	9	317	LHG	C4-O6-P-O5
27	a	845	LHG	C3-O3-P-O5
27	a	846	LHG	C4-O6-P-O5
23	a	830	CLA	C8-C10-C11-C12
24	1	315	SQD	C13-C14-C15-C16
23	9	308	CLA	C10-C11-C12-C13
23	3	311	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	a	846	LHG	C10-C11-C12-C13
23	2	310	CLA	C16-C17-C18-C20
23	b	808	CLA	C16-C17-C18-C20
25	8	304	A1L1F	C47-C48-C49-C50
23	5	311	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	315	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	835	CLA	CAD-CBD-CGD-O1D
23	b	836	CLA	CAD-CBD-CGD-O1D
23	f	802	CLA	CAD-CBD-CGD-O1D
25	6	304	A1L1F	O13-C26-C30-C31
23	4	312	CLA	CBA-CGA-O2A-C1
23	b	840	CLA	C15-C16-C17-C18
23	5	307	CLA	C11-C10-C8-C7
23	9	316	CLA	C3A-C2A-CAA-CBA
23	8	307	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	806	CLA	C11-C12-C13-C15
23	b	825	CLA	C11-C10-C8-C7
23	b	827	CLA	C11-C10-C8-C7
23	b	829	CLA	C11-C12-C13-C15
23	b	829	CLA	C12-C13-C15-C16
23	b	832	CLA	C12-C13-C15-C16
27	9	317	LHG	O6-C4-C5-O7
30	a	843	PQN	C22-C23-C25-C26
23	b	818	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	a	834	CLA	C5-C6-C7-C8
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	316	SQD	C44-C45-C46-O48
24	5	316	SQD	O47-C45-C46-O48
24	1	315	SQD	O6-C44-C45-O47
27	a	846	LHG	O7-C5-C6-O8
27	b	847	LHG	O7-C5-C6-O8
23	8	310	CLA	O1A-CGA-O2A-C1
23	b	814	CLA	C3-C5-C6-C7
27	9	317	LHG	C10-C11-C12-C13
23	9	318	CLA	O1A-CGA-O2A-C1
23	1	311	CLA	CBA-CGA-O2A-C1
23	b	839	CLA	C2C-C3C-CAC-CBC
23	5	309	CLA	C6-C7-C8-C9
23	9	308	CLA	C11-C12-C13-C14
23	8	309	CLA	C11-C10-C8-C9
23	4	308	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	b	804	CLA	C11-C12-C13-C14
23	b	813	CLA	C11-C10-C8-C9
23	b	838	CLA	C14-C13-C15-C16
23	3	315	CLA	O1A-CGA-O2A-C1
23	2	308	CLA	C6-C7-C8-C9
23	a	821	CLA	C2A-CAA-CBA-CGA
23	3	308	CLA	CAA-CBA-CGA-O2A
23	a	809	CLA	C10-C11-C12-C13
22	9	306	A1L1G	C32-C33-C34-C35
23	a	854	CLA	CBD-CGD-O2D-CED
27	9	317	LHG	C13-C14-C15-C16
23	b	827	CLA	C10-C11-C12-C13
22	1	301	A1L1G	C37-C38-C39-C28
23	7	308	CLA	C8-C10-C11-C12
23	8	307	CLA	C16-C17-C18-C20
23	a	823	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	b	831	CLA	C1-C2-C3-C4
23	b	803	CLA	C3-C5-C6-C7
23	a	801	CLA	CAA-CBA-CGA-O2A
24	1	315	SQD	C46-C45-O47-C7
23	4	317	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	b	824	CLA	C2A-CAA-CBA-CGA
23	b	827	CLA	C2A-CAA-CBA-CGA
23	b	805	CLA	CBA-CGA-O2A-C1
23	1	311	CLA	O1D-CGD-O2D-CED
23	5	311	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	810	CLA	C2-C1-O2A-CGA
23	b	832	CLA	C2C-C3C-CAC-CBC
24	5	316	SQD	C7-C8-C9-C10
23	1	311	CLA	O1A-CGA-O2A-C1
23	b	822	CLA	C3-C5-C6-C7
27	b	847	LHG	C25-C26-C27-C28
23	b	805	CLA	O1A-CGA-O2A-C1
23	h	204	CLA	C4-C3-C5-C6
31	b	846	BCR	C1-C6-C7-C8
31	f	804	BCR	C23-C24-C25-C30
31	j	104	BCR	C1-C6-C7-C8
23	b	838	CLA	C2-C3-C5-C6
23	1	308	CLA	O1D-CGD-O2D-CED
23	b	817	CLA	CBA-CGA-O2A-C1
23	b	817	CLA	O1A-CGA-O2A-C1
23	a	830	CLA	C16-C17-C18-C19
23	b	808	CLA	C16-C17-C18-C19
23	a	839	CLA	C15-C16-C17-C18
27	9	307	LHG	C4-O6-P-O3
27	9	317	LHG	C4-O6-P-O3
27	a	846	LHG	C3-O3-P-O6
27	a	846	LHG	C4-O6-P-O3
23	a	841	CLA	C4-C3-C5-C6
23	a	854	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	4	308	CLA	C11-C12-C13-C15
23	2	311	CLA	C11-C10-C8-C7
23	f	802	CLA	C6-C7-C8-C10
23	b	801	CLA	O1A-CGA-O2A-C1
23	a	801	CLA	C14-C13-C15-C16
23	a	812	CLA	C6-C7-C8-C9
23	a	842	CLA	C14-C13-C15-C16
23	b	803	CLA	C14-C13-C15-C16
23	b	827	CLA	C11-C10-C8-C9
23	b	828	CLA	C14-C13-C15-C16
30	a	843	PQN	C24-C23-C25-C26
21	4	301	XAT	C29-C30-C31-C32
22	3	302	A1L1G	C36-C37-C38-C39
31	m	101	BCR	C13-C14-C15-C16
23	b	803	CLA	C16-C17-C18-C20
23	5	307	CLA	C8-C10-C11-C12
23	a	830	CLA	C15-C16-C17-C18
23	6	317	CLA	C13-C15-C16-C17
21	7	303	XAT	C11-C12-C13-C20
23	b	801	CLA	CBA-CGA-O2A-C1
23	5	315	CLA	CAA-CBA-CGA-O2A
21	6	303	XAT	C11-C12-C13-C14
22	3	306	A1L1G	C32-C33-C34-C35
23	2	314	CLA	C11-C10-C8-C7
27	a	846	LHG	C1-C2-C3-O3
23	2	314	CLA	C2-C3-C5-C6
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	312	CLA	CBD-CGD-O2D-CED
23	4	310	CLA	CBD-CGD-O2D-CED
23	a	832	CLA	CBD-CGD-O2D-CED
23	a	854	CLA	O1D-CGD-O2D-CED
23	8	305	CLA	CBD-CGD-O2D-CED
23	9	314	CLA	C2A-CAA-CBA-CGA
23	8	307	CLA	C2A-CAA-CBA-CGA
21	6	306	XAT	C29-C30-C31-C32
21	7	301	XAT	C29-C30-C31-C32
21	j	101	XAT	C9-C10-C11-C12
22	3	302	A1L1G	C40-C41-C42-C44
23	a	820	CLA	C13-C15-C16-C17
23	b	839	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	a	812	CLA	C3-C5-C6-C7
27	a	845	LHG	C25-C26-C27-C28
23	5	310	CLA	CAA-CBA-CGA-O1A
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	5	309	CLA	C2A-CAA-CBA-CGA
23	9	316	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	809	CLA	C2A-CAA-CBA-CGA
28	b	848	DGD	O2G-C2G-C3G-O3G
23	3	312	CLA	CBA-CGA-O2A-C1
23	2	310	CLA	C3A-C2A-CAA-CBA
23	b	813	CLA	C3A-C2A-CAA-CBA
23	b	831	CLA	C3A-C2A-CAA-CBA
23	7	313	CLA	O1D-CGD-O2D-CED
29	2	317	LMG	O9-C10-O7-C8
23	b	817	CLA	CBD-CGD-O2D-CED
25	9	302	A1L1F	C3-C8-O7-C54
23	a	802	CLA	C4-C3-C5-C6
23	a	832	CLA	O1D-CGD-O2D-CED
23	5	307	CLA	C11-C10-C8-C9
23	1	310	CLA	C11-C12-C13-C14
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	854	CLA	C11-C10-C8-C9
23	b	808	CLA	C6-C7-C8-C9
23	a	830	CLA	C16-C17-C18-C20
23	5	306	CLA	CAA-CBA-CGA-O1A
23	8	305	CLA	O1D-CGD-O2D-CED
23	8	312	CLA	O1D-CGD-O2D-CED
23	6	310	CLA	C3-C5-C6-C7
31	b	844	BCR	C11-C10-C9-C34
31	b	844	BCR	C20-C21-C22-C37
31	f	804	BCR	C35-C13-C14-C15
31	l	201	BCR	C11-C10-C9-C34
23	3	315	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
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	840	CLA	CBA-CGA-O2A-C1
28	8	315	DGD	O6D-C1D-O3G-C3G
27	a	845	LHG	C14-C15-C16-C17
21	6	302	XAT	C31-C32-C33-C40
21	7	301	XAT	C7-C8-C9-C19
27	9	317	LHG	C15-C16-C17-C18
23	4	311	CLA	C1A-C2A-CAA-CBA
23	4	316	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	822	CLA	C1A-C2A-CAA-CBA
23	b	834	CLA	C1A-C2A-CAA-CBA
23	a	807	CLA	C11-C10-C8-C7
23	a	814	CLA	C11-C10-C8-C7
23	b	802	CLA	C2-C3-C5-C6
23	b	802	CLA	C12-C13-C15-C16
23	3	312	CLA	O1A-CGA-O2A-C1
22	3	306	A1L1G	C30-C31-C32-C33
23	4	310	CLA	O1D-CGD-O2D-CED
23	a	801	CLA	O1A-CGA-O2A-C1
23	b	840	CLA	O1A-CGA-O2A-C1
23	4	314	CLA	CAA-CBA-CGA-O2A
23	a	817	CLA	CAA-CBA-CGA-O1A
23	a	817	CLA	CAA-CBA-CGA-O2A
23	b	839	CLA	C4C-C3C-CAC-CBC
23	6	317	CLA	C8-C10-C11-C12
29	a	853	LMG	C11-C12-C13-C14
23	1	305	CLA	C3-C5-C6-C7
23	4	314	CLA	CAA-CBA-CGA-O1A
23	4	310	CLA	C13-C15-C16-C17
23	1	307	CLA	C6-C7-C8-C9
23	a	841	CLA	C2-C3-C5-C6
31	b	844	BCR	C11-C10-C9-C8
31	b	844	BCR	C20-C21-C22-C23
31	f	804	BCR	C12-C13-C14-C15
31	l	201	BCR	C11-C10-C9-C8
23	5	307	CLA	C2A-CAA-CBA-CGA
22	9	301	A1L1G	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
22	7	302	A1L1G	C36-C37-C38-C39
22	1	301	A1L1G	C40-C41-C42-C44
23	5	313	CLA	CAA-CBA-CGA-O1A
29	2	317	LMG	C11-C10-O7-C8
23	b	817	CLA	O1D-CGD-O2D-CED
23	5	310	CLA	CBA-CGA-O2A-C1
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	b	808	CLA	C14-C13-C15-C16
23	5	306	CLA	CAA-CBA-CGA-O2A
28	b	848	DGD	C1B-C2B-C3B-C4B
23	5	311	CLA	C4-C3-C5-C6
23	a	819	CLA	CAA-CBA-CGA-O2A
24	1	315	SQD	C15-C16-C17-C18
23	4	306	CLA	C2A-CAA-CBA-CGA
23	6	307	CLA	C2A-CAA-CBA-CGA
23	a	839	CLA	C2A-CAA-CBA-CGA
23	a	842	CLA	O1A-CGA-O2A-C1
26	9	305	45D	C03-C07-C19-C23
31	h	202	BCR	C23-C24-C25-C30
31	m	101	BCR	C23-C24-C25-C30
23	b	835	CLA	C4C-C3C-CAC-CBC
27	9	317	LHG	O1-C1-C2-C3
23	a	830	CLA	O1A-CGA-O2A-C1
25	h	203	A1L1F	C36-C37-C38-C39
26	9	305	45D	C36-C38-C42-C41
21	2	304	XAT	C7-C8-C9-C10
21	a	852	XAT	C31-C32-C33-C34
26	9	305	45D	C31-C33-C35-C37
23	b	802	CLA	C10-C11-C12-C13
23	9	312	CLA	CAA-CBA-CGA-O2A
23	a	813	CLA	C6-C7-C8-C9
23	7	307	CLA	CAA-CBA-CGA-O2A
23	a	804	CLA	O1A-CGA-O2A-C1
23	5	307	CLA	C11-C12-C13-C14
23	b	813	CLA	C16-C17-C18-C19
23	b	813	CLA	C5-C6-C7-C8
23	5	313	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

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Mol	Chain	Res	Type	Atoms
23	a	830	CLA	CBA-CGA-O2A-C1
23	a	842	CLA	CBA-CGA-O2A-C1
23	a	826	CLA	C13-C15-C16-C17
23	7	317	CLA	CAA-CBA-CGA-O2A
23	2	314	CLA	O1A-CGA-O2A-C1
23	8	311	CLA	C6-C7-C8-C10
23	b	802	CLA	C11-C10-C8-C7
28	8	315	DGD	C2D-C1D-O3G-C3G
25	6	304	A1L1F	C3-C8-O7-C54
23	4	308	CLA	C3-C5-C6-C7
23	1	314	CLA	CAA-CBA-CGA-O1A
23	4	309	CLA	CAA-CBA-CGA-O2A
23	1	306	CLA	C16-C17-C18-C19
27	9	317	LHG	C35-C36-C37-C38
29	j	105	LMG	C11-C12-C13-C14
23	a	804	CLA	CBA-CGA-O2A-C1
23	9	316	CLA	C8-C10-C11-C12
23	5	314	CLA	C4-C3-C5-C6
23	b	808	CLA	C4-C3-C5-C6
23	a	830	CLA	C2-C3-C5-C6
22	3	306	A1L1G	C14-C29-C30-C31
25	h	203	A1L1F	C14-C29-C30-C31
23	8	307	CLA	C6-C7-C8-C9
23	4	308	CLA	C6-C7-C8-C9
23	6	309	CLA	C11-C10-C8-C9
23	a	801	CLA	C11-C10-C8-C9
23	b	806	CLA	C11-C12-C13-C14
23	b	829	CLA	C11-C12-C13-C14
23	9	311	CLA	C3A-C2A-CAA-CBA
23	4	306	CLA	C3A-C2A-CAA-CBA
23	2	316	CLA	C3A-C2A-CAA-CBA
23	1	310	CLA	C3A-C2A-CAA-CBA
23	b	809	CLA	C3A-C2A-CAA-CBA
23	b	837	CLA	CAA-CBA-CGA-O2A
23	5	306	CLA	CAD-CBD-CGD-O2D
23	5	311	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	311	CLA	CAD-CBD-CGD-O2D
23	3	314	CLA	CAD-CBD-CGD-O2D
23	6	312	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	2	316	CLA	CAD-CBD-CGD-O2D
23	7	307	CLA	CAD-CBD-CGD-O2D
23	7	311	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	837	CLA	CAD-CBD-CGD-O2D
23	l	204	CLA	CAD-CBD-CGD-O2D
21	8	302	XAT	C9-C10-C11-C12
23	b	818	CLA	C2A-CAA-CBA-CGA
23	b	813	CLA	C13-C15-C16-C17
23	a	818	CLA	CAA-CBA-CGA-O2A
23	b	803	CLA	C10-C11-C12-C13
23	a	835	CLA	C4-C3-C5-C6
23	b	833	CLA	C4-C3-C5-C6
23	a	804	CLA	C6-C7-C8-C9
23	7	317	CLA	CAA-CBA-CGA-O1A
23	b	808	CLA	C2-C3-C5-C6
23	b	801	CLA	CAA-CBA-CGA-O2A
23	l	204	CLA	CAA-CBA-CGA-O2A
31	f	801	BCR	C17-C18-C19-C20
21	5	301	XAT	O4-C6-C7-C8
21	5	304	XAT	O24-C26-C27-C28
21	9	303	XAT	O24-C26-C27-C28
21	8	301	XAT	O24-C26-C27-C28
21	4	301	XAT	O4-C6-C7-C8
21	4	305	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
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	4	309	CLA	O2A-C1-C2-C3
23	3	310	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
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	308	CLA	C2A-CAA-CBA-CGA
23	2	308	CLA	C2A-CAA-CBA-CGA
23	b	833	CLA	C15-C16-C17-C18
30	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	310	CLA	CHA-CBD-CGD-O1D
23	4	314	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
23	b	801	CLA	CHA-CBD-CGD-O2D
23	b	805	CLA	CHA-CBD-CGD-O1D
23	b	805	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

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Mol	Chain	Res	Type	Atoms
23	b	835	CLA	CHA-CBD-CGD-O2D
23	j	102	CLA	CHA-CBD-CGD-O2D
23	4	306	CLA	CAA-CBA-CGA-O2A
23	b	807	CLA	CAA-CBA-CGA-O2A
25	6	304	A1L1F	O13-C45-C47-C48
23	a	835	CLA	C2-C3-C5-C6
25	9	302	A1L1F	C50-C51-C52-C53
23	b	807	CLA	C16-C17-C18-C19
23	a	827	CLA	C10-C11-C12-C13
23	4	312	CLA	O1A-CGA-O2A-C1
23	a	810	CLA	CAA-CBA-CGA-O2A
23	h	204	CLA	CAA-CBA-CGA-O2A
27	9	307	LHG	O7-C5-C6-O8
23	b	803	CLA	CAA-CBA-CGA-O2A
23	a	829	CLA	C2A-CAA-CBA-CGA
23	2	314	CLA	CBA-CGA-O2A-C1
23	9	308	CLA	C11-C10-C8-C7
23	a	801	CLA	C11-C10-C8-C7
23	a	835	CLA	C11-C12-C13-C15
23	b	810	CLA	C2-C3-C5-C6
23	b	824	CLA	C10-C11-C12-C13
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	809	CLA	CAA-CBA-CGA-O2A
23	b	817	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
21	7	304	XAT	C9-C10-C11-C12
23	1	312	CLA	CAA-CBA-CGA-O2A
23	b	832	CLA	CAA-CBA-CGA-O2A
24	5	316	SQD	C4-C5-C6-S
25	9	302	A1L1F	O13-C26-C30-C29
25	6	304	A1L1F	O13-C26-C30-C29
23	a	841	CLA	C2A-CAA-CBA-CGA
23	b	837	CLA	CAA-CBA-CGA-O1A
27	a	845	LHG	O8-C23-C24-C25
23	4	309	CLA	CAA-CBA-CGA-O1A
25	8	304	A1L1F	C3-C8-O7-C54
23	j	102	CLA	CAA-CBA-CGA-O2A
23	b	810	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
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
31	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	825	CLA	C1A-C2A-CAA-CBA
23	b	831	CLA	C1A-C2A-CAA-CBA
23	j	102	CLA	C10-C11-C12-C13
23	b	819	CLA	C6-C7-C8-C9
23	a	818	CLA	CAA-CBA-CGA-O1A
23	b	801	CLA	CAA-CBA-CGA-O1A
23	a	827	CLA	C2-C1-O2A-CGA
23	a	829	CLA	C2-C1-O2A-CGA
23	b	807	CLA	C2-C1-O2A-CGA
23	b	834	CLA	C2-C1-O2A-CGA
23	4	306	CLA	CAA-CBA-CGA-O1A
29	j	105	LMG	C7-C8-C9-O8
23	b	804	CLA	C4C-C3C-CAC-CBC
23	b	803	CLA	C5-C6-C7-C8
27	9	317	LHG	C30-C31-C32-C33
25	6	301	A1L1F	O13-C45-C47-C48
23	b	809	CLA	CAA-CBA-CGA-O1A
23	h	204	CLA	C2-C3-C5-C6
23	a	826	CLA	C10-C11-C12-C13
27	a	846	LHG	C3-O3-P-O5
27	9	317	LHG	C27-C28-C29-C30
23	b	832	CLA	CAA-CBA-CGA-O1A
23	3	312	CLA	CAA-CBA-CGA-O2A
26	9	305	45D	C15-C07-C19-C23
31	b	849	BCR	C1-C6-C7-C8
31	h	202	BCR	C23-C24-C25-C26
31	j	104	BCR	C5-C6-C7-C8
31	m	101	BCR	C23-C24-C25-C26
23	a	836	CLA	CAA-CBA-CGA-O1A
23	b	807	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	h	204	CLA	CAA-CBA-CGA-O1A
25	6	304	A1L1F	O46-C45-C47-C48
23	b	804	CLA	CAA-CBA-CGA-O2A
23	a	814	CLA	C16-C17-C18-C19
23	b	810	CLA	C16-C17-C18-C20
23	7	309	CLA	CBA-CGA-O2A-C1
23	7	308	CLA	C2A-CAA-CBA-CGA
23	1	312	CLA	CAA-CBA-CGA-O1A
25	9	302	A1L1F	O46-C45-O13-C26
23	3	313	CLA	C4-C3-C5-C6
23	9	315	CLA	C2C-C3C-CAC-CBC
23	a	834	CLA	C10-C11-C12-C13
23	4	310	CLA	CAD-CBD-CGD-O1D
23	4	316	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	316	SQD	O5-C5-C6-S
27	9	307	LHG	C6-C5-O7-C7
23	a	820	CLA	CBD-CGD-O2D-CED
23	b	813	CLA	CBD-CGD-O2D-CED
23	7	309	CLA	O1A-CGA-O2A-C1
23	a	813	CLA	CAA-CBA-CGA-O2A
23	b	805	CLA	C11-C12-C13-C14
23	b	806	CLA	C11-C10-C8-C9
23	j	102	CLA	C11-C10-C8-C9
23	4	310	CLA	C8-C10-C11-C12
25	9	302	A1L1F	C47-C45-O13-C26
23	a	810	CLA	C16-C17-C18-C20
23	9	314	CLA	CAA-CBA-CGA-O2A
23	6	316	CLA	CAA-CBA-CGA-O2A
23	7	308	CLA	CAA-CBA-CGA-O2A
23	a	813	CLA	CBD-CGD-O2D-CED
24	5	316	SQD	C10-C11-C12-C13
23	a	810	CLA	CAA-CBA-CGA-O1A
23	3	309	CLA	C2A-CAA-CBA-CGA
23	4	310	CLA	CAA-CBA-CGA-O2A
23	7	309	CLA	CAA-CBA-CGA-O2A
23	7	316	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	a	835	CLA	CAA-CBA-CGA-O2A
23	a	854	CLA	CAA-CBA-CGA-O2A
23	5	309	CLA	C15-C16-C17-C18
23	a	801	CLA	C5-C6-C7-C8
23	b	824	CLA	C15-C16-C17-C18
23	8	308	CLA	C4-C3-C5-C6
23	b	810	CLA	C4-C3-C5-C6
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	1	310	CLA	C12-C13-C15-C16
23	a	834	CLA	C11-C12-C13-C15
23	b	805	CLA	C11-C12-C13-C15
23	b	818	CLA	C11-C10-C8-C7
23	l	203	CLA	C6-C7-C8-C10
23	j	102	CLA	CAA-CBA-CGA-O1A
23	5	309	CLA	CAA-CBA-CGA-O2A
23	2	307	CLA	CAA-CBA-CGA-O2A
23	a	826	CLA	CAA-CBA-CGA-O2A
23	j	102	CLA	C3-C5-C6-C7
21	7	303	XAT	C11-C12-C13-C14
31	b	845	BCR	C7-C8-C9-C10
23	3	312	CLA	CAA-CBA-CGA-O1A
23	7	308	CLA	CAA-CBA-CGA-O1A
23	a	813	CLA	CAA-CBA-CGA-O1A
24	1	315	SQD	C12-C13-C14-C15
23	7	310	CLA	CAA-CBA-CGA-O2A
23	5	309	CLA	CAA-CBA-CGA-O1A
23	7	316	CLA	CAA-CBA-CGA-O1A
23	a	835	CLA	CAA-CBA-CGA-O1A
25	6	301	A1L1F	O46-C45-C47-C48
23	6	314	CLA	CAA-CBA-CGA-O2A
27	a	845	LHG	O10-C23-C24-C25
23	7	314	CLA	CAA-CBA-CGA-O2A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	h	203	A1L1F	C1-C11-C3-C4-C6-C8

235 monomers are involved in 722 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	310	CLA	6	0
23	b	820	CLA	3	0
22	7	302	A1L1G	2	0
23	a	839	CLA	4	0
21	3	301	XAT	8	0
23	7	311	CLA	3	0
23	7	313	CLA	4	0
31	l	205	BCR	10	0
23	3	308	CLA	2	0
23	5	312	CLA	3	0
22	9	301	A1L1G	2	0
23	f	802	CLA	2	0
23	a	804	CLA	5	0
21	5	301	XAT	4	0
23	a	825	CLA	5	0
23	j	102	CLA	8	0
21	7	301	XAT	3	0
28	b	848	DGD	6	0
31	f	804	BCR	6	0
21	6	302	XAT	3	0
21	7	304	XAT	11	0
31	b	844	BCR	5	0
23	7	308	CLA	6	0
25	6	301	A1L1F	2	0
31	a	847	BCR	3	0
25	6	304	A1L1F	4	0
23	8	307	CLA	6	0
23	2	307	CLA	1	0
23	a	840	CLA	6	0
21	8	302	XAT	6	0
21	8	301	XAT	3	0
23	b	802	CLA	3	0
23	b	832	CLA	3	0
31	b	842	BCR	4	0
23	b	826	CLA	5	0
23	a	820	CLA	5	0
21	9	303	XAT	6	0
23	8	312	CLA	3	0
23	a	841	CLA	7	0
23	a	801	CLA	6	0
21	4	301	XAT	3	0
23	a	822	CLA	5	0
23	4	308	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	1	310	CLA	1	0
23	b	812	CLA	4	0
31	f	801	BCR	9	0
23	4	316	CLA	1	0
23	b	806	CLA	2	0
23	3	309	CLA	1	0
30	a	843	PQN	5	0
23	l	203	CLA	2	0
23	a	816	CLA	2	0
23	5	311	CLA	1	0
21	4	302	XAT	4	0
21	6	305	XAT	5	0
23	5	314	CLA	1	0
23	a	831	CLA	5	0
23	4	313	CLA	4	0
23	a	836	CLA	1	0
23	b	824	CLA	5	0
25	9	302	A1L1F	2	0
25	8	304	A1L1F	2	0
29	a	853	LMG	10	0
31	i	101	BCR	2	0
31	a	848	BCR	7	0
23	b	805	CLA	3	0
23	a	803	CLA	4	0
21	8	303	XAT	7	0
21	9	304	XAT	8	0
23	b	816	CLA	6	0
29	j	105	LMG	6	0
23	4	312	CLA	1	0
23	b	813	CLA	7	0
23	8	311	CLA	3	0
23	4	306	CLA	2	0
23	a	827	CLA	3	0
23	b	829	CLA	4	0
23	a	818	CLA	11	0
23	b	835	CLA	5	0
23	7	307	CLA	1	0
30	b	841	PQN	3	0
23	a	819	CLA	6	0
23	a	802	CLA	5	0
23	b	819	CLA	1	0
23	b	801	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	9	316	CLA	7	0
23	h	204	CLA	3	0
23	3	312	CLA	1	0
31	l	201	BCR	4	0
23	a	823	CLA	3	0
23	b	814	CLA	3	0
23	7	314	CLA	2	0
31	b	849	BCR	7	0
23	8	314	CLA	1	0
23	2	314	CLA	1	0
23	4	317	CLA	7	0
23	b	823	CLA	6	0
27	b	847	LHG	1	0
23	a	807	CLA	4	0
23	a	808	CLA	1	0
23	a	832	CLA	2	0
31	b	846	BCR	3	0
23	l	202	CLA	1	0
31	m	101	BCR	1	0
23	a	813	CLA	1	0
23	b	838	CLA	6	0
23	6	309	CLA	1	0
23	1	308	CLA	3	0
23	a	835	CLA	5	0
21	4	303	XAT	10	0
23	6	308	CLA	4	0
29	2	317	LMG	3	0
22	5	303	A1L1G	1	0
24	5	316	SQD	1	0
22	9	306	A1L1G	1	0
23	9	311	CLA	3	0
25	h	203	A1L1F	4	0
23	9	314	CLA	7	0
28	8	315	DGD	2	0
23	2	316	CLA	2	0
23	6	315	CLA	3	0
21	7	303	XAT	13	0
23	a	806	CLA	9	0
21	j	101	XAT	7	0
23	3	313	CLA	3	0
23	4	311	CLA	1	0
23	4	314	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	7	312	CLA	1	0
32	c	102	SF4	3	0
23	a	833	CLA	2	0
23	1	306	CLA	5	0
23	b	809	CLA	4	0
23	b	810	CLA	1	0
21	4	304	XAT	5	0
23	2	308	CLA	4	0
23	a	826	CLA	6	0
23	b	839	CLA	5	0
24	1	315	SQD	2	0
23	a	838	CLA	1	0
23	1	312	CLA	2	0
21	2	301	XAT	3	0
23	a	828	CLA	6	0
23	5	310	CLA	1	0
23	9	312	CLA	3	0
23	b	803	CLA	3	0
23	a	837	CLA	1	0
31	b	845	BCR	6	0
21	2	302	XAT	1	0
23	b	808	CLA	1	0
23	a	814	CLA	3	0
23	5	315	CLA	2	0
23	7	315	CLA	2	0
21	6	303	XAT	9	0
23	7	316	CLA	2	0
21	3	304	XAT	4	0
23	2	310	CLA	4	0
23	a	842	CLA	4	0
31	h	202	BCR	6	0
23	b	825	CLA	3	0
21	3	303	XAT	3	0
23	9	318	CLA	5	0
23	1	311	CLA	2	0
23	6	317	CLA	4	0
23	a	844	CLA	5	0
23	5	309	CLA	4	0
23	9	315	CLA	1	0
23	a	824	CLA	1	0
23	5	308	CLA	2	0
23	9	310	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	a	852	XAT	4	0
23	4	307	CLA	1	0
23	a	812	CLA	1	0
23	6	313	CLA	2	0
31	a	849	BCR	4	0
31	j	104	BCR	9	0
23	3	311	CLA	1	0
23	b	828	CLA	4	0
27	9	317	LHG	3	0
23	b	831	CLA	2	0
23	5	305	CLA	3	0
28	4	318	DGD	11	0
21	7	305	XAT	2	0
21	1	302	XAT	2	0
21	2	304	XAT	3	0
21	2	305	XAT	5	0
25	1	304	A1L1F	2	0
23	j	103	CLA	2	0
21	1	303	XAT	3	0
23	b	811	CLA	3	0
23	8	313	CLA	3	0
23	b	822	CLA	6	0
23	b	840	CLA	5	0
23	7	306	CLA	2	0
26	9	305	45D	8	0
27	a	845	LHG	4	0
23	b	830	CLA	5	0
23	a	810	CLA	4	0
23	b	833	CLA	6	0
23	a	854	CLA	3	0
23	8	308	CLA	1	0
23	b	817	CLA	9	0
23	b	821	CLA	2	0
23	4	315	CLA	1	0
22	1	301	A1L1G	1	0
23	8	305	CLA	5	0
23	b	818	CLA	3	0
23	b	807	CLA	6	0
27	a	846	LHG	3	0
31	a	850	BCR	2	0
23	a	809	CLA	2	0
23	9	309	CLA	1	0

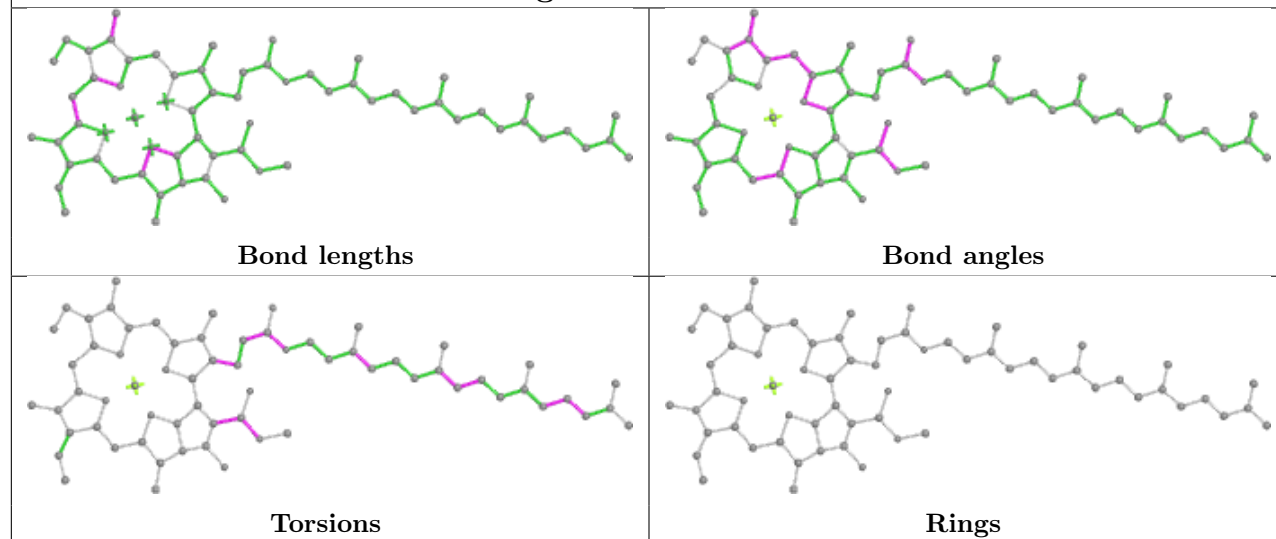
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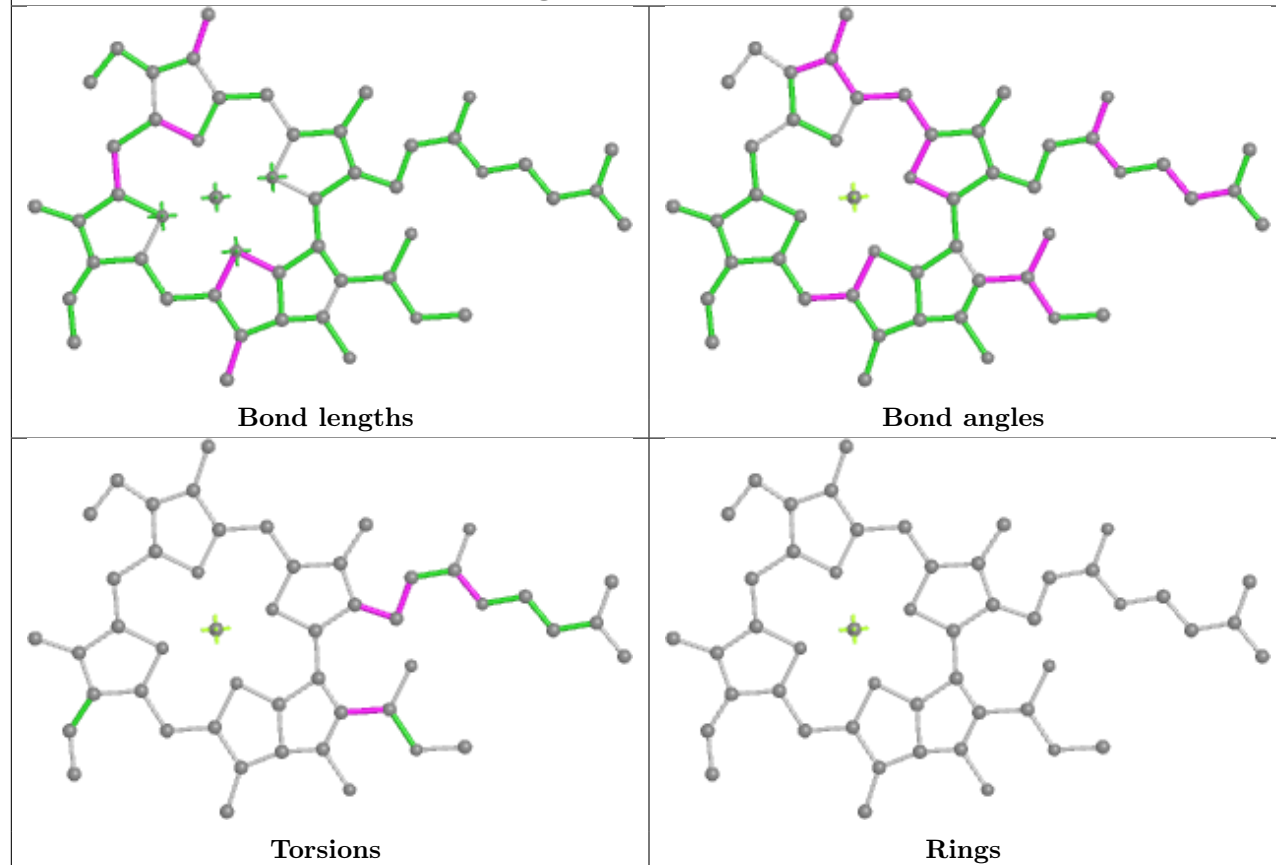
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	804	CLA	5	0
23	1	314	CLA	1	0
21	2	303	XAT	11	0
21	4	305	XAT	4	0
23	9	308	CLA	7	0
23	b	827	CLA	5	0
23	6	314	CLA	1	0
23	b	837	CLA	5	0
23	b	836	CLA	6	0
27	9	307	LHG	2	0
23	a	829	CLA	8	0
23	8	306	CLA	1	0
23	5	307	CLA	7	0
23	4	309	CLA	3	0
21	6	306	XAT	3	0
21	5	302	XAT	9	0
23	a	830	CLA	7	0
31	b	843	BCR	1	0
23	9	313	CLA	2	0
21	3	305	XAT	4	0
23	a	834	CLA	6	0
23	a	805	CLA	1	0
31	h	201	BCR	2	0
21	5	304	XAT	5	0

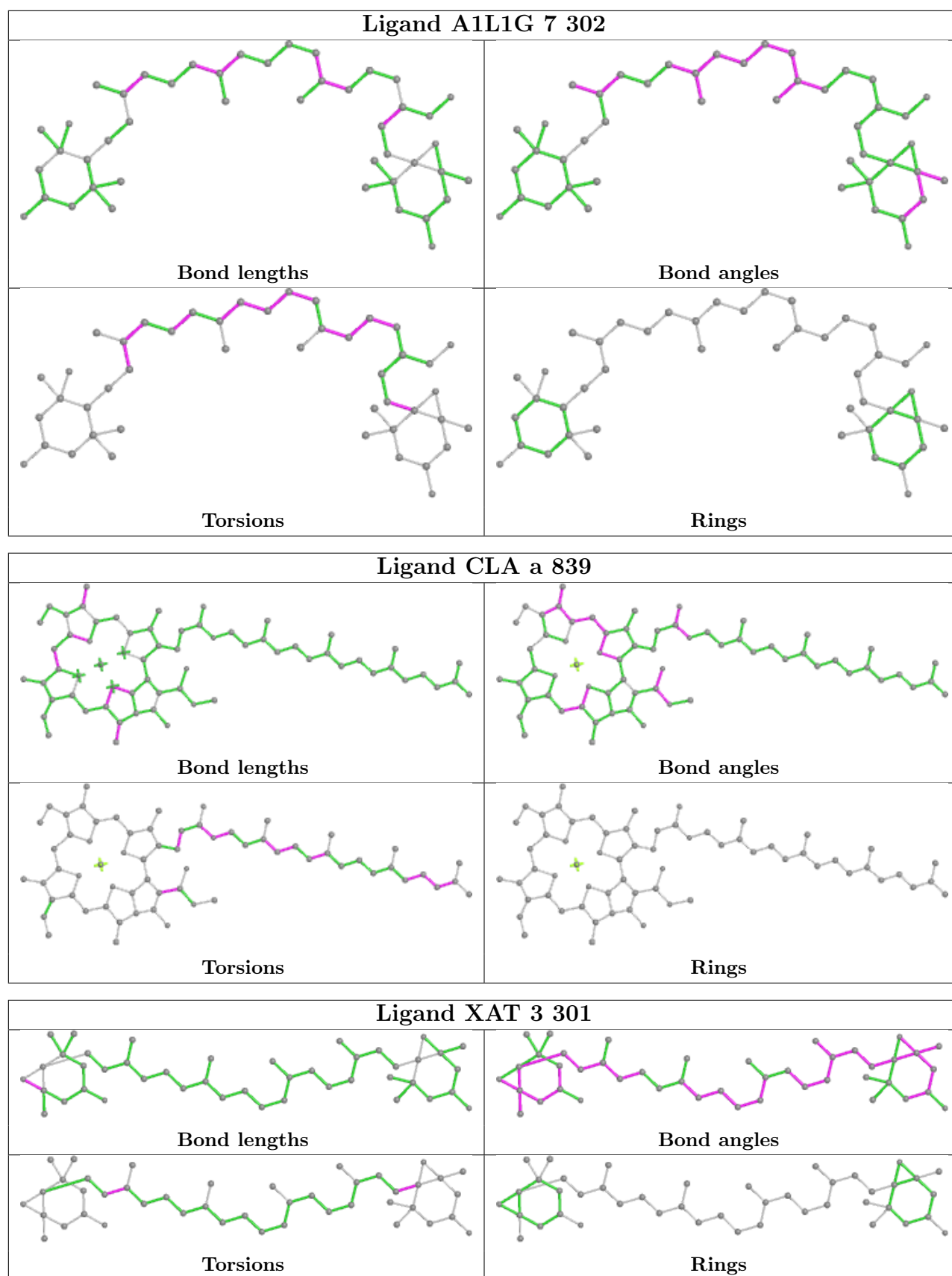
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 4 310

