



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:22 PM UTC

PDB ID : 8ZOA / pdb_00008zoa
EMDB ID : EMD-60286
Title : Structure of the wild-type PSI-8VCPI supercomplex in Nannochloropsis oceanica
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 2.95 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:

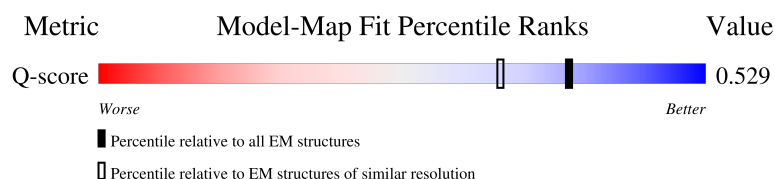
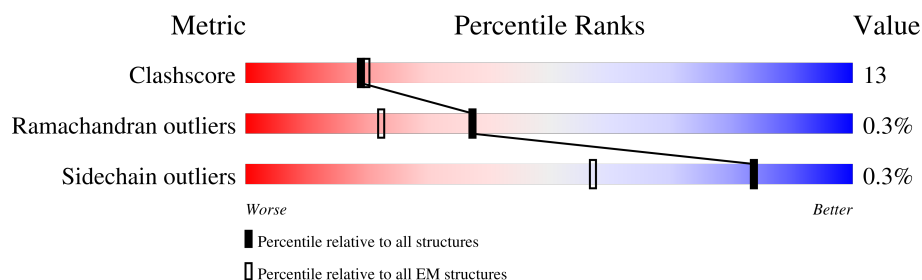
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.95 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13114 (2.45 - 3.45)

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	2	223	
7	1	208	
8	a	745	
9	b	737	
10	d	136	
11	e	67	
12	f	185	
13	h	128	
14	i	45	
15	j	41	
16	l	172	
17	m	30	
18	g	55	
19	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
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	1	311	X	-	-	-
22	CLA	1	312	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	1	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	306	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	2	309	X	-	-	-
22	CLA	2	310	X	-	-	-
22	CLA	2	311	X	-	-	-
22	CLA	2	312	X	-	-	-
22	CLA	2	313	X	-	-	-
22	CLA	2	314	X	-	-	-
22	CLA	2	315	X	-	-	-
22	CLA	2	316	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	314	X	-	-	-
22	CLA	3	315	X	-	-	-
22	CLA	4	306	X	-	-	-
22	CLA	4	307	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	4	311	X	-	-	-
22	CLA	4	312	X	-	-	-
22	CLA	4	313	X	-	-	-
22	CLA	4	314	X	-	-	-
22	CLA	4	315	X	-	-	-
22	CLA	4	316	X	-	-	-
22	CLA	4	317	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	306	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	5	312	X	-	-	-
22	CLA	5	313	X	-	-	-
22	CLA	5	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	315	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	308	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-
22	CLA	8	305	X	-	-	-
22	CLA	8	306	X	-	-	-
22	CLA	8	307	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	8	311	X	-	-	-
22	CLA	8	312	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	314	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	312	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	9	314	X	-	-	-
22	CLA	9	315	X	-	-	-
22	CLA	9	316	X	-	-	-
22	CLA	9	318	X	-	-	-
22	CLA	a	801	X	-	-	-
22	CLA	a	802	X	-	-	-
22	CLA	a	803	X	-	-	-
22	CLA	a	804	X	-	-	-
22	CLA	a	805	X	-	-	-
22	CLA	a	806	X	-	-	-
22	CLA	a	807	X	-	-	-
22	CLA	a	808	X	-	-	-
22	CLA	a	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	810	X	-	-	-
22	CLA	a	811	X	-	-	-
22	CLA	a	812	X	-	-	-
22	CLA	a	813	X	-	-	-
22	CLA	a	814	X	-	-	-
22	CLA	a	815	X	-	-	-
22	CLA	a	816	X	-	-	-
22	CLA	a	817	X	-	-	-
22	CLA	a	818	X	-	-	-
22	CLA	a	819	X	-	-	-
22	CLA	a	820	X	-	-	-
22	CLA	a	821	X	-	-	-
22	CLA	a	822	X	-	-	-
22	CLA	a	823	X	-	-	-
22	CLA	a	824	X	-	-	-
22	CLA	a	825	X	-	-	-
22	CLA	a	826	X	-	-	-
22	CLA	a	827	X	-	-	-
22	CLA	a	828	X	-	-	-
22	CLA	a	829	X	-	-	-
22	CLA	a	830	X	-	-	-
22	CLA	a	831	X	-	-	-
22	CLA	a	832	X	-	-	-
22	CLA	a	833	X	-	-	-
22	CLA	a	834	X	-	-	-
22	CLA	a	835	X	-	-	-
22	CLA	a	836	X	-	-	-
22	CLA	a	837	X	-	-	-
22	CLA	a	838	X	-	-	-
22	CLA	a	839	X	-	-	-
22	CLA	a	840	X	-	-	-
22	CLA	a	841	X	-	-	-
22	CLA	a	842	X	-	-	-
22	CLA	a	844	X	-	-	-
22	CLA	a	854	X	-	-	-
22	CLA	b	801	X	-	-	-
22	CLA	b	802	X	-	-	-
22	CLA	b	803	X	-	-	-
22	CLA	b	804	X	-	-	-
22	CLA	b	805	X	-	-	-
22	CLA	b	806	X	-	-	-
22	CLA	b	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	b	808	X	-	-	-
22	CLA	b	809	X	-	-	-
22	CLA	b	810	X	-	-	-
22	CLA	b	811	X	-	-	-
22	CLA	b	812	X	-	-	-
22	CLA	b	813	X	-	-	-
22	CLA	b	814	X	-	-	-
22	CLA	b	815	X	-	-	-
22	CLA	b	816	X	-	-	-
22	CLA	b	817	X	-	-	-
22	CLA	b	818	X	-	-	-
22	CLA	b	819	X	-	-	-
22	CLA	b	820	X	-	-	-
22	CLA	b	821	X	-	-	-
22	CLA	b	822	X	-	-	-
22	CLA	b	823	X	-	-	-
22	CLA	b	824	X	-	-	-
22	CLA	b	825	X	-	-	-
22	CLA	b	826	X	-	-	-
22	CLA	b	827	X	-	-	-
22	CLA	b	828	X	-	-	-
22	CLA	b	829	X	-	-	-
22	CLA	b	830	X	-	-	-
22	CLA	b	831	X	-	-	-
22	CLA	b	832	X	-	-	-
22	CLA	b	833	X	-	-	-
22	CLA	b	834	X	-	-	-
22	CLA	b	835	X	-	-	-
22	CLA	b	836	X	-	-	-
22	CLA	b	837	X	-	-	-
22	CLA	b	838	X	-	-	-
22	CLA	b	839	X	-	-	-
22	CLA	b	840	X	-	-	-
22	CLA	f	802	X	-	-	-
22	CLA	f	803	X	-	-	-
22	CLA	h	203	X	-	-	-
22	CLA	h	205	X	-	-	-
22	CLA	j	102	X	-	-	-
22	CLA	j	103	X	-	-	-
22	CLA	l	202	X	-	-	-
22	CLA	l	203	X	-	-	-
22	CLA	l	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SF4	c	102	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 41637 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-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	185	Total	C	N	O	S	0	0
			1372	892	224	249	7		

- Molecule 7 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

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

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

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

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

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

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

- Molecule 13 is a protein called Psar.

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

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

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

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

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

- Molecule 16 is a protein called PSI subunit V.

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

- Molecule 17 is a protein called PsaM.

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

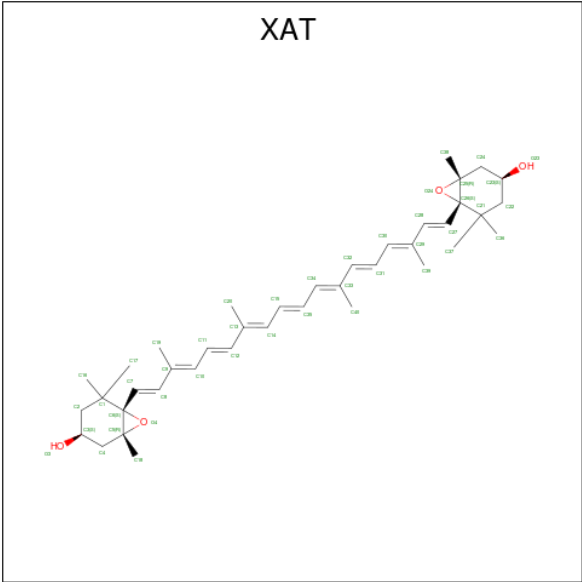
- Molecule 18 is a protein called PsaS.

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

- Molecule 19 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 20 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).



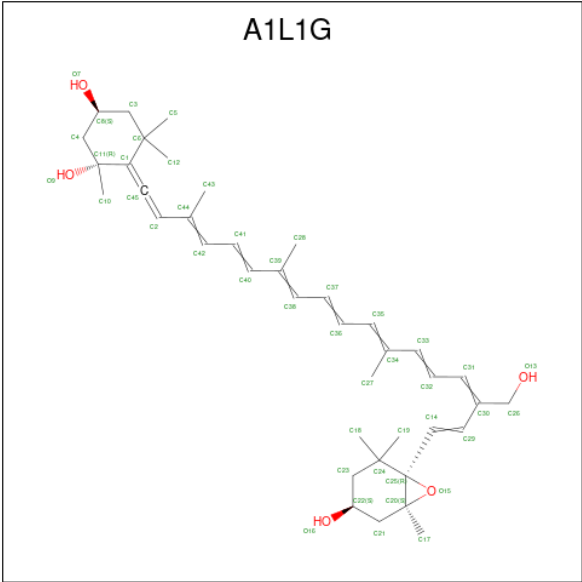
Mol	Chain	Residues	Atoms			AltConf
20	5	1	Total	C	O	0
			44	40	4	
20	5	1	Total	C	O	0
			44	40	4	
20	5	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	9	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	8	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	

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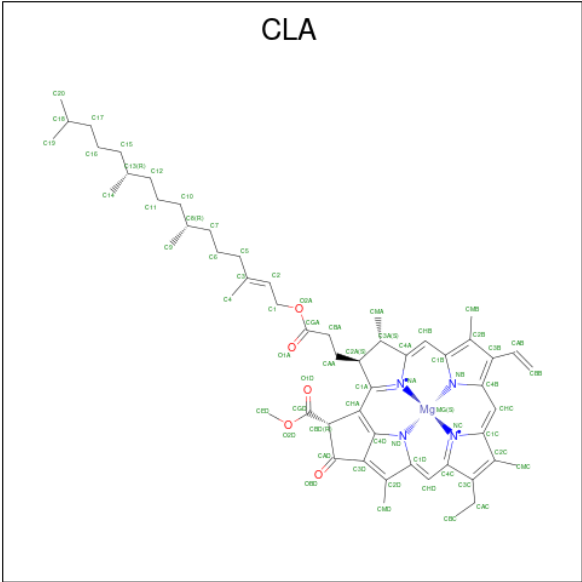
Mol	Chain	Residues	Atoms			AltConf
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	7	1	Total	C	O	0
			44	40	4	
20	1	1	Total	C	O	0
			44	40	4	
20	1	1	Total	C	O	0
			44	40	4	
20	a	1	Total	C	O	0
			44	40	4	
20	j	1	Total	C	O	0
			44	40	4	

- Molecule 21 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxa bicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	5	1	Total	C	O	0
			45	40	5	
21	9	1	Total	C	O	0
			45	40	5	
21	9	1	Total	C	O	0
			45	40	5	
21	3	1	Total	C	O	0
			45	40	5	
21	3	1	Total	C	O	0
			45	40	5	
21	7	1	Total	C	O	0
			45	40	5	
21	1	1	Total	C	O	0
			45	40	5	