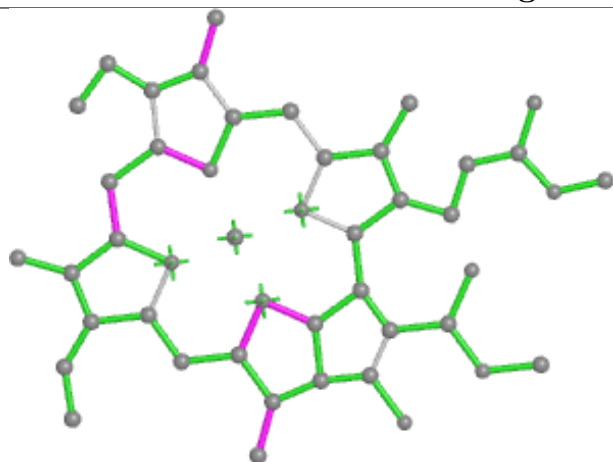


Ligand CLA b 820

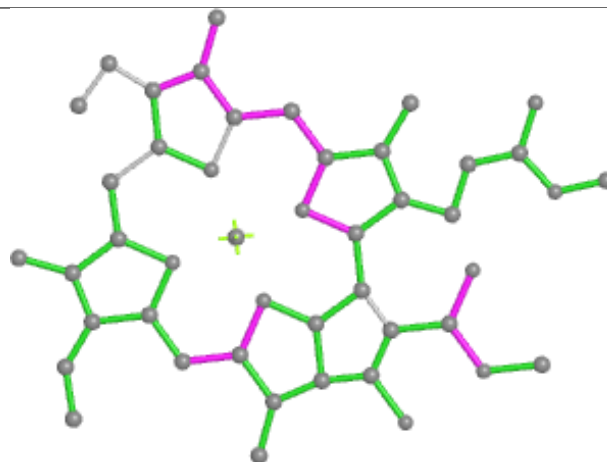




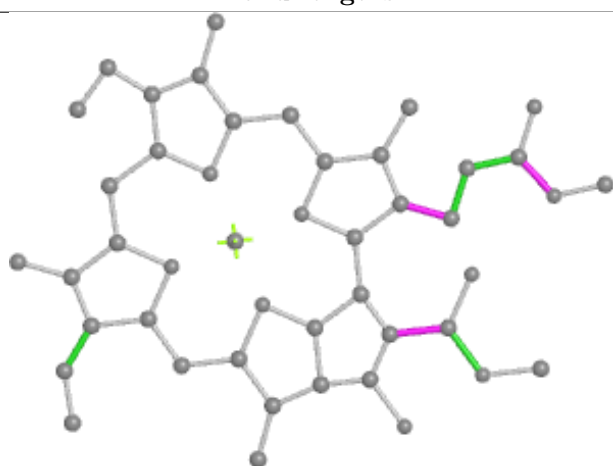
Ligand CLA 7 311



Bond lengths



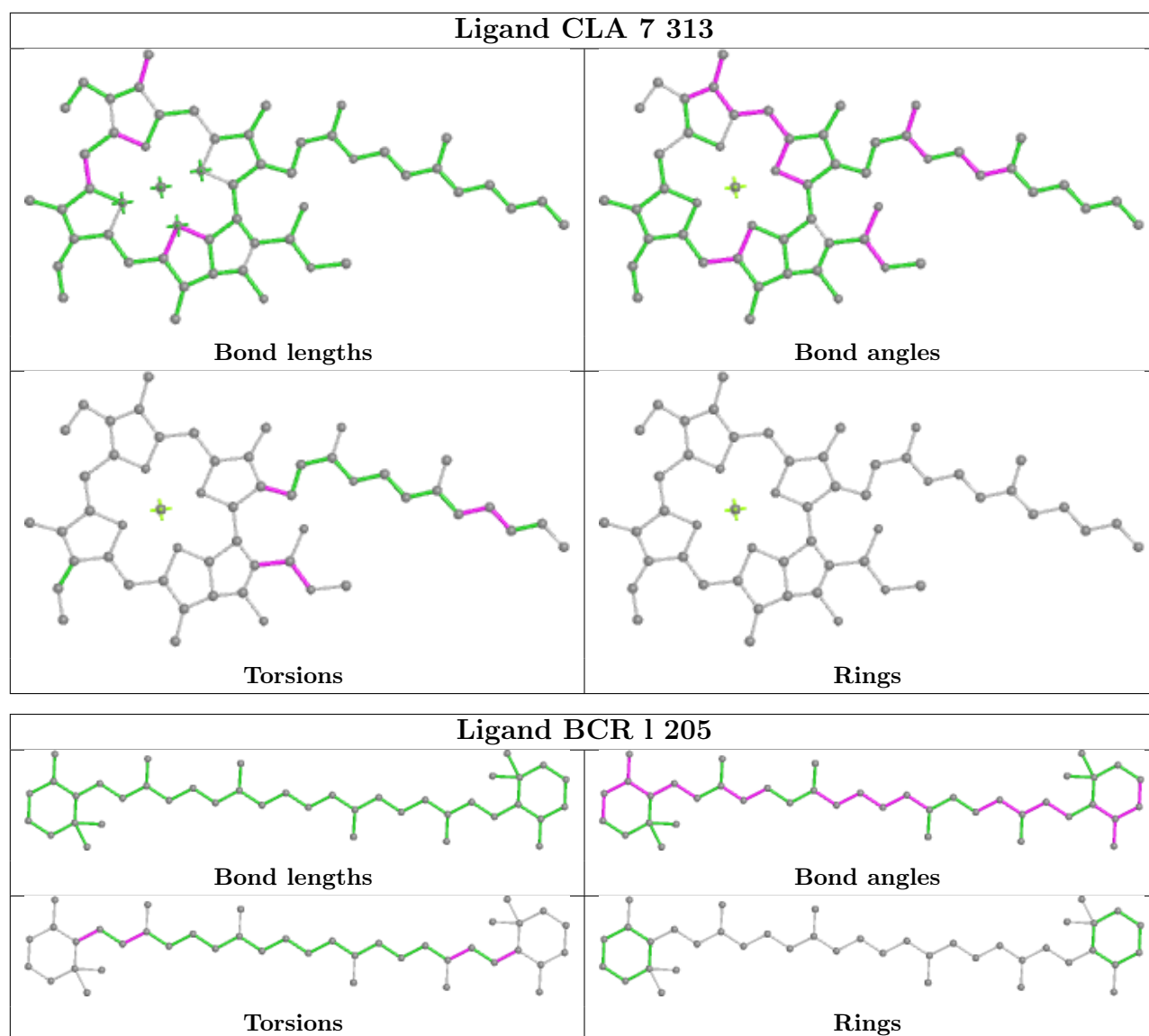
Bond angles



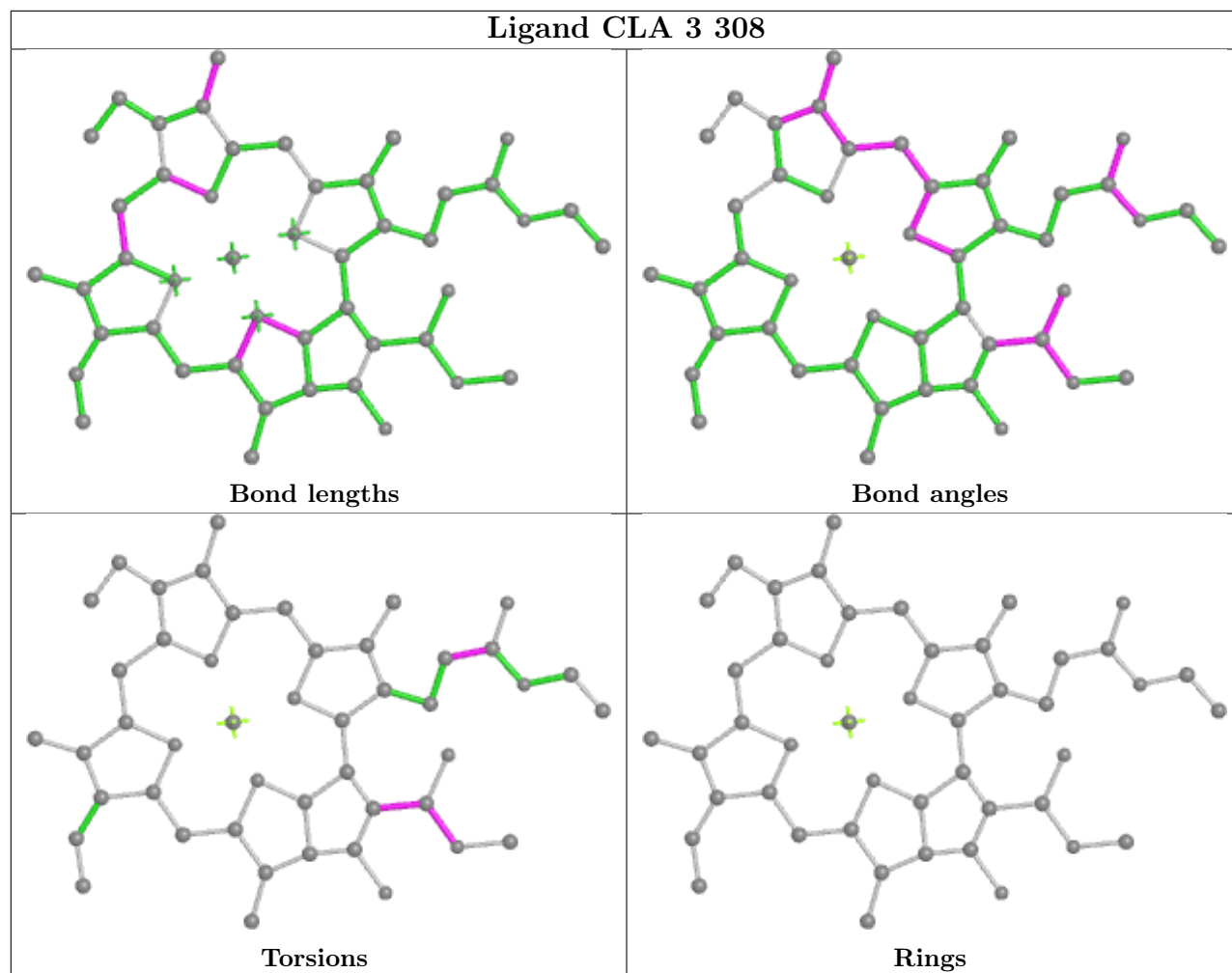
Torsions



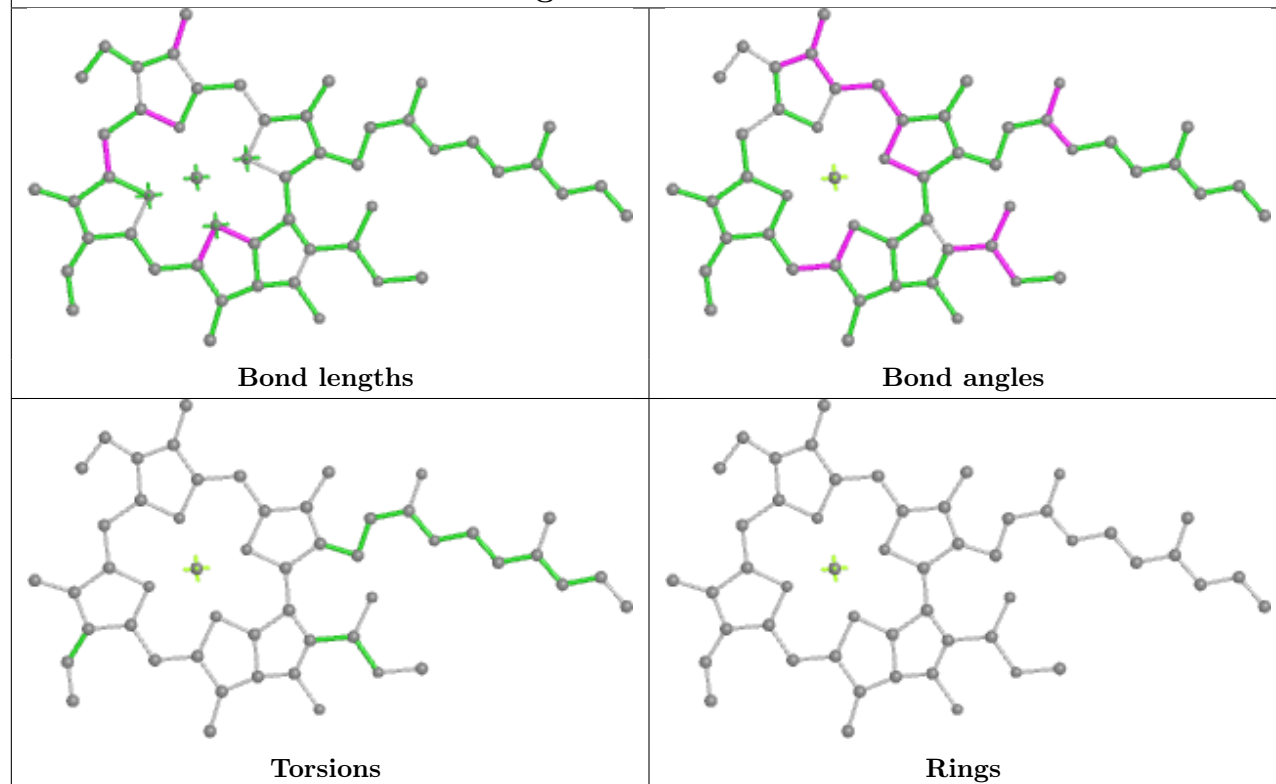
Rings



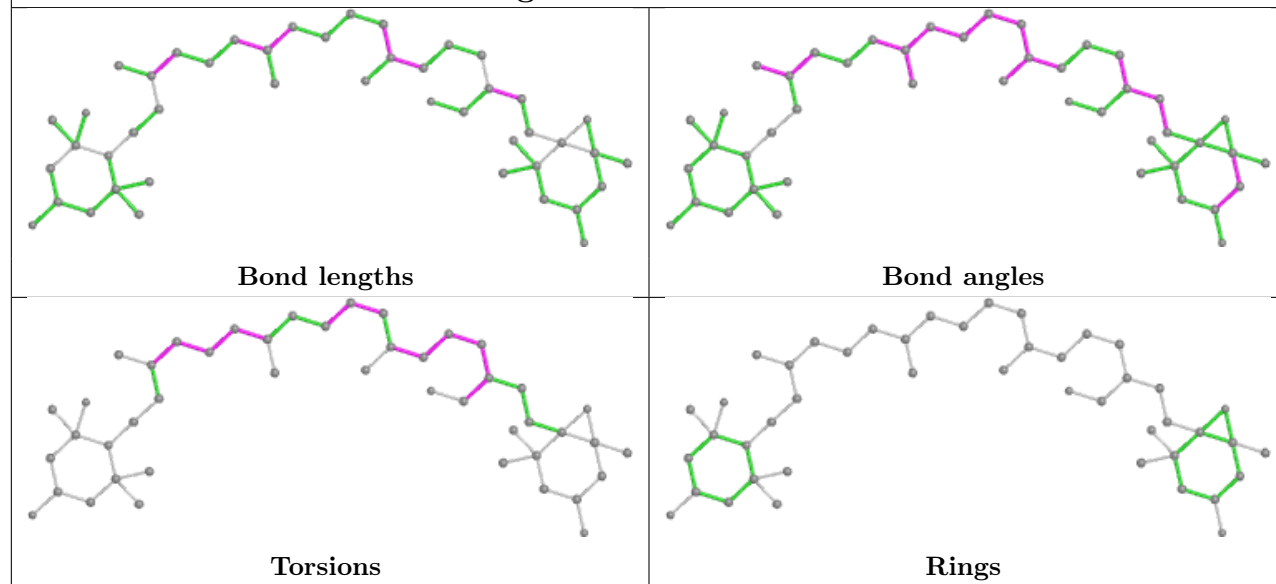
Ligand CLA 3 308



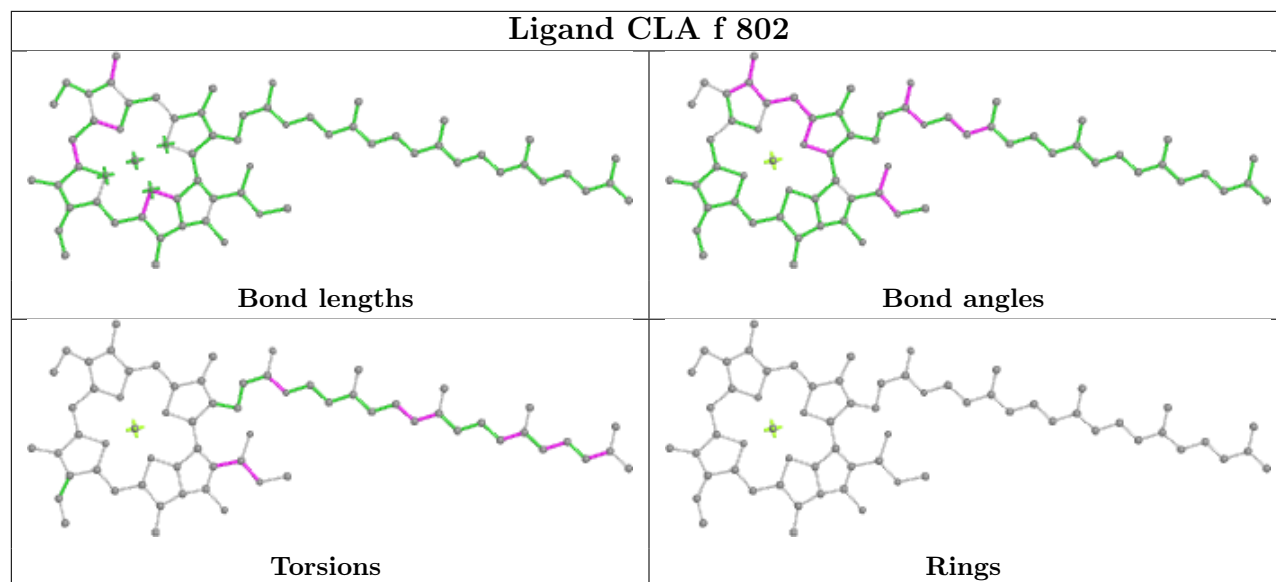
Ligand CLA 5 312



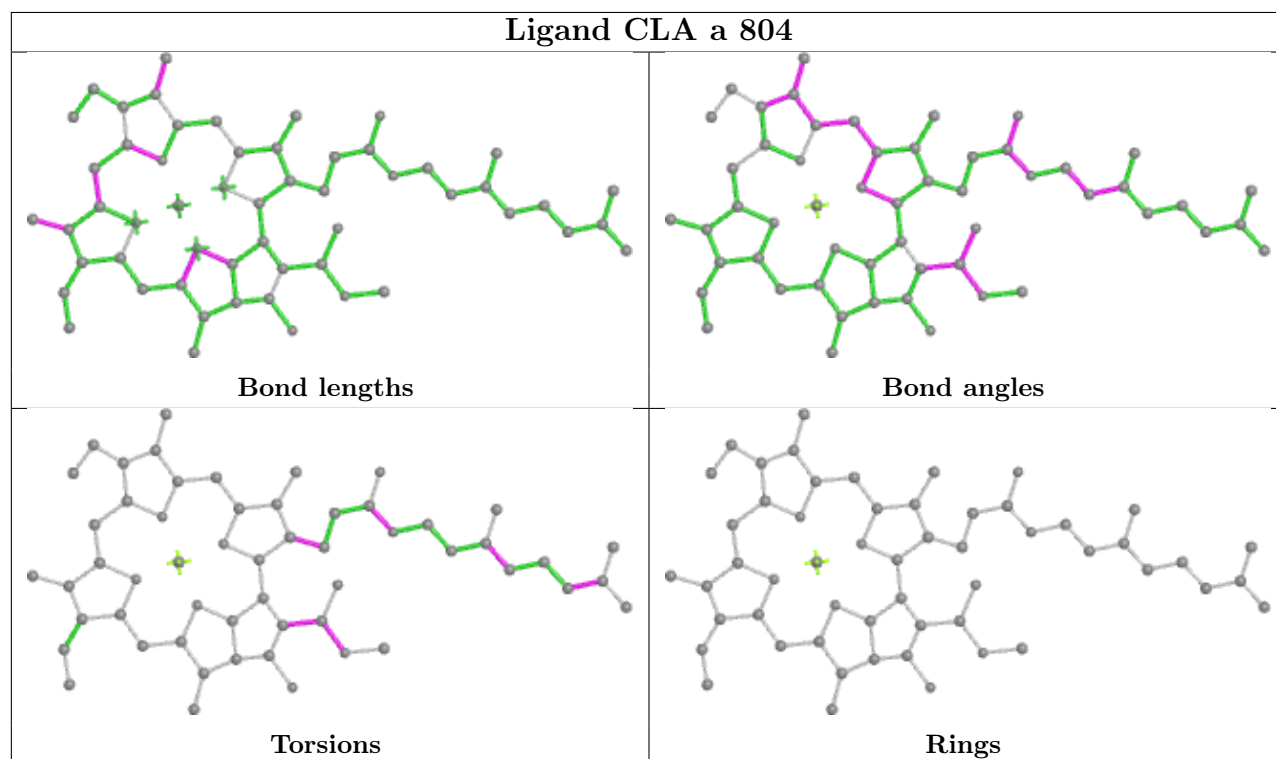
Ligand A1L1G 9 301



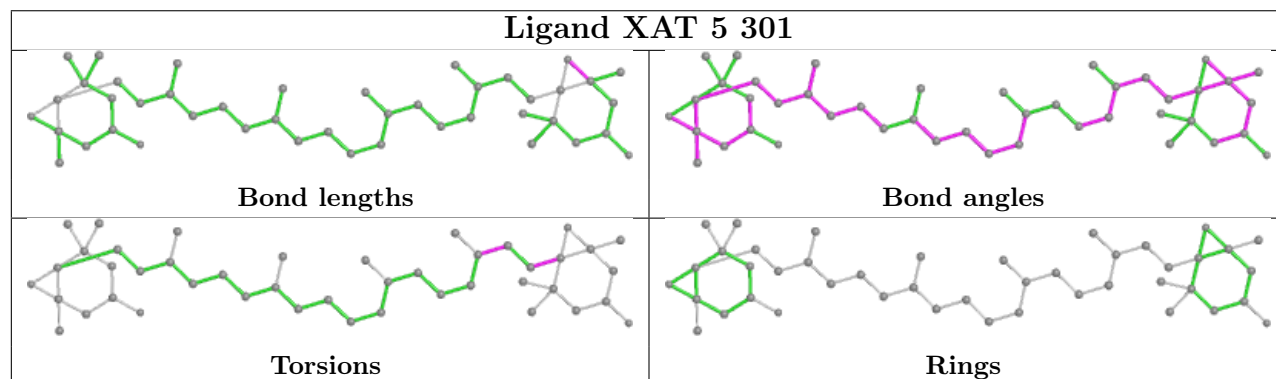
Ligand CLA f 802



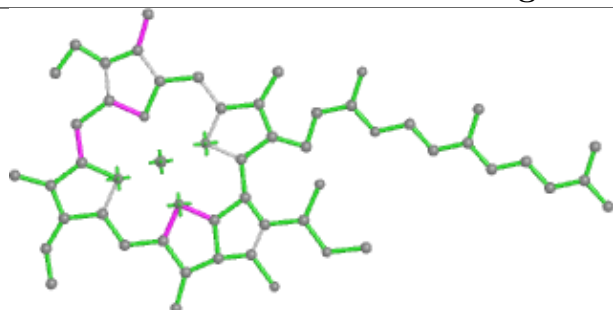
Ligand CLA a 804



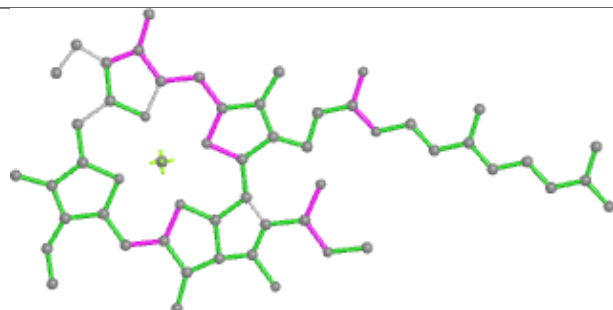
Ligand XAT 5 301



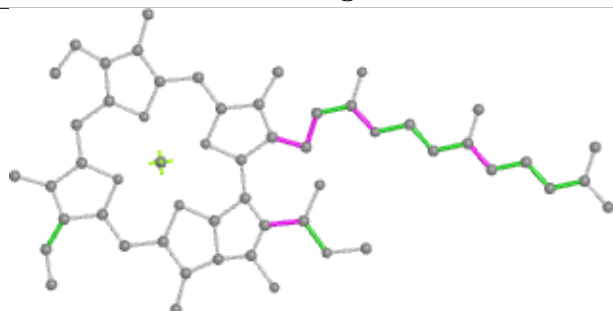
Ligand CLA a 825



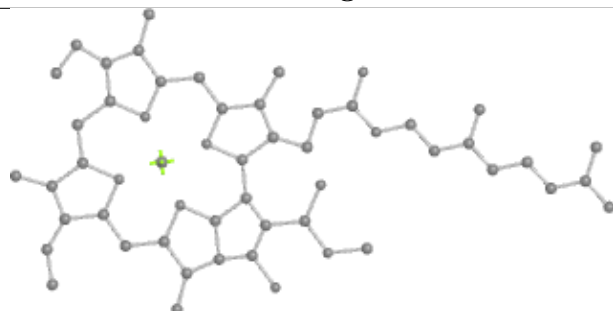
Bond lengths



Bond angles

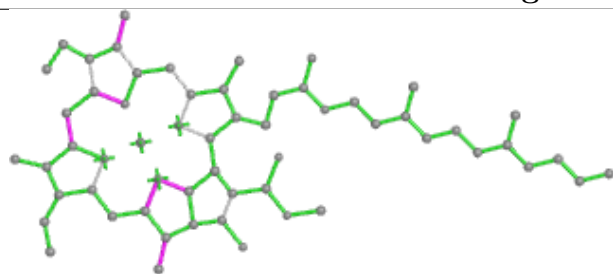


Torsions

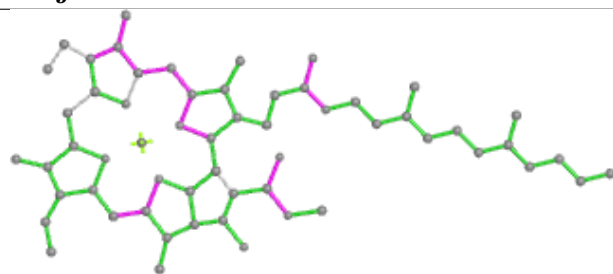


Rings

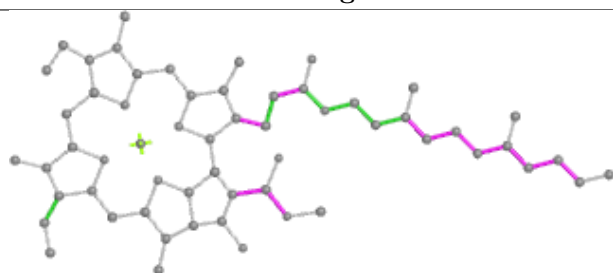
Ligand CLA j 102



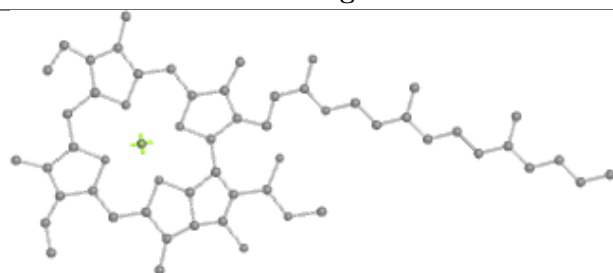
Bond lengths



Bond angles

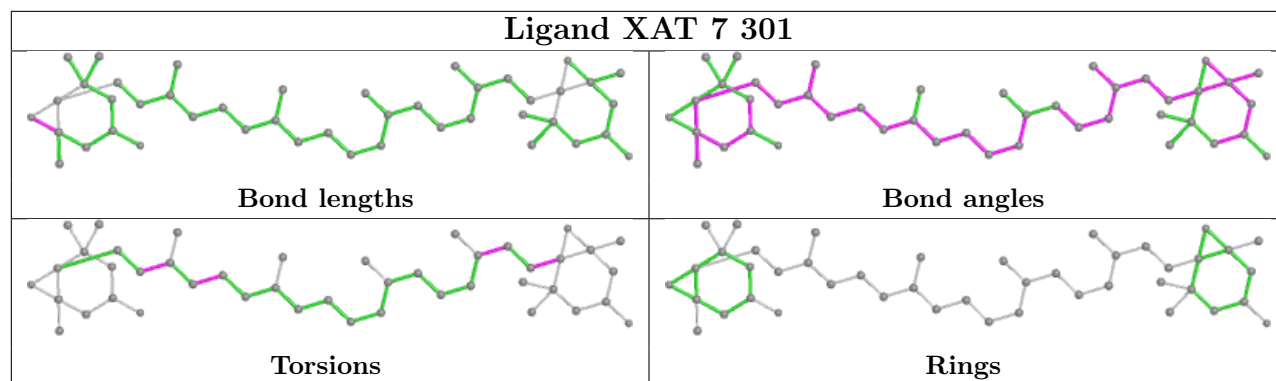


Torsions

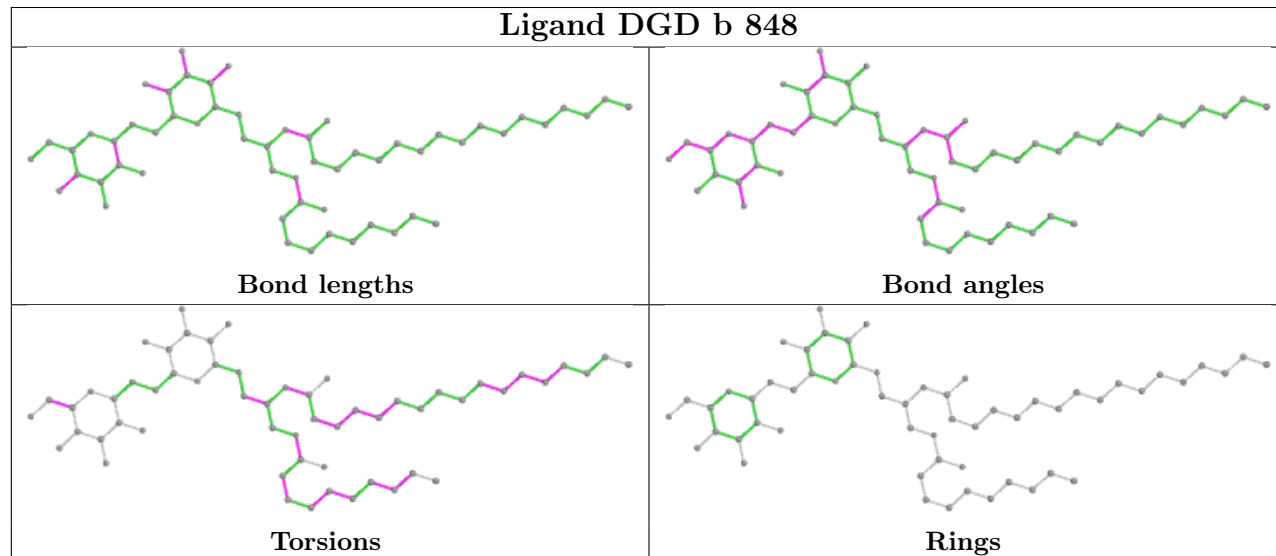


Rings

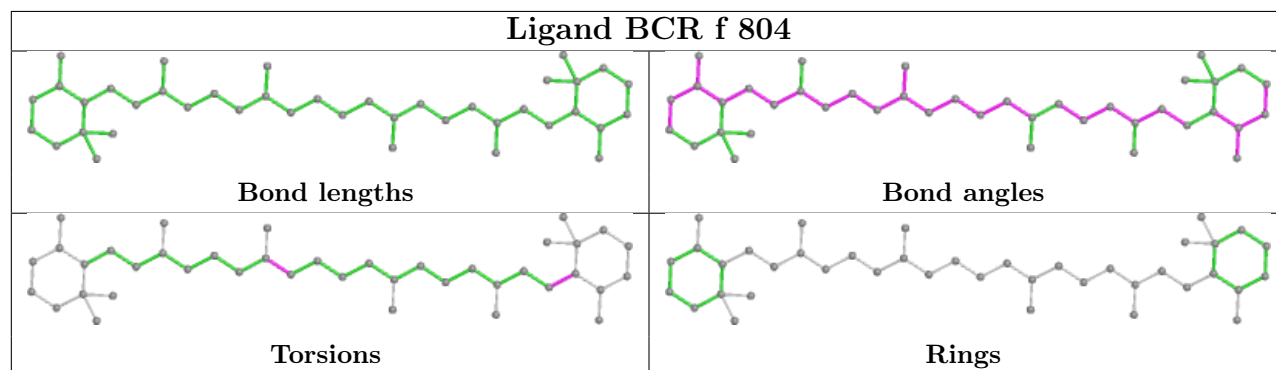
Ligand XAT 7 301



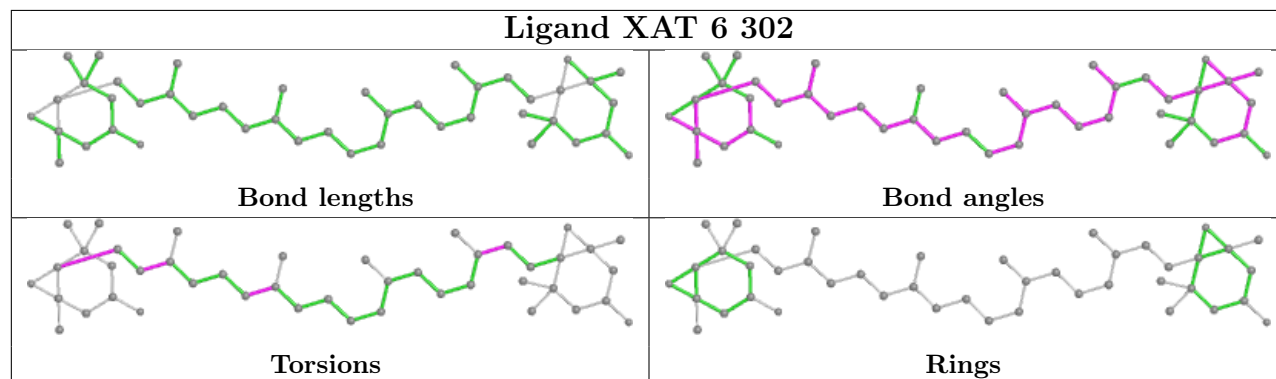
Ligand DGD b 848



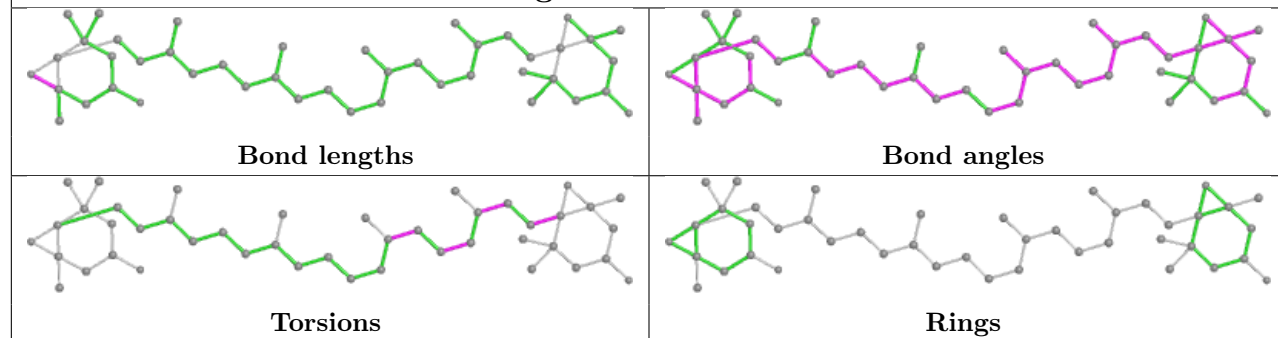
Ligand BCR f 804



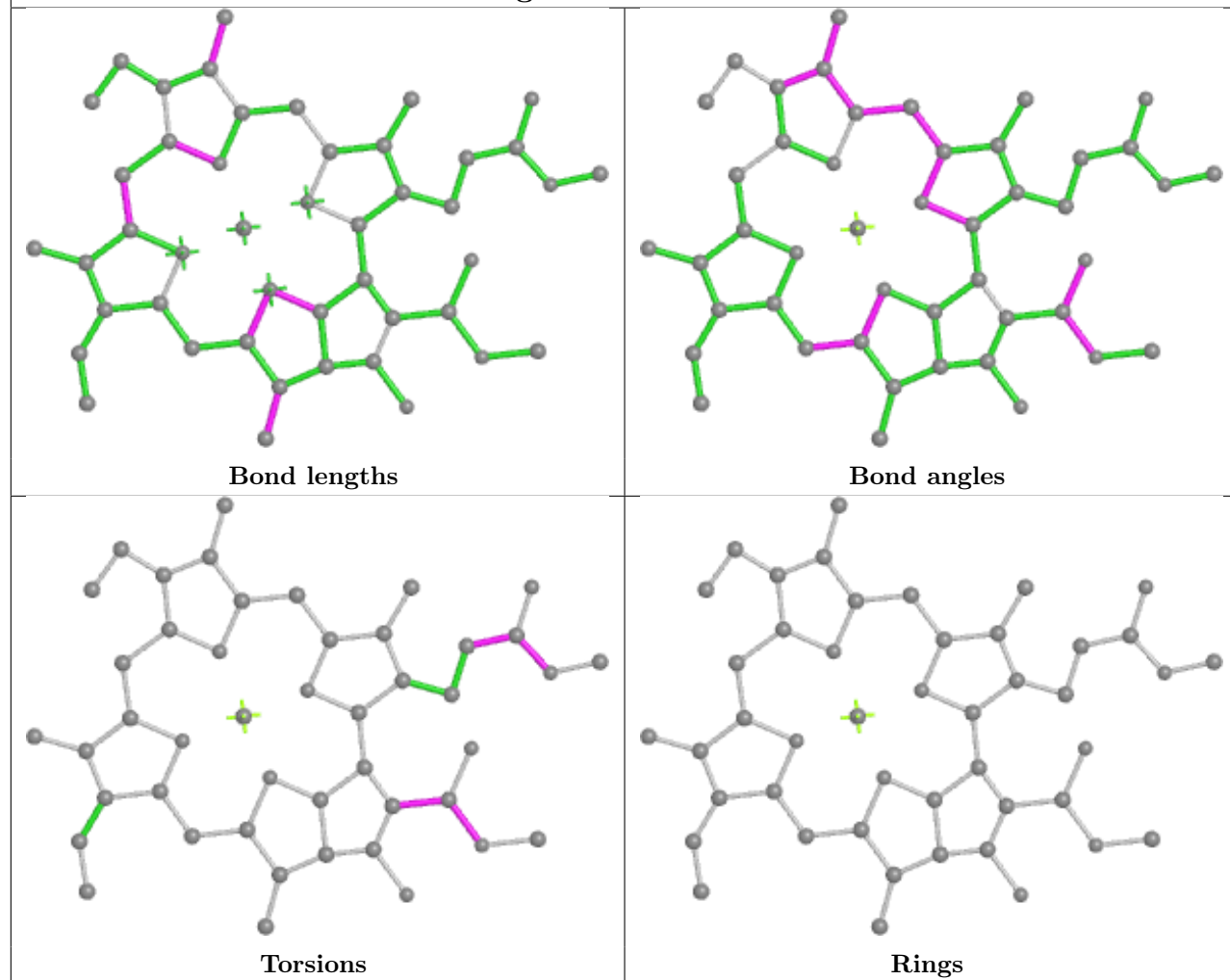
Ligand XAT 6 302

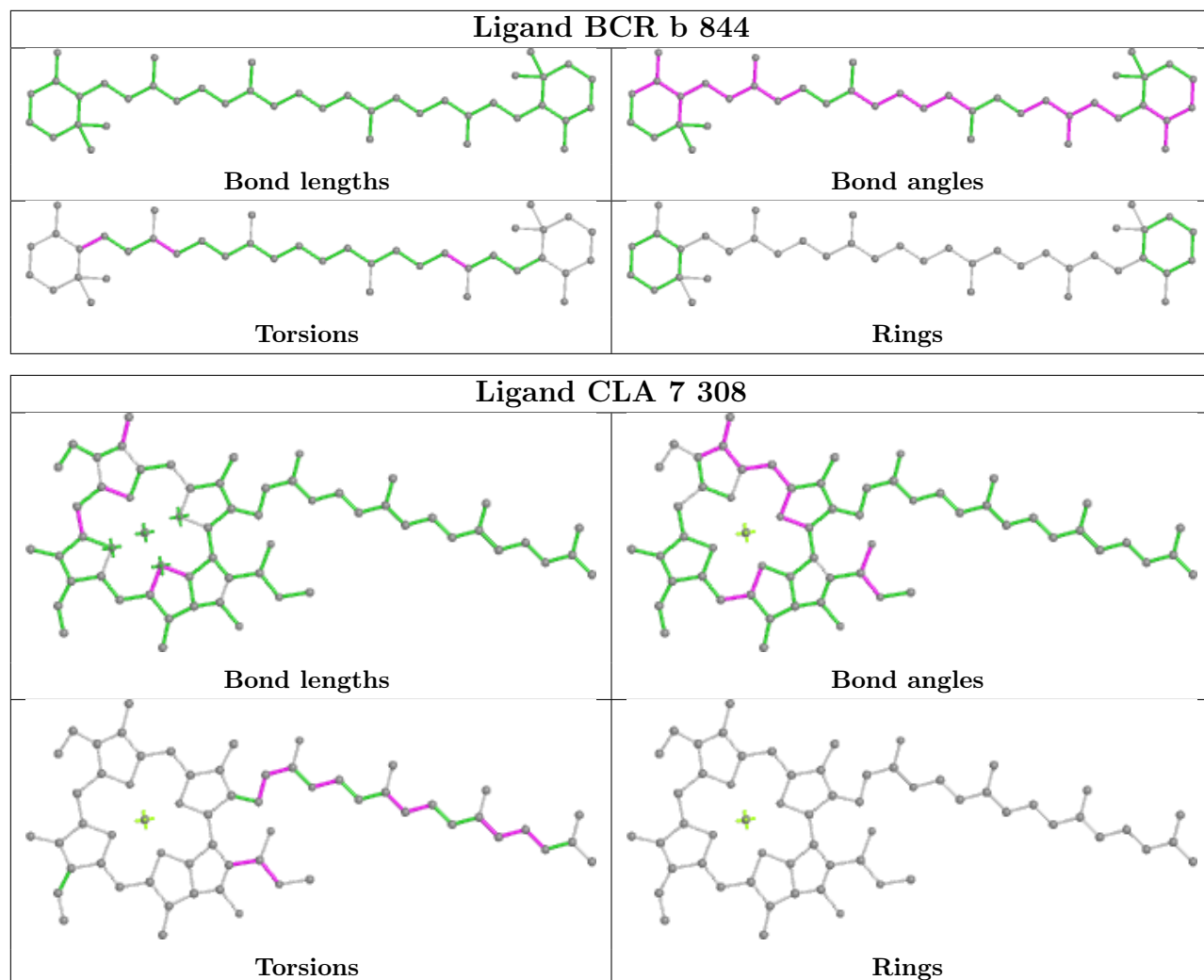


Ligand XAT 7 304

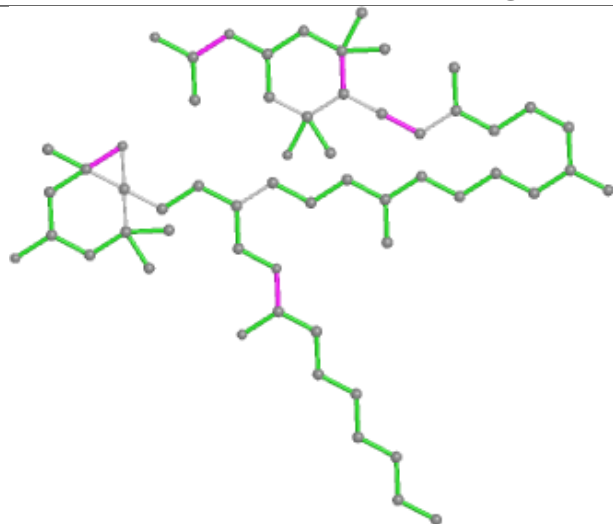


Ligand CLA 1 309

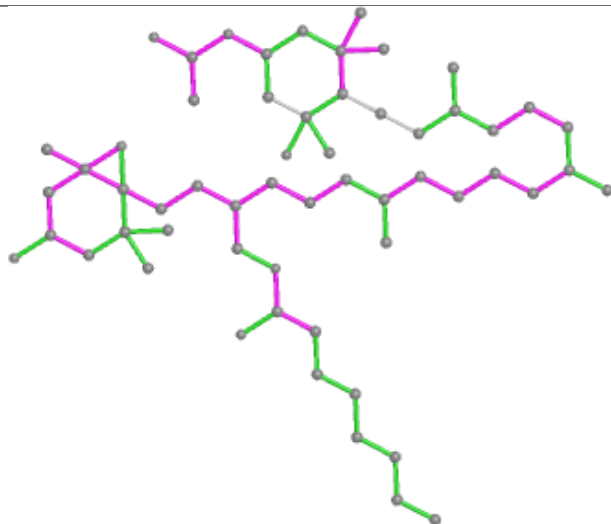




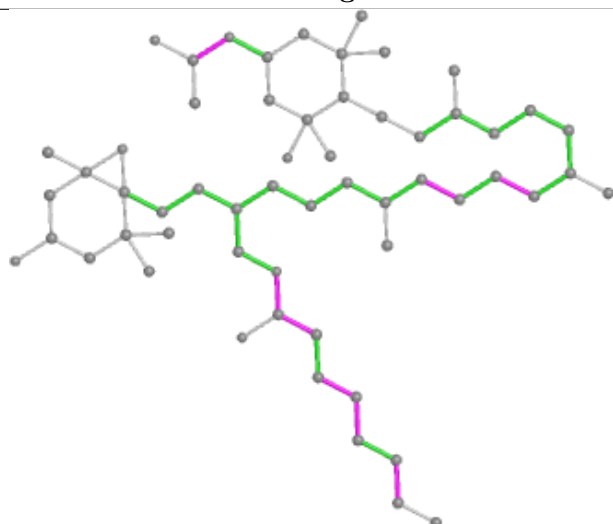
Ligand A1L1F 6 301



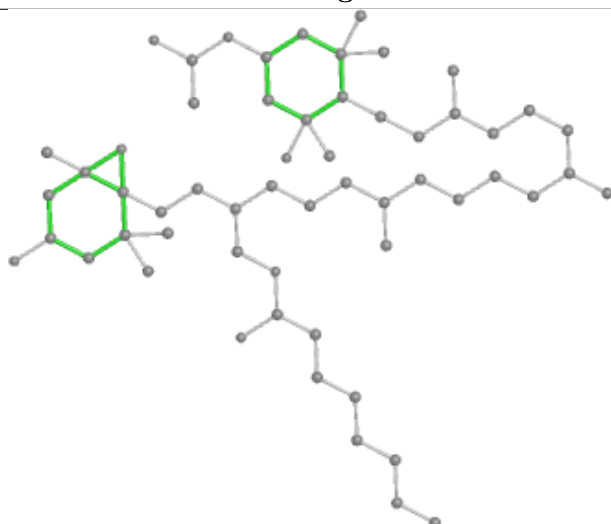
Bond lengths



Bond angles

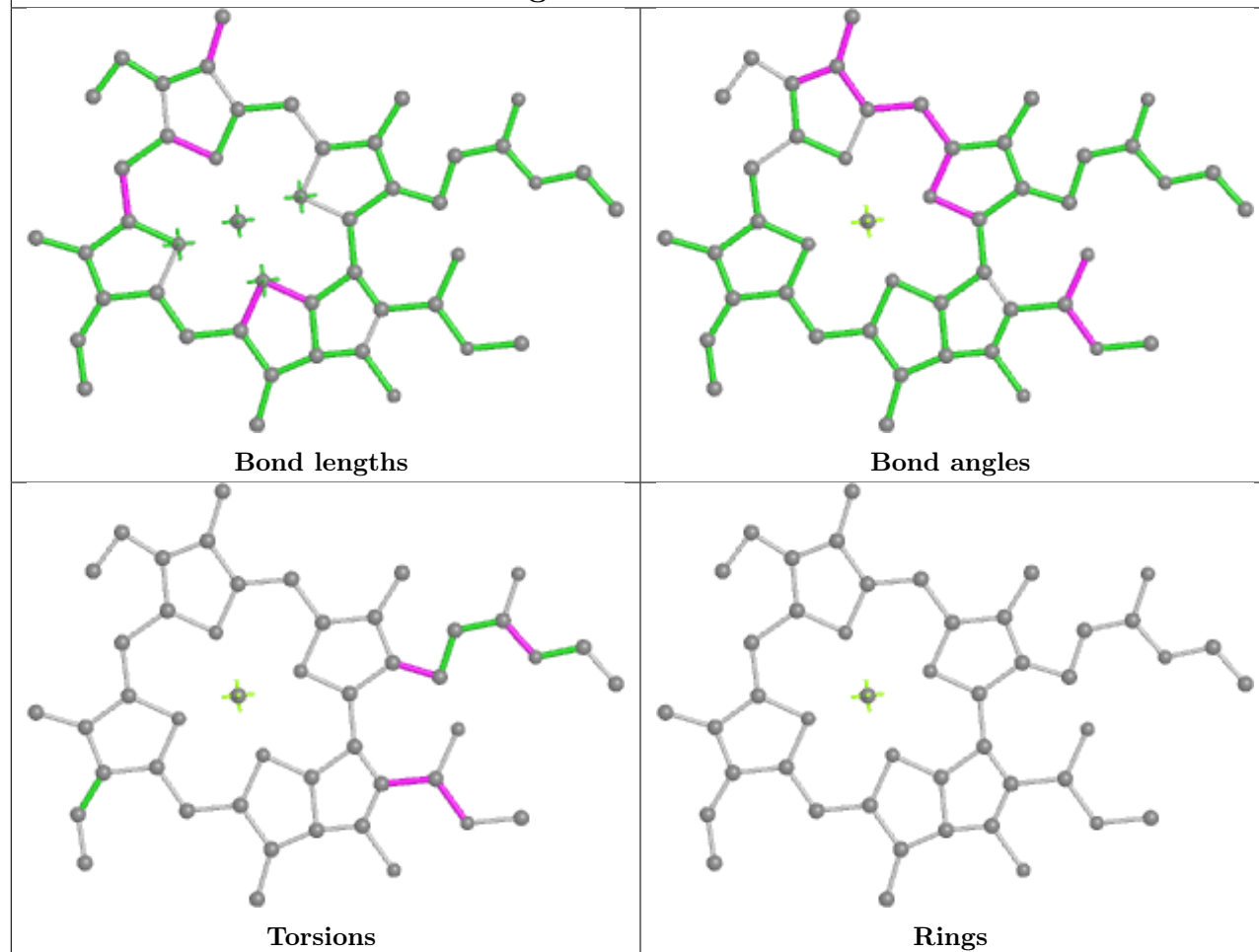


Torsions

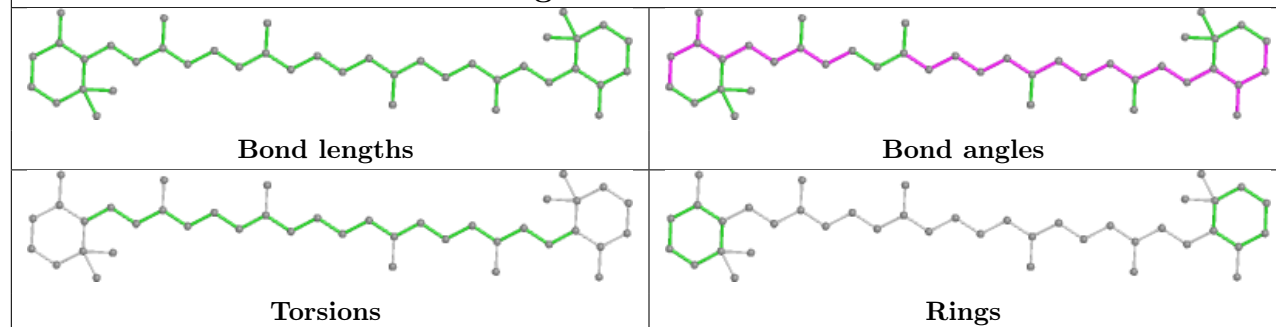


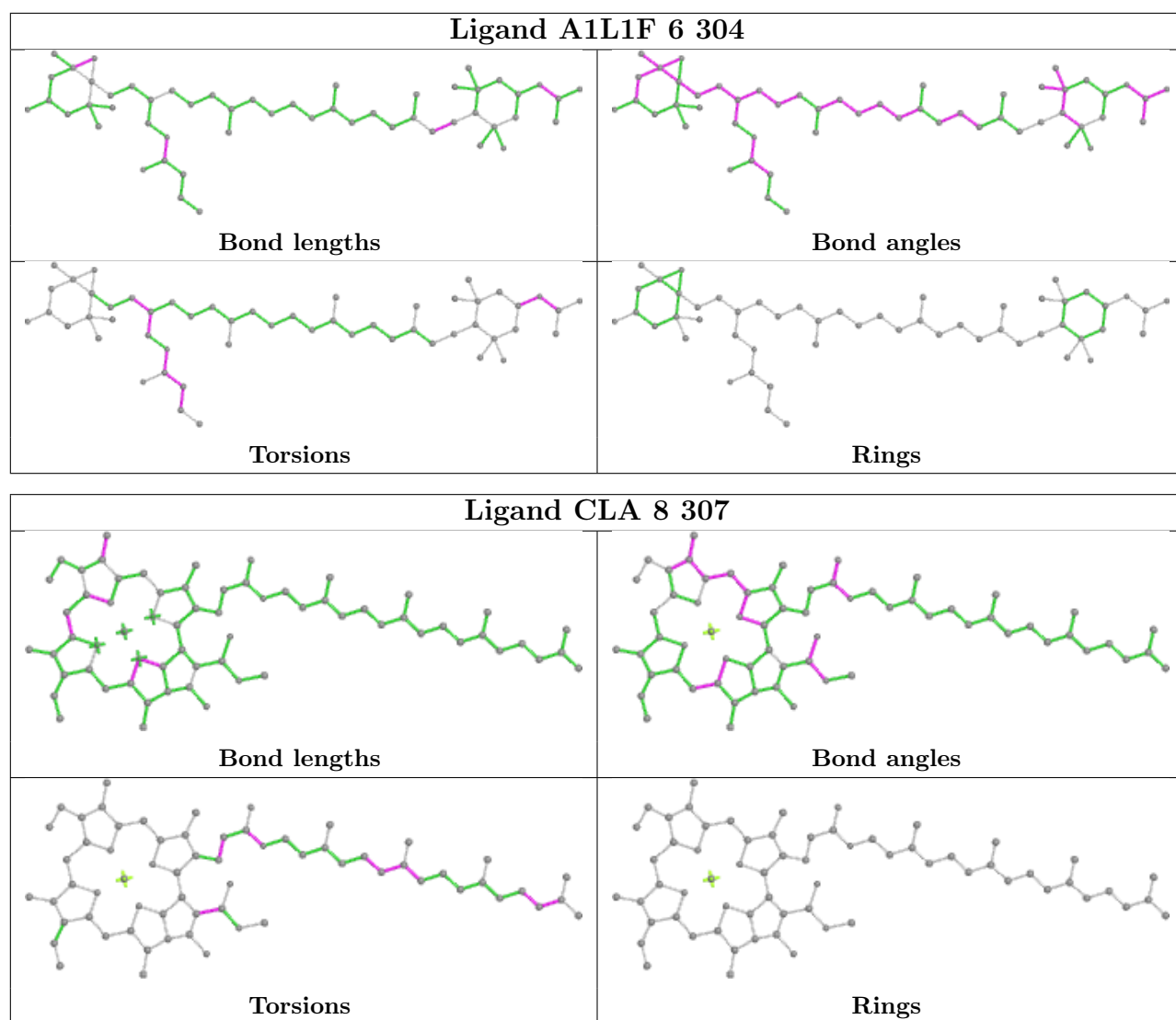
Rings

Ligand CLA 3 314

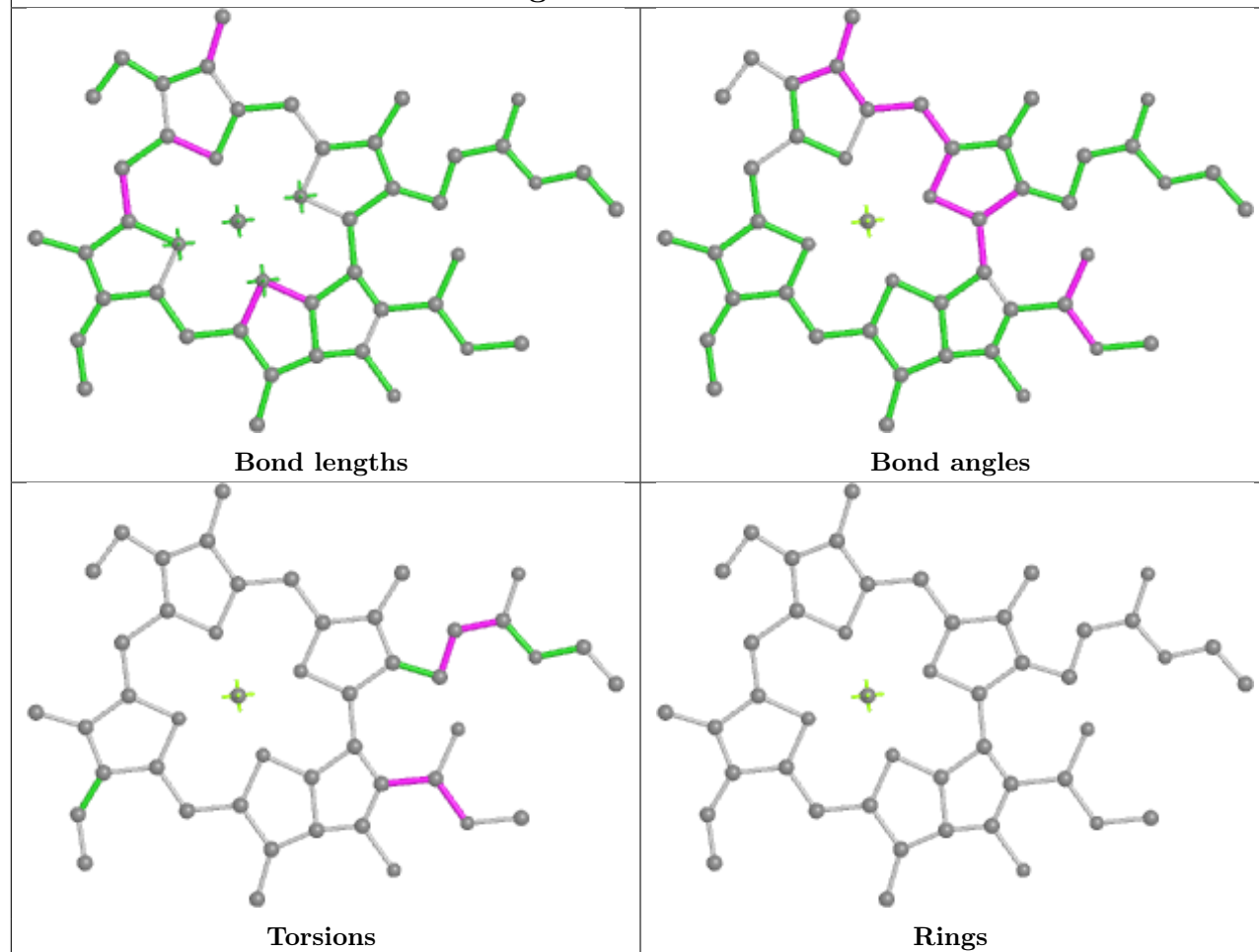


Ligand BCR a 847

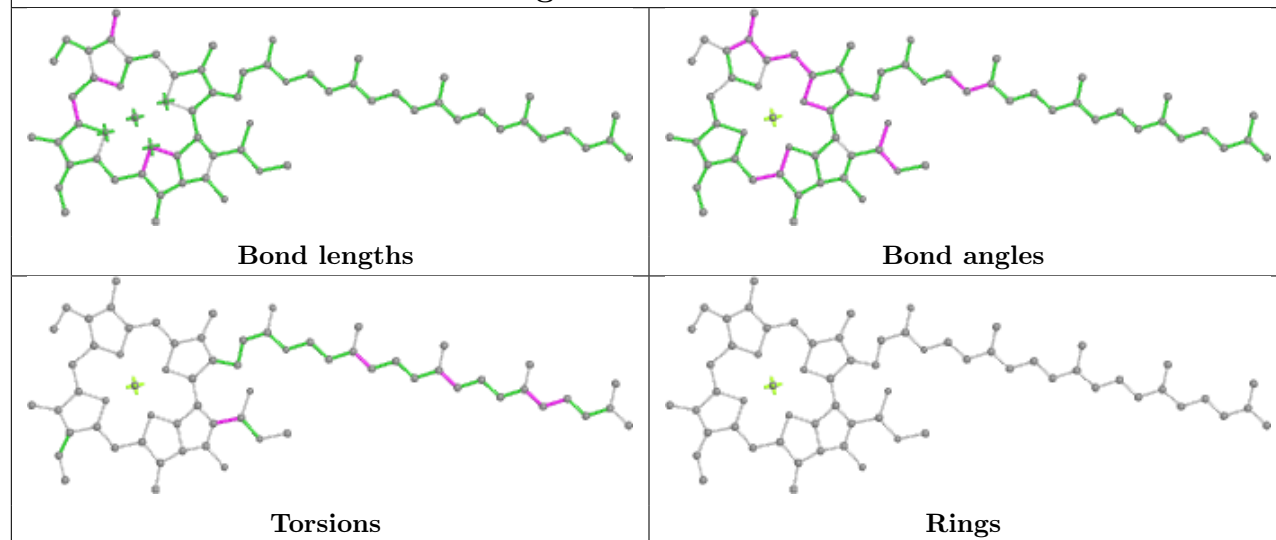


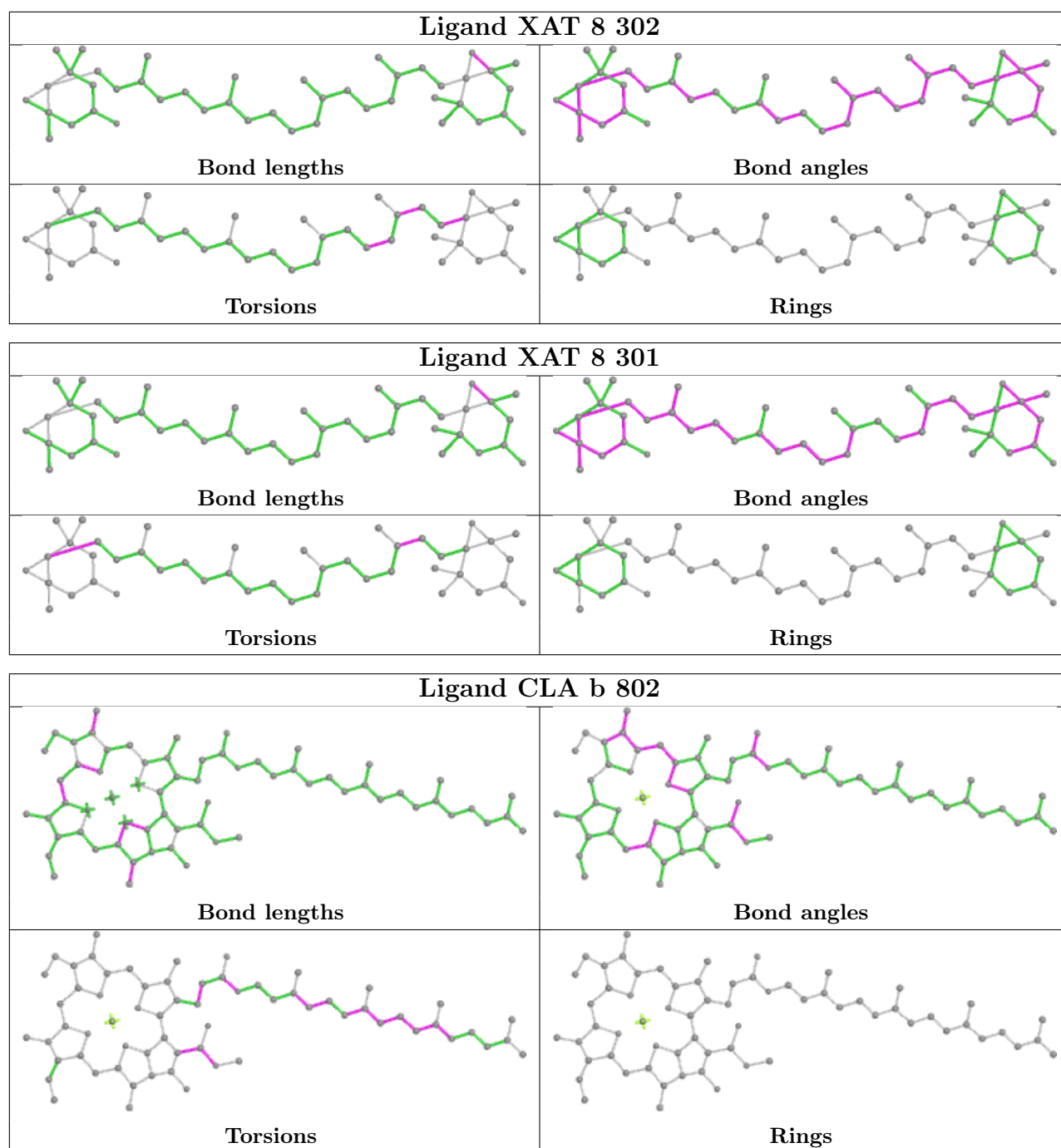


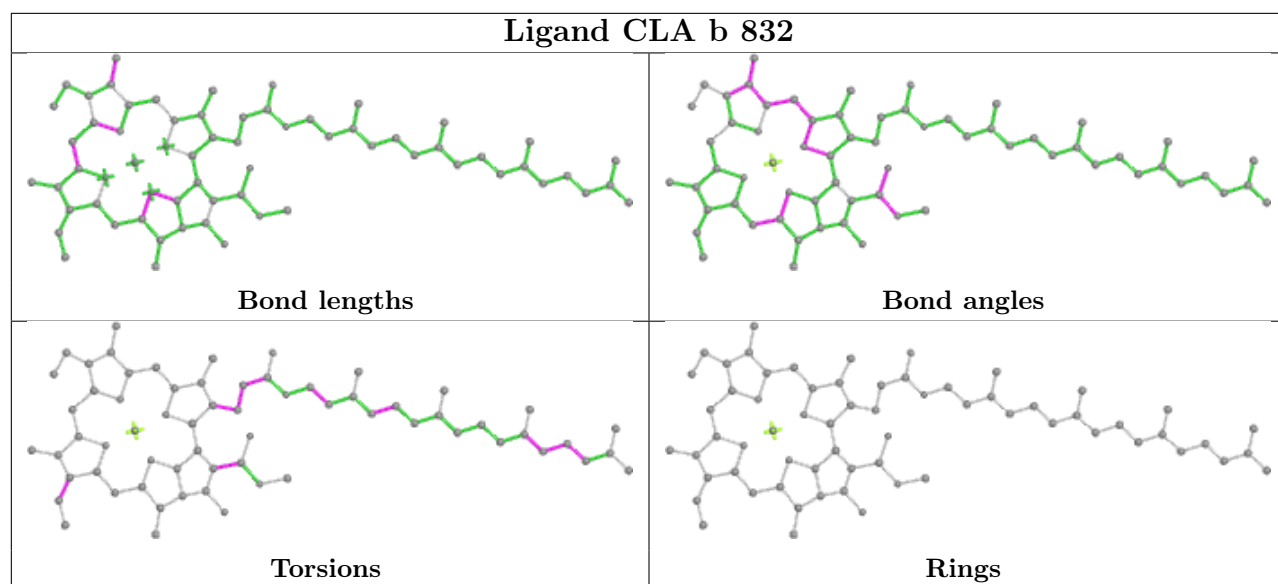
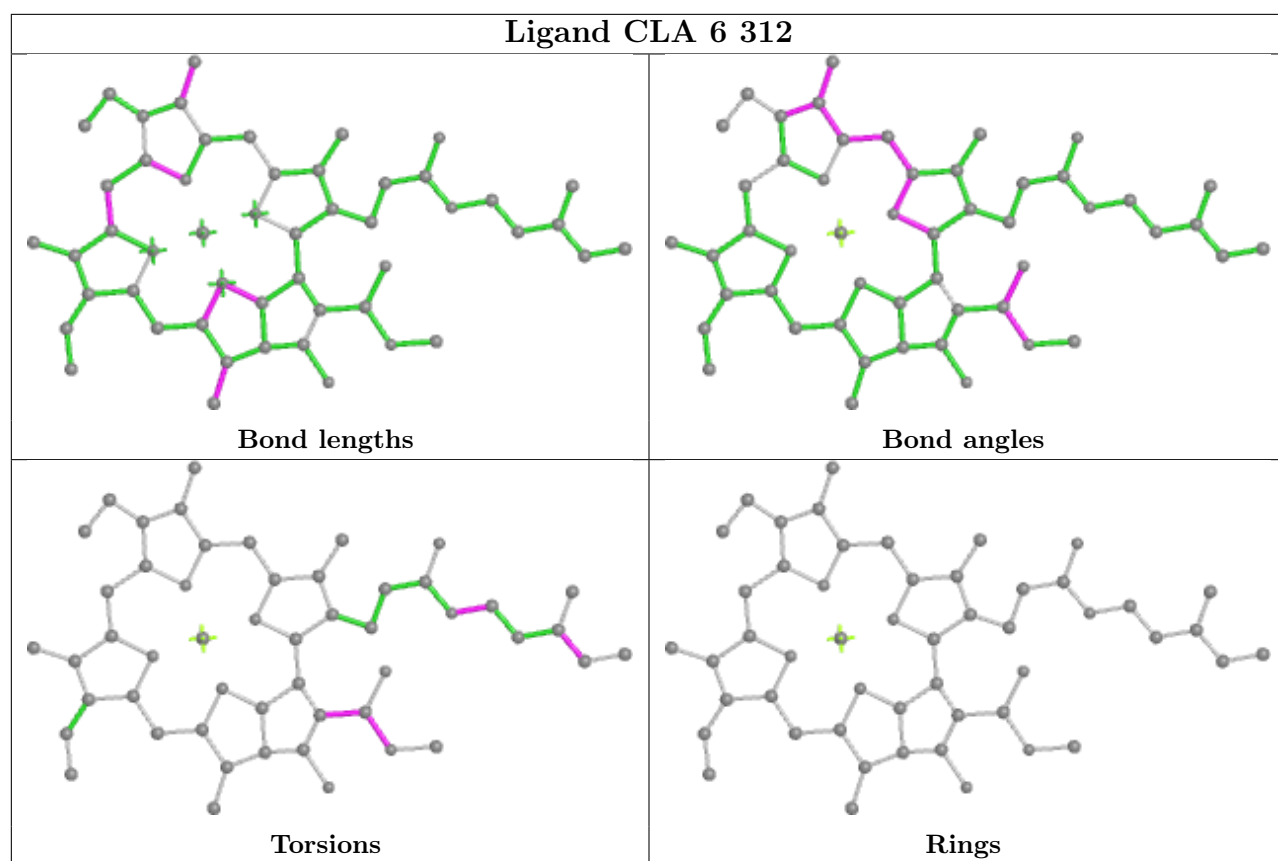
Ligand CLA 2 307

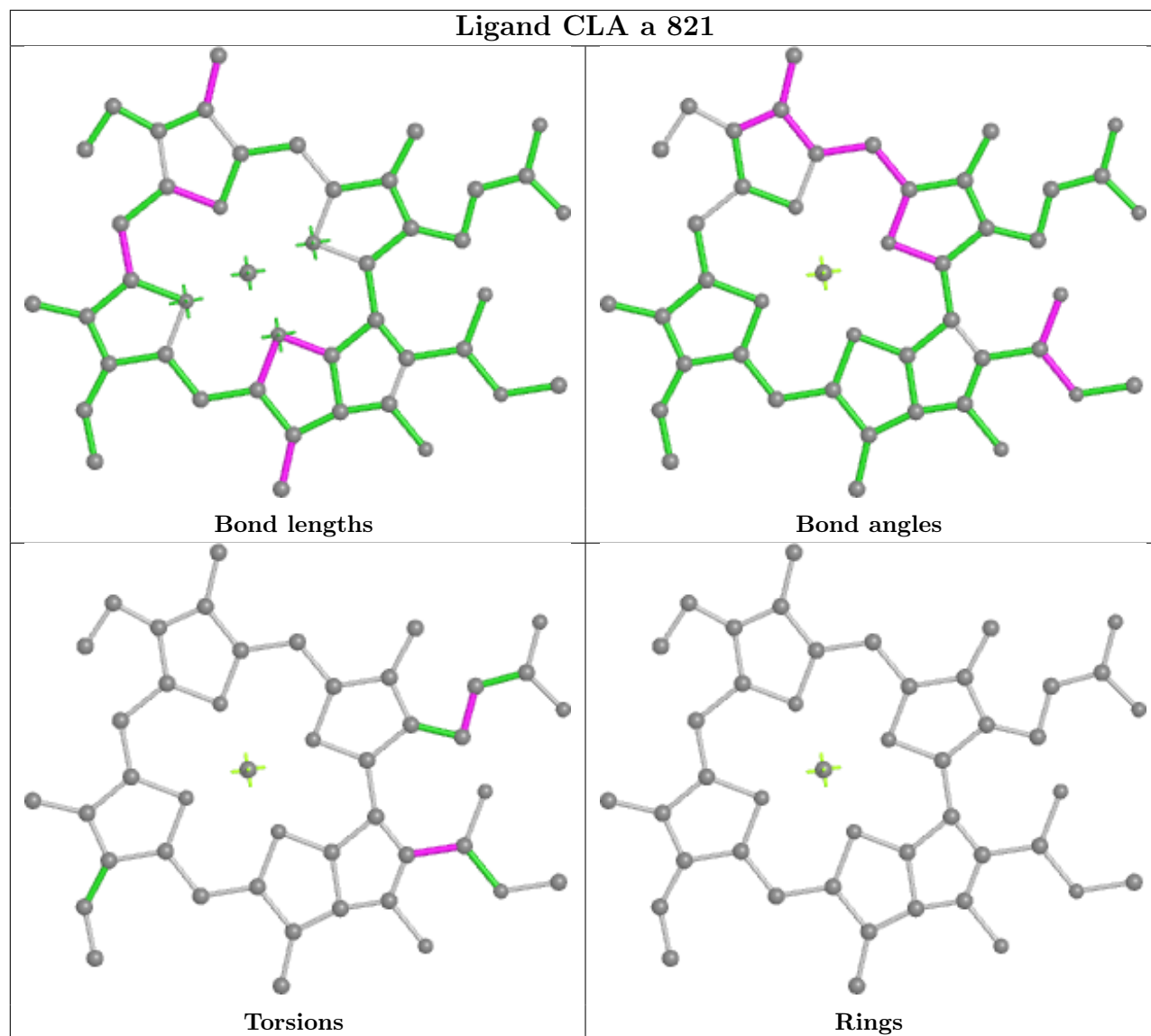
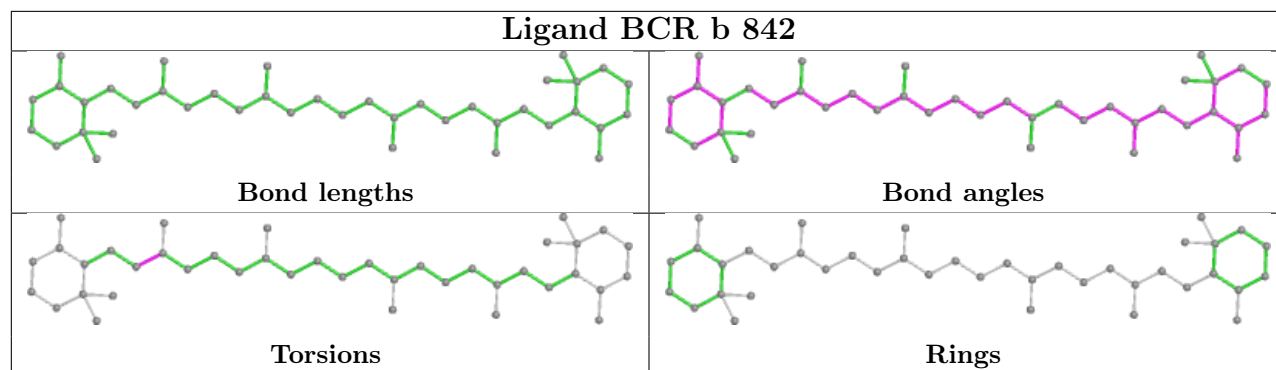


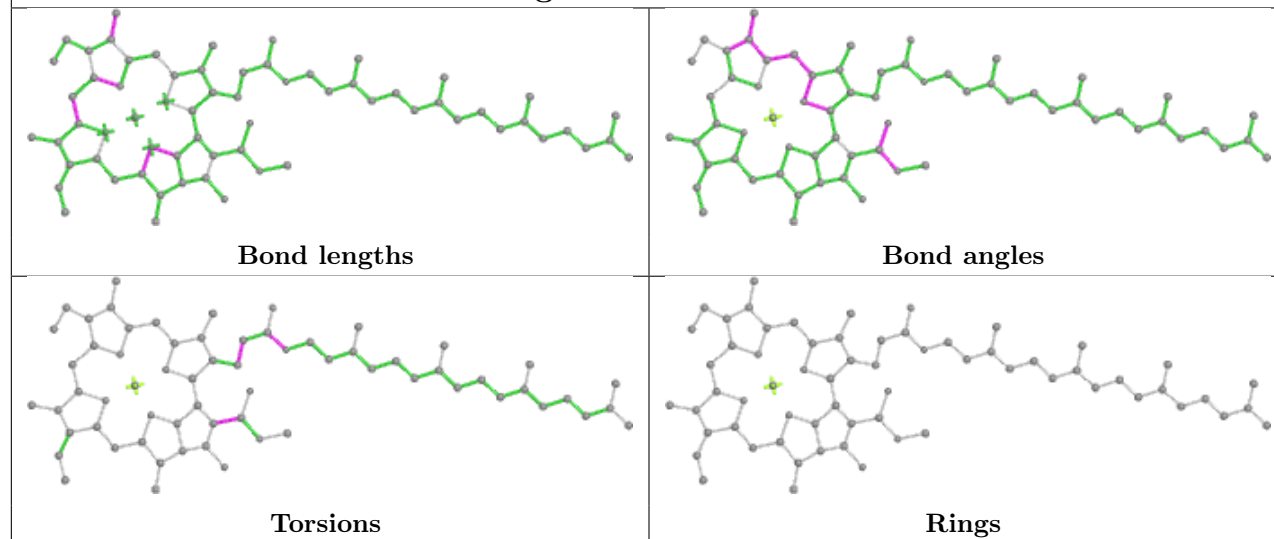
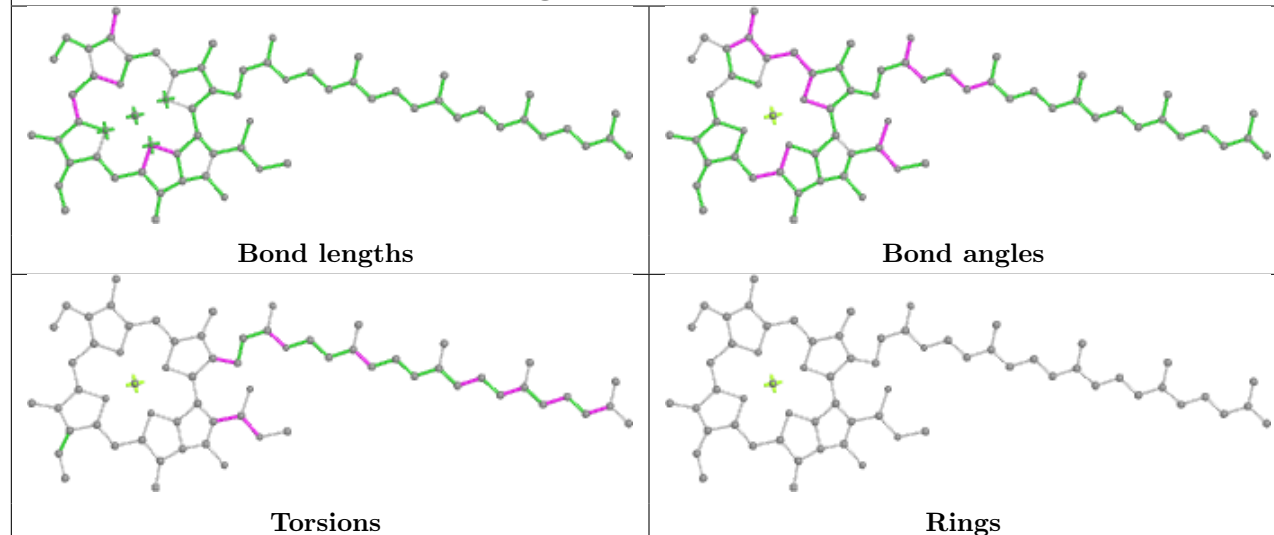
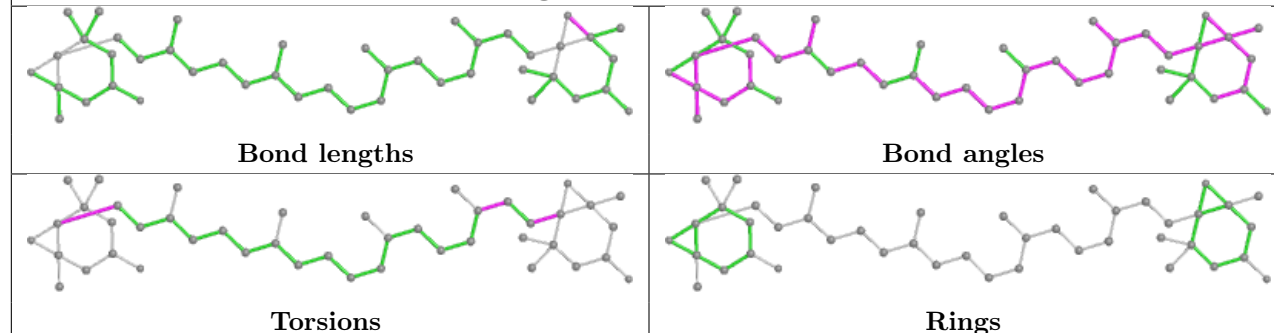
Ligand CLA a 840

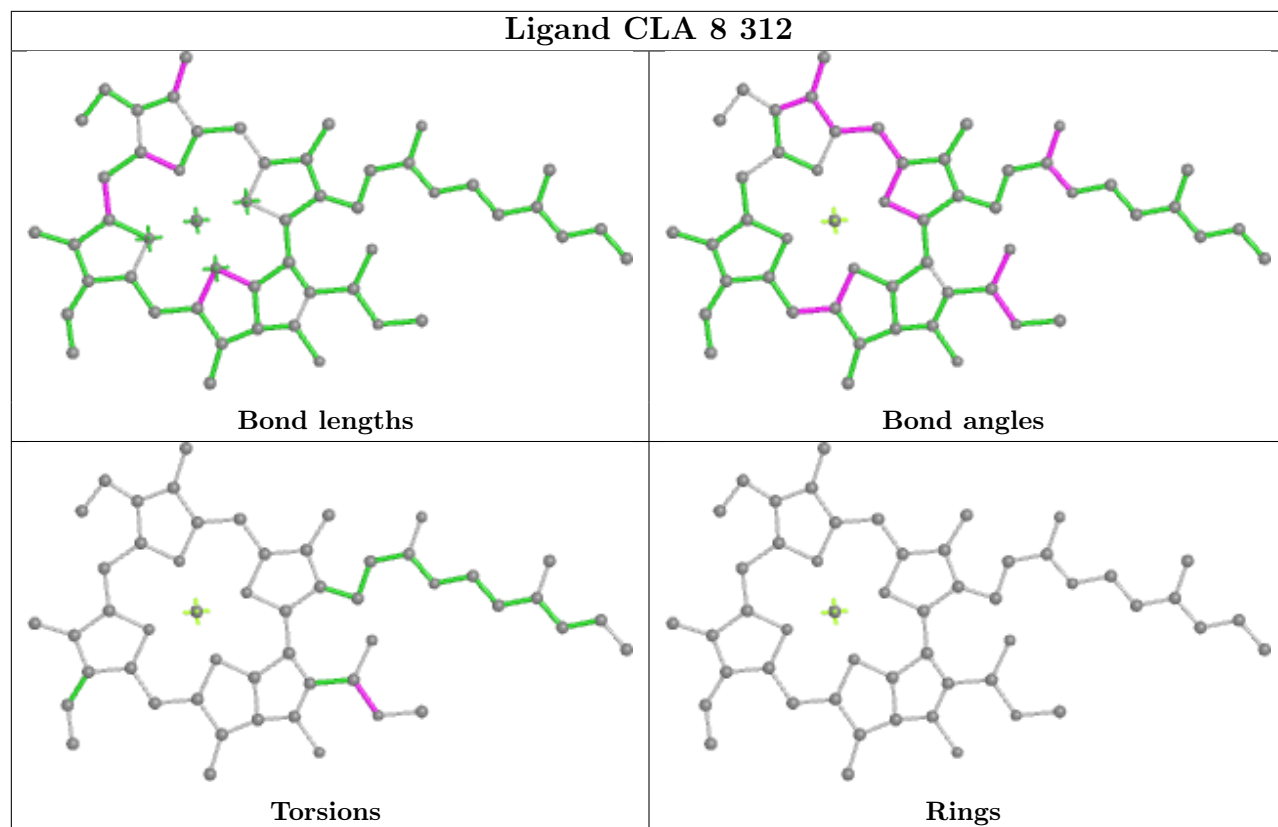




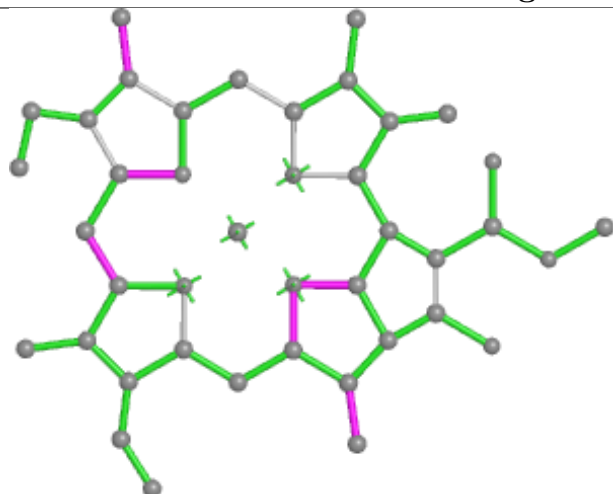




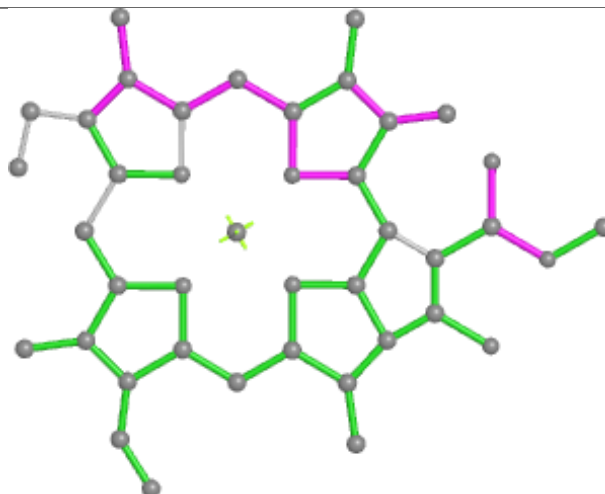
Ligand CLA b 826**Ligand CLA a 820****Ligand XAT 9 303**



Ligand CLA 1 313



Bond lengths



Bond angles

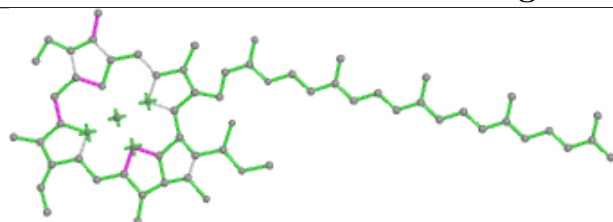


Torsions

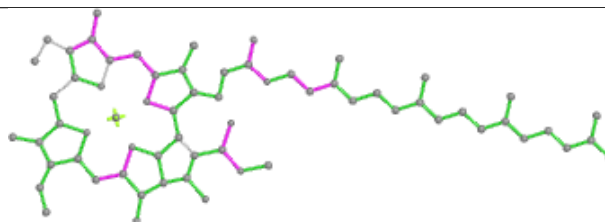


Rings

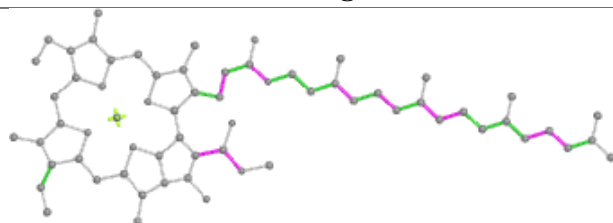
Ligand CLA a 841



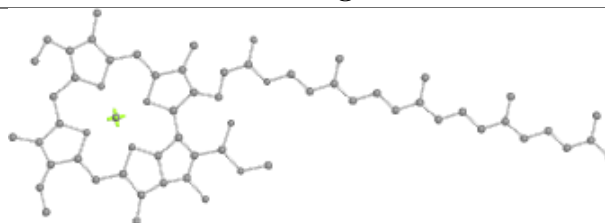
Bond lengths



Bond angles

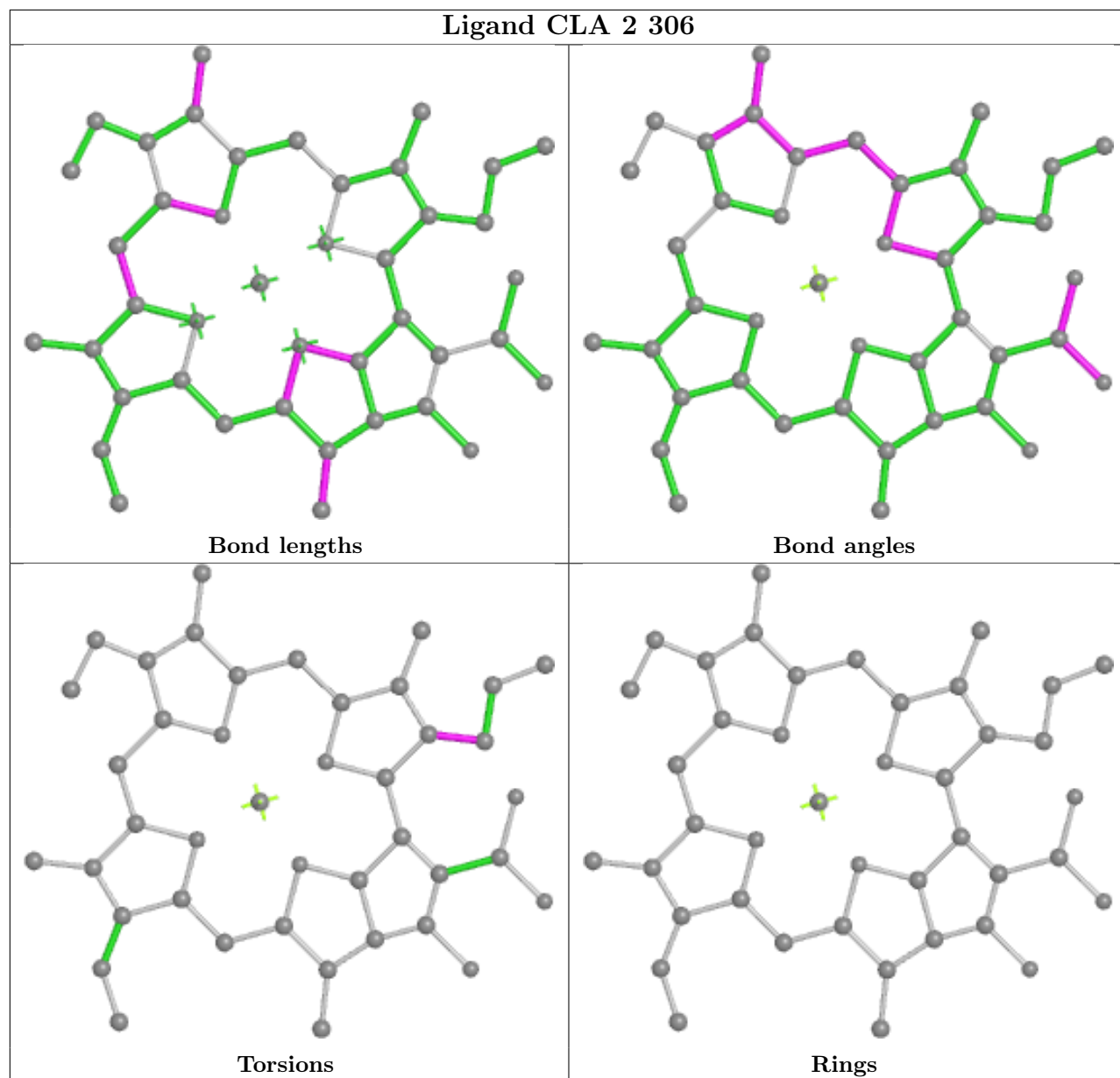


Torsions

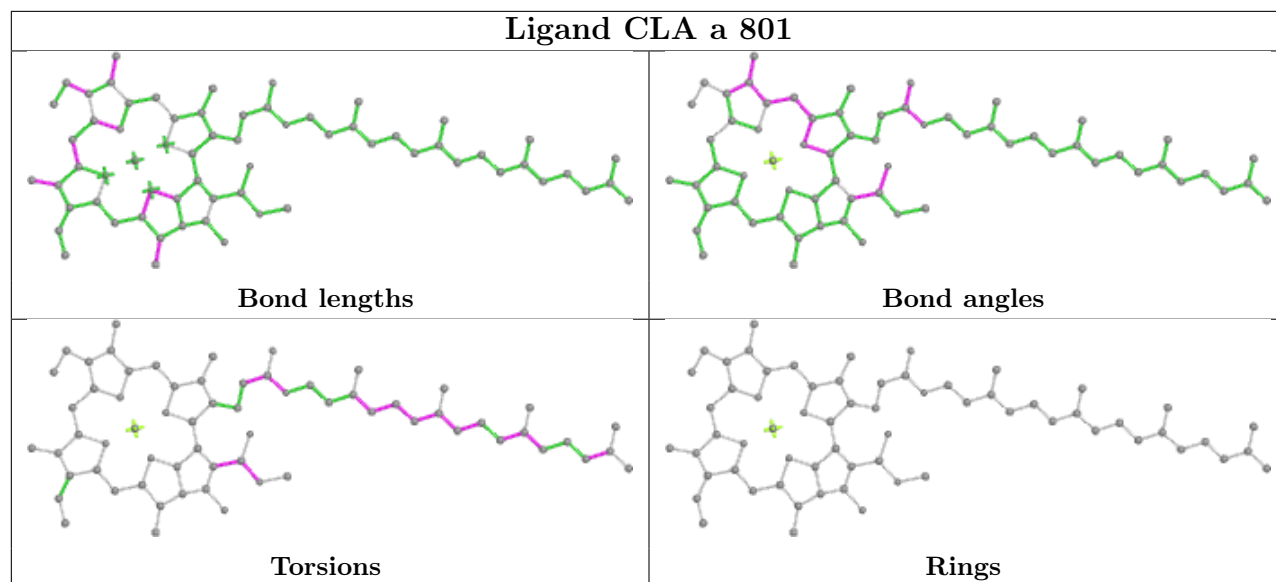


Rings

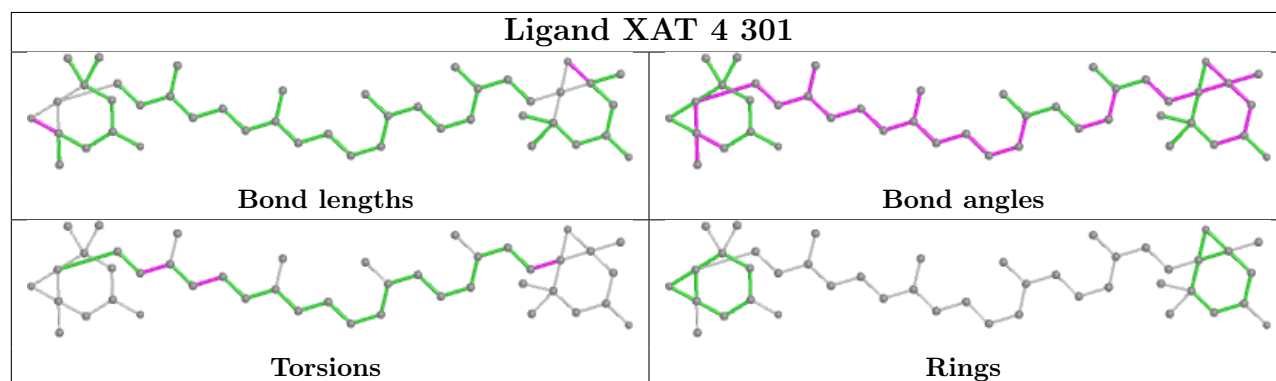
Ligand CLA 2 306



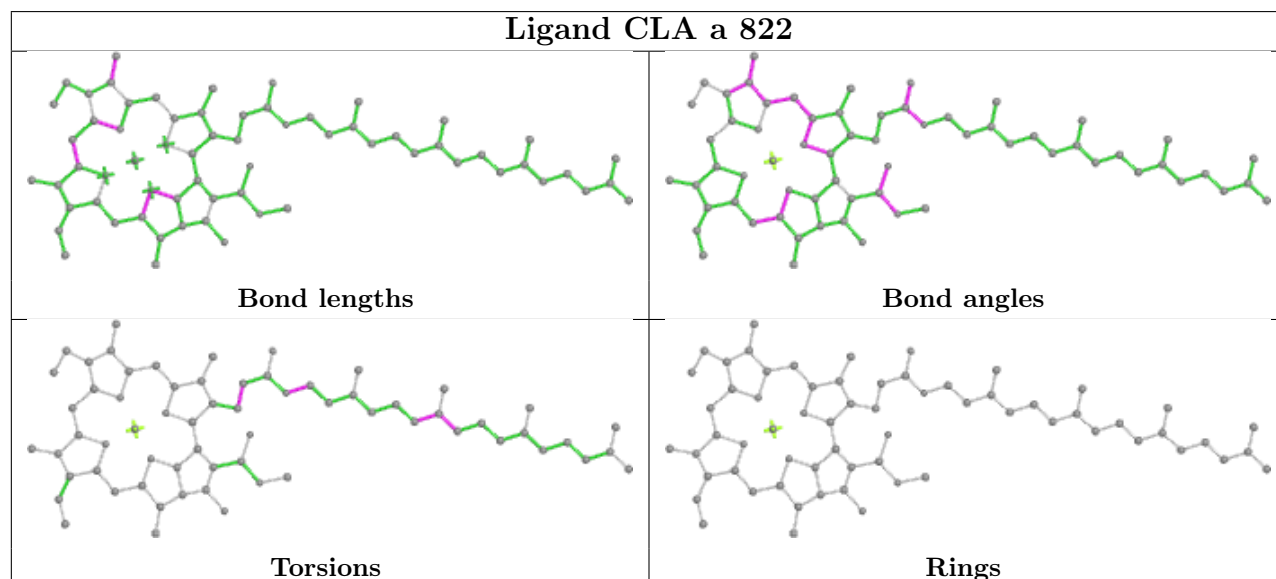
Ligand CLA a 801



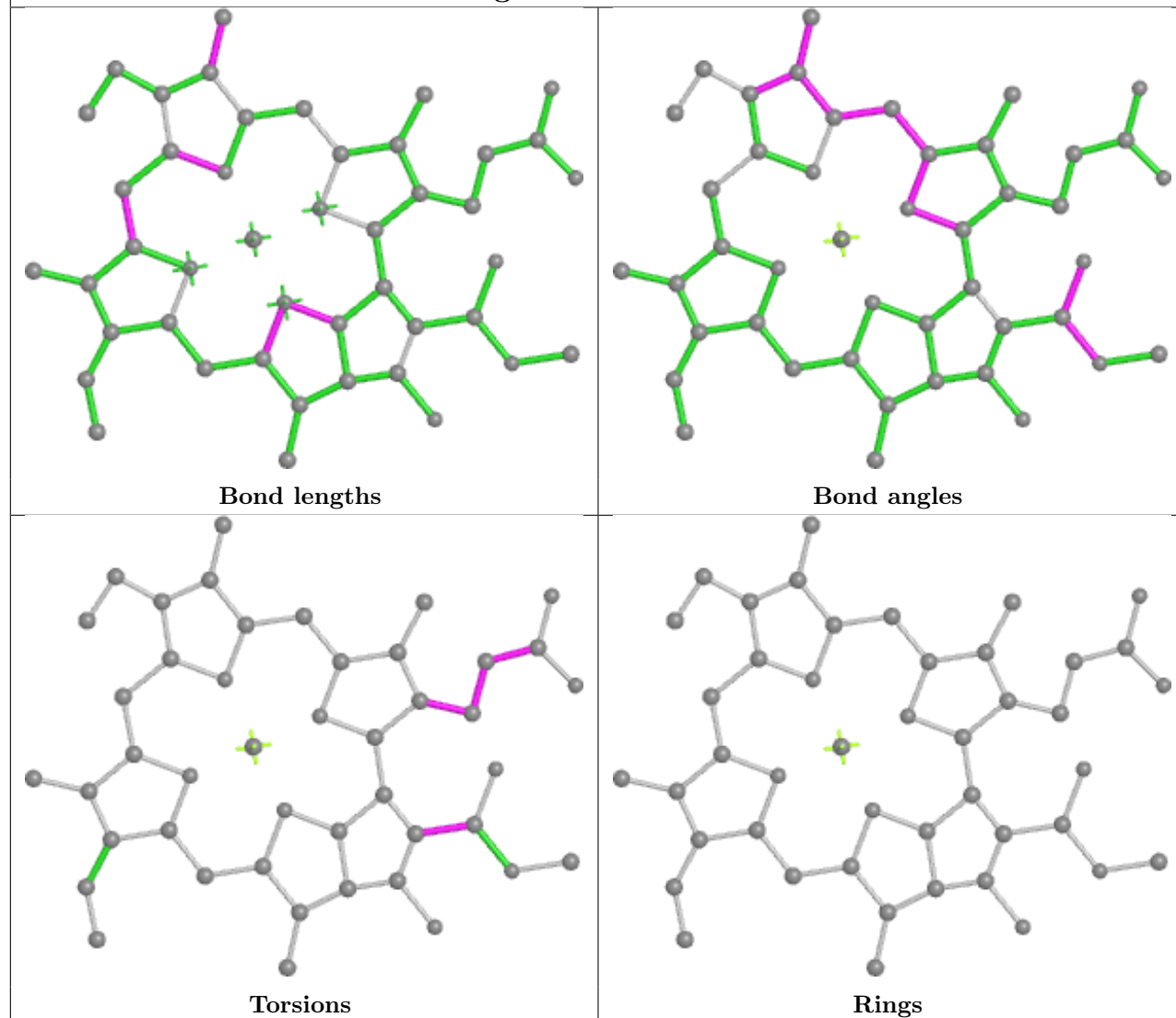
Ligand XAT 4 301



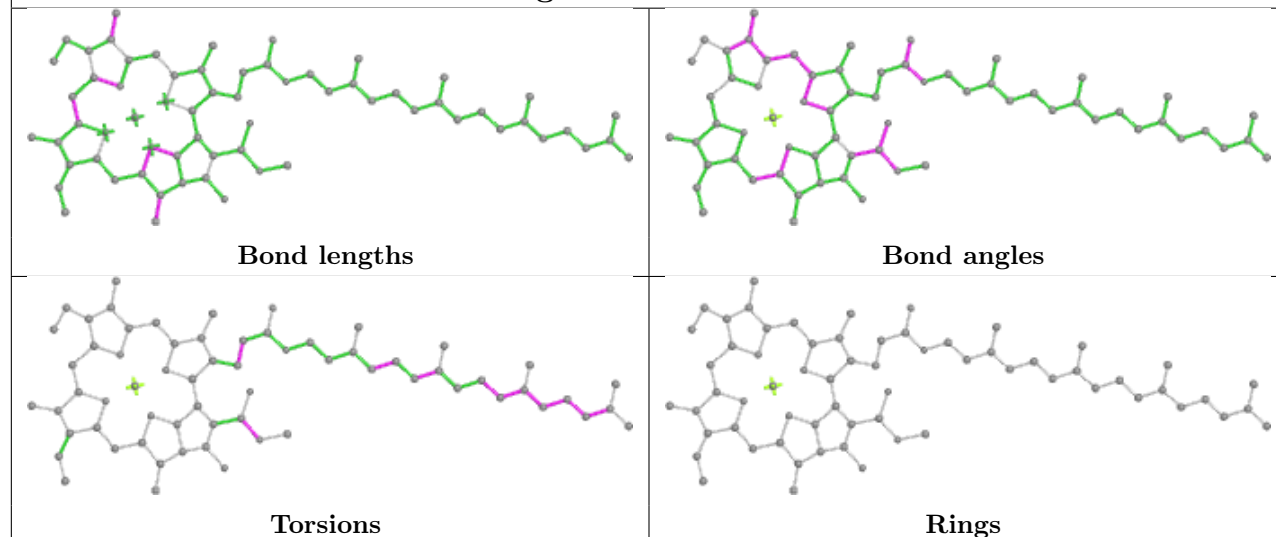
Ligand CLA a 822



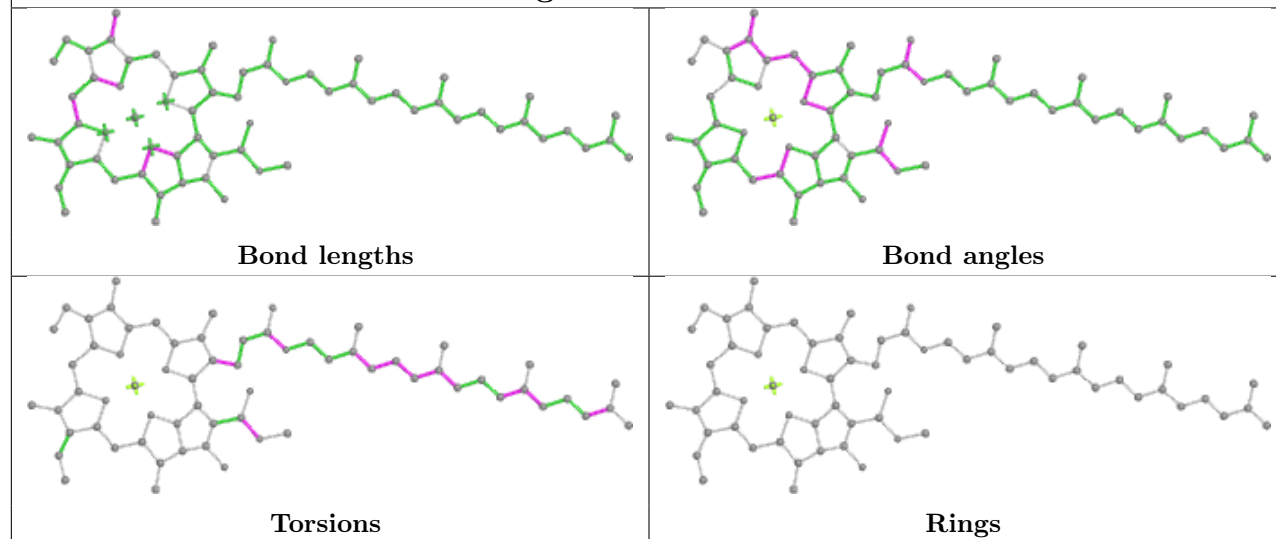
Ligand CLA a 817



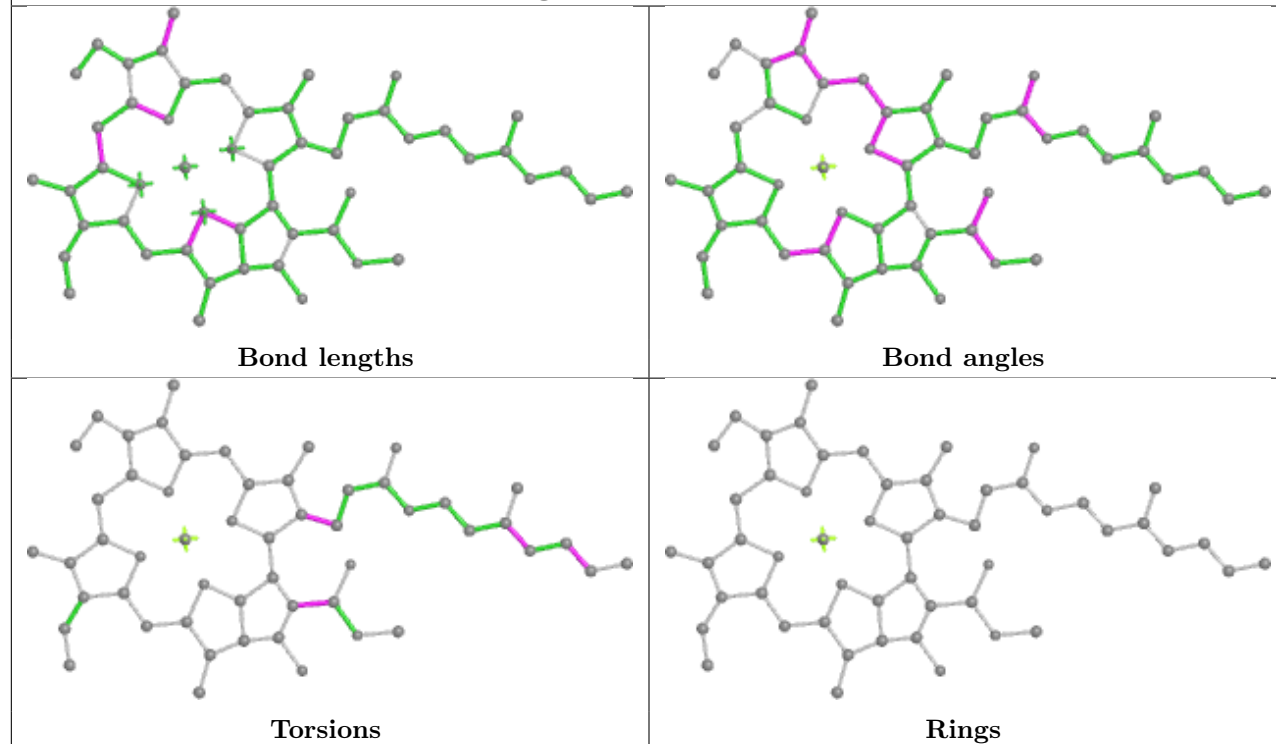
Ligand CLA 4 308



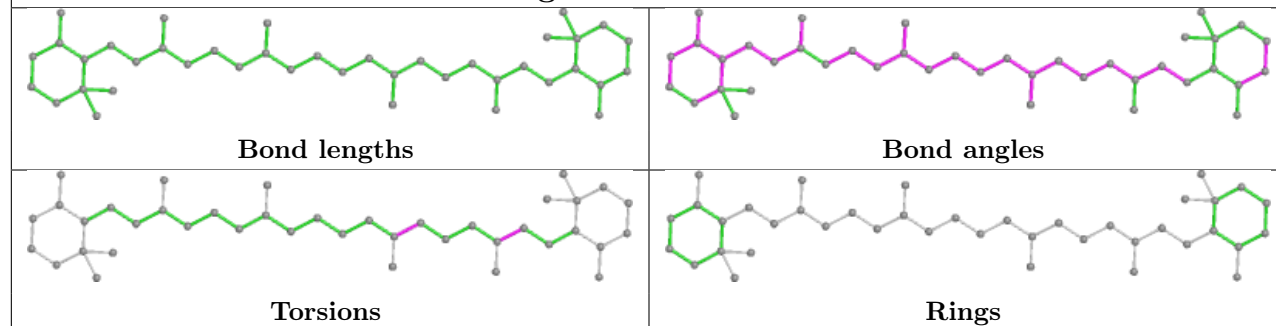
Ligand CLA 1 310



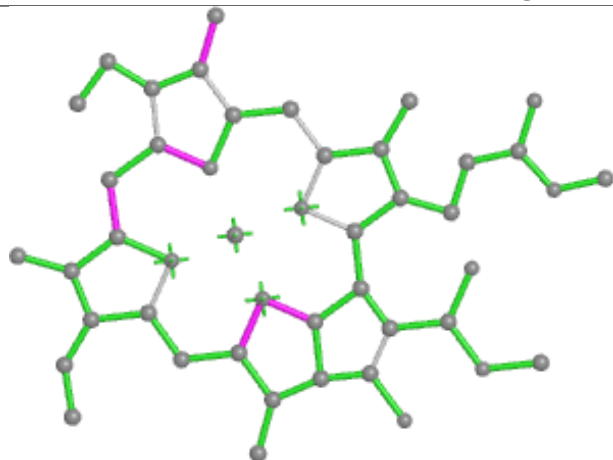
Ligand CLA b 812



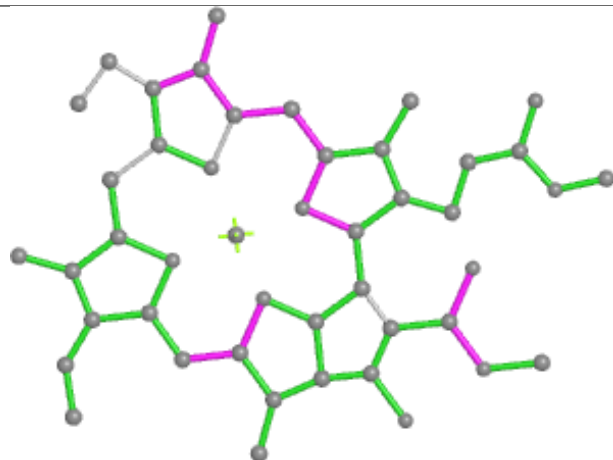
Ligand BCR f 801



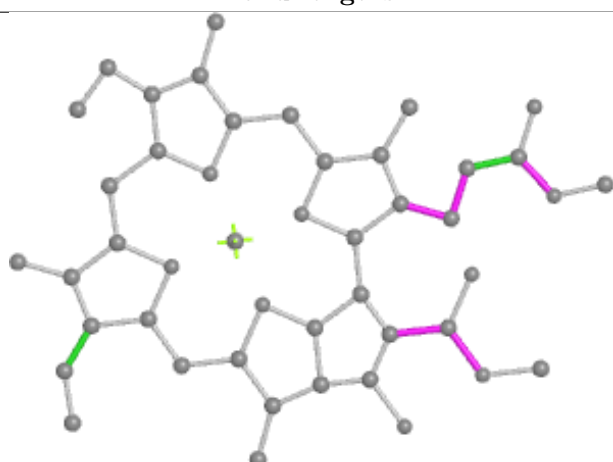
Ligand CLA 4 316



Bond lengths



Bond angles

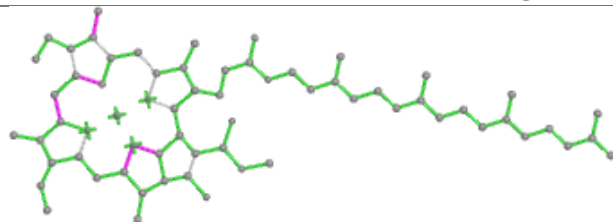


Torsions

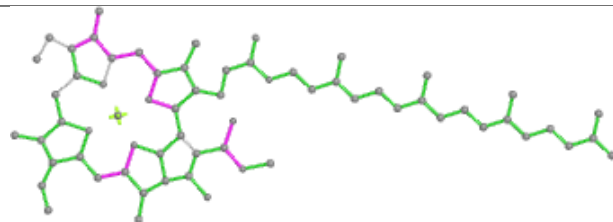


Rings

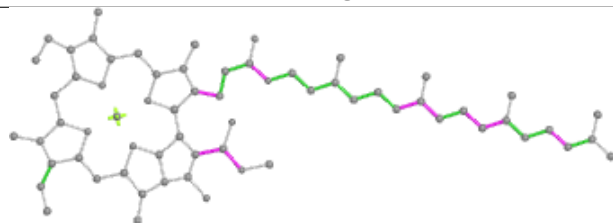
Ligand CLA b 806



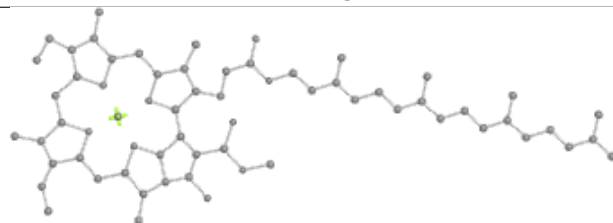
Bond lengths



Bond angles

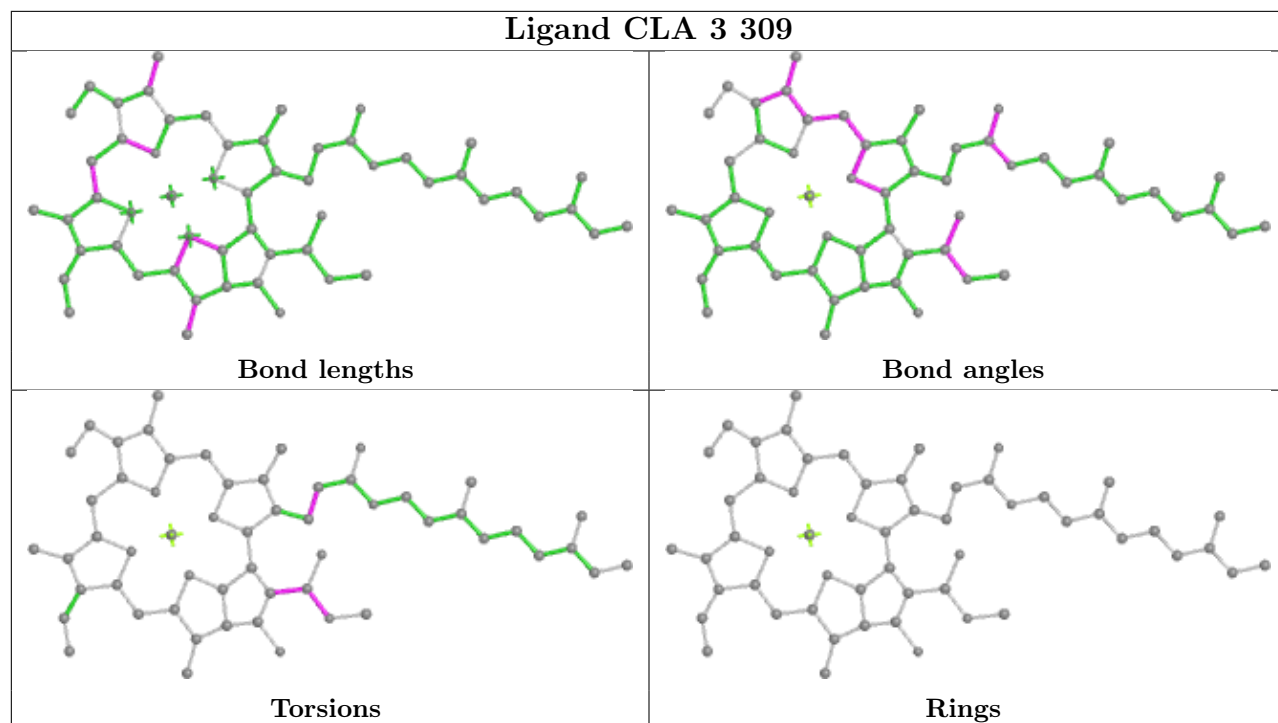


Torsions

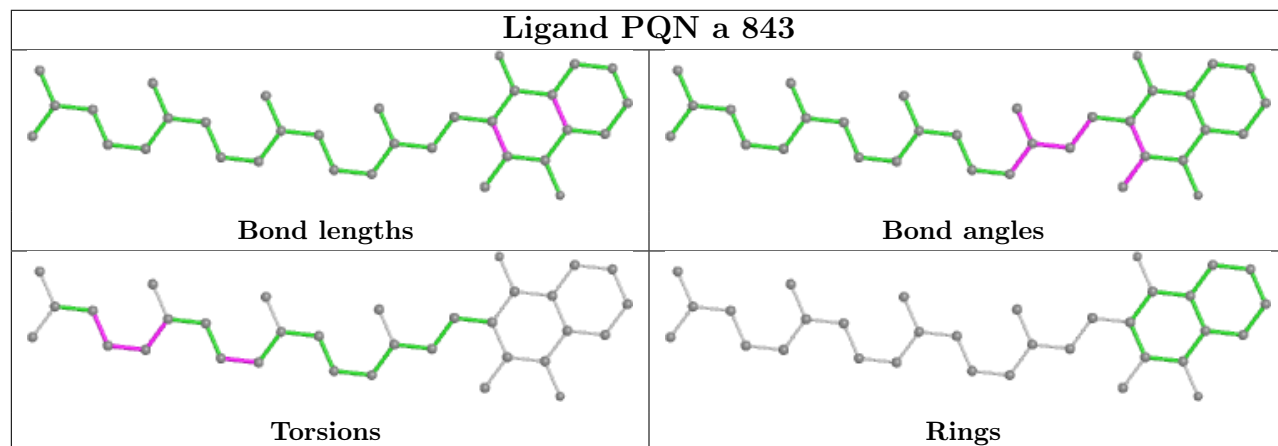


Rings

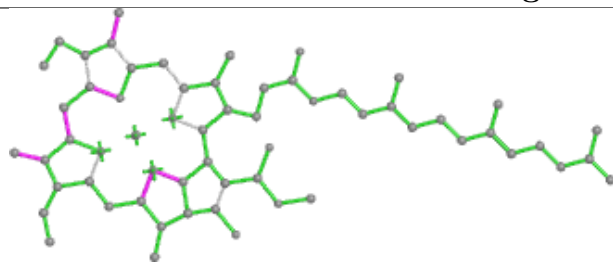
Ligand CLA 3 309



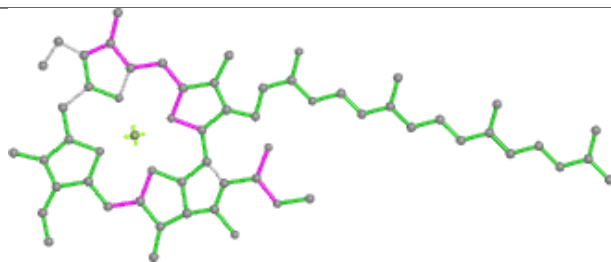
Ligand PQN a 843



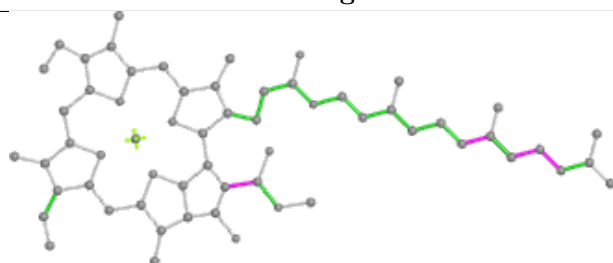
Ligand CLA 1 203



Bond lengths



Bond angles

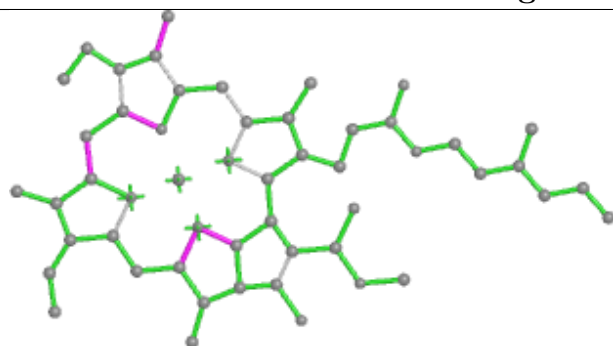


Torsions

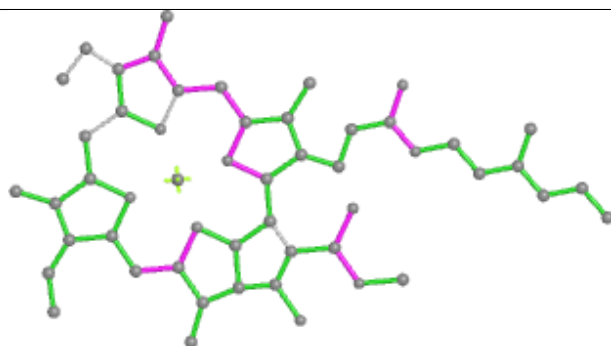


Rings

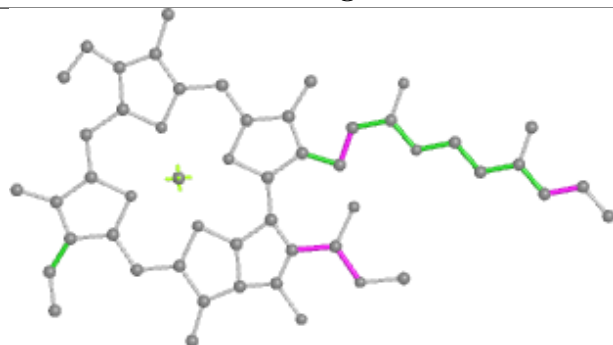
Ligand CLA 6 310



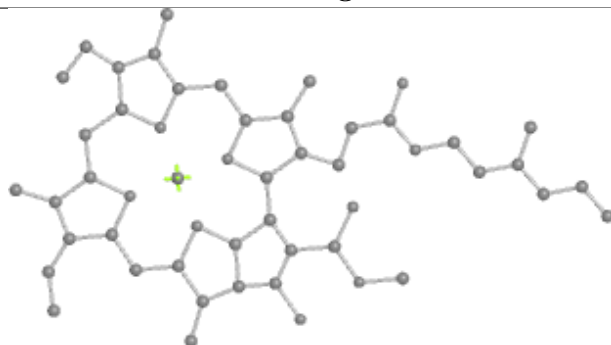
Bond lengths



Bond angles

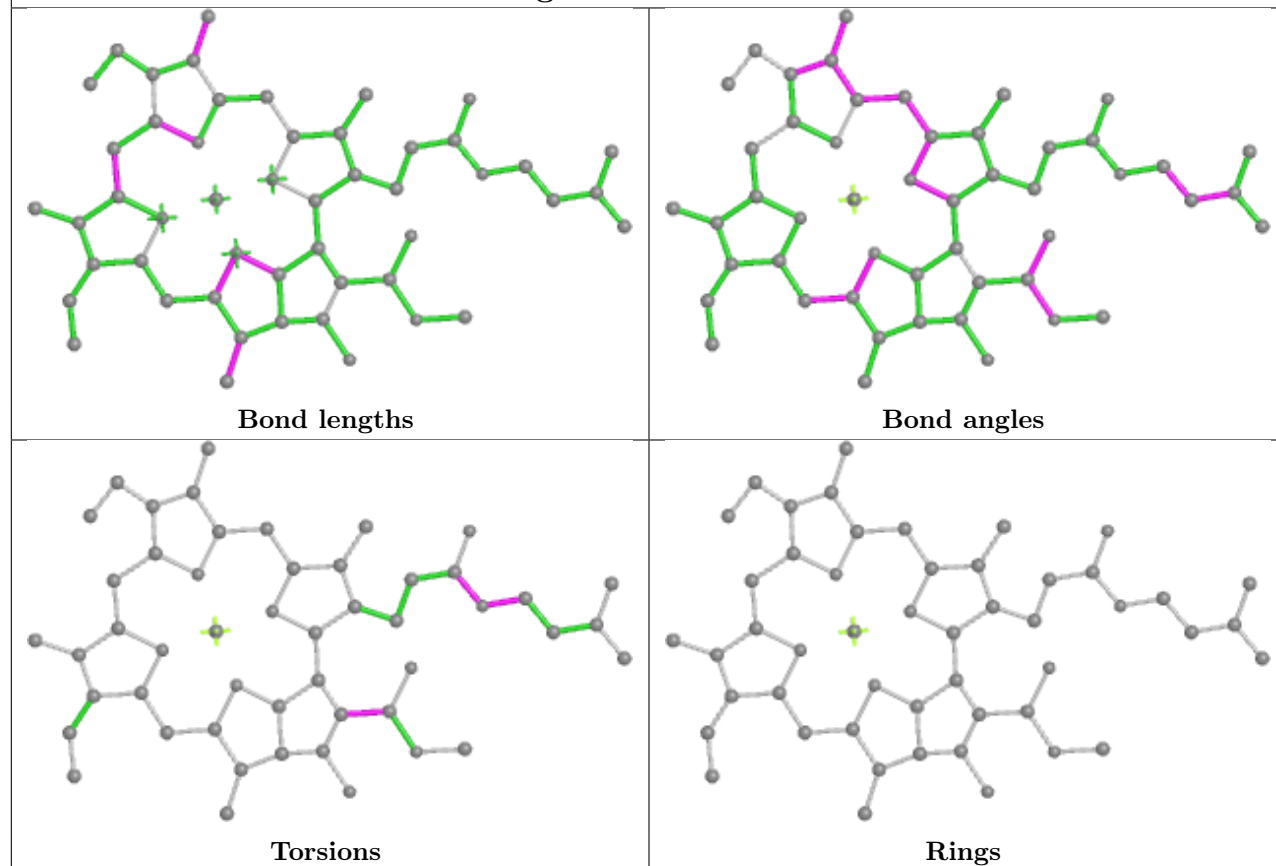


Torsions

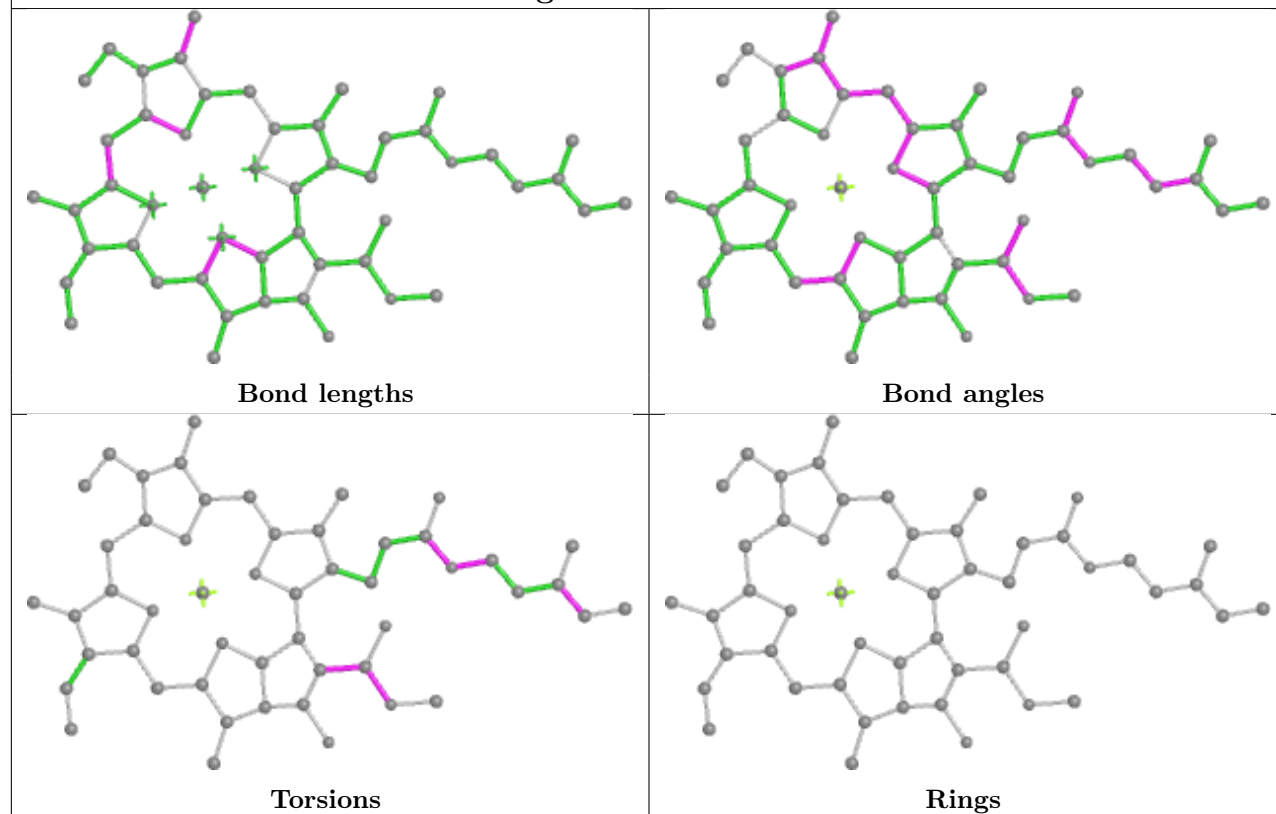


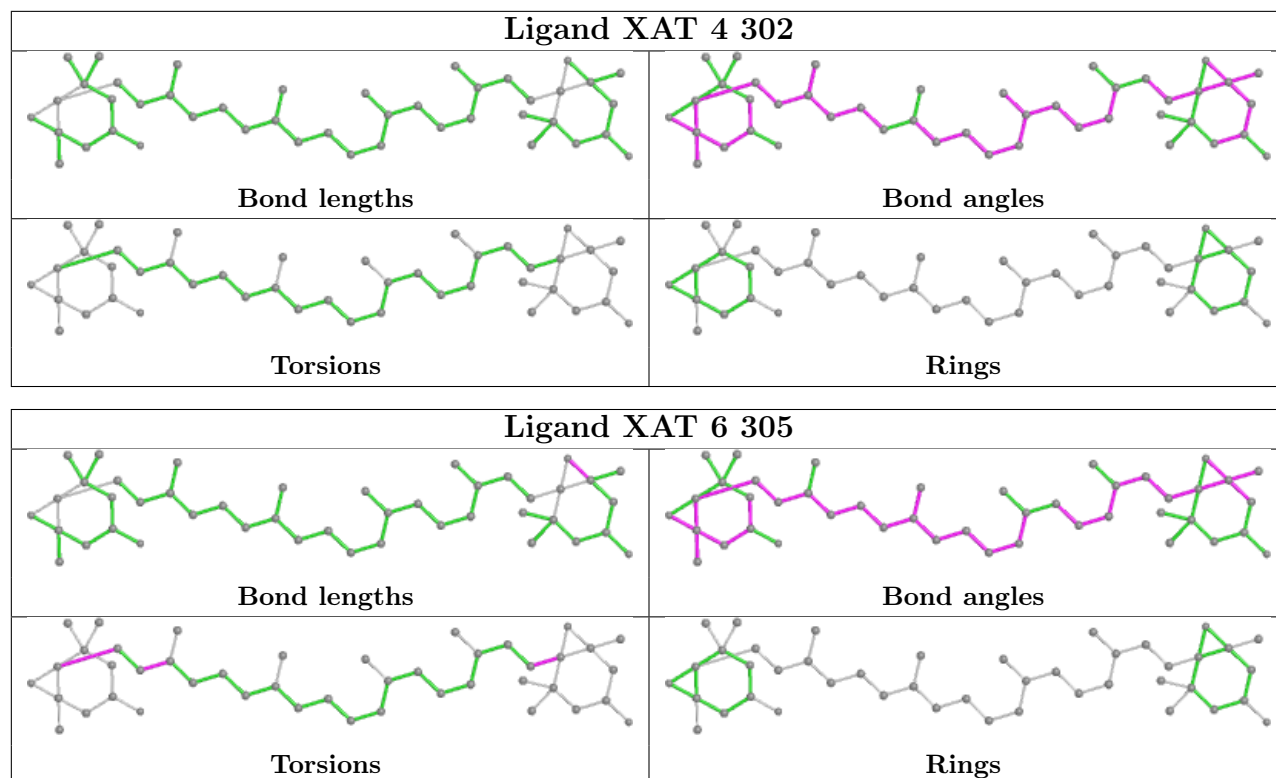
Rings

Ligand CLA a 816

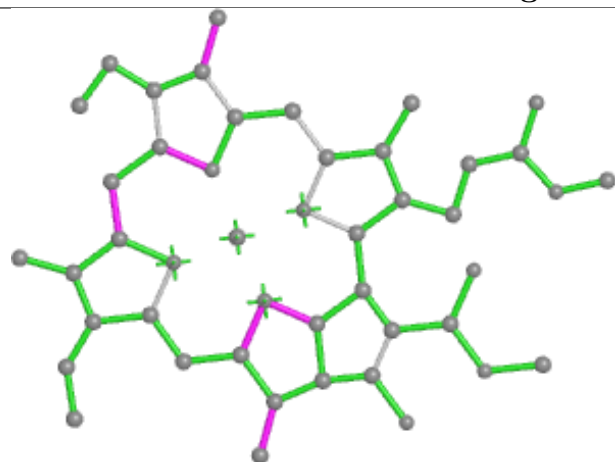


Ligand CLA 5 311

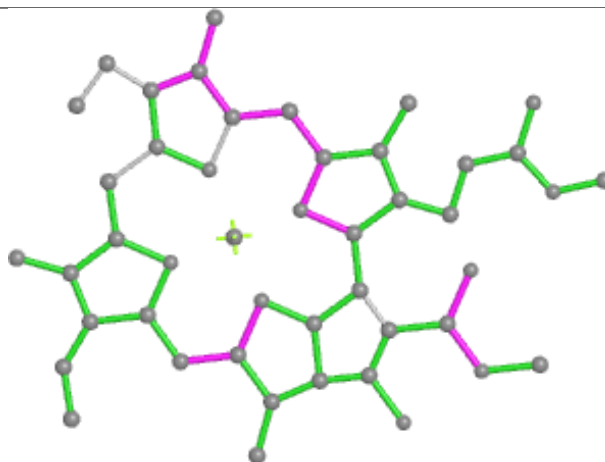




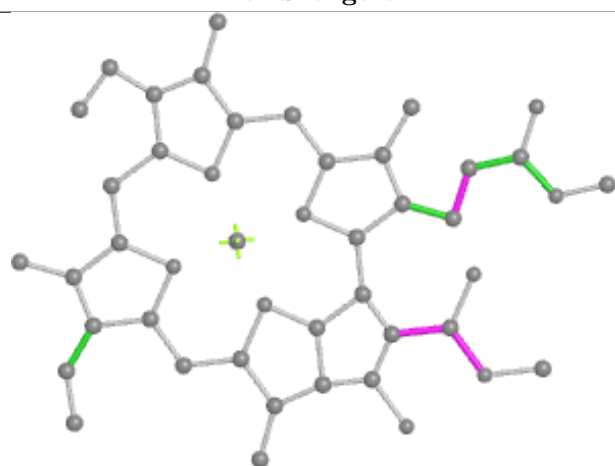
Ligand CLA 2 309



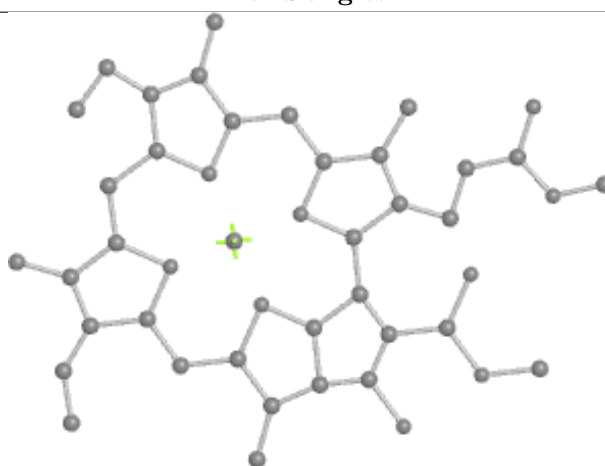
Bond lengths



Bond angles

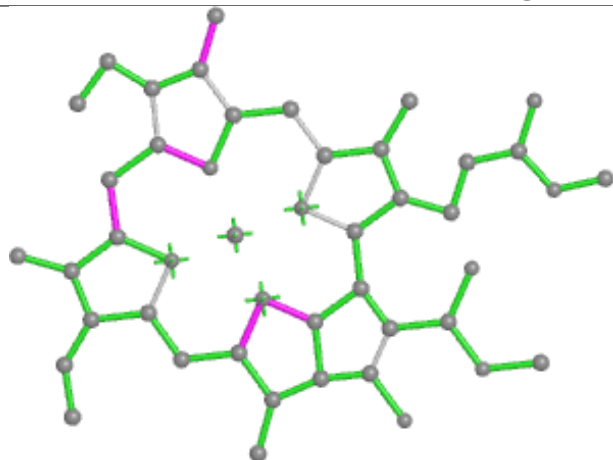


Torsions

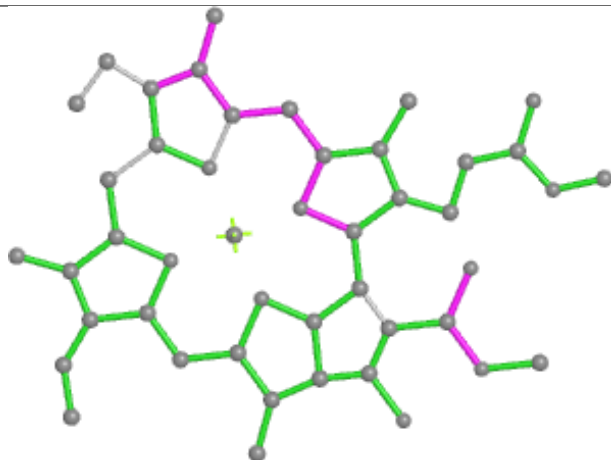


Rings

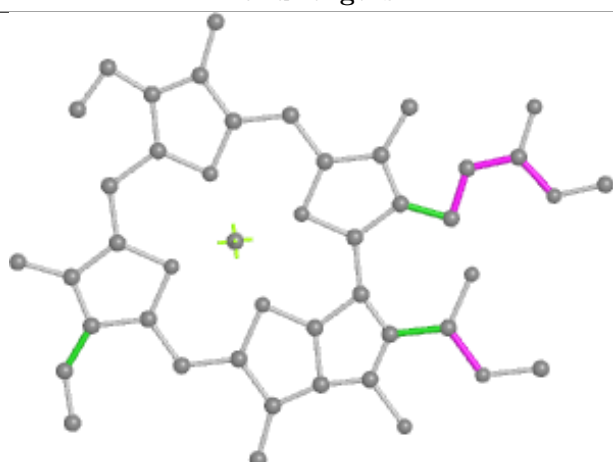
Ligand CLA 7 310



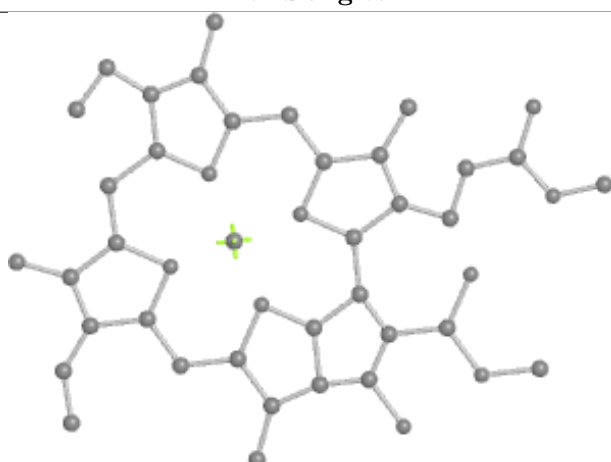
Bond lengths



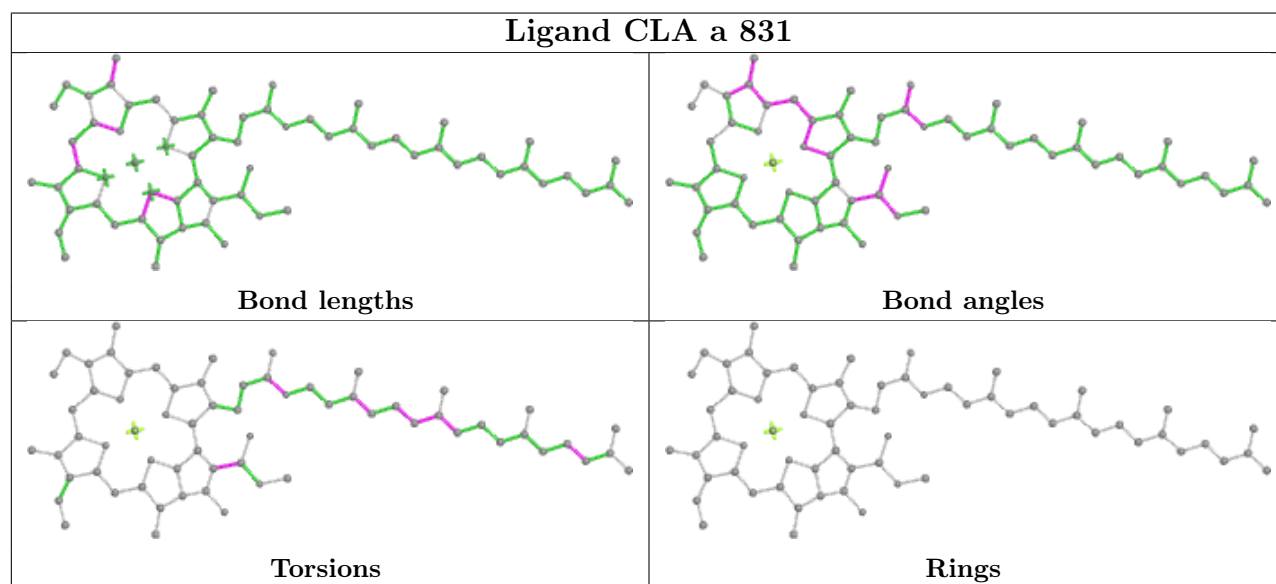
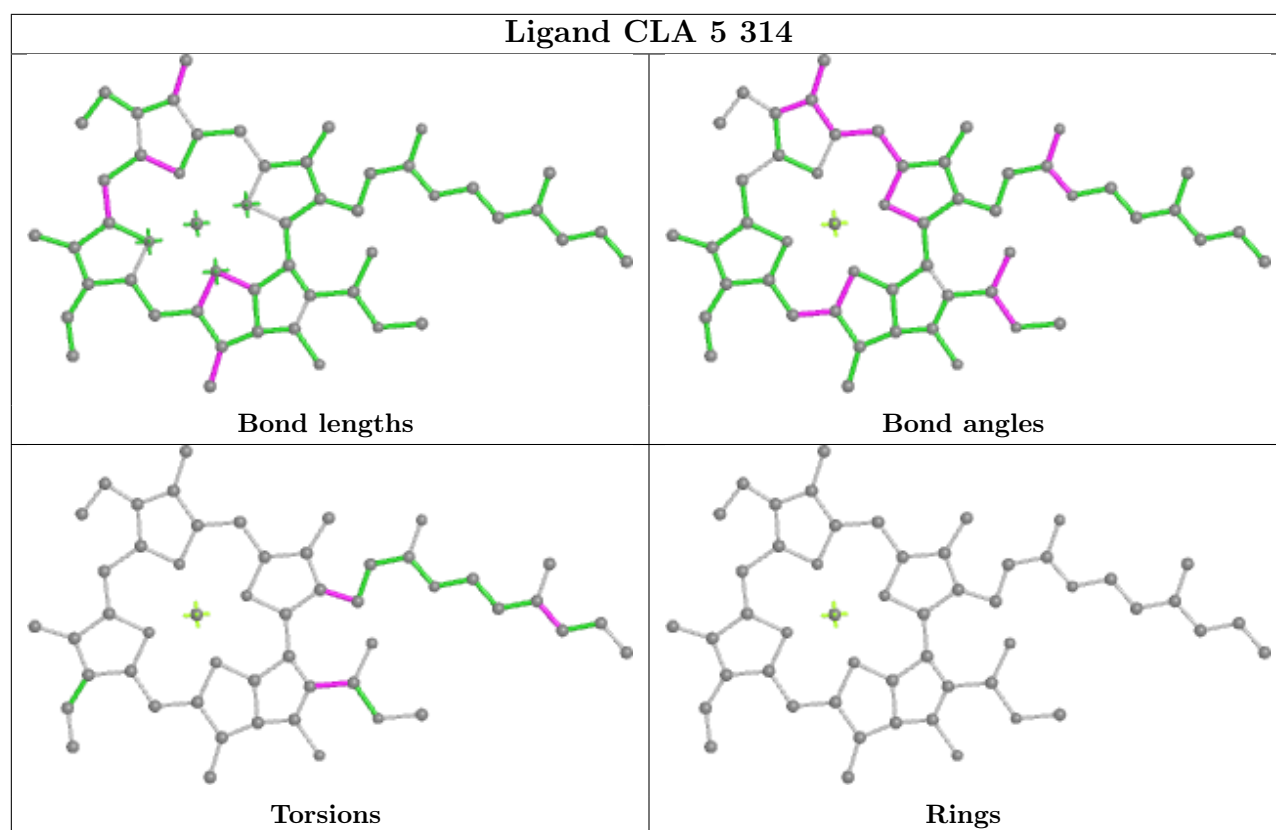
Bond angles