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	2	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	2	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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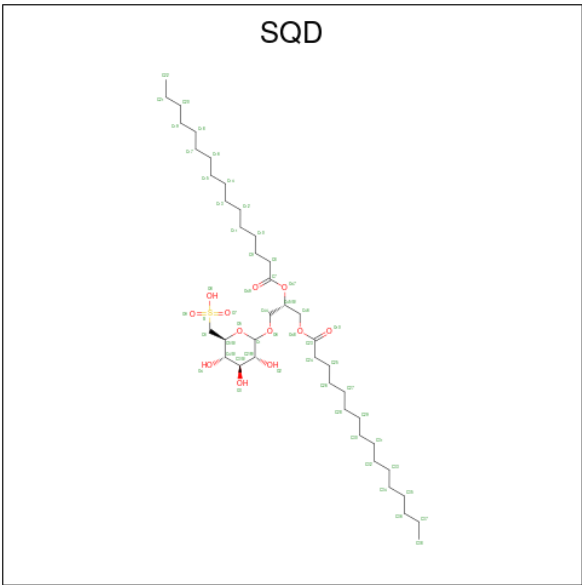
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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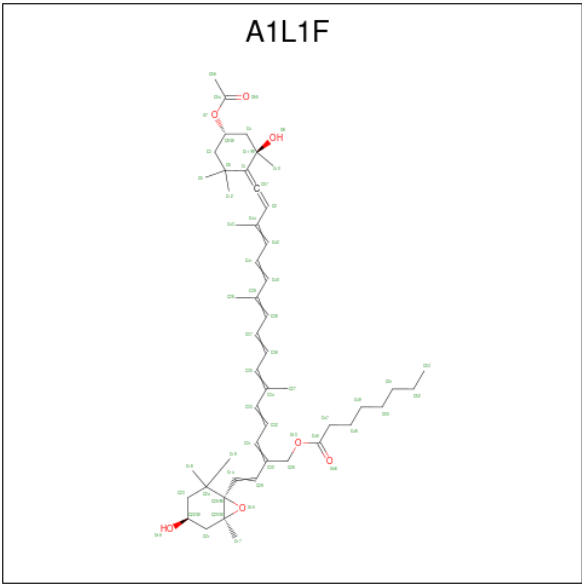
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



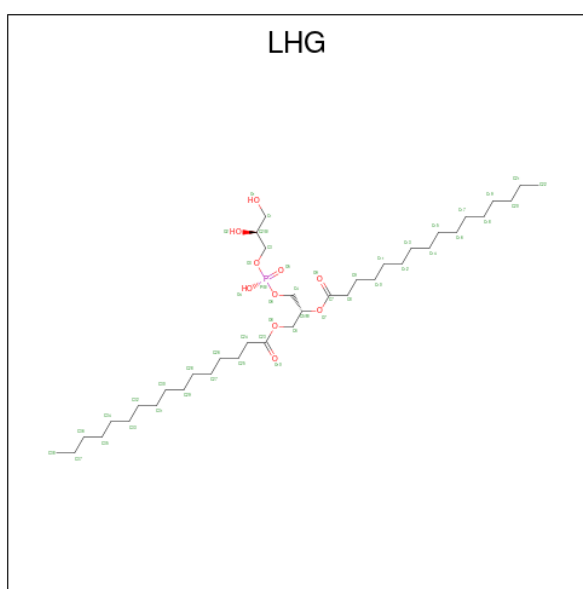
Mol	Chain	Residues	Atoms				AltConf
23	5	1	Total	C	O	S	0
			35	22	12	1	
23	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 24 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyl oxy-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-2,4,6,8,1 0,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: C₅₀H₇₂O₇) (labeled as "Ligand of Interest" by depositor).



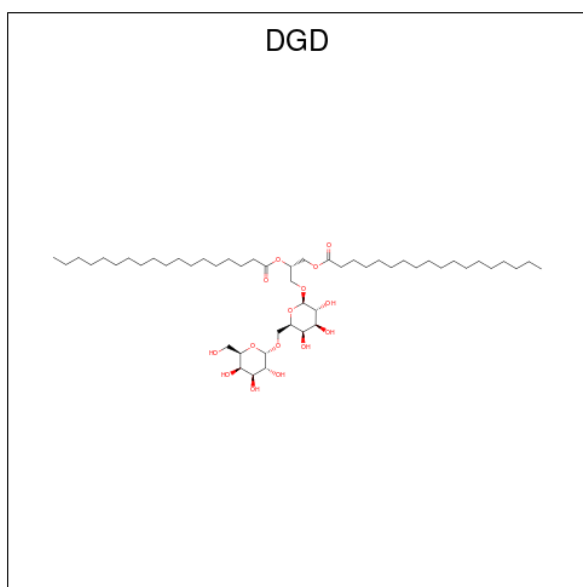
Mol	Chain	Residues	Atoms			AltConf
24	9	1	Total	C	O	0
			57	50	7	
24	8	1	Total	C	O	0
			57	50	7	
24	1	1	Total	C	O	0
			57	50	7	
24	h	1	Total	C	O	0
			57	50	7	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



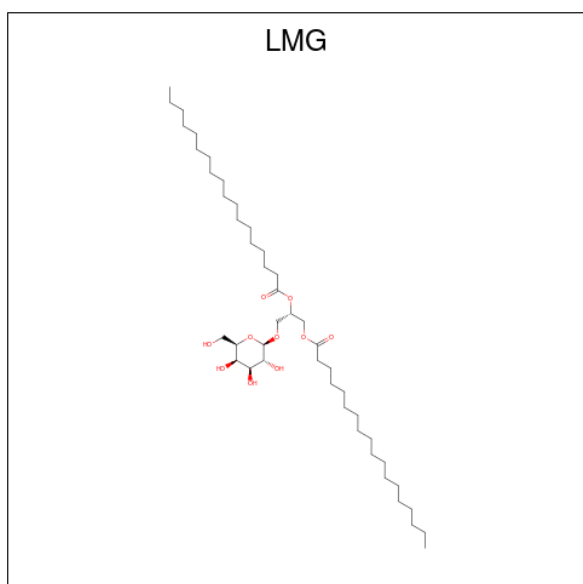
Mol	Chain	Residues	Atoms				AltConf
25	9	1	Total	C	O	P	0
			36	25	10	1	
25	9	1	Total	C	O	P	0
			46	35	10	1	
25	a	1	Total	C	O	P	0
			48	37	10	1	
25	a	1	Total	C	O	P	0
			27	16	10	1	
25	b	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



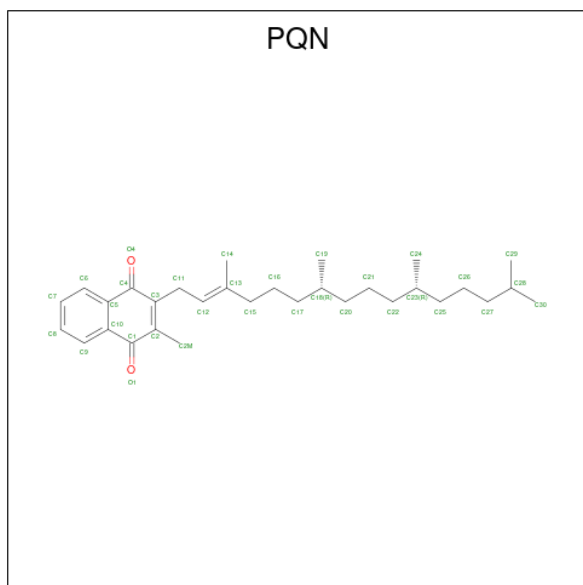
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	8	1	40	25	15	0
26	4	1	40	25	15	0
26	b	1	57	42	15	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



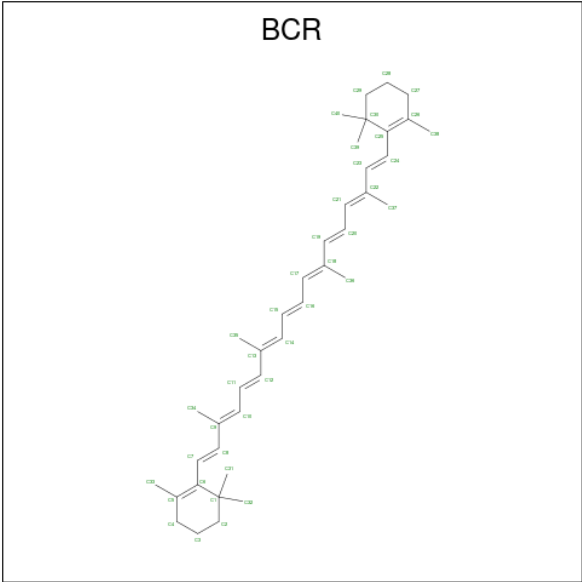
Mol	Chain	Residues	Atoms			AltConf
27	2	1	Total	C	O	0
			35	25	10	
27	a	1	Total	C	O	0
			34	24	10	
27	j	1	Total	C	O	0
			32	22	10	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



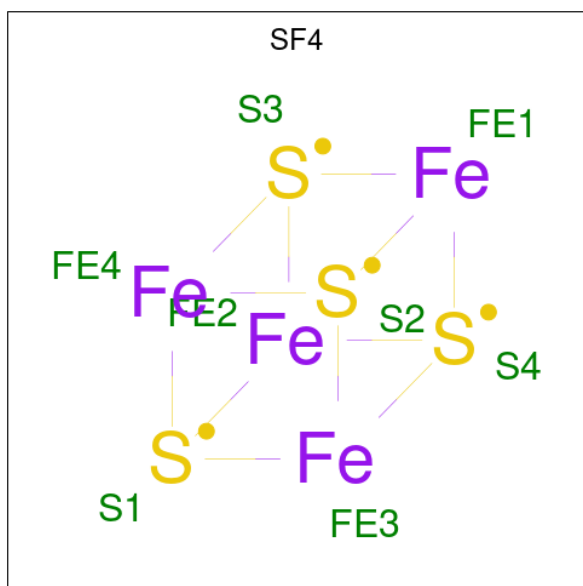
Mol	Chain	Residues	Atoms	AltConf
29	a	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	f	1	Total C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

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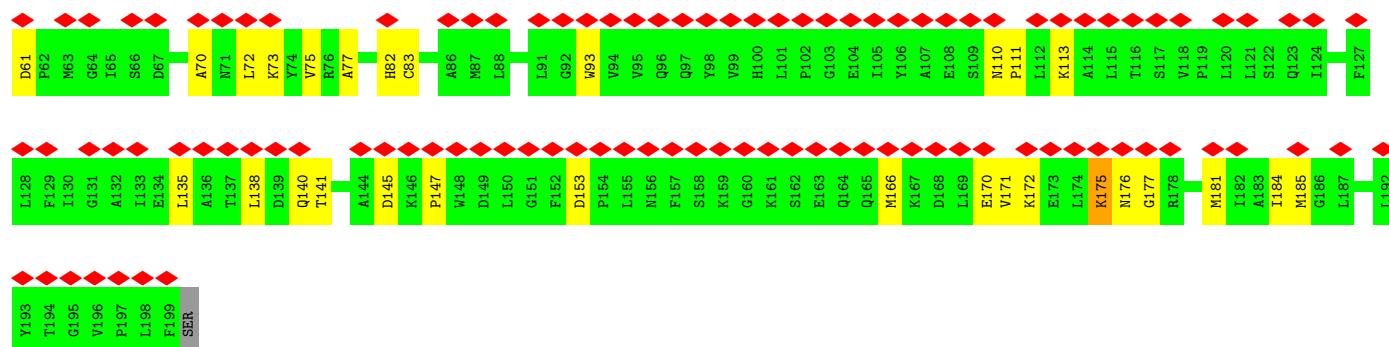
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Mol	Chain	Residues	Atoms	AltConf
29	i	1	Total C 40 40	0
29	j	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	l	1	Total C 40 40	0
29	m	1	Total C 40 40	0

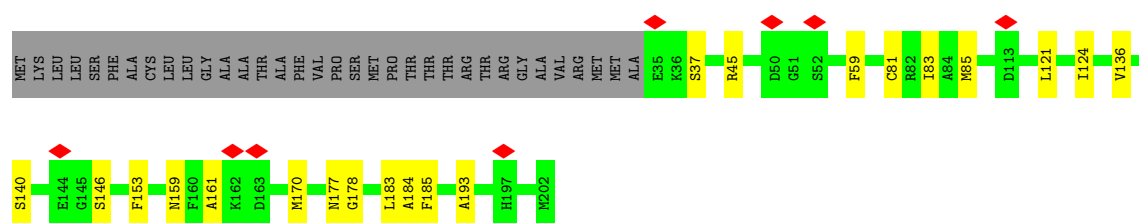
- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



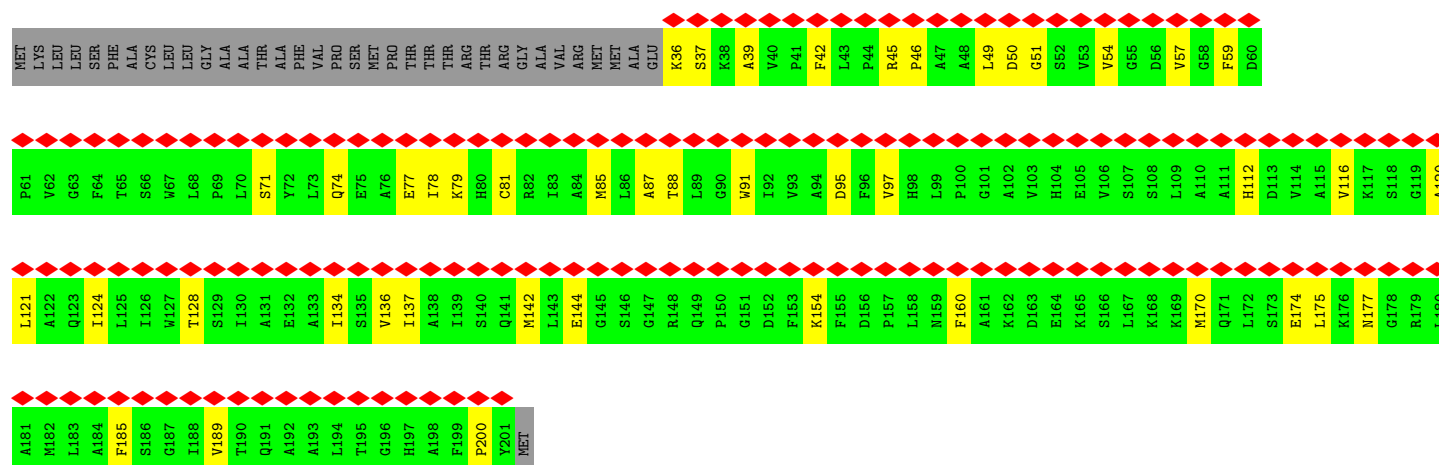
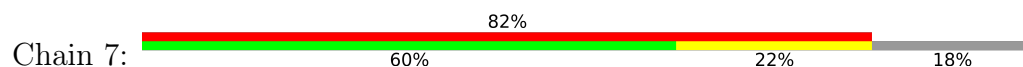
Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total Fe S 8 4 4	0
30	c	1	Total Fe S 8 4 4	0
30	c	1	Total Fe S 8 4 4	0



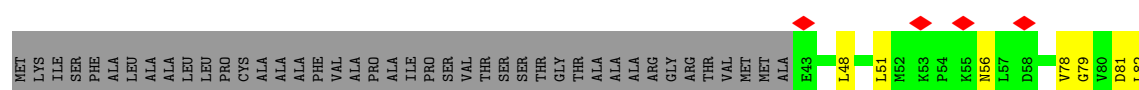
• Molecule 4: VCPI-4/7

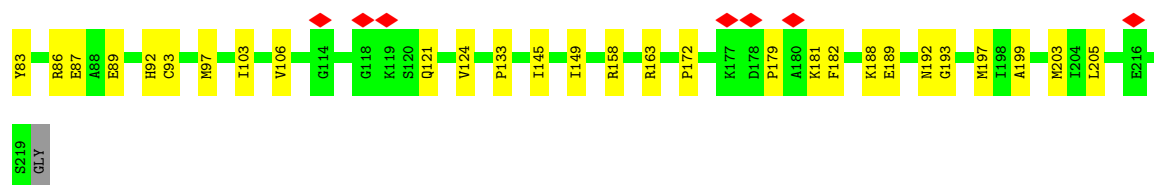


• Molecule 4: VCPI-4/7

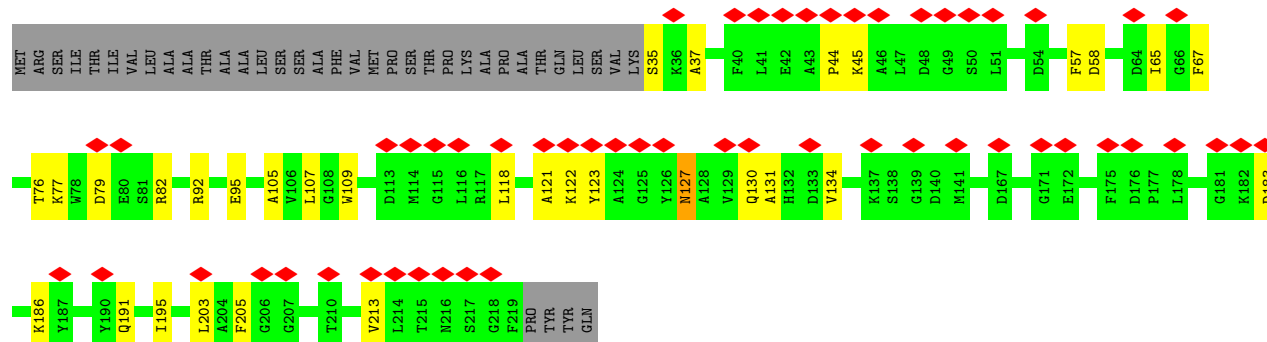


• Molecule 5: VCPI-3

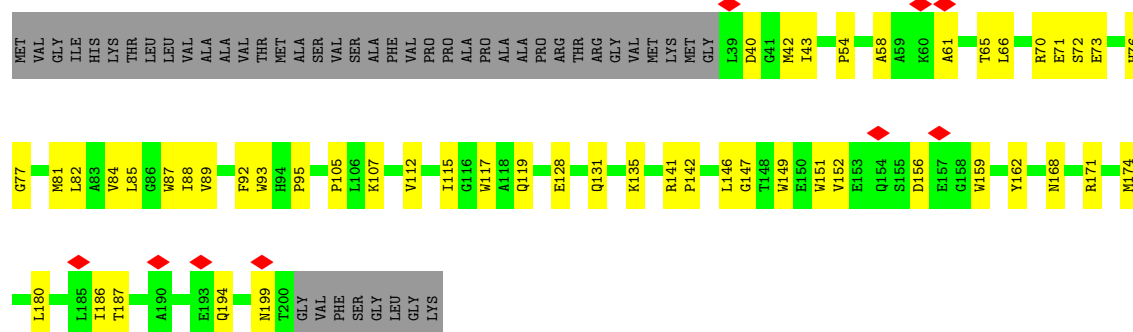




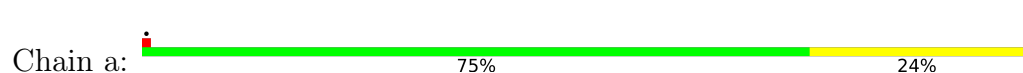
• Molecule 6: VCPI-2

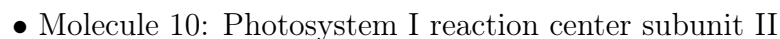


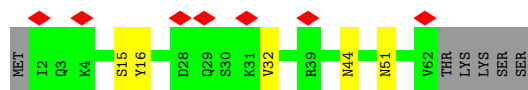
• Molecule 7: VCPI-1



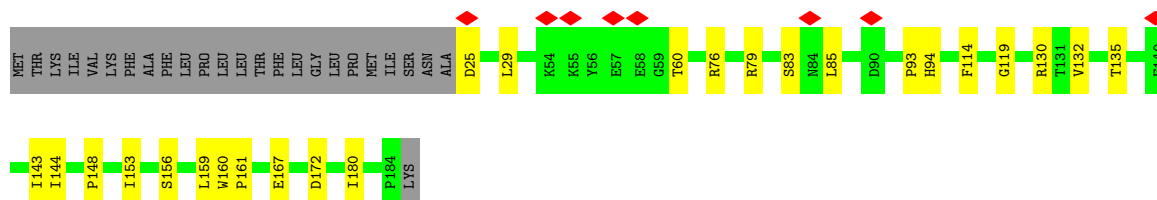
• Molecule 8: Photosystem I P700 chlorophyll a apoprotein A1



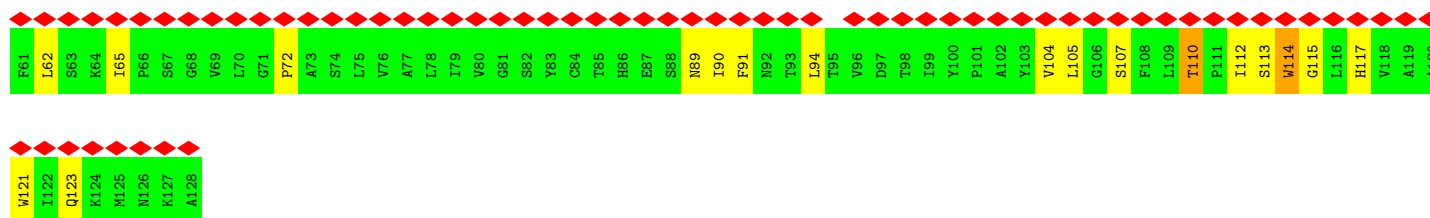
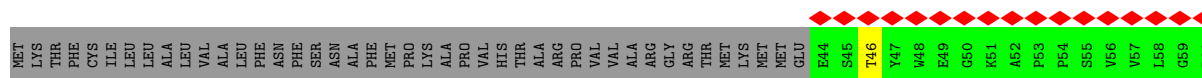




- Molecule 12: Photosystem I reaction center subunit III



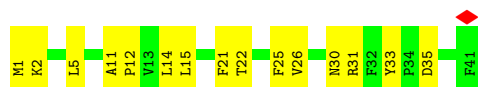
- Molecule 13: PsaR



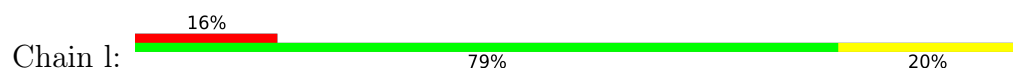
- Molecule 14: Photosystem I reaction center subunit VIII