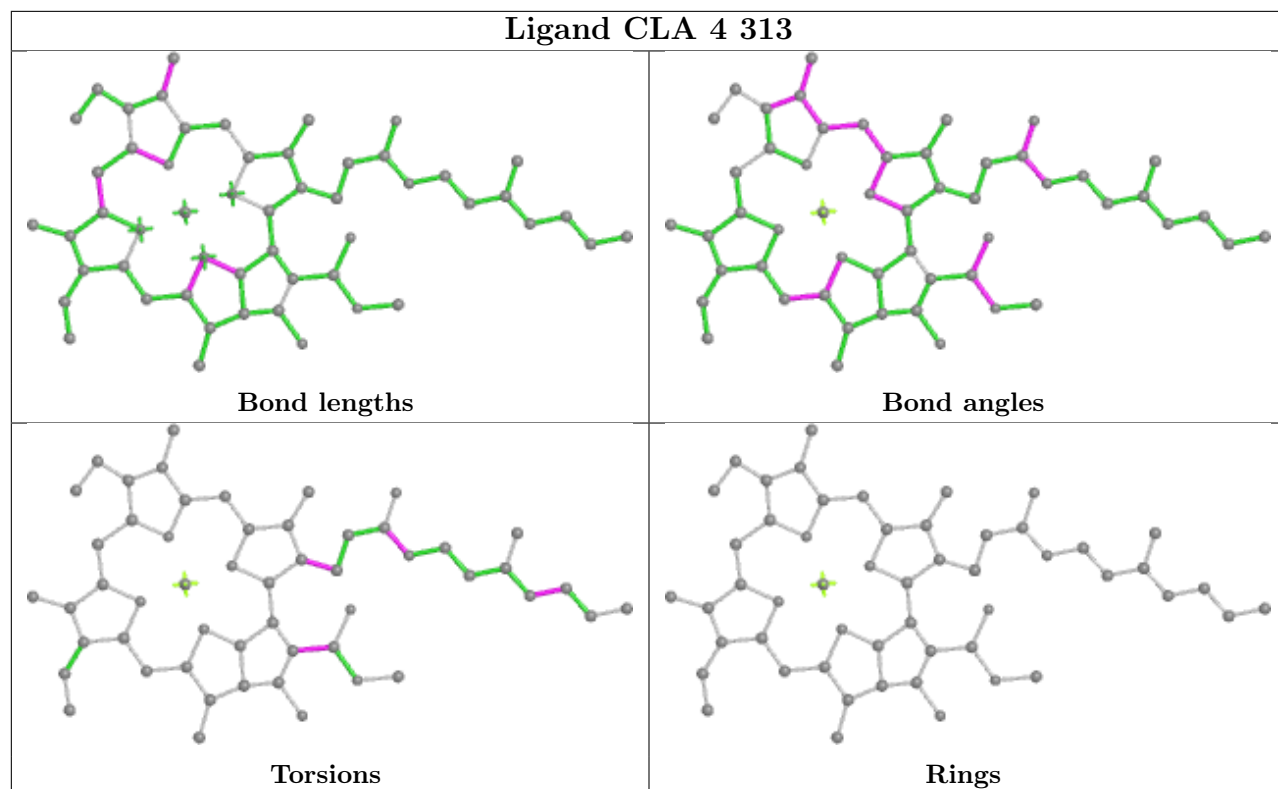
Torsions



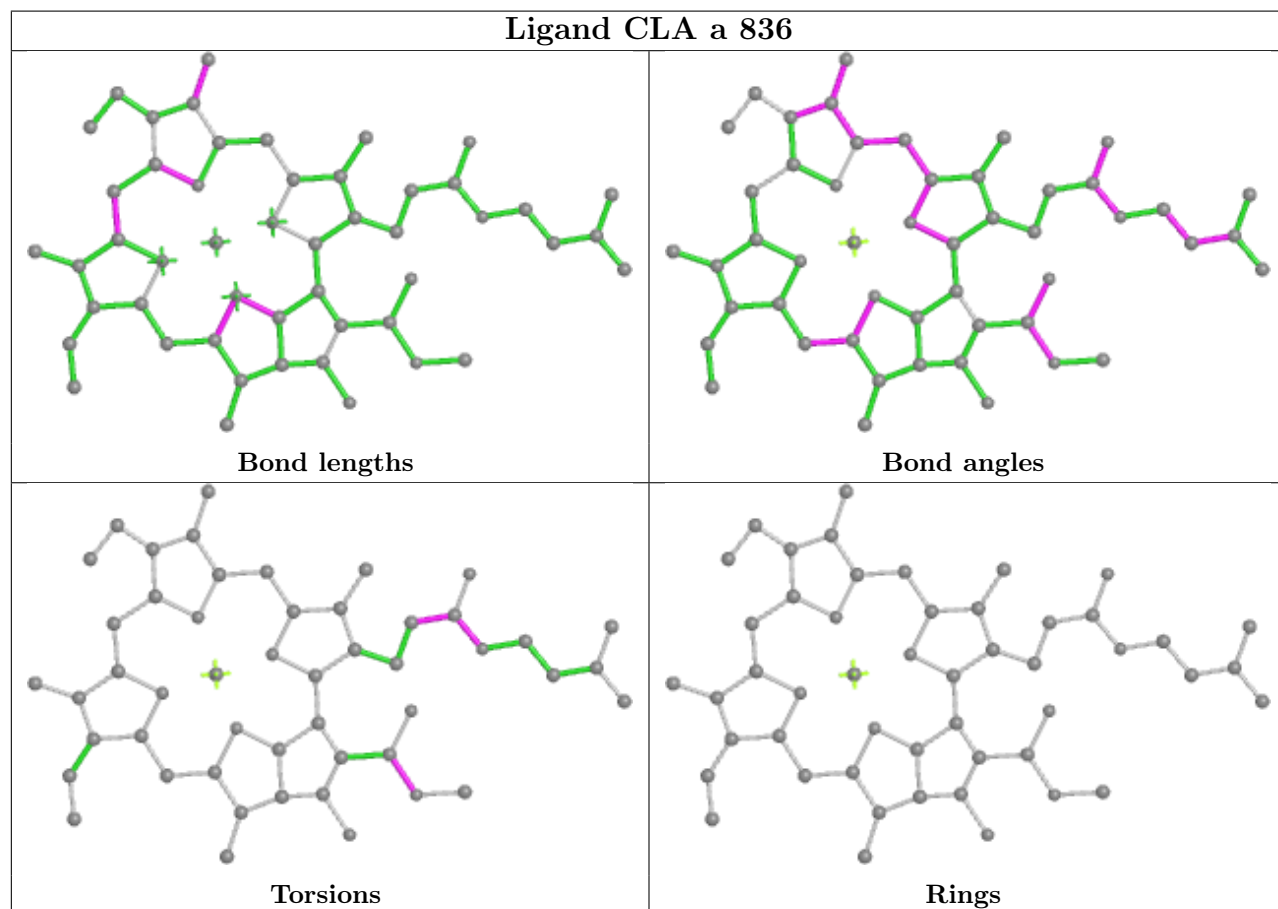
Rings

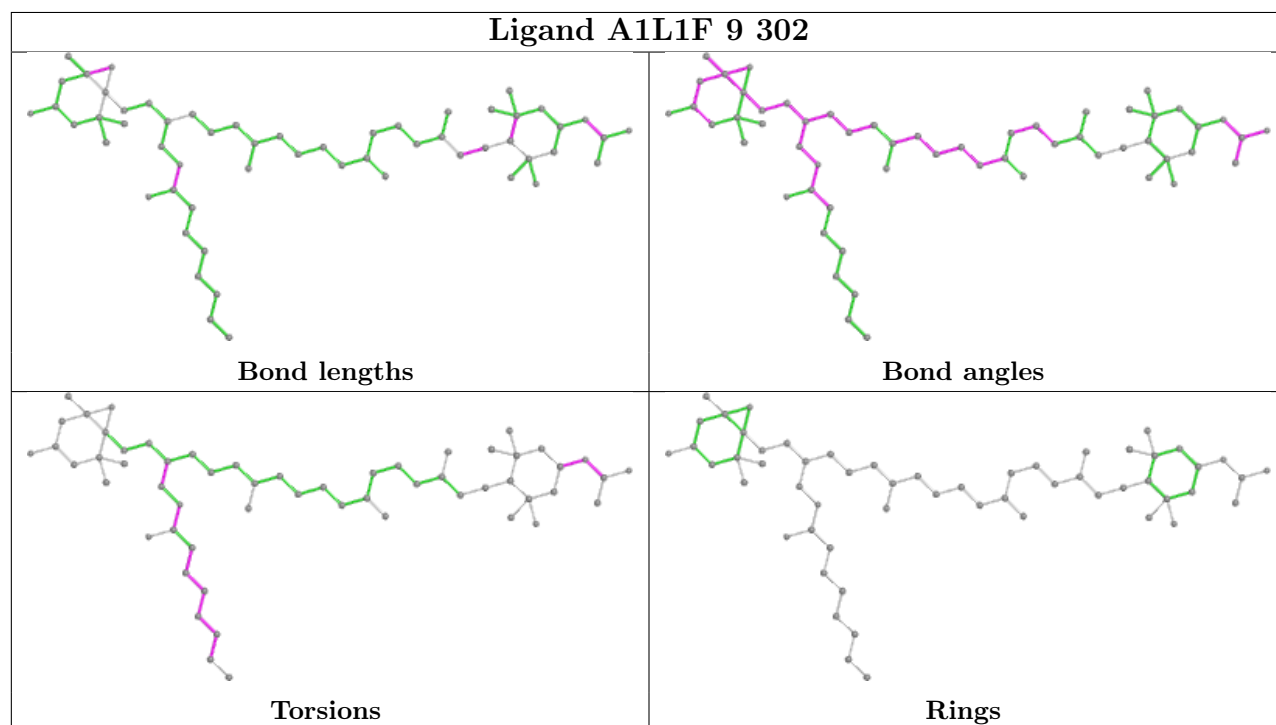
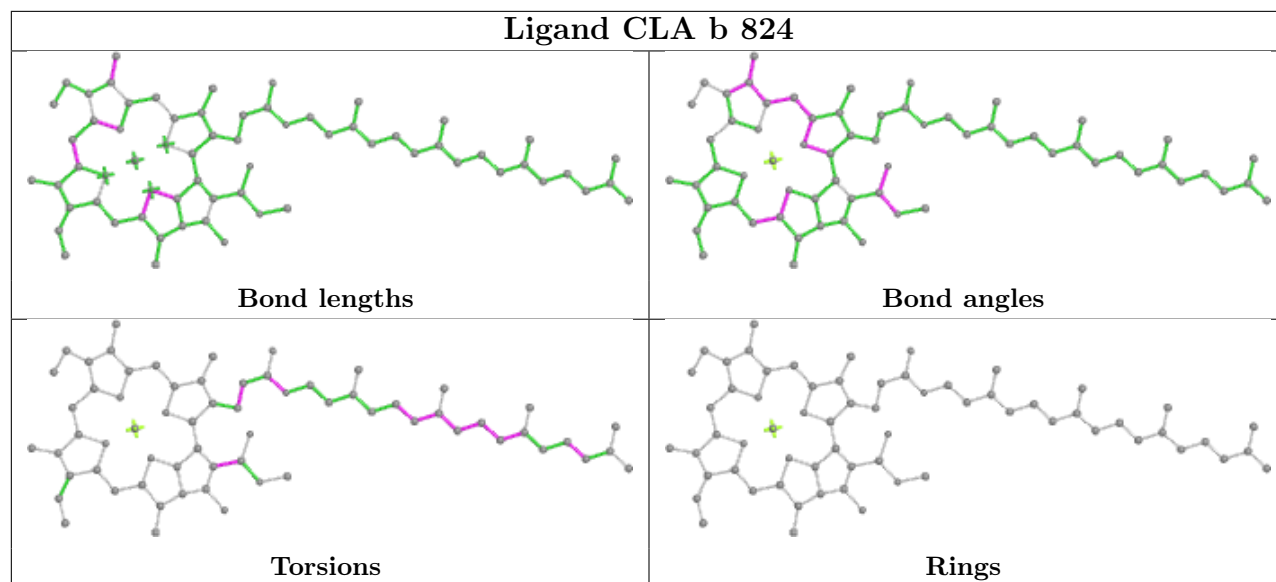


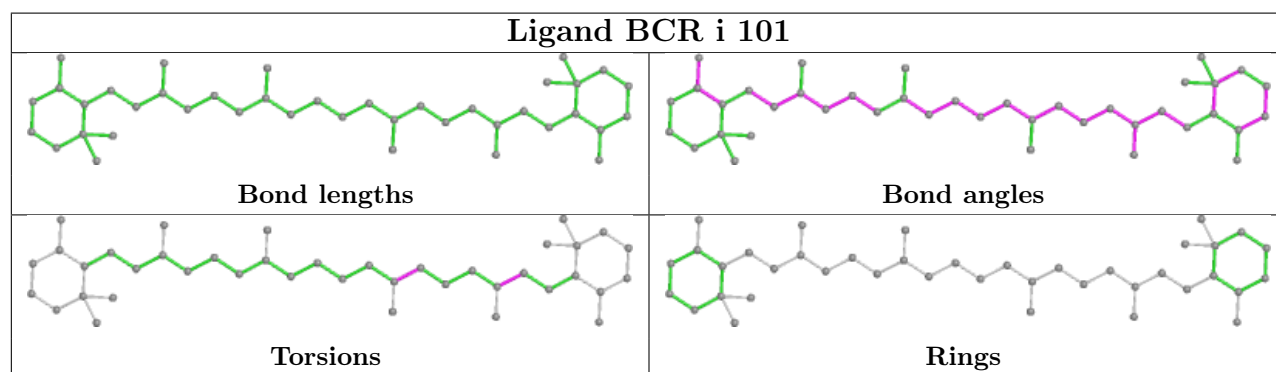
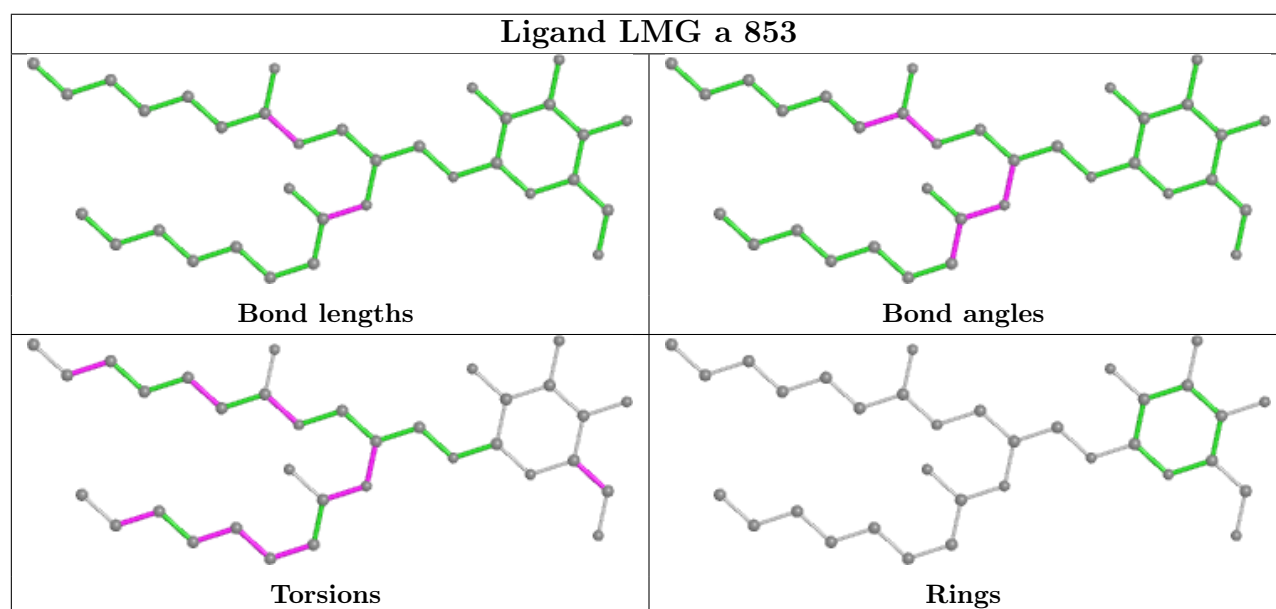
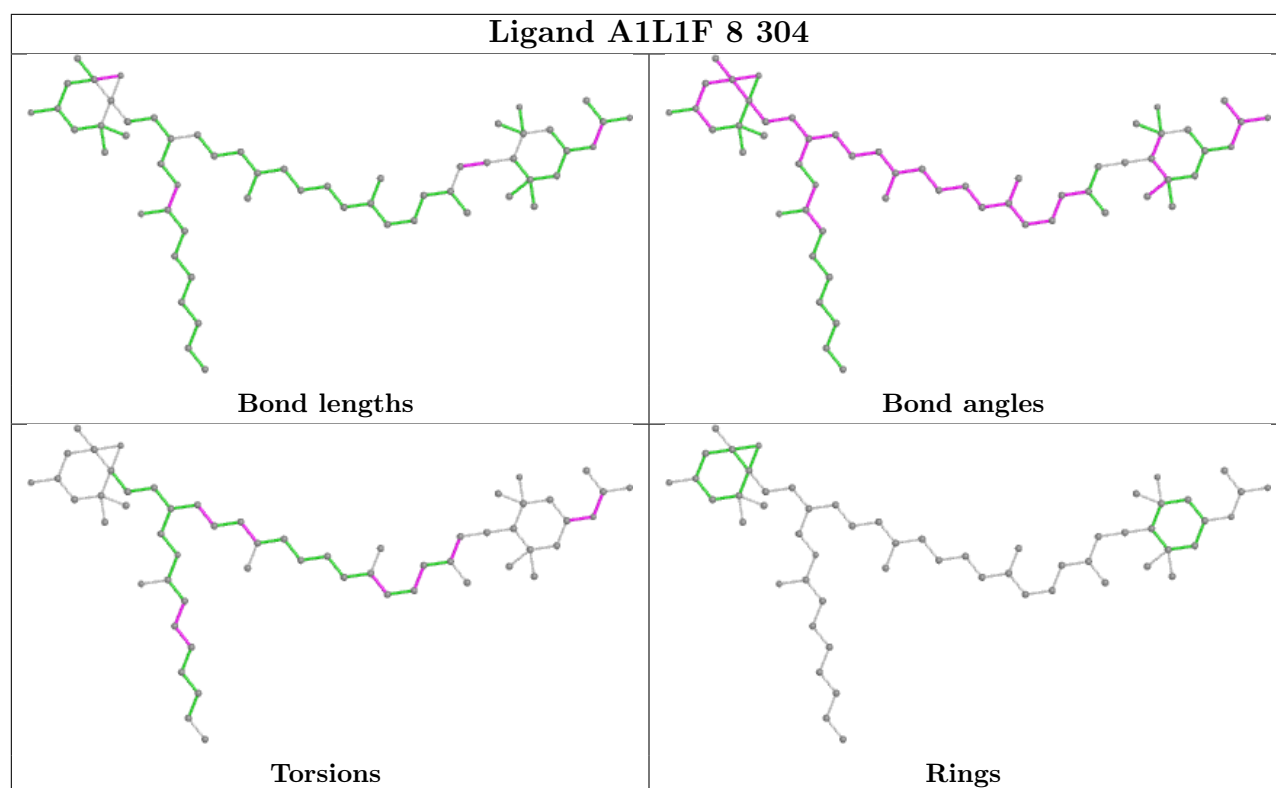
Ligand CLA 4 313

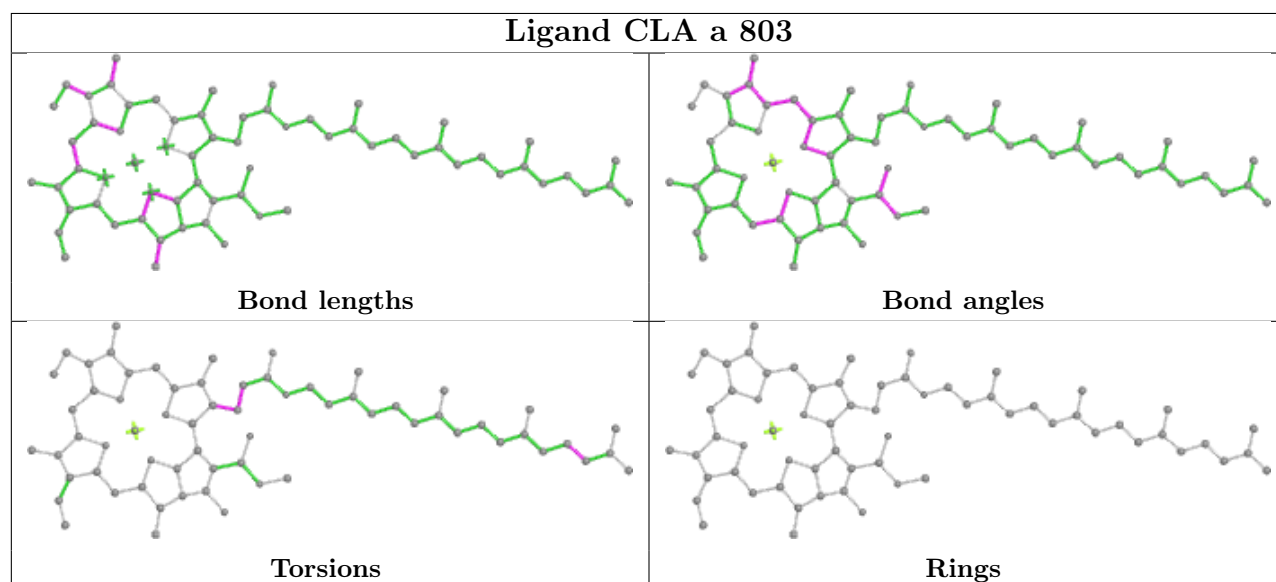
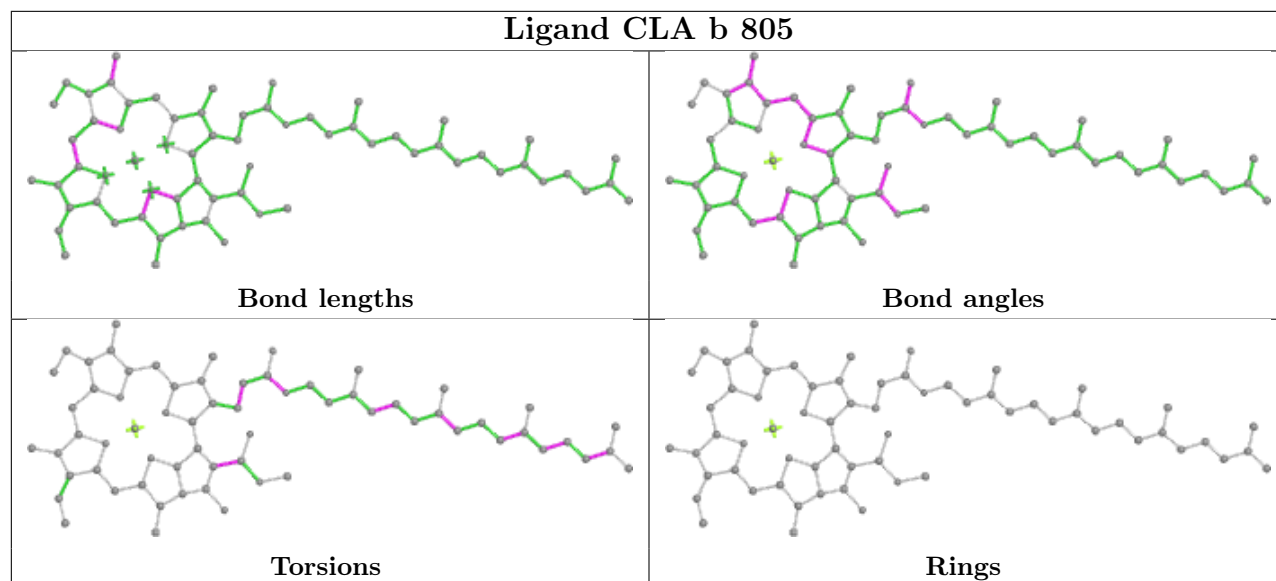
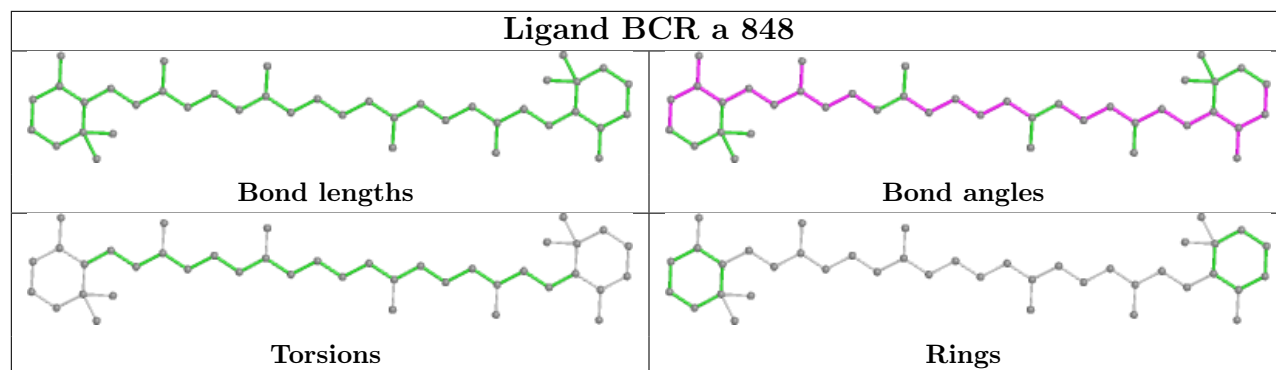


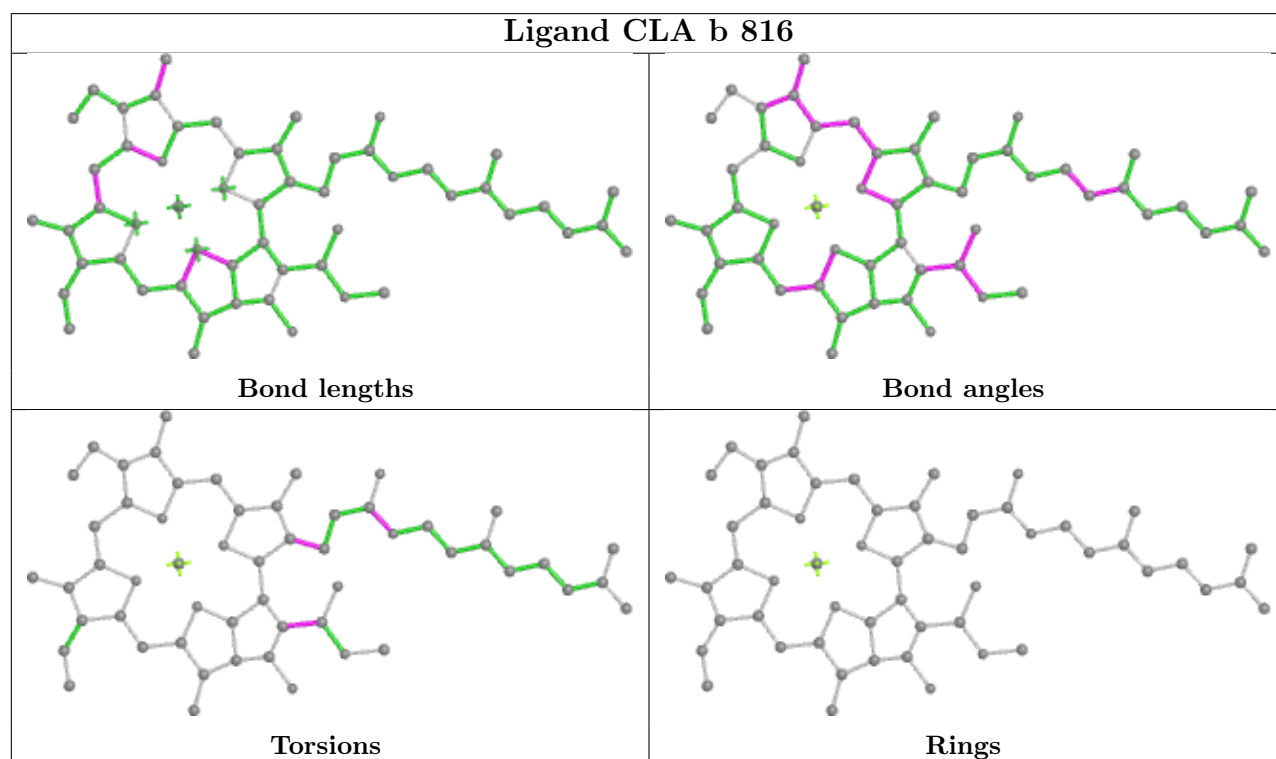
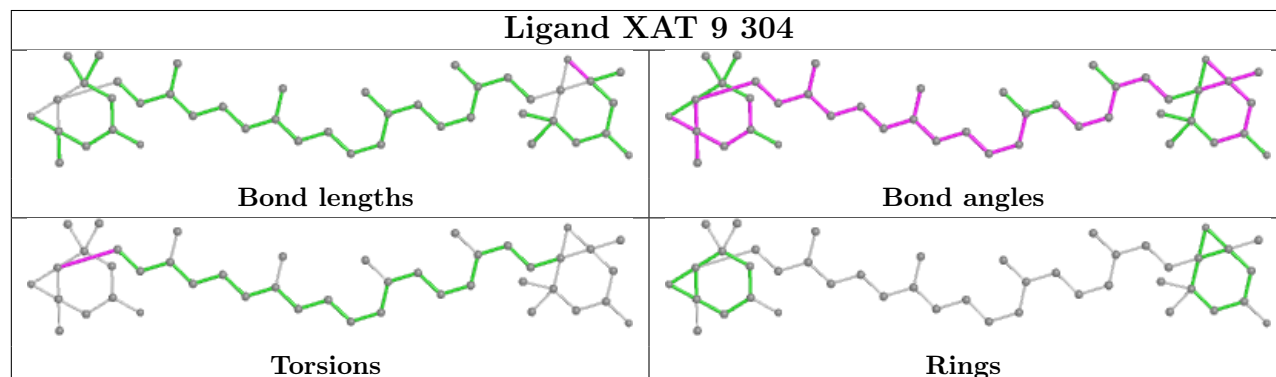
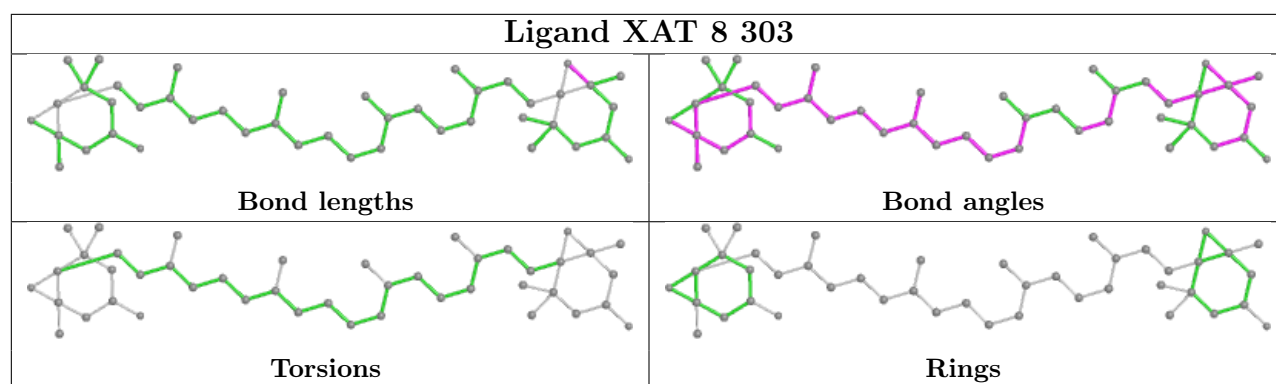
Ligand CLA a 836



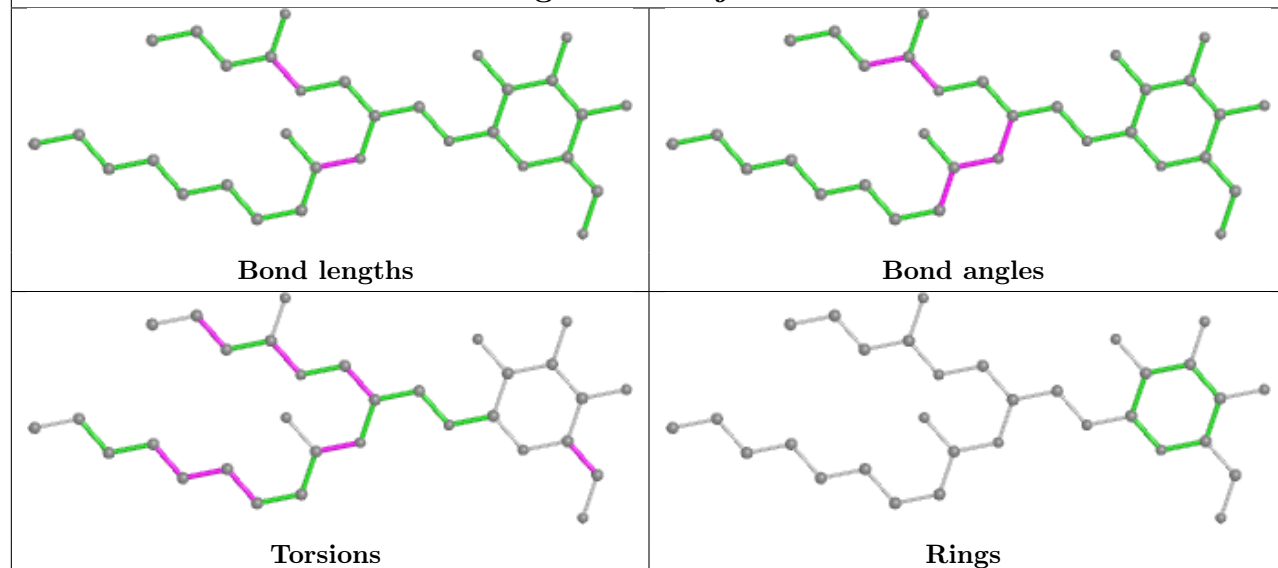




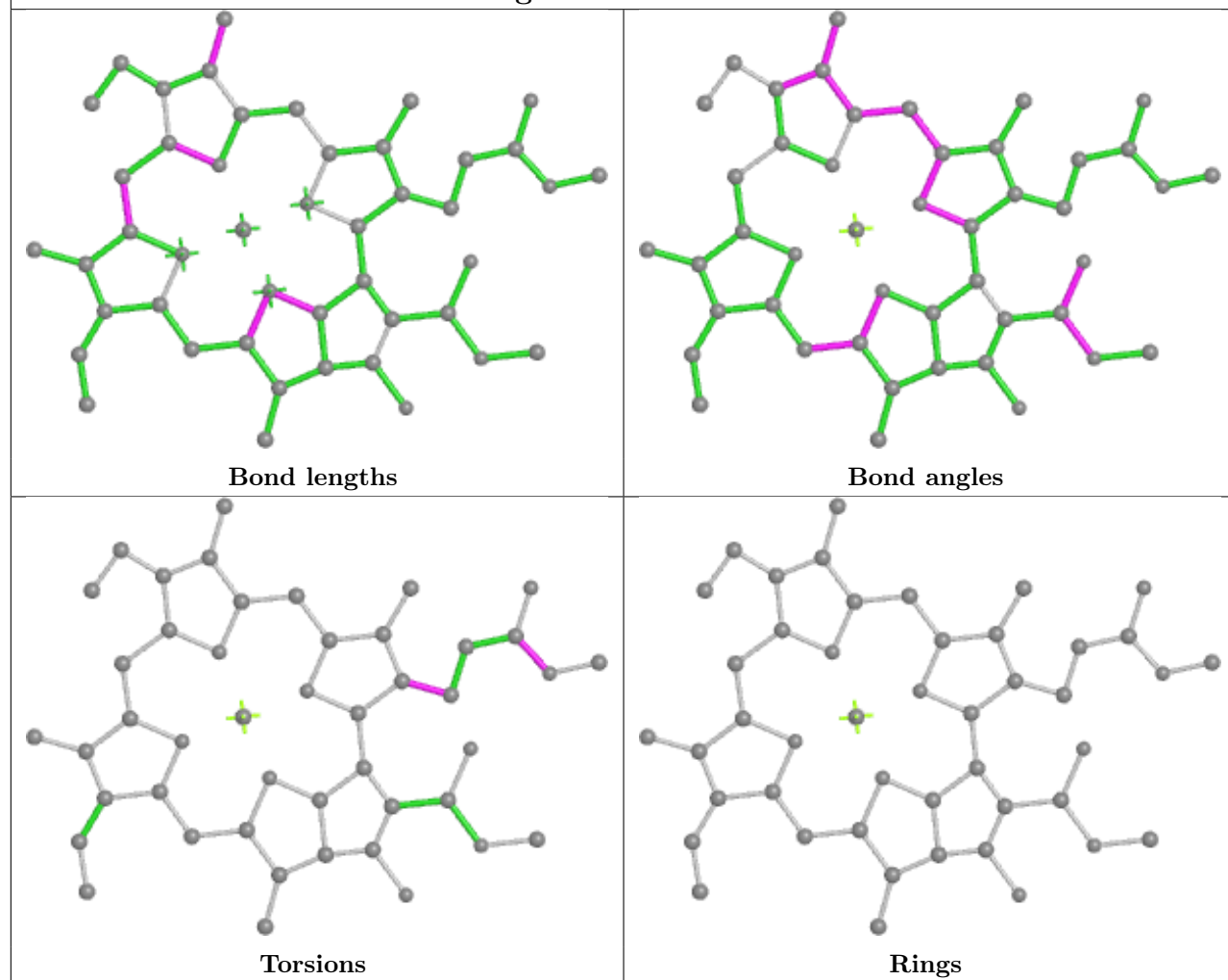




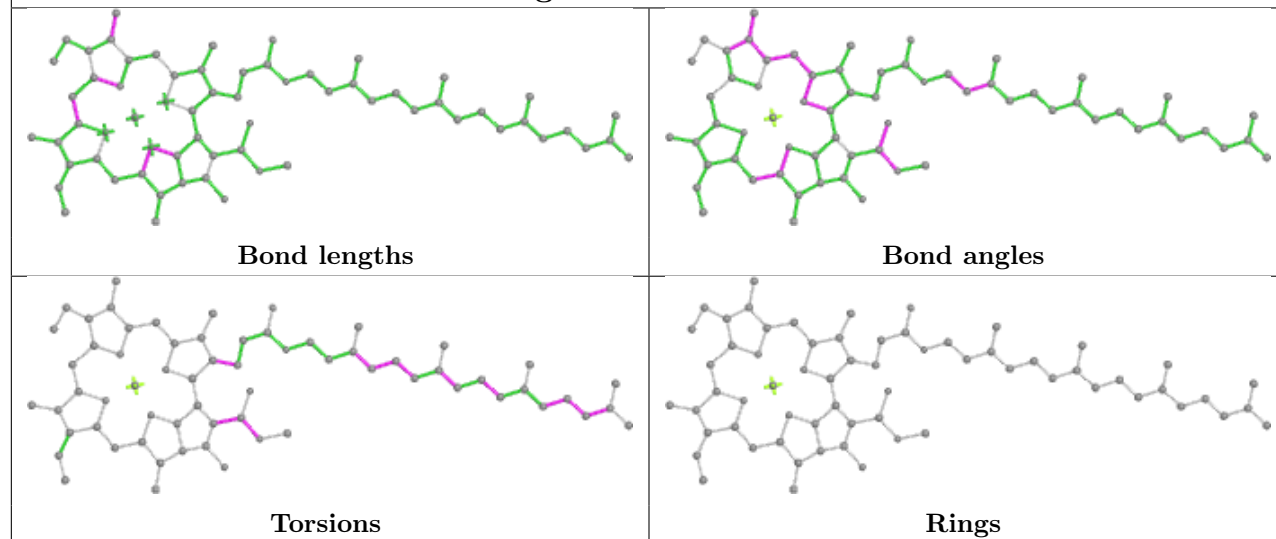
Ligand LMG j 105



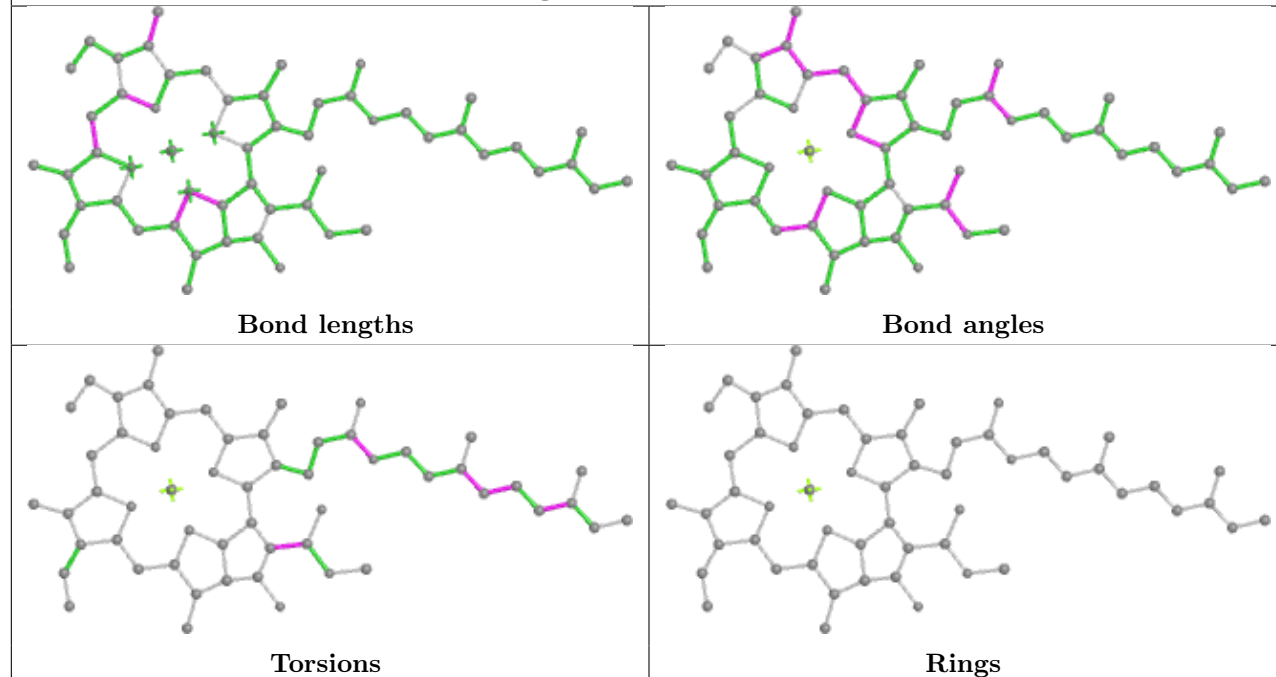
Ligand CLA 4 312



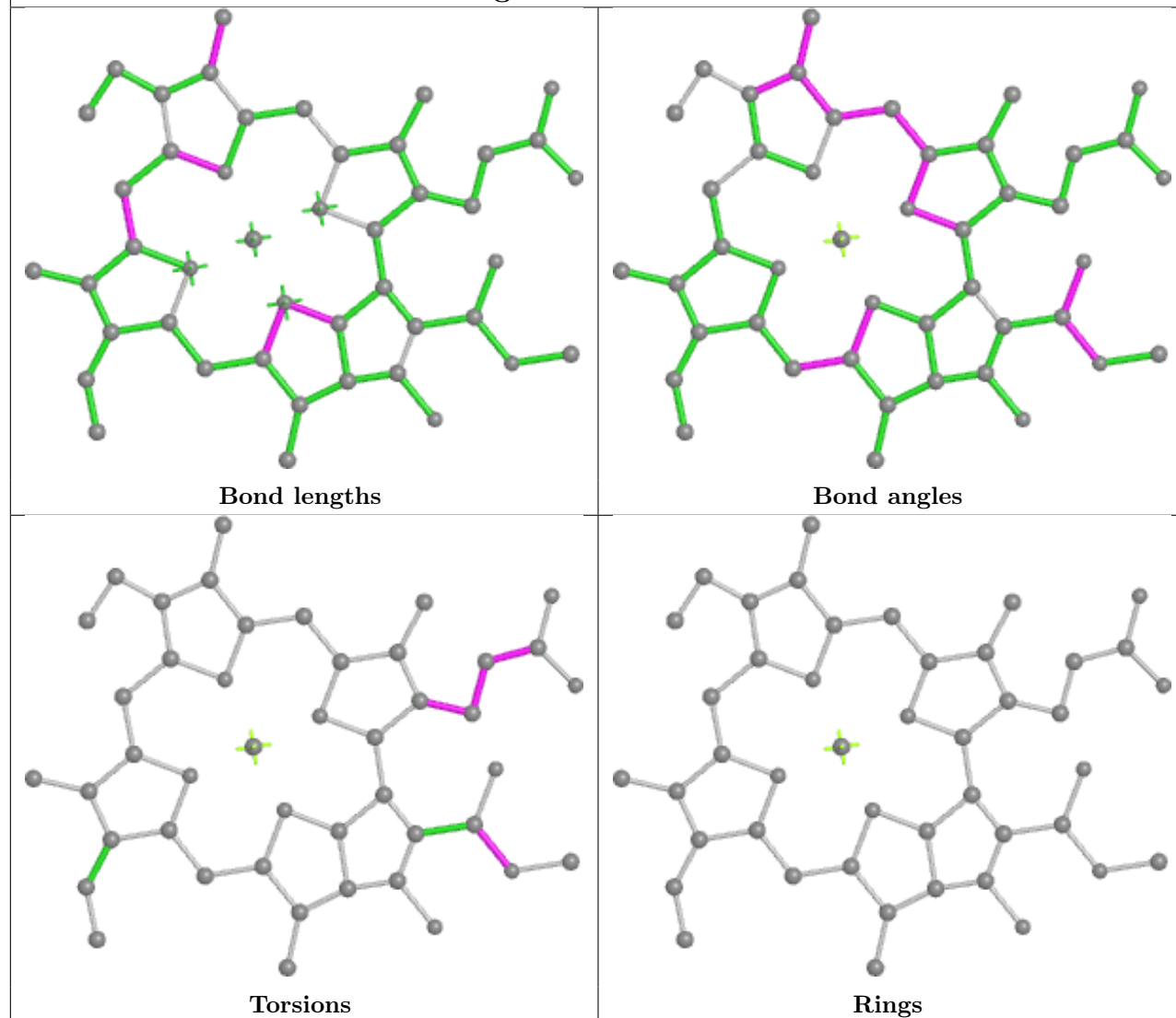
Ligand CLA b 813



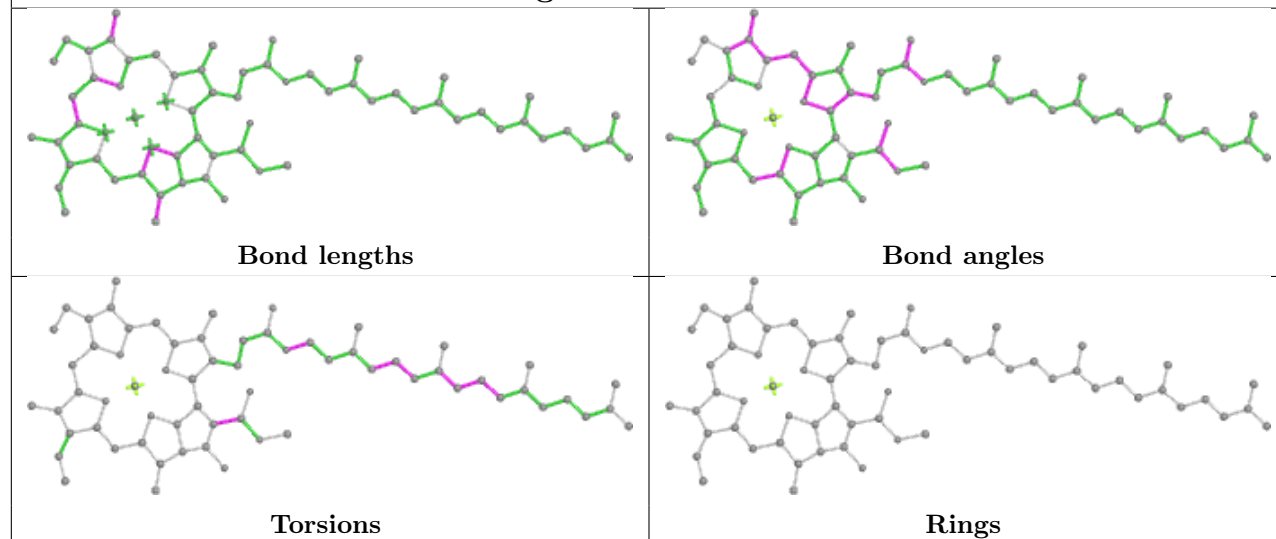
Ligand CLA 8 311



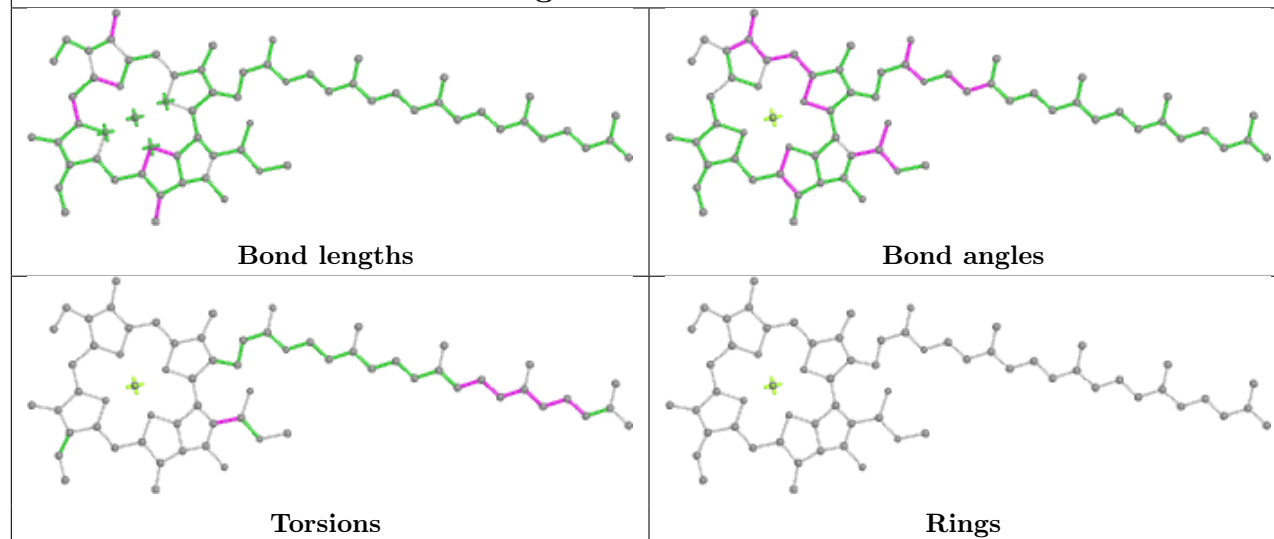
Ligand CLA 4 306



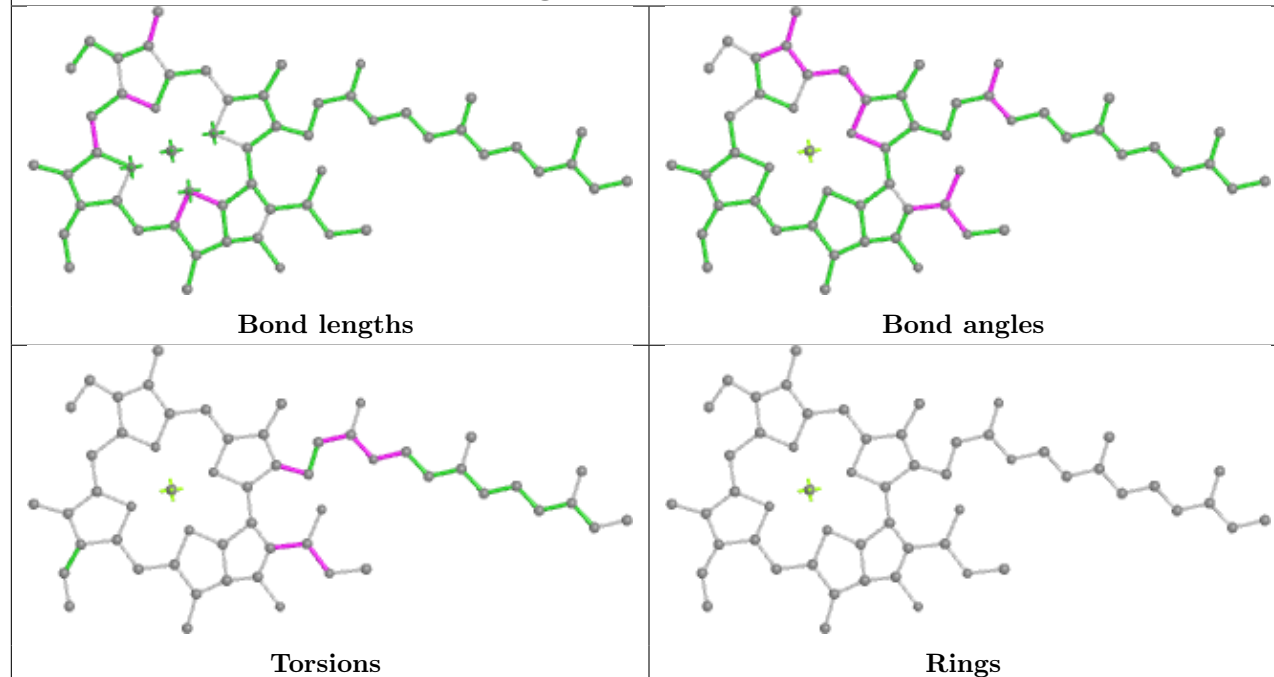
Ligand CLA a 827

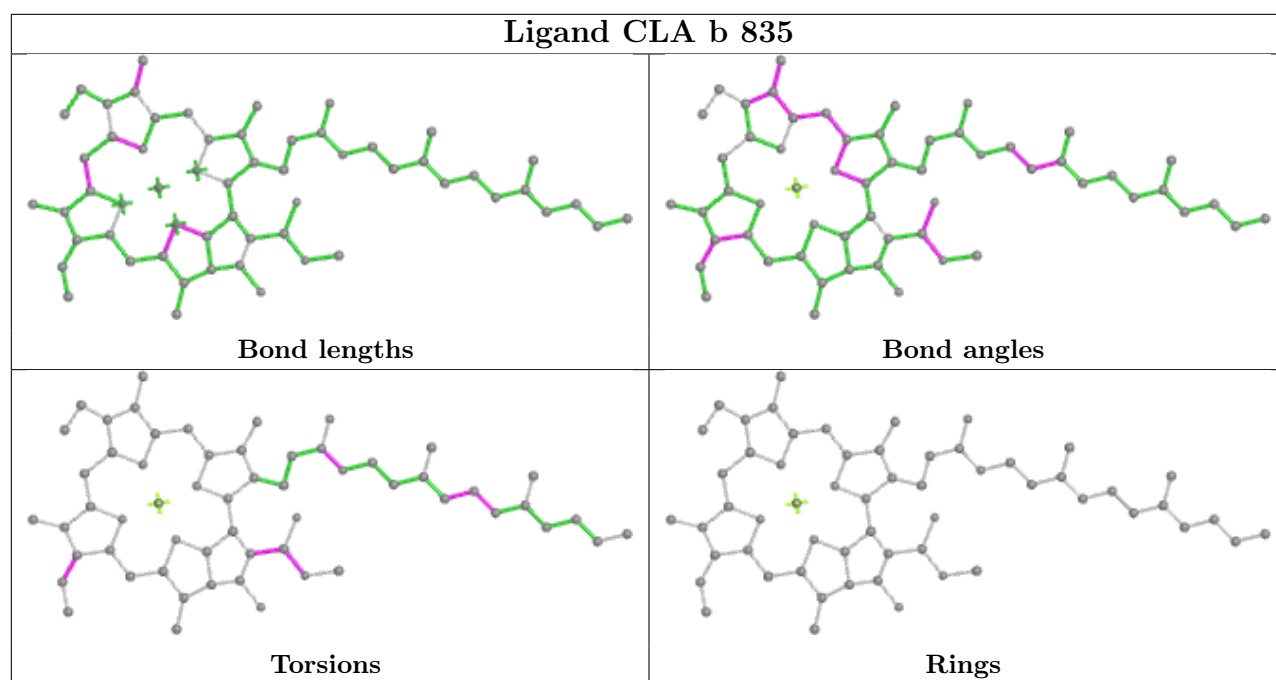


Ligand CLA b 829

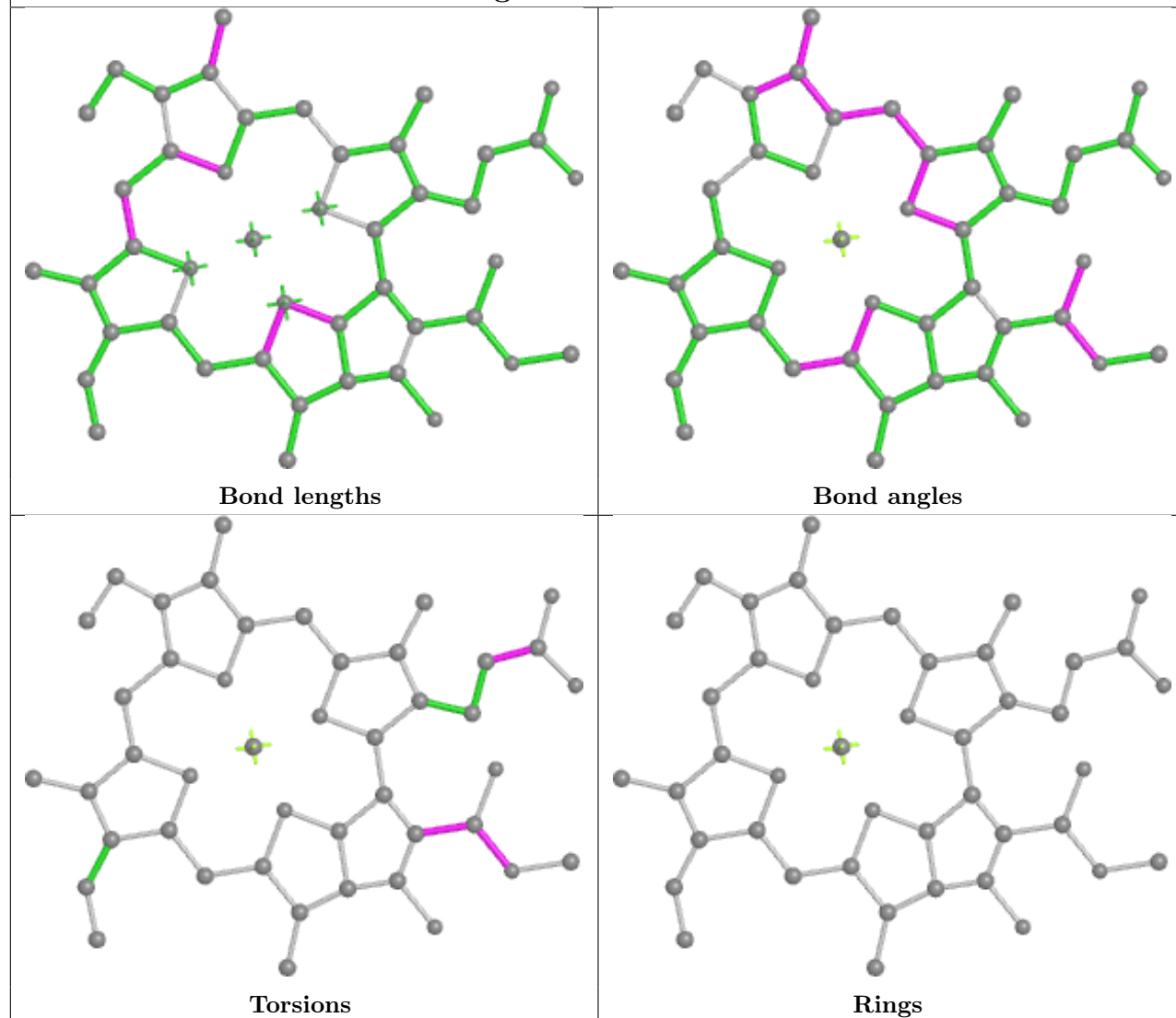


Ligand CLA a 818

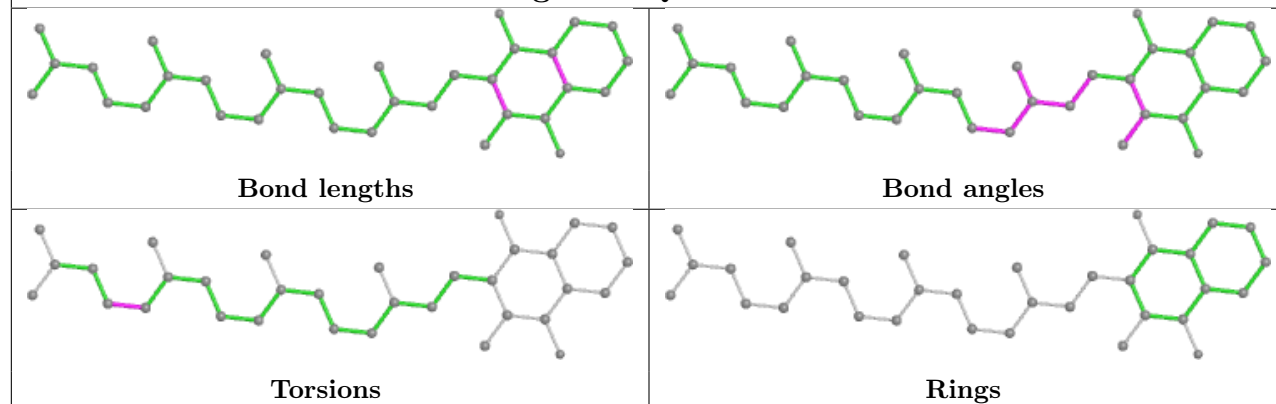




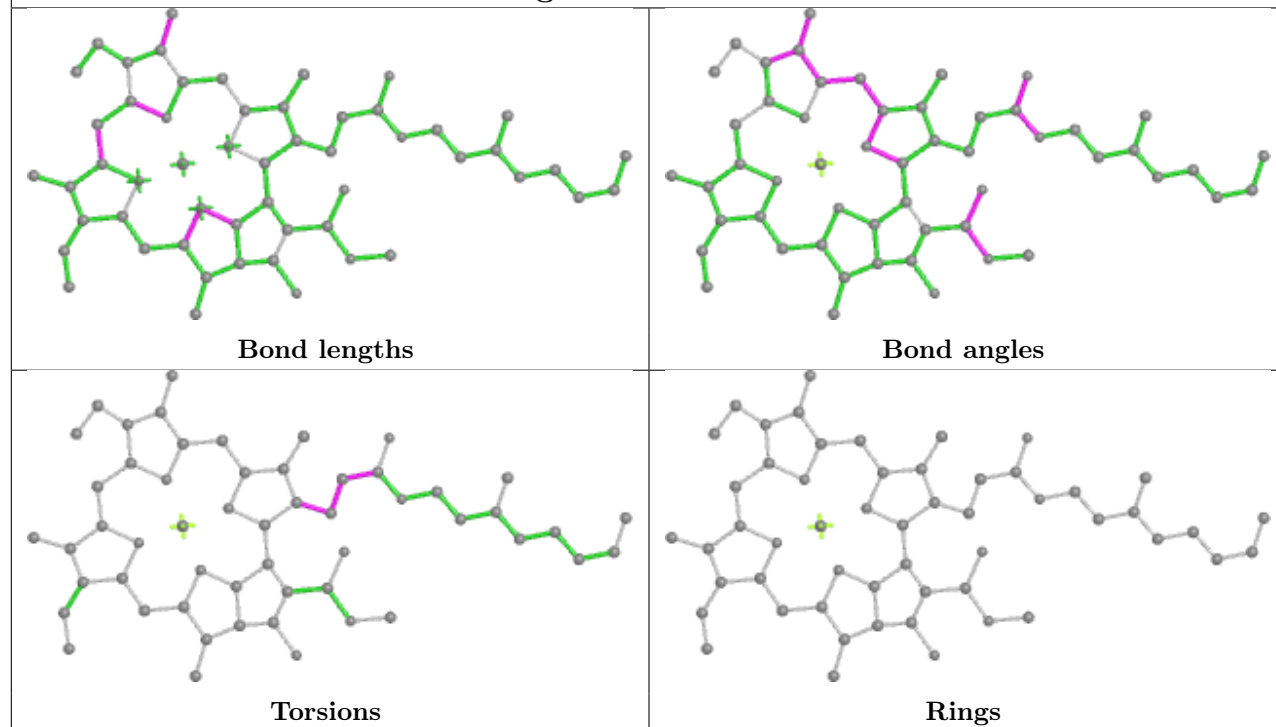
Ligand CLA 7 307



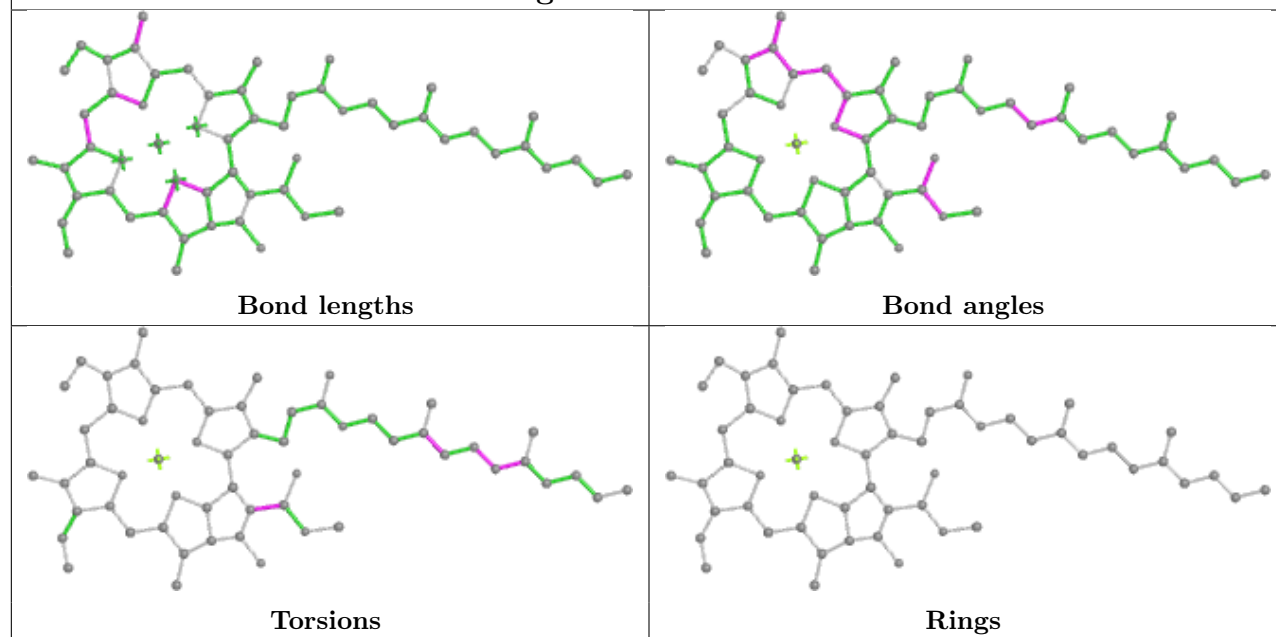
Ligand PQN b 841



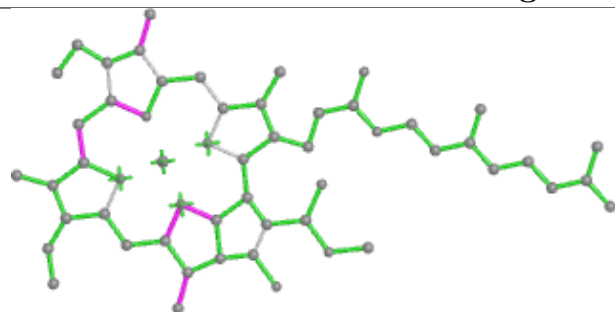
Ligand CLA a 819



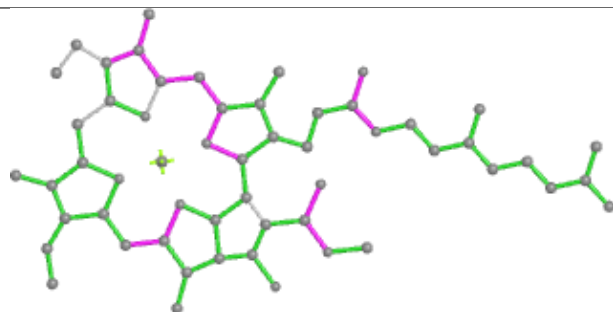
Ligand CLA a 802



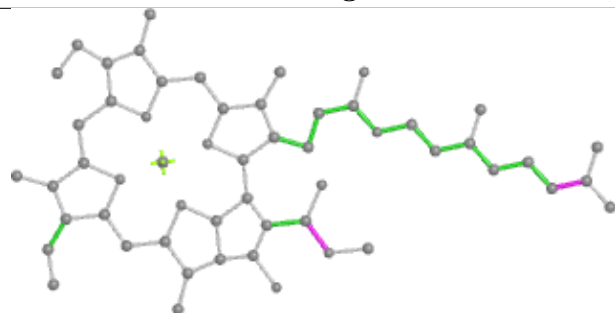
Ligand CLA b 819



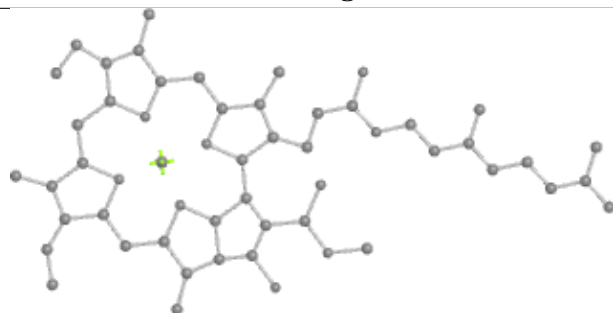
Bond lengths



Bond angles

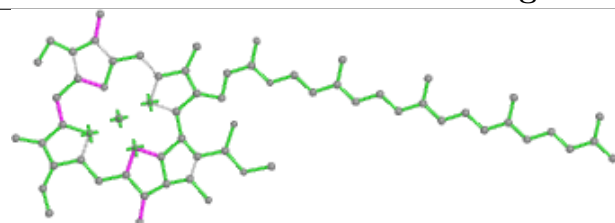


Torsions

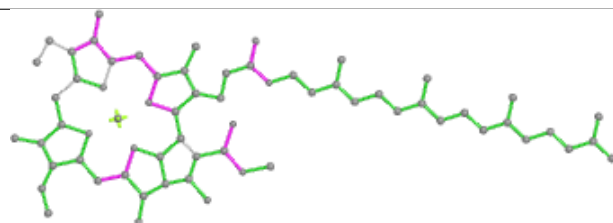


Rings

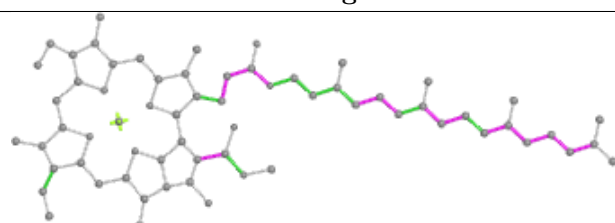
Ligand CLA b 801



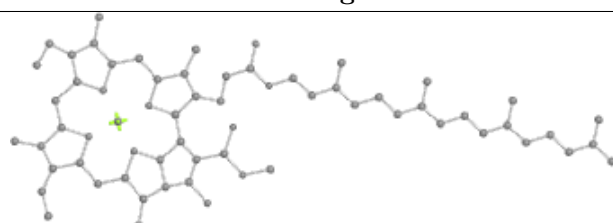
Bond lengths



Bond angles

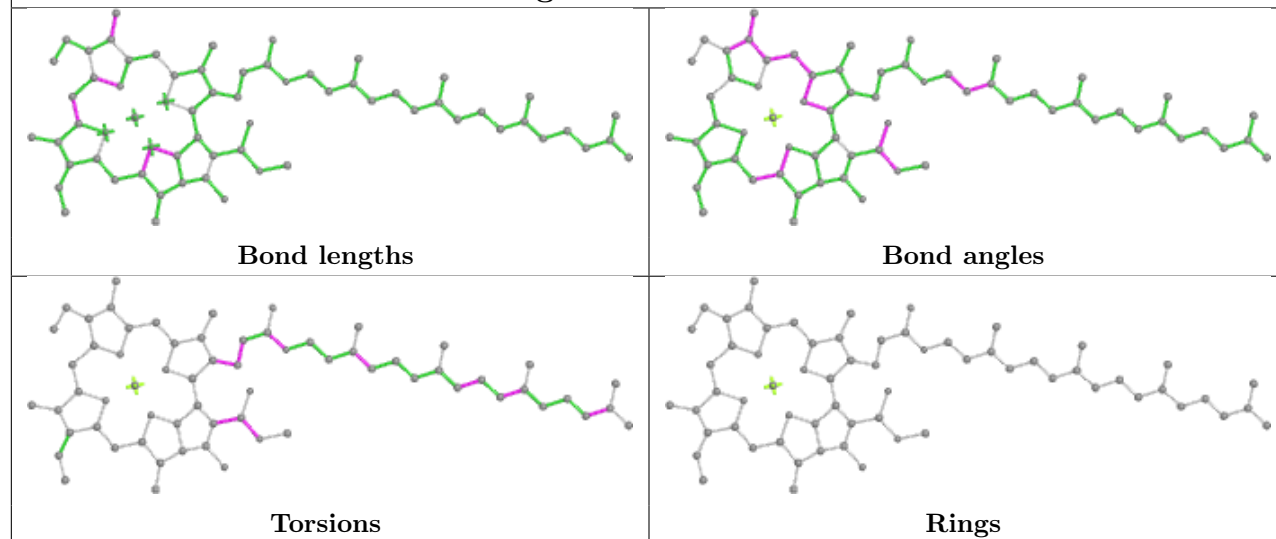


Torsions

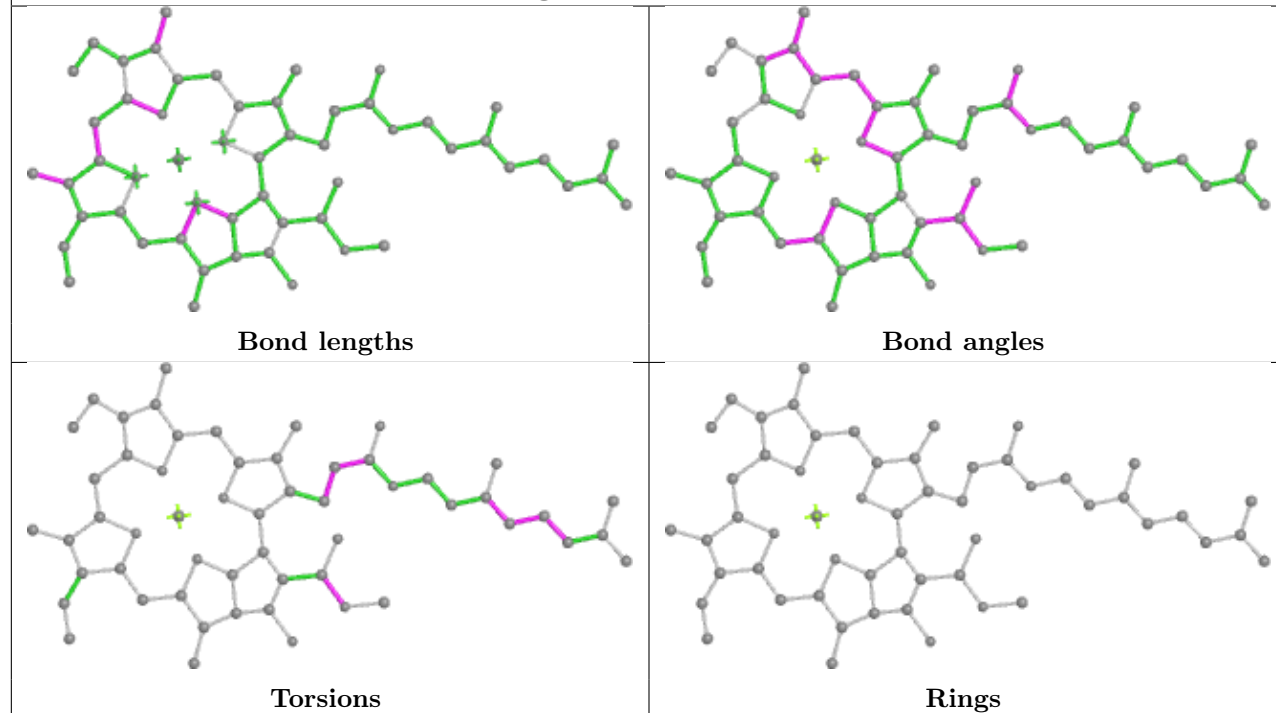


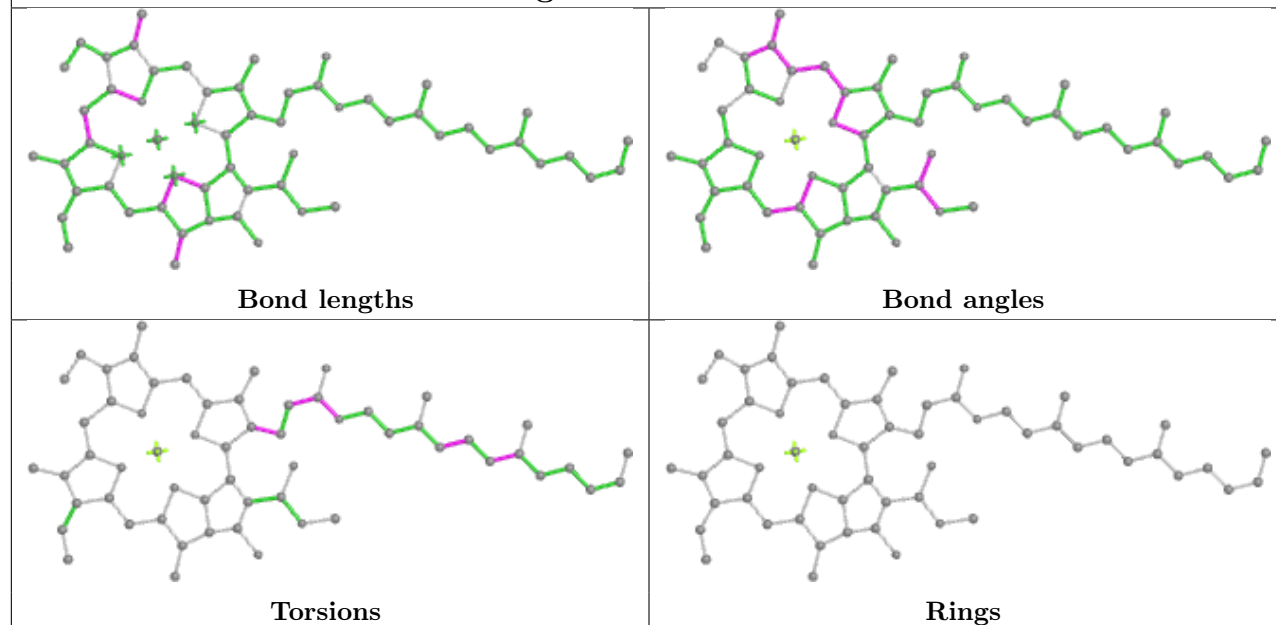
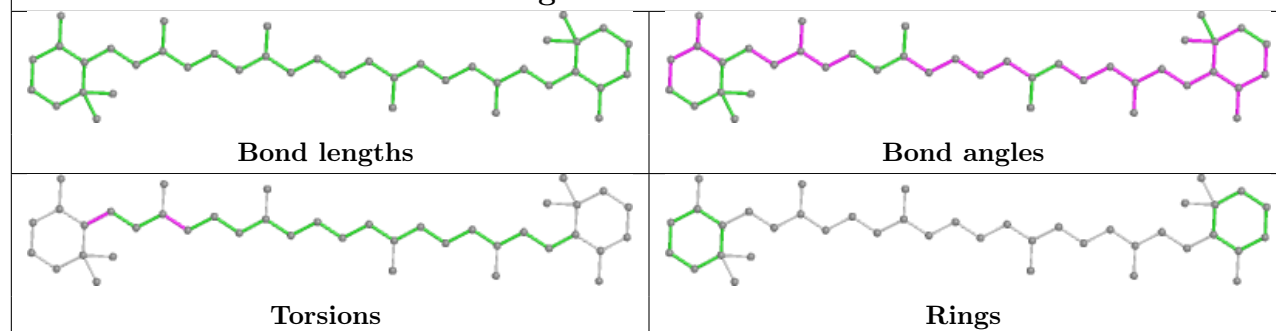
Rings