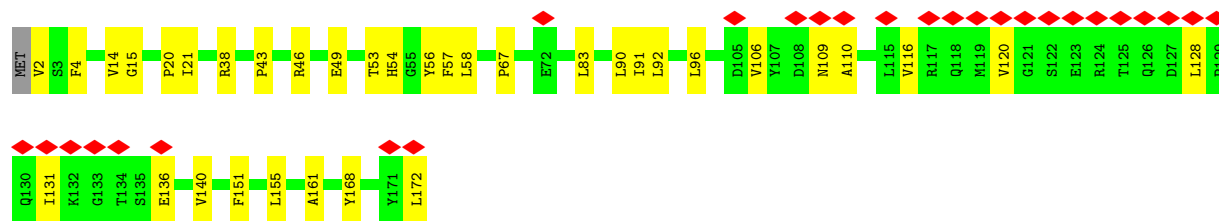


- Molecule 15: Photosystem I reaction center subunit IX



- Molecule 16: PSI subunit V





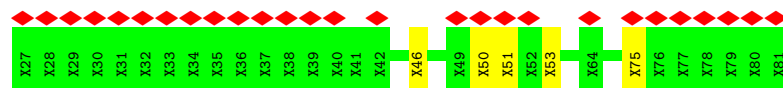
• Molecule 17: Psam

Chain m: 90% 10%



• Molecule 18: PsaS

Chain g: 49% 91% 9%



• Molecule 19: Photosystem I iron-sulfur center

Chain c: 70% 28%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60260	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	1.545	Depositor
Minimum map value	-0.339	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.295	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: BCR, PQN, A1L1F, SF4, DGD, LMG, XAT, SQD, LHG, A1L1G, CLA

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	0.34	0/1496	0.34	0/2032
3	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
4	4	0.17	0/1298	0.31	0/1761
4	7	0.19	0/1248	0.37	0/1700
5	3	0.12	0/1350	0.27	0/1821
6	2	0.14	0/1405	0.36	0/1904
7	1	0.13	0/1293	0.33	0/1759
8	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
9	b	0.20	0/6080	0.32	1/8302 (0.0%)
10	d	0.12	0/1040	0.32	0/1402
11	e	0.09	0/502	0.20	0/681
12	f	0.14	0/1297	0.30	0/1762
13	h	0.52	1/667 (0.1%)	0.52	0/915
14	i	0.15	0/278	0.33	0/378
15	j	0.15	0/351	0.36	0/478
16	l	0.14	0/1315	0.31	0/1796
17	m	0.09	0/210	0.28	0/288
19	c	0.13	0/606	0.34	0/822
All	All	0.24	5/29099 (0.0%)	0.33	8/39586 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	580	SER	CA-C	-7.02	1.43	1.52
3	8	44	LEU	C-O	-6.16	1.15	1.23
8	a	581	ALA	CA-C	-5.42	1.45	1.52
13	h	114	TRP	C-O	-5.28	1.18	1.24
8	a	582	TRP	CA-C	-5.08	1.45	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	581	ALA	N-CA-C	-8.63	102.50	113.72
8	a	448	LEU	N-CA-C	-6.11	104.18	111.69
3	8	39	LYS	N-CA-C	-6.10	105.66	113.23
8	a	584	HIS	N-CA-C	-5.81	106.53	113.97
9	b	672	TYR	N-CA-C	-5.59	106.30	113.23
3	8	41	LEU	CA-C-N	5.09	124.80	119.82
3	8	41	LEU	C-N-CA	5.09	124.80	119.82
8	a	585	VAL	N-CA-C	-5.07	105.45	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	37	0
2	9	1466	0	1470	46	0
3	8	1258	0	1280	33	0
4	4	1268	0	1288	22	0
4	7	1220	0	1209	41	0
5	3	1324	0	1340	25	0
6	2	1372	0	1347	21	0
7	1	1262	0	1237	37	0
8	a	5827	0	5697	140	0
9	b	5865	0	5710	157	0
10	d	1014	0	1015	22	0
11	e	494	0	495	5	0
12	f	1266	0	1262	21	0
13	h	646	0	649	18	0
14	i	271	0	292	12	0
15	j	339	0	342	20	0
16	l	1283	0	1278	28	0
17	m	210	0	226	3	0
18	g	275	0	62	3	0
19	c	596	0	583	20	0
20	1	88	0	112	7	0
20	2	220	0	280	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	3	176	0	224	19	0
20	4	220	0	280	31	0
20	5	132	0	168	13	0
20	7	176	0	224	25	0
20	8	132	0	168	12	0
20	9	132	0	168	17	0
20	a	44	0	56	6	0
20	j	44	0	56	7	0
21	1	45	0	0	1	0
21	3	90	0	0	0	0
21	5	45	0	0	1	0
21	7	45	0	0	2	0
21	9	90	0	0	3	0
22	1	547	0	508	15	0
22	2	544	0	452	13	0
22	3	458	0	378	9	0
22	4	613	0	522	32	0
22	5	563	0	472	22	0
22	7	576	0	444	23	0
22	8	507	0	429	20	0
22	9	519	0	452	34	0
22	a	2579	0	2562	138	0
22	b	2410	0	2464	133	0
22	f	117	0	115	2	0
22	h	120	0	121	6	0
22	j	100	0	86	9	0
22	l	148	0	123	3	0
23	1	45	0	54	2	0
23	5	35	0	34	1	0
24	1	57	0	0	2	0
24	8	57	0	0	2	0
24	9	57	0	0	2	0
24	h	57	0	0	4	0
25	9	82	0	110	5	0
25	a	75	0	93	6	0
25	b	31	0	32	0	0
26	4	40	0	38	11	0
26	8	40	0	38	2	0
26	b	57	0	72	6	0
27	2	35	0	40	3	0
27	a	34	0	38	10	0
27	j	32	0	34	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	33	0	46	4	0
28	b	33	0	46	3	0
29	a	160	0	224	12	0
29	b	240	0	336	24	0
29	f	80	0	112	14	0
29	h	80	0	112	6	0
29	i	40	0	56	3	0
29	j	40	0	56	9	0
29	l	80	0	112	14	0
29	m	40	0	56	2	0
30	a	8	0	0	0	0
30	c	16	0	0	3	0
All	All	41637	0	40703	1052	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 (1052) 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	26:4:318:DGD:HE62	1.13	1.13
4:4:193:ALA:HB1	26:4:318:DGD:C6E	1.84	1.07
26:4:318:DGD:O4E	26:4:318:DGD:O5E	1.61	0.91
20:2:303:XAT:H32	22:2:308:CLA:HAB	1.52	0.90
20:5:302:XAT:H12	22:5:307:CLA:HAB	1.53	0.89
22:a:806:CLA:O1A	22:a:814:CLA:HBA1	1.81	0.80
8:a:531:ILE:HD12	22:a:801:CLA:H172	1.63	0.80
20:4:303:XAT:H12	22:4:308:CLA:HAB	1.67	0.77
22:b:825:CLA:HMA1	29:b:845:BCR:H17C	1.66	0.76
20:8:303:XAT:H12	22:8:312:CLA:HAB	1.67	0.76
22:1:312:CLA:HHC	22:1:312:CLA:HBB1	1.69	0.74
4:4:193:ALA:CB	26:4:318:DGD:HE62	2.07	0.74
20:2:303:XAT:H181	22:2:314:CLA:HBB1	1.70	0.72
22:b:833:CLA:H72	29:b:845:BCR:H391	1.72	0.71
7:1:43:ILE:O	7:1:70:ARG:NH2	2.25	0.70
22:4:317:CLA:H2A	26:4:318:DGD:HE62	1.73	0.69
22:b:807:CLA:H151	22:b:828:CLA:HBB2	1.74	0.69
15:j:22:THR:HA	15:j:25:PHE:CE1	2.28	0.69
29:a:847:BCR:H362	29:a:848:BCR:H21C	1.73	0.69
12:f:167:GLU:HG3	12:f:172:ASP:HB3	1.73	0.68
1:5:179:LEU:HD12	12:f:159:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:302:XAT:H14	22:4:310:CLA:H12	1.76	0.68
9:b:273:HIS:HD1	22:b:817:CLA:HAB	1.58	0.68
8:a:569:ASP:OD2	8:a:573:ARG:NH2	2.27	0.68
8:a:363:HIS:ND1	22:a:819:CLA:OBD	2.26	0.67
7:1:70:ARG:NH1	7:1:73:GLU:OE1	2.28	0.67
9:b:295:ILE:HG13	22:b:820:CLA:HED1	1.77	0.67
22:4:317:CLA:HAA2	26:4:318:DGD:HE5	1.77	0.66
8:a:112:TRP:HB3	20:j:101:XAT:H373	1.77	0.66
15:j:31:ARG:HD3	20:j:101:XAT:H222	1.77	0.66
7:1:194:GLN:HG3	7:1:199:ASN:HB3	1.77	0.66
9:b:304:GLU:HG2	9:b:318:ILE:HG13	1.78	0.66
22:a:804:CLA:HED1	15:j:15:LEU:HD22	1.76	0.65
1:5:113:ARG:NH1	1:5:116:GLU:OE1	2.29	0.65
22:a:808:CLA:HMB2	29:j:104:BCR:HC8	1.78	0.65
9:b:336:LEU:HD21	22:b:829:CLA:HAB	1.78	0.65
7:1:146:LEU:HD13	22:a:844:CLA:H91	1.77	0.65
8:a:197:GLY:O	8:a:201:LEU:HB2	1.97	0.65
9:b:9:SER:HB2	26:b:848:DGD:HE62	1.78	0.65
13:h:114:TRP:HA	13:h:117:HIS:NE2	2.11	0.65
2:9:191:ALA:O	2:9:195:ASN:ND2	2.30	0.64
12:f:25:ASP:N	12:f:29:LEU:O	2.30	0.64
4:7:120:ALA:HB1	22:7:311:CLA:HMD1	1.78	0.64
8:a:356:LEU:HD11	22:a:820:CLA:H71	1.78	0.64
20:4:303:XAT:H193	22:4:308:CLA:H142	1.78	0.64
9:b:115:LEU:HA	9:b:365:THR:HG22	1.80	0.64
20:3:305:XAT:H32	22:3:313:CLA:HAB	1.79	0.64
22:a:834:CLA:H142	29:b:846:BCR:H15C	1.79	0.64
14:i:29:TYR:HA	14:i:32:LYS:HE2	1.78	0.64
8:a:684:ARG:H	9:b:570:CYS:HB2	1.63	0.64
9:b:129:THR:HG22	9:b:131:ASN:H	1.63	0.63
22:b:813:CLA:H121	22:b:818:CLA:H72	1.79	0.63
4:7:50:ASP:OD1	4:7:51:GLY:N	2.32	0.63
12:f:79:ARG:NH1	15:j:35:ASP:O	2.30	0.63
22:b:823:CLA:HBB1	22:b:837:CLA:H151	1.79	0.63
4:7:136:VAL:HG22	22:7:312:CLA:HMA1	1.81	0.63
1:5:120:GLY:O	1:5:124:MET:HG3	1.98	0.63
8:a:362:HIS:HA	8:a:365:TYR:CE1	2.33	0.63
15:j:26:VAL:HG11	29:j:104:BCR:H24C	1.81	0.62
1:5:130:PHE:CE1	20:5:302:XAT:O24	2.52	0.62
8:a:114:ILE:HB	20:j:101:XAT:H372	1.81	0.62
20:4:304:XAT:H32	22:4:313:CLA:HAB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:7:303:XAT:H362	22:7:308:CLA:H51	1.81	0.62
8:a:298:PHE:HE1	22:a:822:CLA:HAB	1.64	0.62
2:9:182:ALA:HB3	2:9:190:GLU:HG2	1.82	0.62
9:b:424:LEU:HD13	9:b:534:LEU:HA	1.81	0.62
10:d:12:LYS:HB2	10:d:51:LYS:HB3	1.82	0.62
15:j:21:PHE:HA	22:j:103:CLA:HBB2	1.80	0.62
20:4:305:XAT:H363	20:3:301:XAT:H10	1.80	0.62
10:d:88:TYR:HB2	10:d:92:ASP:HB2	1.81	0.62
24:h:204:A1L1F:C12	24:h:204:A1L1F:C4	2.78	0.62
22:a:818:CLA:C3D	27:a:853:LMG:HC91	2.30	0.61
22:8:305:CLA:CGA	26:8:315:DGD:HE5	2.29	0.61
8:a:70:HIS:ND1	22:a:814:CLA:OBD	2.31	0.61
8:a:162:ALA:O	8:a:166:MET:HG2	2.00	0.61
8:a:298:PHE:CE1	22:a:822:CLA:HAB	2.35	0.61
9:b:660:ALA:HB3	22:b:804:CLA:HBB2	1.83	0.61
1:5:190:ARG:NH1	1:5:191:GLU:O	2.34	0.61
22:4:317:CLA:H2A	26:4:318:DGD:C6E	2.30	0.61
8:a:121:ASN:HB3	8:a:129:GLN:HB3	1.82	0.61
8:a:589:LEU:HD21	22:a:831:CLA:HBC1	1.81	0.61
10:d:86:ARG:HB2	10:d:96:LEU:HD11	1.82	0.61
4:7:136:VAL:HG11	22:b:820:CLA:HBA1	1.81	0.61
9:b:561:CYS:SG	9:b:563:GLY:N	2.71	0.61
22:b:830:CLA:HAB	22:b:837:CLA:HBB2	1.82	0.61
6:2:44:PRO:HG3	6:2:58:ASP:HB3	1.83	0.61
4:7:144:GLU:HB2	9:b:294:LEU:HD11	1.82	0.61
9:b:15:ASP:HB3	9:b:20:ARG:HB2	1.82	0.61
23:5:316:SQD:H2	20:4:301:XAT:H373	1.82	0.60
6:2:76:THR:O	6:2:82:ARG:NH1	2.33	0.60
22:b:823:CLA:HAB	22:b:830:CLA:HMD2	1.83	0.60
22:b:831:CLA:HBC3	29:f:804:BCR:H362	1.83	0.60
24:1:304:A1L1F:C2	22:a:844:CLA:H11	2.31	0.60
22:8:305:CLA:HAA2	26:8:315:DGD:HE5	1.82	0.60
8:a:429:ALA:O	8:a:433:HIS:ND1	2.31	0.60
22:a:833:CLA:HBC2	22:a:840:CLA:HMC2	1.83	0.60
1:5:225:ILE:HG22	22:5:314:CLA:HAB	1.82	0.60
20:2:303:XAT:H363	22:2:308:CLA:H2	1.84	0.60
8:a:53:ASP:OD2	8:a:343:HIS:NE2	2.35	0.60
9:b:412:ARG:NH2	22:b:830:CLA:O1D	2.35	0.60
5:3:92:HIS:HB3	5:3:197:MET:SD	2.42	0.60
5:3:199:ALA:O	5:3:203:MET:HG3	2.01	0.60
8:a:167:LEU:HD11	22:a:810:CLA:H193	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:302:XAT:H162	22:5:307:CLA:H2	1.82	0.59
7:1:186:ILE:HG13	7:1:187:THR:HG23	1.83	0.59
5:3:83:TYR:OH	5:3:163:ARG:NH1	2.35	0.59
21:1:301:A1L1G:C18	22:1:306:CLA:HAC2	2.32	0.59
4:4:185:PHE:CZ	20:4:303:XAT:H30	2.37	0.59
3:8:185:MET:HE2	22:8:308:CLA:HBB2	1.83	0.59
16:l:38:ARG:O	16:l:46:ARG:NH2	2.35	0.58
2:9:185:PRO:HA	22:9:313:CLA:HBA2	1.85	0.58