Ligand CLA 9 316

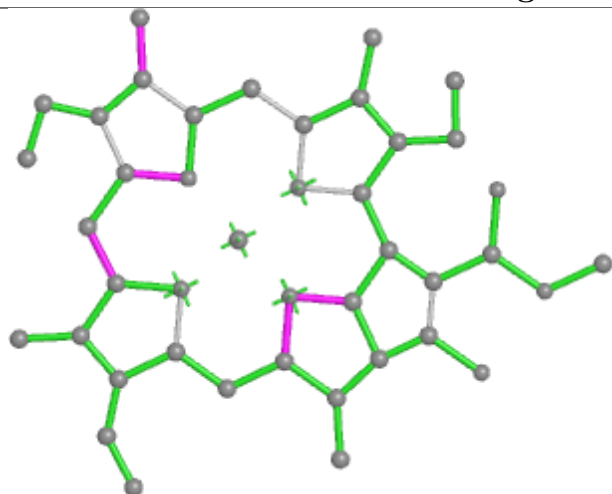


Ligand CLA h 204

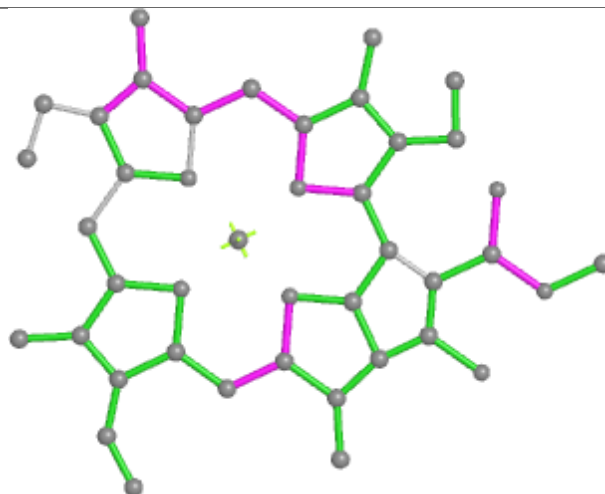


Ligand CLA 3 312**Ligand BCR 1 201**

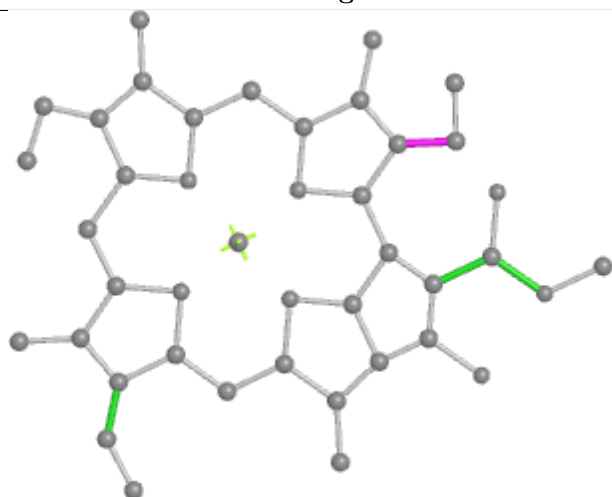
Ligand CLA 2 315



Bond lengths



Bond angles

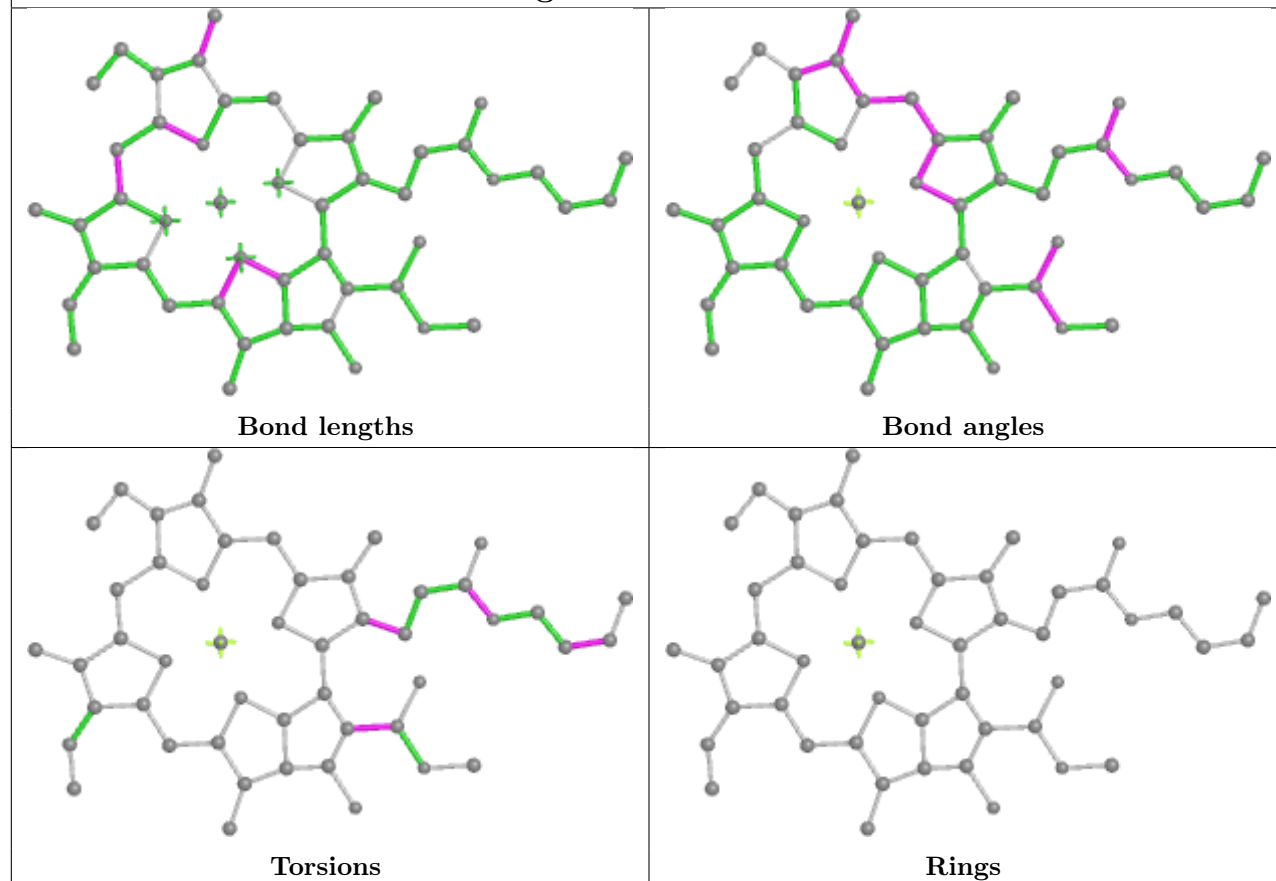


Torsions

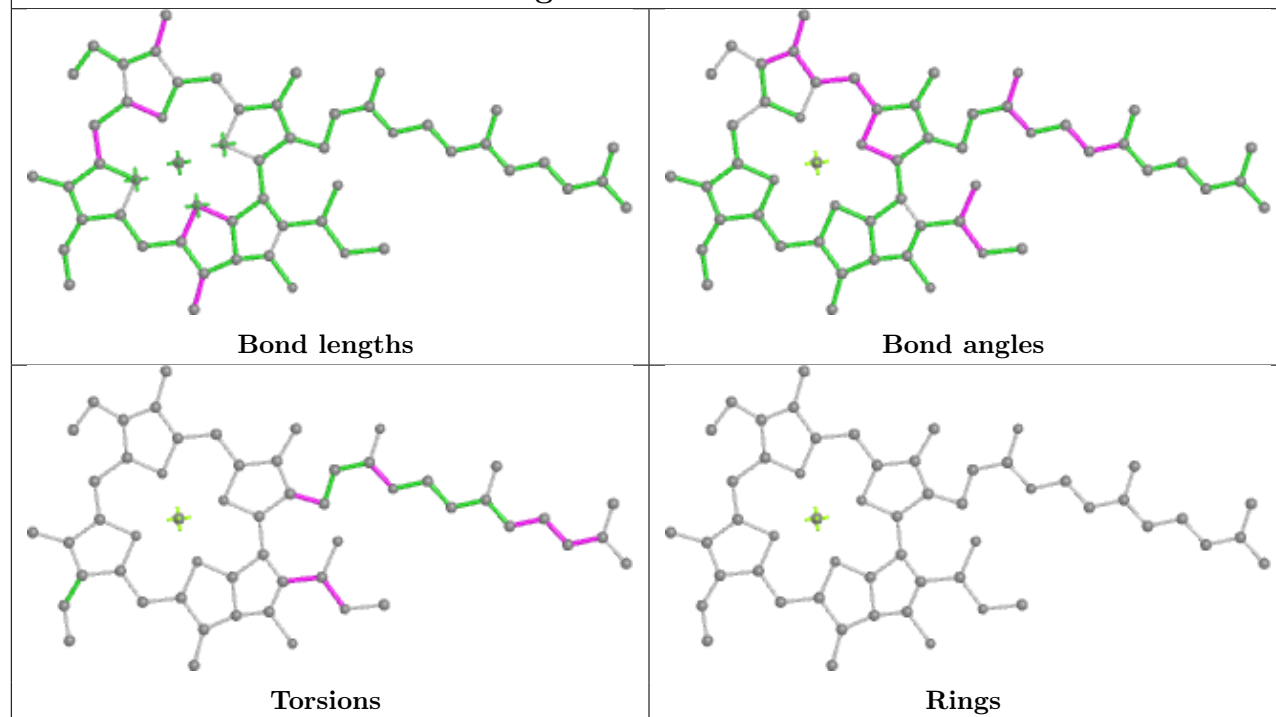


Rings

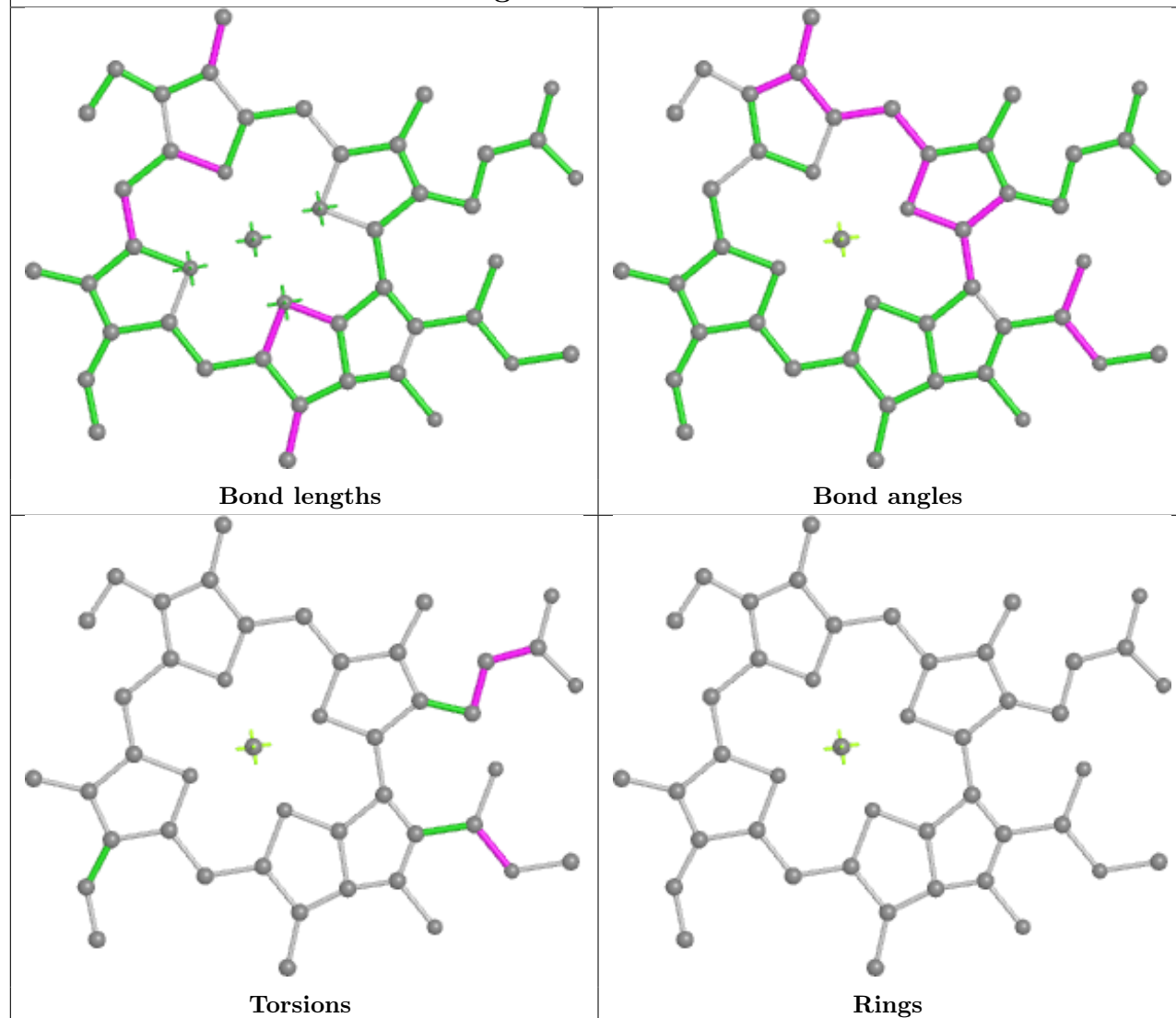
Ligand CLA a 823



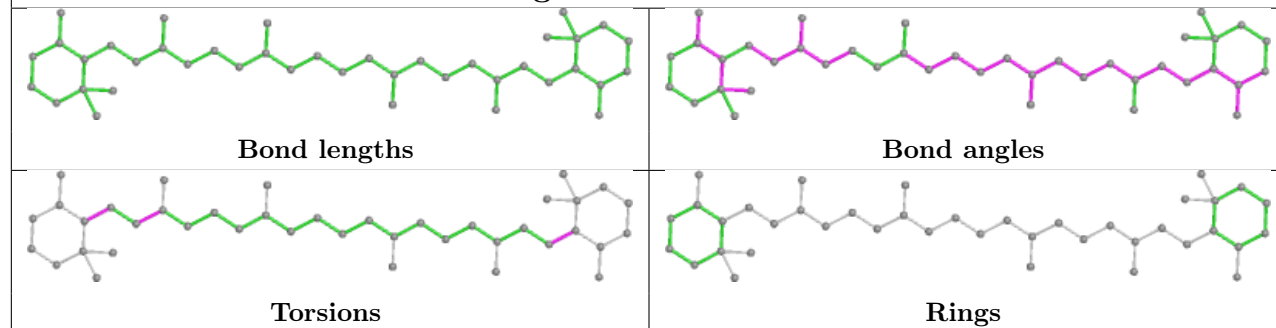
Ligand CLA b 814



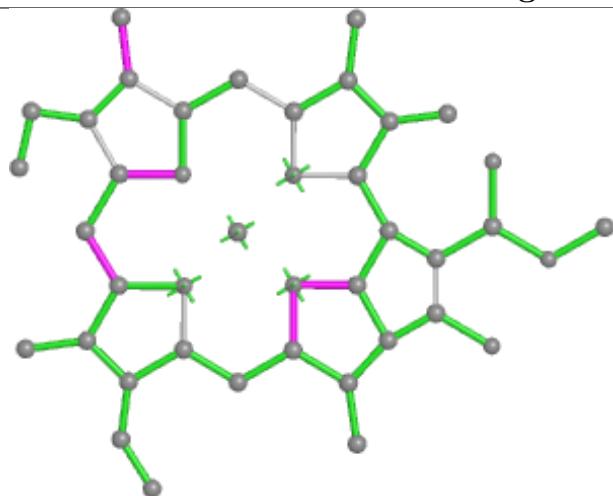
Ligand CLA 7 314



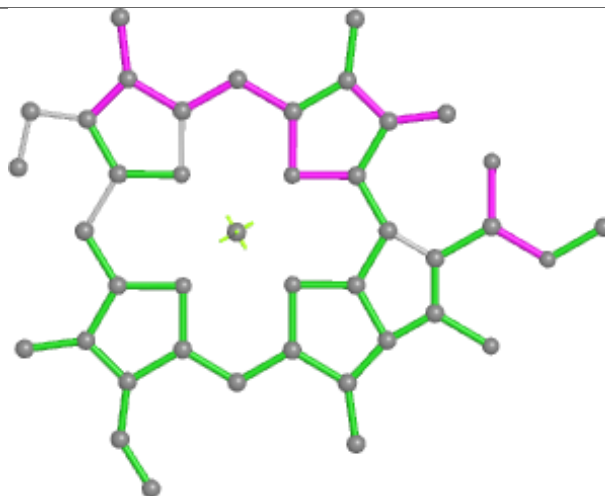
Ligand BCR b 849



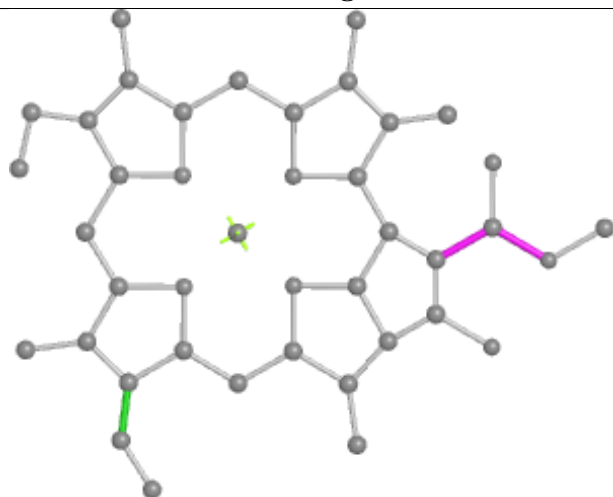
Ligand CLA 8 314



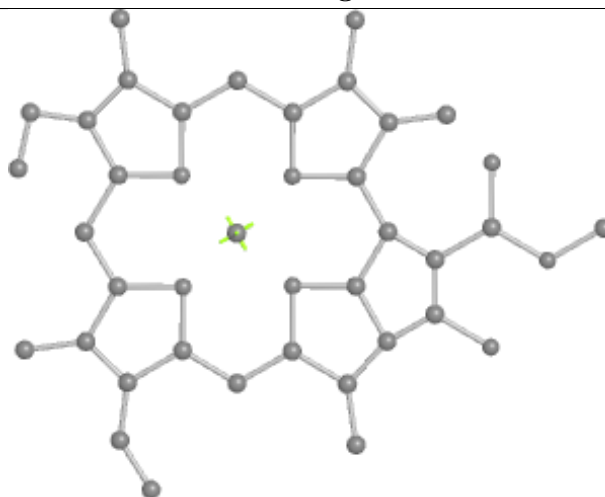
Bond lengths



Bond angles

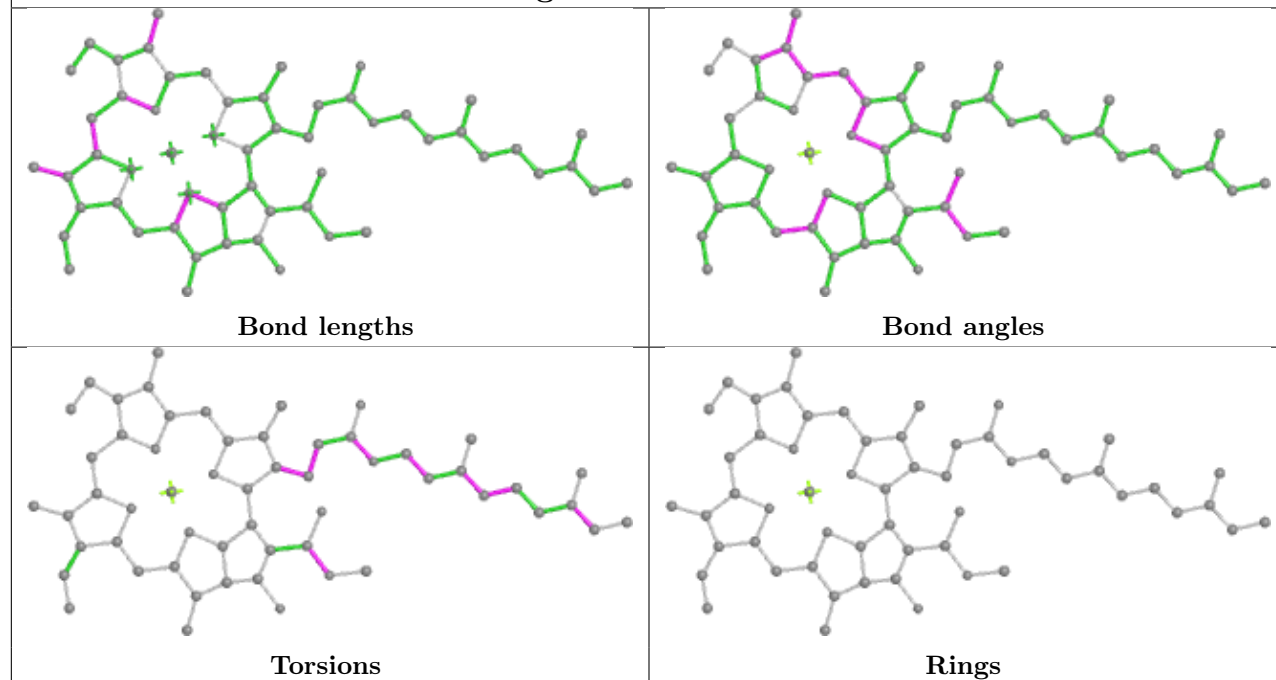


Torsions

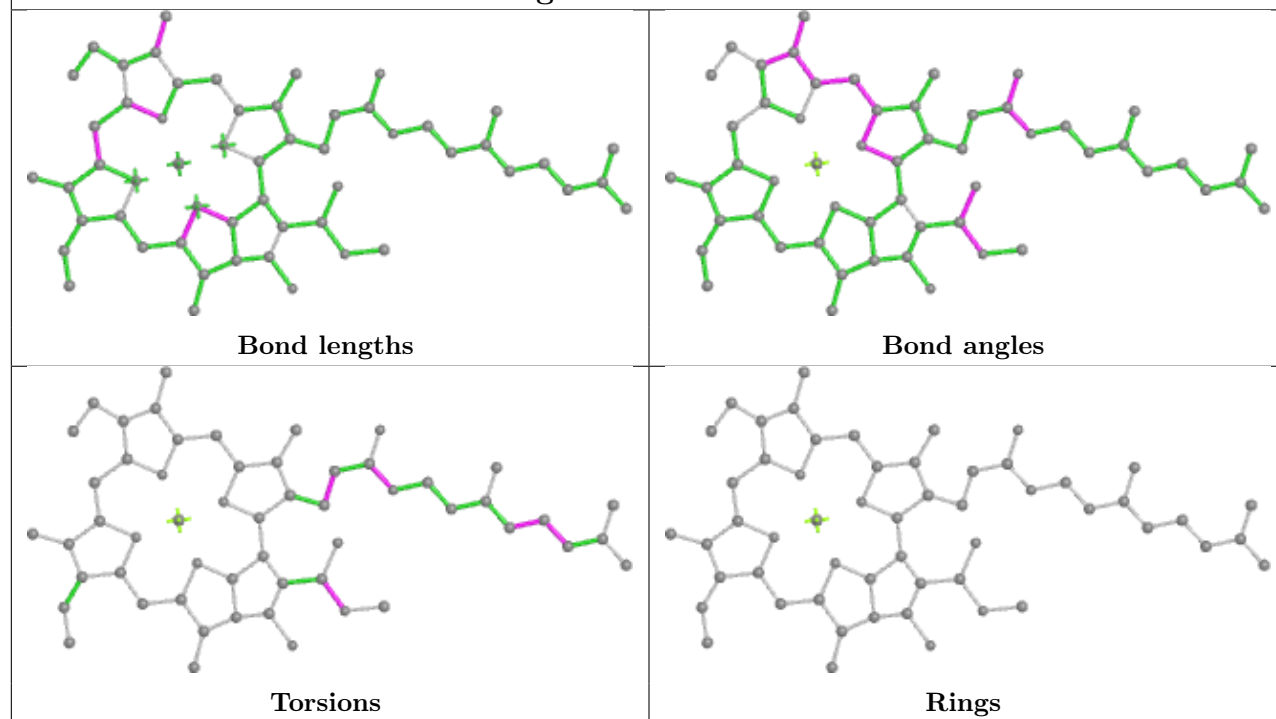


Rings

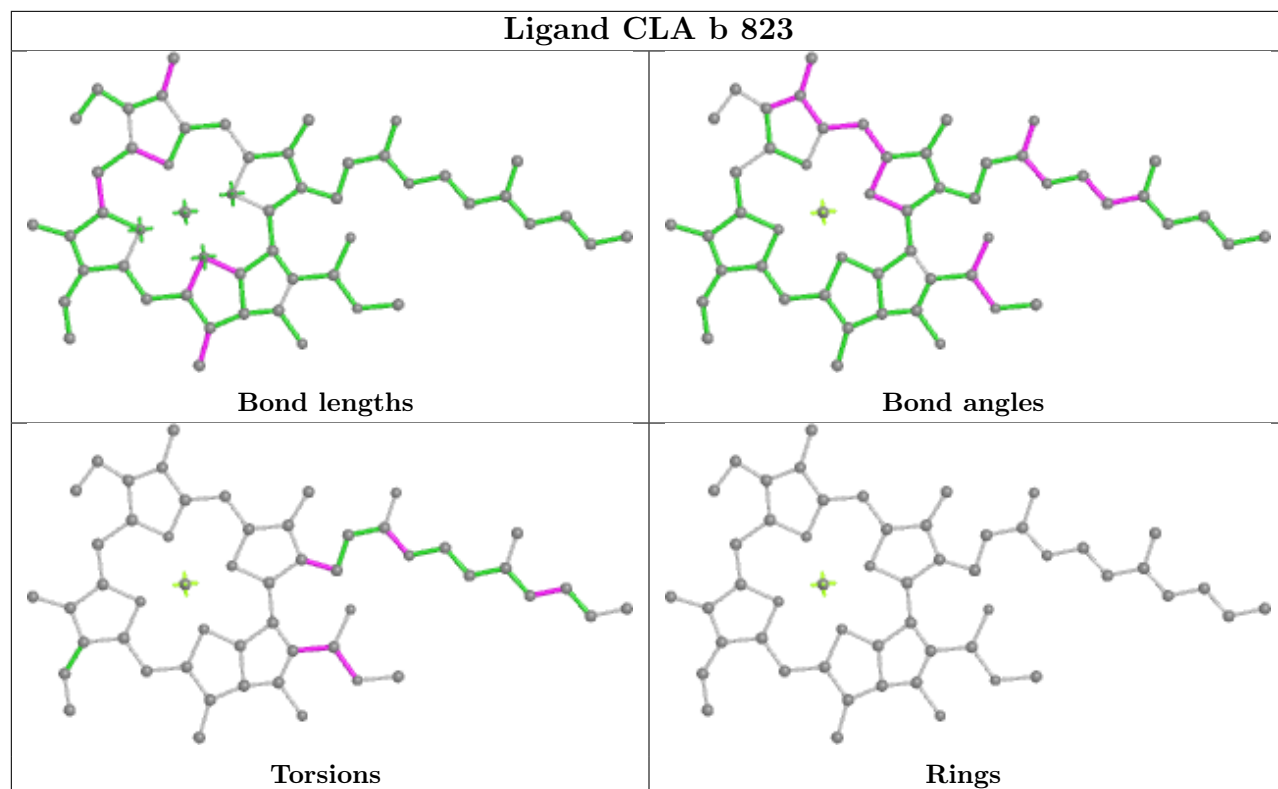
Ligand CLA 2 314



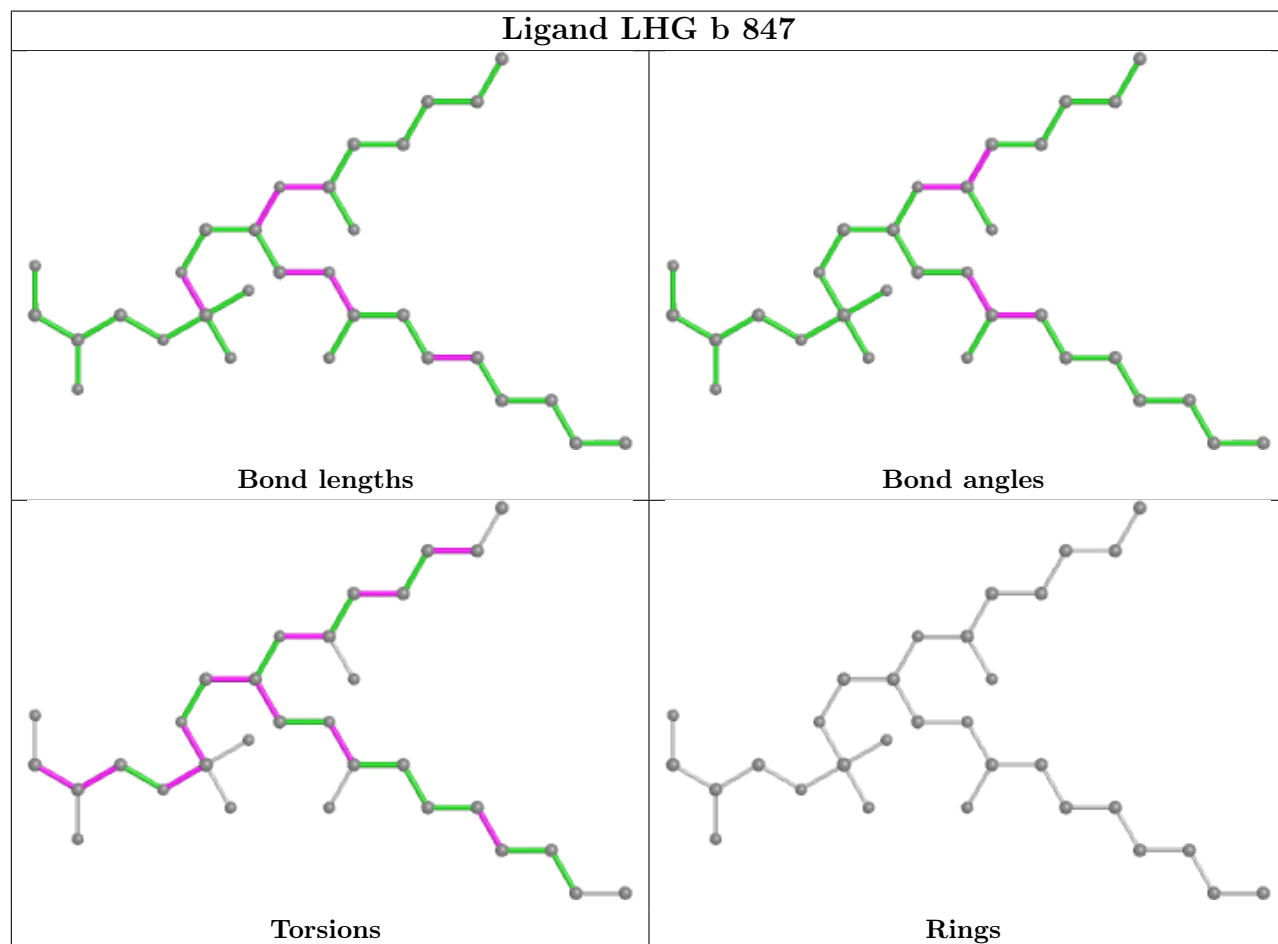
Ligand CLA 4 317



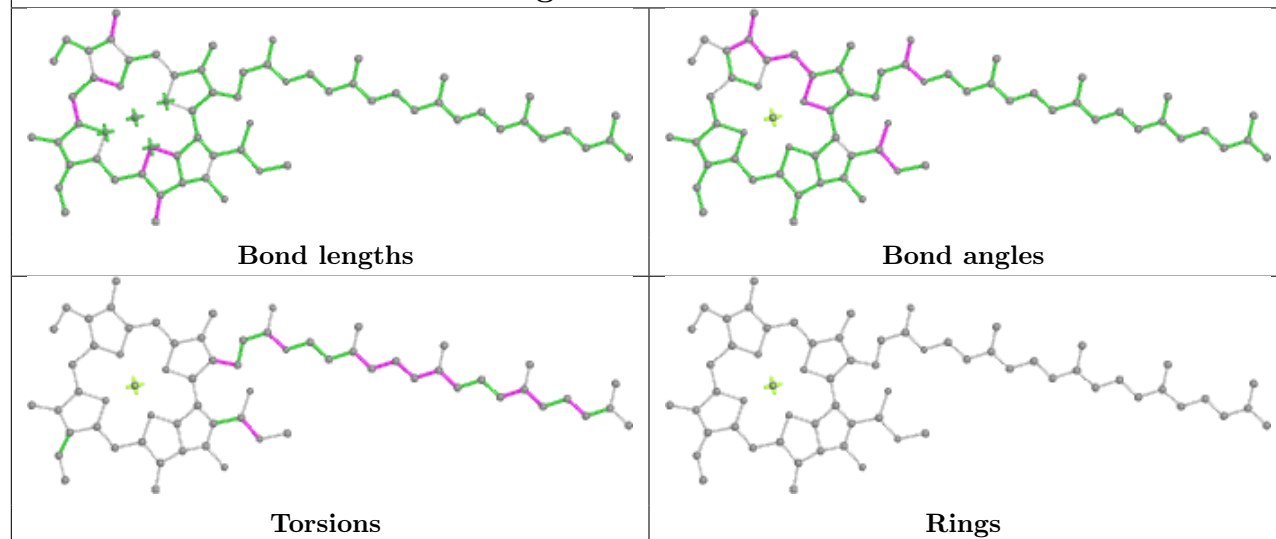
Ligand CLA b 823



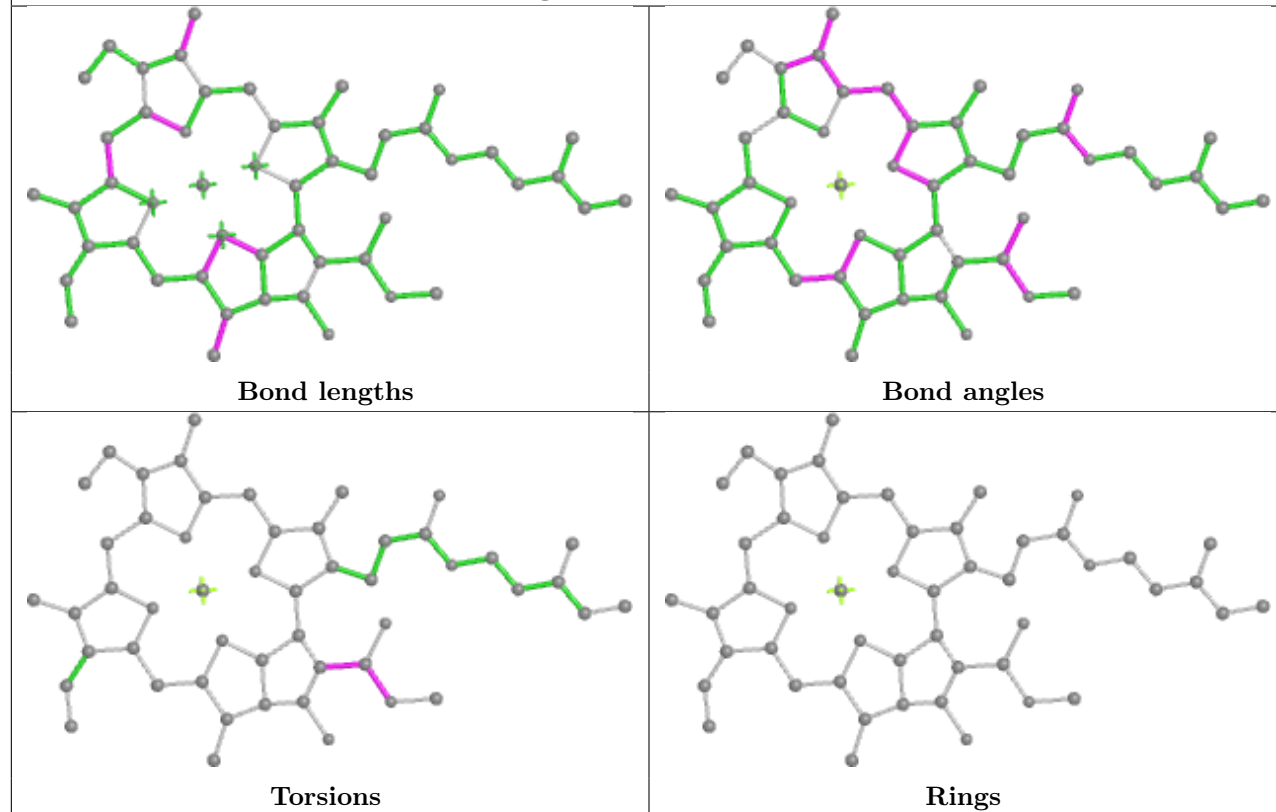
Ligand LHG b 847

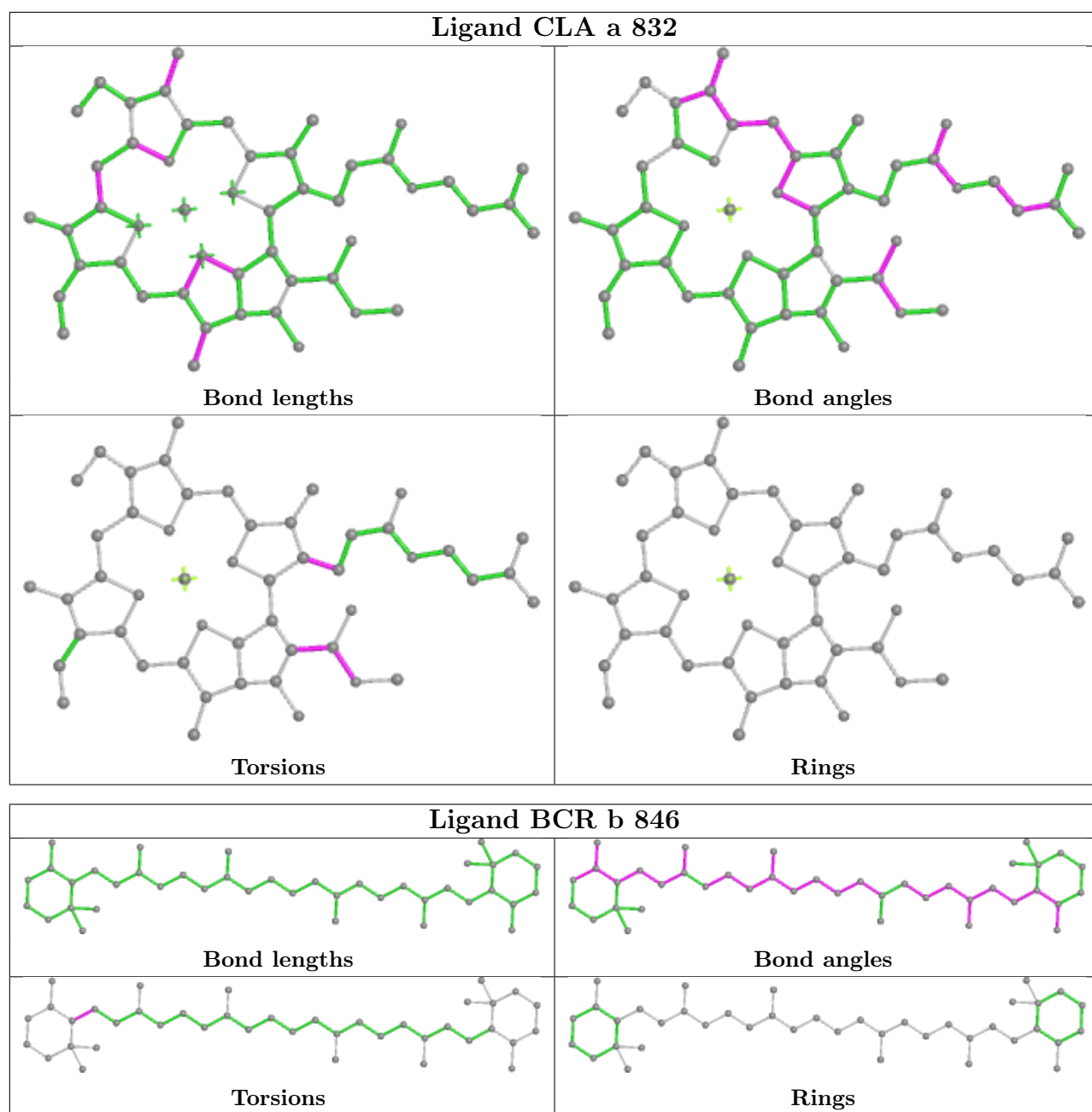


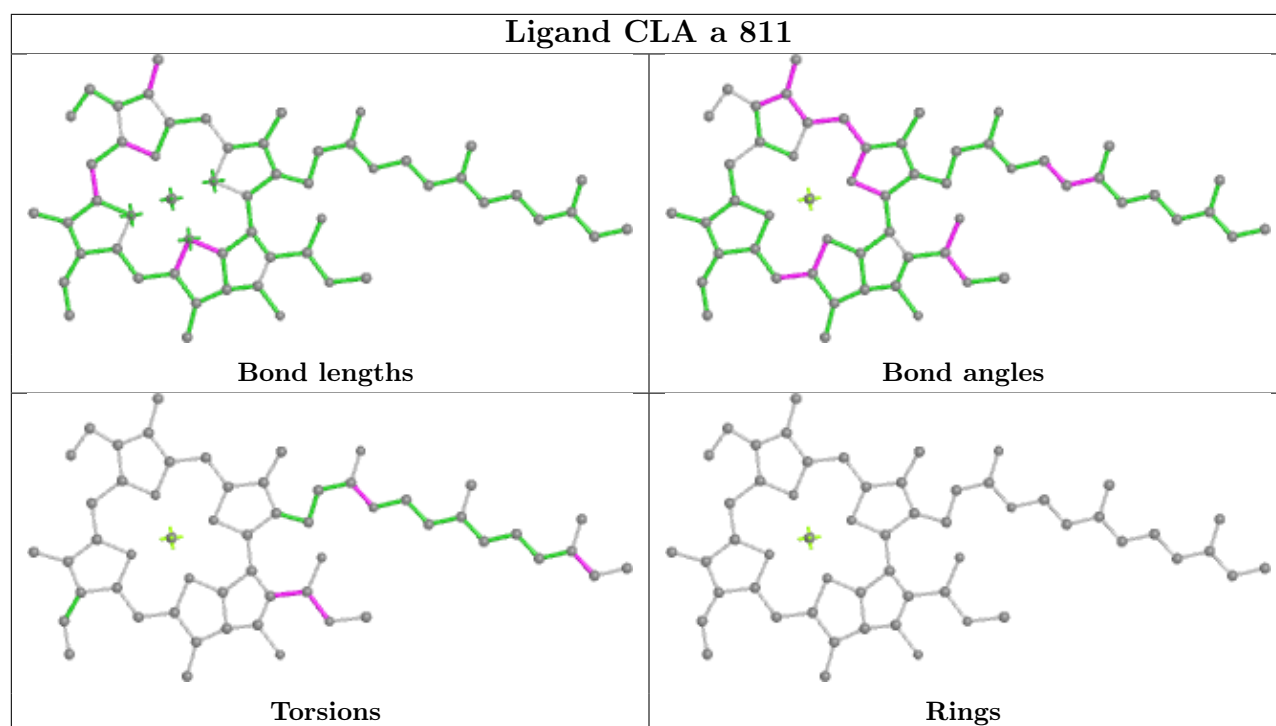
Ligand CLA a 807



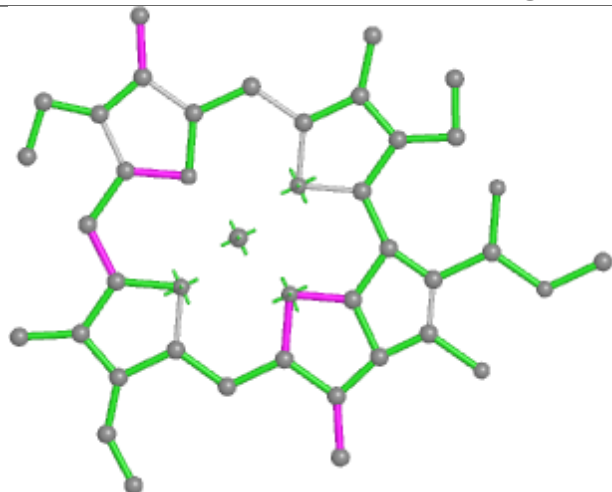
Ligand CLA a 808



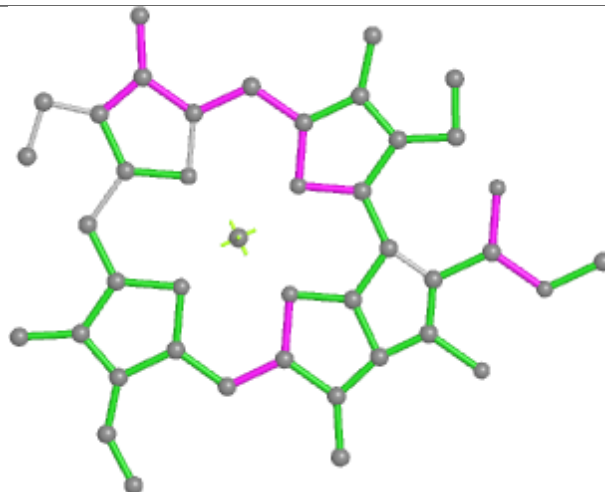




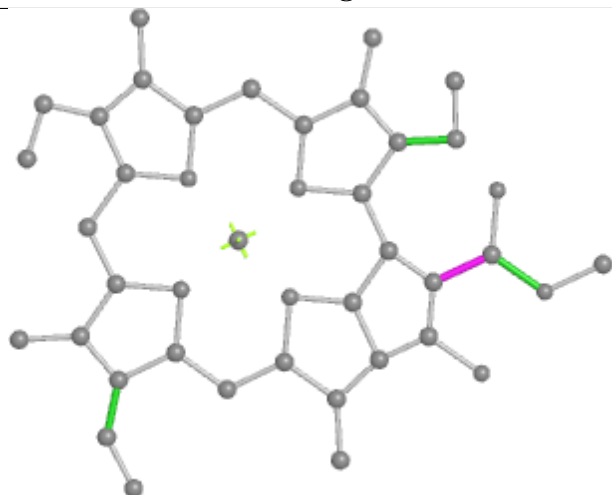
Ligand CLA 1 202



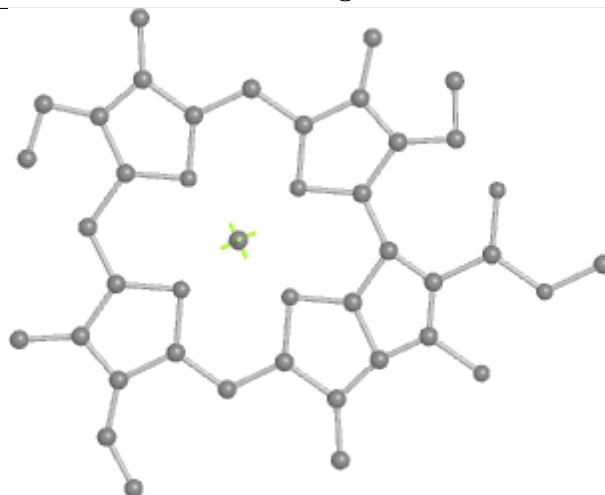
Bond lengths



Bond angles

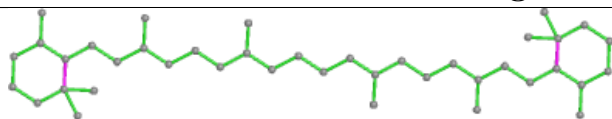


Torsions

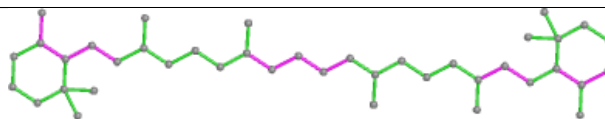


Rings

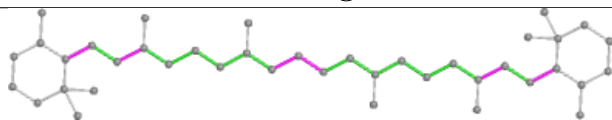
Ligand BCR m 101



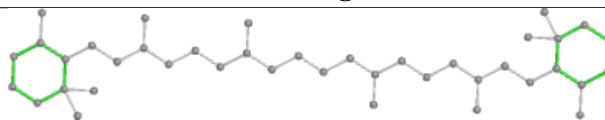
Bond lengths



Bond angles

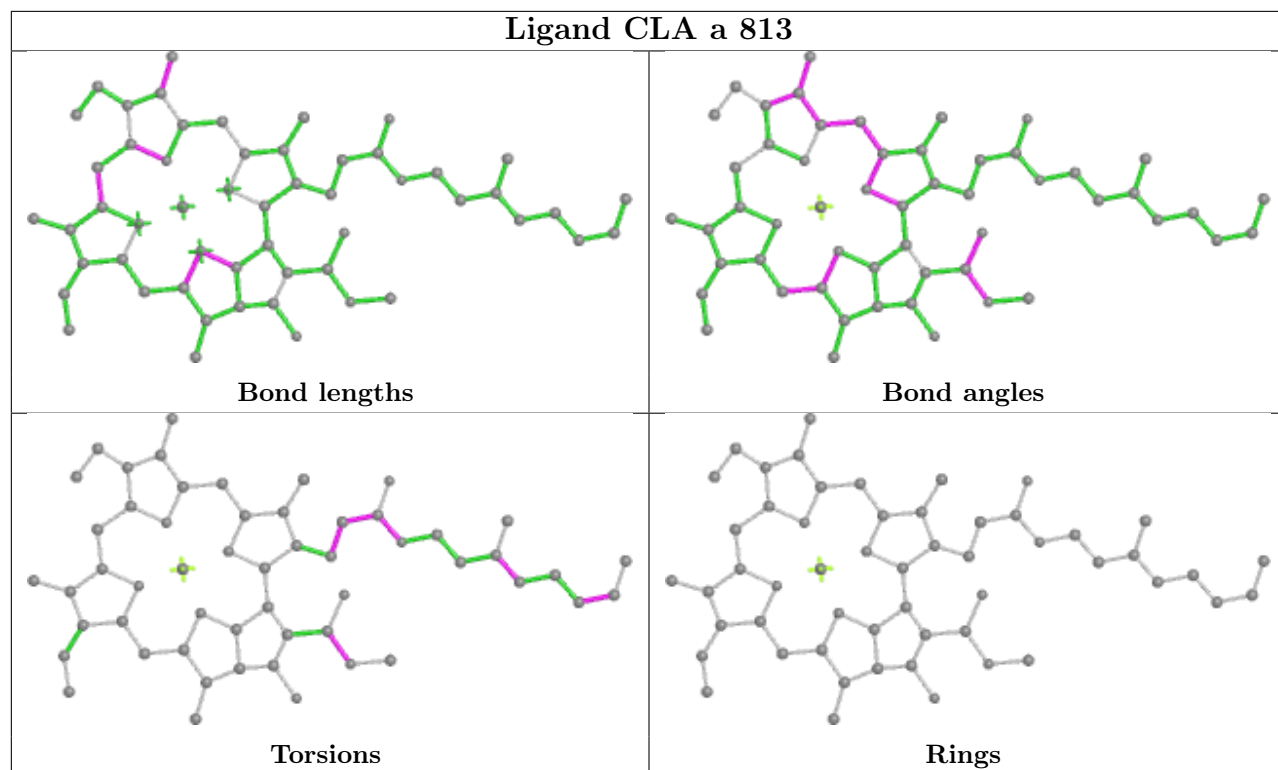


Torsions

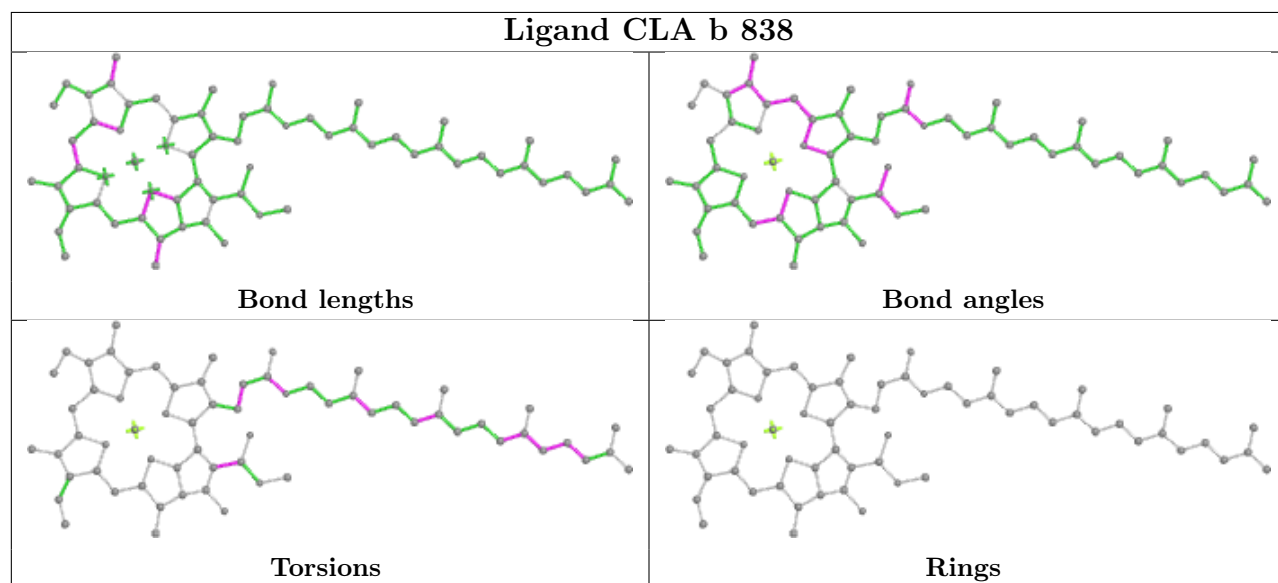


Rings

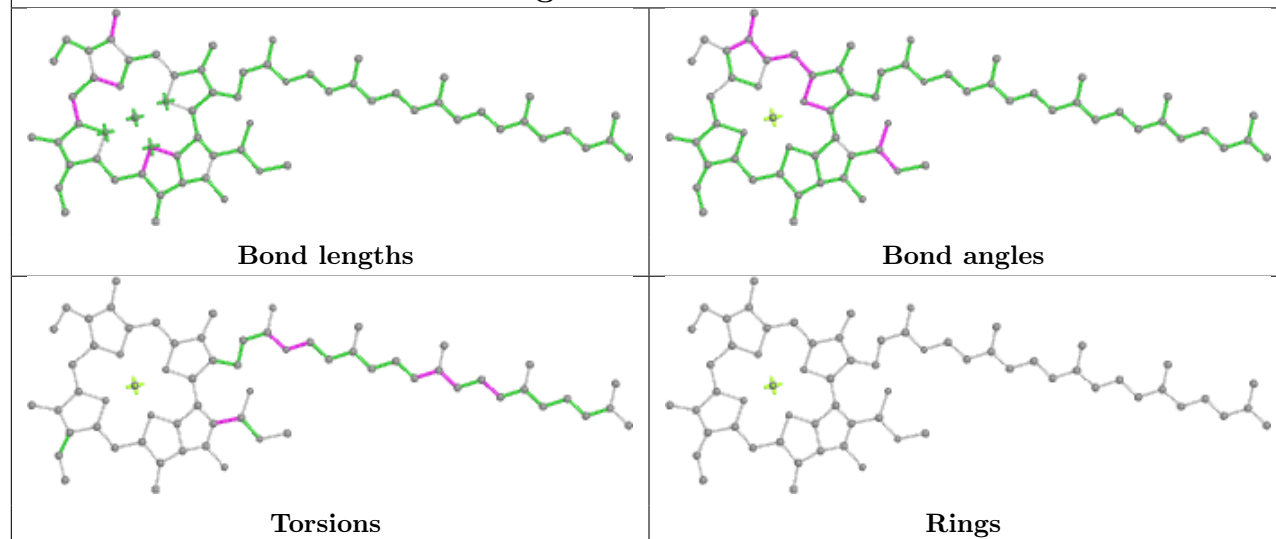
Ligand CLA a 813



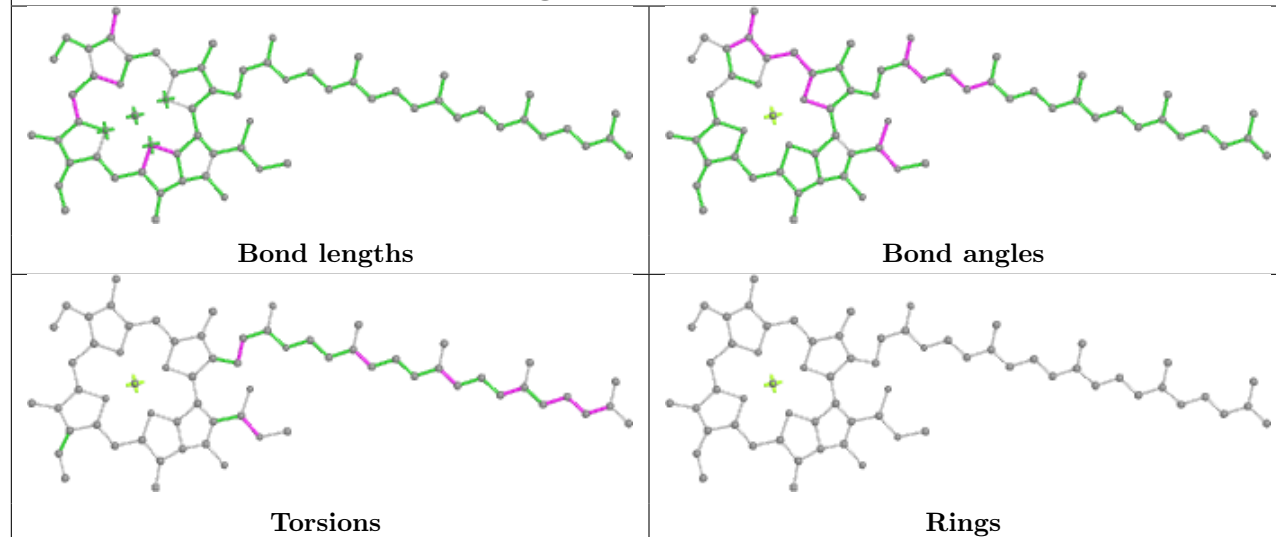
Ligand CLA b 838



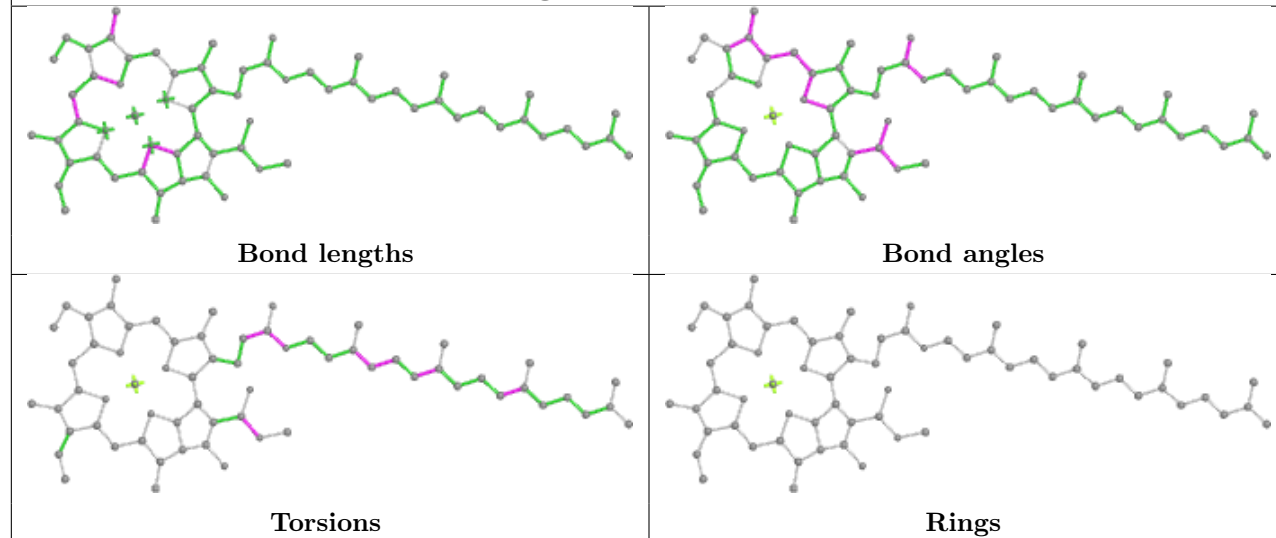
Ligand CLA 6 309



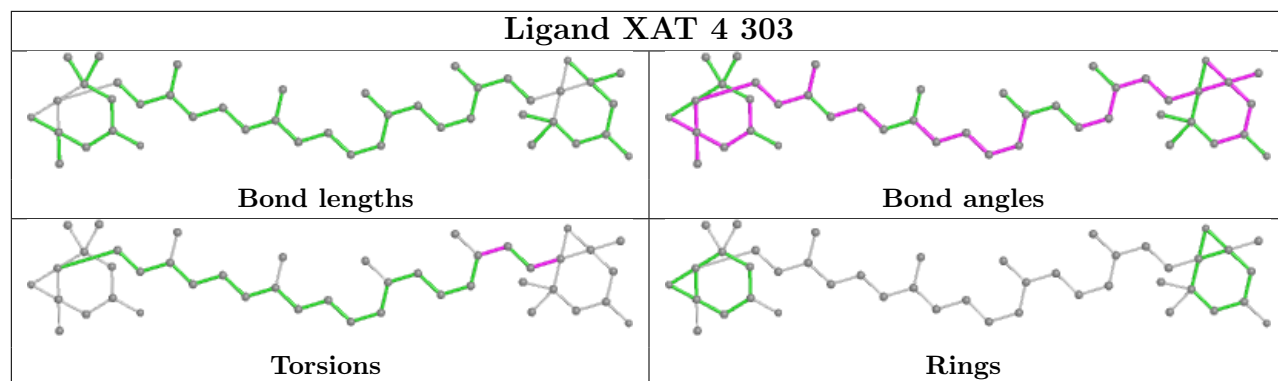
Ligand CLA 1 308



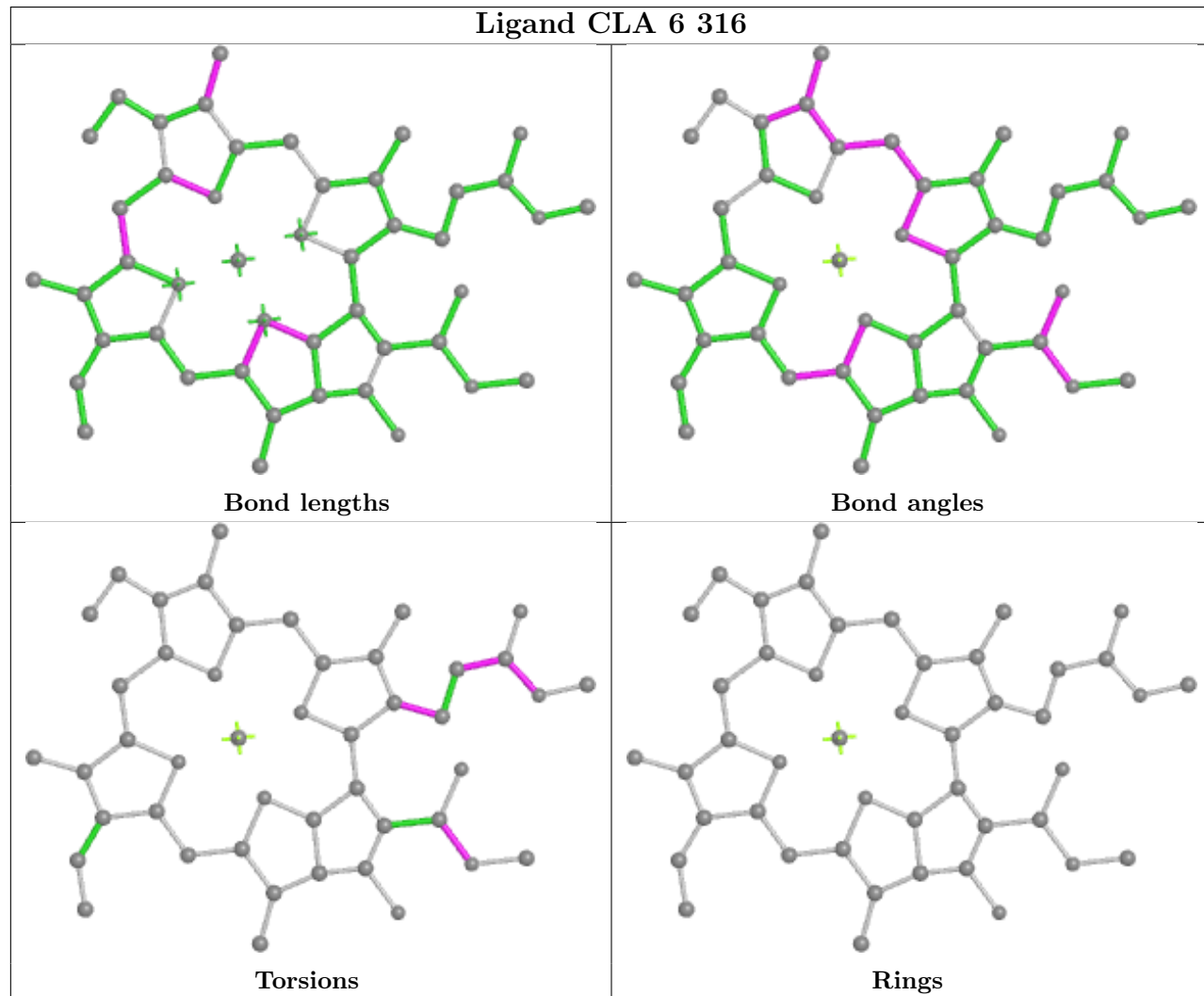
Ligand CLA a 835



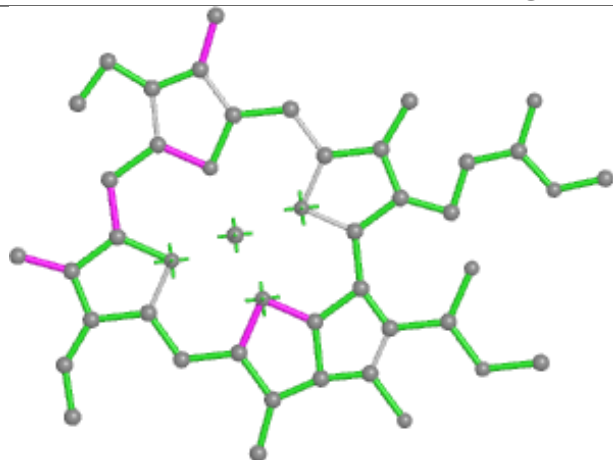
Ligand XAT 4 303



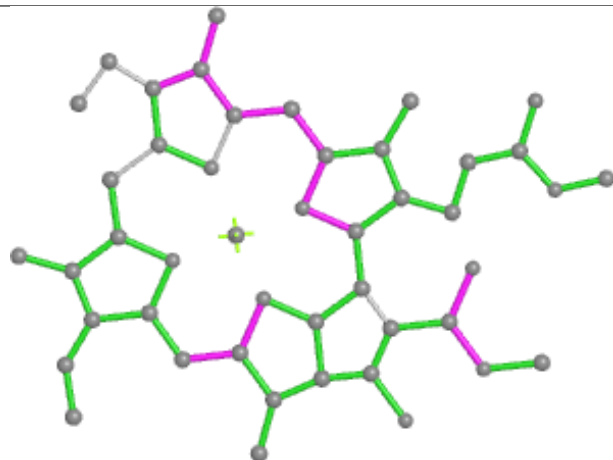
Ligand CLA 6 316



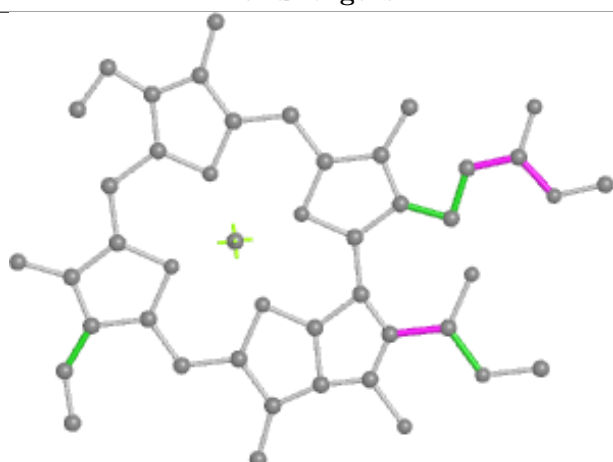
Ligand CLA 1 204



Bond lengths



Bond angles

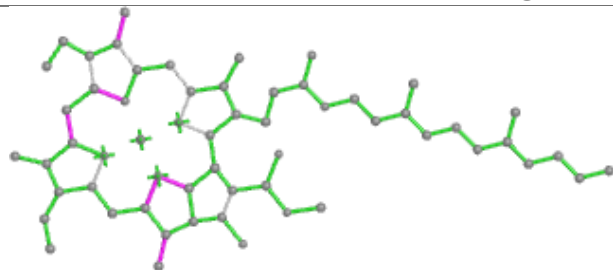


Torsions

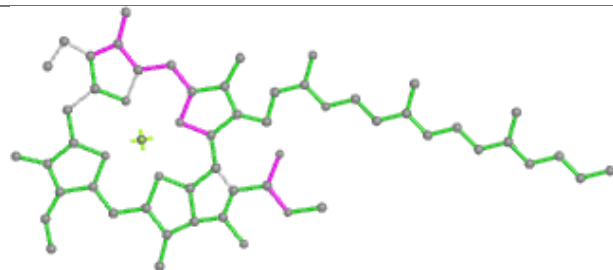


Rings

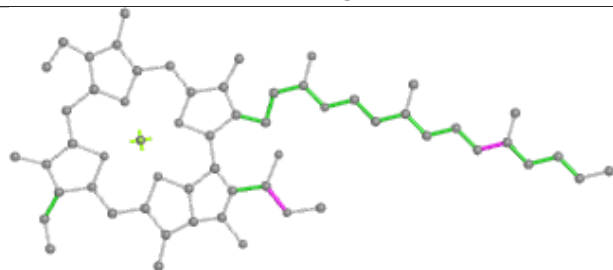
Ligand CLA 6 308



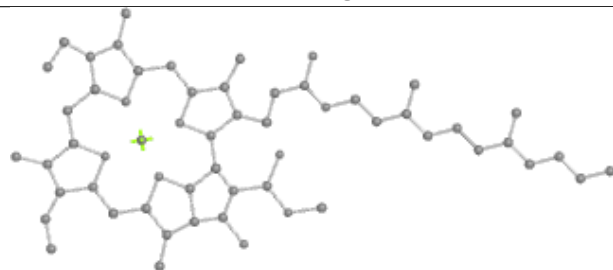
Bond lengths



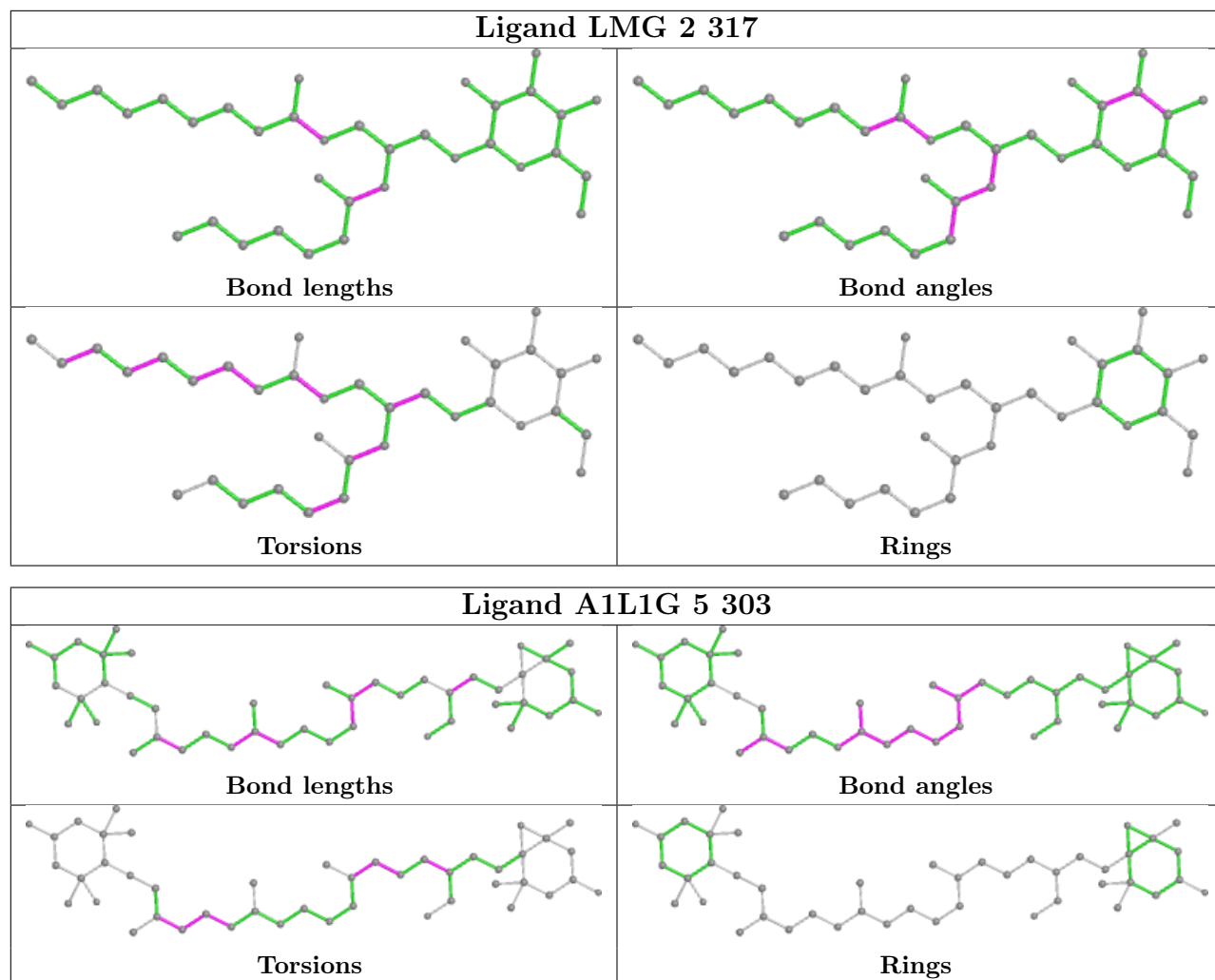
Bond angles



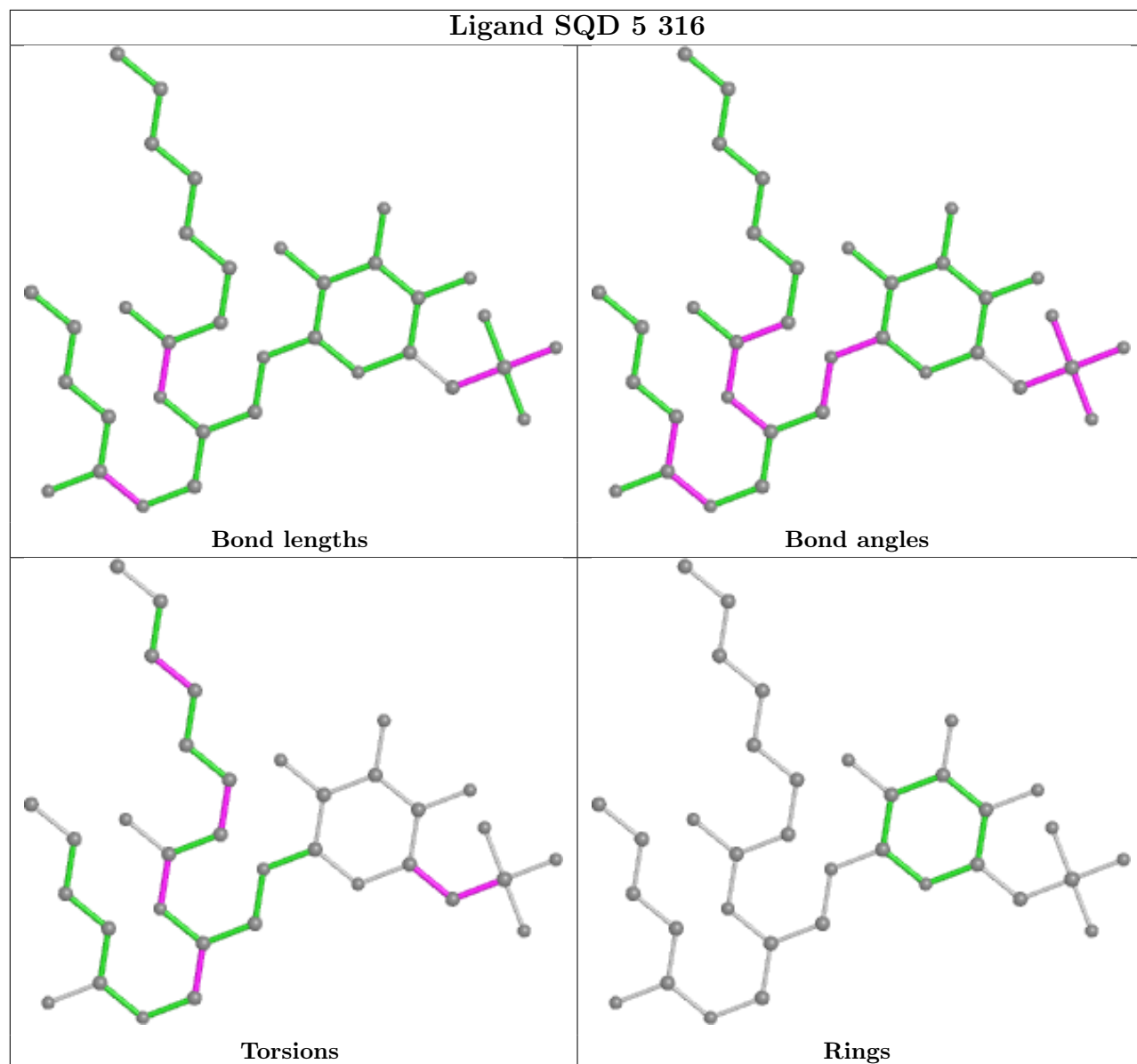
Torsions



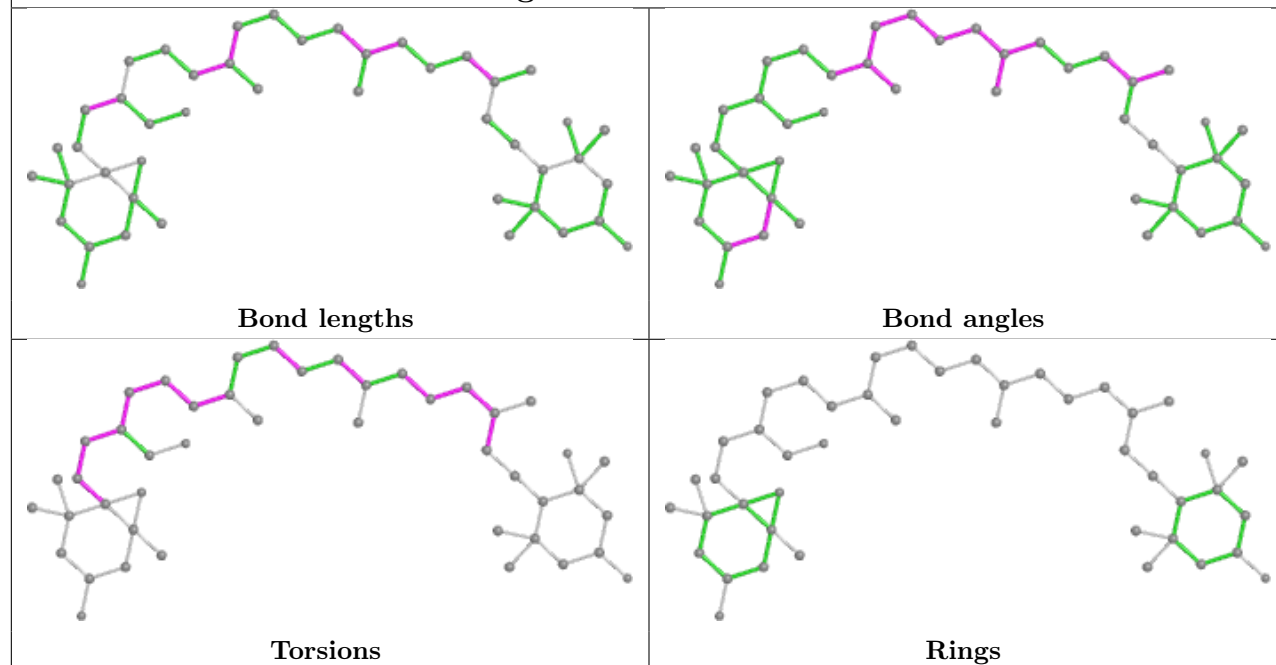
Rings



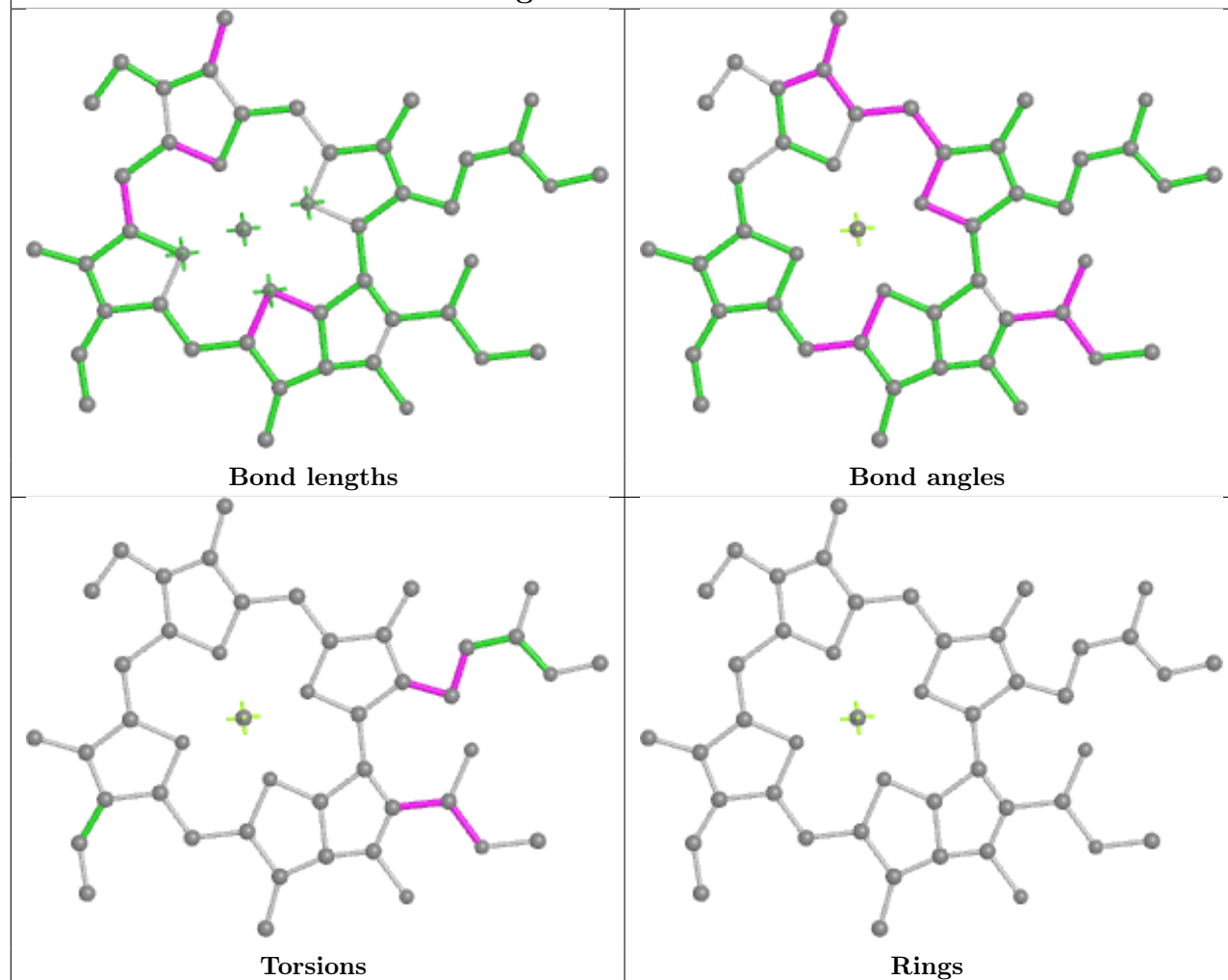
Ligand SQD 5 316



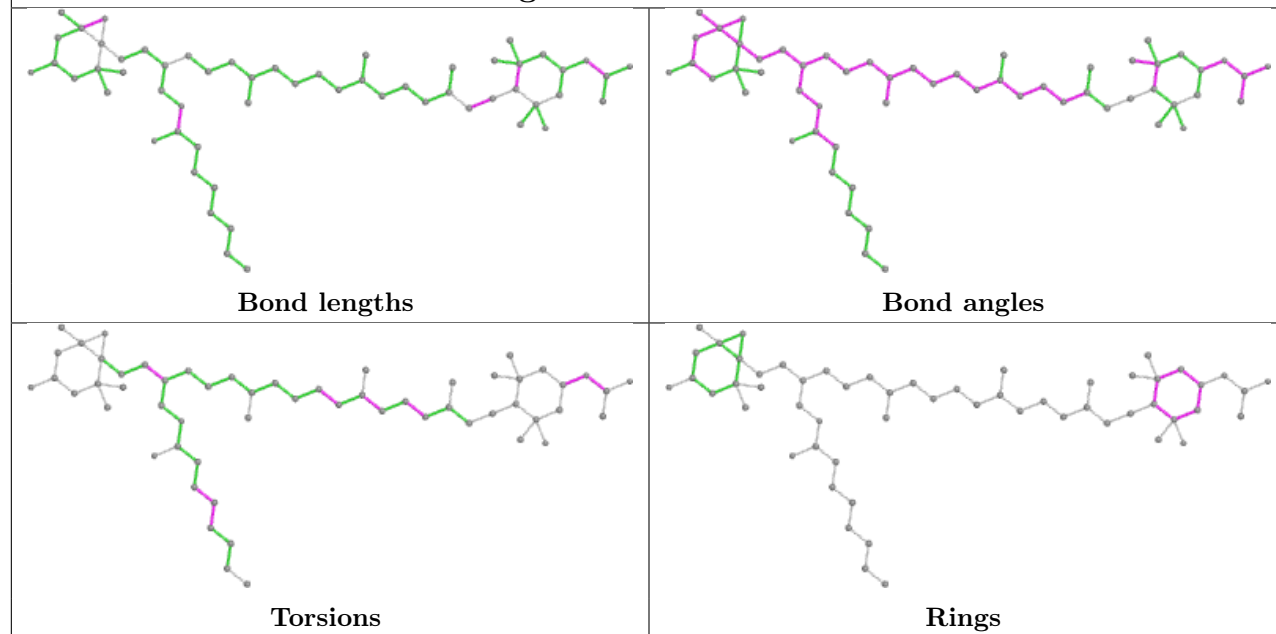
Ligand A1L1G 9 306



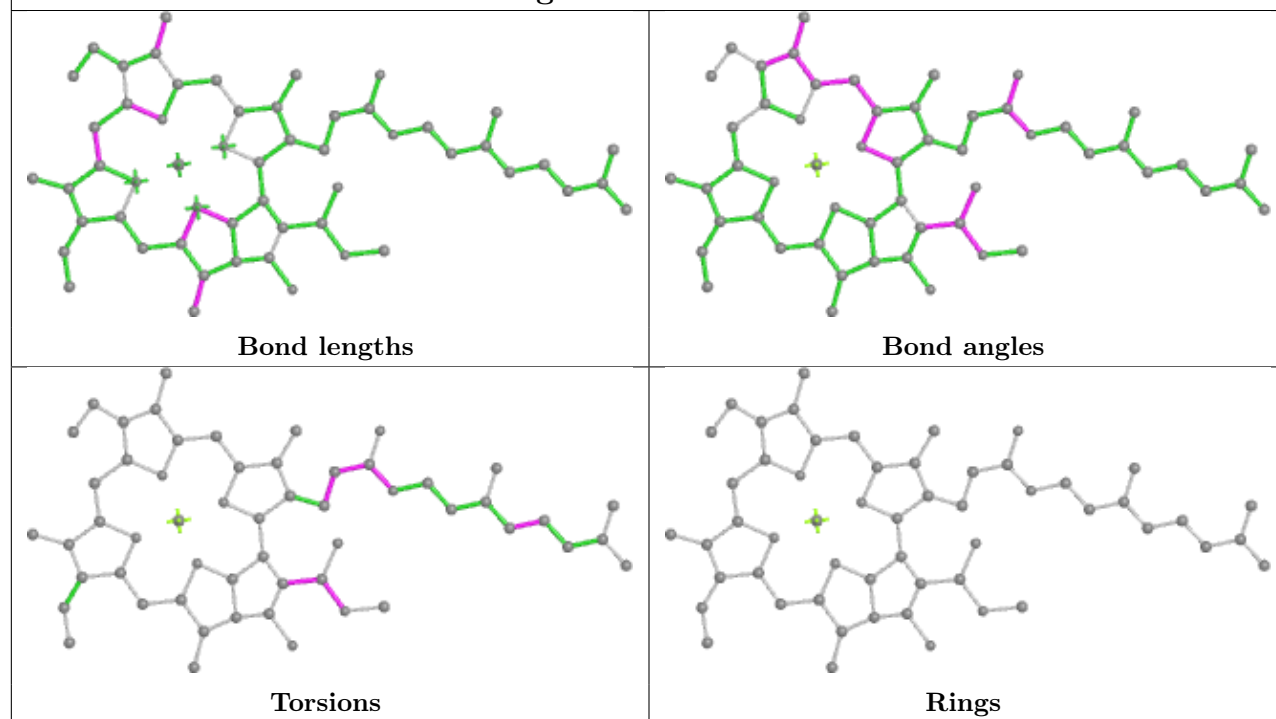
Ligand CLA 9 311



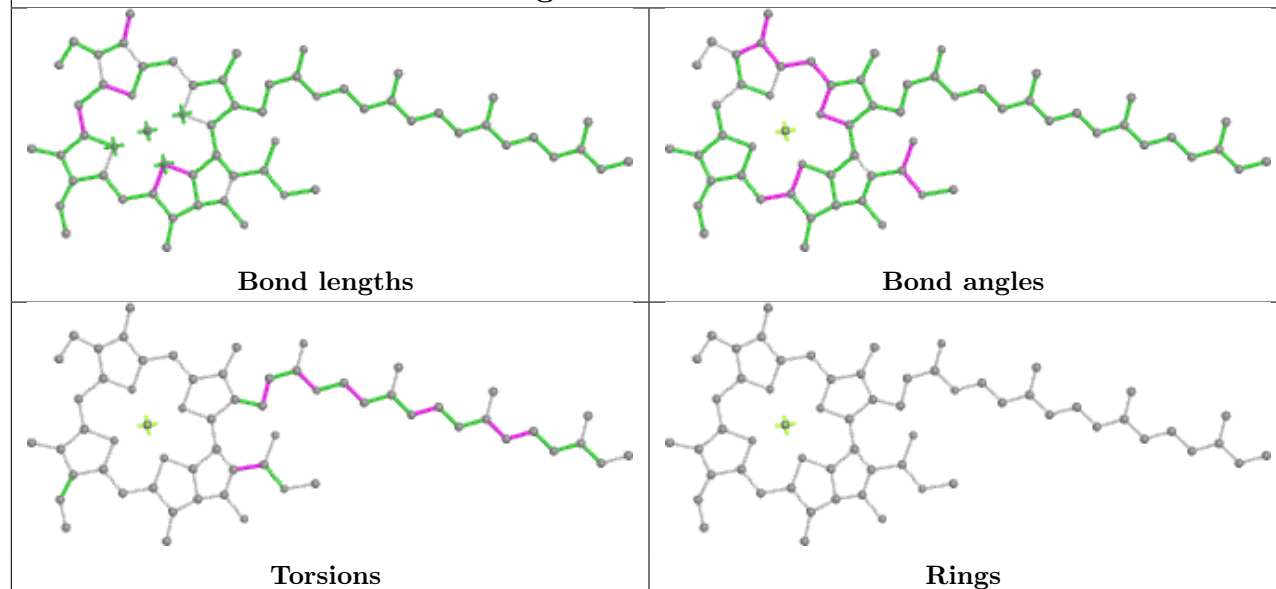
Ligand A1L1F h 203



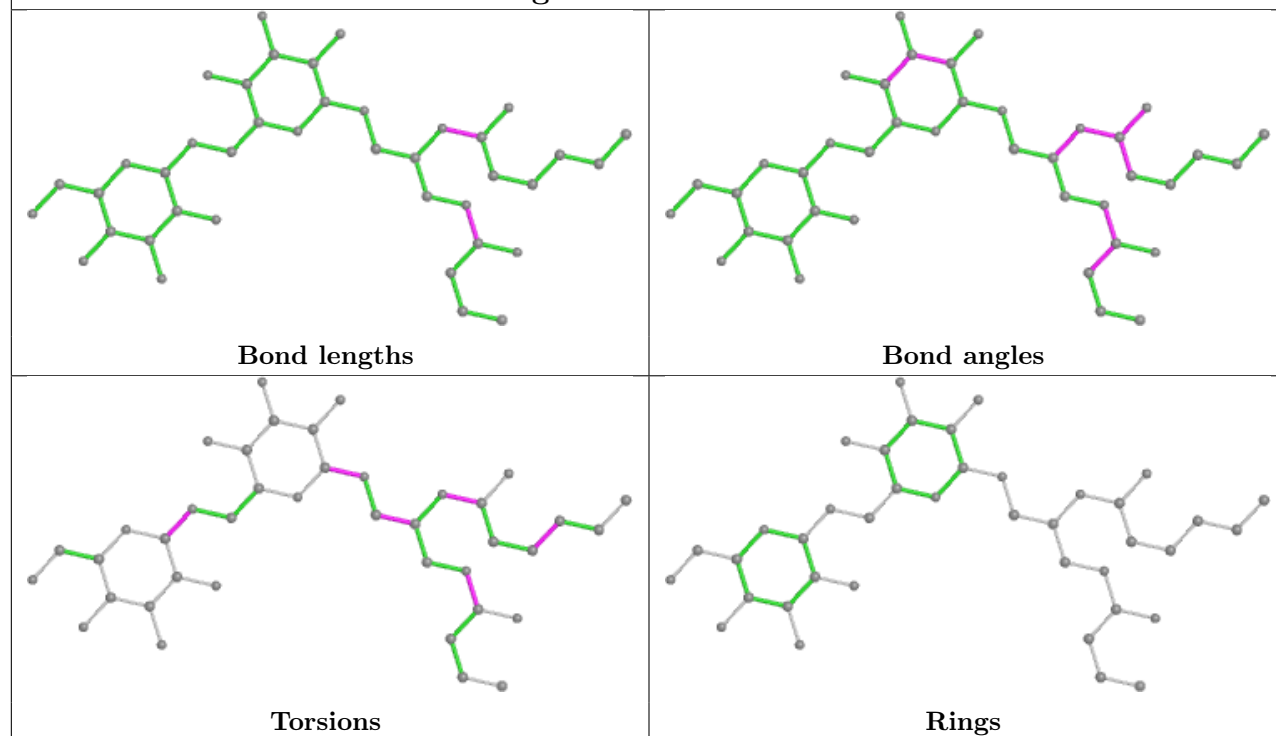
Ligand CLA 9 314



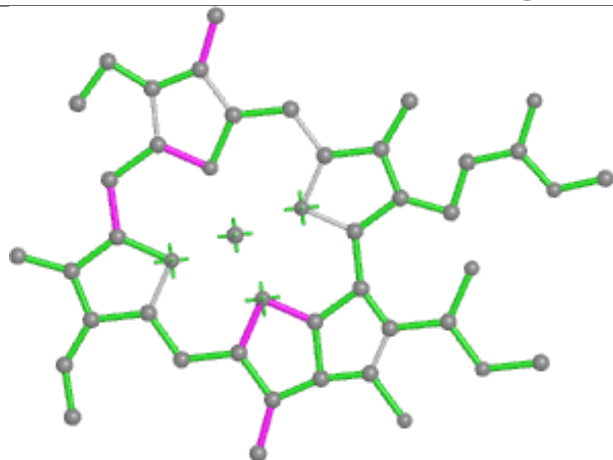
Ligand CLA 1 305



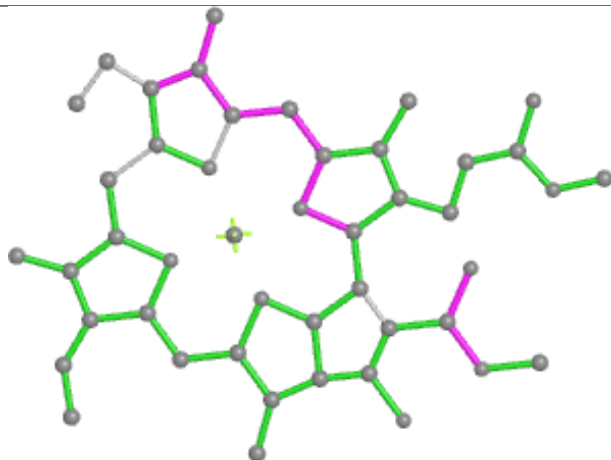
Ligand DGD 8 315



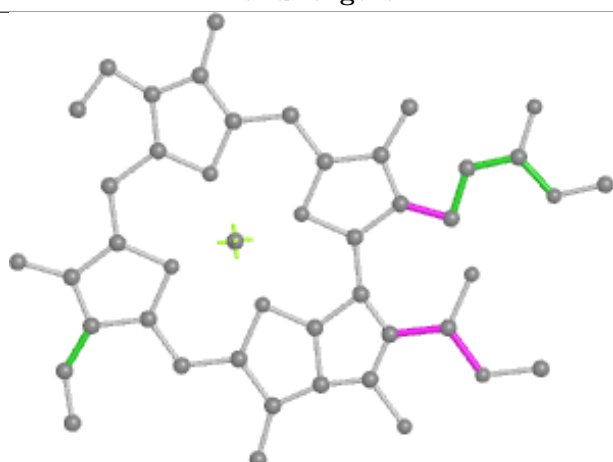
Ligand CLA 2 316



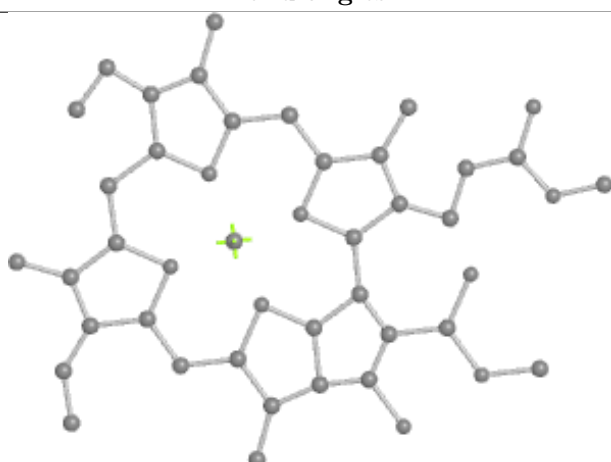
Bond lengths



Bond angles

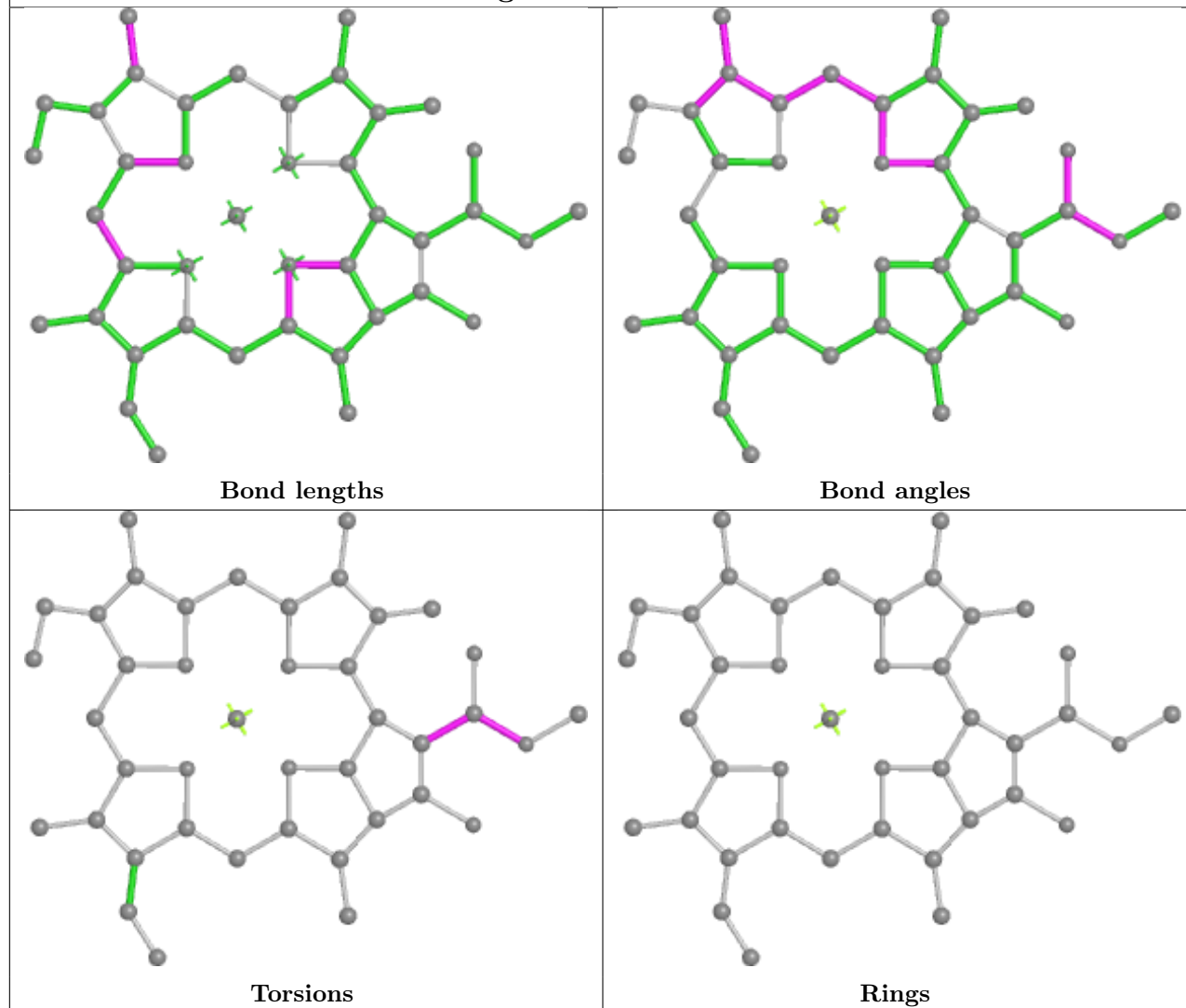


Torsions

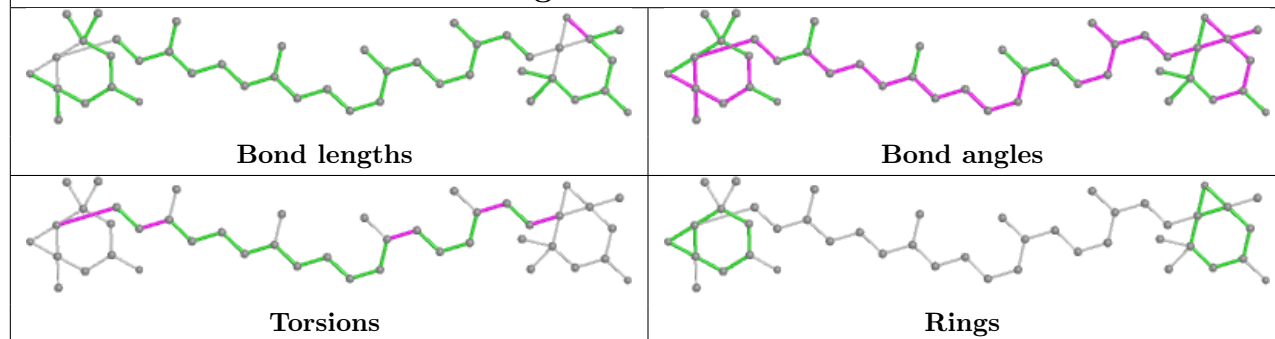