4:7:88:THR:HG21	20:7:304:XAT:H12	1.85	0.58
22:a:820:CLA:H92	22:a:830:CLA:H91	1.84	0.58
8:a:107:SER:HB2	8:a:124:VAL:HG11	1.85	0.58
22:a:804:CLA:ND	15:j:12:PRO:HG3	2.17	0.58
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.58
10:d:97:HIS:HB3	10:d:98:PRO:HD3	1.86	0.58
22:a:818:CLA:C1D	27:a:853:LMG:H291	2.34	0.58
13:h:121:TRP:CD1	22:h:203:CLA:HAA1	2.39	0.58
20:8:302:XAT:H32	22:8:307:CLA:HAB	1.85	0.58
22:b:804:CLA:CGA	22:b:804:CLA:H3A	2.34	0.58
8:a:292:LEU:HD21	22:a:818:CLA:CAB	2.34	0.57
8:a:507:VAL:HG22	8:a:517:MET:HG3	1.85	0.57
1:5:155:VAL:HG21	22:5:309:CLA:HAA2	1.86	0.57
4:4:170:MET:HE1	22:4:313:CLA:H43	1.84	0.57
22:a:802:CLA:CGA	22:a:802:CLA:H3A	2.35	0.57
20:5:301:XAT:H14	22:5:309:CLA:H12	1.86	0.57
9:b:178:SER:HB3	9:b:286:GLY:HA3	1.86	0.57
29:f:801:BCR:HC32	22:j:102:CLA:H43	1.86	0.57
5:3:86:ARG:NH1	5:3:89:GLU:OE1	2.38	0.57
8:a:7:SER:H	8:a:12:PHE:HE2	1.53	0.57
9:b:29:HIS:ND1	22:b:807:CLA:O1A	2.28	0.57
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.57
8:a:598:ILE:HG13	22:a:801:CLA:H192	1.86	0.57
2:9:107:LEU:HD11	2:9:140:ILE:HD11	1.87	0.57
2:9:222:ASP:HB2	2:9:230:LEU:HD13	1.86	0.57
3:8:60:PHE:HE1	22:8:305:CLA:HBC3	1.70	0.57
4:7:185:PHE:CD2	20:7:303:XAT:H12	2.39	0.57
22:b:840:CLA:HBB2	22:h:203:CLA:C2	2.34	0.57
29:b:842:BCR:H23C	29:h:202:BCR:H323	1.86	0.57
1:5:112:LEU:HD22	22:5:307:CLA:H12	1.86	0.57
22:3:312:CLA:H42	29:a:848:BCR:H272	1.85	0.57
8:a:517:MET:HE1	8:a:623:HIS:NE2	2.19	0.57
22:a:826:CLA:HBA1	22:a:830:CLA:H193	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:69:ALA:HB2	9:b:133:LEU:HB2	1.86	0.56
8:a:324:GLY:HA3	25:a:846:LHG:HC32	1.87	0.56
20:9:303: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
20:2:303:XAT:C36	22:2:308:CLA:H2	2.35	0.56
27:a:853:LMG:O8	27:a:853:LMG:H112	2.05	0.56
9:b:582:MET:HG3	9:b:712:LEU:HD21	1.87	0.56
9:b:693:VAL:HG11	22:b:801:CLA:HAB	1.87	0.56
22:b:805:CLA:H18	14:i:14:VAL:HG22	1.86	0.56
4:4:140:SER:OG	15:j:1:MET:SD	2.57	0.56
9:b:39:GLU:HB3	9:b:163:LEU:HD11	1.87	0.56
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.56
8:a:441:LEU:HB3	8:a:534:PHE:HB2	1.88	0.56
22:a:818:CLA:CHD	27:a:853:LMG:H291	2.36	0.56
22:a:841:CLA:H92	29:f:801:BCR:H15C	1.88	0.56
9:b:74:PHE:O	9:b:78:ILE:HG12	2.04	0.56
14:i:26:LEU:HD13	29:l:205:BCR:HC8	1.86	0.56
4:4:136:VAL:HG22	22:4:312:CLA:HMA1	1.87	0.56
8:a:114:ILE:HG13	8:a:115:VAL:HG13	1.87	0.56
10:d:105:GLU:HG2	19:c:19:ARG:HB3	1.88	0.56
16:l:54:HIS:HA	16:l:57:PHE:CE2	2.41	0.56
27:a:853:LMG:H112	27:a:853:LMG:C9	2.35	0.56
5:3:182:PHE:HZ	22:3:313:CLA:HED3	1.70	0.56
8:a:651:VAL:HG22	8:a:739:ALA:HB3	1.87	0.56
1:5:111:TRP:NE1	22:5:308:CLA:O1A	2.32	0.55
22:a:841:CLA:H72	29:f:801:BCR:H17C	1.88	0.55
22:b:821:CLA:HHB	22:b:822:CLA:H2	1.88	0.55
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.55
7:1:88:ILE:HG22	7:1:92:PHE:HE1	1.71	0.55
22:a:825:CLA:H12	29:a:849:BCR:H14C	1.88	0.55
8:a:734:TRP:NE1	22:a:829:CLA:O1A	2.36	0.55
9:b:521:VAL:HG21	9:b:595:TYR:HB2	1.89	0.55
8:a:651:VAL:HG21	8:a:736:PHE:HA	1.87	0.55
2:9:85:GLY:O	2:9:89:MET:HG3	2.07	0.55
2:9:93:ILE:HG13	20:9:304:XAT:H8	1.89	0.55
8:a:213:ILE:HG23	8:a:233:PRO:HB3	1.87	0.55
2:9:153:PHE:HA	16:l:151:PHE:HE2	1.71	0.55
4:4:185:PHE:CE2	20:4:303:XAT:H30	2.42	0.55
8:a:686:TYR:OH	22:a:802:CLA:OBD	2.22	0.55
22:b:806:CLA:HBA1	22:b:813:CLA:HBA1	1.87	0.55
6:2:35:SER:OG	6:2:37:ALA:O	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:93:ASP:OD1	9:b:95:HIS:ND1	2.33	0.55
8:a:197:GLY:HA3	22:a:814:CLA:HBB1	1.89	0.54
8:a:667:LEU:HD11	9:b:619:MET:HB2	1.89	0.54
15:j:14:LEU:HD21	27:j:105:LMG:H141	1.89	0.54
16:l:92:LEU:HB3	29:l:205:BCR:H401	1.88	0.54
2:9:117:TRP:O	2:9:120:TRP:CD1	2.60	0.54
7:1:115:ILE:O	7:1:119:GLN:NE2	2.40	0.54
22:a:822:CLA:HBC3	22:a:828:CLA:H172	1.88	0.54
22:a:829:CLA:H101	29:j:104:BCR:H341	1.89	0.54
22:a:854:CLA:H112	15:j:14:LEU:HD22	1.88	0.54
19:c:15:THR:HG22	19:c:28:MET:HG3	1.89	0.54
8:a:210:GLN:HA	8:a:214:ALA:HB3	1.89	0.54
9:b:317:HIS:HB3	9:b:320:LEU:HD12	1.89	0.54
3:8:75:VAL:HG23	22:8:307:CLA:HMA2	1.89	0.54
24:8:304:A1L1F:C2	17:m:23:ARG:HD3	2.38	0.54
8:a:290:HIS:HB2	22:a:819:CLA:C1B	2.37	0.54
8:a:660:SER:HB2	9:b:447:ALA:HB1	1.88	0.54
8:a:573:ARG:HG3	19:c:78:GLY:HA3	1.90	0.54
10:d:63:ARG:NH2	10:d:65:GLU:OE1	2.41	0.54
2:9:149:ALA:O	2:9:153:PHE:HD1	1.89	0.54
8:a:219:LYS:HD3	8:a:246:LEU:HB3	1.90	0.54
7:1:61:ALA:HB1	7:1:65:THR:HB	1.90	0.54
9:b:355:PRO:HG3	22:b:818:CLA:HBA1	1.89	0.54
22:a:820:CLA:HAB	22:a:820:CLA:H8	1.90	0.54
11:e:32:VAL:HG11	19:c:35:LYS:HD3	1.89	0.54
21:5:303:A1L1G:C41	22:5:312:CLA:HMC1	2.37	0.54
8:a:388:VAL:HG12	8:a:596:ILE:HG23	1.89	0.54
9:b:140:LEU:HG	29:b:844:BCR:H382	1.90	0.54
9:b:443:ASP:OD1	9:b:617:TYR:HB2	2.08	0.54
2:9:162:LYS:NZ	22:9:312:CLA:O1A	2.40	0.53
2:9:179:LEU:HD23	22:9:308:CLA:HMD3	1.90	0.53
9:b:22:TRP:CG	9:b:706:GLN:HE22	2.26	0.53
22:9:312:CLA:HBA1	22:9:312:CLA:HBD	1.89	0.53
3:8:36:ALA:N	3:8:44:LEU:O	2.42	0.53
4:7:46:PRO:HG2	4:7:49:LEU:HD12	1.90	0.53
8:a:702:LYS:HB3	12:f:130:ARG:HD3	1.89	0.53
3:8:175:LYS:HB3	22:8:306:CLA:HMD2	1.90	0.53
8:a:591:TRP:HE1	22:b:804:CLA:C1D	2.21	0.53
9:b:5:PHE:HB2	14:i:30:ILE:HA	1.89	0.53
22:a:835:CLA:O2D	22:a:835:CLA:H2A	2.09	0.53
9:b:718:GLY:O	9:b:722:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:823:CLA:HBB2	22:b:840:CLA:H52	1.90	0.53
22:a:825:CLA:HMA3	22:a:844:CLA:HAB	1.90	0.53
9:b:633:LEU:HD22	9:b:726:PHE:HA	1.89	0.53
22:b:816:CLA:H91	13:h:105:LEU:HG	1.91	0.53
2:9:107:LEU:HG	2:9:136:ALA:HB1	1.91	0.53
22:8:305:CLA:HBC2	4:7:134:ILE:HG13	1.91	0.53
22:a:809:CLA:CHC	22:a:810:CLA:HMD2	2.39	0.53
4:4:121:LEU:HD23	4:4:124:ILE:HD12	1.90	0.53
22:a:831:CLA:H42	25:a:845:LHG:H251	1.90	0.53
9:b:661:THR:O	9:b:664:MET:HB3	2.08	0.53
9:b:709:LEU:HD11	26:b:848:DGD:HB41	1.90	0.53
22:b:829:CLA:H42	26:b:848:DGD:HB42	1.91	0.53
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.53
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.91	0.53
4:4:83:ILE:HD11	20:4:302:XAT:H362	1.90	0.53
18:g:51:UNK:O	18:g:53:UNK:N	2.42	0.53
2:9:137:ARG:NH1	22:9:318:CLA:OBD	2.41	0.52
22:4:317:CLA:O2D	26:4:318:DGD:HE61	2.09	0.52
9:b:419:ALA:O	9:b:423:HIS:ND1	2.39	0.52
22:b:801:CLA:H101	22:b:801:CLA:HBB1	1.92	0.52
4:7:128:THR:HG23	21:7:302:A1L1G:C17	2.39	0.52
7:1:72:SER:O	7:1:76:HIS:ND1	2.28	0.52
9:b:50:HIS:ND1	22:b:813:CLA:OBD	2.38	0.52
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.52
3:8:177:GLY:O	3:8:181:MET:HG3	2.09	0.52
8:a:396:VAL:HG11	8:a:589:LEU:HG	1.91	0.52
22:b:836:CLA:HBC3	29:f:804:BCR:H401	1.91	0.52
12:f:143:ILE:HG13	12:f:144:ILE:HG13	1.92	0.52
2:9:192:GLU:HB2	22:9:312:CLA:C1B	2.40	0.52
4:7:200:PRO:O	20:7:304:XAT:O3	2.26	0.52
22:a:810:CLA:HAB	22:j:102:CLA:HMD2	1.91	0.52
22:a:827:CLA:H93	22:a:840:CLA:H52	1.92	0.52
20:5:302:XAT:C16	22:5:307:CLA:H2	2.39	0.52
3:8:70:ALA:H	22:b:811:CLA:HED1	1.75	0.52
5:3:87:GLU:OE2	5:3:163:ARG:NH2	2.31	0.52
7:1:85:LEU:HB3	22:1:308:CLA:HMC2	1.92	0.52
9:b:179:GLY:O	9:b:183:VAL:HB	2.10	0.52
10:d:95:LEU:HD22	18:g:75:UNK:HA	1.91	0.52
12:f:85:LEU:HD13	12:f:93:PRO:HB3	1.92	0.52
5:3:93:CYS:HB3	5:3:193:GLY:HA3	1.92	0.52
9:b:189:THR:HG21	9:b:276:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:662:GLY:O	9:b:666:LEU:HG	2.10	0.52
8:a:577:CYS:O	9:b:671:GLY:HA3	2.11	0.51
4:4:193:ALA:O	26:4:318:DGD:O6E	2.28	0.51
7:1:77:GLY:O	7:1:81:MET:HG3	2.09	0.51
19:c:58:CYS:SG	19:c:63:LEU:HA	2.51	0.51
19:c:11:CYS:SG	19:c:39:ILE:HG13	2.50	0.51
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.51
22:b:836:CLA:HBC3	29:f:804:BCR:H292	1.91	0.51
24:h:204:A1L1F:O46	22:h:205:CLA:H52	2.11	0.51
8:a:422:ARG:O	8:a:426:HIS:ND1	2.41	0.51
22:b:811:CLA:H72	22:b:812:CLA:HBC3	1.93	0.51
2:9:218:LEU:HG	22:9:314:CLA:HMA2	1.92	0.51
4:4:81:CYS:HB3	4:4:178:GLY:HA3	1.91	0.51
20:7:301:XAT:H10	22:7:315:CLA:HMD1	1.93	0.51
9:b:274:HIS:HB2	22:b:817:CLA:C1B	2.41	0.51
22:h:203:CLA:HBA1	22:h:203:CLA:HBD	1.93	0.51
6:2:121:ALA:O	6:2:122:LYS:HG2	2.10	0.51
4:7:121:LEU:HD13	22:7:316:CLA:HBC3	1.92	0.51
22:a:834:CLA:H151	28:b:841:PQN:H202	1.91	0.51
9:b:434:HIS:CD2	29:b:849:BCR:H333	2.46	0.51
22:b:807:CLA:H52	26:b:848:DGD:HB72	1.92	0.51
12:f:160:TRP:CD1	12:f:161:PRO:HD3	2.46	0.51
5:3:79:GLY:O	5:3:158:ARG:NH1	2.43	0.51
10:d:33:ILE:HG22	10:d:58:VAL:HG22	1.92	0.51
8:a:431:ILE:HG13	8:a:549:TYR:HE1	1.74	0.51
9:b:722:THR:HG23	22:b:803:CLA:O1D	2.11	0.51
24:1:304:A1L1F:C56	25:a:846:LHG:H241	2.41	0.50
22:a:818:CLA:HHC	22:a:818:CLA:HBB1	1.93	0.50
27:a:853:LMG:H131	27:a:853:LMG:H292	1.94	0.50
9:b:273:HIS:ND1	22:b:817:CLA:HAB	2.25	0.50
9:b:342:ALA:O	9:b:346:THR:HG23	2.11	0.50
20:4:303:XAT:C16	22:4:308:CLA:H2	2.41	0.50
6:2:77:LYS:O	6:2:79:ASP:N	2.43	0.50
8:a:440:PHE:HE2	22:a:839:CLA:HAB	1.76	0.50
9:b:305:ALA:HB2	13:h:46:THR:HB	1.94	0.50
9:b:602:THR:HG21	9:b:611:PHE:HB2	1.93	0.50
19:c:17:CYS:SG	19:c:18:VAL:N	2.85	0.50
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.50
20:5:301:XAT:H193	22:5:310:CLA:HBA2	1.94	0.50
22:5:312:CLA:CGA	22:5:312:CLA:H3A	2.41	0.50
27:a:853:LMG:HC92	27:a:853:LMG:C11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:50:LEU:HD11	3:8:61:ASP:HB2	1.93	0.50
8:a:460:ARG:NH2	22:a:835:CLA:O1D	2.44	0.50
9:b:478:LEU:HG	9:b:479:LEU:HG	1.93	0.50
19:c:13:GLY:O	19:c:38:GLN:NE2	2.44	0.50
1:5:130:PHE:HE1	20:5:302:XAT:O24	1.94	0.50
4:7:45:ARG:NH1	4:7:49:LEU:O	2.42	0.50
4:7:54:VAL:HG21	4:7:74:GLN:HE21	1.77	0.50
8:a:425:ARG:NH2	10:d:15:GLY:O	2.44	0.50
22:b:832:CLA:HBB2	29:f:801:BCR:HC41	1.94	0.50
2:9:117:TRP:O	2:9:120:TRP:NE1	2.45	0.50
22:3:308:CLA:HED2	22:3:308:CLA:H2A	1.94	0.50
2:9:32:THR:H	2:9:33:PRO:HD2	1.77	0.49
21:9:301:A1L1G:C44	22:9:315:CLA:HBC3	2.41	0.49
9:b:26:ALA:HA	22:b:829:CLA:H43	1.93	0.49
9:b:492:SER:HA	9:b:496:LEU:HD12	1.94	0.49
9:b:562:ASP:OD2	9:b:566:ARG:NH2	2.38	0.49
8:a:565:ARG:HG2	8:a:715:THR:HG21	1.93	0.49
29:b:849:BCR:H23C	15:j:33:TYR:CD2	2.47	0.49
8:a:292:LEU:HD12	22:a:816:CLA:HMC3	1.95	0.49
22:a:803:CLA:H2	9:b:657:LEU:HD22	1.95	0.49
9:b:3:TYR:HB2	14:i:33:GLU:HA	1.95	0.49
9:b:25:ILE:HG12	29:l:205:BCR:H312	1.94	0.49
6:2:183:ASP:O	6:2:186:LYS:N	2.44	0.49
8:a:615:VAL:HG22	8:a:621:VAL:HG22	1.95	0.49
16:l:106:VAL:H	16:l:140:VAL:HG23	1.77	0.49
18:g:46:UNK:O	18:g:50:UNK:N	2.45	0.49
2:9:191:ALA:HB1	22:9:313:CLA:HAA1	1.93	0.49
7:1:112:VAL:HB	7:1:117:TRP:NE1	2.27	0.49
8:a:423:VAL:HA	8:a:426:HIS:CE1	2.47	0.49
4:7:42:PHE:HE2	22:7:306:CLA:HAB	1.77	0.49
22:a:818:CLA:CHD	22:a:819:CLA:HBB2	2.43	0.49
19:c:17:CYS:HB3	30:c:102:SF4:S4	2.52	0.49
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.49
4:7:185:PHE:O	4:7:189:VAL:HG22	2.13	0.49
9:b:443:ASP:OD1	9:b:618:ILE:N	2.46	0.49
3:8:60:PHE:CE1	22:8:305:CLA:HBC3	2.47	0.49
4:4:159:ASN:C	4:4:161:ALA:H	2.20	0.49
5:3:203:MET:HE2	20:3:305:XAT:O4	2.13	0.49
4:7:91:TRP:CE3	20:7:303:XAT:H22	2.48	0.49
4:7:97:VAL:O	4:7:97:VAL:HG13	2.13	0.49
8:a:637:ASN:HB2	9:b:653:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:802:CLA:H41	9:b:436:LEU:HD22	1.95	0.49
2:9:88:ALA:HA	20:9:303:XAT:H8	1.95	0.49
22:a:818:CLA:O1A	27:a:853:LMG:O10	2.30	0.49
9:b:65:LEU:HD11	29:b:844:BCR:H281	1.95	0.48
9:b:181:PHE:HE2	22:b:819:CLA:HAB	1.78	0.48
22:b:823:CLA:H2A	22:b:823:CLA:HED3	1.95	0.48
22:b:824:CLA:H141	22:b:824:CLA:H193	1.95	0.48
14:i:26:LEU:HD22	29:l:205:BCR:H323	1.94	0.48
16:l:43:PRO:HD3	16:l:136:GLU:CD	2.38	0.48
16:l:109:ASN:OD1	16:l:110:ALA:N	2.35	0.48
3:8:73:LYS:HD3	3:8:145:ASP:HA	1.95	0.48
24:8:304:A1L1F:C36	22:8:311:CLA:H51	2.43	0.48
22:4:309:CLA:HAC1	22:4:316:CLA:HAB	1.95	0.48
8:a:674:ALA:HB3	22:a:802:CLA:HBB2	1.94	0.48
9:b:166:PHE:O	9:b:172:ARG:NH2	2.46	0.48
9:b:271:MET:O	9:b:275:HIS:ND1	2.47	0.48
9:b:412:ARG:HH21	22:b:830:CLA:CGD	2.27	0.48
8:a:712:LEU:N	28:a:843:PQN:O4	2.45	0.48
9:b:526:ALA:O	9:b:530:HIS:ND1	2.37	0.48
3:8:172:LYS:O	3:8:176:ASN:ND2	2.39	0.48
22:a:832:CLA:HAB	22:a:840:CLA:HBB2	1.96	0.48
22:b:821:CLA:CHB	22:b:822:CLA:H2	2.44	0.48
13:h:89:ASN:O	13:h:91:PHE:N	2.46	0.48
22:9:311:CLA:H2A	22:9:311:CLA:O2D	2.14	0.48
5:3:81:ASP:N	5:3:81:ASP:OD1	2.46	0.48
4:7:81:CYS:O	4:7:85:MET:HG3	2.13	0.48
8:a:554:ARG:HB2	9:b:678:GLU:OE1	2.13	0.48
9:b:407:LYS:HB3	9:b:411:ALA:HB3	1.95	0.48
13:h:72:PRO:HG3	24:h:204:A1L1F:C56	2.43	0.48
29:b:849:BCR:H23C	15:j:33:TYR:HD2	1.79	0.48
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.48
6:2:107:LEU:HB3	22:2:310:CLA:HMC2	1.94	0.48
22:2:316:CLA:C2C	27:2:317:LMG:H111	2.44	0.48
4:7:185:PHE:HE1	20:7:303:XAT:H162	1.79	0.48
22:a:820:CLA:H203	22:a:828:CLA:H3A	1.96	0.48
22:a:839:CLA:H62	22:a:839:CLA:H41	1.54	0.48
9:b:266:LEU:HD22	22:b:817:CLA:HBA1	1.95	0.48
9:b:597:HIS:CE1	9:b:601:LEU:HD11	2.49	0.48
15:j:2:LYS:O	27:j:105:LMG:HC61	2.13	0.48
15:j:5:LEU:HB3	27:j:105:LMG:HC72	1.96	0.48
1:5:171:GLU:HG3	22:5:311:CLA:NB	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:92:ARG:NH1	6:2:95:GLU:OE1	2.47	0.48
9:b:277:ALA:HA	22:b:816:CLA:HMC2	1.96	0.48
22:b:839:CLA:H13	29:i:101:BCR:H19C	1.95	0.48
9:b:595:TYR:CZ	22:b:835:CLA:HBC3	2.49	0.48
20:2:303:XAT:H11	20:2:303:XAT:H191	1.66	0.47
7:1:42:MET:HE1	7:1:66:LEU:HD22	1.95	0.47
7:1:88:ILE:HG22	7:1:92:PHE:CE1	2.49	0.47
8:a:712:LEU:HD21	28:a:843:PQN:H151	1.95	0.47
22:a:825:CLA:H71	22:a:840:CLA:H62	1.96	0.47
9:b:8:PHE:HB2	9:b:34:HIS:CG	2.49	0.47
9:b:432:GLY:HA2	9:b:527:LEU:HD22	1.96	0.47
9:b:670:ARG:C	9:b:672:TYR:H	2.22	0.47
22:b:838:CLA:HAB	28:b:841:PQN:H172	1.96	0.47
10:d:95:LEU:HD11	10:d:98:PRO:HD2	1.95	0.47
14:i:26:LEU:HB3	29:l:205:BCR:H323	1.96	0.47
5:3:145:ILE:O	5:3:149:ILE:HG12	2.13	0.47
4:7:124:ILE:HA	22:7:311:CLA:HBC3	1.96	0.47
20:7:303:XAT:H191	20:7:303:XAT:H11	1.70	0.47
8:a:514:ILE:HD11	8:a:621:VAL:HG13	1.96	0.47
3:8:36:ALA:HB3	3:8:45:LYS:HZ2	1.78	0.47
7:1:84:VAL:O	7:1:88:ILE:HG12	2.14	0.47
8:a:38:THR:HB	8:a:710:ARG:HG3	1.97	0.47
8:a:114:ILE:HG23	8:a:115:VAL:HG22	1.95	0.47
20:5:304:XAT:C10	22:5:315:CLA:HBC3	2.43	0.47
2:9:91:GLY:HA3	20:9:303:XAT:H173	1.94	0.47
25:9:307:LHG:H341	16:l:91:ILE:HD11	1.96	0.47
20:3:304:XAT:H15	20:3:304:XAT:H201	1.78	0.47
8:a:127:ASN:HD21	12:f:60:THR:HG21	1.79	0.47
8:a:287:THR:HG23	22:a:820:CLA:HMA3	1.96	0.47
8:a:375:ILE:HG21	8:a:510:VAL:HB	1.96	0.47
22:9:316:CLA:H202	16:l:90:LEU:HD22	1.96	0.47
4:4:184:ALA:HA	22:4:315:CLA:HBB1	1.96	0.47
5:3:78:VAL:HG12	5:3:78:VAL:O	2.13	0.47
22:1:306:CLA:H93	22:1:306:CLA:H61	1.70	0.47
8:a:354:GLY:HA2	8:a:391:GLY:HA2	1.97	0.47
9:b:385:PHE:HB3	9:b:536:LEU:HB3	1.97	0.47
22:b:839:CLA:H92	22:b:839:CLA:H61	1.73	0.47
6:2:65:ILE:HG22	6:2:67:PHE:H	1.80	0.47
8:a:290:HIS:HB2	22:a:819:CLA:CHB	2.44	0.47
9:b:176:HIS:O	9:b:180:LEU:HB3	2.14	0.47
2:9:201:LEU:HD21	20:9:304:XAT:H371	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:316:CLA:H71	16:l:83:LEU:HG	1.97	0.47
22:8:311:CLA:HBB1	22:8:311:CLA:HMB3	1.97	0.47
22:3:308:CLA:H2A	22:3:308:CLA:CED	2.44	0.47
20:7:304:XAT:H191	22:7:314:CLA:HAB	1.97	0.47
8:a:476:PHE:HB3	22:a:838:CLA:H11	1.96	0.47
22:a:841:CLA:H61	22:b:832:CLA:H42	1.95	0.47
29:a:848:BCR:H15C	29:a:848:BCR:H351	1.78	0.47
9:b:127:MET:HE1	29:b:844:BCR:H282	1.97	0.47
9:b:143:LEU:HD23	9:b:146:LEU:HD12	1.97	0.47
9:b:538:LYS:O	9:b:542:ASP:HB2	2.15	0.47
9:b:586:LEU:HD21	9:b:716:THR:HG23	1.96	0.47
22:b:812:CLA:H41	22:b:812:CLA:H62	1.62	0.47
22:b:822:CLA:H43	13:h:115:GLY:C	2.40	0.47
10:d:20:TRP:CZ2	16:l:14:VAL:HG12	2.50	0.47
13:h:114:TRP:HA	13:h:117:HIS:CD2	2.49	0.47
22:a:834:CLA:CAD	29:l:201:BCR:H10C	2.45	0.47
22:b:807:CLA:H192	22:b:807:CLA:H161	1.72	0.47
22:b:812:CLA:H3A	22:b:812:CLA:HBA2	1.61	0.47
22:b:830:CLA:HAB	22:b:837:CLA:CBB	2.44	0.47
2:9:49:MET:HA	2:9:52:LYS:HD3	1.97	0.47
22:b:822:CLA:H42	13:h:62:LEU:HD11	1.97	0.47
22:b:837:CLA:H101	22:b:837:CLA:H13	1.78	0.47
11:e:51:ASN:CG	19:c:61:ASP:HB2	2.39	0.47
22:j:102:CLA:NB	29:j:104:BCR:H281	2.30	0.47
22:4:317:CLA:CGD	26:4:318:DGD:HE61	2.45	0.47
20:2:303:XAT:H15	20:2:303:XAT:H201	1.79	0.47
8:a:677:LEU:HB2	22:a:802:CLA:HMC2	1.97	0.47
2:9:187:LEU:HA	22:9:312:CLA:HMB1	1.96	0.46
6:2:191:GLN:O	6:2:195:ILE:HD12	2.15	0.46
27:2:317:LMG:H321	27:2:317:LMG:H292	1.35	0.46
22:b:838:CLA:H162	22:b:838:CLA:H192	1.73	0.46
16:l:168:TYR:O	16:l:172:LEU:HB2	2.15	0.46
4:4:185:PHE:CZ	20:4:303:XAT:H28	2.50	0.46
20:4:301:XAT:H15	20:4:301:XAT:H201	1.80	0.46