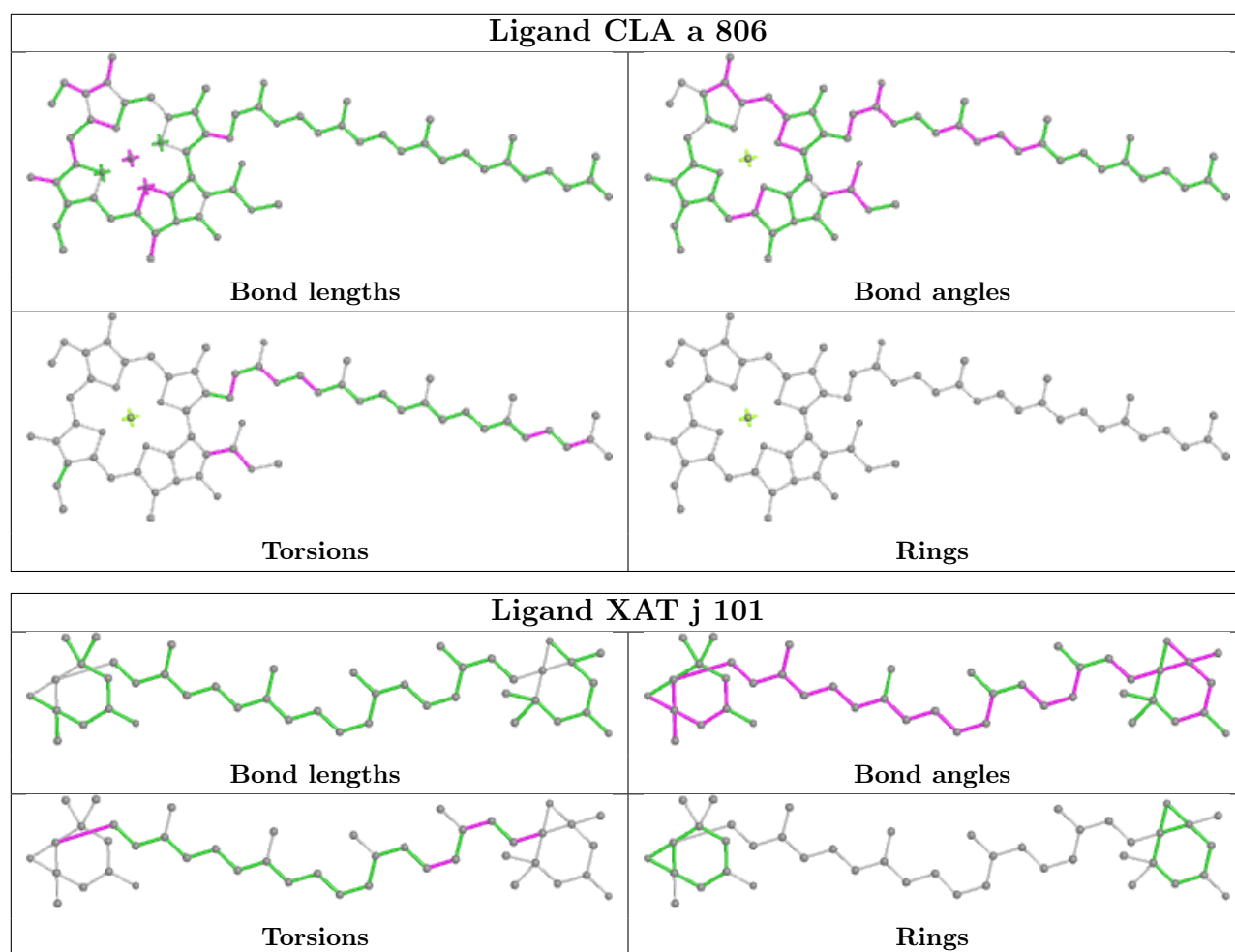
Rings

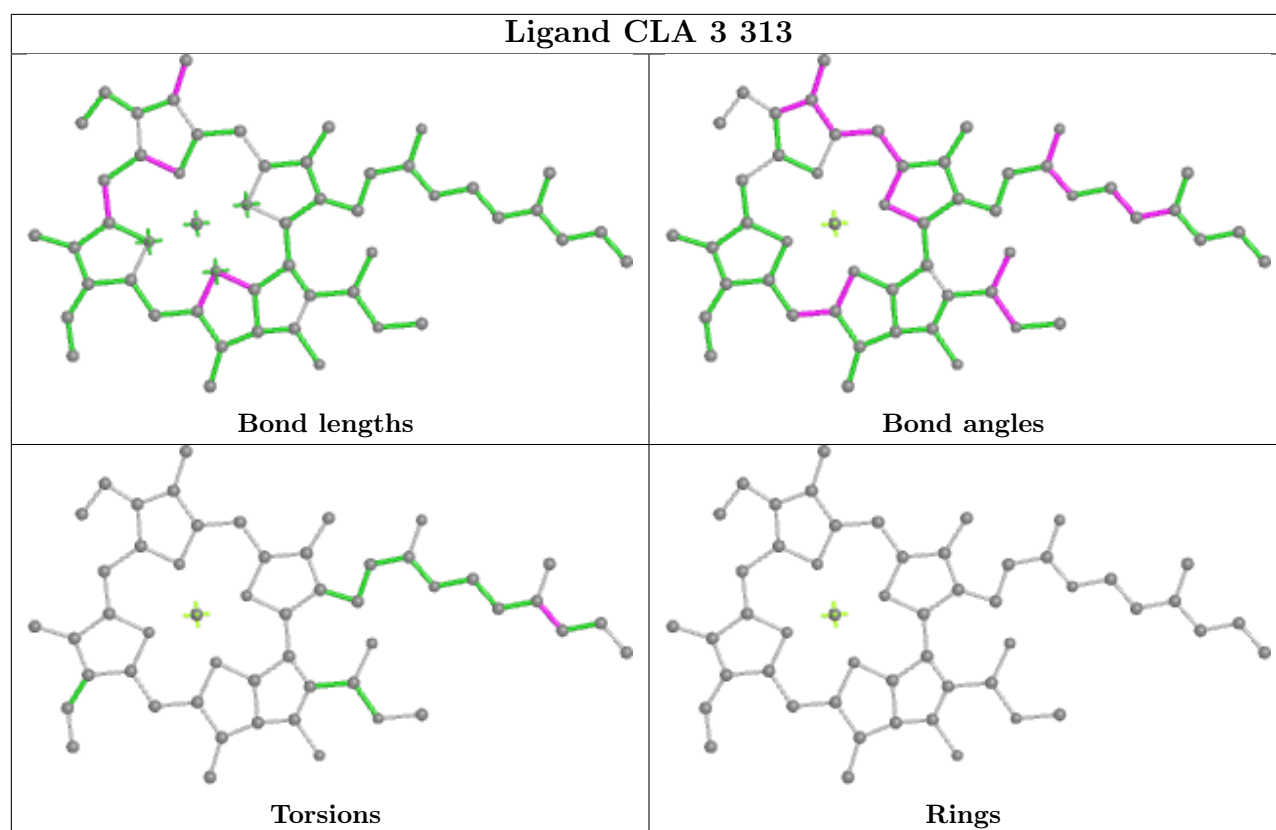
Ligand CLA 6 315



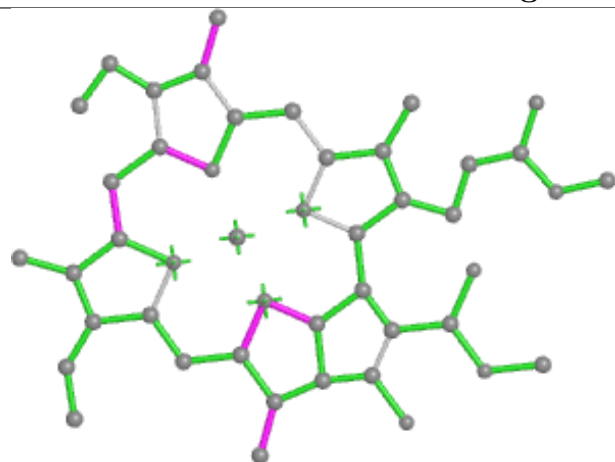
Ligand XAT 7 303



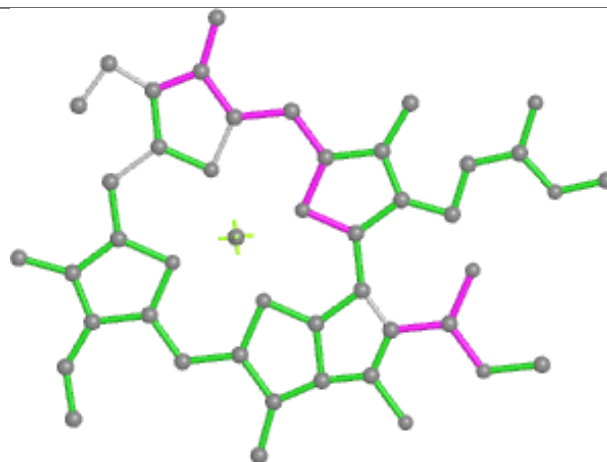




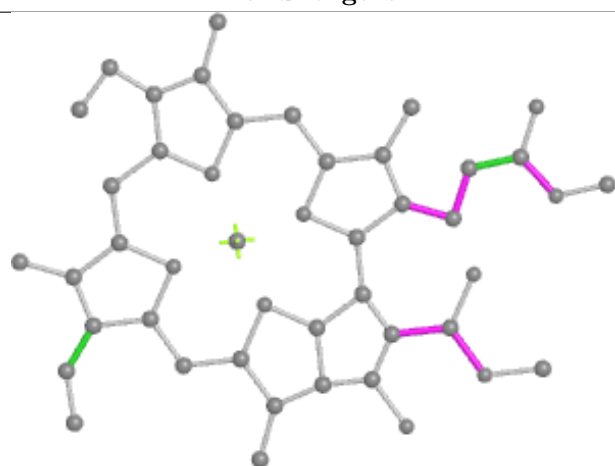
Ligand CLA 4 311



Bond lengths



Bond angles

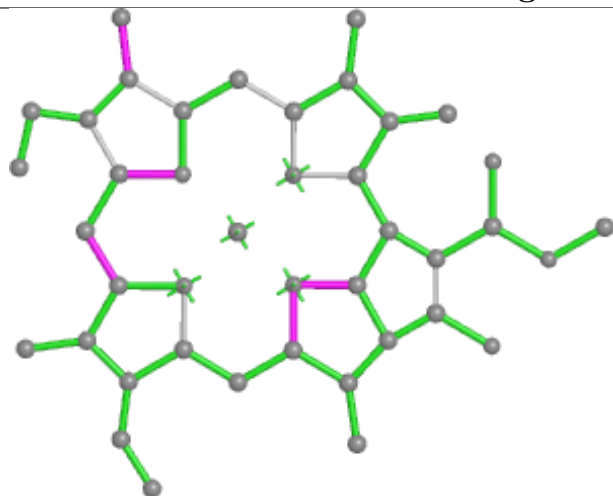


Torsions

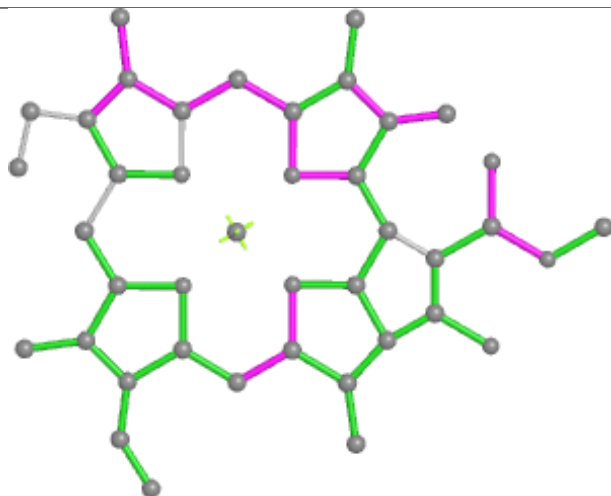


Rings

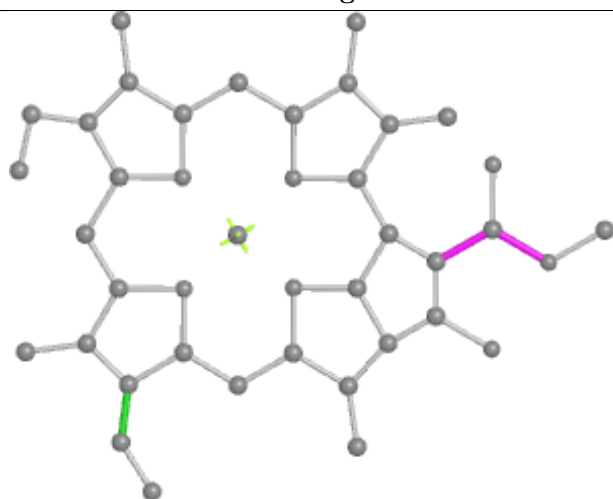
Ligand CLA 2 313



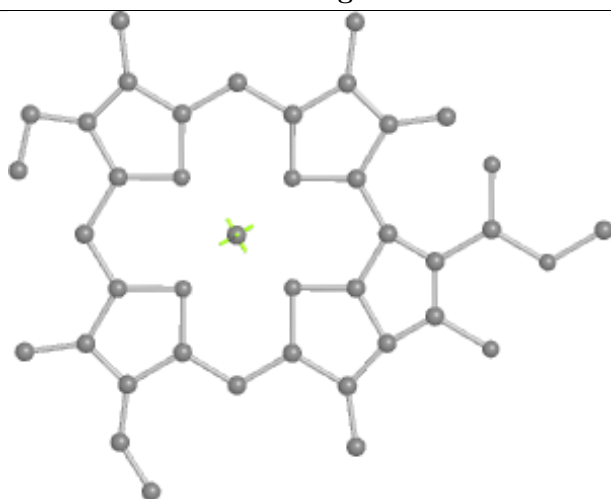
Bond lengths



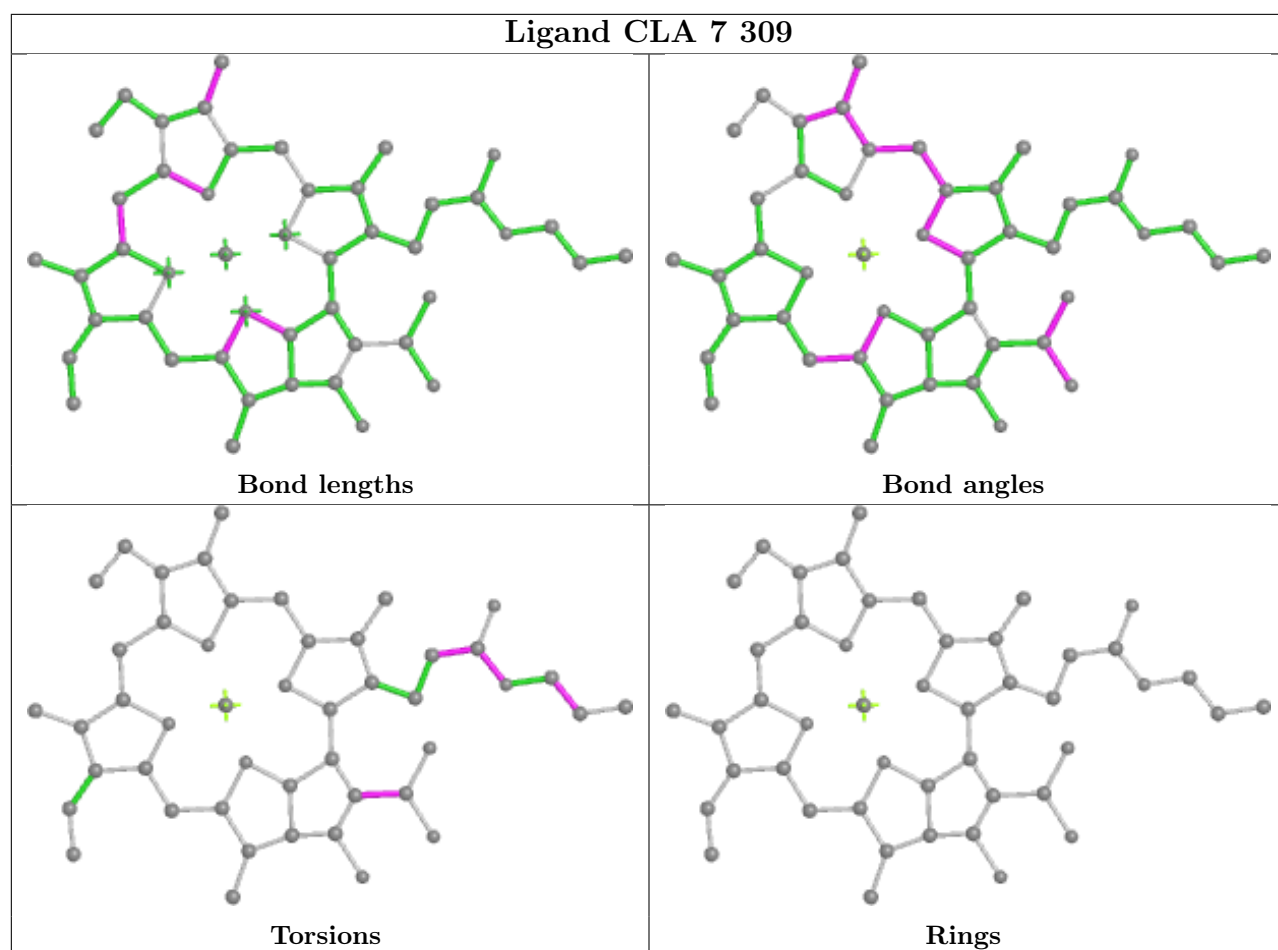
Bond angles



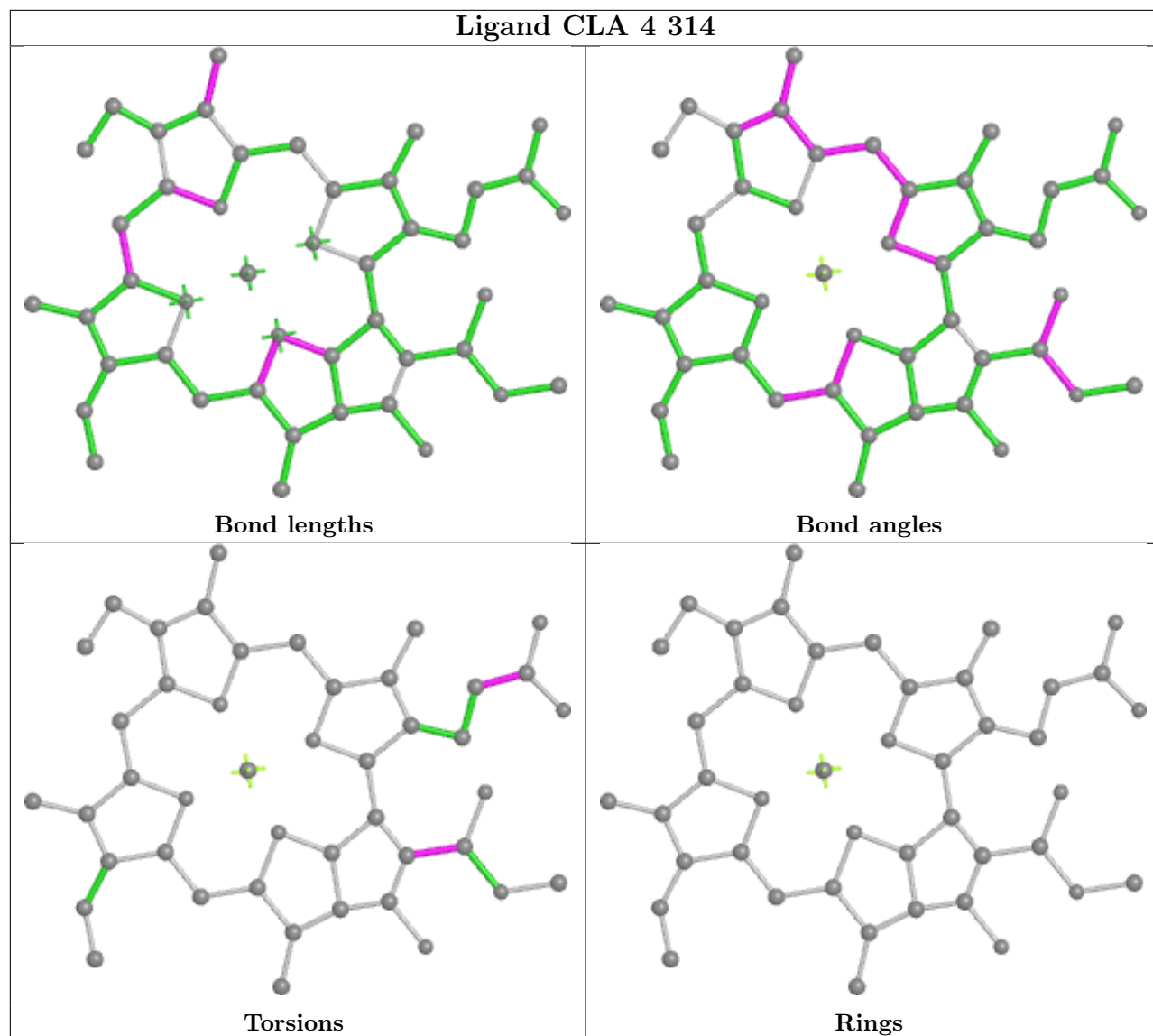
Torsions

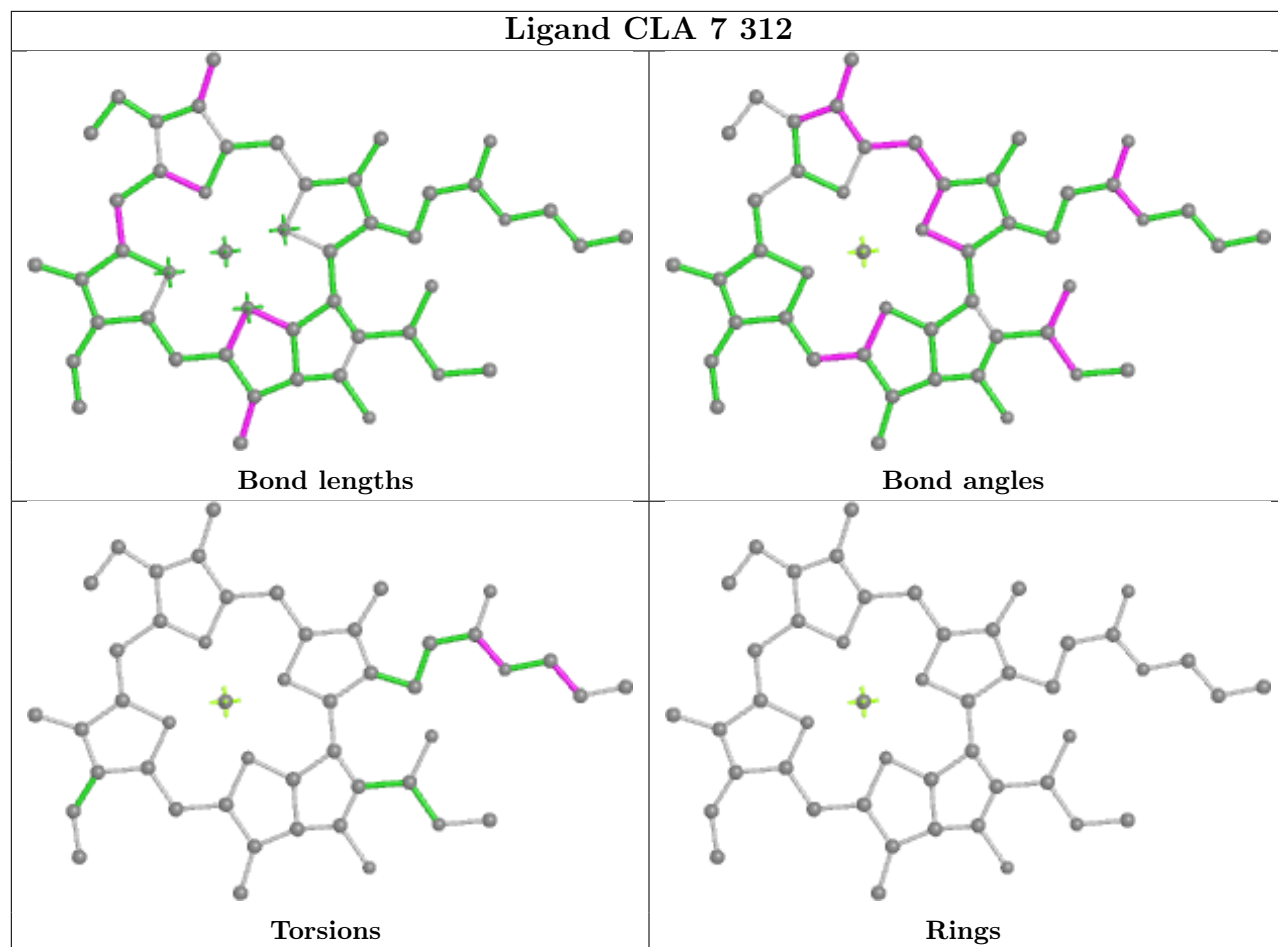


Rings

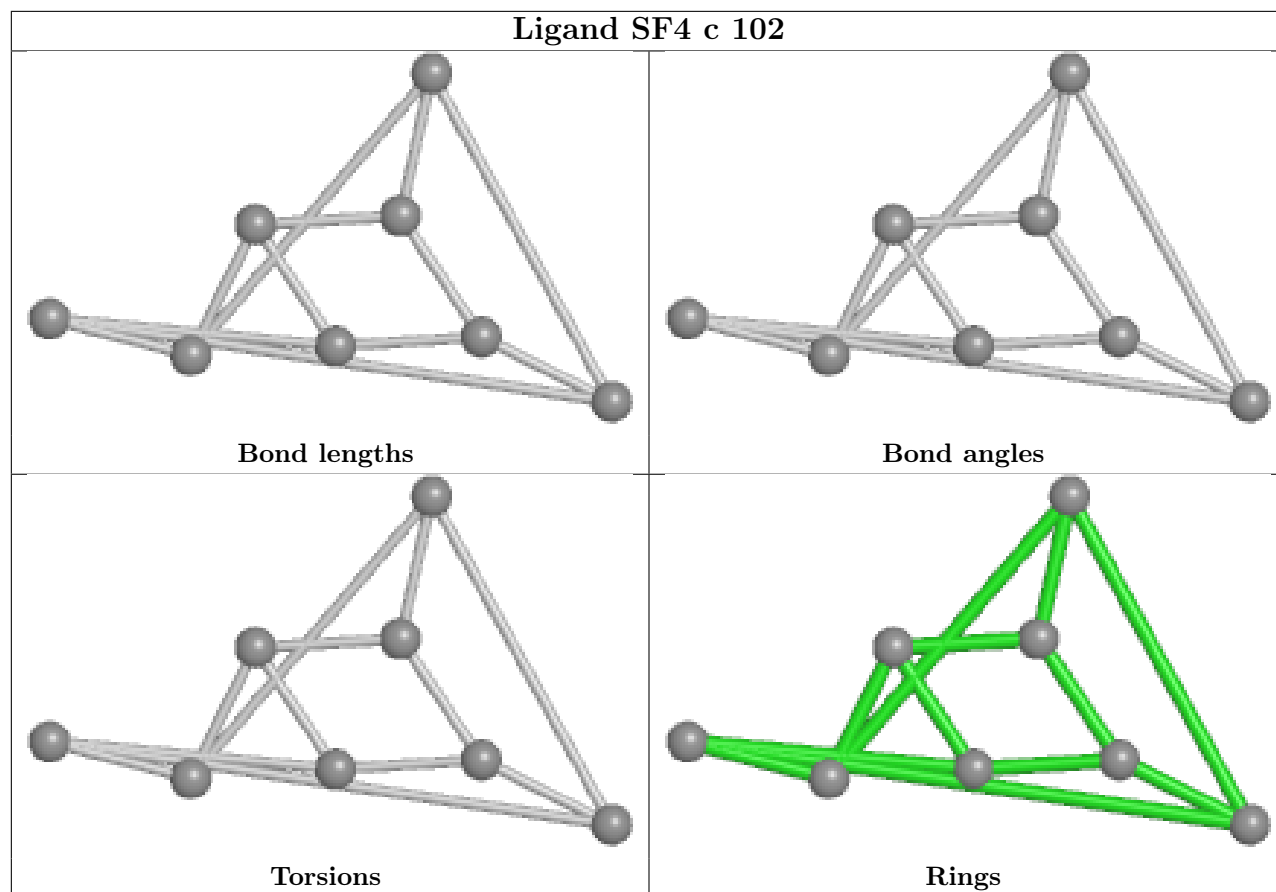


Ligand CLA 4 314

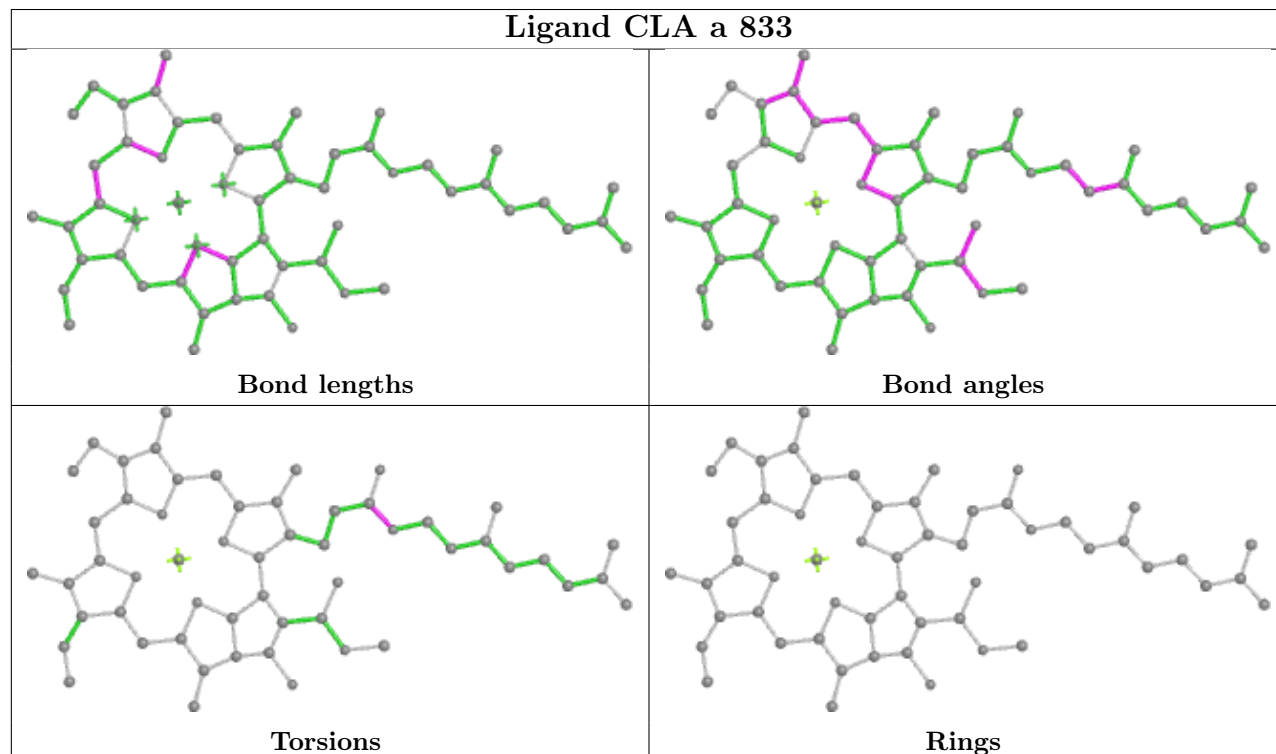




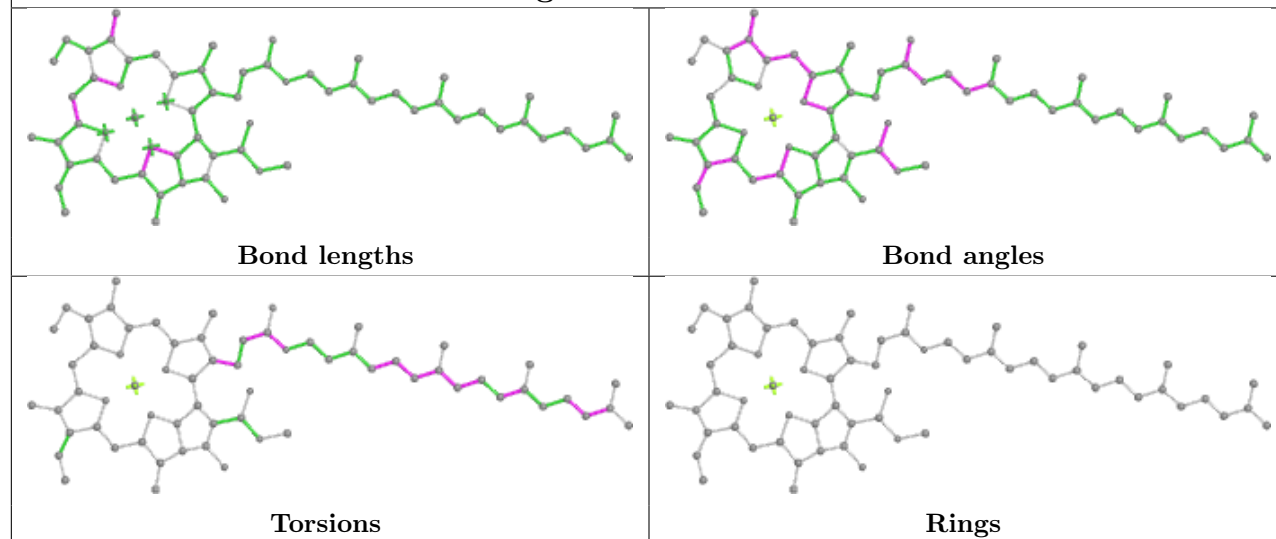
Ligand SF4 c 102



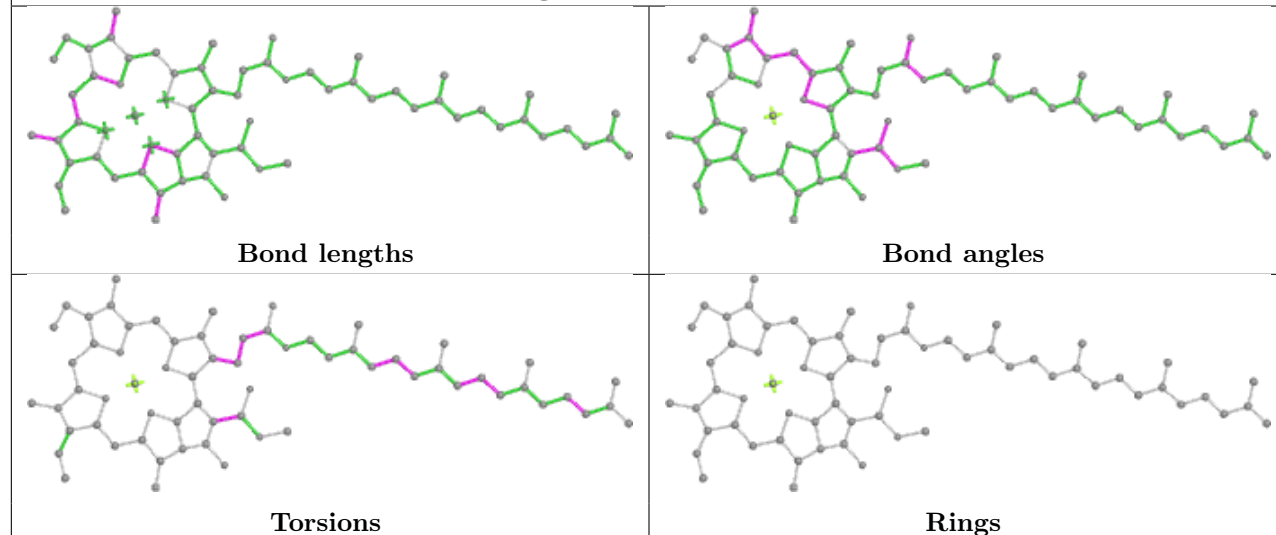
Ligand CLA a 833



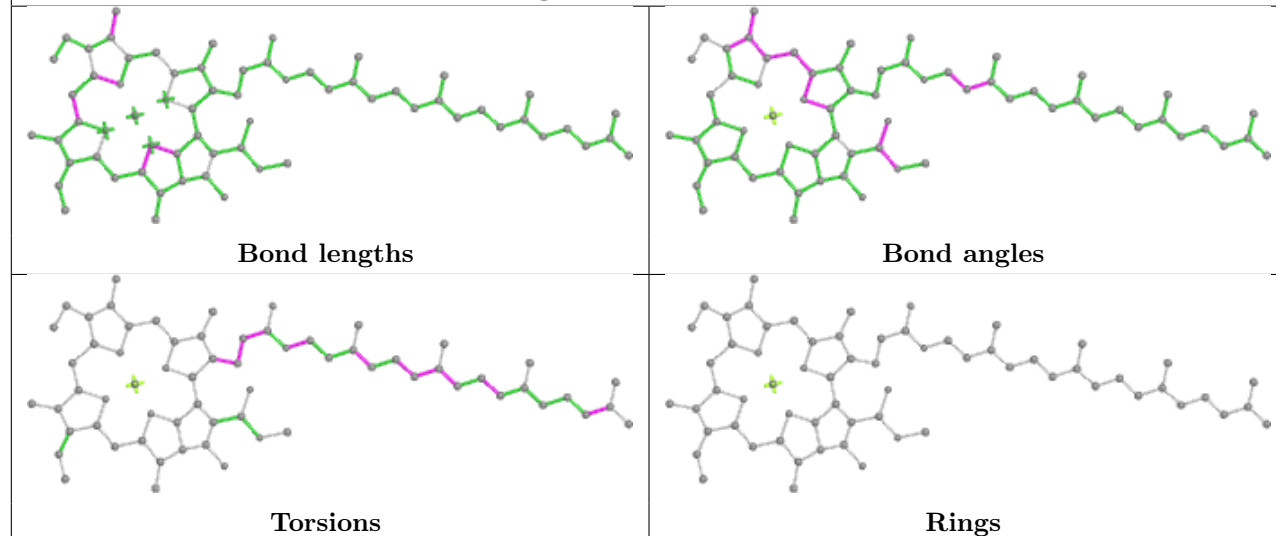
Ligand CLA 1 306

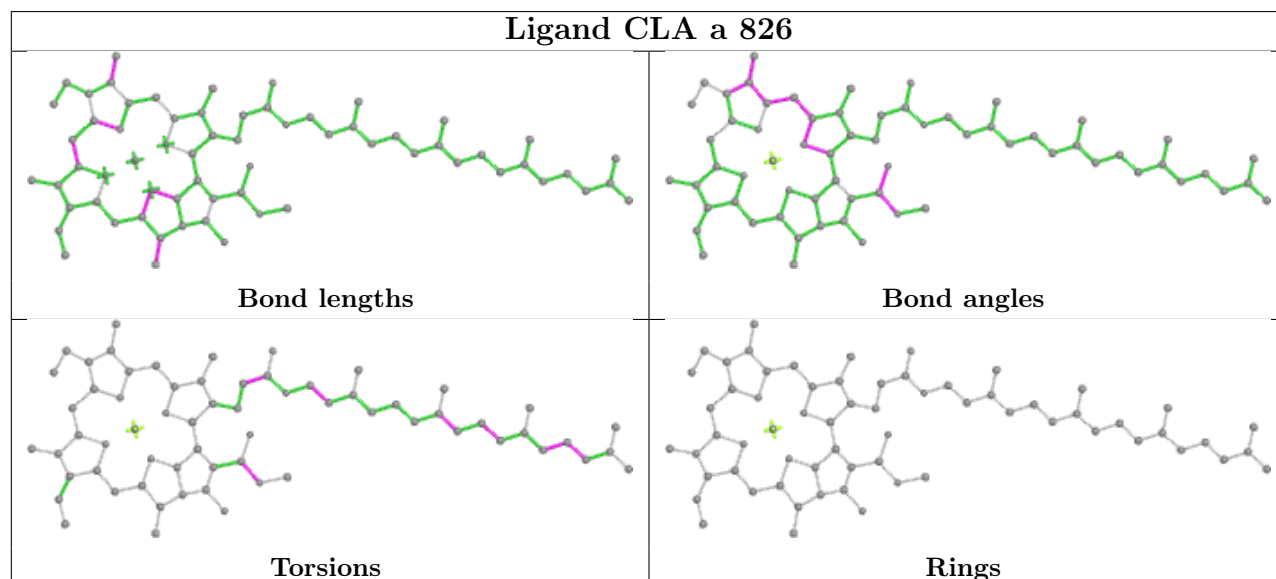
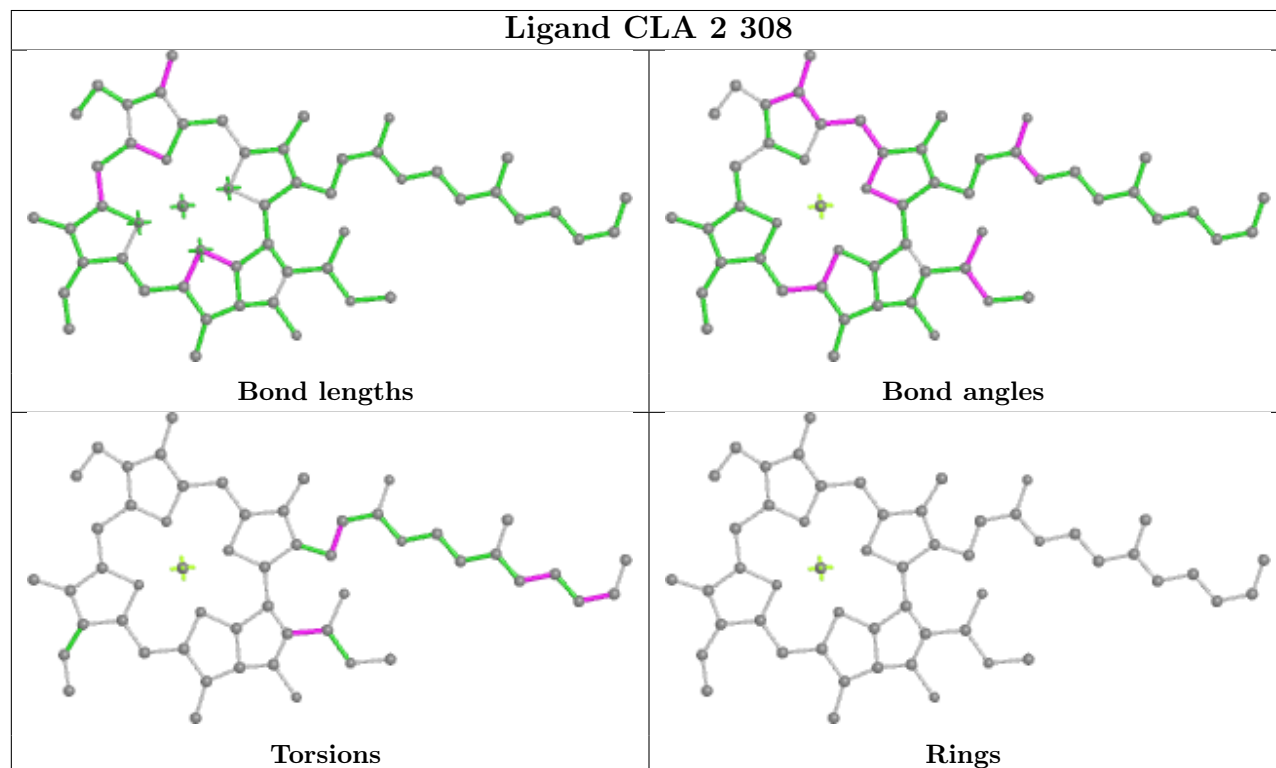
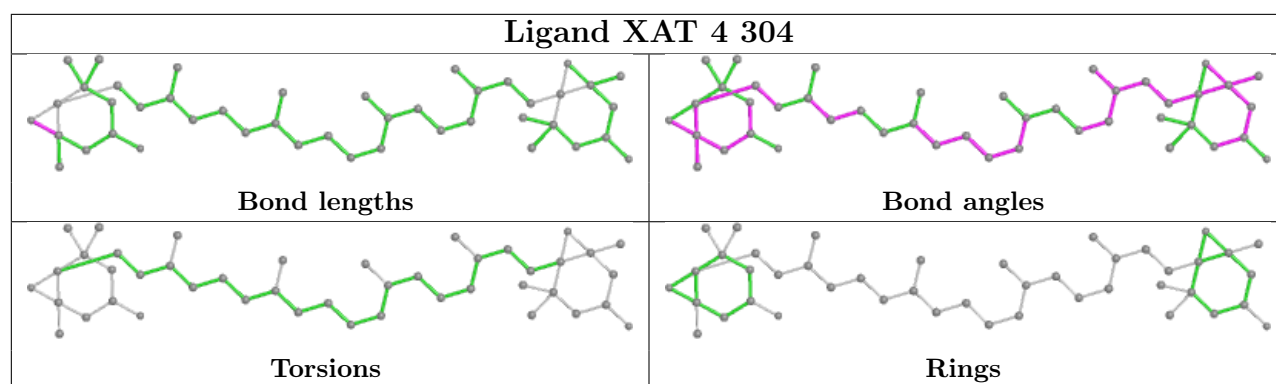


Ligand CLA b 809

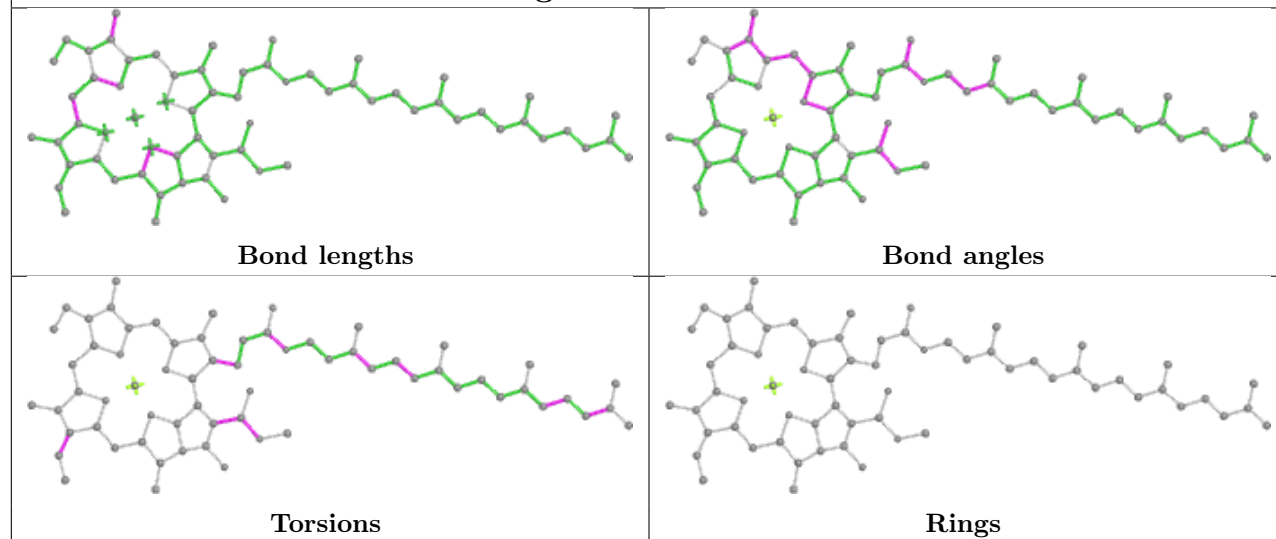


Ligand CLA b 810

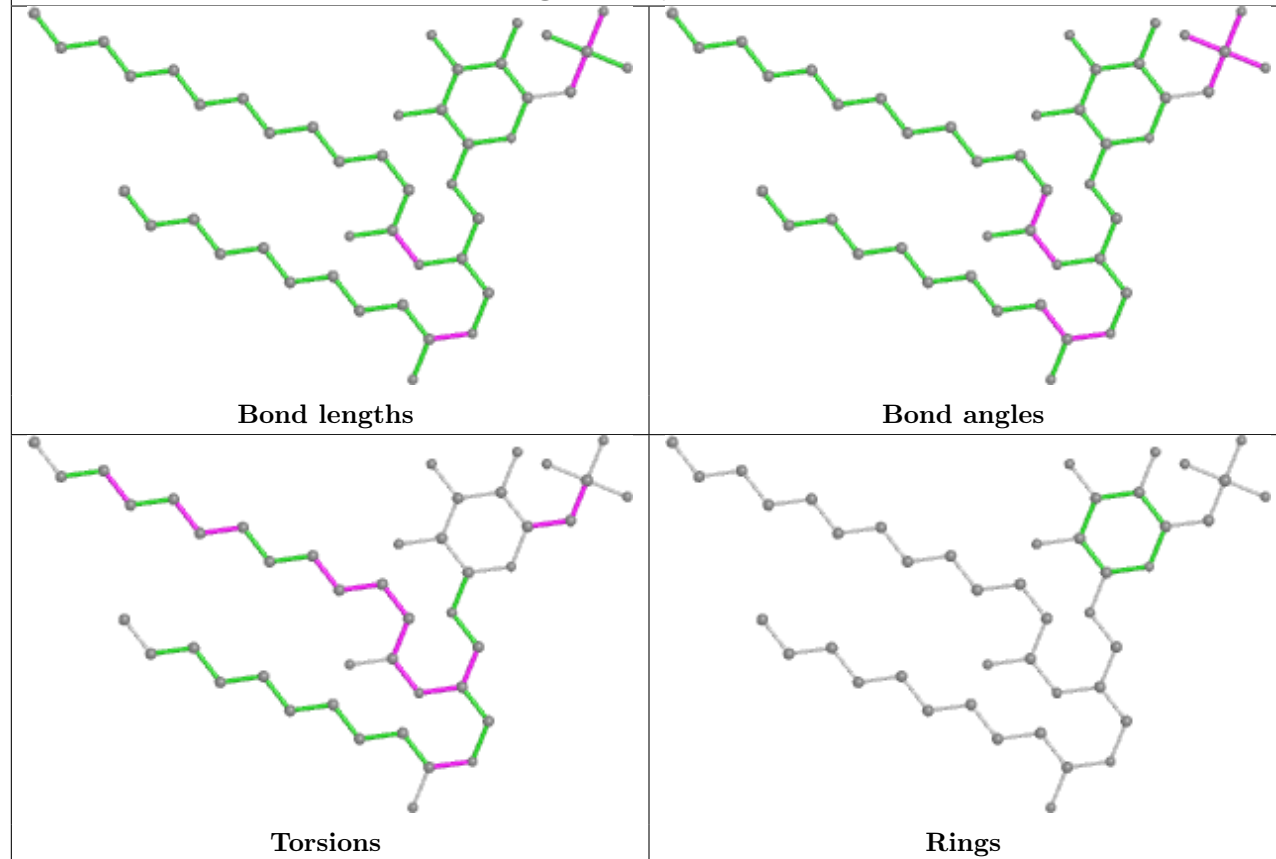




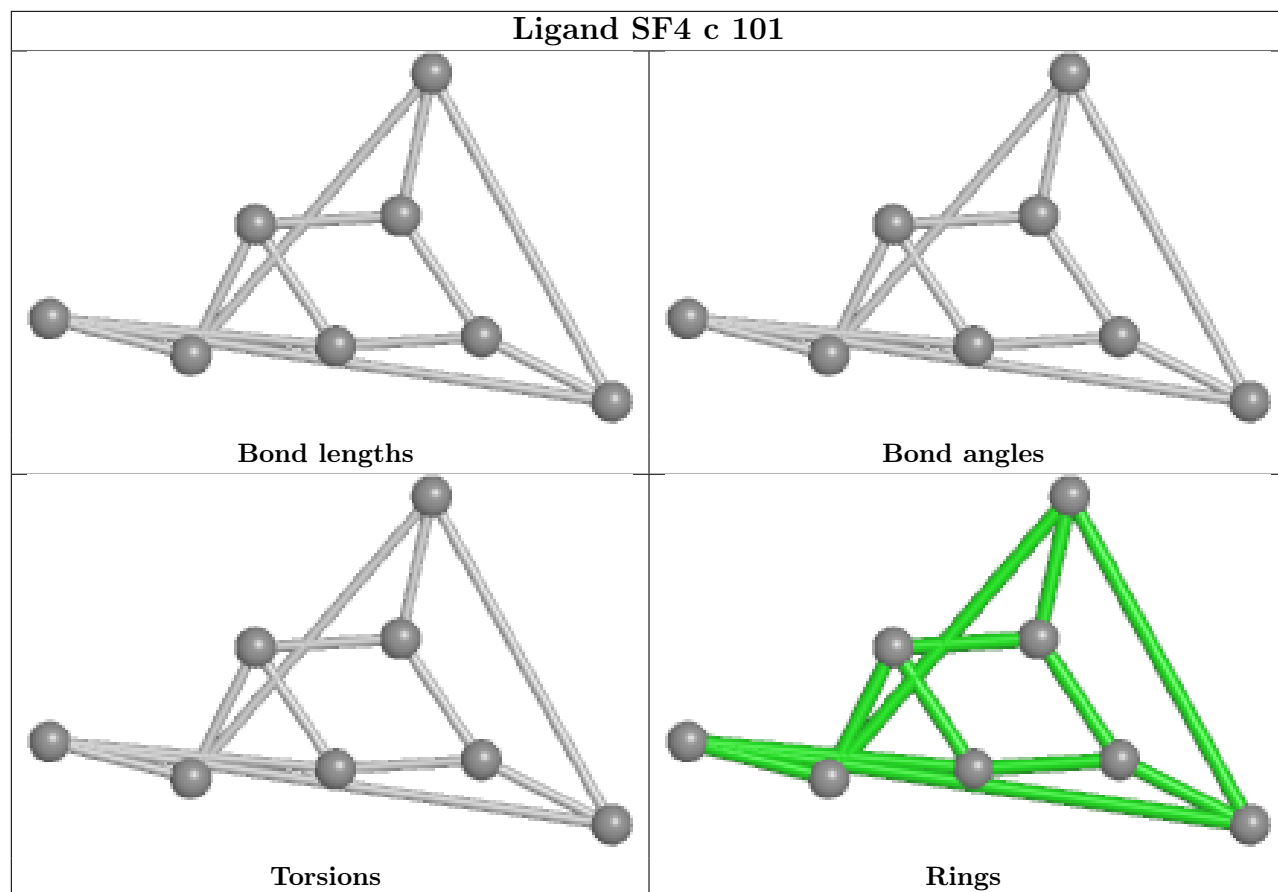
Ligand CLA b 839



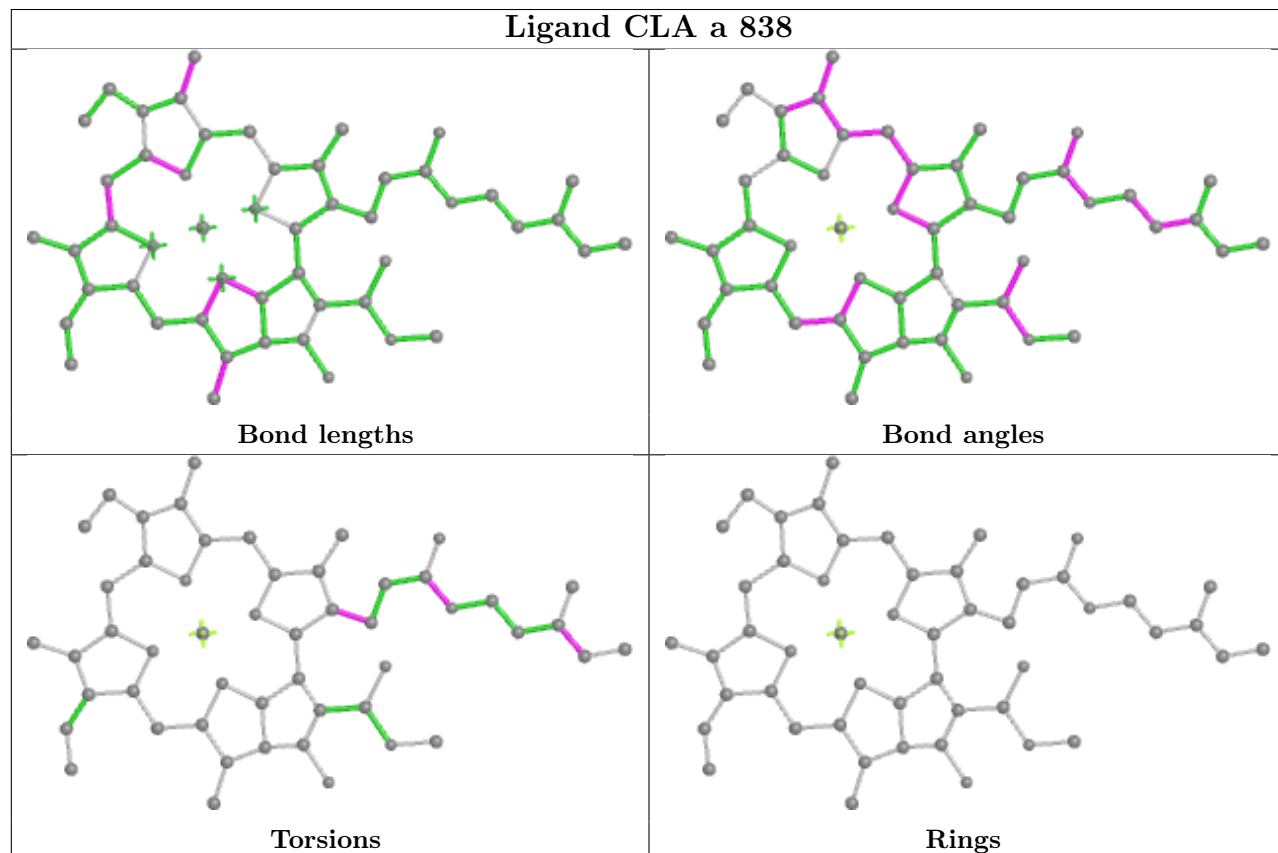
Ligand SQD 1 315

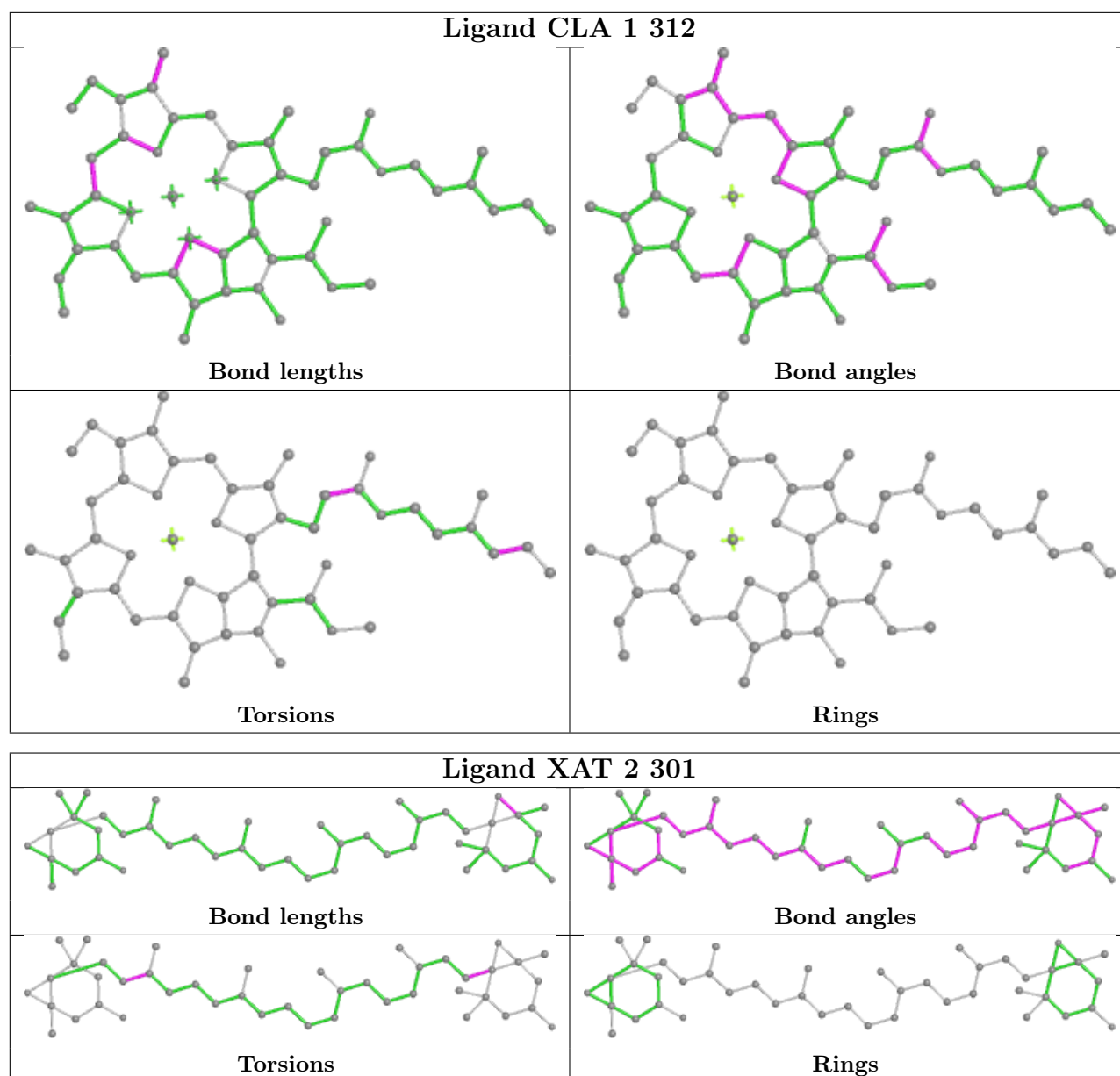


Ligand SF4 c 101

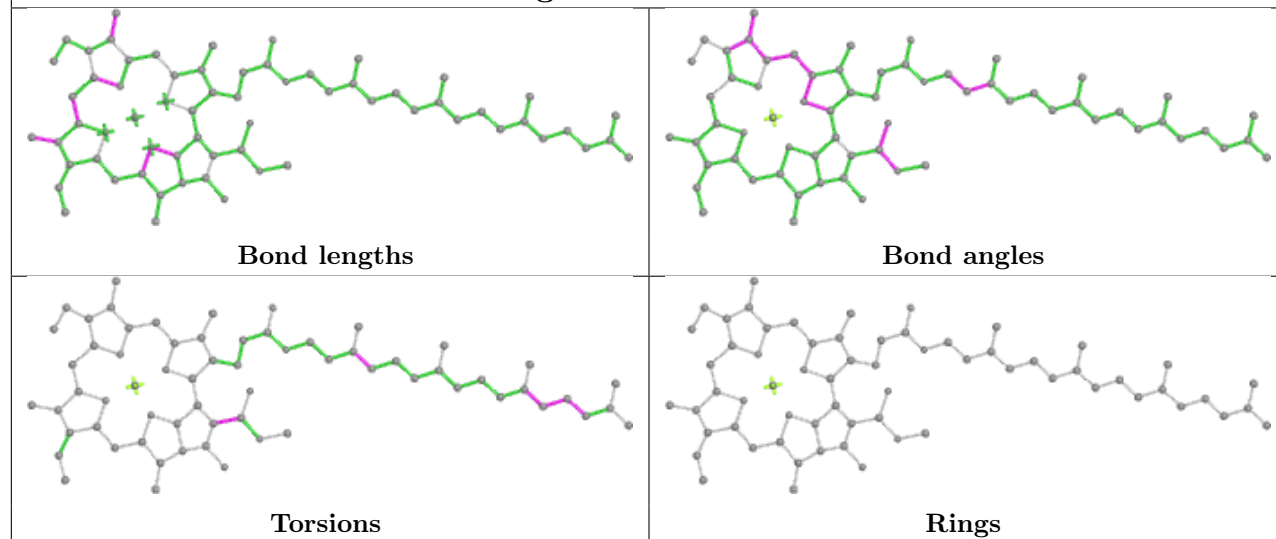


Ligand CLA a 838

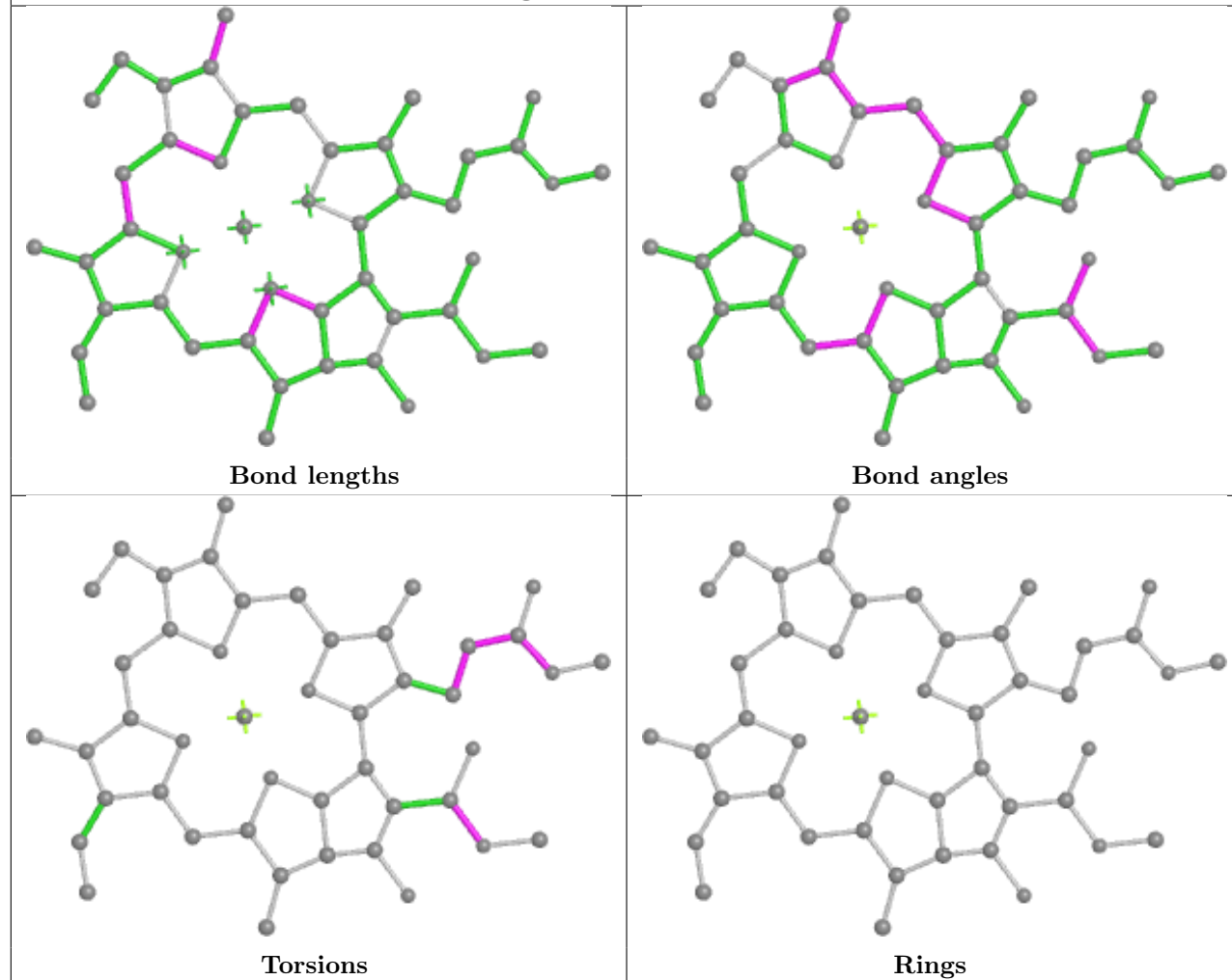




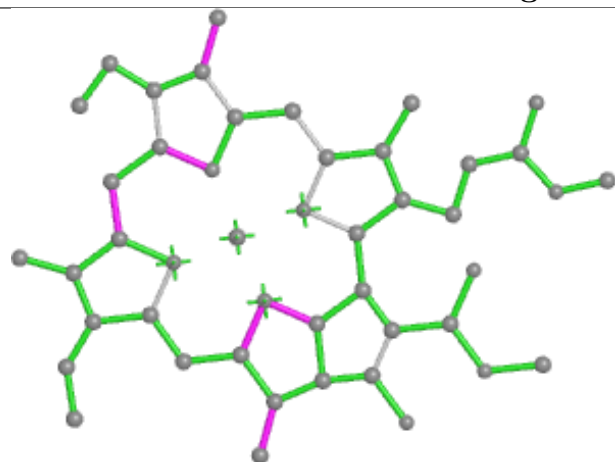
Ligand CLA a 828



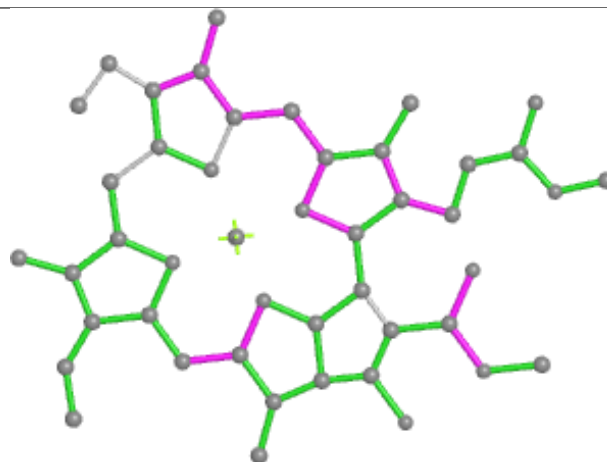
Ligand CLA 5 310



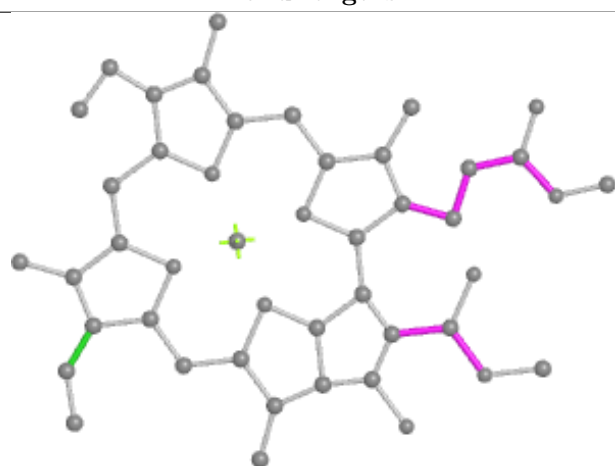
Ligand CLA 9 312



Bond lengths



Bond angles

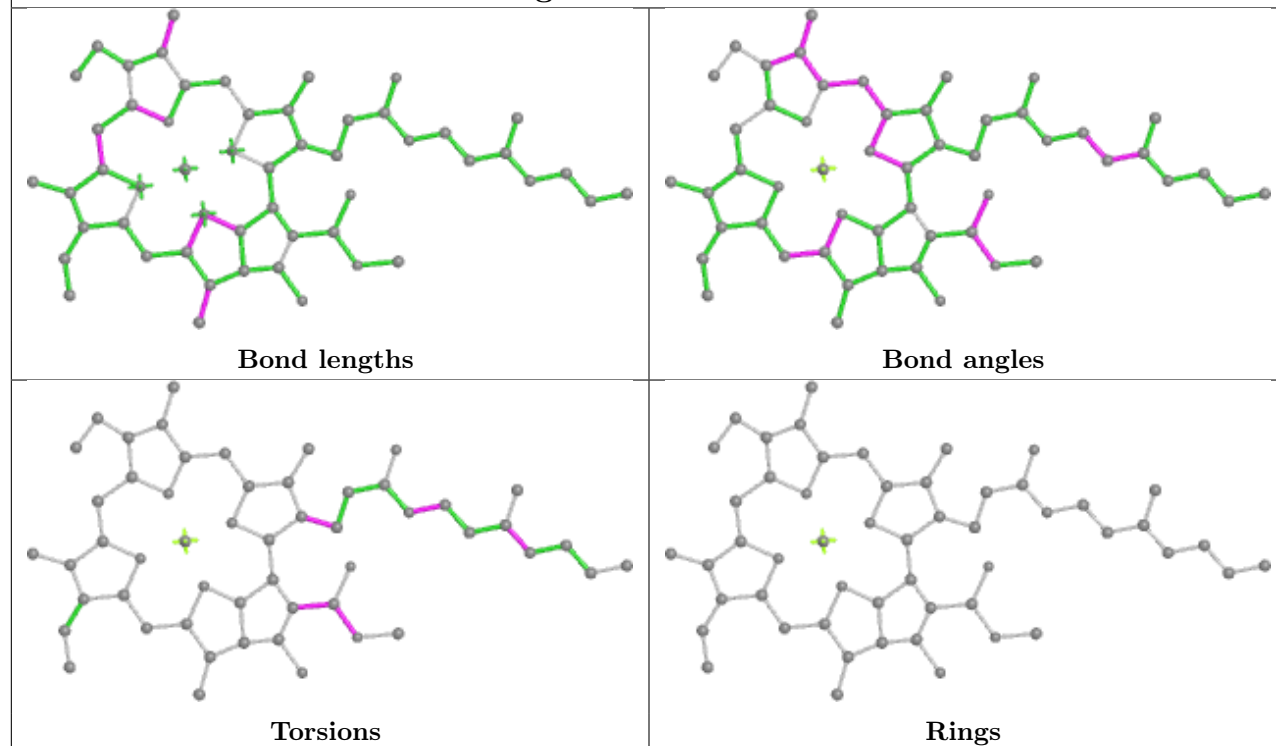


Torsions

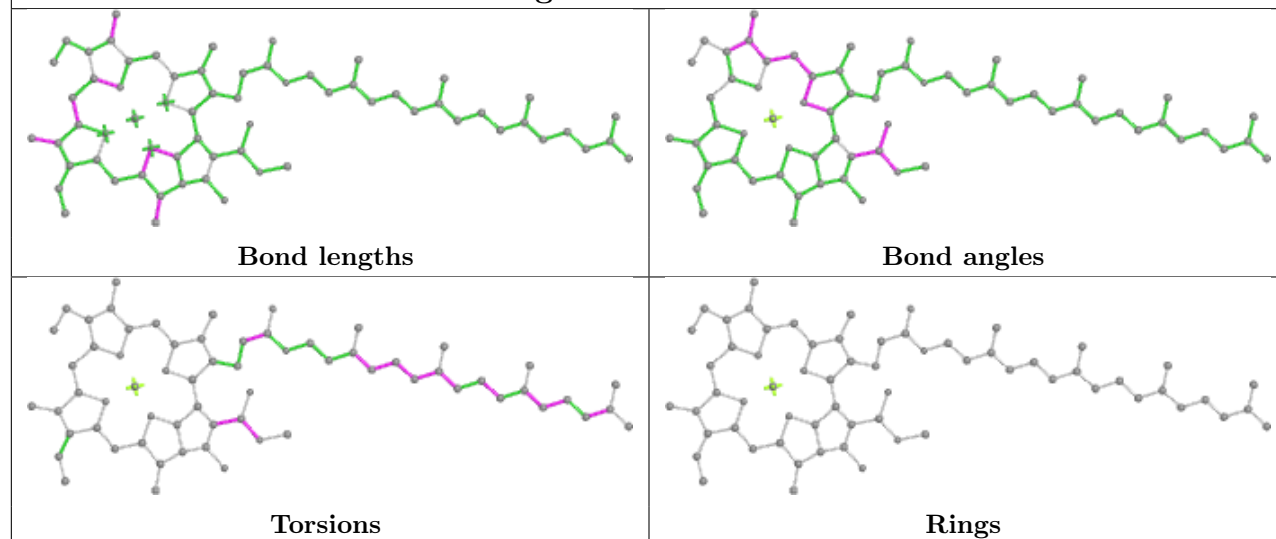


Rings

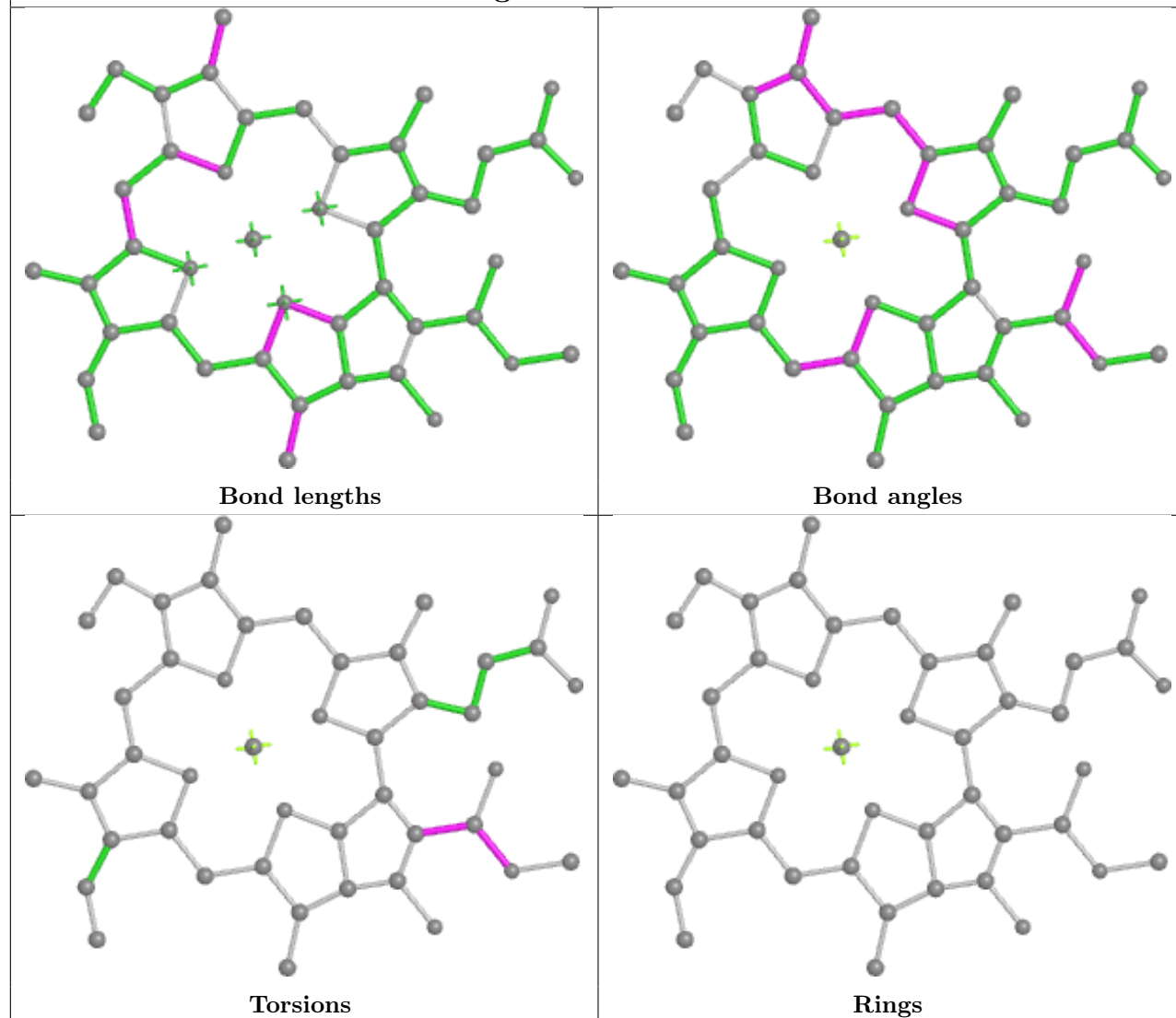
Ligand CLA b 834



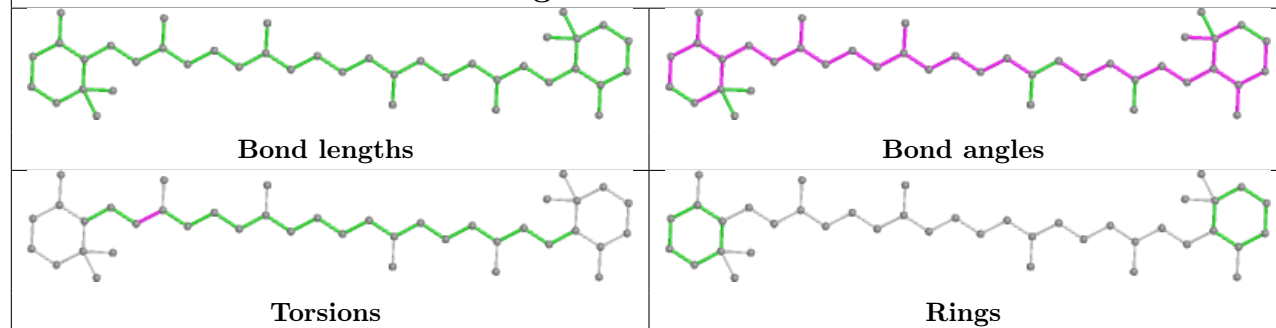
Ligand CLA b 803

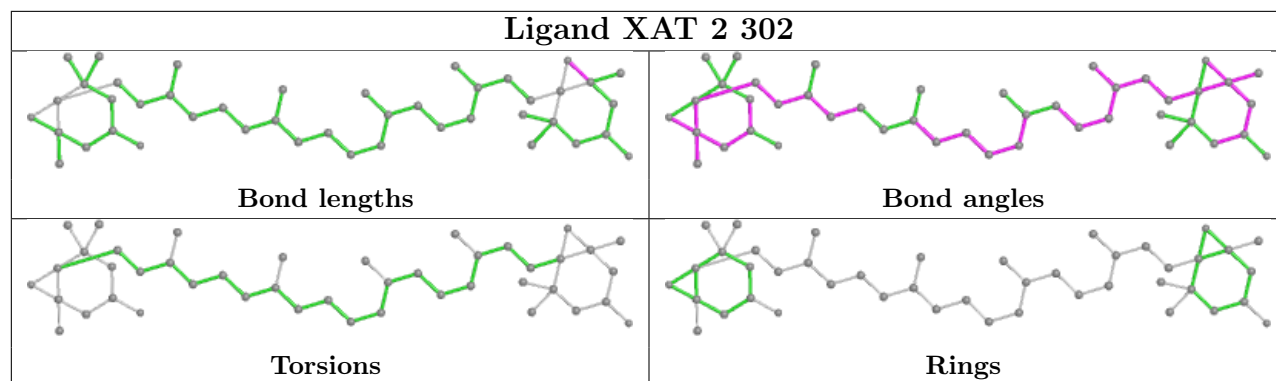
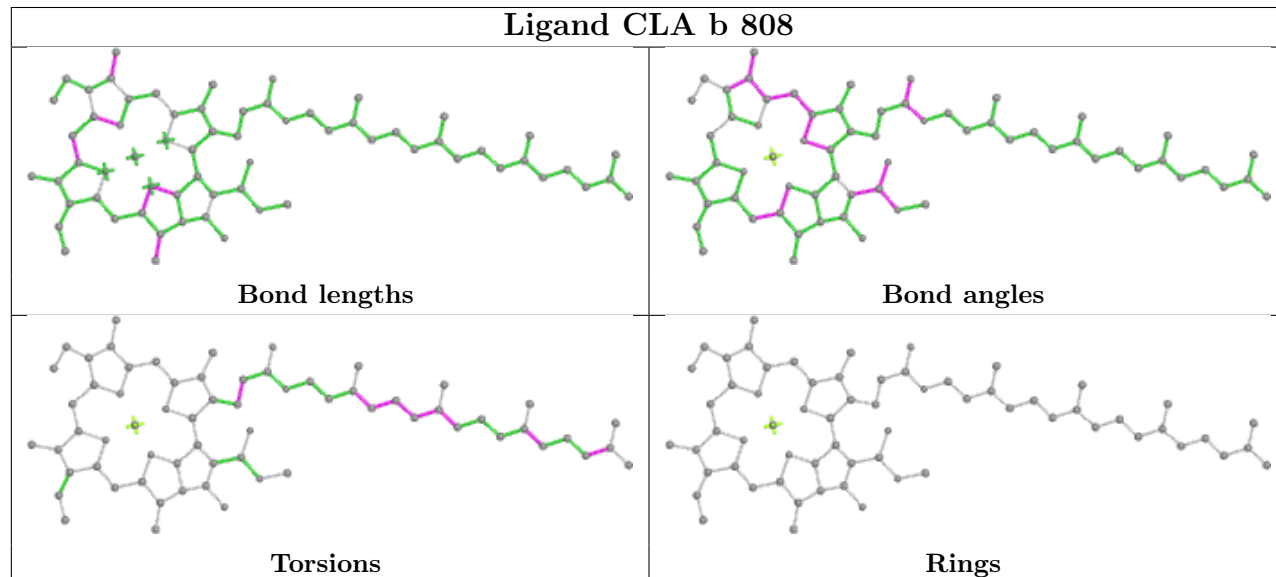
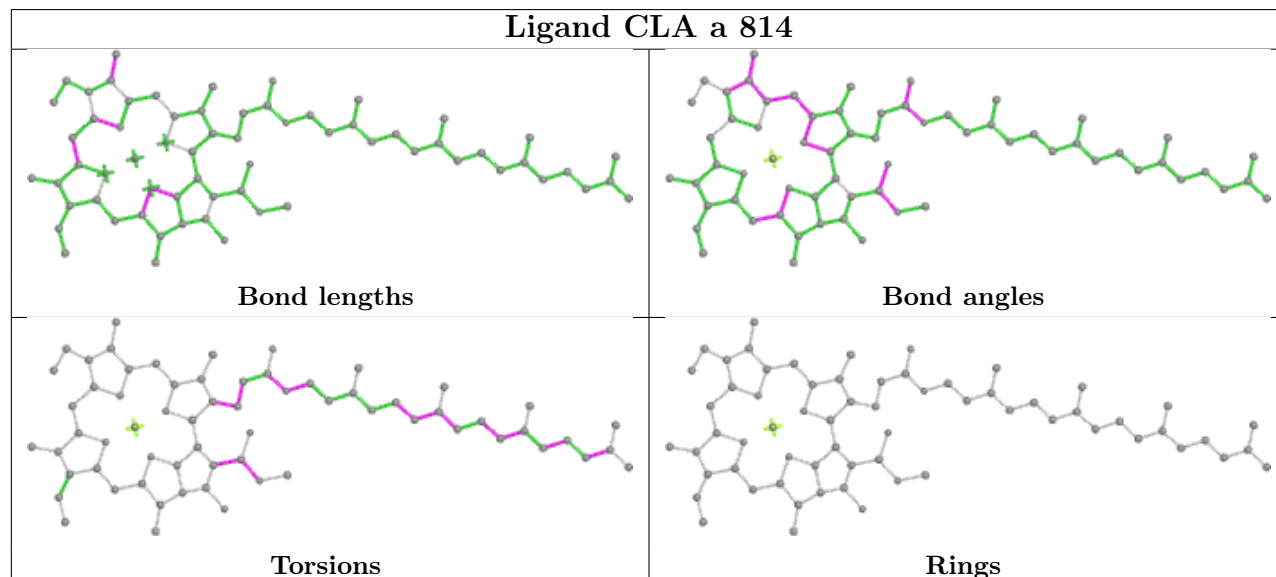


Ligand CLA a 837

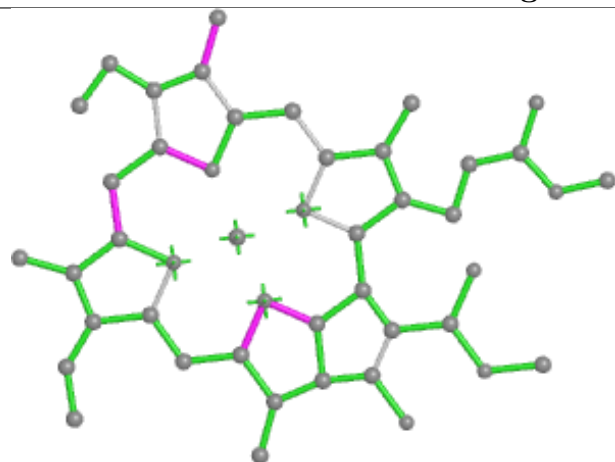


Ligand BCR b 845

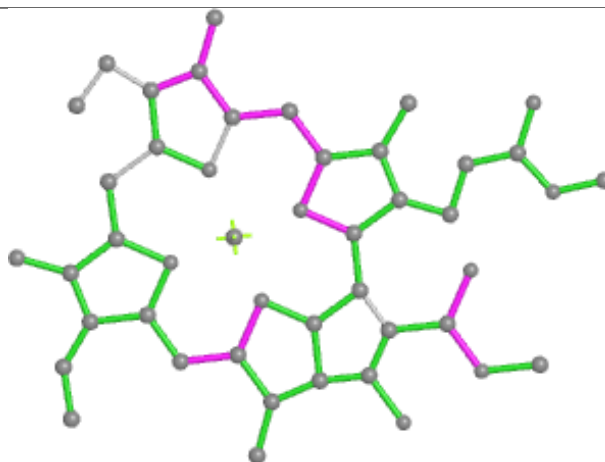


Ligand XAT 2 302**Ligand CLA b 808****Ligand CLA a 814**

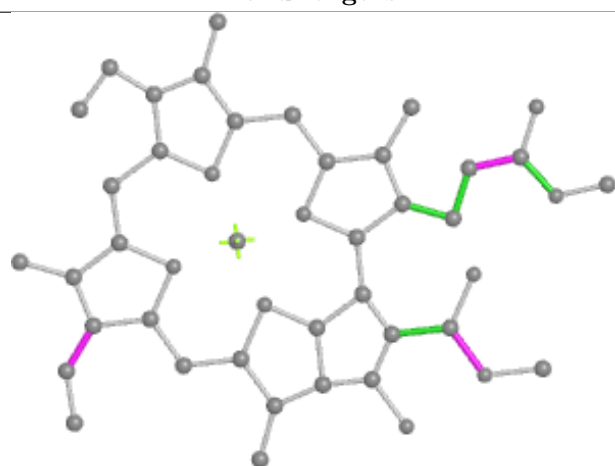
Ligand CLA 5 315



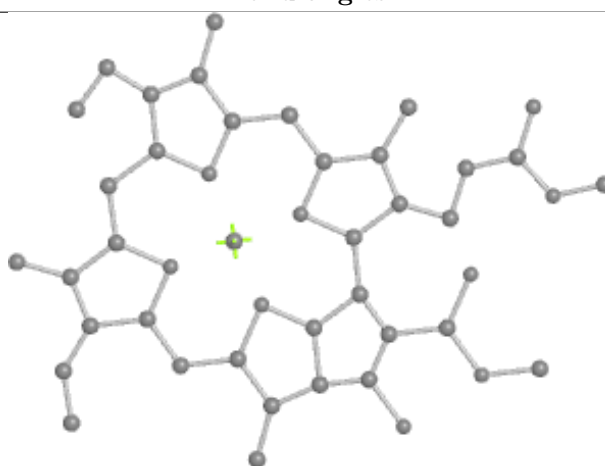
Bond lengths



Bond angles

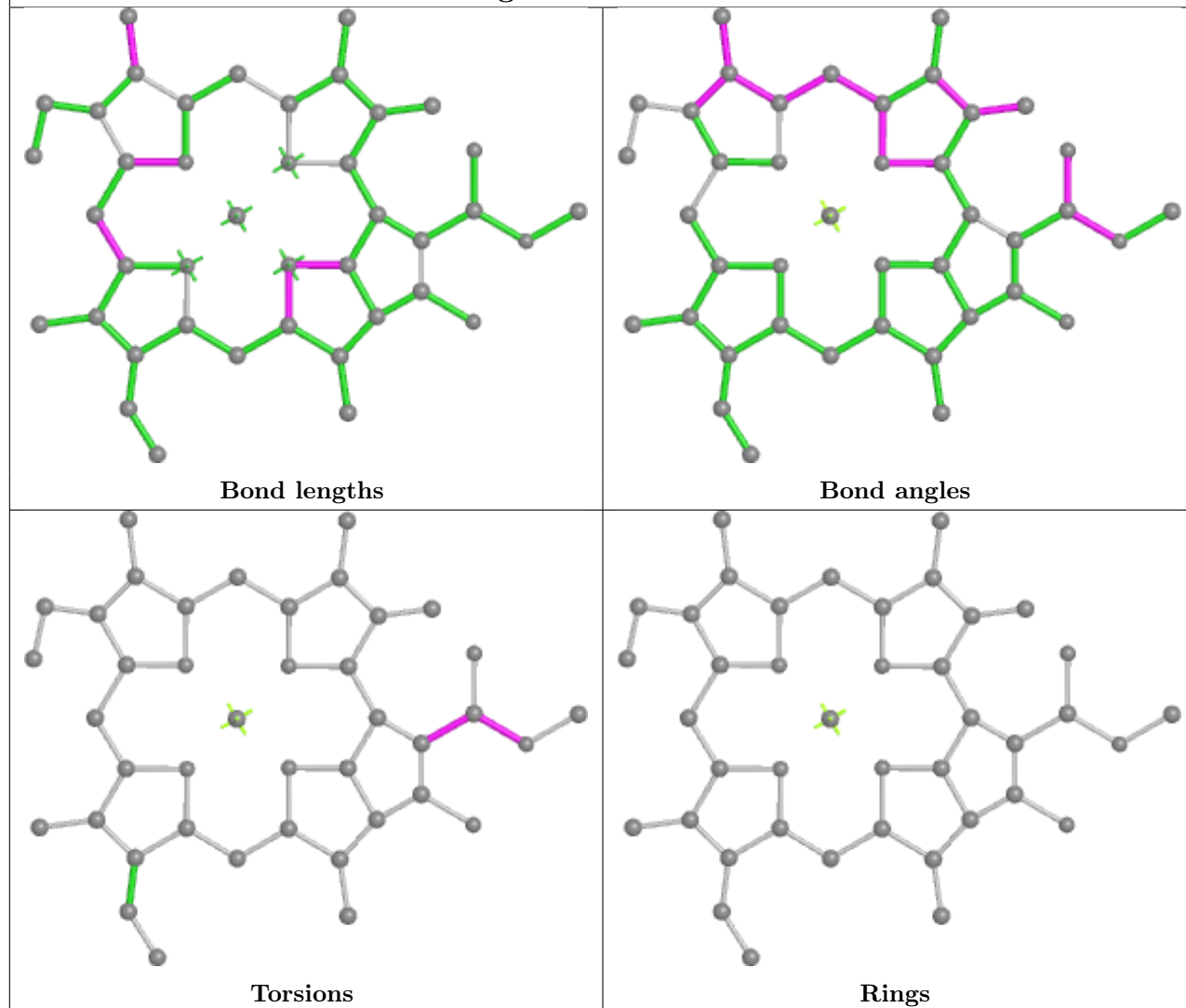


Torsions

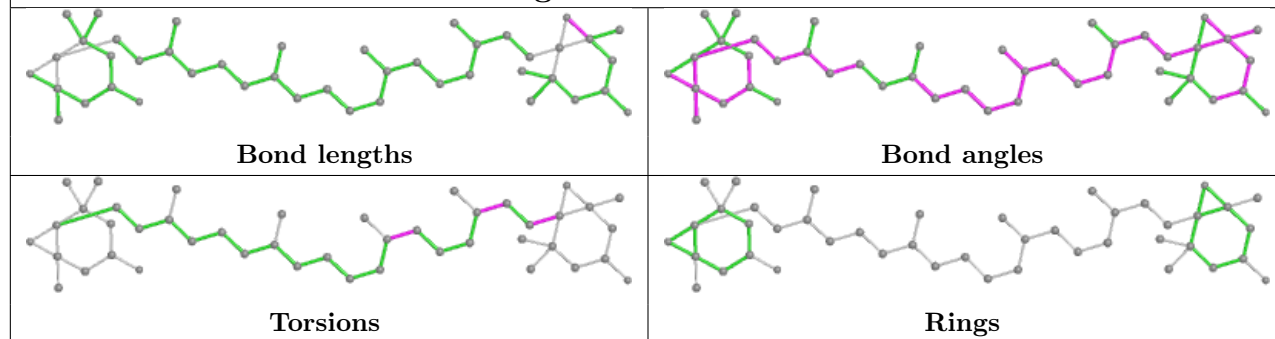


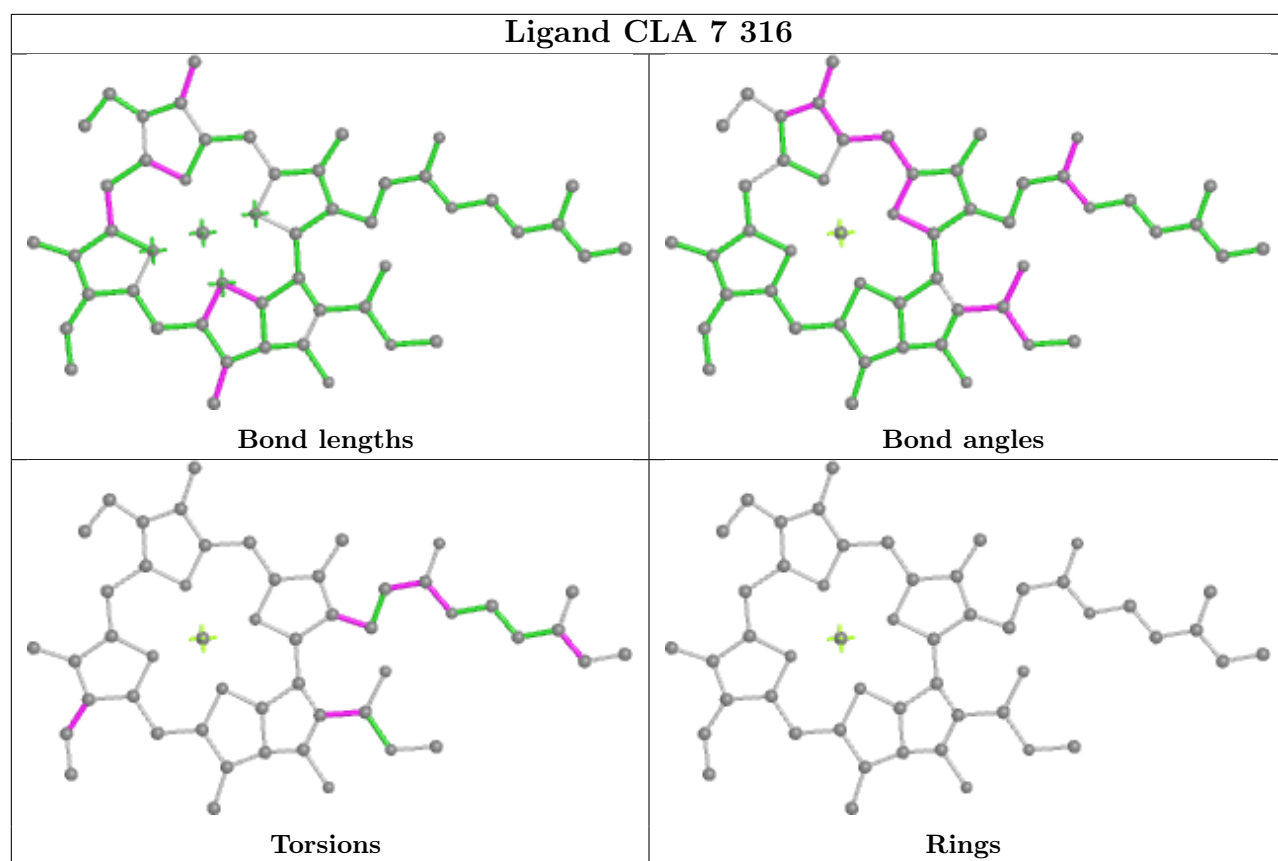
Rings

Ligand CLA 7 315

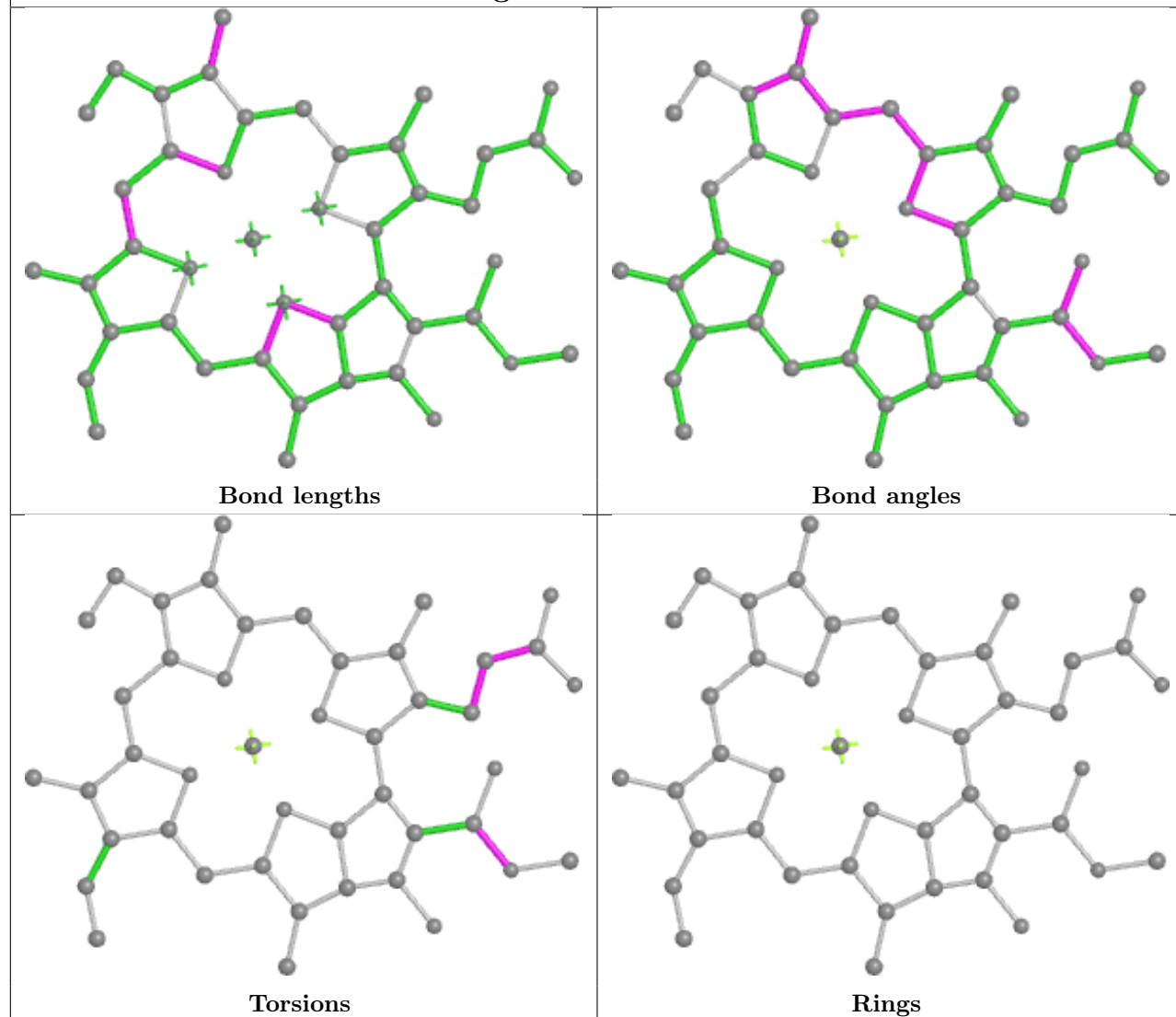


Ligand XAT 6 303

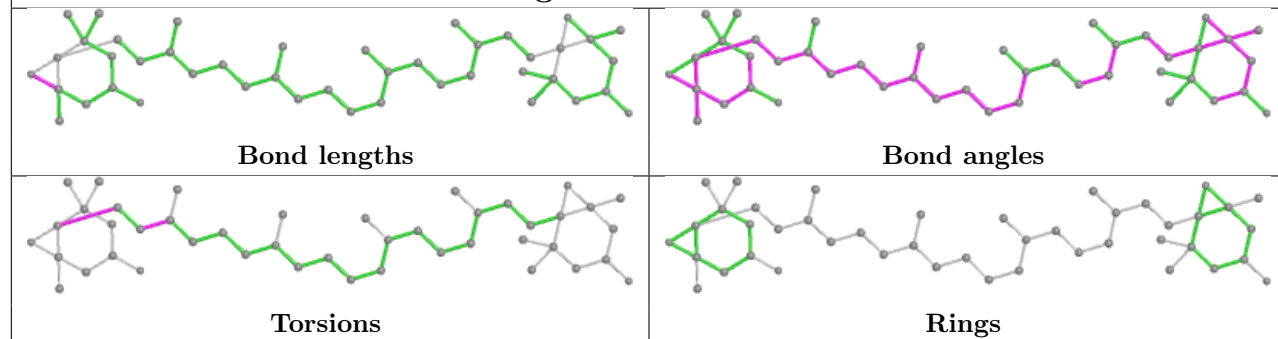


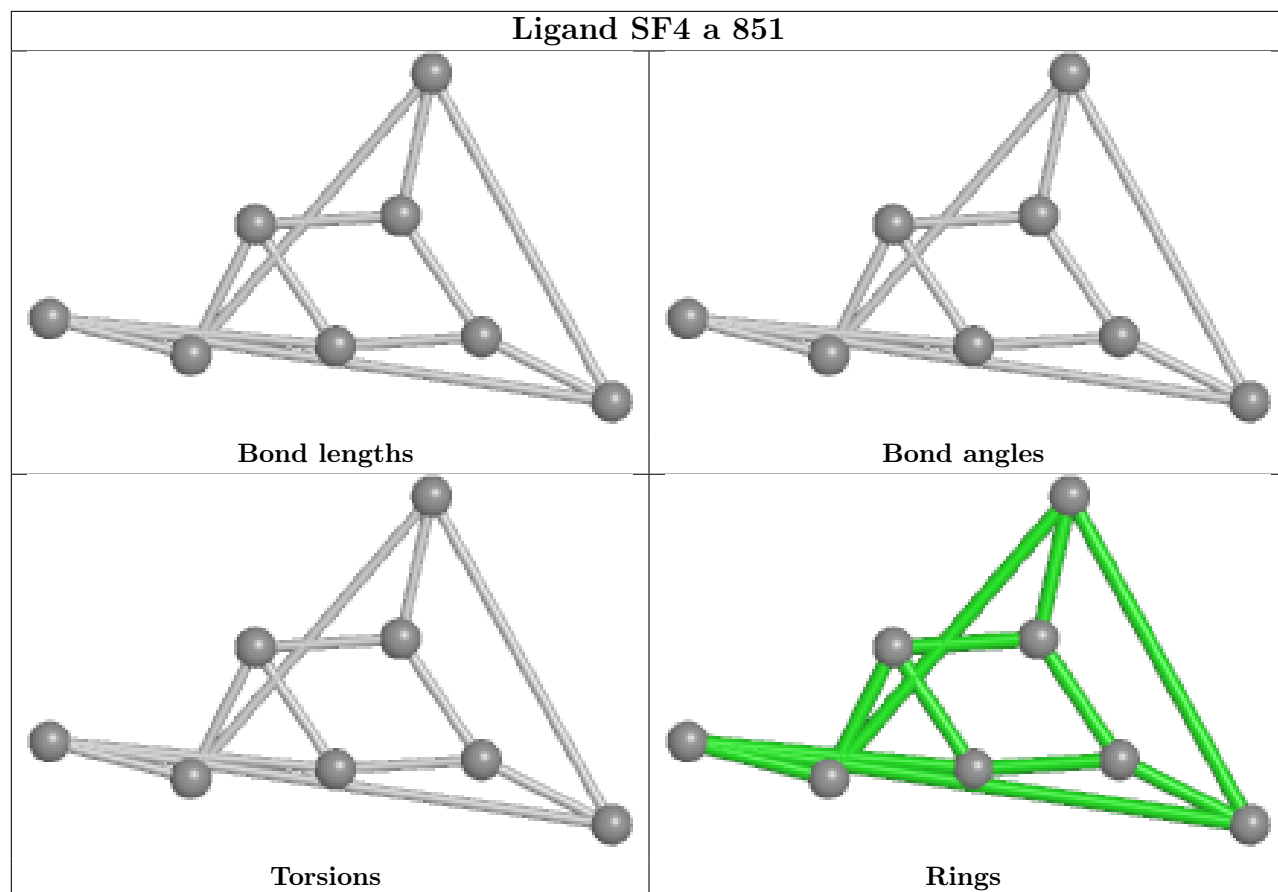


Ligand CLA 7 317

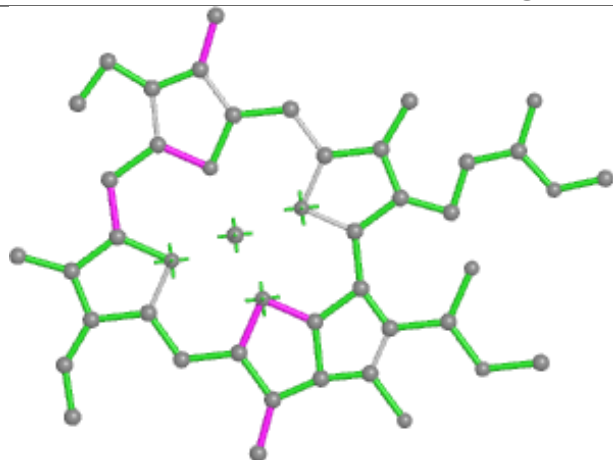


Ligand XAT 3 304

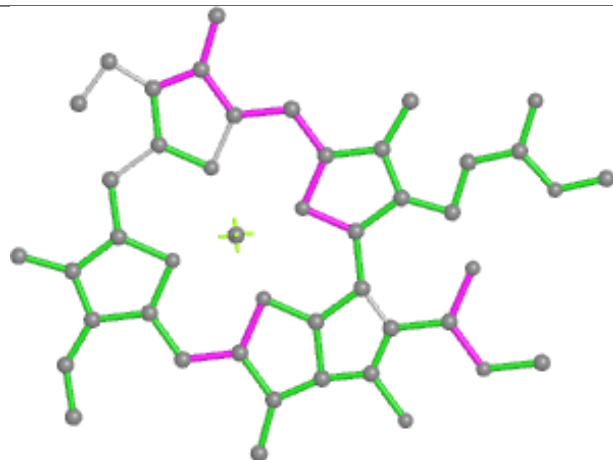




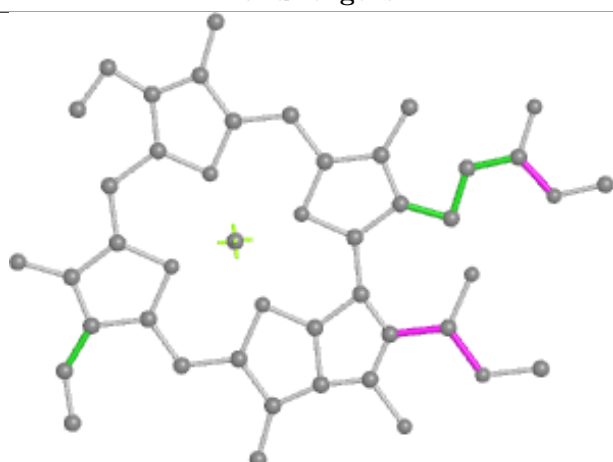
Ligand CLA 8 310



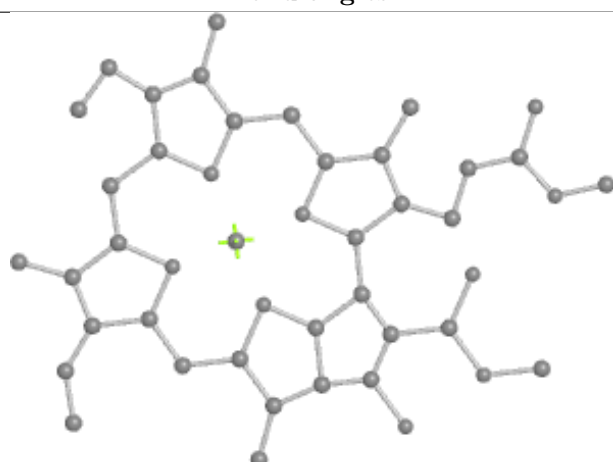
Bond lengths



Bond angles

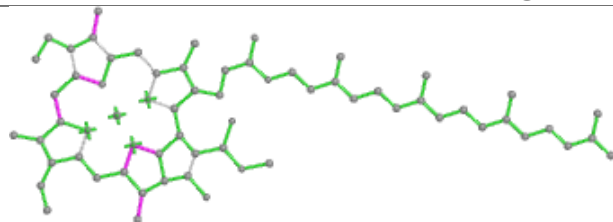


Torsions

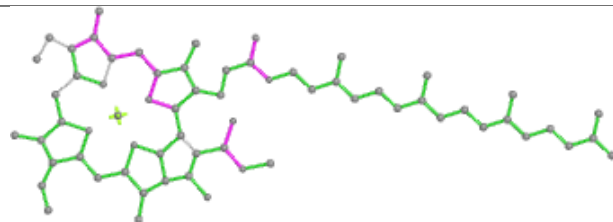


Rings

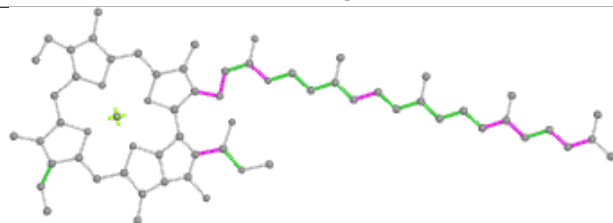
Ligand CLA 2 310



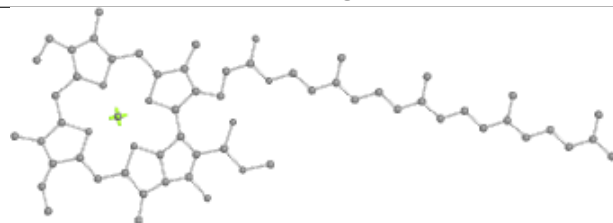
Bond lengths



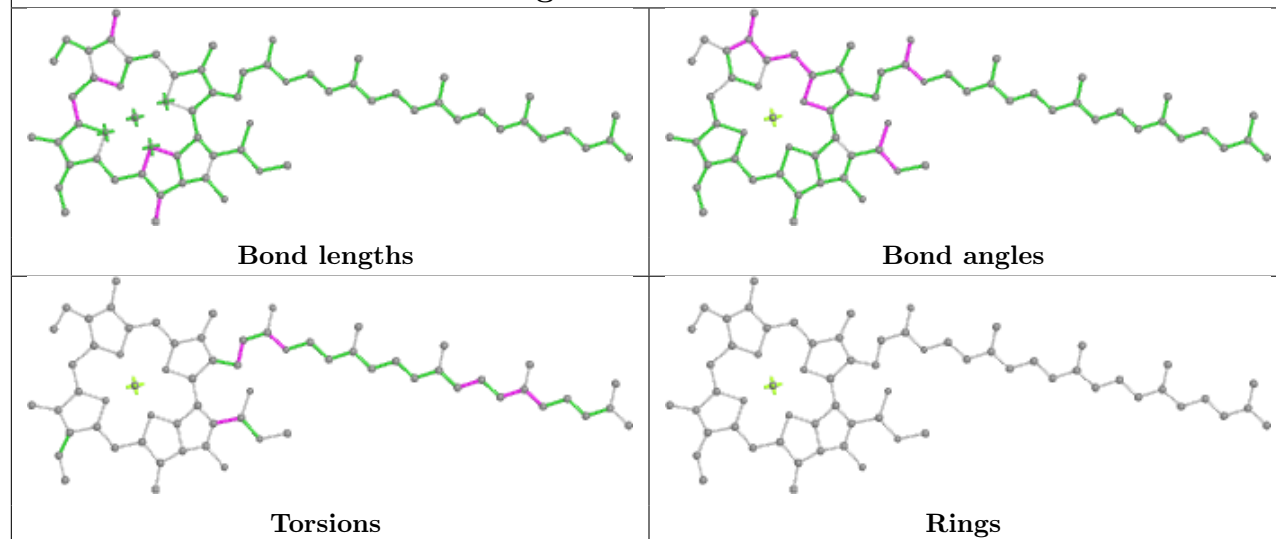
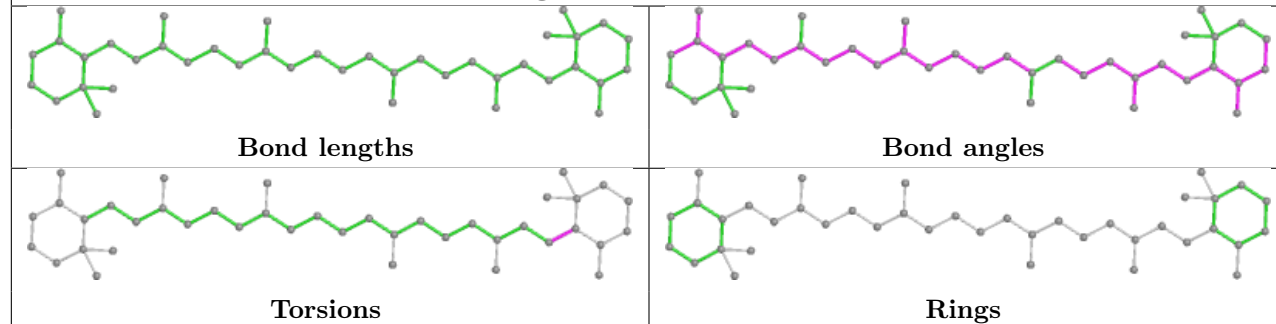
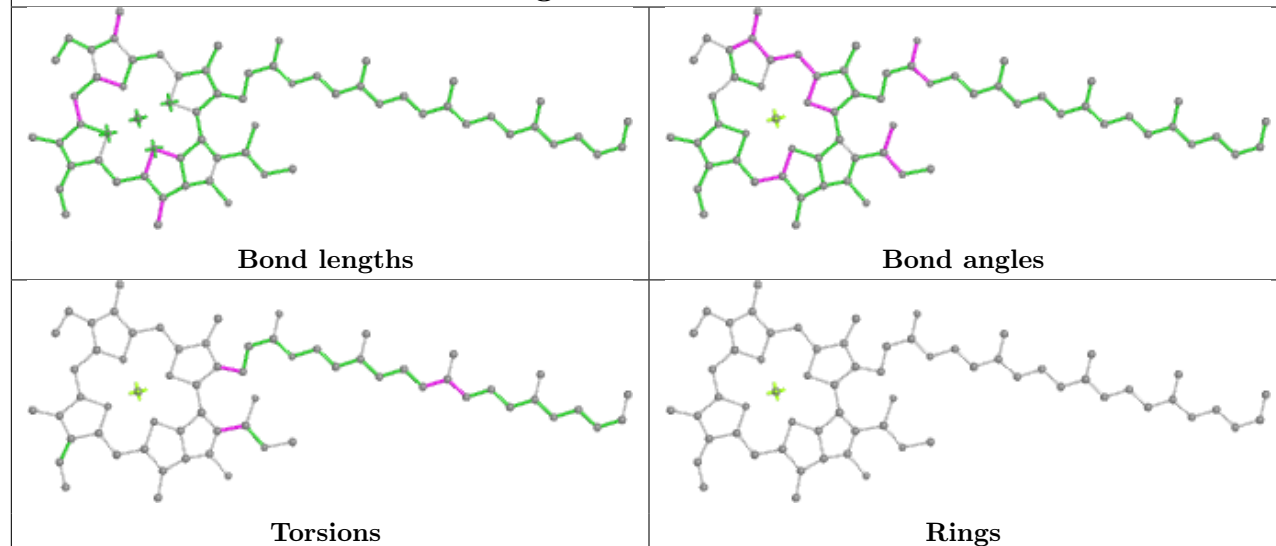
Bond angles



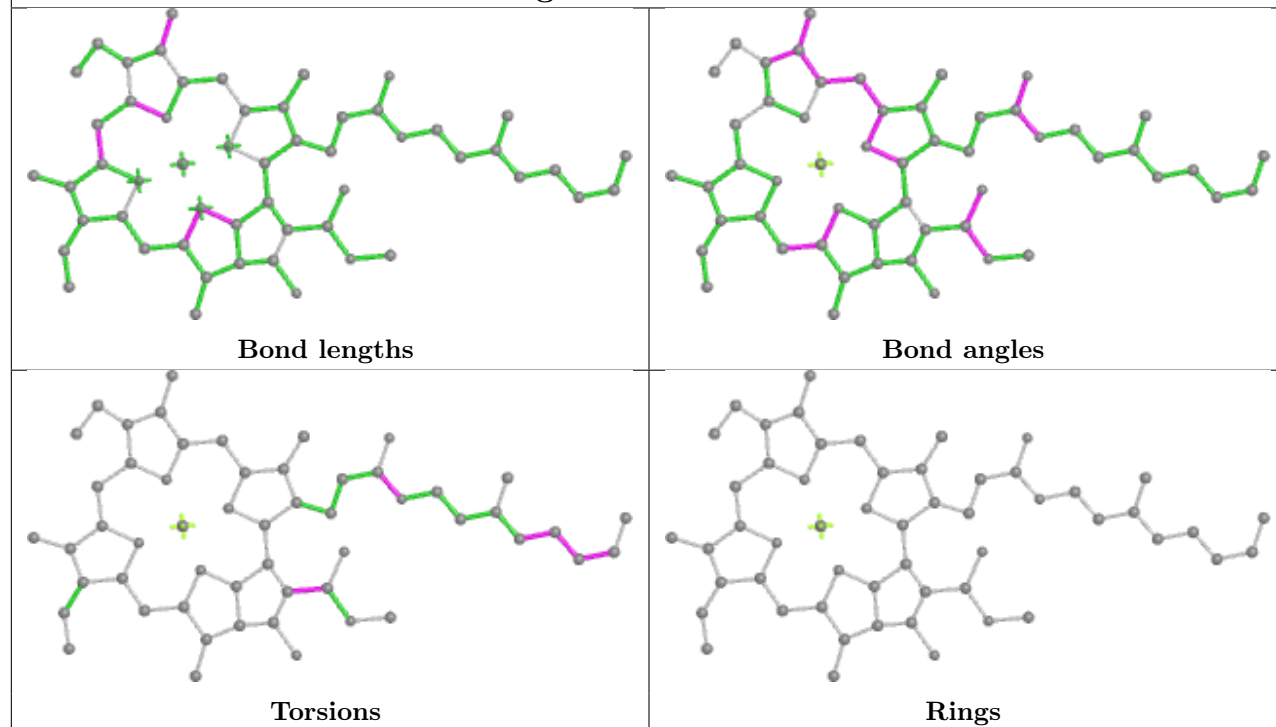
Torsions



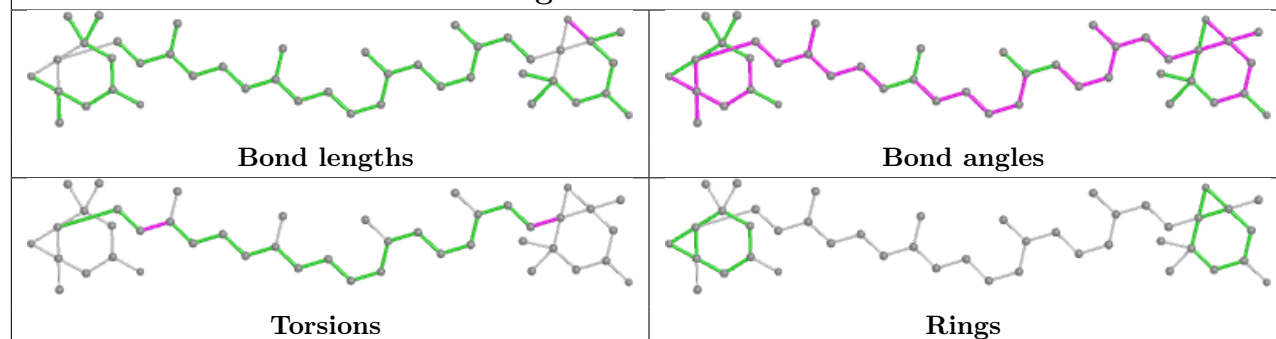
Rings

Ligand CLA a 842**Ligand BCR h 202****Ligand CLA b 825**

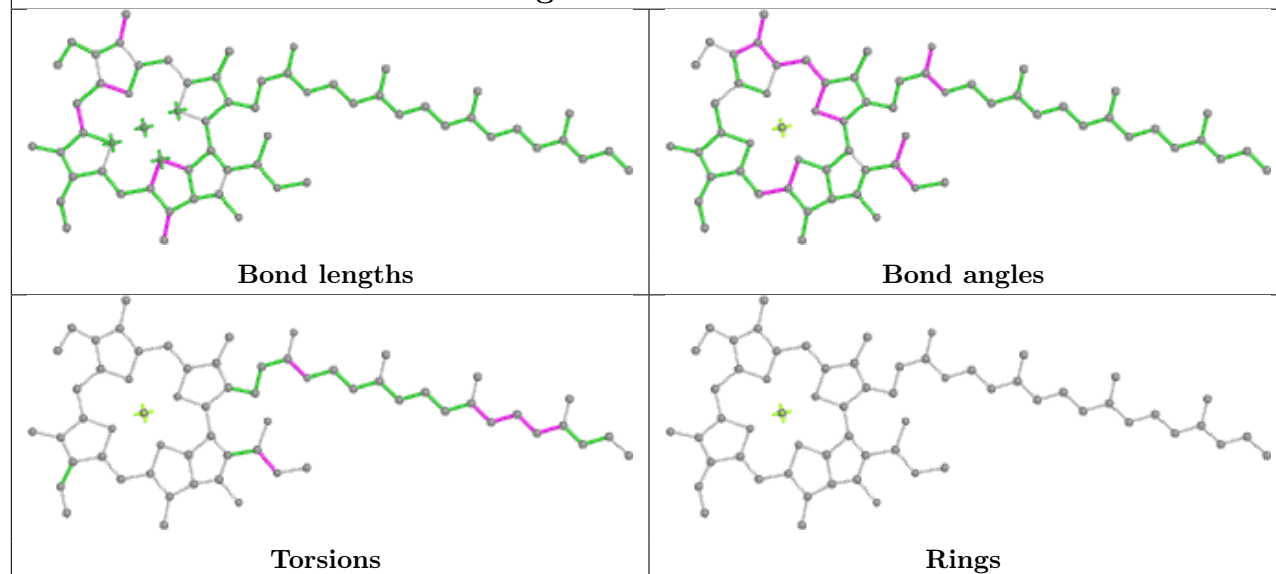
Ligand CLA 1 307



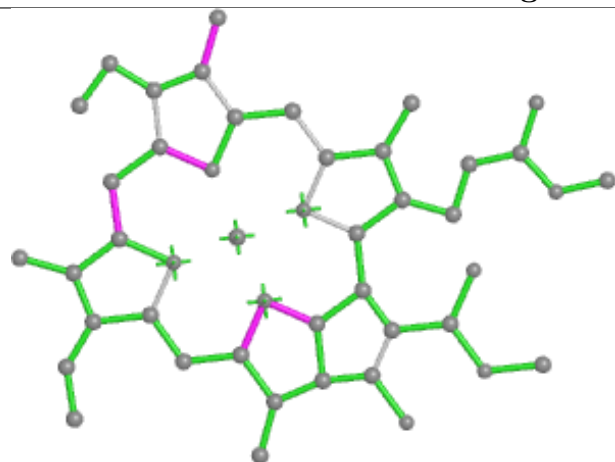
Ligand XAT 3 303



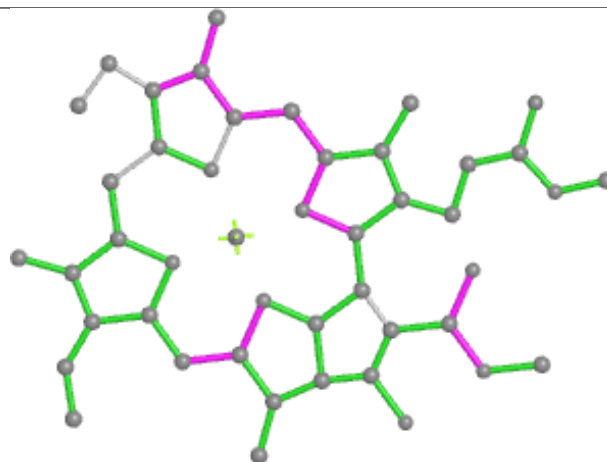
Ligand CLA 9 318



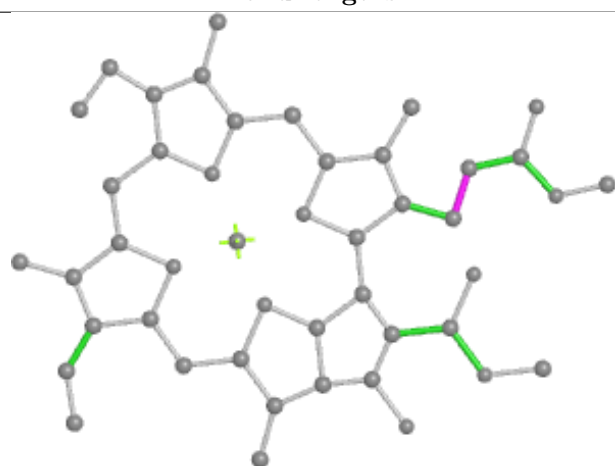
Ligand CLA 6 307



Bond lengths



Bond angles

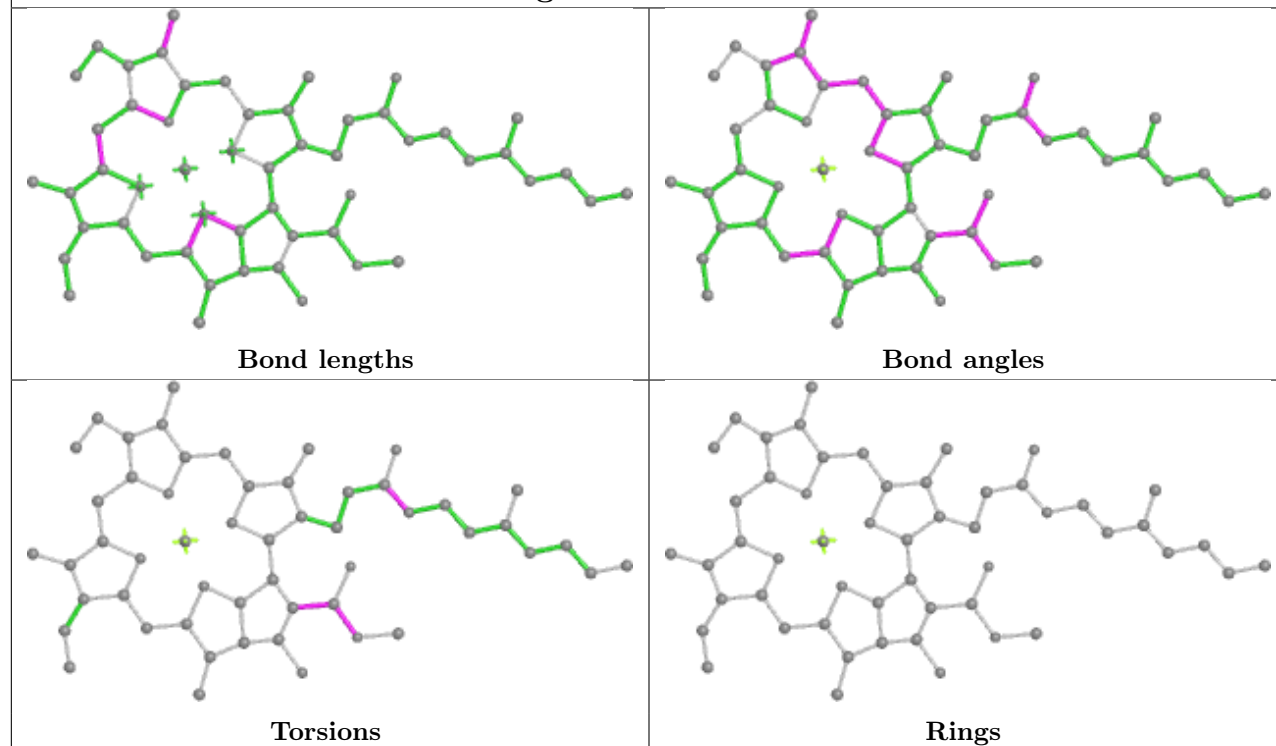


Torsions

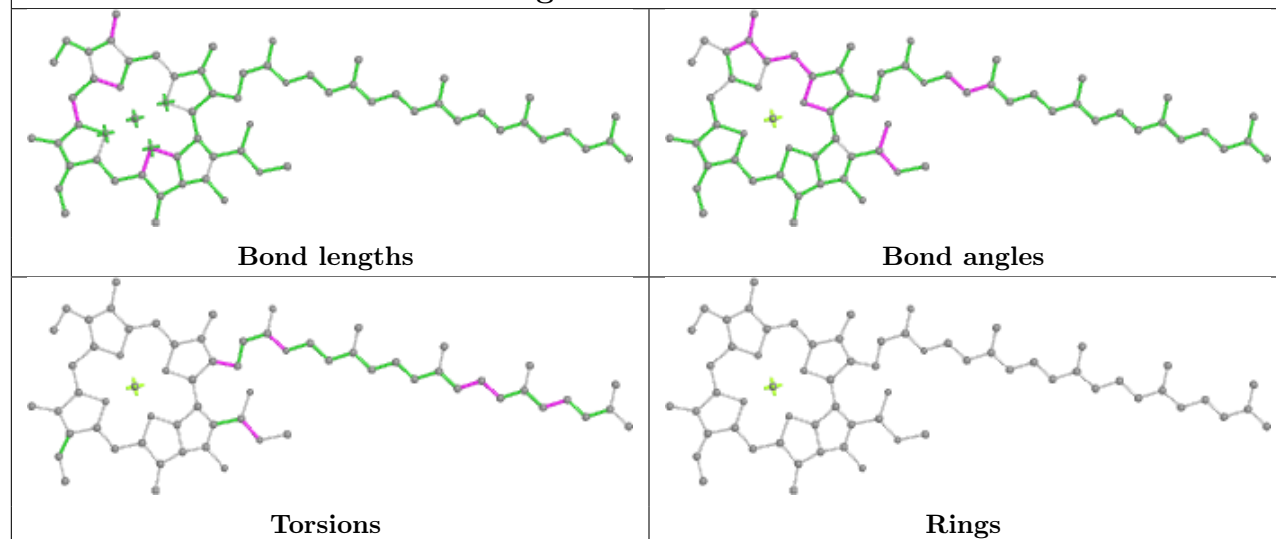


Rings

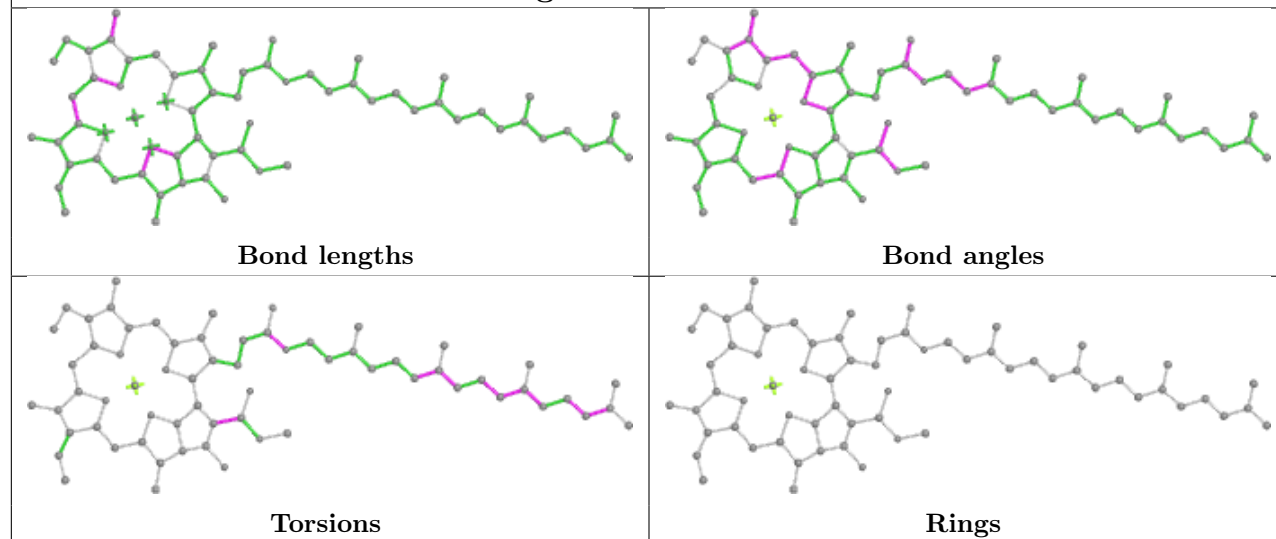
Ligand CLA 1 311



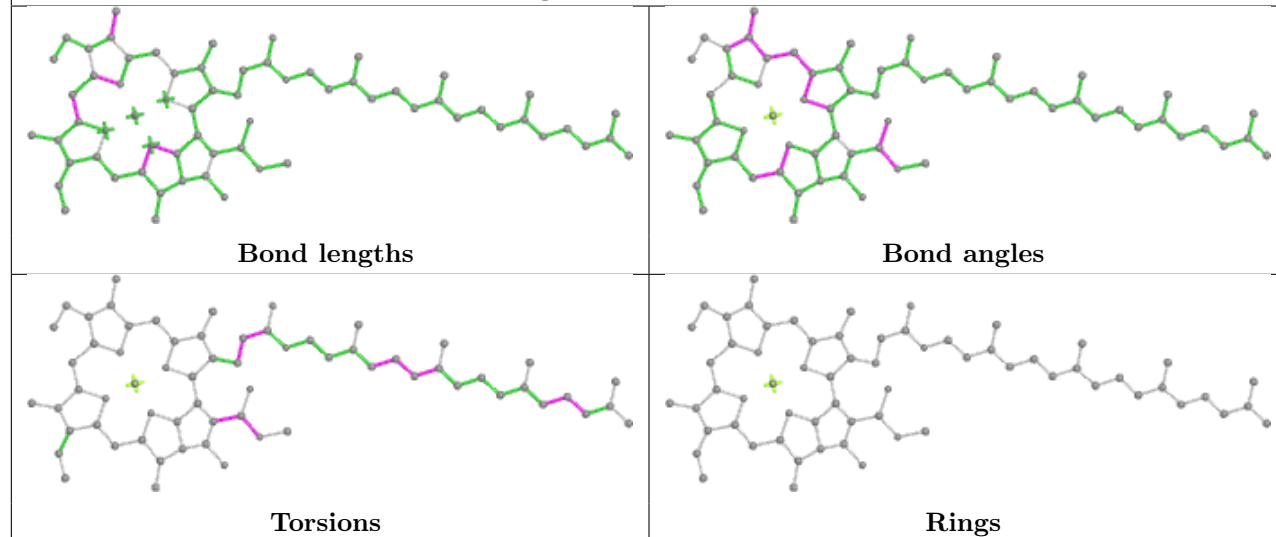
Ligand CLA 6 317



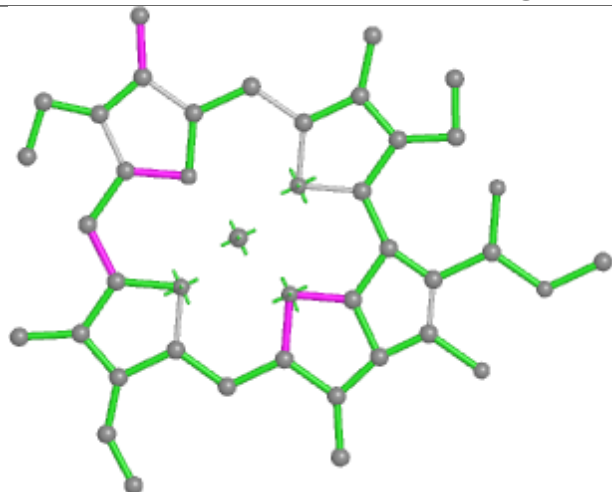
Ligand CLA a 844



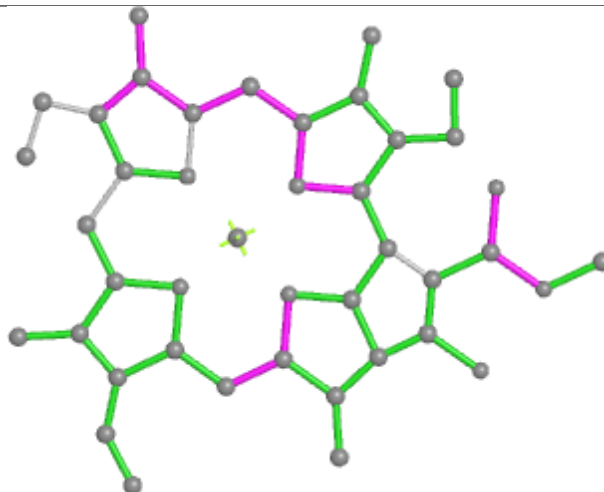
Ligand CLA 5 309



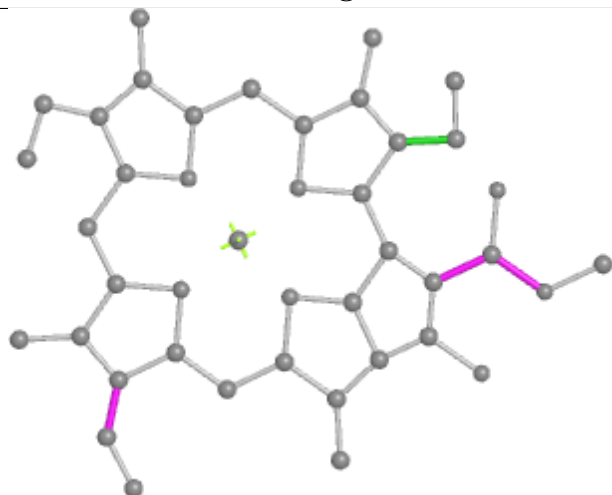
Ligand CLA 9 315



Bond lengths



Bond angles

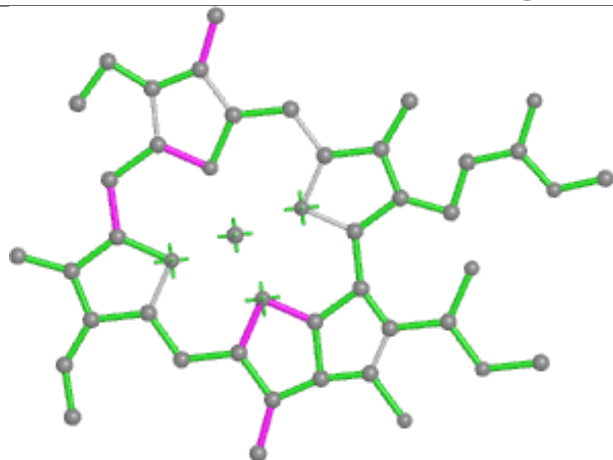


Torsions

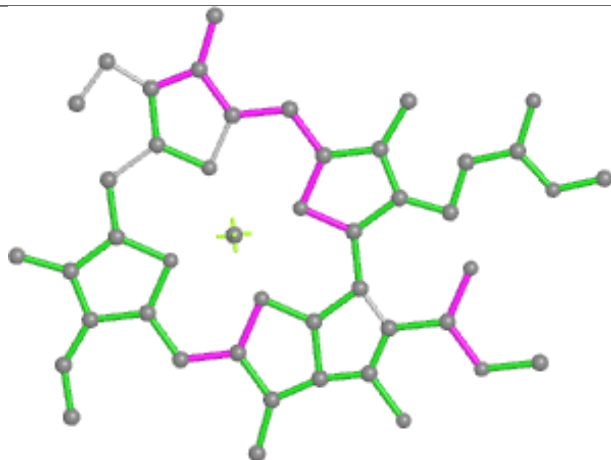


Rings

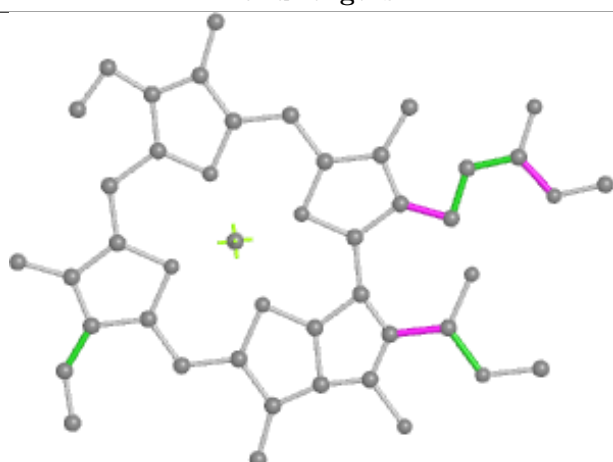
Ligand CLA a 824



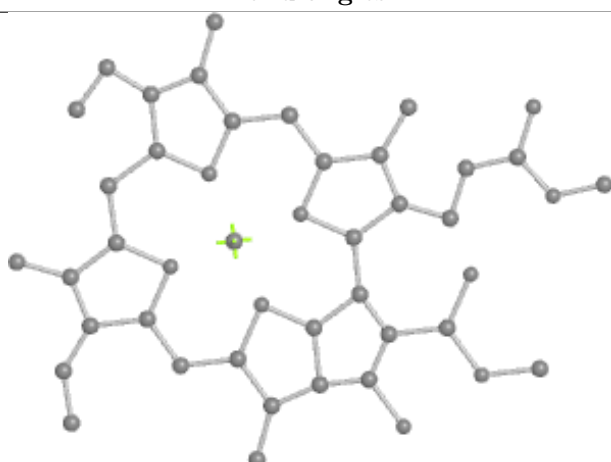
Bond lengths



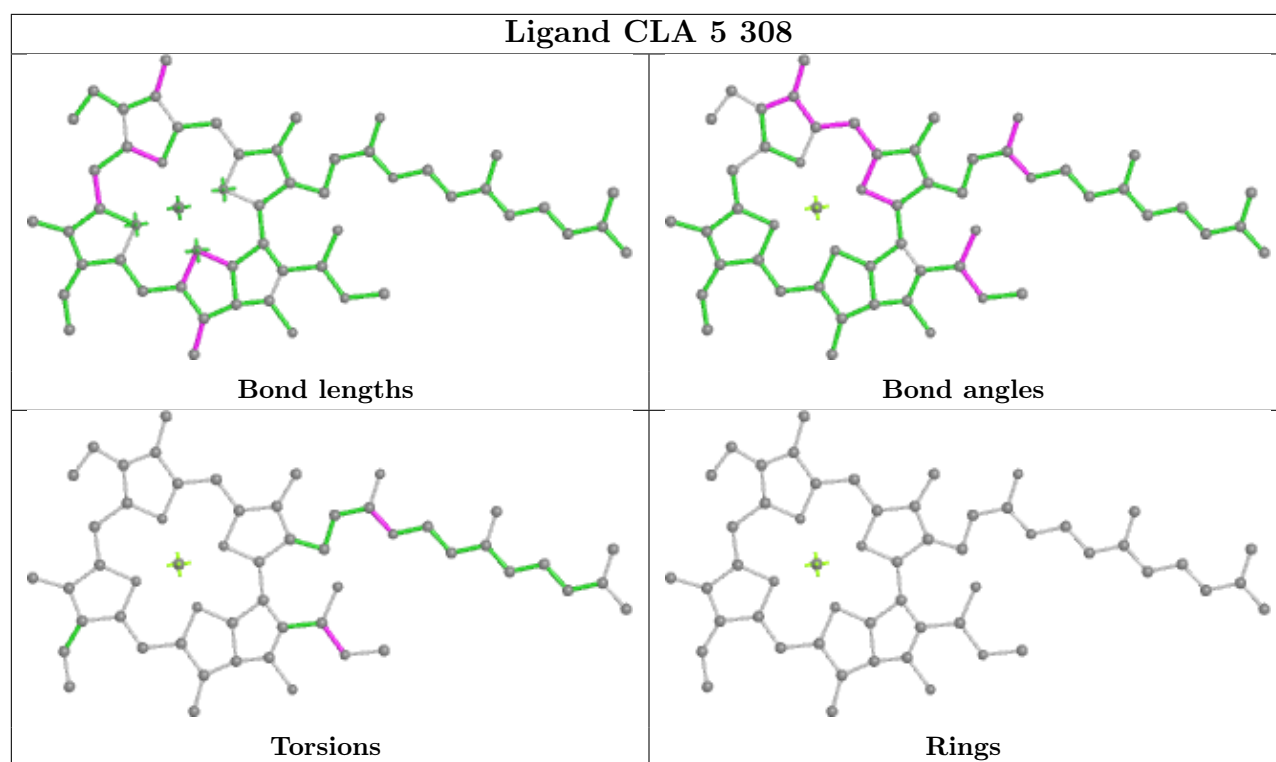
Bond angles



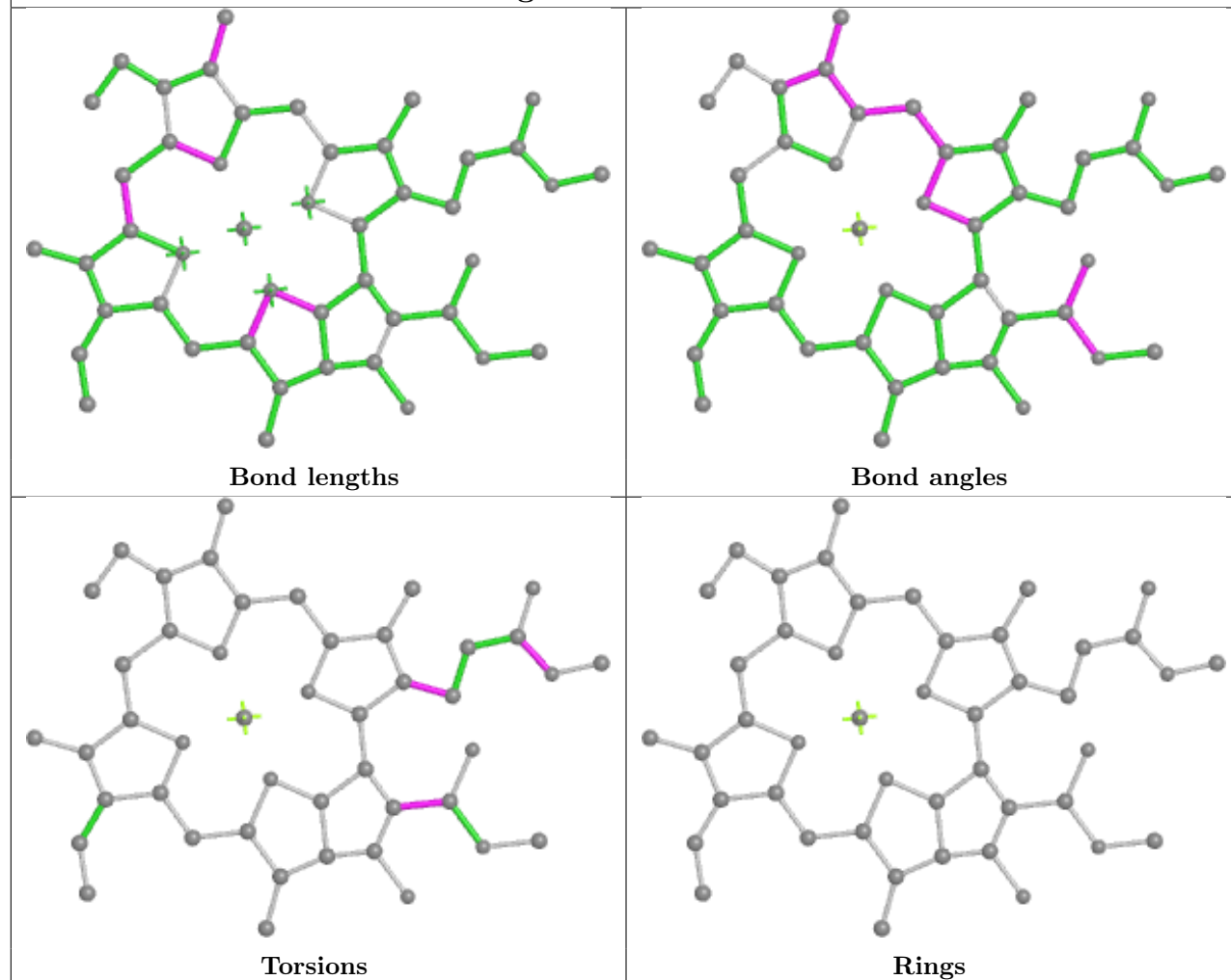
Torsions



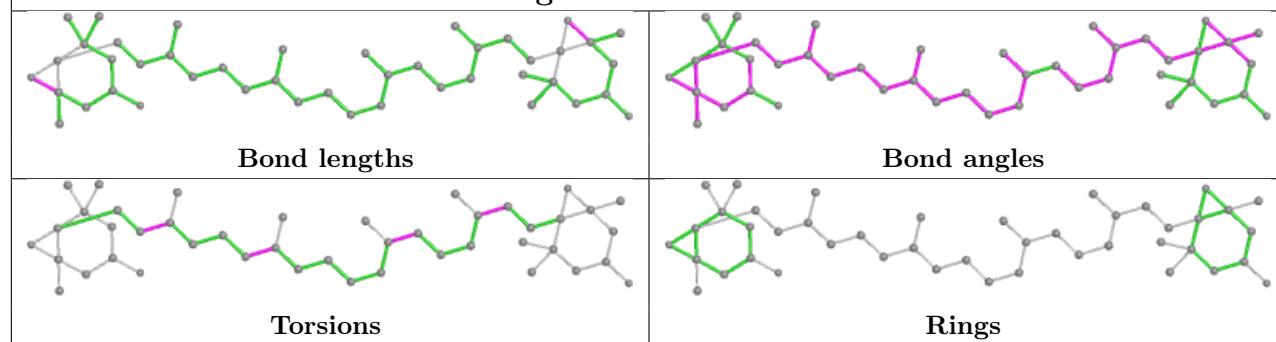
Rings



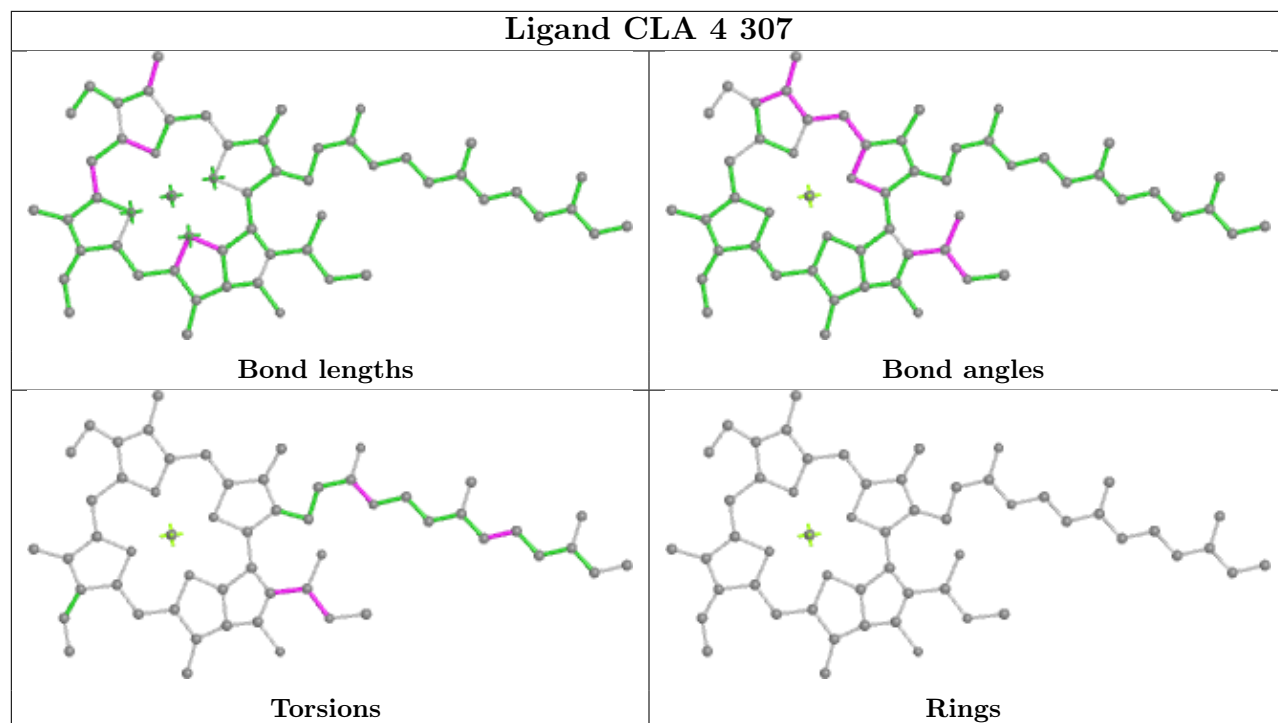
Ligand CLA 9 310



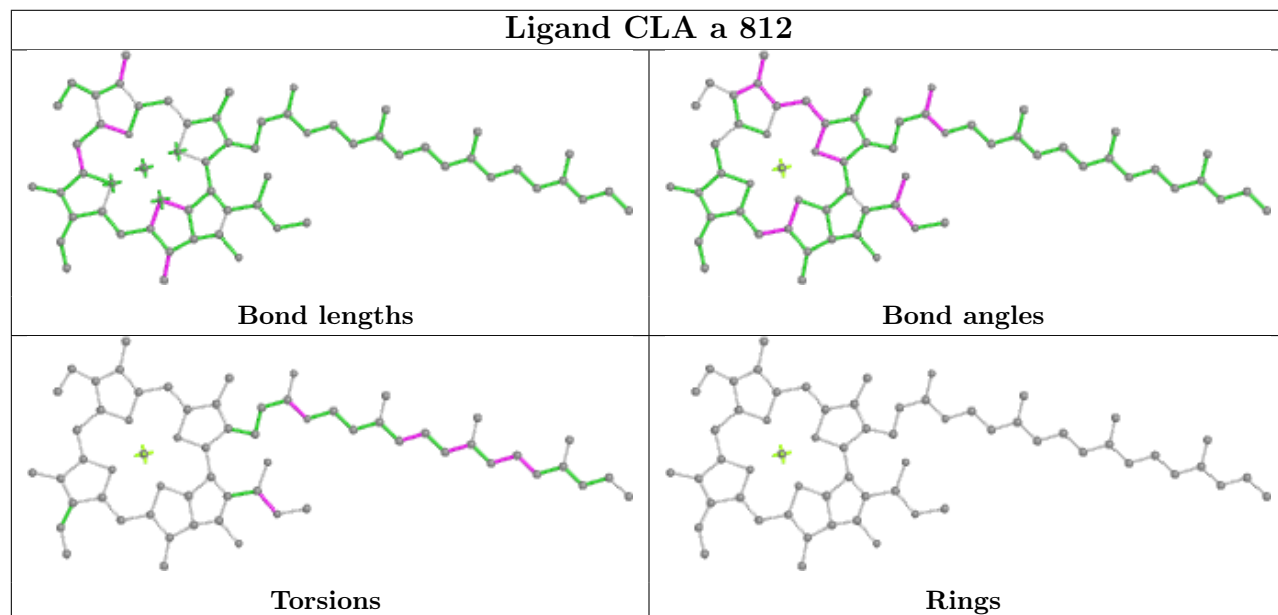
Ligand XAT a 852

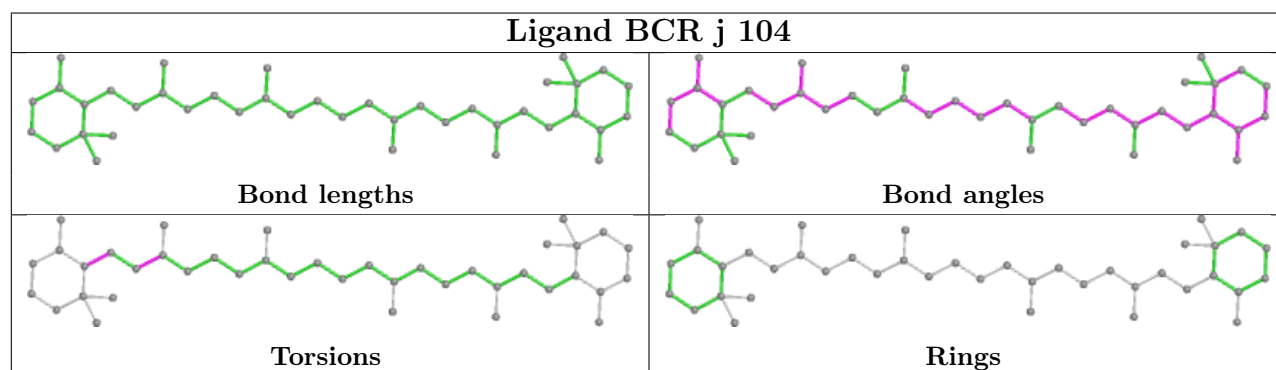
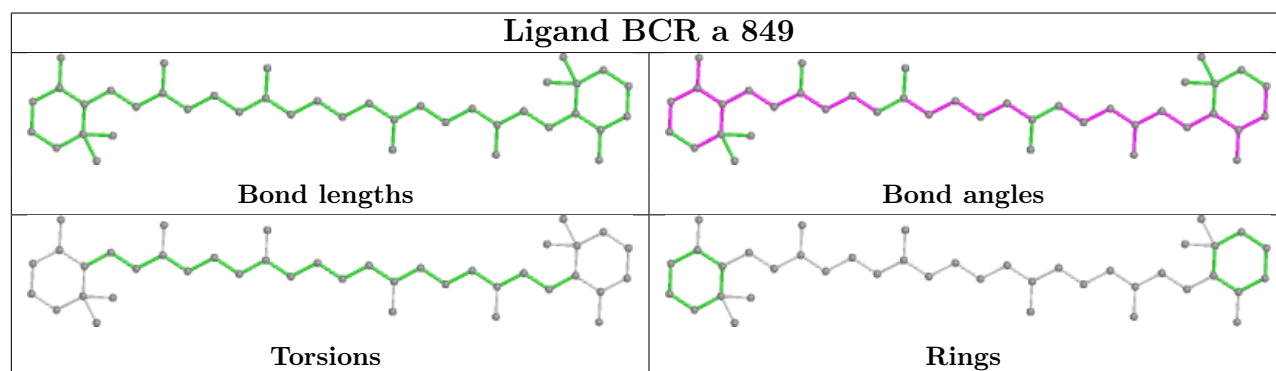
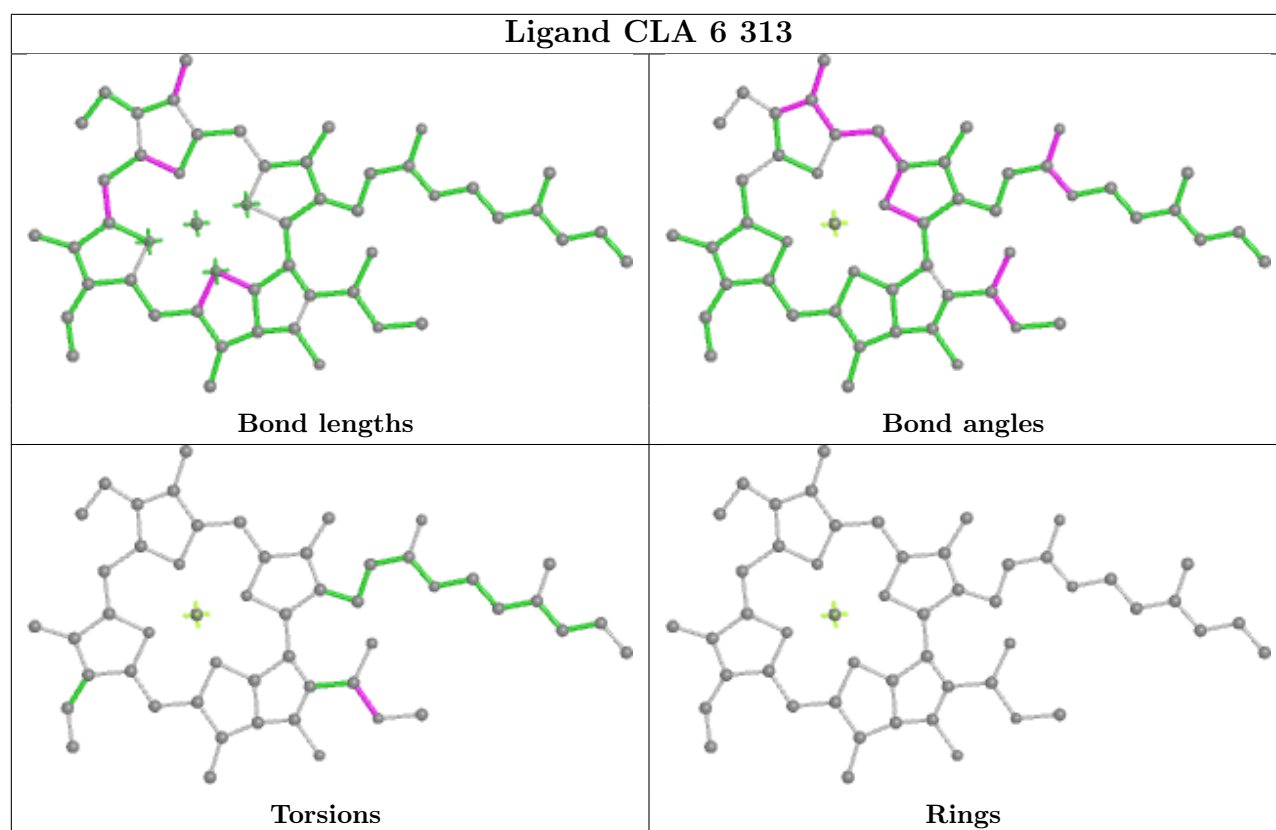


Ligand CLA 4 307

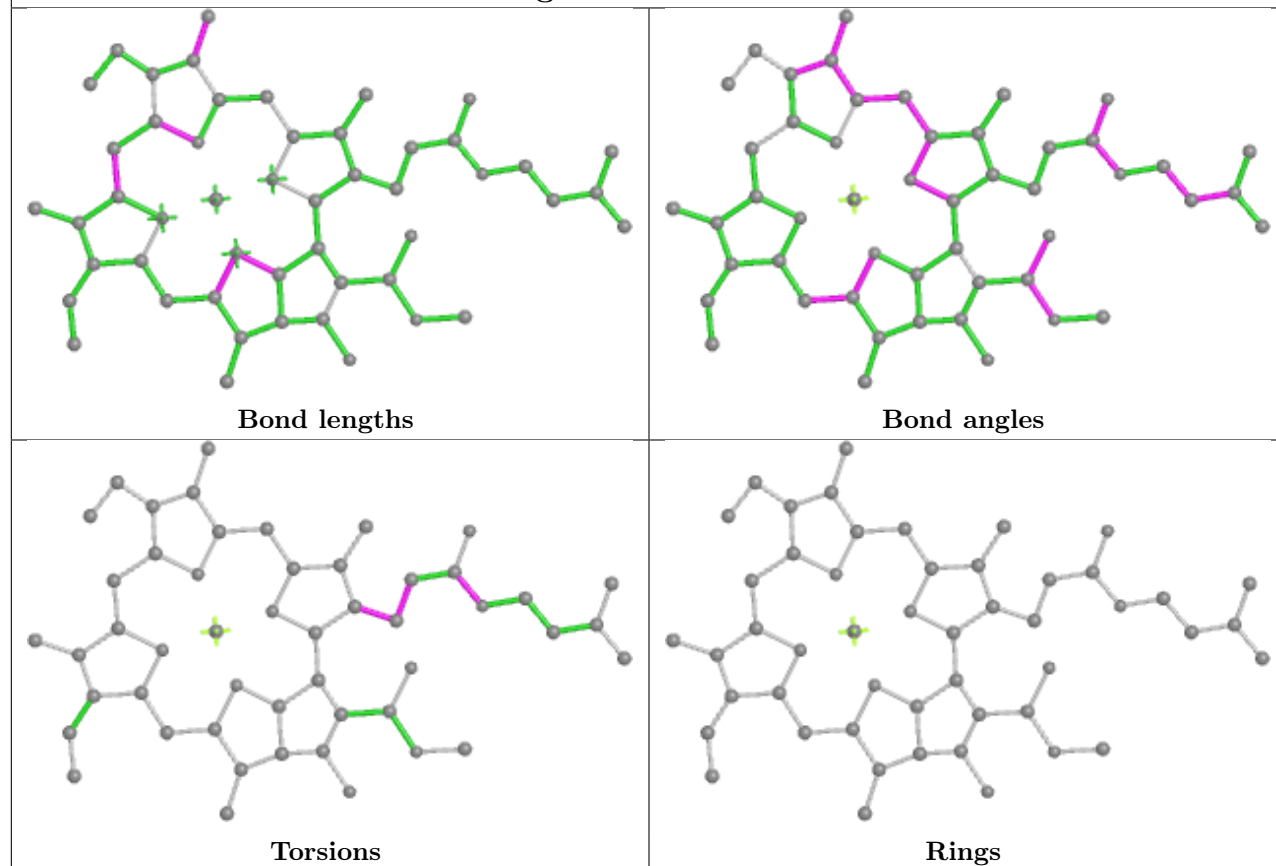


Ligand CLA a 812

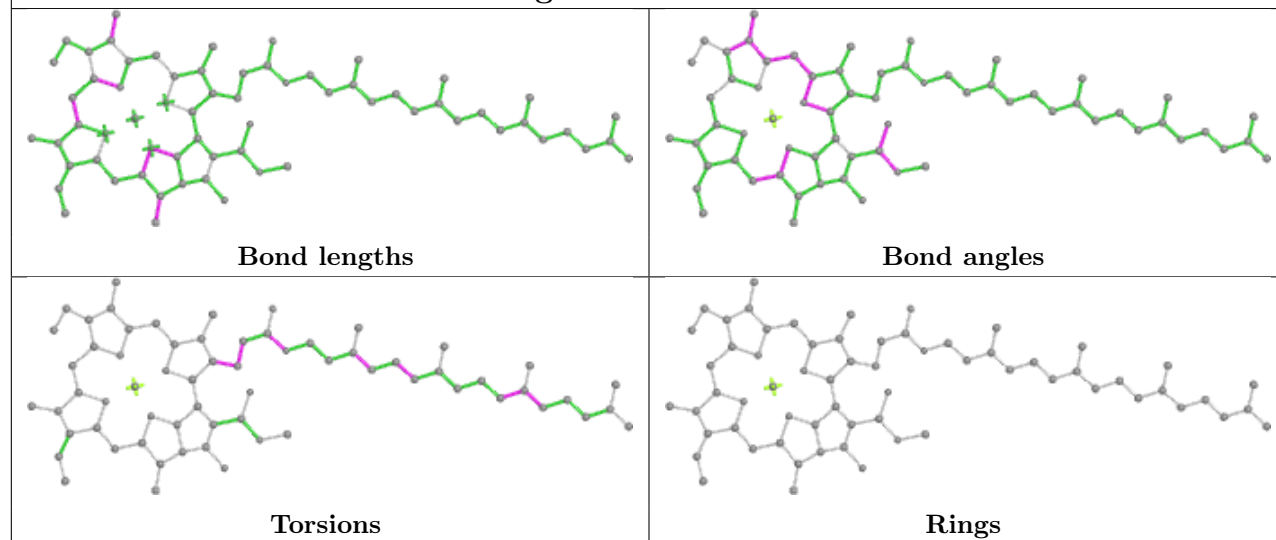




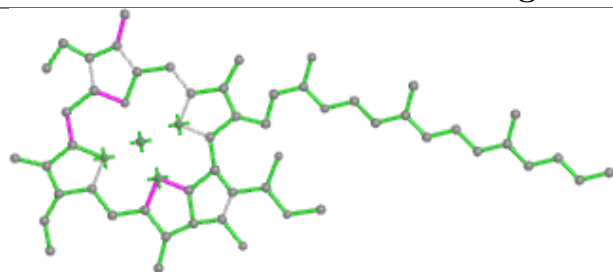
Ligand CLA 3 311



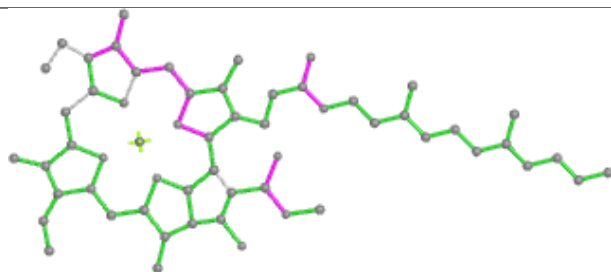
Ligand CLA b 828



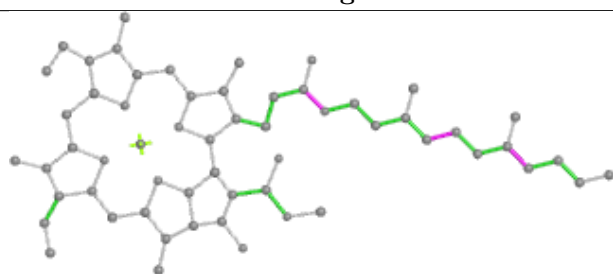
Ligand CLA 2 311



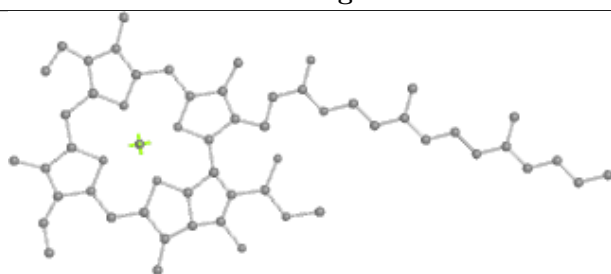
Bond lengths



Bond angles

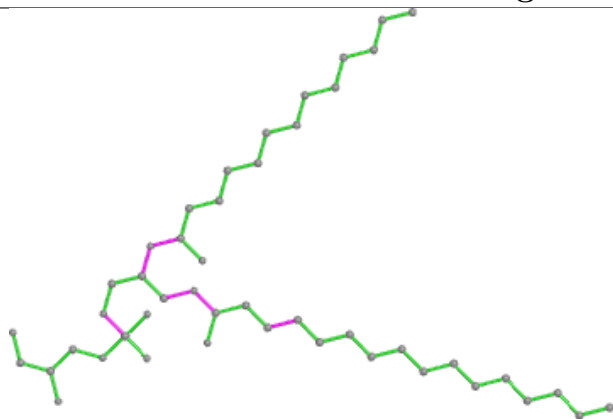


Torsions

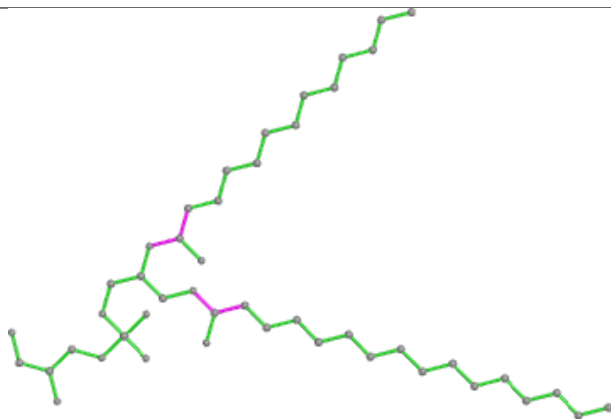


Rings

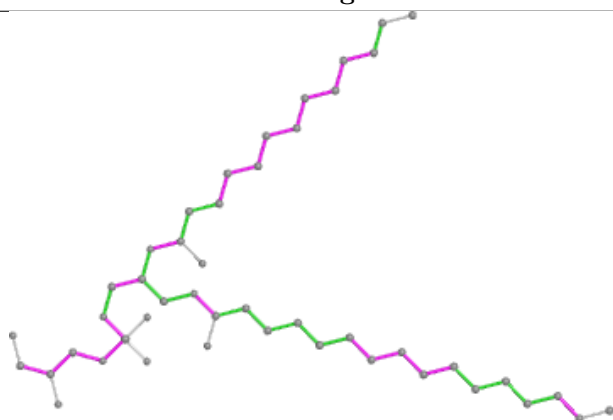
Ligand LHG 9 317



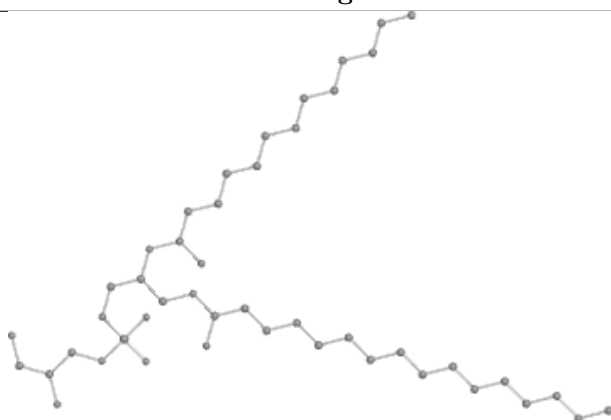
Bond lengths



Bond angles

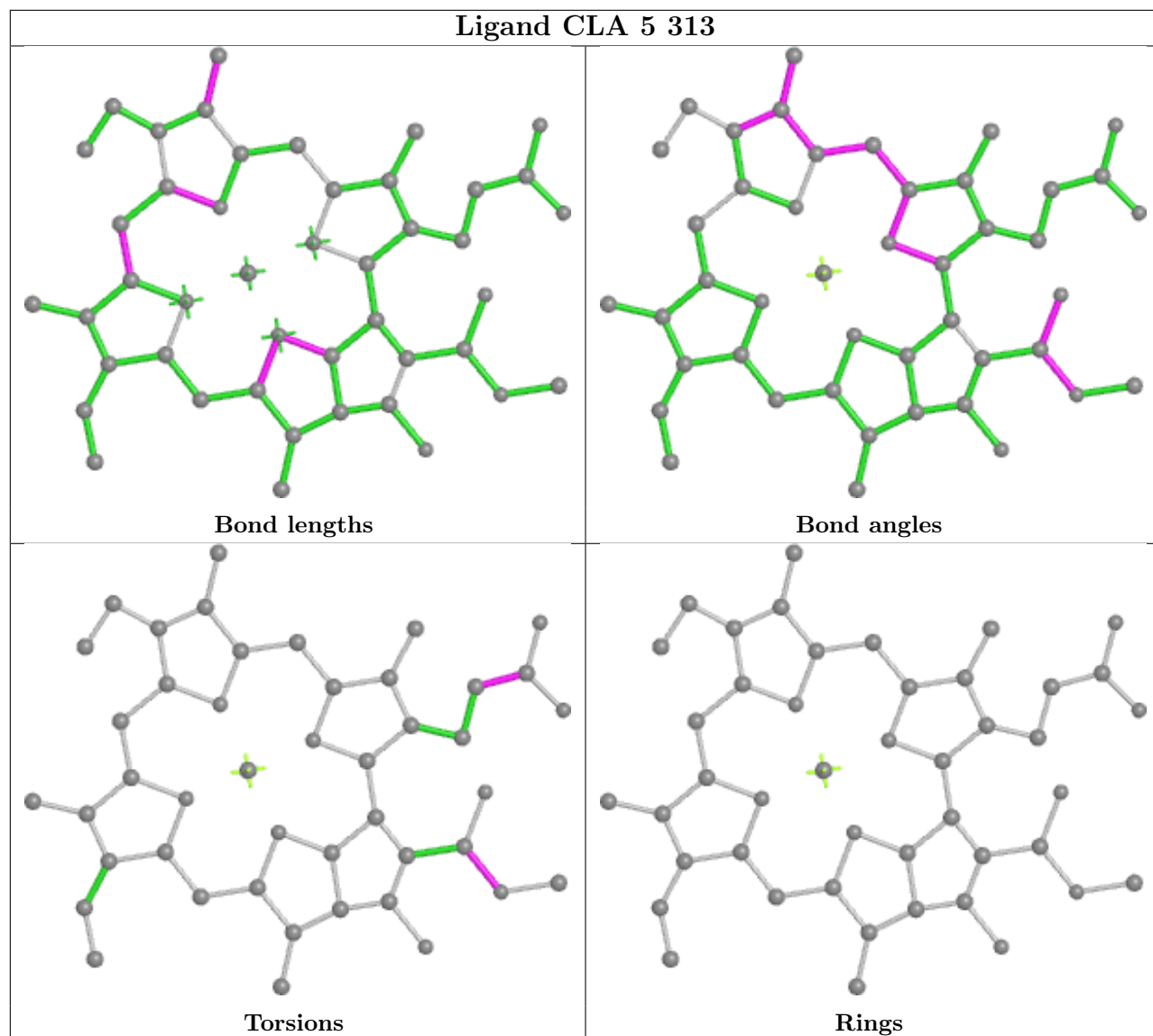


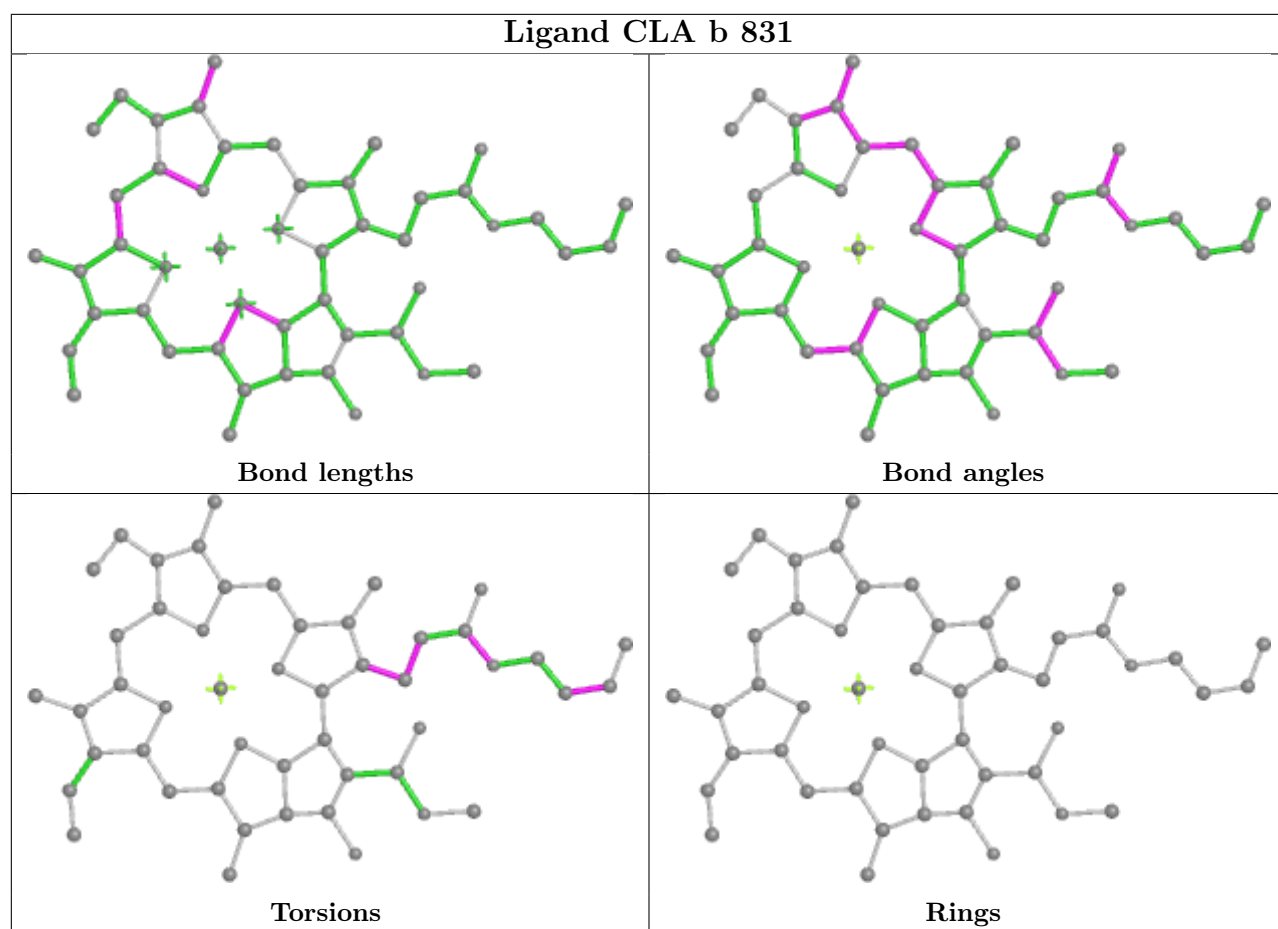
Torsions



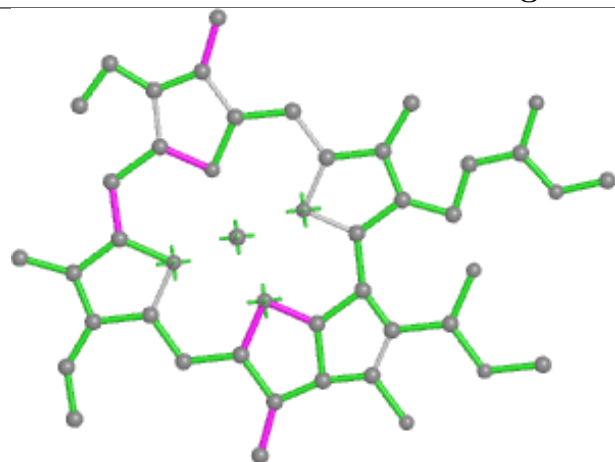
Rings

Ligand CLA 5 313

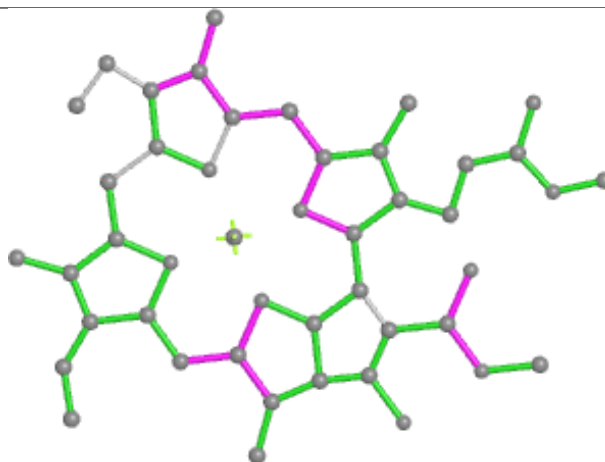




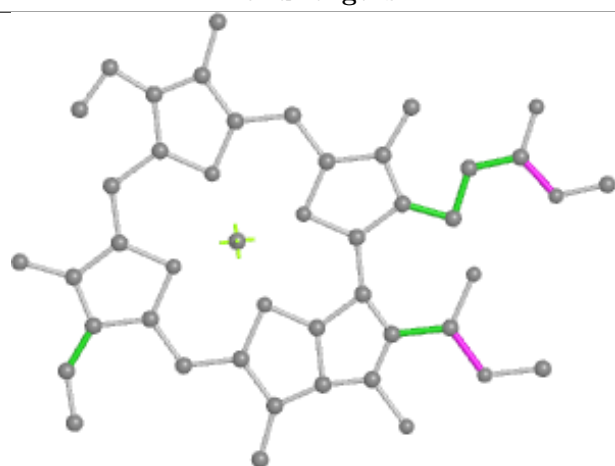
Ligand CLA 5 305



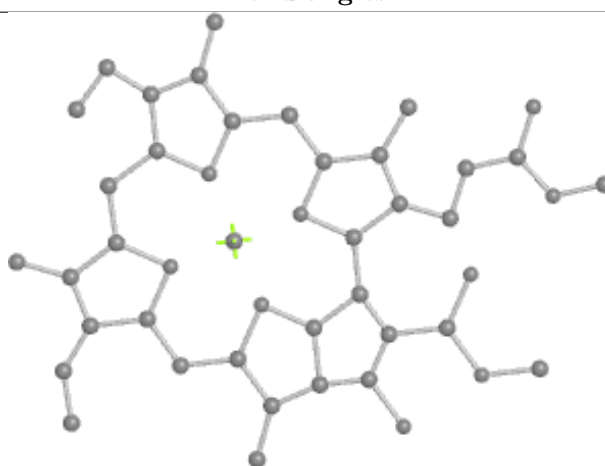
Bond lengths



Bond angles

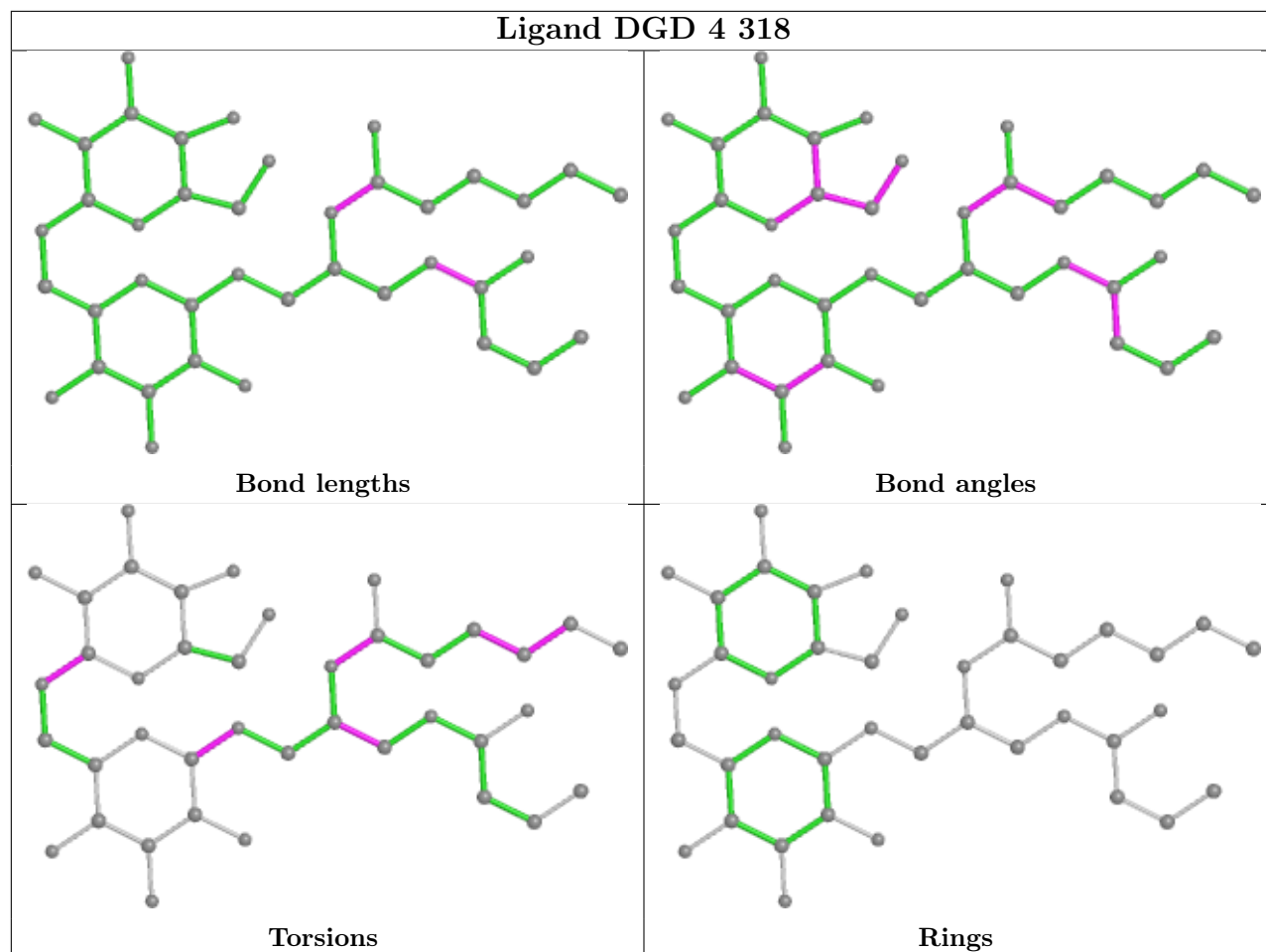


Torsions

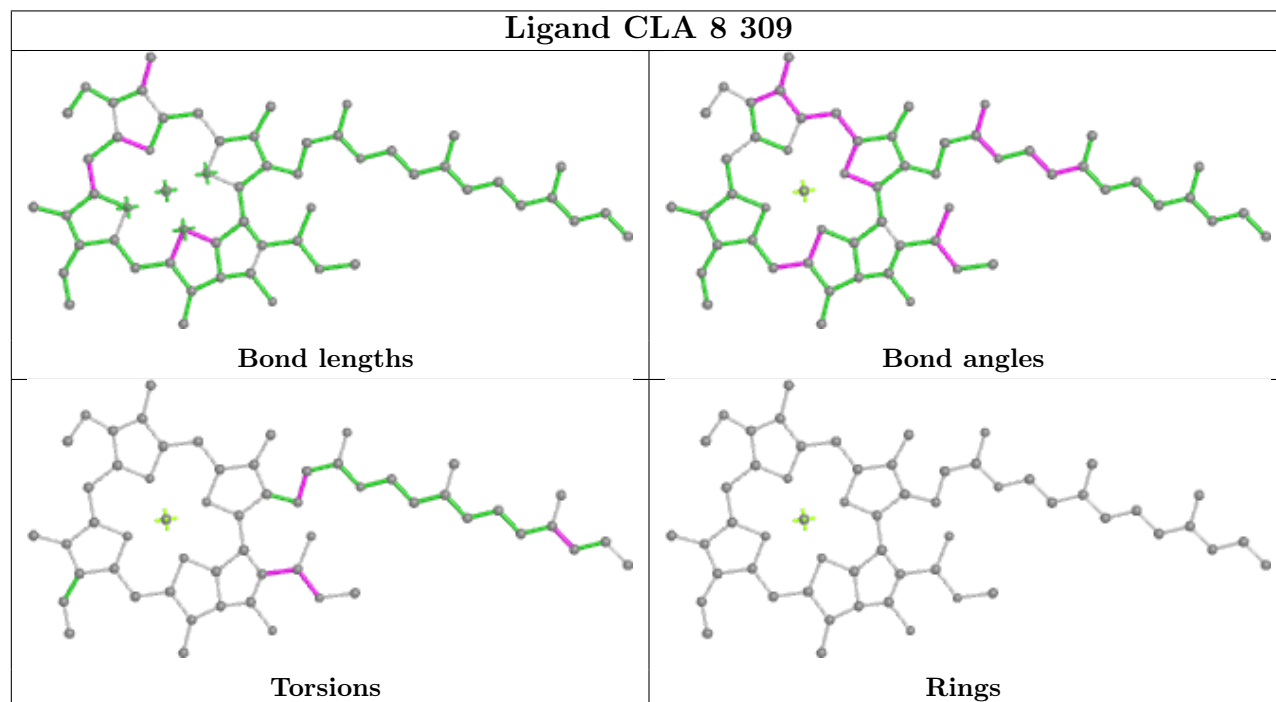


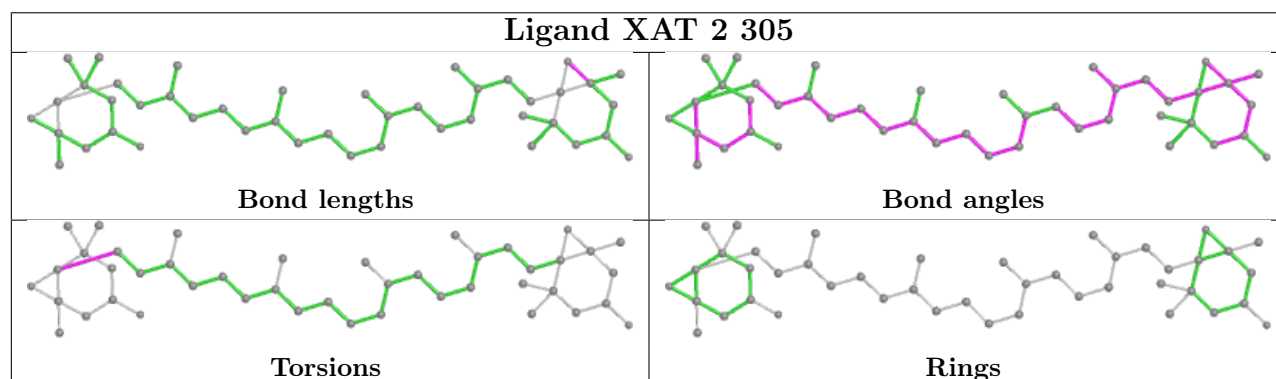
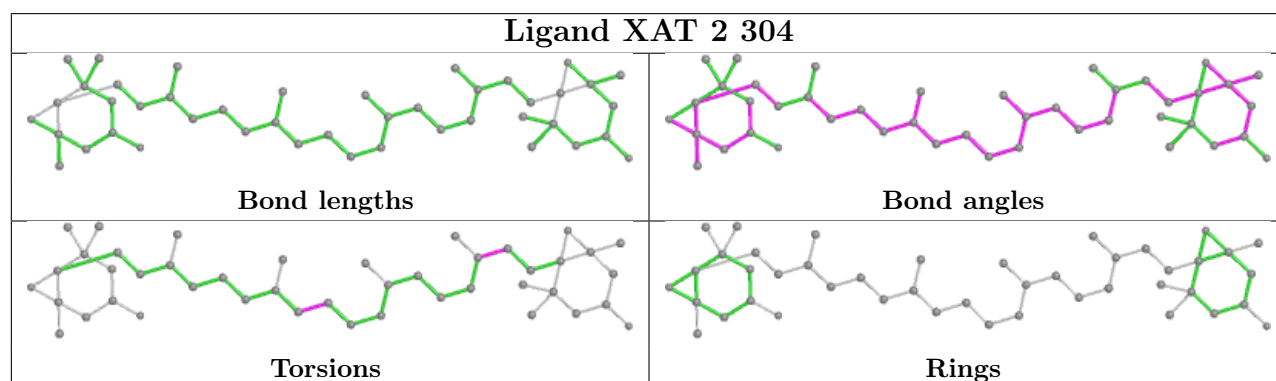
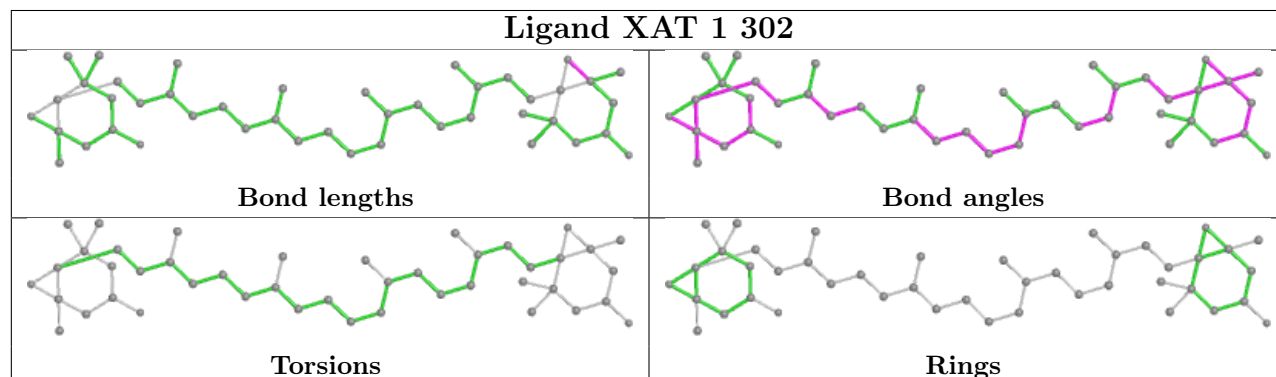
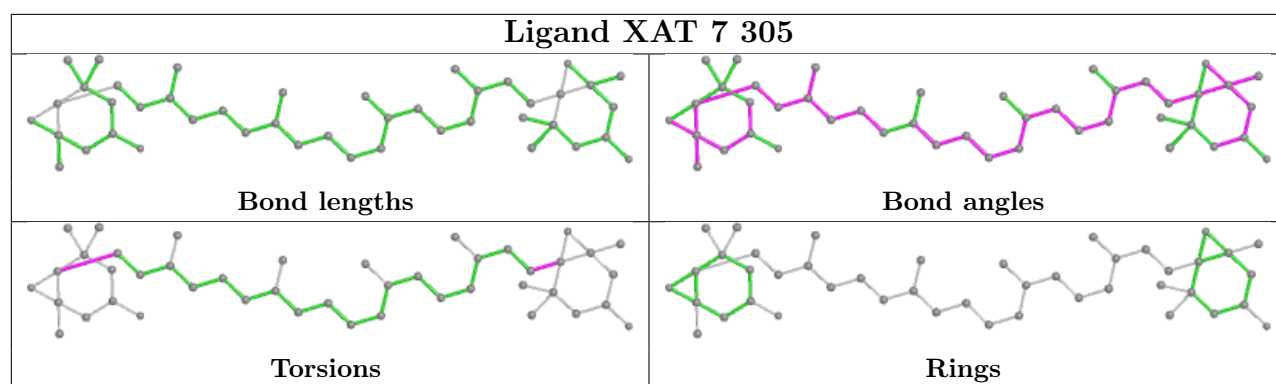
Rings

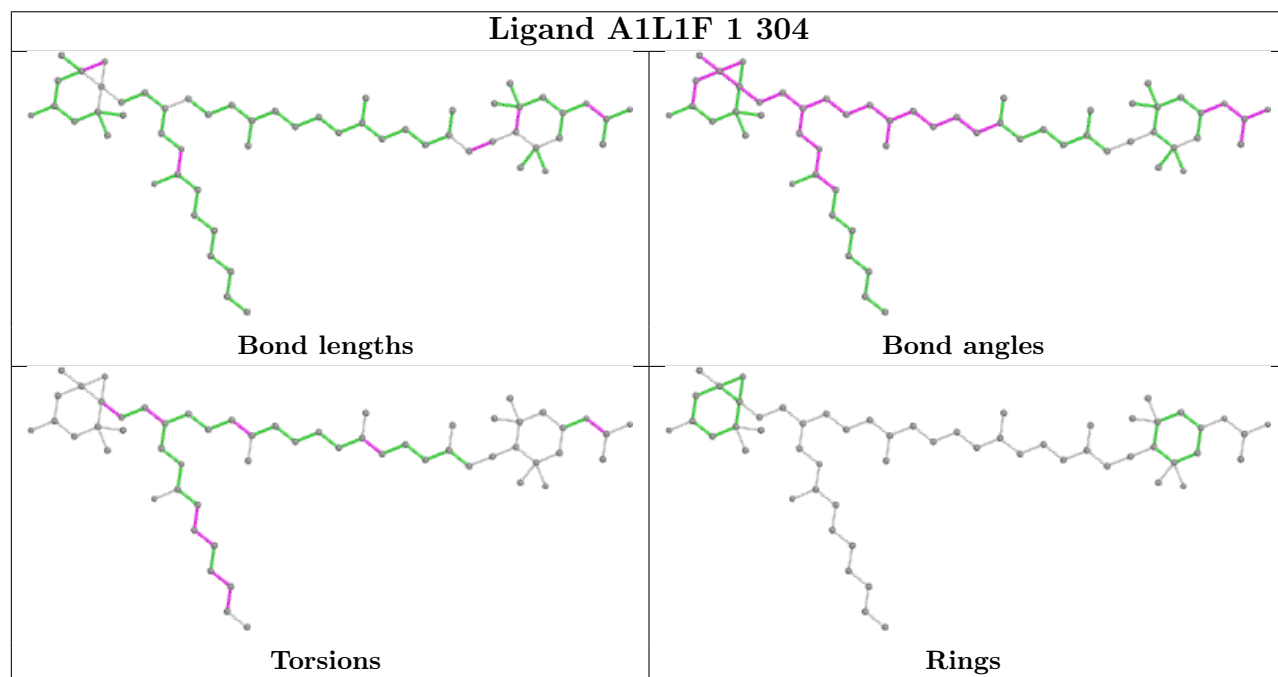
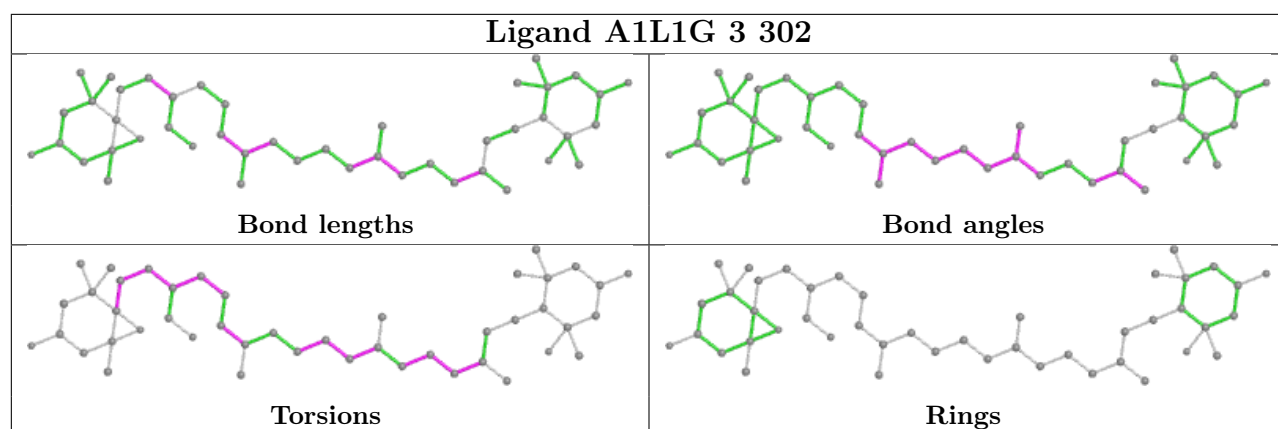
Ligand DGD 4 318



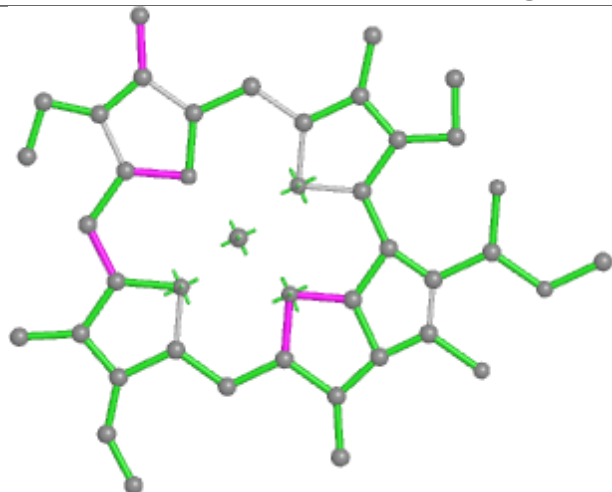
Ligand CLA 8 309



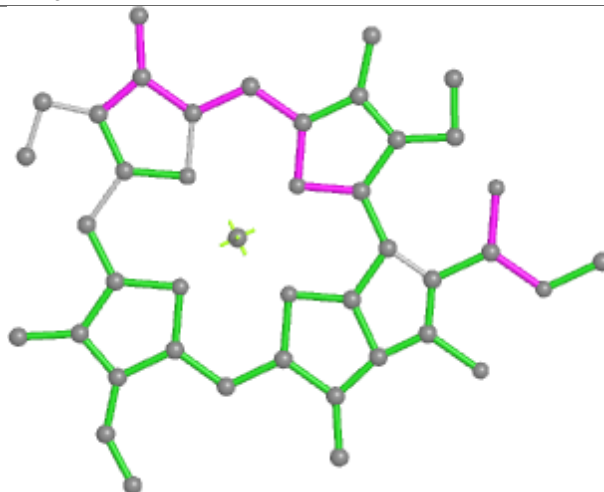




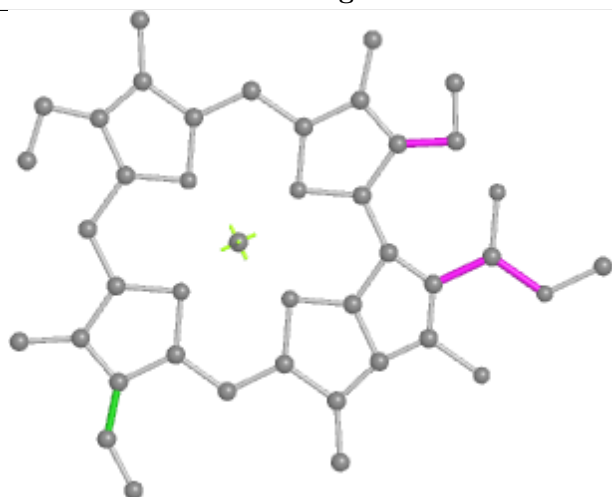
Ligand CLA j 103



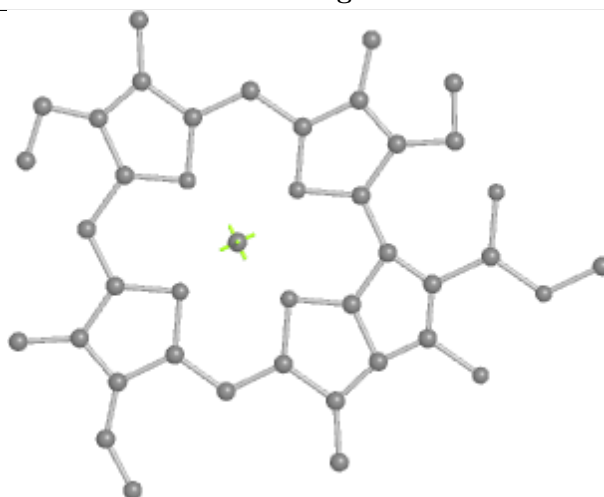
Bond lengths



Bond angles

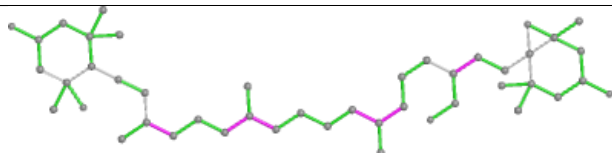


Torsions

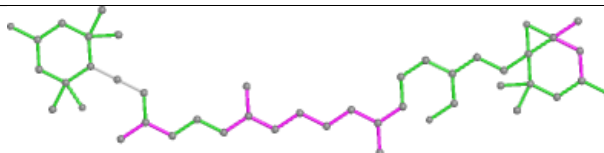


Rings

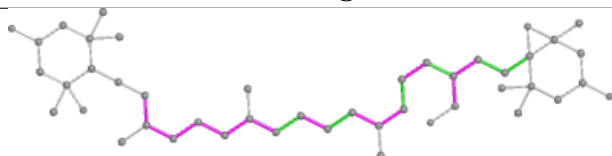
Ligand A1L1G 3 306



Bond lengths



Bond angles

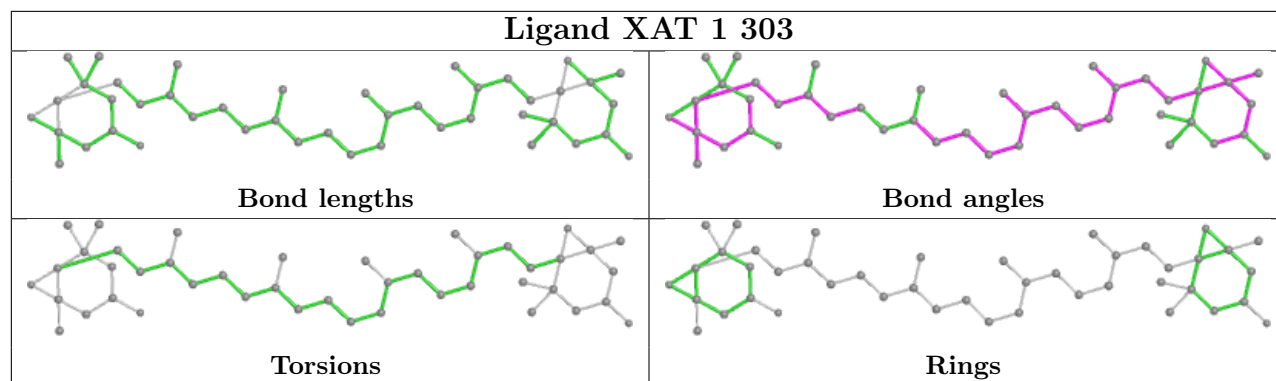


Torsions

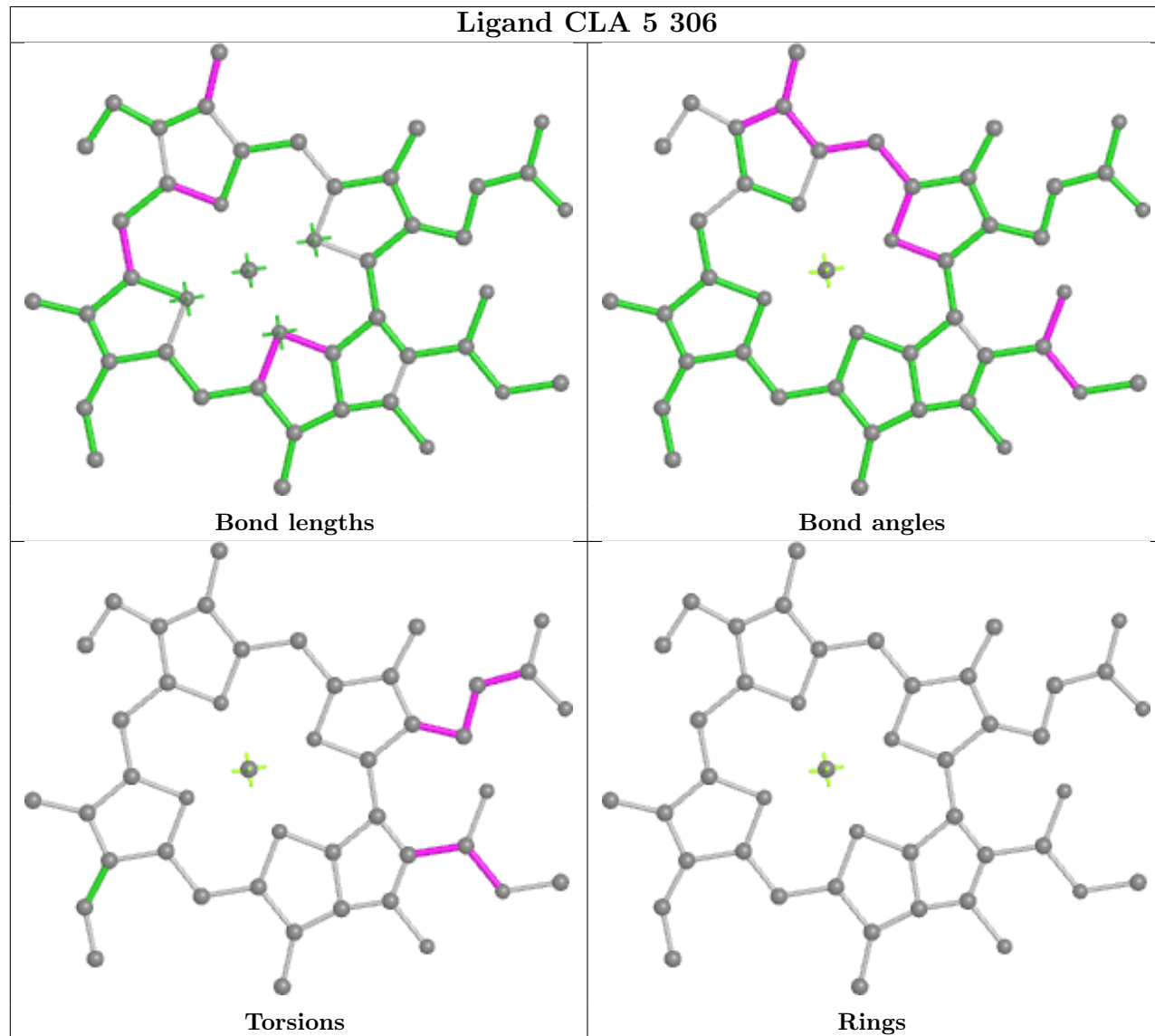


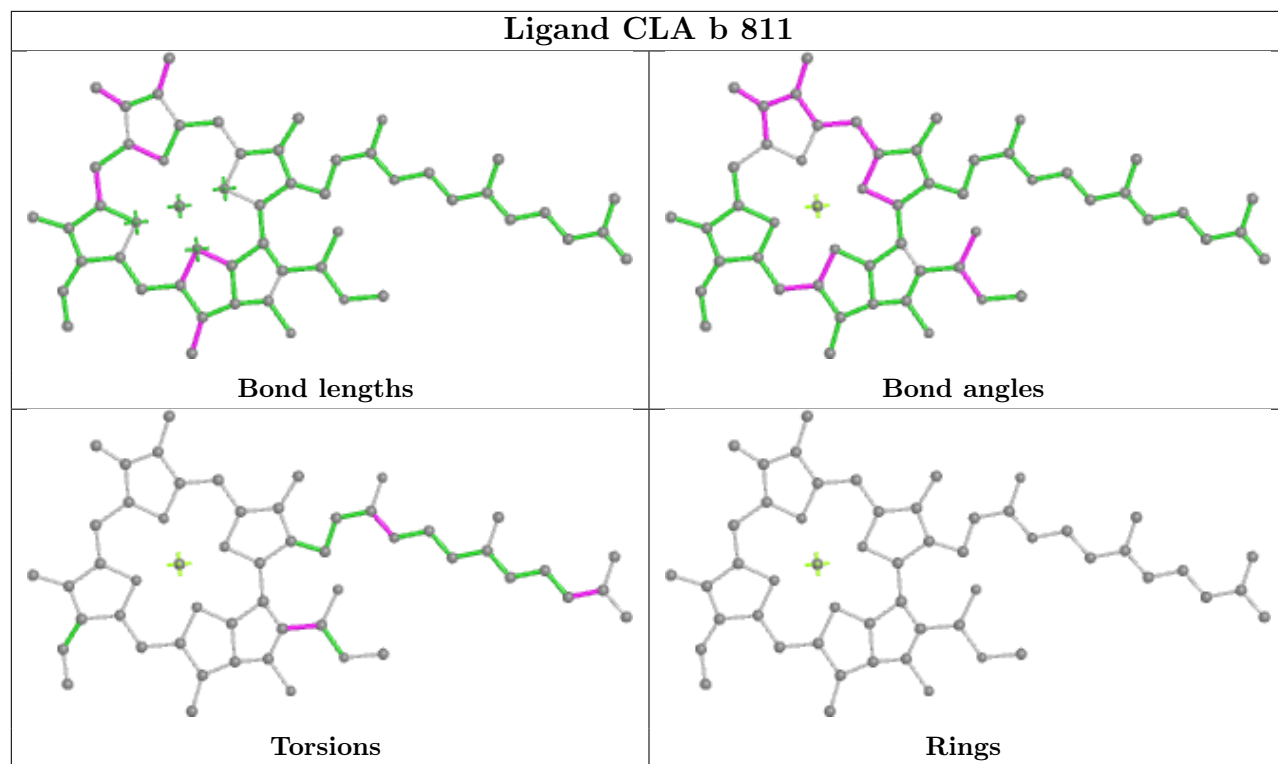
Rings

Ligand XAT 1 303

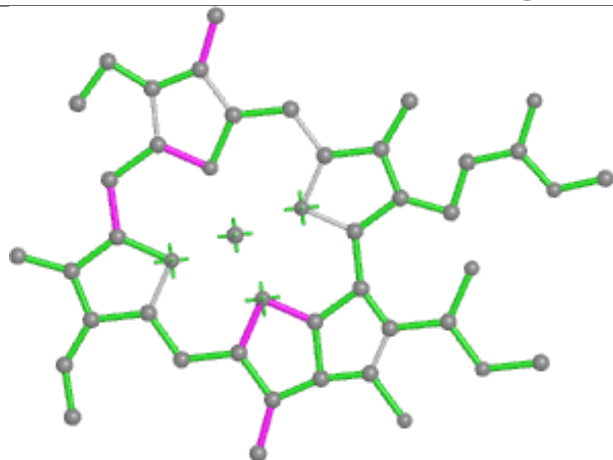


Ligand CLA 5 306

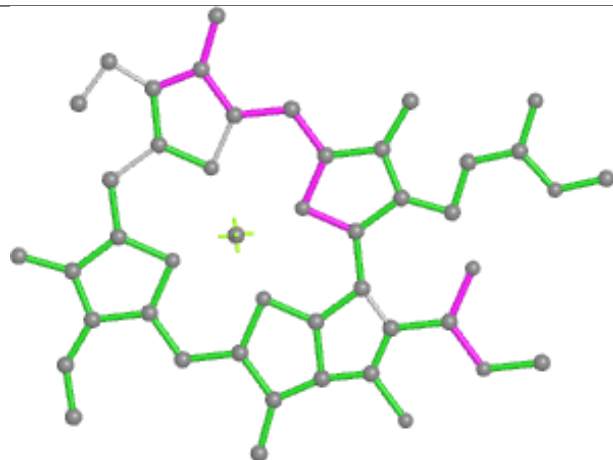




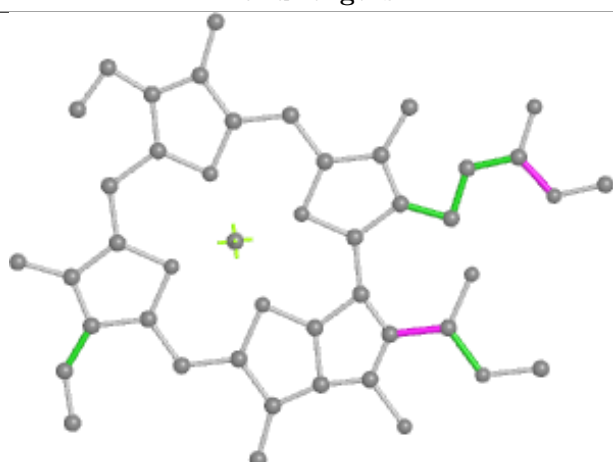
Ligand CLA 8 313



Bond lengths



Bond angles

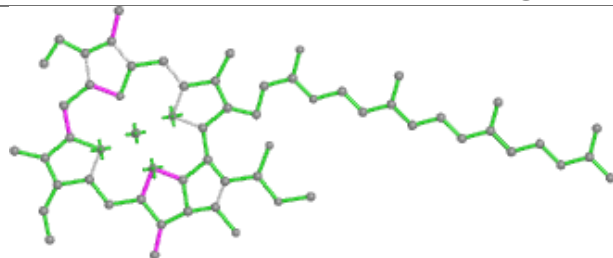


Torsions

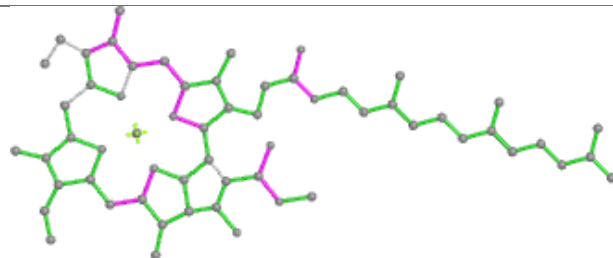


Rings

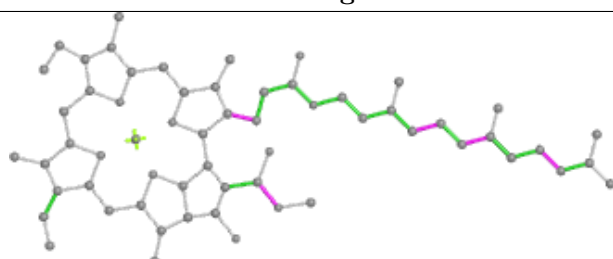
Ligand CLA b 822



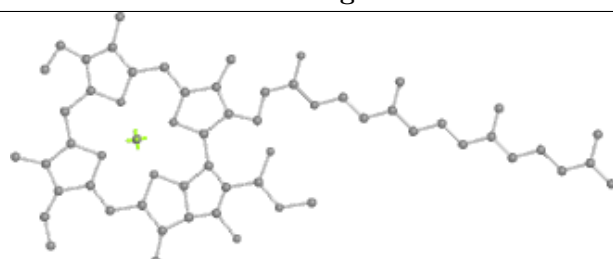
Bond lengths



Bond angles

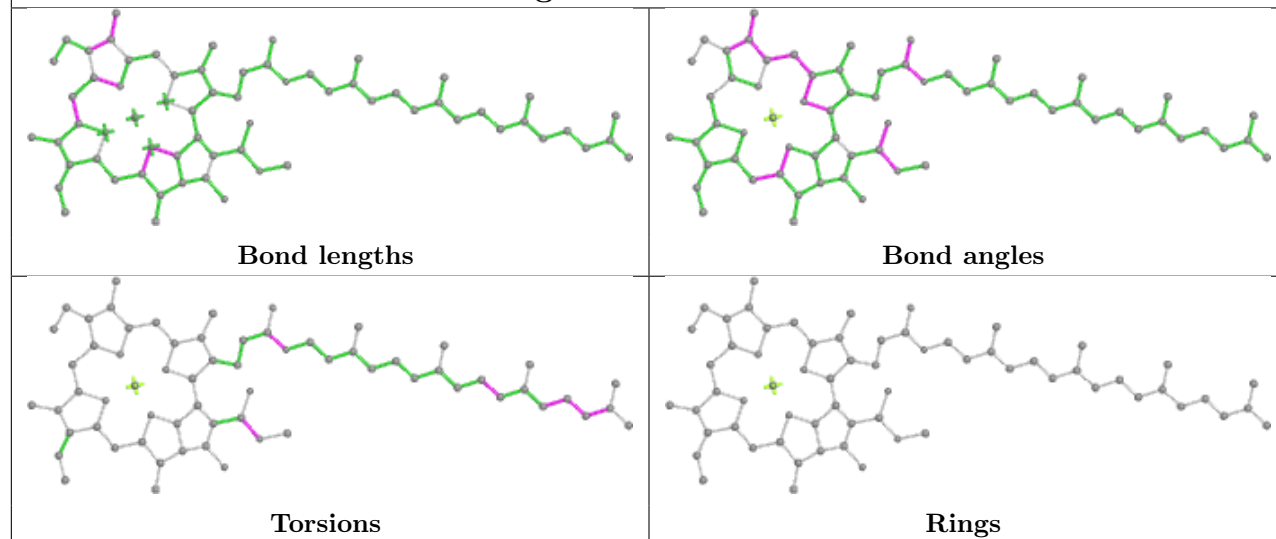


Torsions

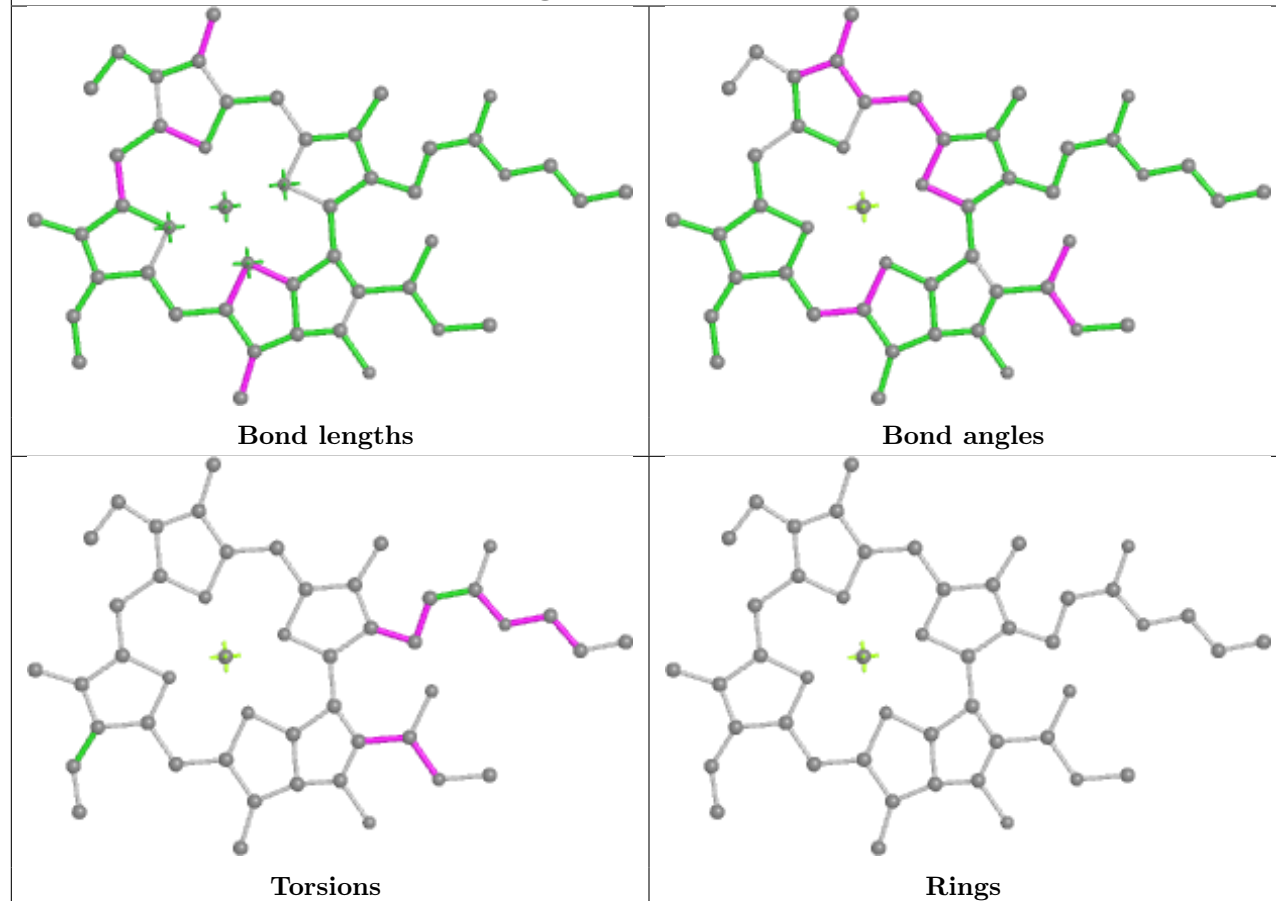


Rings

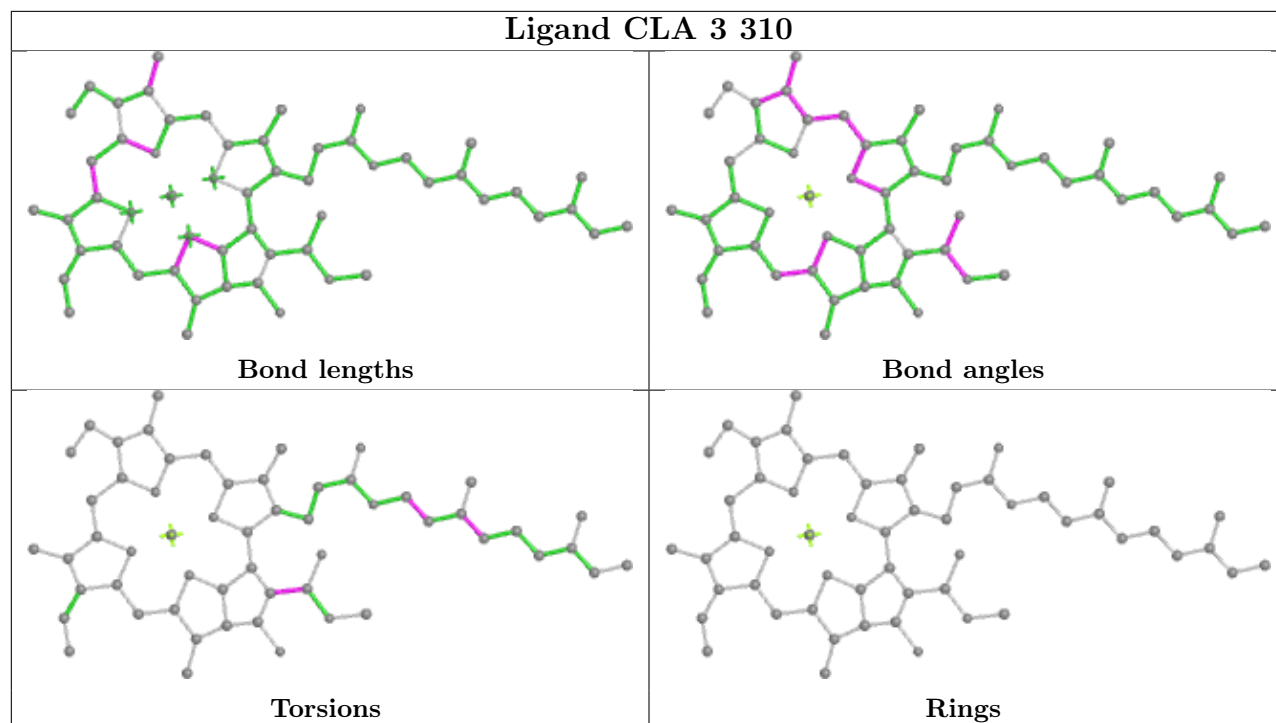
Ligand CLA b 840



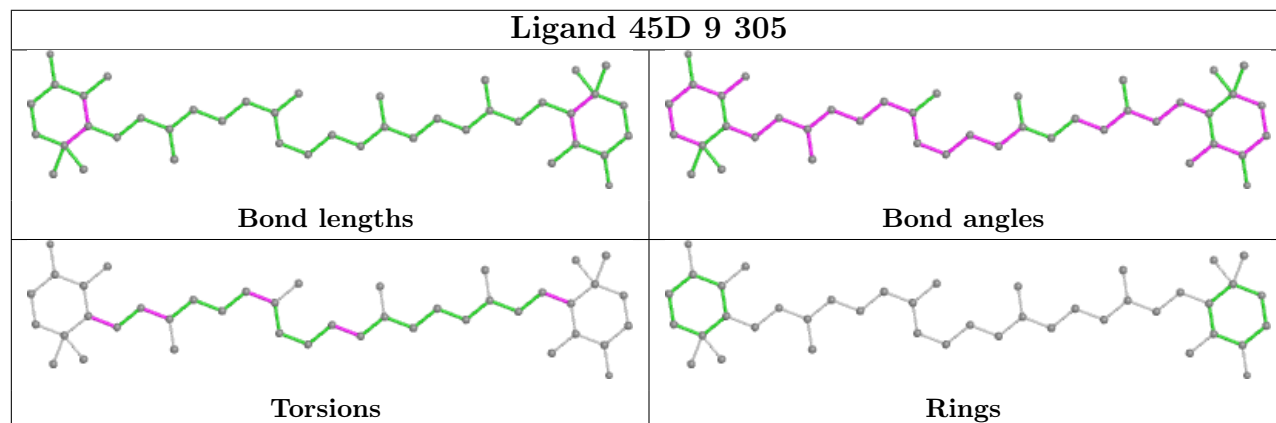
Ligand CLA 7 306

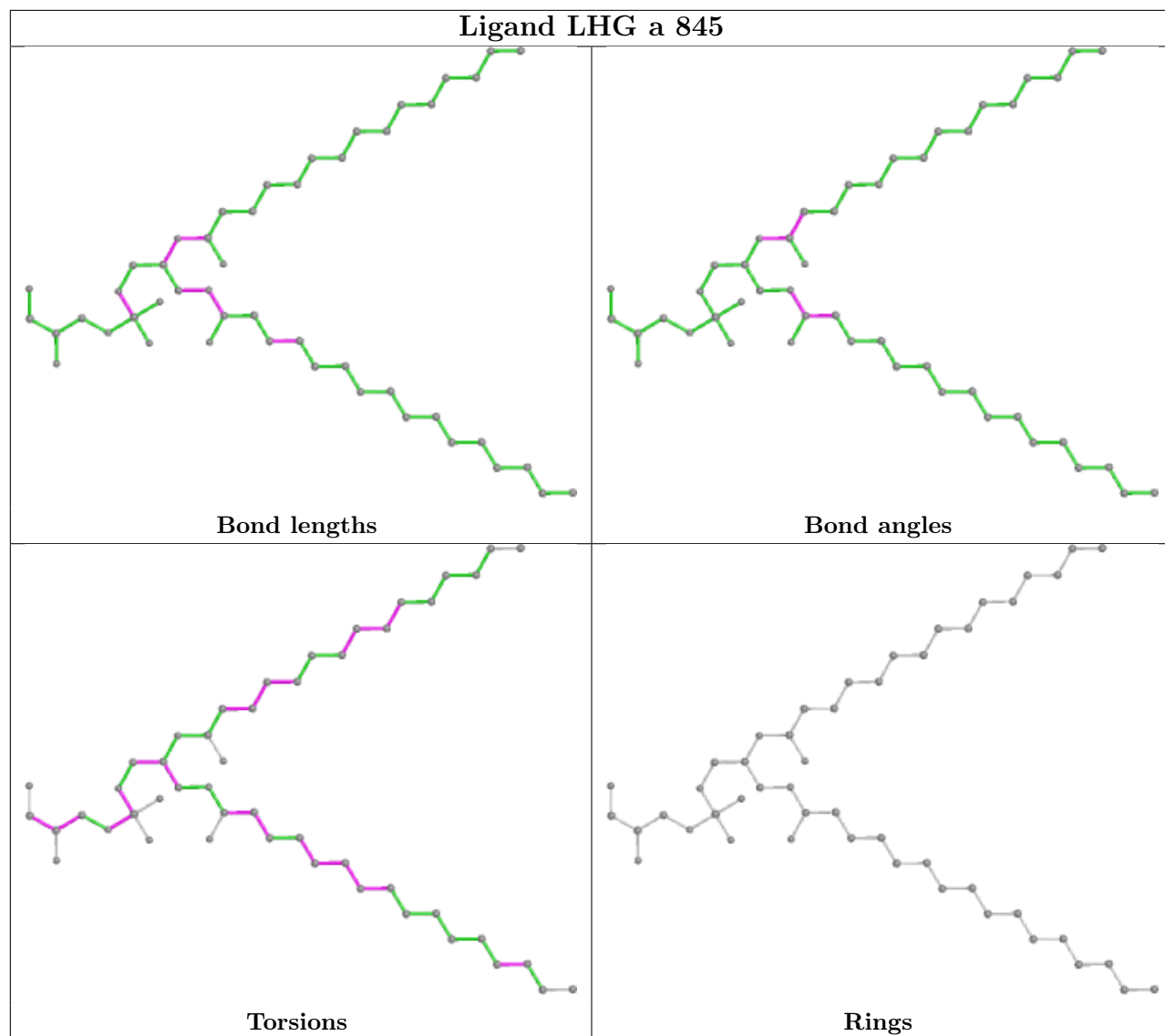


Ligand CLA 3 310

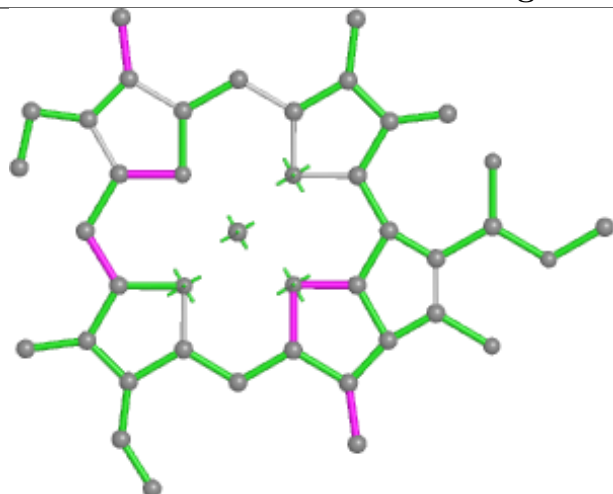


Ligand 45D 9 305

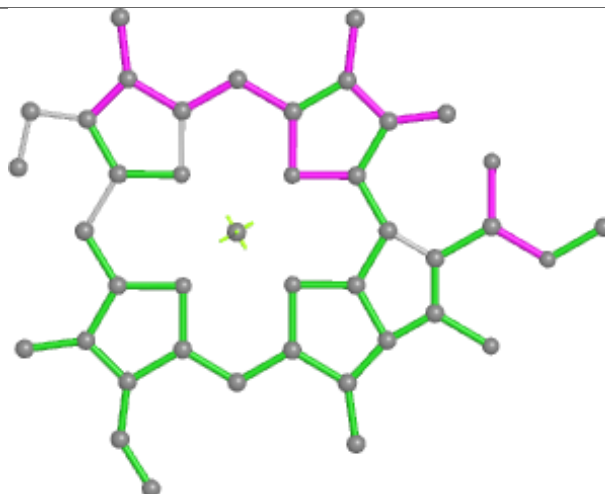




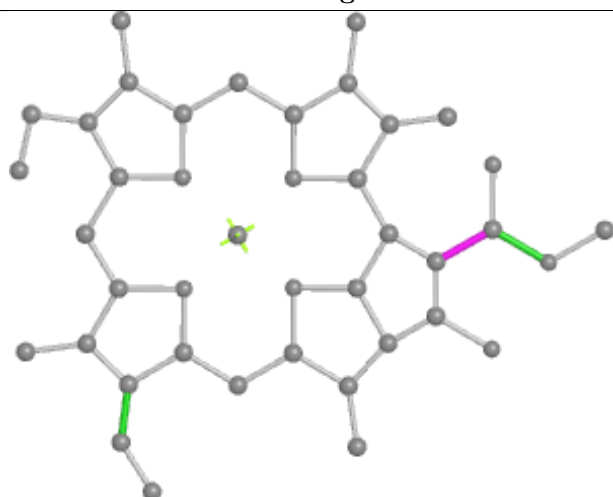
Ligand CLA b 830



Bond lengths



Bond angles

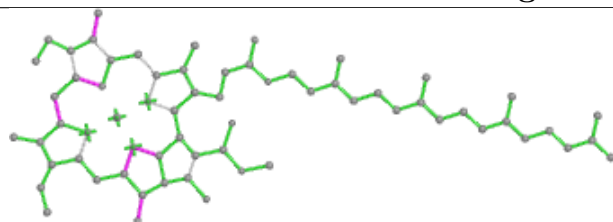


Torsions

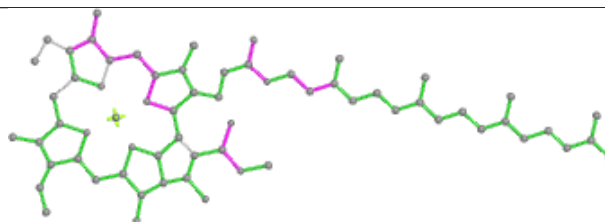


Rings

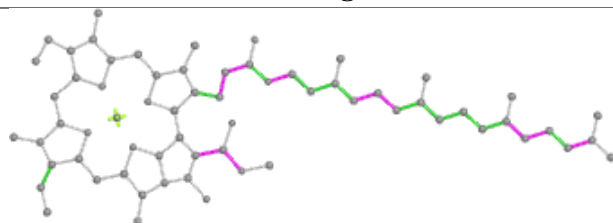
Ligand CLA a 810



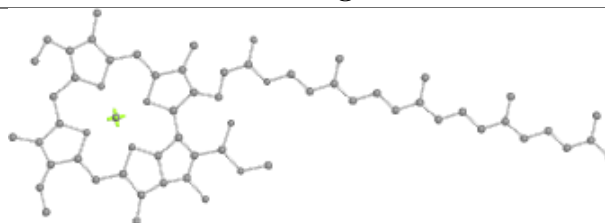
Bond lengths



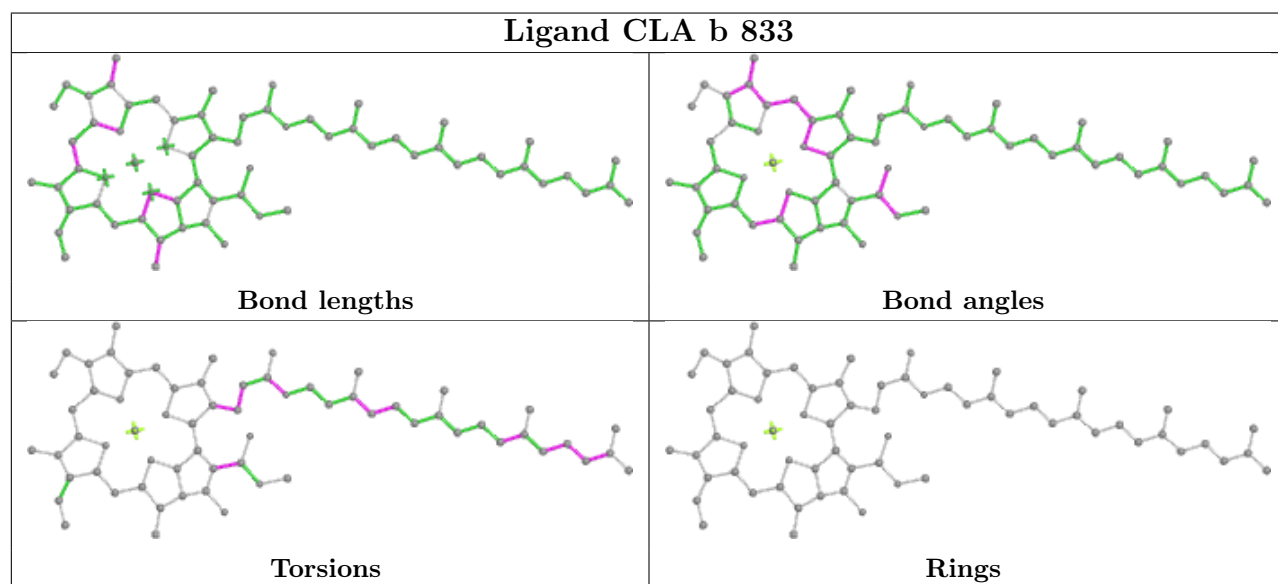
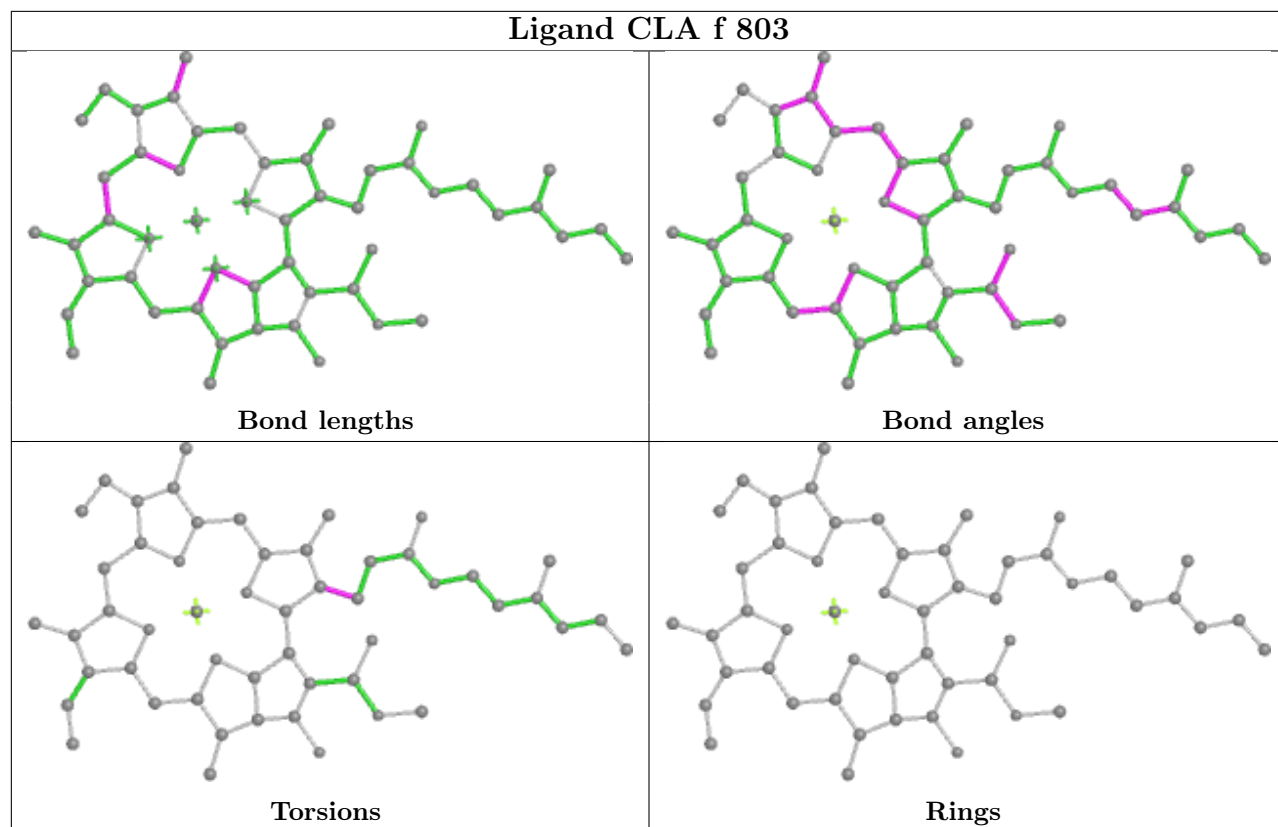
Bond angles



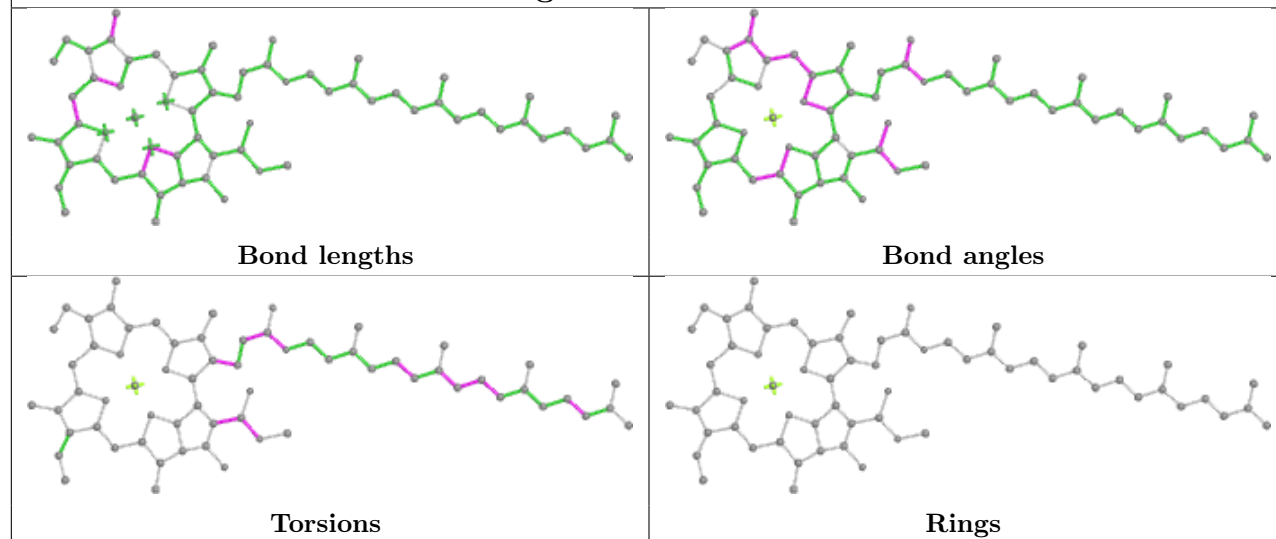
Torsions



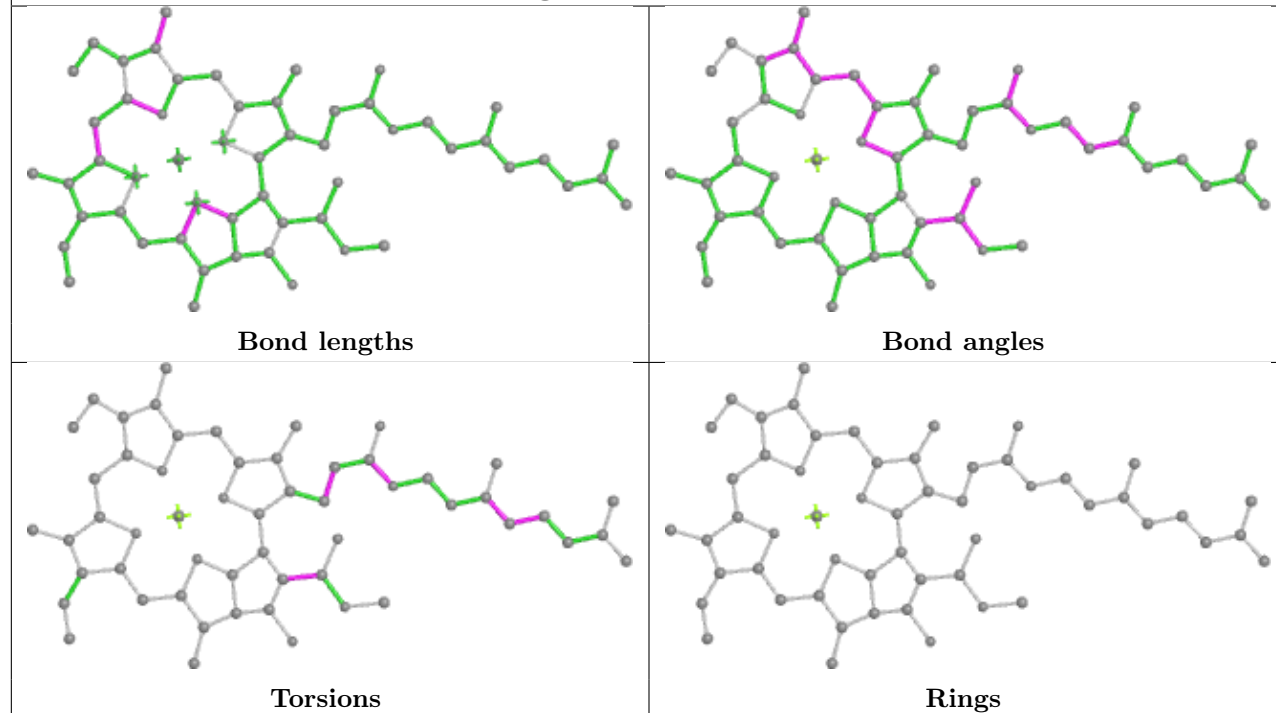
Rings



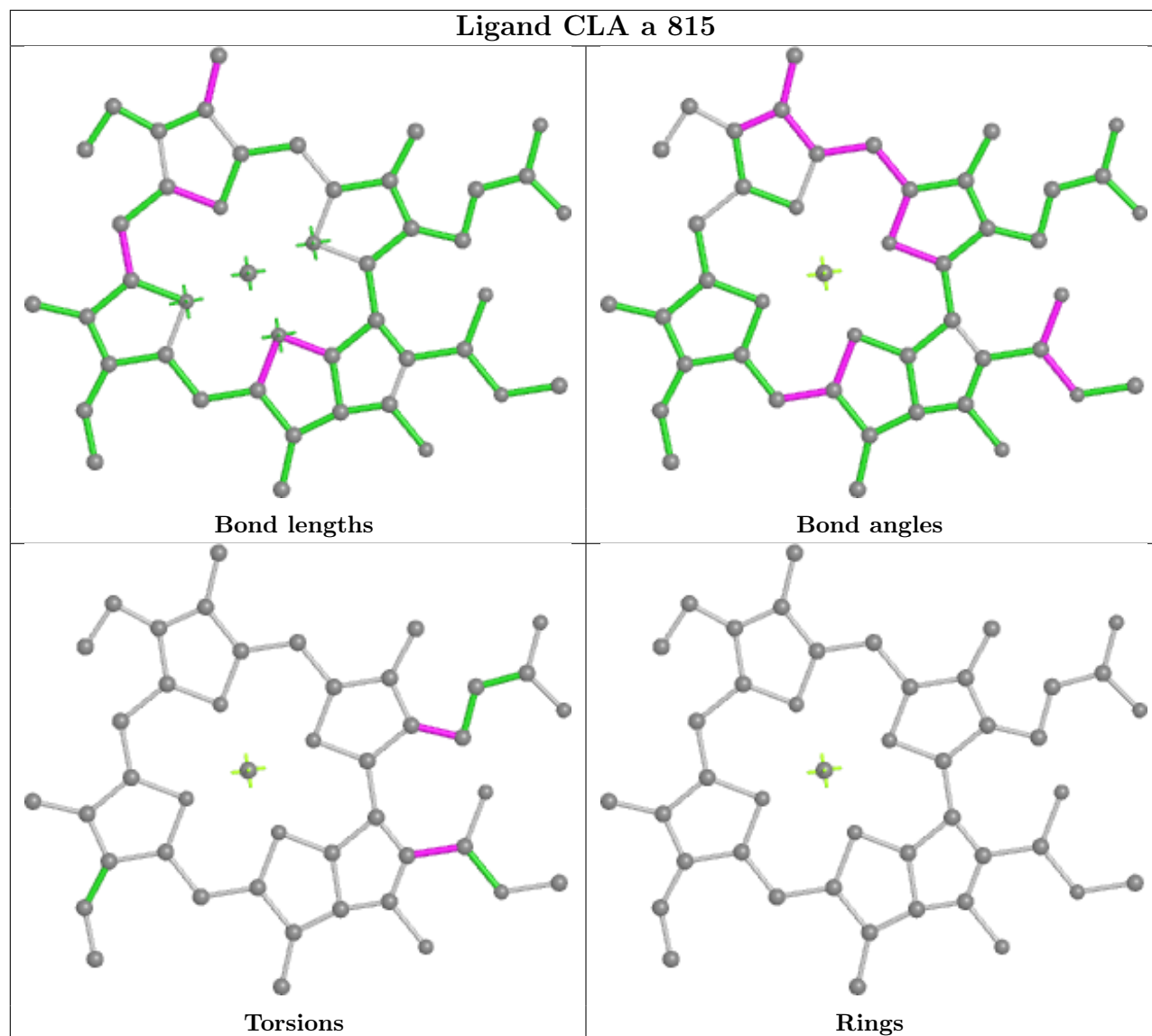
Ligand CLA a 854



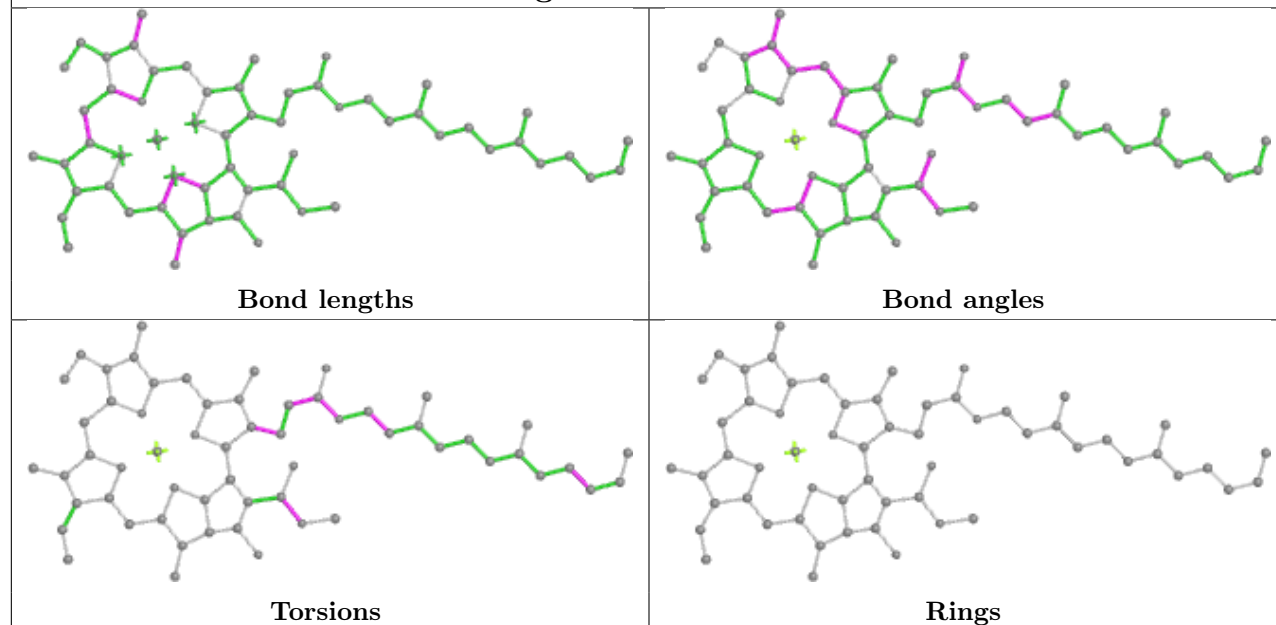
Ligand CLA 8 308



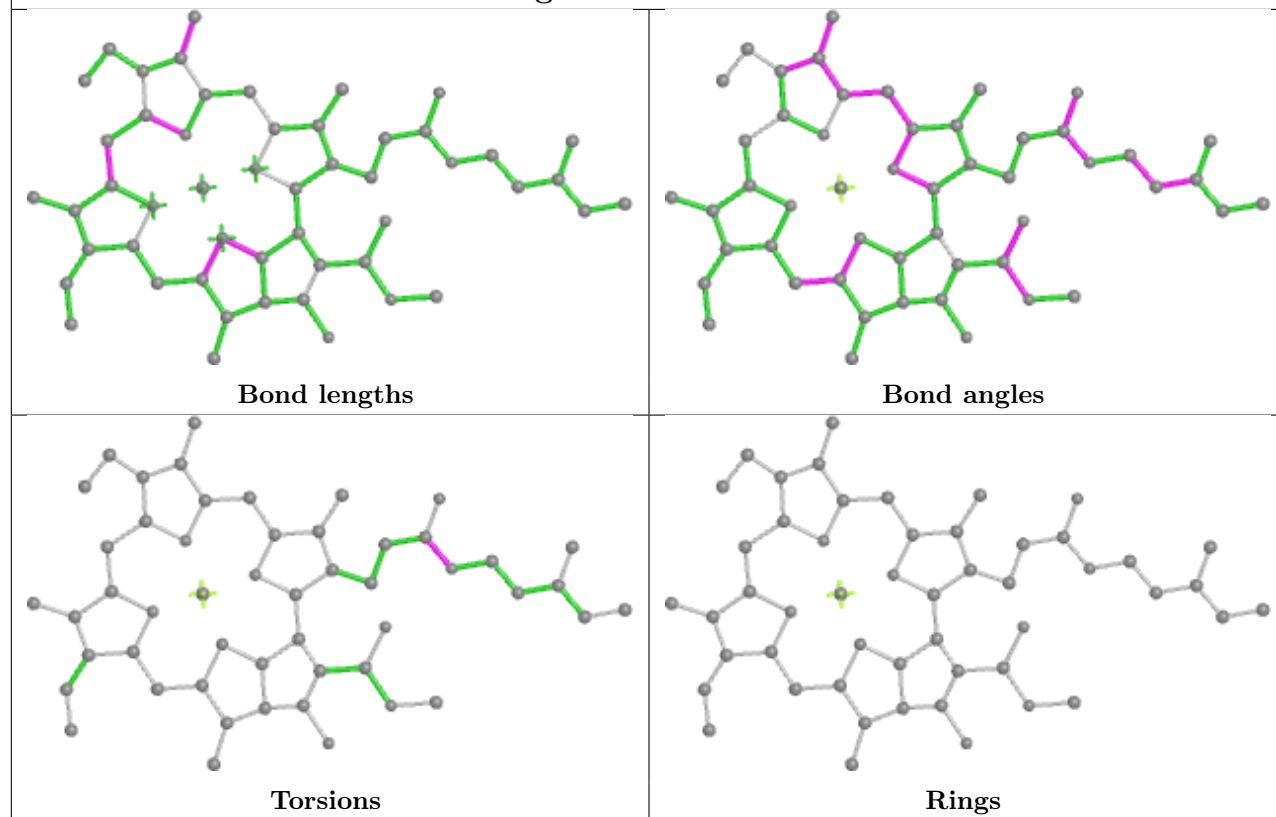
Ligand CLA a 815



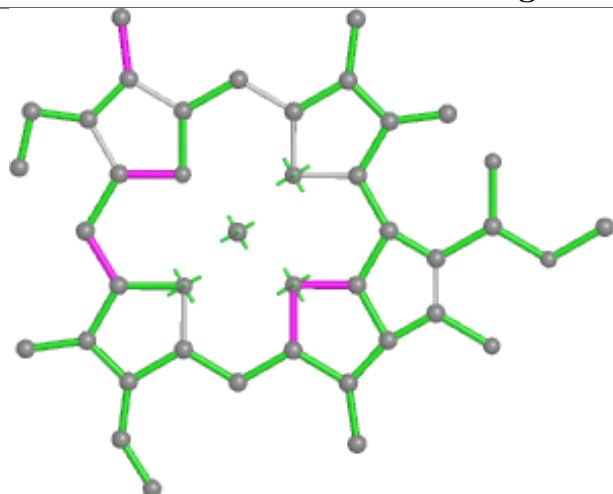
Ligand CLA b 817



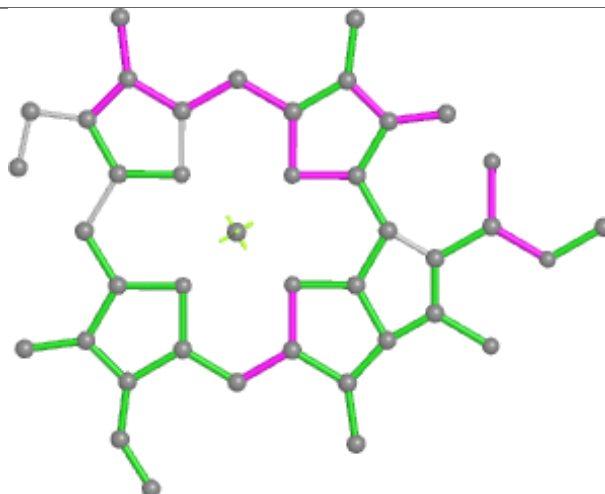
Ligand CLA b 821



Ligand CLA 4 315



Bond lengths



Bond angles

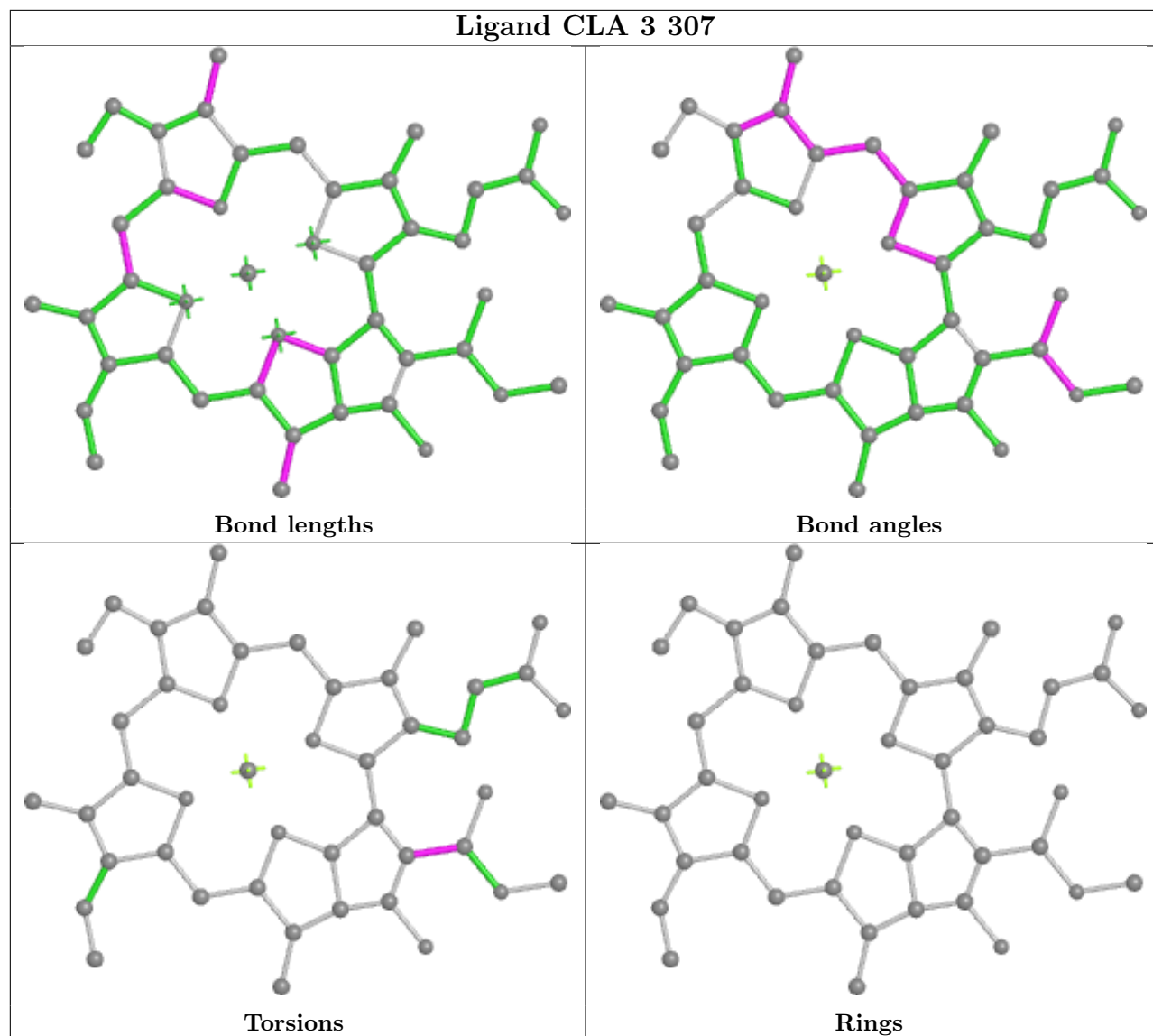


Torsions

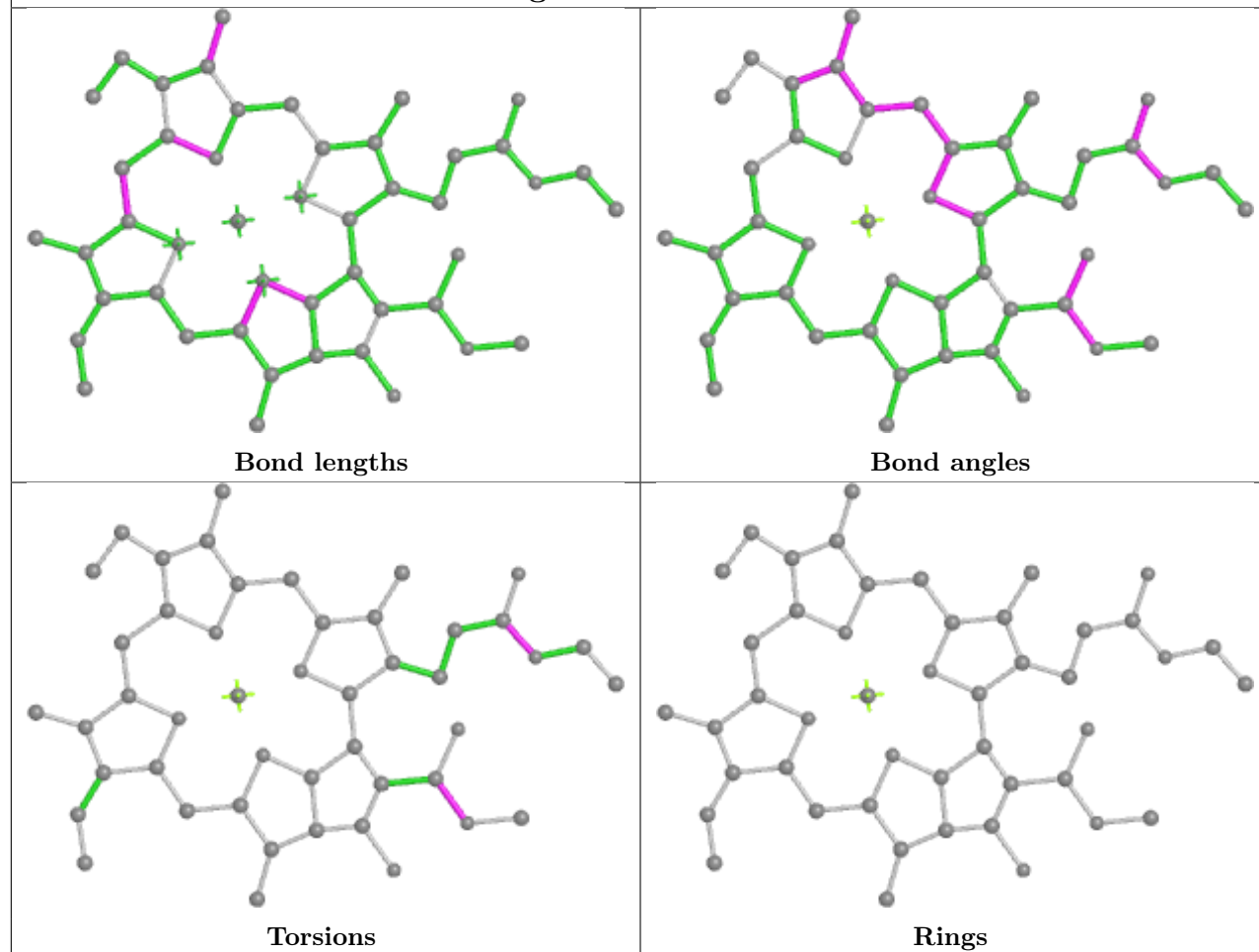


Rings

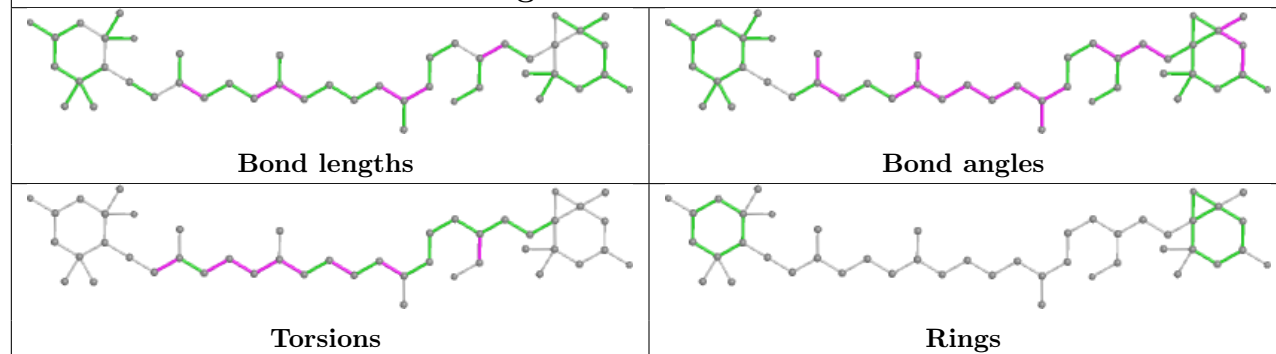
Ligand CLA 3 307



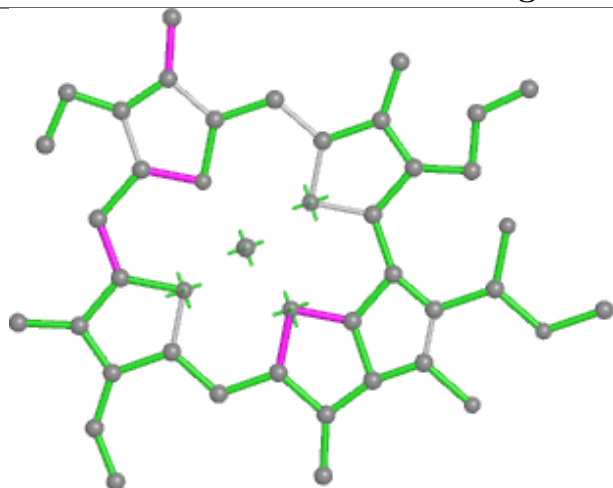
Ligand CLA 2 312



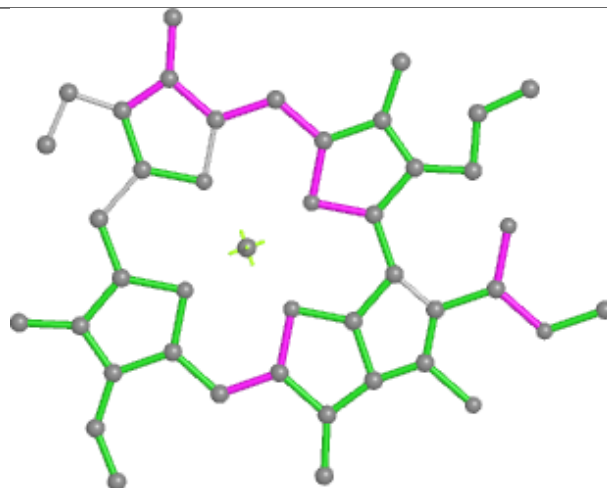
Ligand A1L1G 1 301



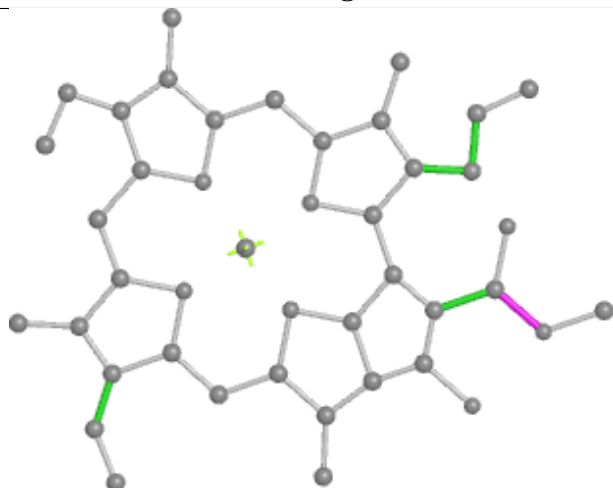
Ligand CLA 8 305



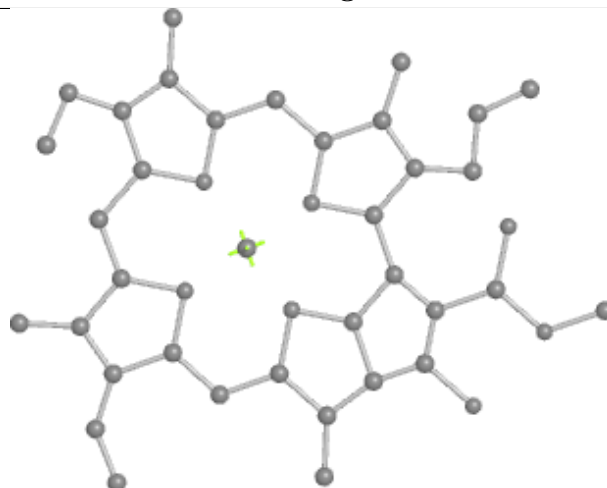
Bond lengths



Bond angles

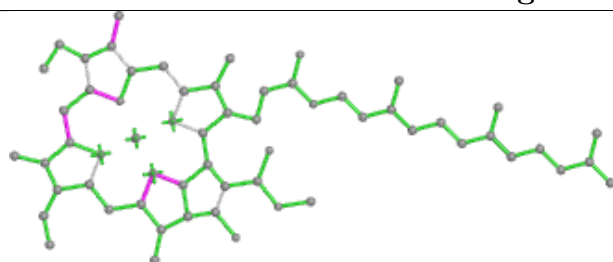


Torsions

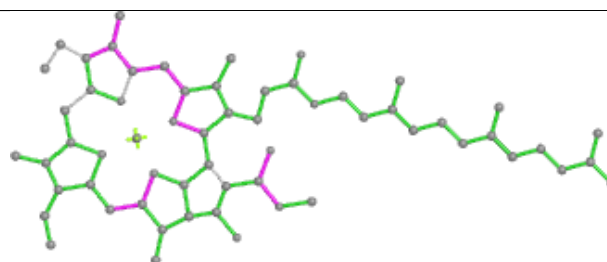


Rings

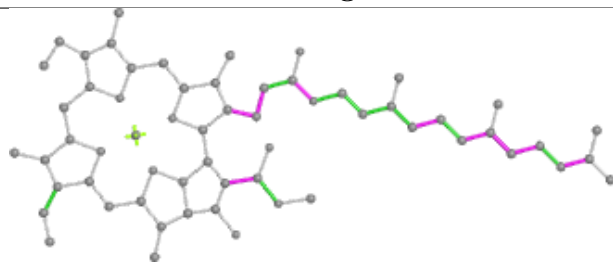
Ligand CLA b 818



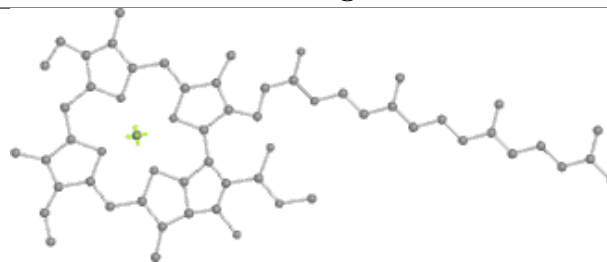
Bond lengths



Bond angles

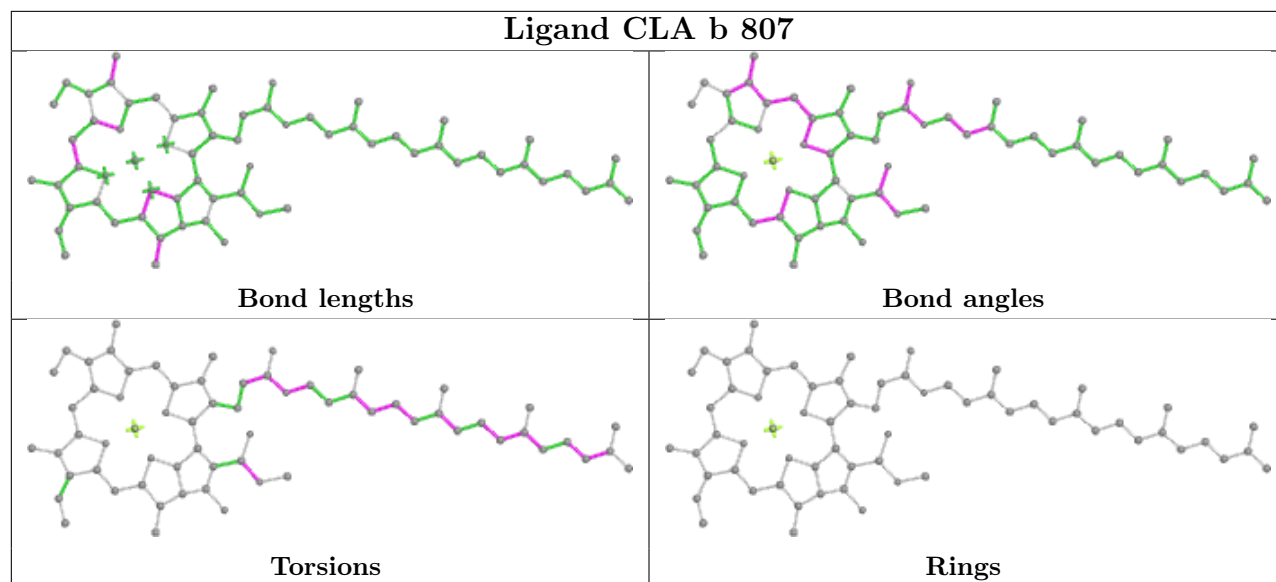


Torsions

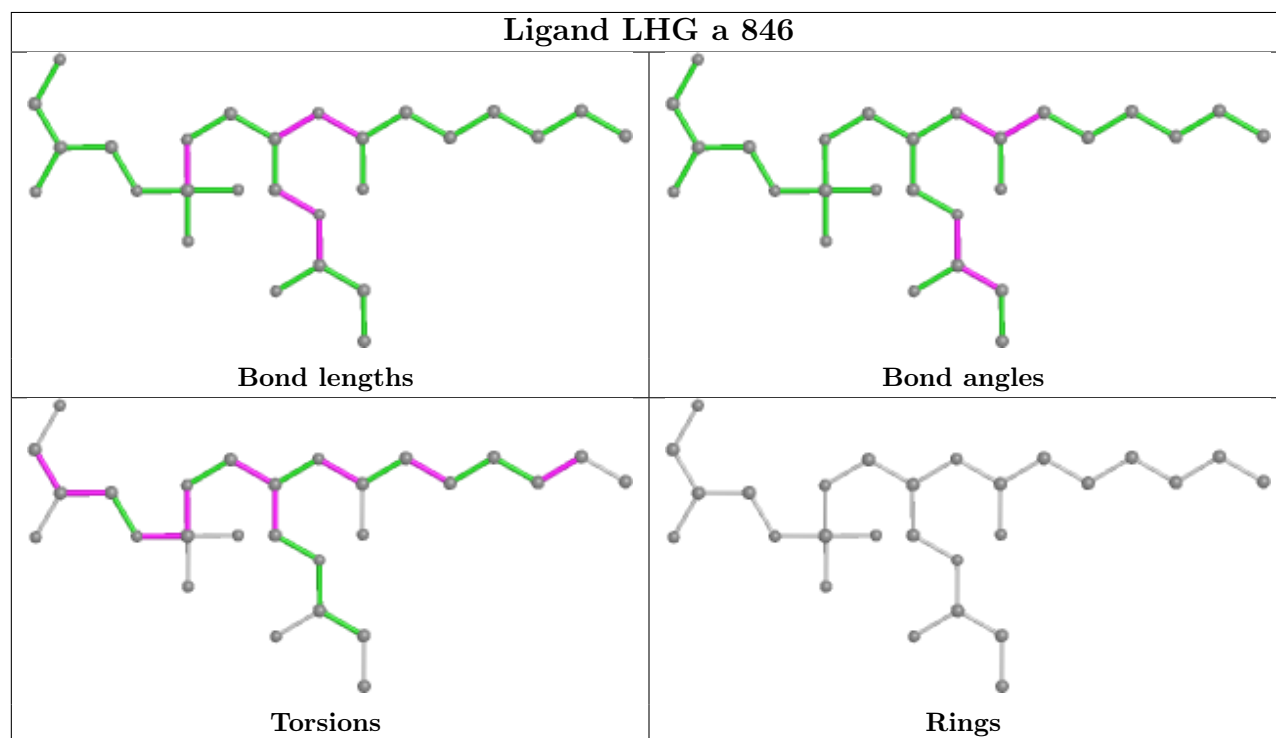


Rings

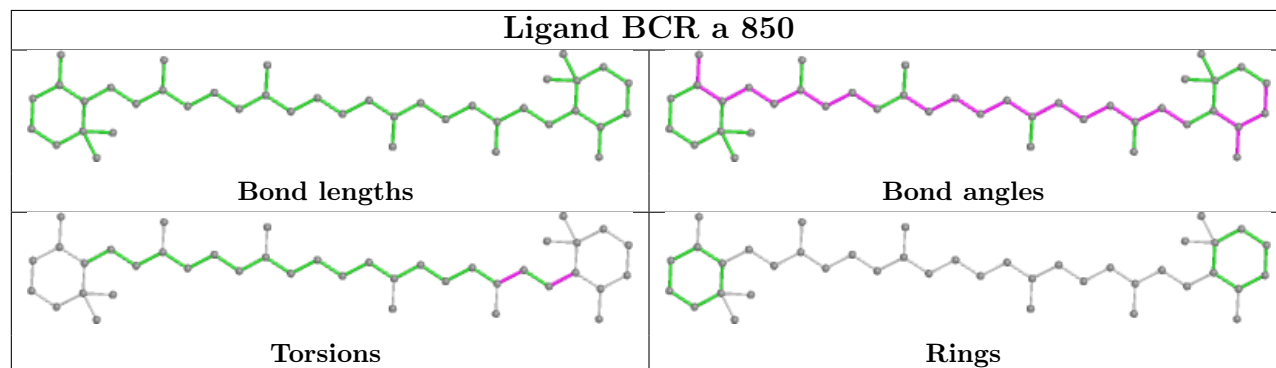
Ligand CLA b 807



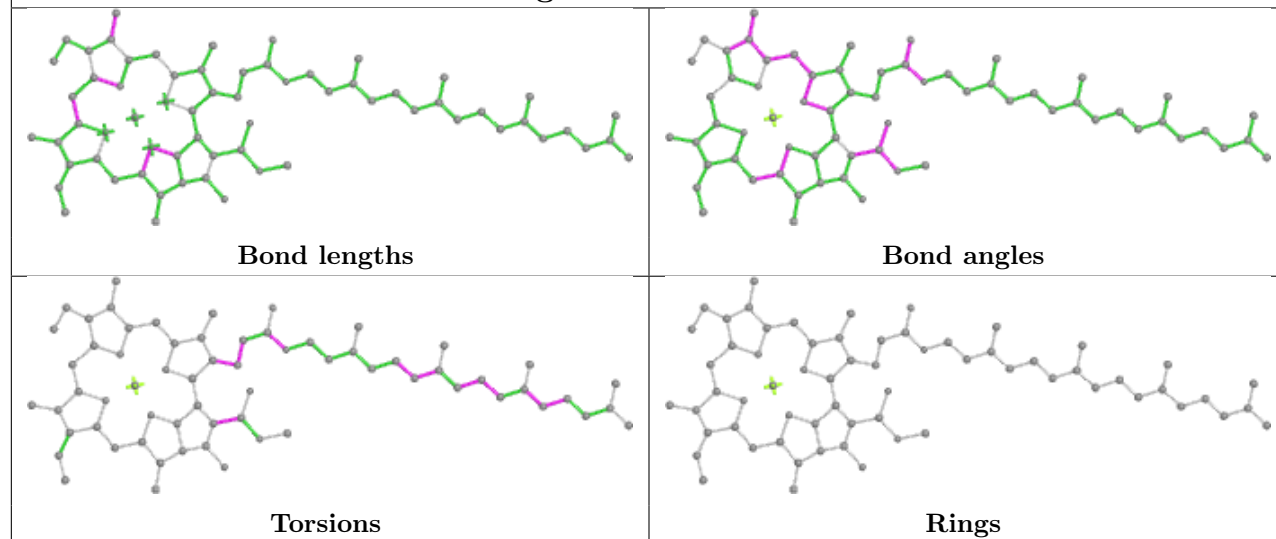
Ligand LHG a 846



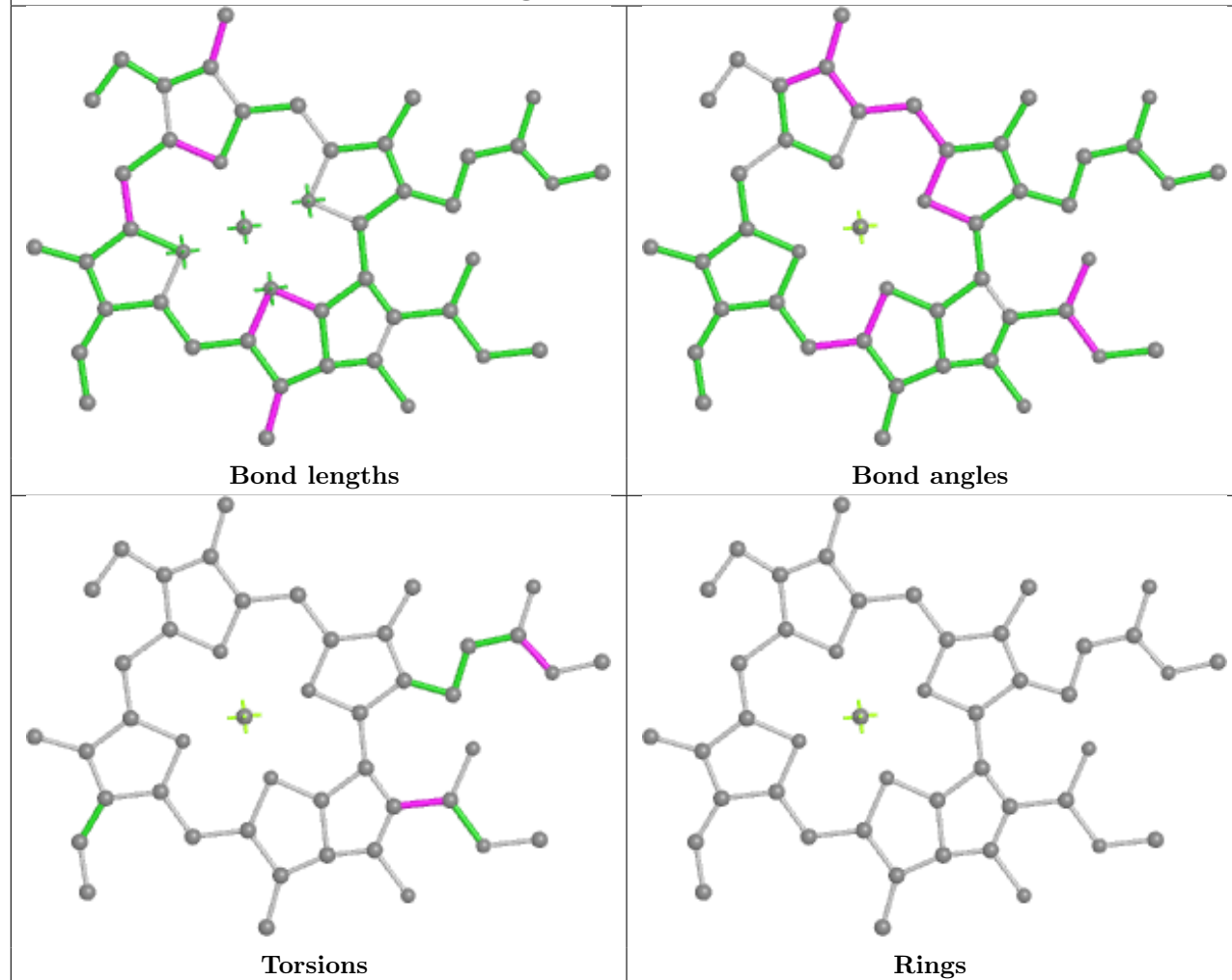
Ligand BCR a 850



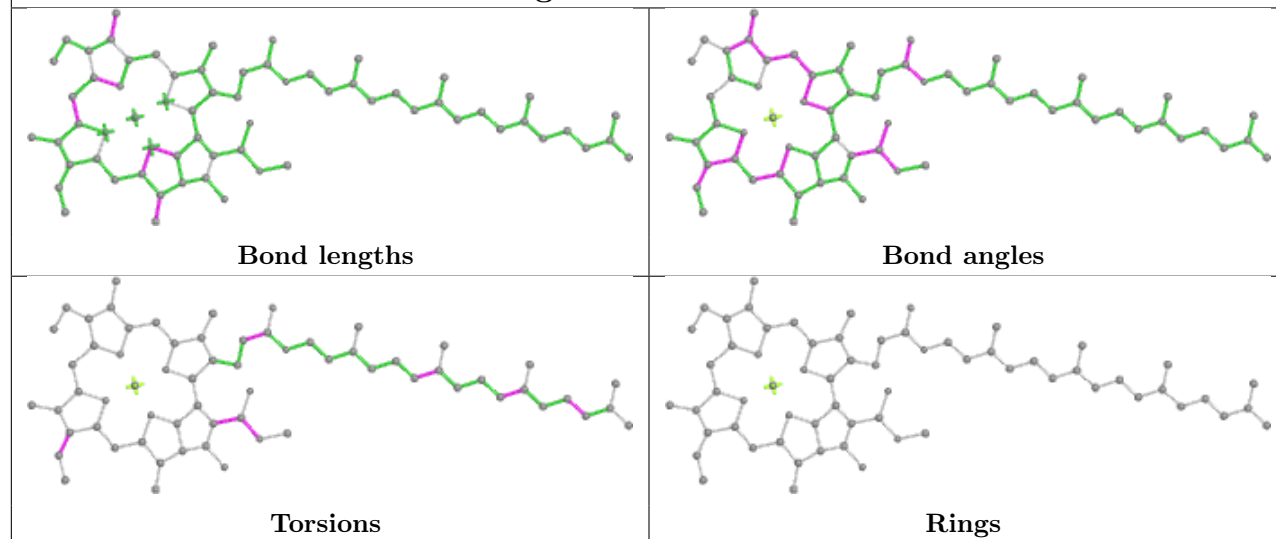
Ligand CLA a 809



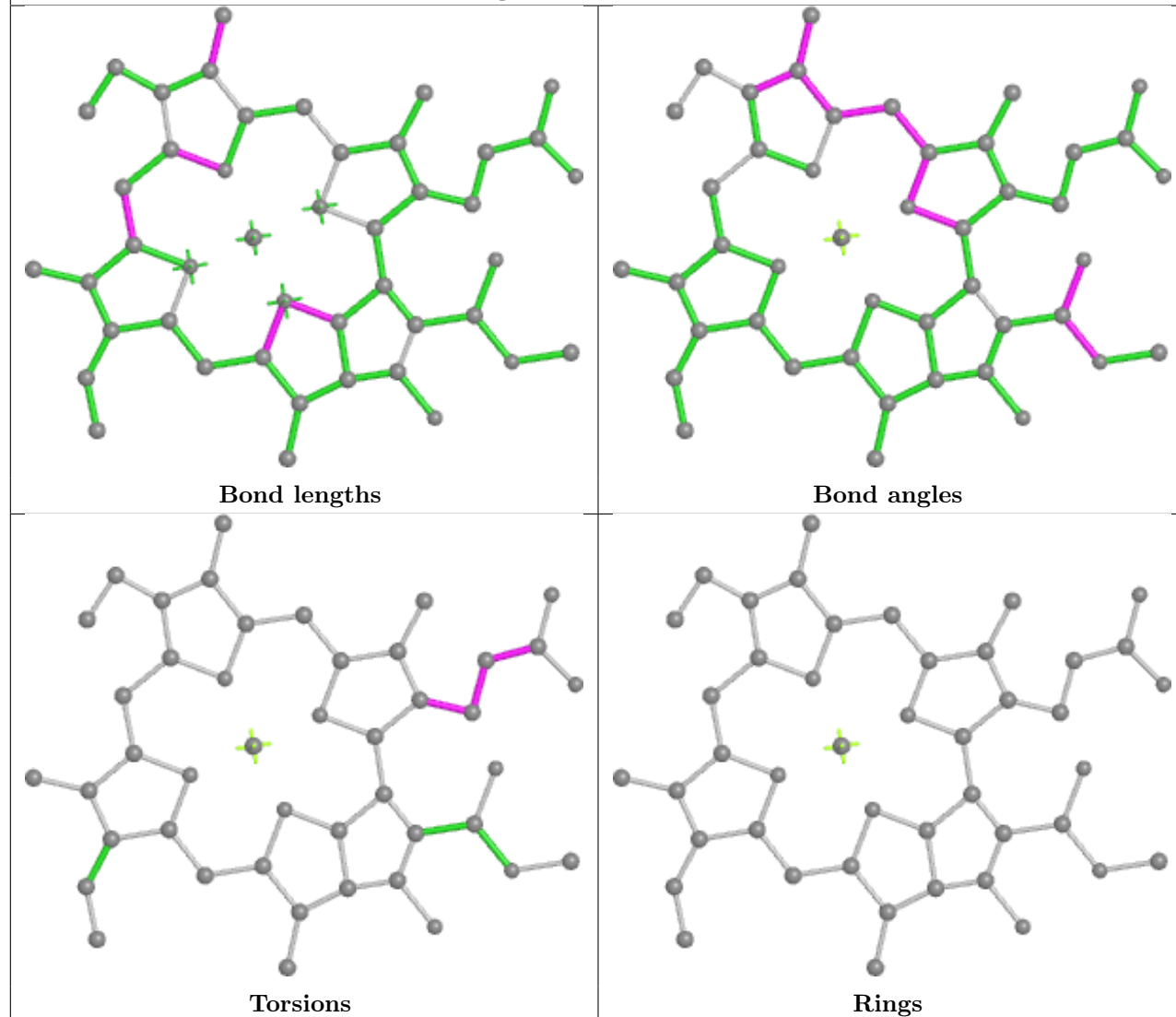
Ligand CLA 9 309

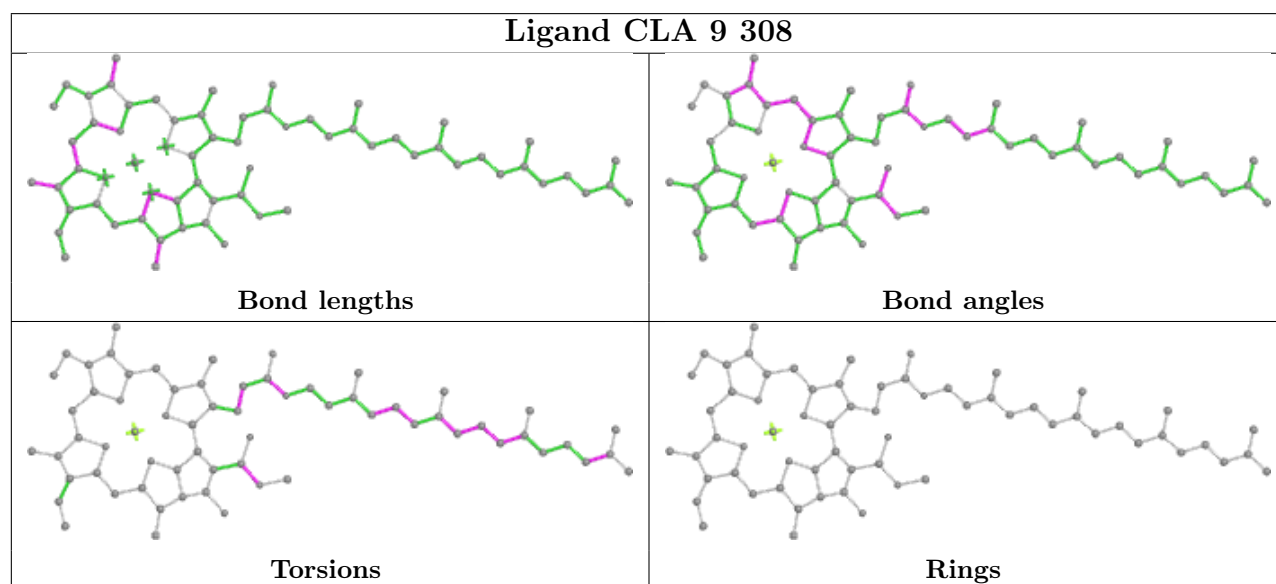
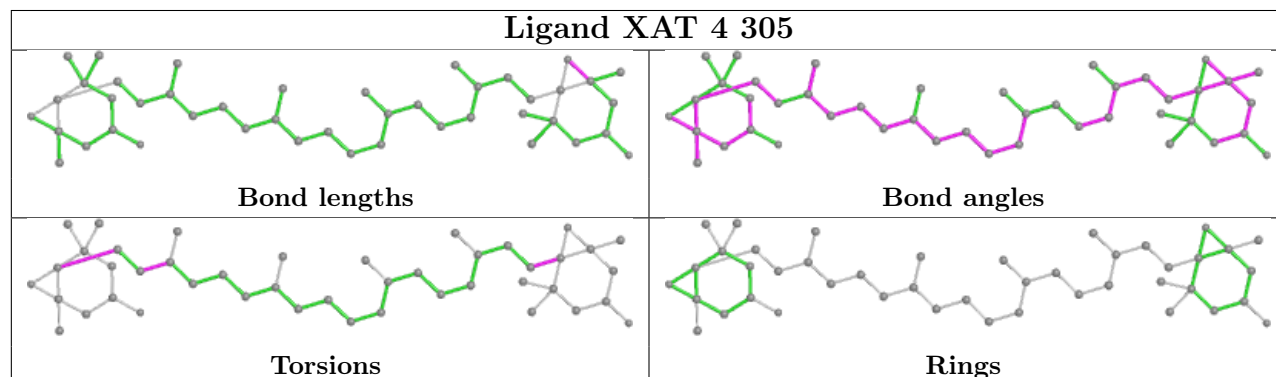
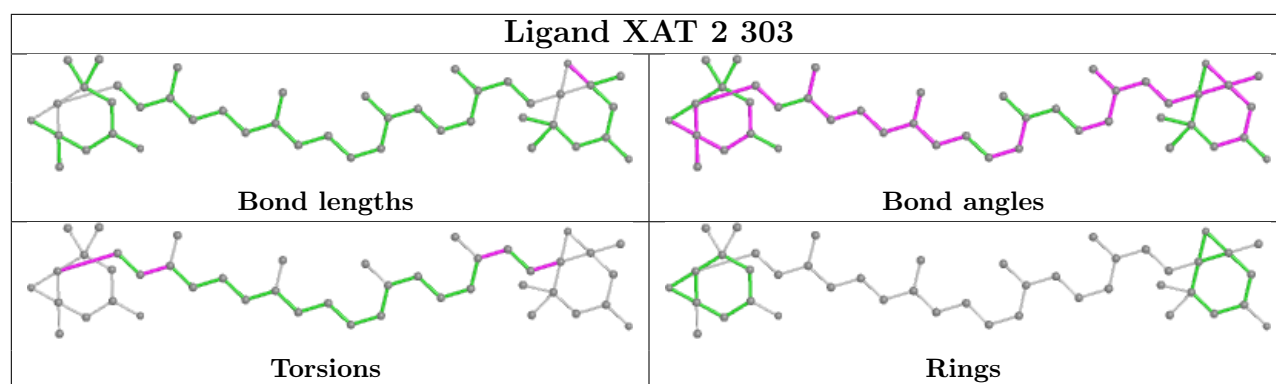


Ligand CLA b 804

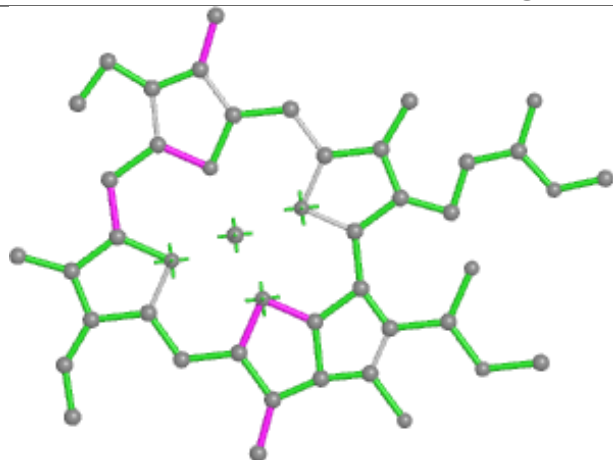


Ligand CLA 1 314

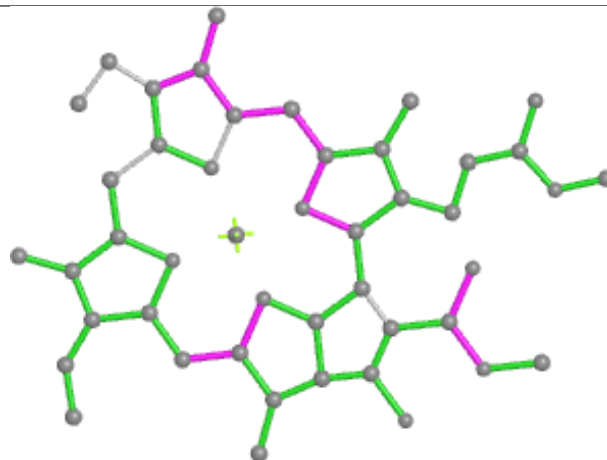




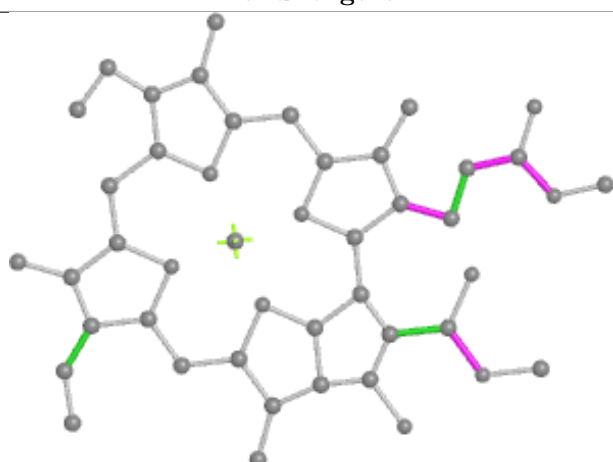
Ligand CLA 3 315



Bond lengths



Bond angles

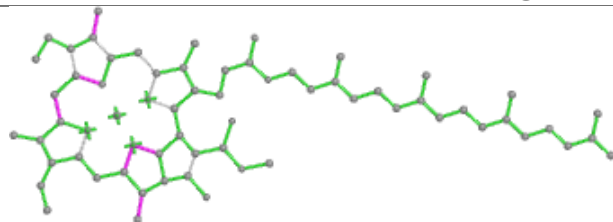


Torsions

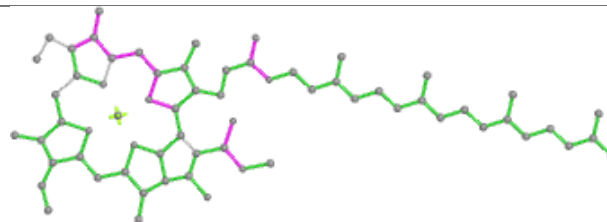


Rings

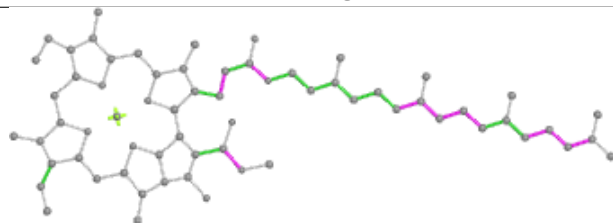
Ligand CLA b 827



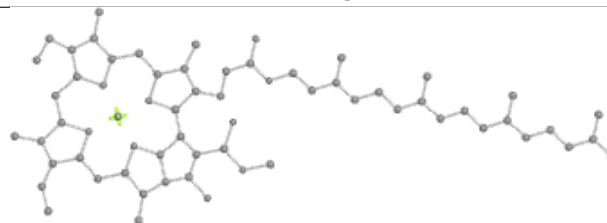
Bond lengths



Bond angles

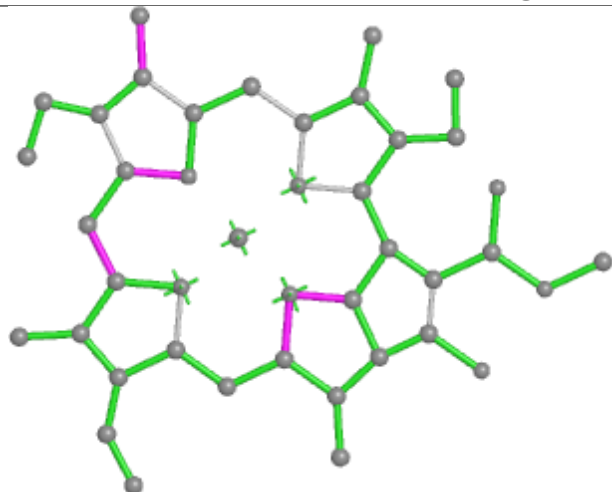


Torsions

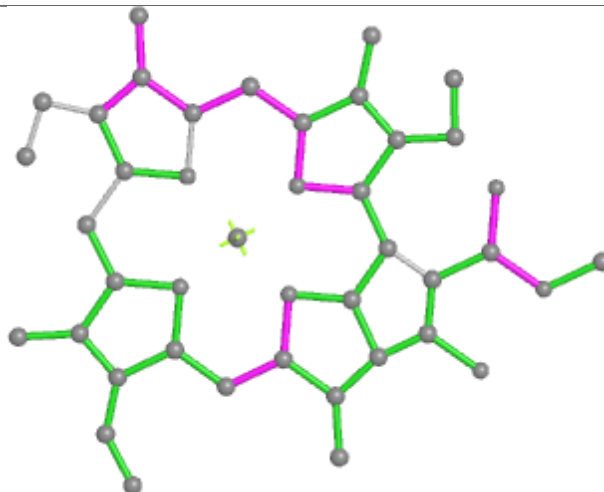


Rings

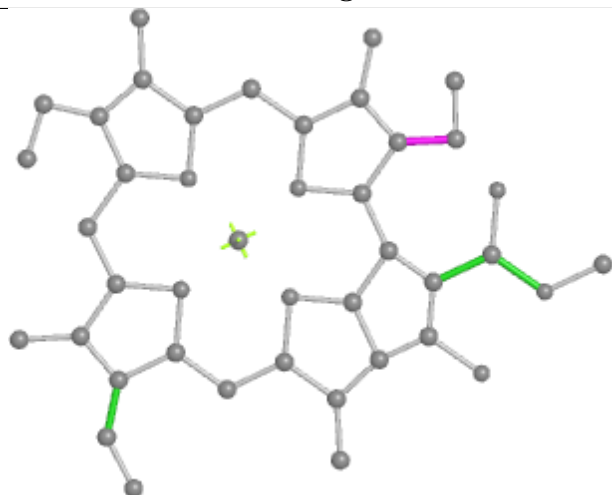
Ligand CLA 6 311



Bond lengths



Bond angles

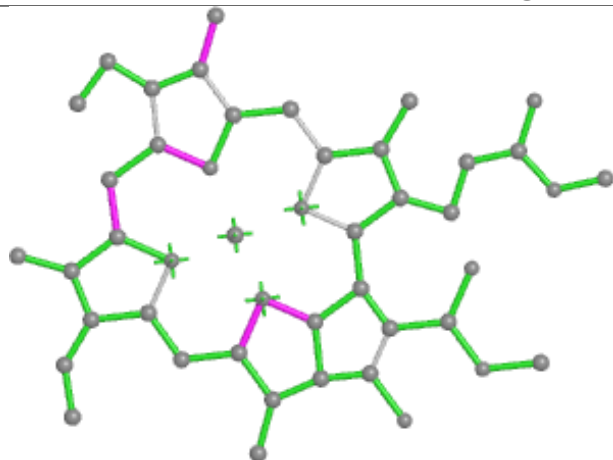


Torsions

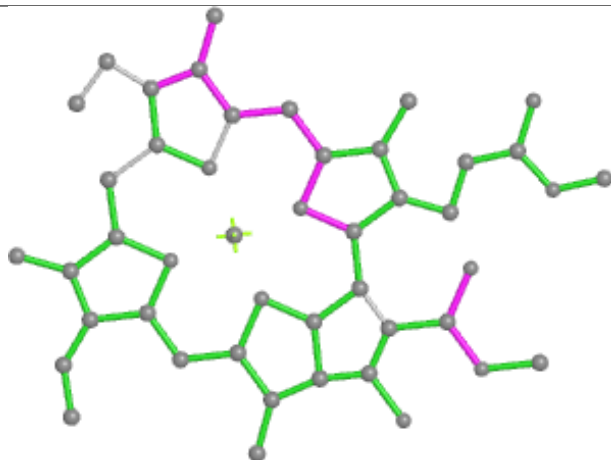


Rings

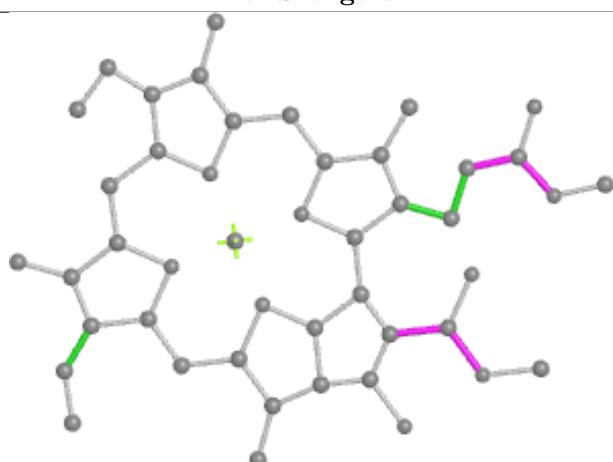
Ligand CLA 6 314



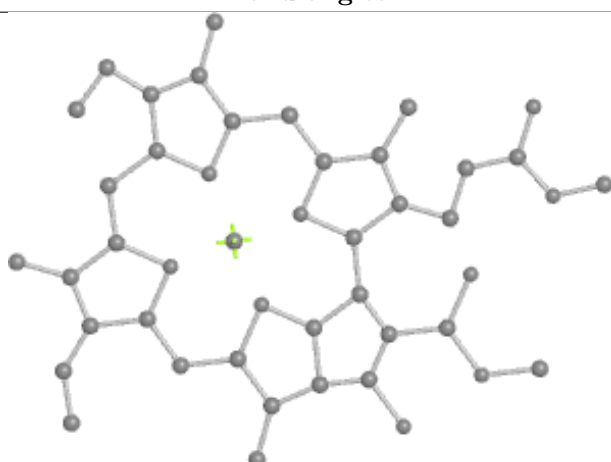
Bond lengths



Bond angles

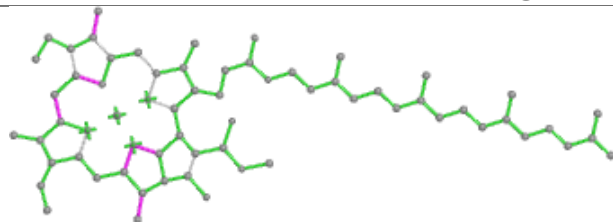


Torsions

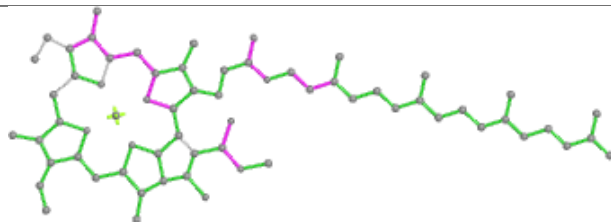


Rings

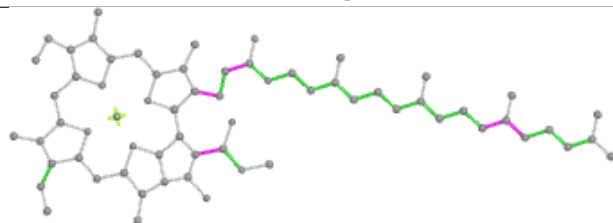
Ligand CLA b 837



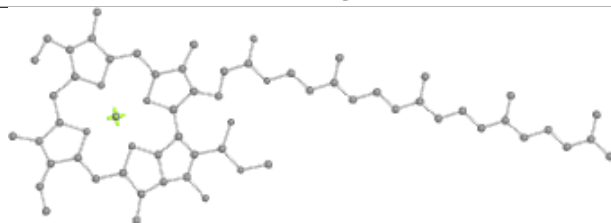
Bond lengths



Bond angles

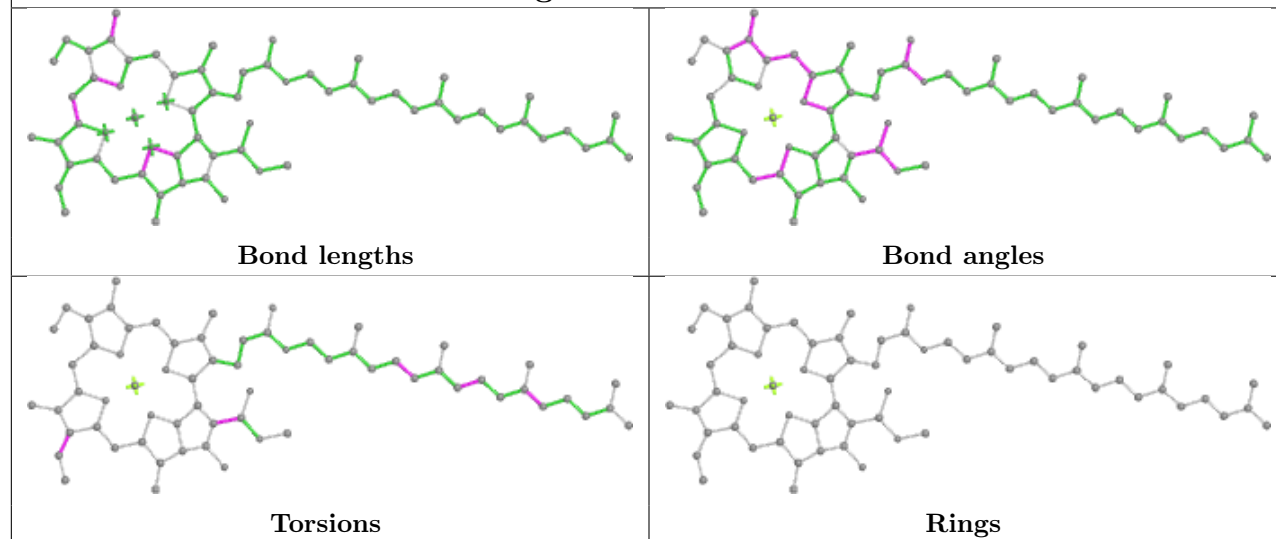


Torsions

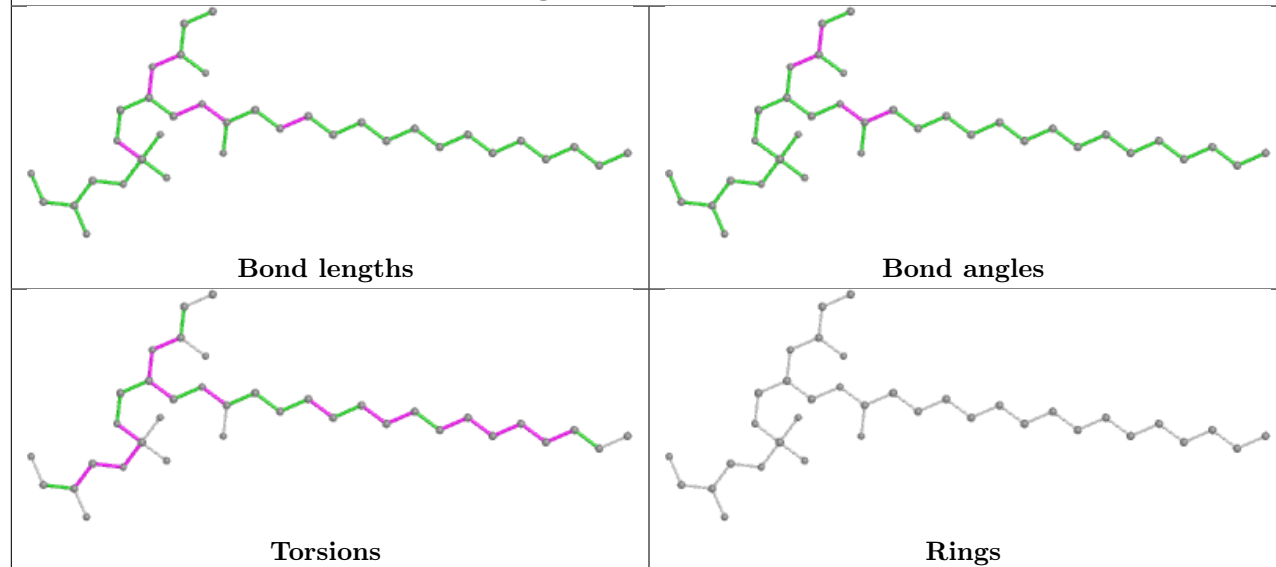


Rings

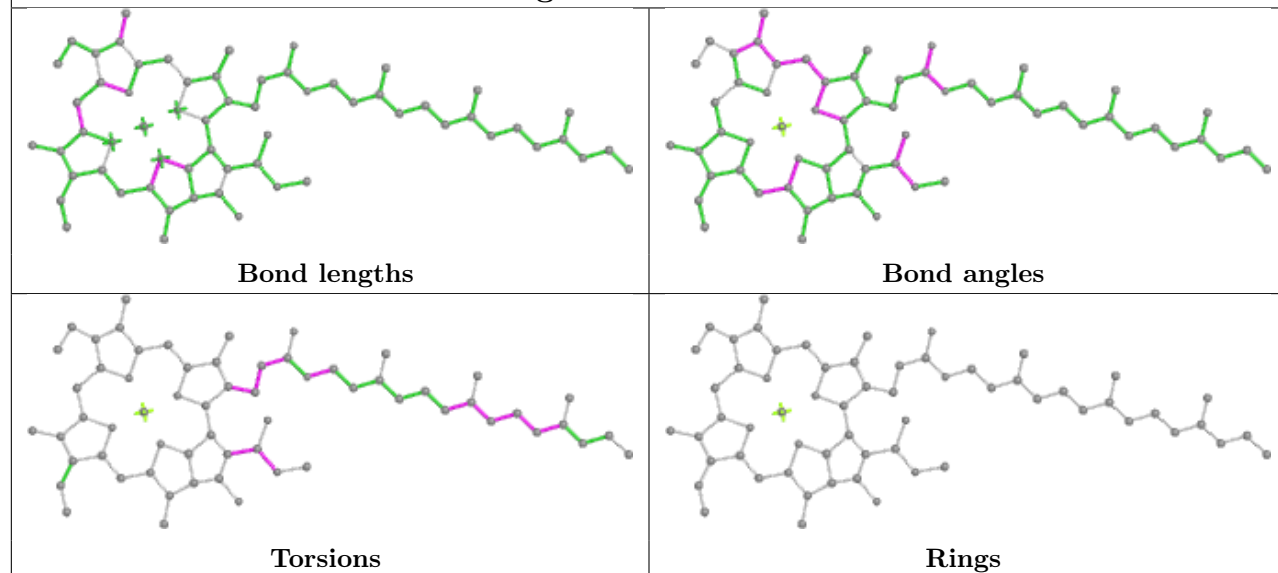
Ligand CLA b 836



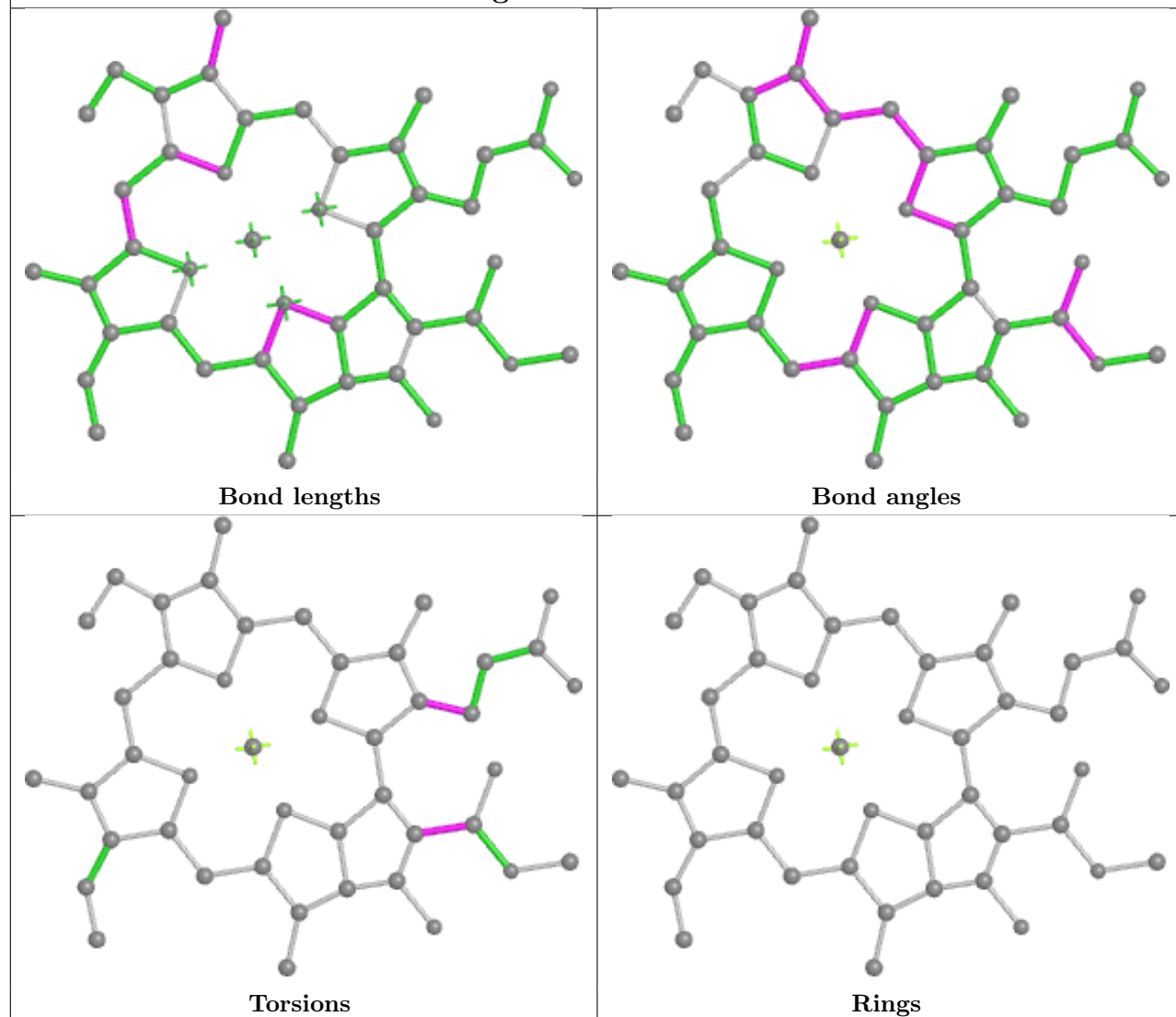
Ligand LHG 9 307



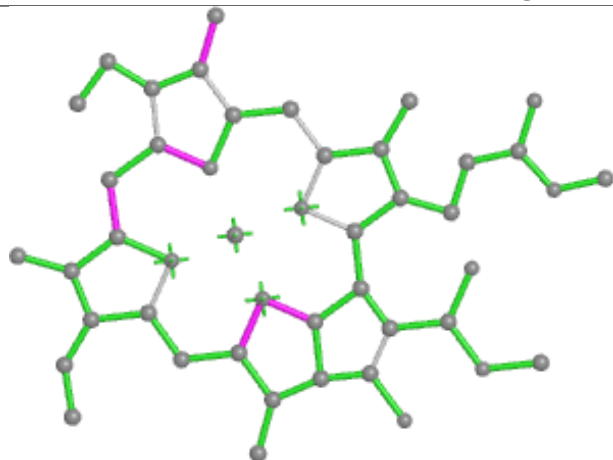
Ligand CLA a 829



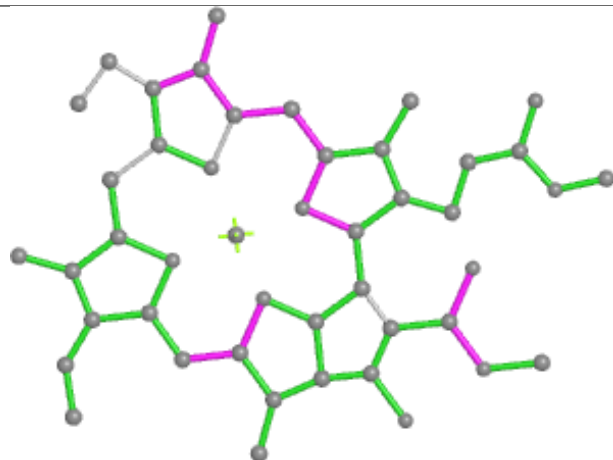
Ligand CLA b 815



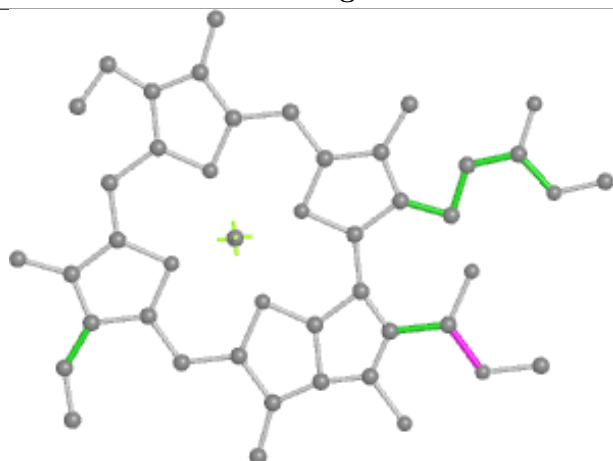
Ligand CLA 8 306



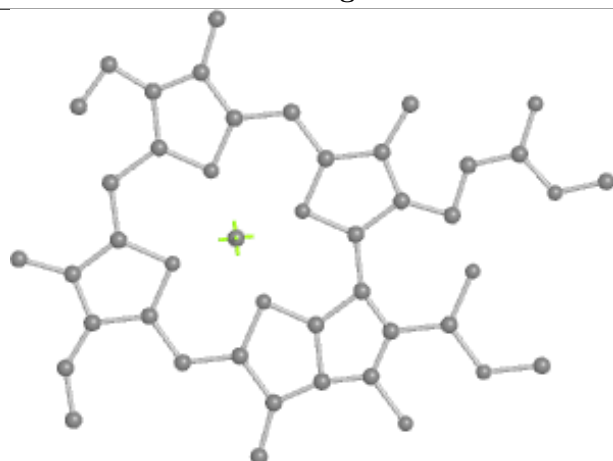
Bond lengths



Bond angles

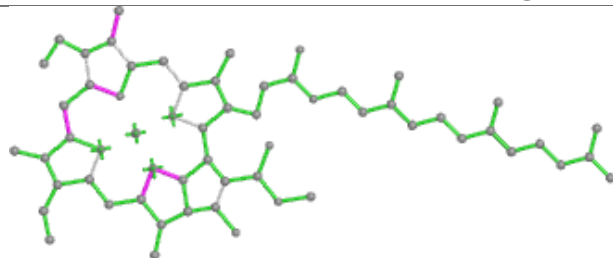


Torsions

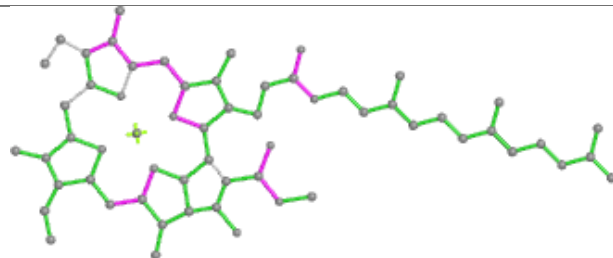


Rings

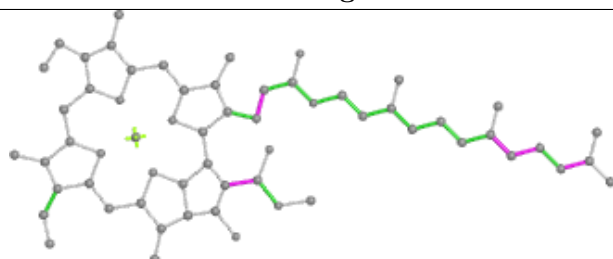
Ligand CLA 5 307



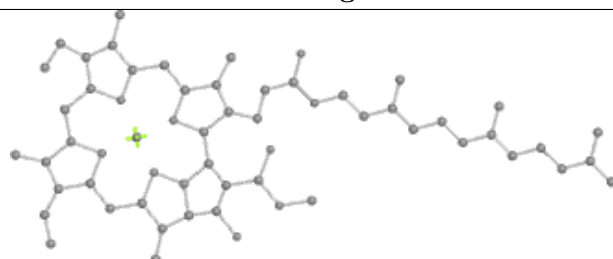
Bond lengths



Bond angles

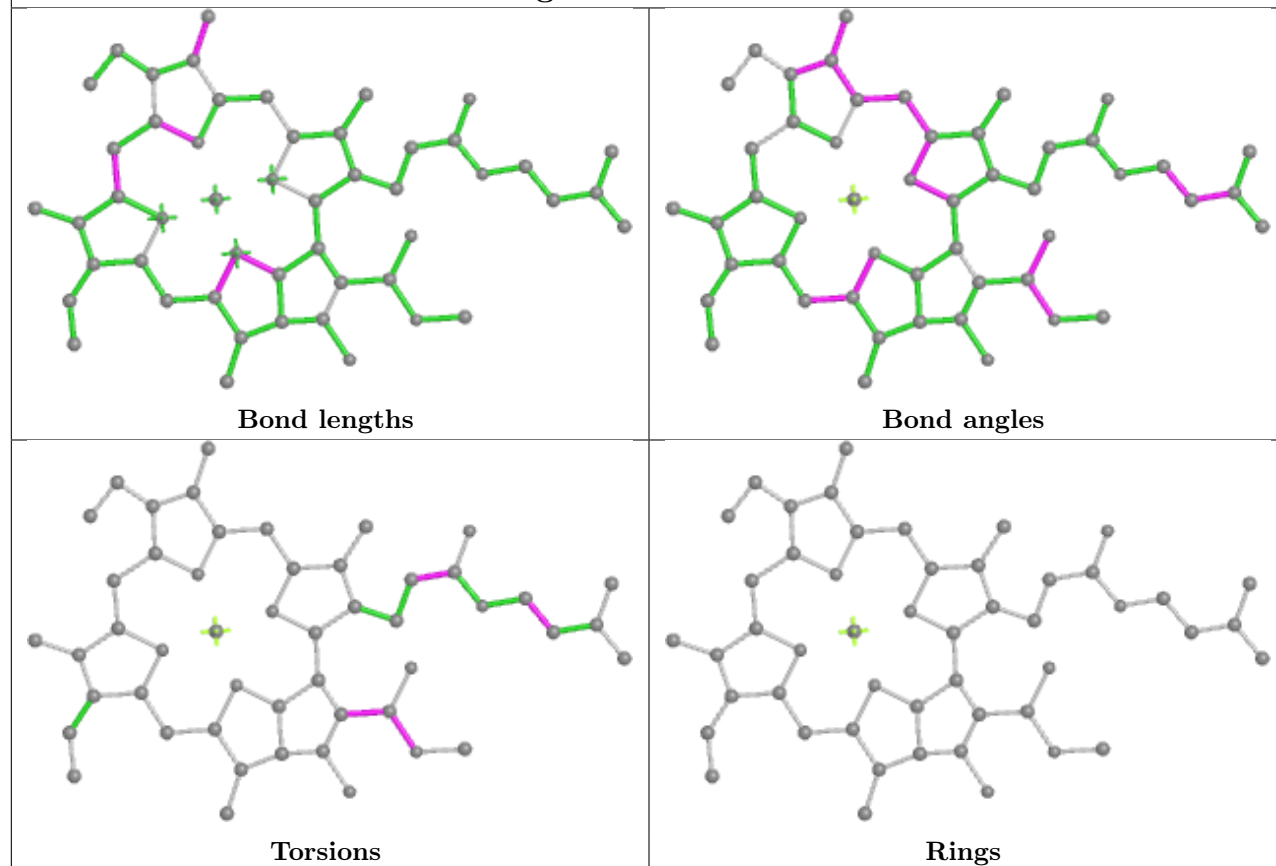


Torsions

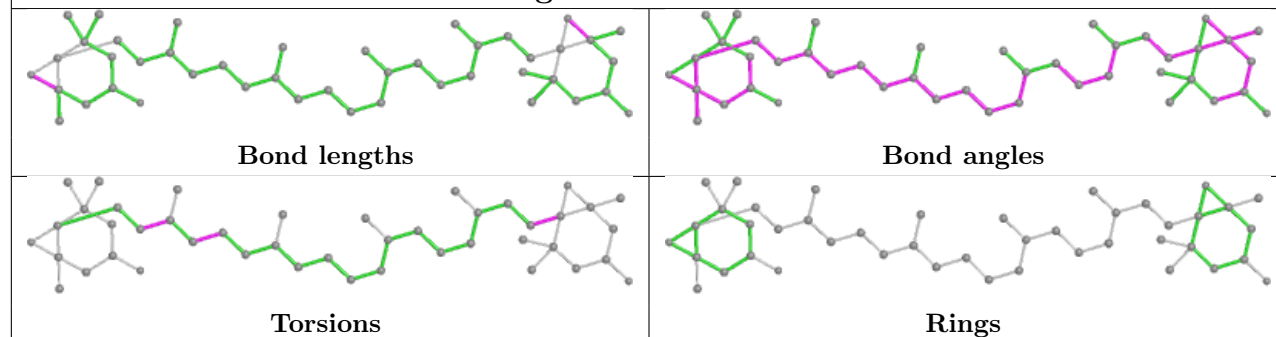


Rings

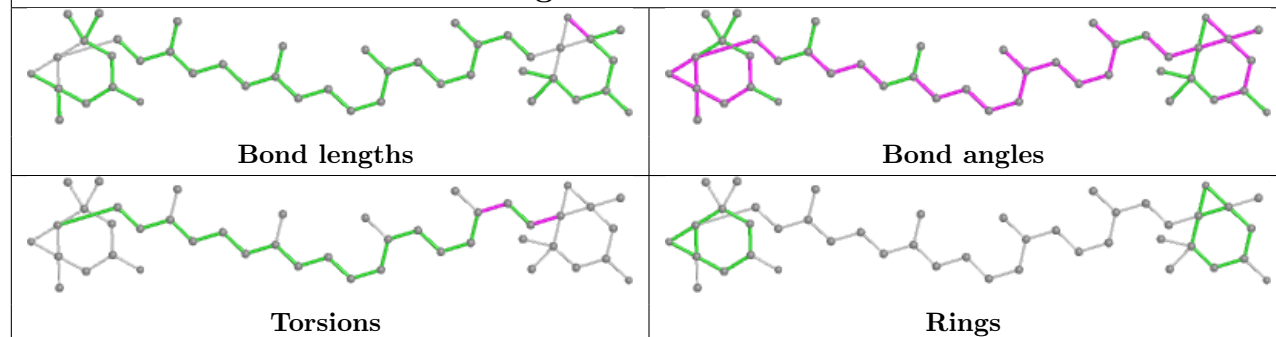
Ligand CLA 4 309

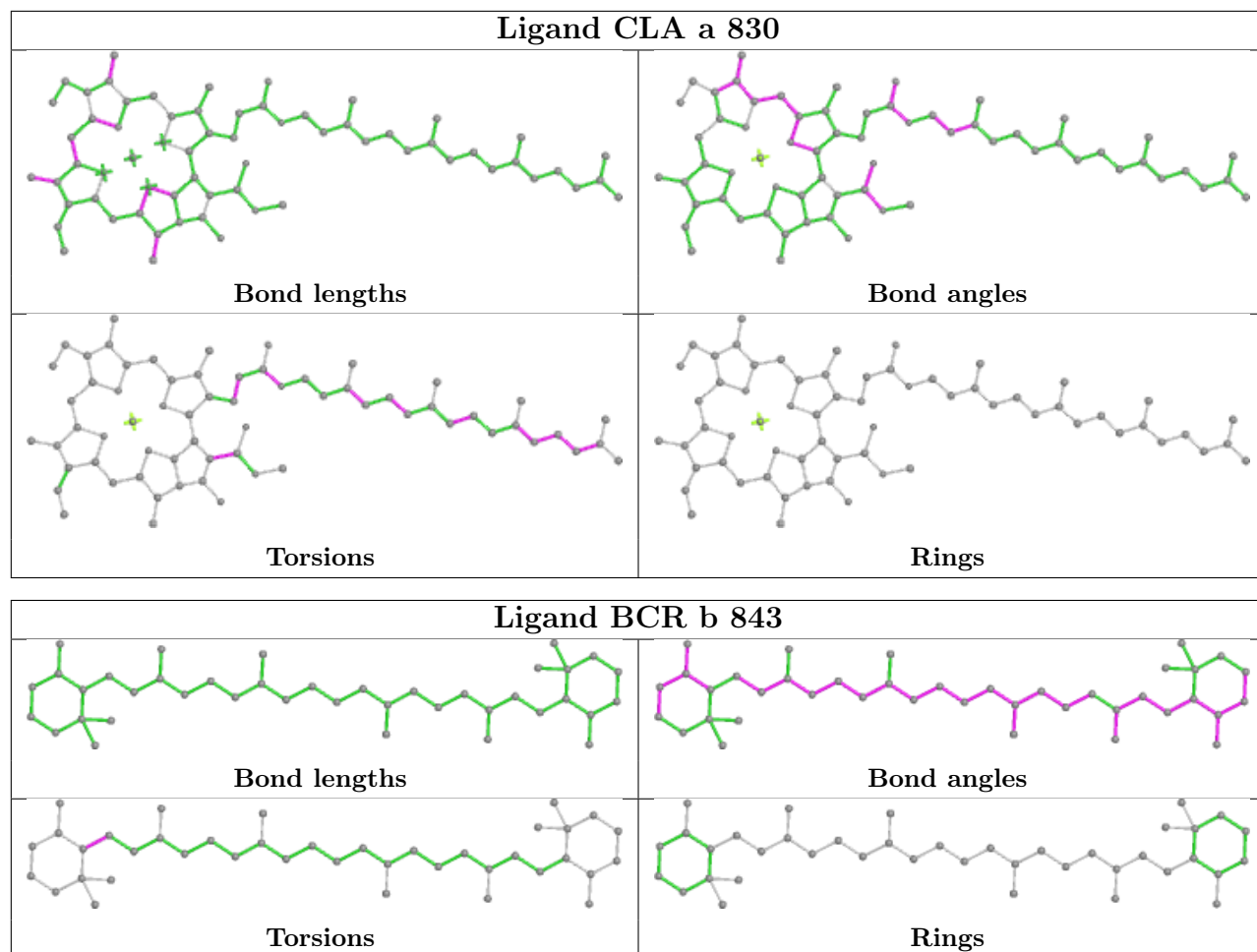


Ligand XAT 6 306

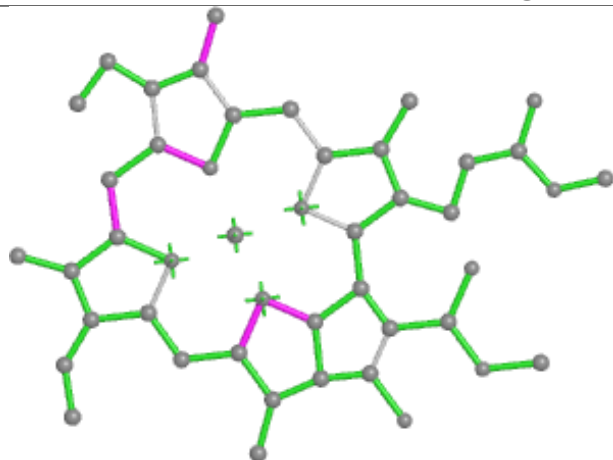


Ligand XAT 5 302

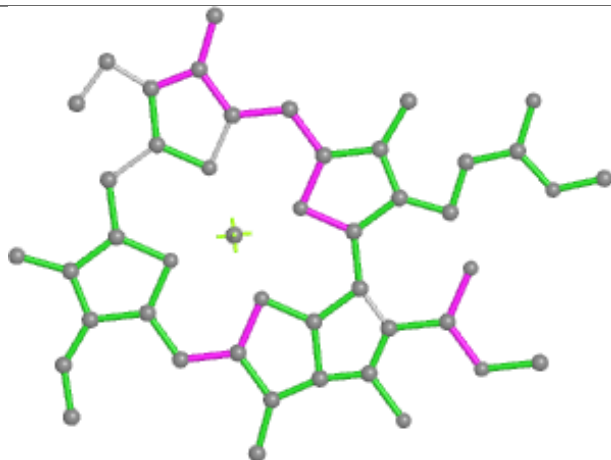




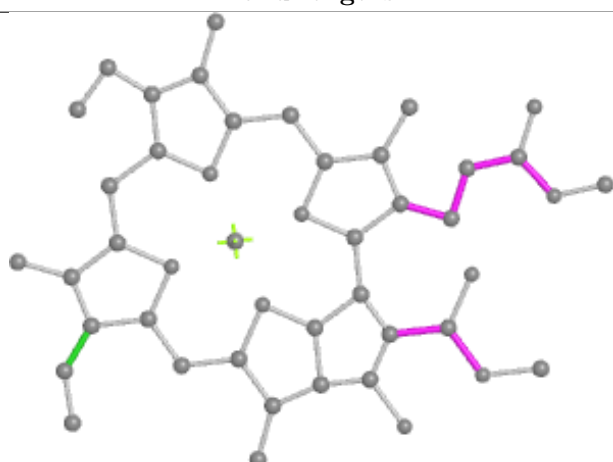
Ligand CLA 9 313



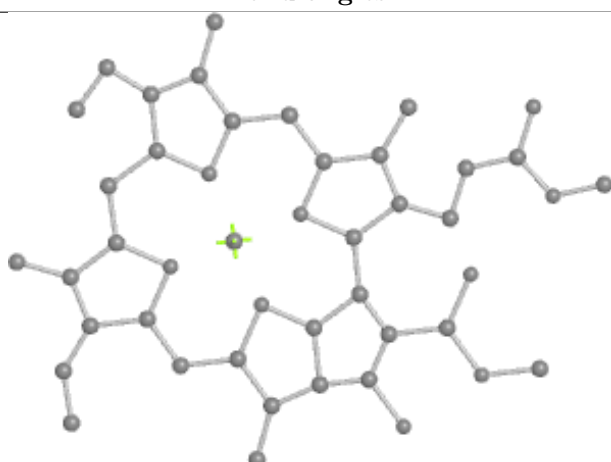
Bond lengths



Bond angles

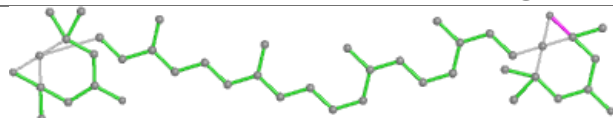


Torsions

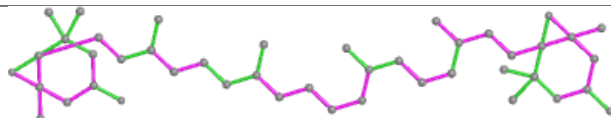


Rings

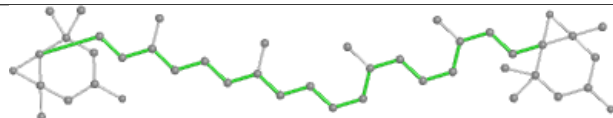
Ligand XAT 3 305



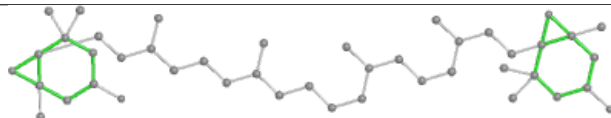
Bond lengths



Bond angles

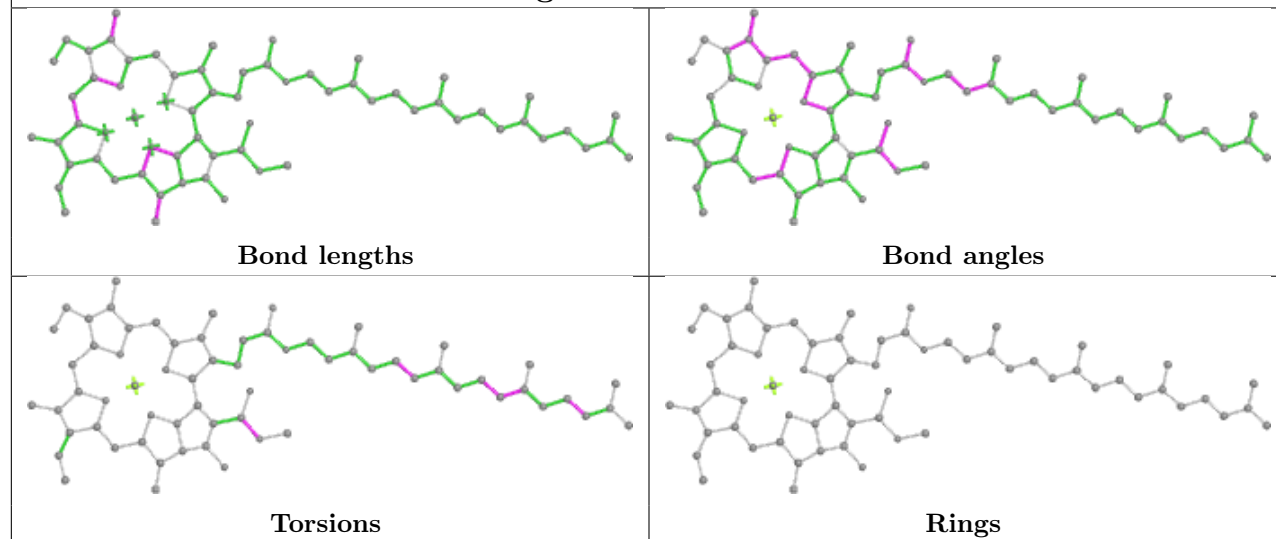


Torsions

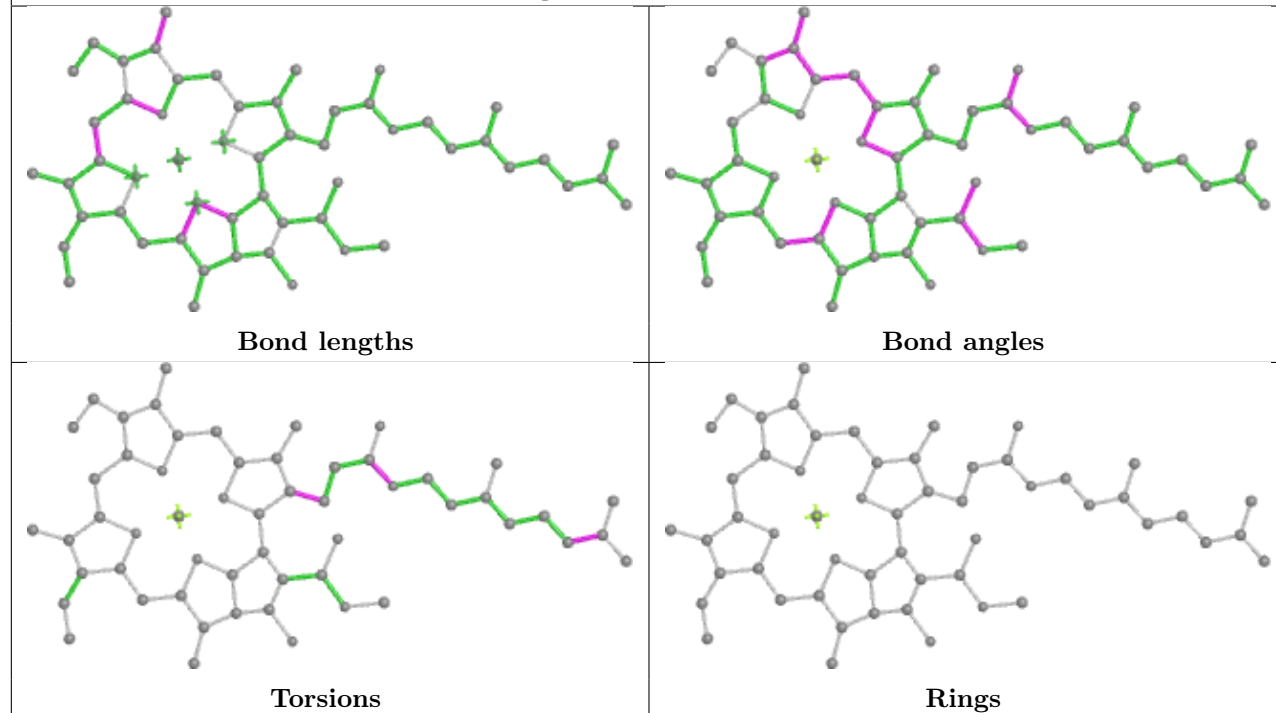


Rings

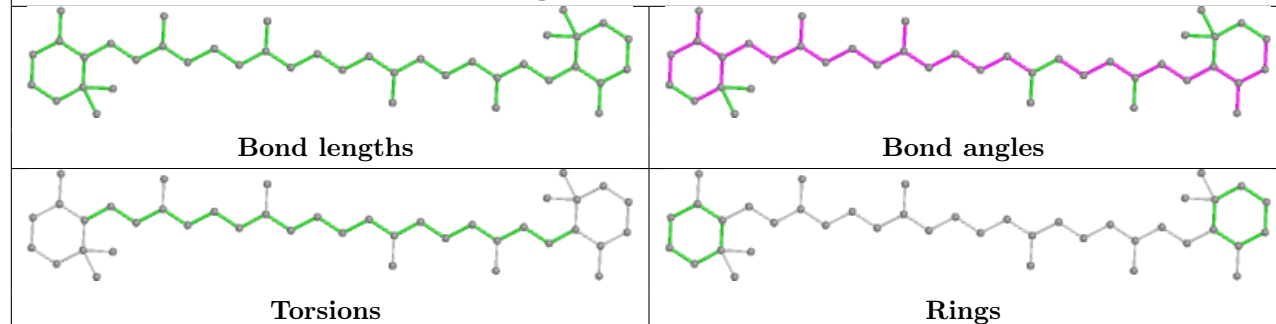
Ligand CLA a 834

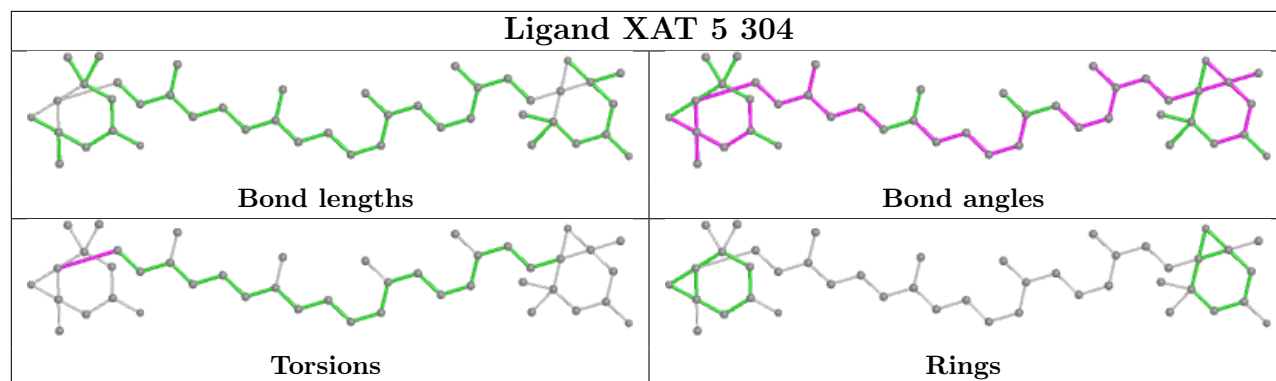


Ligand CLA a 805



Ligand BCR h 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

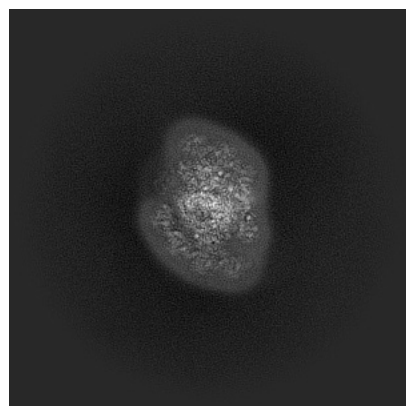
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60288. These allow visual inspection of the internal detail of the map and identification of artifacts.

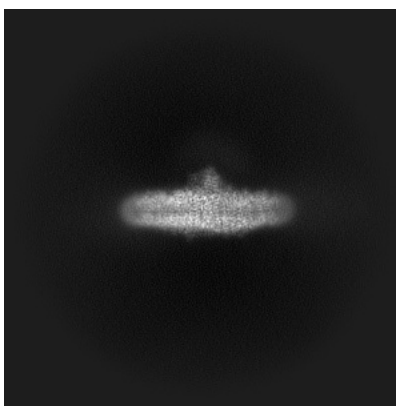
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

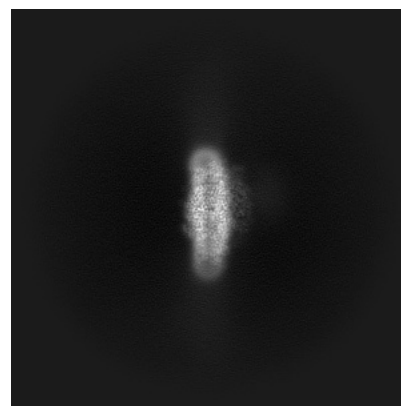
6.1.1 Primary map



X

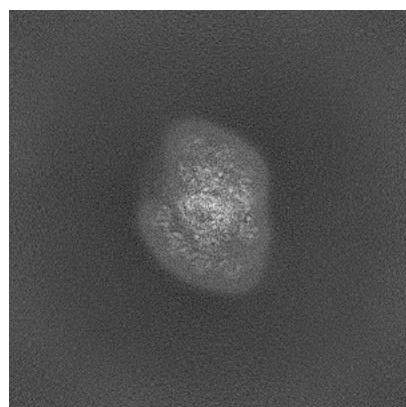


Y

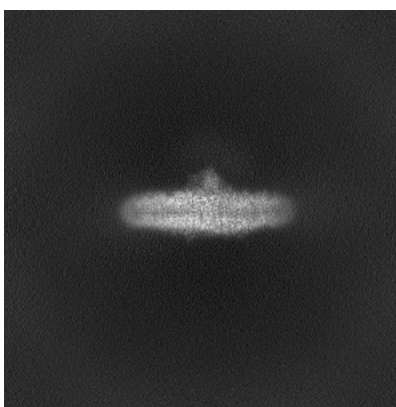


Z

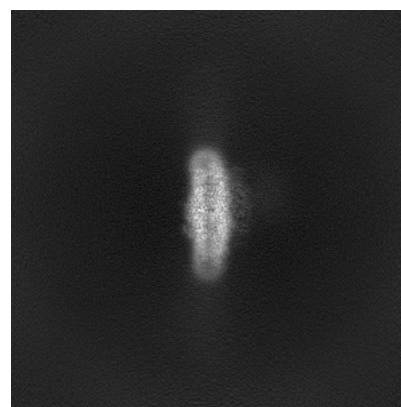
6.1.2 Raw map



X



Y

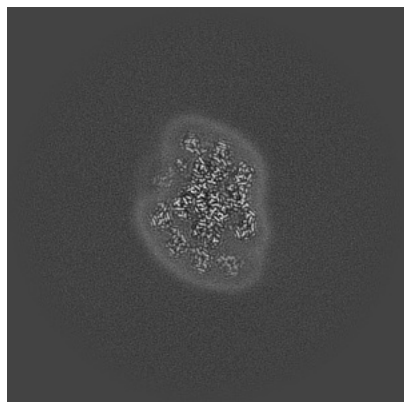


Z

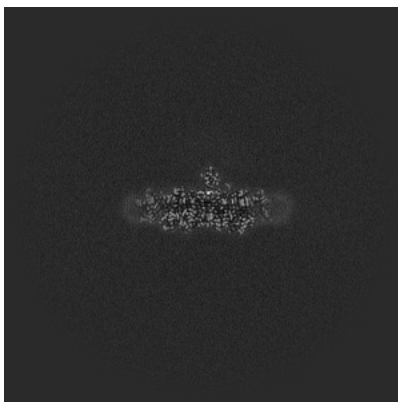
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

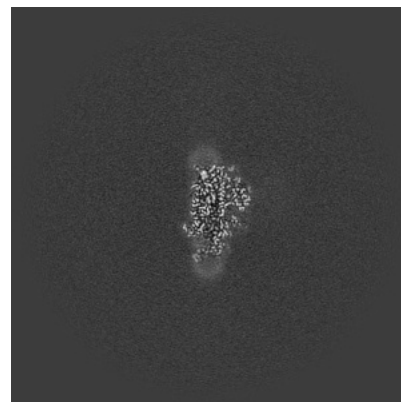
6.2.1 Primary map



X Index: 256

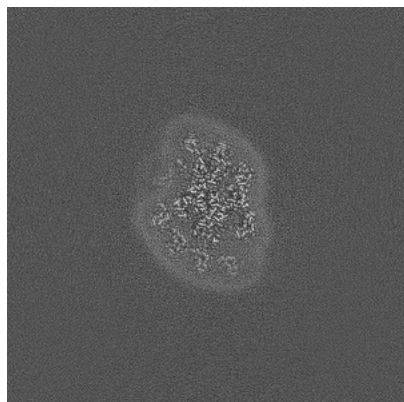


Y Index: 256

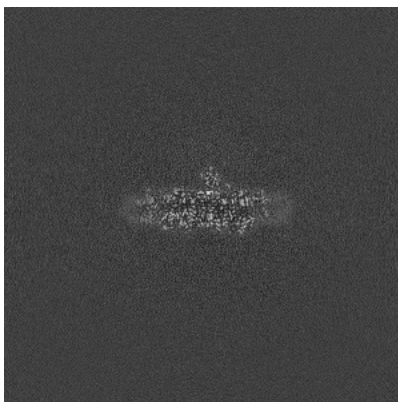


Z Index: 256

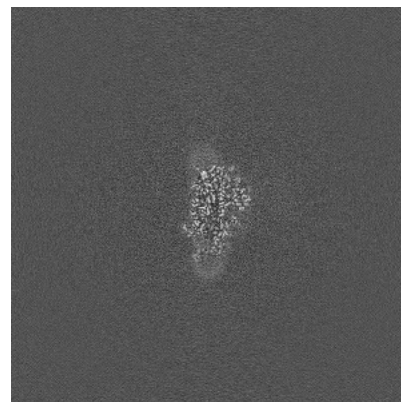
6.2.2 Raw map



X Index: 256



Y Index: 256

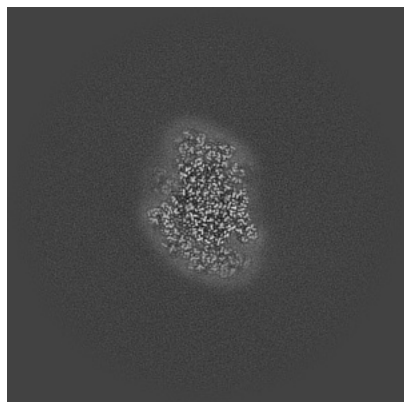


Z Index: 256

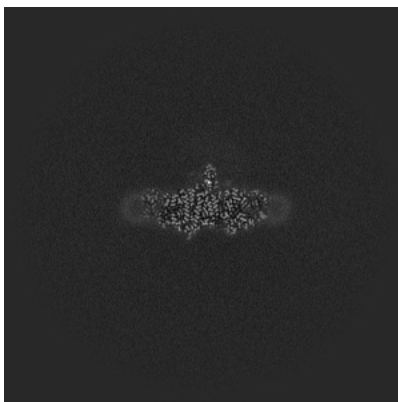
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

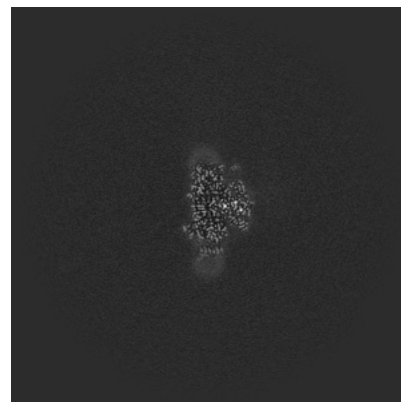
6.3.1 Primary map



X Index: 268

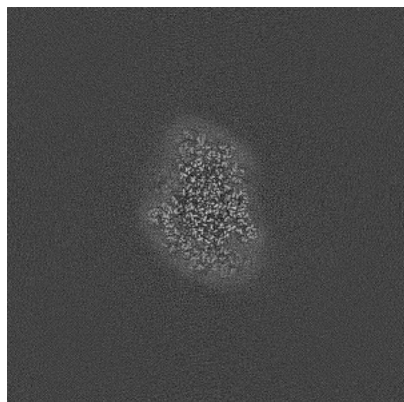


Y Index: 262

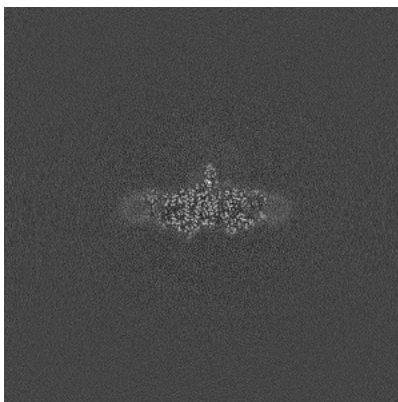


Z Index: 261

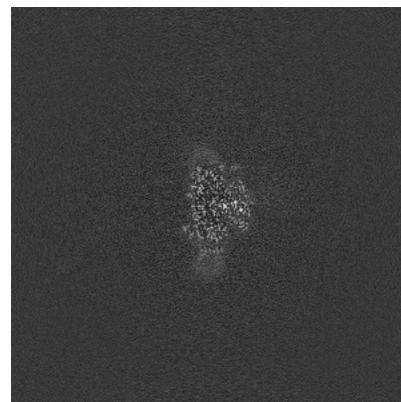
6.3.2 Raw map



X Index: 268



Y Index: 262

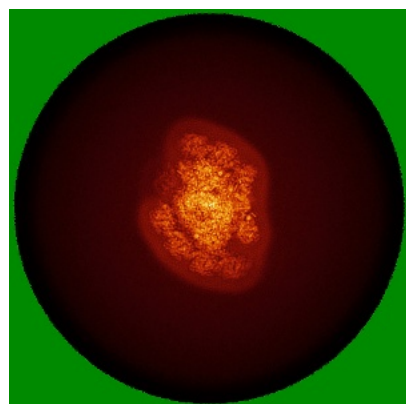


Z Index: 261

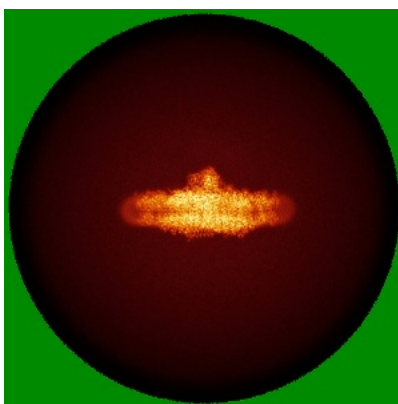
The images above show the largest variance slices of the map in three orthogonal directions.

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

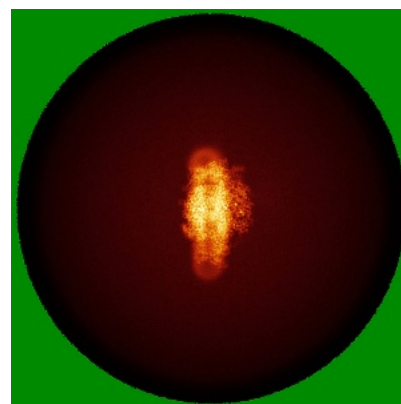
6.4.1 Primary map



X

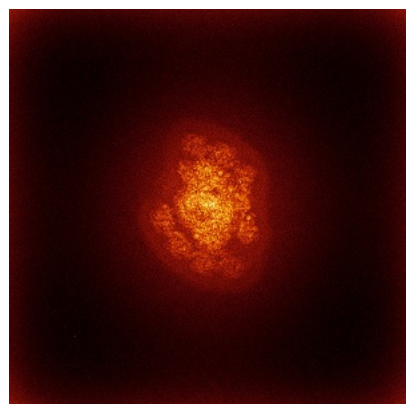


Y

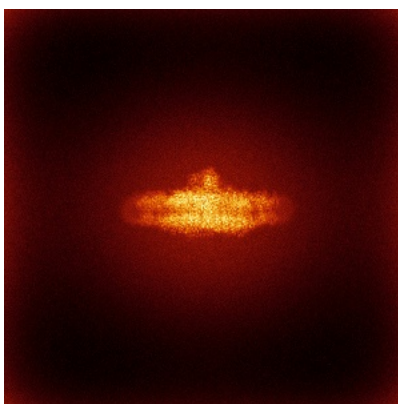


Z

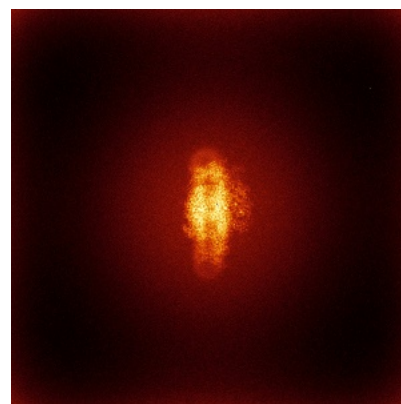
6.4.2 Raw map



X



Y

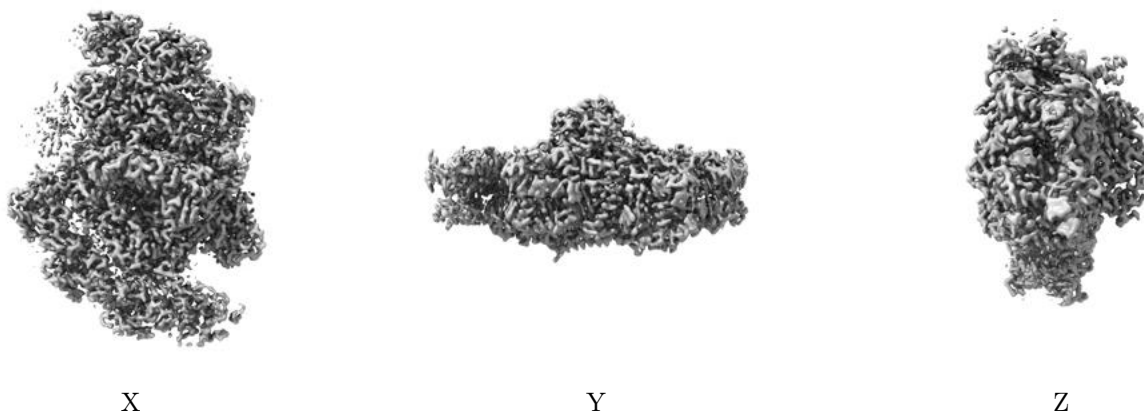


Z

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.

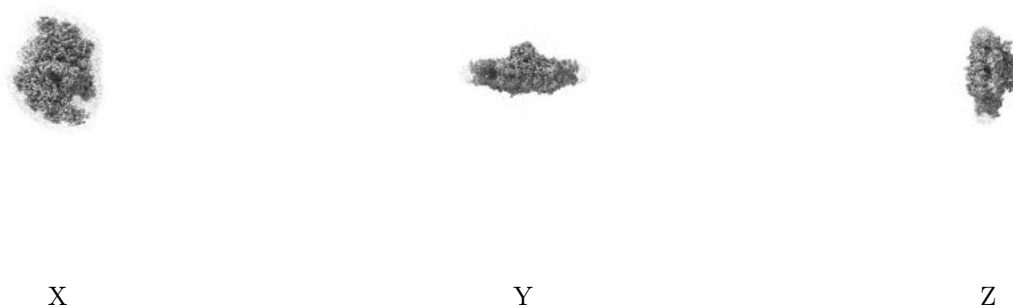
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.287. 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.

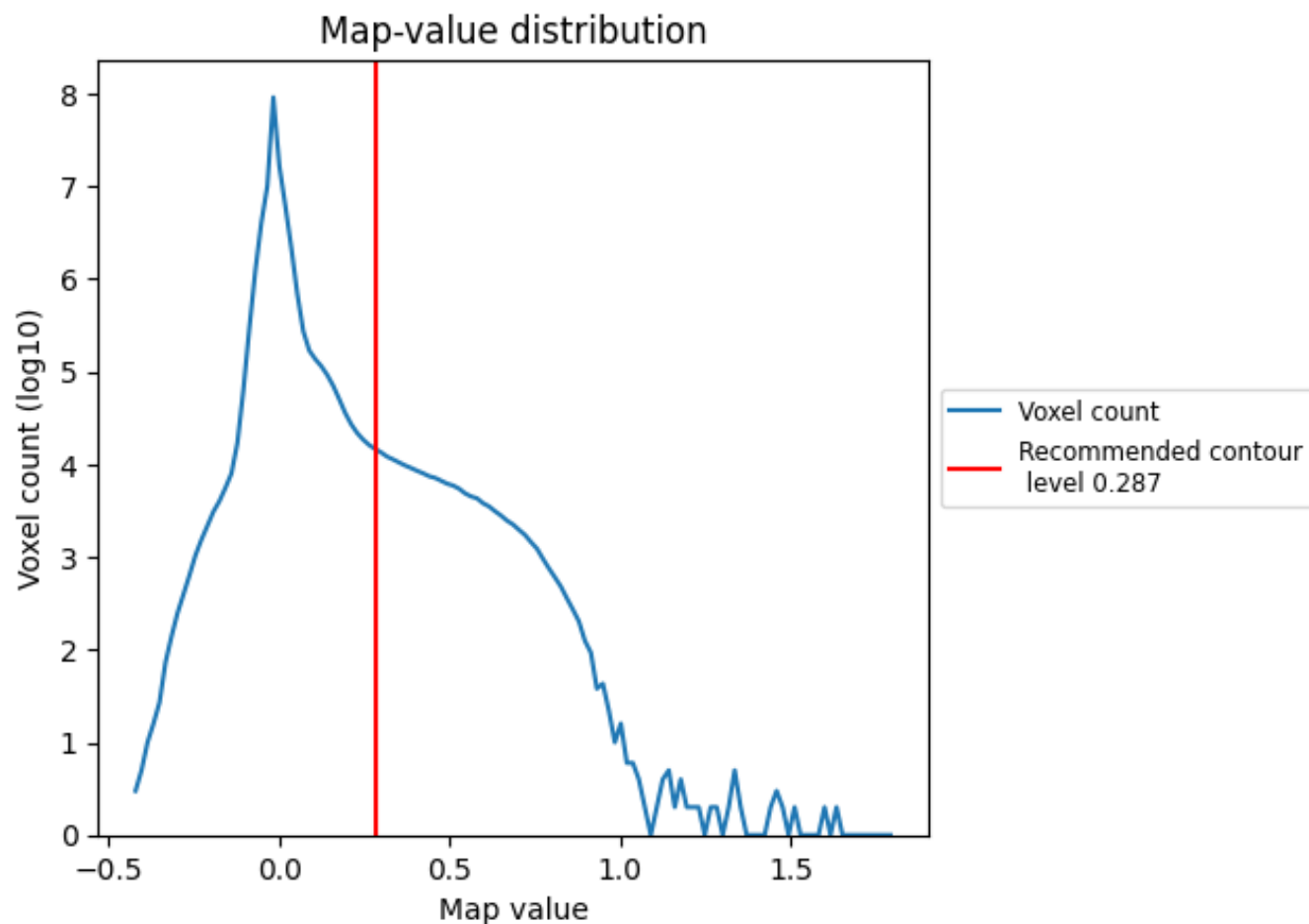
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

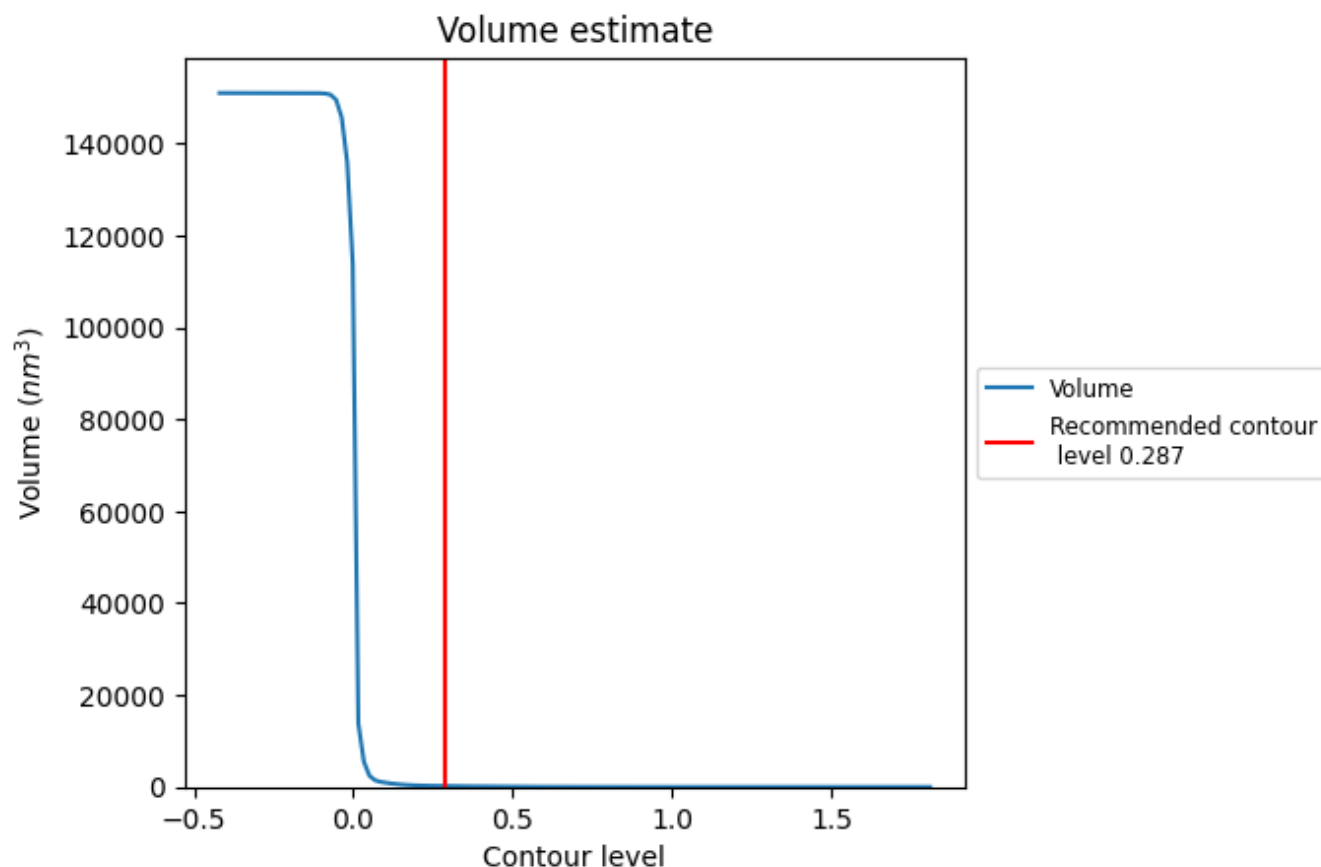
This section contains the results of statistical analysis of the map.

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.

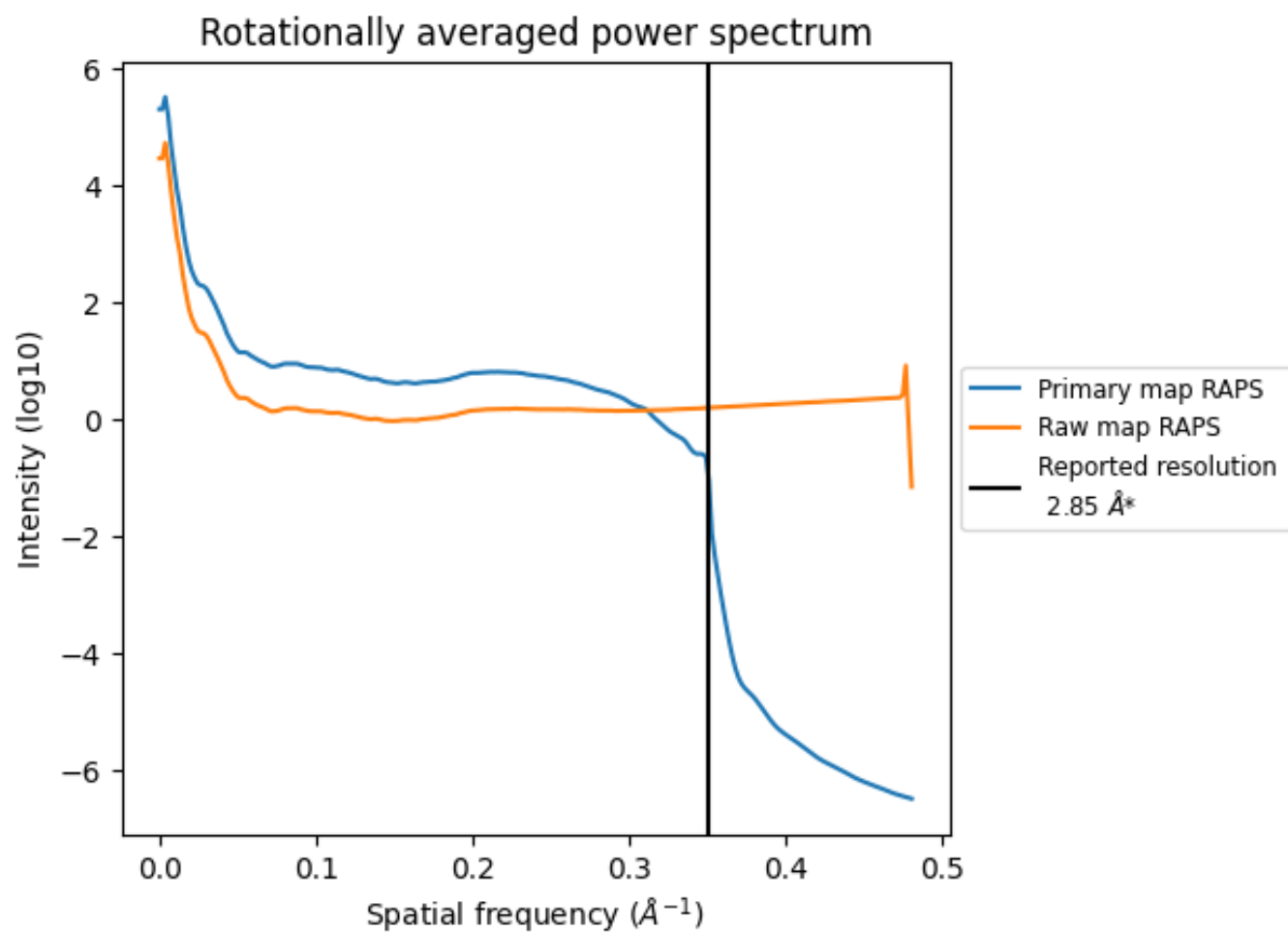
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm^3 ; this corresponds to an approximate mass of 178 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

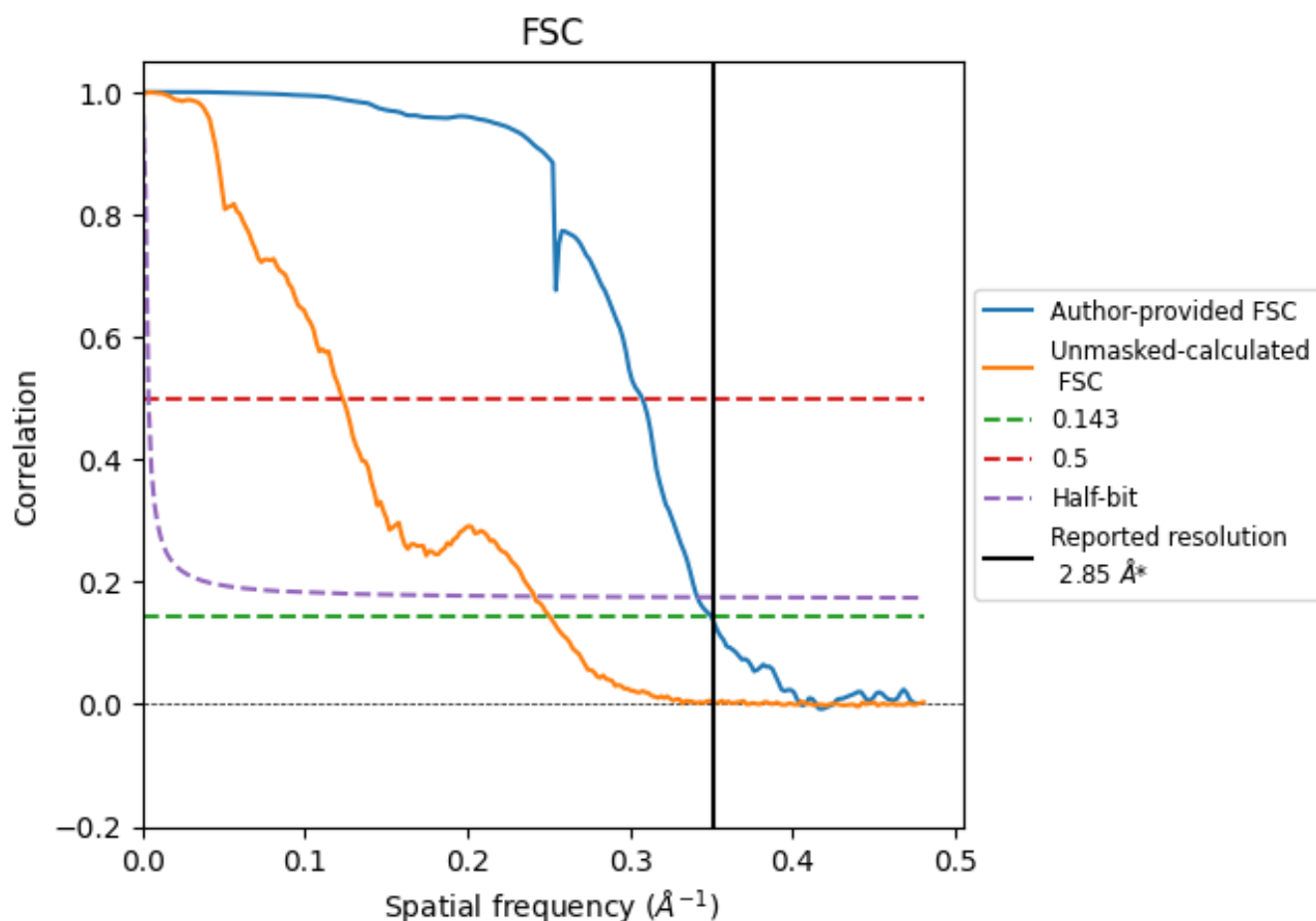


*Reported resolution corresponds to spatial frequency of 0.351 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.351 \AA^{-1}

8.2 Resolution estimates [i](#)

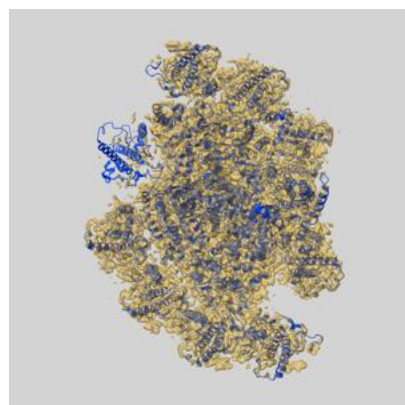
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.25	2.93
Unmasked-calculated*	3.99	8.12	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 2.85 by more than 10 %

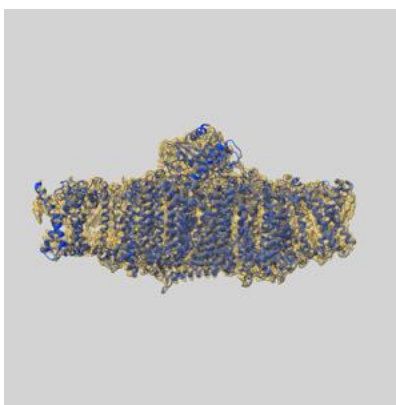
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60288 and PDB model 8ZOC. Per-residue inclusion information can be found in section 3 on page 32.

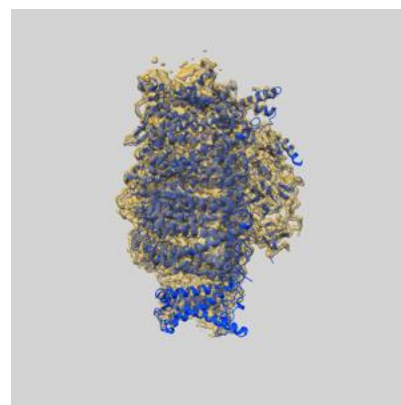
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.287 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



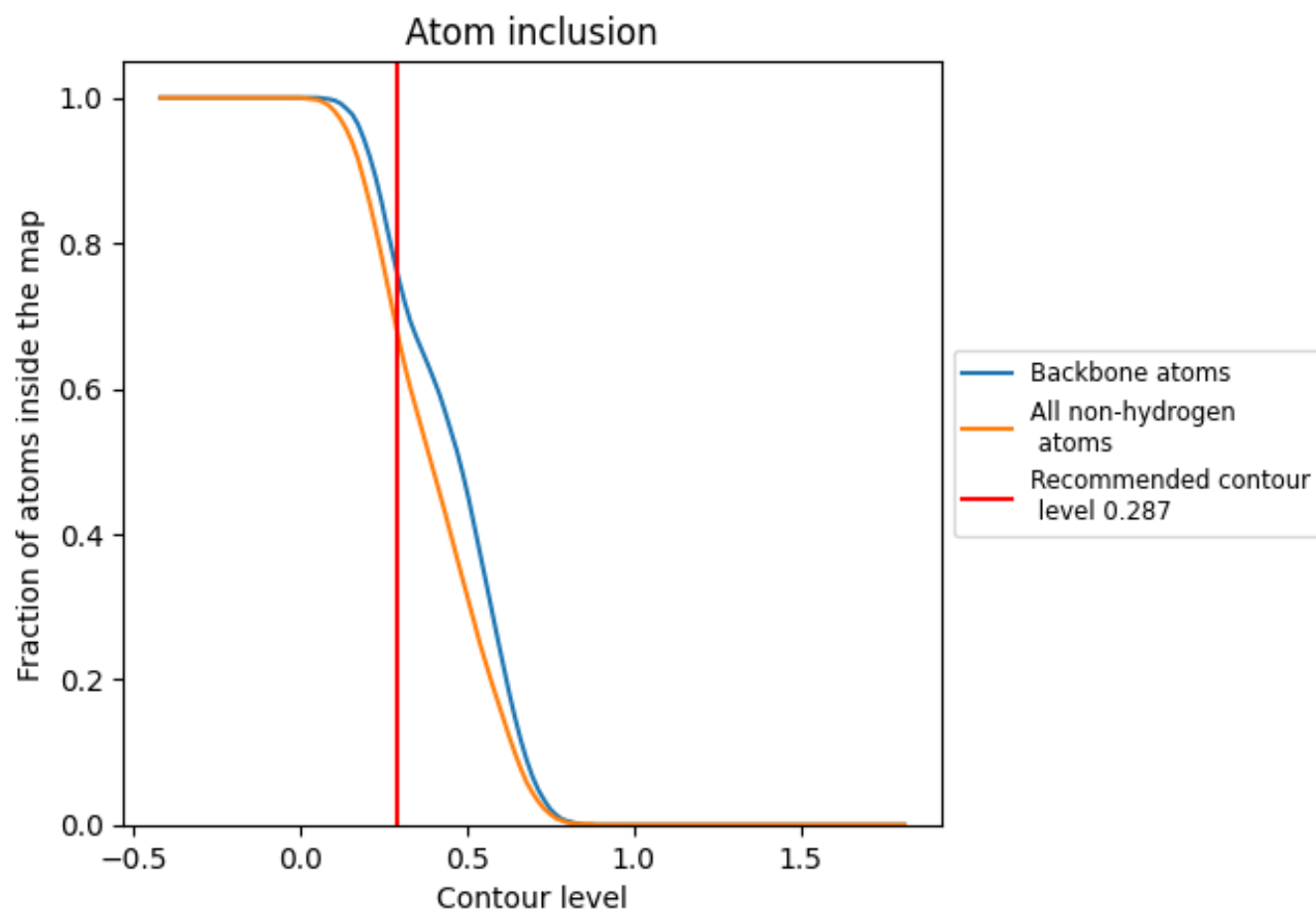
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.287).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.287) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6840	<div></div> 0.5420
1	<div></div> 0.6930	<div></div> 0.5420
2	<div></div> 0.4040	<div></div> 0.4440
3	<div></div> 0.6100	<div></div> 0.5280
4	<div></div> 0.6630	<div></div> 0.5280
5	<div></div> 0.6730	<div></div> 0.5220
6	<div></div> 0.0880	<div></div> 0.4270
7	<div></div> 0.5460	<div></div> 0.4920
8	<div></div> 0.6920	<div></div> 0.5440
9	<div></div> 0.6930	<div></div> 0.5420
a	<div></div> 0.8030	<div></div> 0.5800
b	<div></div> 0.8030	<div></div> 0.5790
c	<div></div> 0.8380	<div></div> 0.5620
d	<div></div> 0.7520	<div></div> 0.5590
e	<div></div> 0.7320	<div></div> 0.5630
f	<div></div> 0.7270	<div></div> 0.5470
g	<div></div> 0.5380	<div></div> 0.4440
h	<div></div> 0.6160	<div></div> 0.5330
i	<div></div> 0.7580	<div></div> 0.5460
j	<div></div> 0.7420	<div></div> 0.5680
l	<div></div> 0.7230	<div></div> 0.5360
m	<div></div> 0.7530	<div></div> 0.5310