8:a:114:ILE:O	8:a:117:GLN:HG2	2.16	0.46
8:a:144:GLU:HG2	8:a:206:TRP:HH2	1.80	0.46
8:a:400:ALA:HB2	8:a:585:VAL:HG11	1.96	0.46
22:a:801:CLA:H61	22:a:803:CLA:O1D	2.15	0.46
22:a:854:CLA:H143	27:j:105:LMG:H142	1.98	0.46
9:b:297:HIS:HB3	9:b:302:ILE:HD11	1.97	0.46
9:b:452:GLU:OE2	12:f:76:ARG:NE	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:28:LEU:O	14:i:32:LYS:HG3	2.15	0.46
22:4:309:CLA:HED2	22:4:309:CLA:HBD	1.83	0.46
20:3:304:XAT:H31	20:3:304:XAT:H391	1.78	0.46
4:7:37:SER:HB2	4:7:45:ARG:HA	1.97	0.46
7:1:40:ASP:HB2	7:1:42:MET:HG3	1.98	0.46
7:1:73:GLU:HB2	22:1:306:CLA:C1B	2.45	0.46
22:1:306:CLA:H202	22:1:306:CLA:H162	1.69	0.46
8:a:68:SER:OG	8:a:174:TYR:HB2	2.14	0.46
22:b:823:CLA:HBA1	29:h:201:BCR:H16C	1.98	0.46
3:8:58:PHE:HZ	3:8:175:LYS:HZ1	1.62	0.46
6:2:118:LEU:N	22:2:310:CLA:OBD	2.47	0.46
22:h:205:CLA:HED3	22:h:205:CLA:H2A	1.97	0.46
22:j:102:CLA:H41	22:j:102:CLA:H61	1.64	0.46
4:7:120:ALA:O	4:7:124:ILE:HG13	2.16	0.46
22:a:807:CLA:H92	22:a:807:CLA:H61	1.69	0.46
22:a:829:CLA:HBB1	22:a:829:CLA:HMB1	1.97	0.46
22:b:822:CLA:HHC	22:b:840:CLA:HED1	1.98	0.46
22:9:314:CLA:CED	22:9:314:CLA:H2A	2.45	0.46
3:8:166:MET:O	3:8:170:GLU:HG3	2.16	0.46
20:7:303:XAT:H32	22:7:308:CLA:HAB	1.96	0.46
22:a:832:CLA:HBA1	22:a:832:CLA:H3A	1.80	0.46
9:b:339:LEU:O	9:b:343:THR:HG22	2.16	0.46
9:b:372:HIS:HB2	22:b:827:CLA:C1B	2.45	0.46
29:b:844:BCR:HC8	29:b:844:BCR:H311	1.97	0.46
1:5:96:VAL:HG12	22:5:307:CLA:OBD	2.15	0.46
21:9:306:A1L1G:C31	22:9:310:CLA:HBD	2.46	0.46
3:8:82:HIS:HB3	3:8:181:MET:SD	2.56	0.46
3:8:141:THR:HA	3:8:147:PRO:HB3	1.97	0.46
20:8:303:XAT:H34	22:8:313:CLA:HBB1	1.96	0.46
8:a:689:GLU:OE2	9:b:546:SER:OG	2.30	0.46
9:b:280:VAL:HG21	22:b:816:CLA:HAB	1.98	0.46
9:b:687:THR:HG23	9:b:690:ALA:HB3	1.97	0.46
22:b:817:CLA:H41	22:b:833:CLA:HAA2	1.98	0.46
3:8:171:VAL:HG13	3:8:175:LYS:HE3	1.97	0.46
4:4:37:SER:HB3	4:4:45:ARG:HA	1.98	0.46
22:a:818:CLA:NC	27:a:853:LMG:H302	2.31	0.46
9:b:392:PHE:CE2	29:b:845:BCR:HC42	2.51	0.46
12:f:143:ILE:O	15:j:11:ALA:N	2.48	0.46
2:9:80:ALA:O	2:9:84:ASN:ND2	2.49	0.46
22:9:316:CLA:HBC3	22:a:803:CLA:H151	1.97	0.46
3:8:110:ASN:HB3	3:8:113:LYS:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:806:CLA:H72	29:a:848:BCR:HC8	1.98	0.46
10:d:83:LYS:HG2	10:d:98:PRO:HG2	1.97	0.46
1:5:116:GLU:HB2	22:5:307:CLA:C1B	2.46	0.45
22:9:318:CLA:H91	22:9:318:CLA:H112	1.69	0.45
20:4:302:XAT:H30	22:4:310:CLA:H151	1.98	0.45
22:2:310:CLA:H141	22:2:310:CLA:H162	1.74	0.45
22:1:306:CLA:H91	22:1:306:CLA:H112	1.69	0.45
8:a:312:GLY:HA2	22:a:823:CLA:HMD2	1.99	0.45
8:a:665:ILE:HG23	22:a:809:CLA:H171	1.98	0.45
22:b:808:CLA:H93	22:b:808:CLA:H61	1.71	0.45
12:f:119:GLY:HA3	12:f:160:TRP:CE2	2.51	0.45
27:j:105:LMG:H292	27:j:105:LMG:H111	1.98	0.45
16:l:38:ARG:NH1	16:l:49:GLU:OE1	2.40	0.45
22:9:316:CLA:HBA2	16:l:67:PRO:HG3	1.97	0.45
6:2:127:ASN:OD1	6:2:130:GLN:N	2.46	0.45
4:7:160:PHE:HE2	20:7:304:XAT:H373	1.81	0.45
20:7:304:XAT:H32	22:7:313:CLA:HAB	1.98	0.45
22:a:801:CLA:CED	22:a:801:CLA:HAA2	2.46	0.45
22:a:827:CLA:H13	22:a:827:CLA:H172	1.77	0.45
27:a:853:LMG:H112	27:a:853:LMG:HC92	1.98	0.45
9:b:433:PHE:HZ	29:f:801:BCR:H372	1.80	0.45
20:7:305:XAT:H201	20:7:305:XAT:H15	1.69	0.45
8:a:25:PRO:HB2	8:a:41:TRP:HH2	1.81	0.45
8:a:342:TRP:CD1	22:a:826:CLA:H192	2.51	0.45
29:a:848:BCR:H11C	29:a:848:BCR:H341	1.86	0.45
9:b:228:TRP:HZ3	29:h:202:BCR:H363	1.81	0.45
9:b:268:LEU:HD23	9:b:271:MET:HE3	1.98	0.45
22:b:802:CLA:H162	22:b:802:CLA:H122	1.61	0.45
22:b:811:CLA:H51	22:b:812:CLA:H43	1.97	0.45
22:b:832:CLA:H18	29:f:804:BCR:H17C	1.98	0.45
22:b:838:CLA:H12	29:l:205:BCR:H15C	1.98	0.45
14:i:14:VAL:O	14:i:19:PRO:HD2	2.17	0.45
20:1:303:XAT:H183	22:1:308:CLA:C2B	2.47	0.45
8:a:502:ALA:HB2	8:a:516:MET:HE2	1.97	0.45
19:c:3:HIS:HB2	19:c:48:CYS:SG	2.57	0.45
3:8:93:TRP:CE2	3:8:111:PRO:HG2	2.51	0.45
4:4:193:ALA:HB1	26:4:318:DGD:O5E	2.16	0.45
20:a:852:XAT:H35	20:a:852:XAT:H401	1.85	0.45
22:b:813:CLA:H143	22:b:824:CLA:H51	1.99	0.45
22:b:825:CLA:HAA2	22:b:826:CLA:OBD	2.16	0.45
29:j:104:BCR:H15C	29:j:104:BCR:H351	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:124:MET:HE3	22:5:312:CLA:HMC2	1.98	0.45
1:5:164:PHE:HE1	22:f:802:CLA:H121	1.81	0.45
2:9:126:THR:OG1	2:9:129:GLU:OE2	2.34	0.45
29:b:849:BCR:H361	29:b:849:BCR:H20C	1.76	0.45
15:j:26:VAL:CG1	29:j:104:BCR:H403	2.47	0.45
2:9:153:PHE:CG	16:l:151:PHE:HE2	2.34	0.45
3:8:72:LEU:HD13	22:8:307:CLA:HED1	1.99	0.45
22:4:317:CLA:H62	22:4:317:CLA:H92	1.83	0.45
5:3:179:PRO:C	5:3:181:LYS:H	2.24	0.45
20:2:301:XAT:H15	20:2:301:XAT:H201	1.77	0.45
22:1:312:CLA:HMA2	23:1:315:SQD:H141	1.99	0.45
8:a:71:PHE:HD1	8:a:166:MET:HE3	1.82	0.45
22:a:835:CLA:H61	29:l:201:BCR:H363	1.99	0.45
20:4:305:XAT:H15	20:4:305:XAT:H201	1.71	0.45
20:2:303:XAT:H31	20:2:303:XAT:H391	1.70	0.45
20:7:304:XAT:H171	22:7:315:CLA:HBB1	1.99	0.45
20:1:302:XAT:H35	20:1:302:XAT:H401	1.72	0.45
22:a:834:CLA:H201	29:l:205:BCR:H343	1.98	0.45
13:h:65:ILE:O	13:h:123:GLN:NE2	2.49	0.45
13:h:112:ILE:O	13:h:115:GLY:N	2.49	0.45
4:7:170:MET:HE2	22:7:313:CLA:H12	1.99	0.45
8:a:686:TYR:CE1	9:b:538:LYS:HD2	2.52	0.45
22:a:804:CLA:H41	22:a:841:CLA:HMC1	1.98	0.45
9:b:458:GLU:OE1	12:f:94:HIS:ND1	2.46	0.45
9:b:547:LYS:NZ	11:e:15:SER:O	2.45	0.45
22:b:824:CLA:H92	22:b:824:CLA:H61	1.72	0.45
3:8:83:CYS:HB3	3:8:177:GLY:HA3	1.97	0.45
4:4:170:MET:CE	22:4:313:CLA:H12	2.47	0.45
20:7:301:XAT:H31	20:7:301:XAT:H391	1.79	0.45
22:a:826:CLA:HMB3	22:a:826:CLA:HBB1	1.99	0.45
9:b:678:GLU:HG2	19:c:81:TYR:HE1	1.82	0.45
22:b:823:CLA:HHB	22:b:840:CLA:O1D	2.16	0.45
1:5:232:HIS:HE1	20:5:304:XAT:H14	1.81	0.44
20:3:303:XAT:H35	20:3:303:XAT:H401	1.79	0.44
4:7:77:GLU:HB2	22:7:308:CLA:CHB	2.48	0.44
4:7:78:ILE:HG12	4:7:175:LEU:HD21	1.99	0.44
7:1:95:PRO:HD2	22:1:308:CLA:HMD3	1.99	0.44
8:a:407:VAL:HG11	8:a:564:PHE:N	2.32	0.44
8:a:411:ASN:ND2	8:a:414:ASN:OD1	2.37	0.44
8:a:447:GLY:HA3	22:a:835:CLA:HAB	1.98	0.44
8:a:580:SER:HB2	8:a:582:TRP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:50:HIS:HE1	22:b:806:CLA:H171	1.81	0.44
9:b:654:PHE:O	9:b:658:VAL:HG23	2.17	0.44
29:l:205:BCR:H15C	29:l:205:BCR:H351	1.74	0.44
1:5:106:PHE:HB2	12:f:148:PRO:HG3	1.99	0.44
22:9:318:CLA:H111	22:9:318:CLA:H142	1.61	0.44
20:4:303:XAT:H11	20:4:303:XAT:H191	1.74	0.44
4:7:85:MET:HE3	4:7:177:ASN:HB3	1.99	0.44
7:1:156:ASP:OD2	16:l:2:VAL:N	2.51	0.44
8:a:304:MET:HG3	22:a:823:CLA:C3C	2.47	0.44
8:a:738:LEU:HD23	8:a:738:LEU:HA	1.80	0.44
22:a:822:CLA:H12	22:a:825:CLA:HBA2	1.99	0.44
9:b:172:ARG:HB2	22:b:813:CLA:HBC2	2.00	0.44
9:b:259:PHE:CZ	9:b:510:LEU:HD12	2.52	0.44
22:h:203:CLA:H141	22:h:203:CLA:H162	1.77	0.44
29:l:205:BCR:H11C	29:l:205:BCR:H341	1.84	0.44
2:9:93:ILE:CG1	20:9:304:XAT:H8	2.47	0.44
2:9:153:PHE:HA	16:l:151:PHE:CE2	2.51	0.44
22:4:310:CLA:H112	22:4:310:CLA:H142	1.78	0.44
4:7:36:LYS:HB2	4:7:45:ARG:H	1.83	0.44
7:1:89:VAL:O	7:1:93:TRP:N	2.49	0.44
8:a:194:HIS:ND1	22:a:826:CLA:OBD	2.48	0.44
22:a:831:CLA:H92	22:a:831:CLA:H61	1.70	0.44
9:b:201:ARG:HG2	9:b:248:SER:HB2	1.99	0.44
9:b:208:ASP:OD1	9:b:208:ASP:N	2.43	0.44
20:j:101:XAT:H35	20:j:101:XAT:H401	1.80	0.44
16:l:116:VAL:HG11	16:l:128:LEU:C	2.42	0.44
20:5:302:XAT:H383	22:5:309:CLA:C2B	2.48	0.44
2:9:144:HIS:CD2	22:9:314:CLA:HBC3	2.53	0.44
2:9:207:VAL:HG21	22:9:308:CLA:H191	1.99	0.44
22:9:308:CLA:H92	22:9:308:CLA:H61	1.76	0.44
20:8:302:XAT:H31	20:8:302:XAT:H391	1.88	0.44
22:4:311:CLA:H2A	22:4:311:CLA:O2D	2.16	0.44
5:3:121:GLN:HA	5:3:124:VAL:HG12	1.99	0.44
5:3:133:PRO:HB2	20:3:301:XAT:H23	2.00	0.44
6:2:131:ALA:HA	6:2:134:VAL:HG12	1.98	0.44
20:2:301:XAT:H35	20:2:301:XAT:H401	1.76	0.44
7:1:105:PRO:C	7:1:107:LYS:H	2.24	0.44
8:a:578:GLN:HA	8:a:583:ASP:OD2	2.18	0.44
22:a:807:CLA:H43	25:a:845:LHG:H252	2.00	0.44
22:b:827:CLA:H61	22:b:827:CLA:H102	1.85	0.44
12:f:153:ILE:O	12:f:156:SER:OG	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:9:301:A1L1G:O13	20:9:304:XAT:H28	2.16	0.44
22:4:308:CLA:H112	22:4:308:CLA:H143	1.66	0.44
6:2:105:ALA:HB1	20:2:303:XAT:H161	1.98	0.44
20:7:304:XAT:H401	20:7:304:XAT:H35	1.74	0.44
22:1:310:CLA:H92	22:1:310:CLA:H61	1.73	0.44
8:a:415:ASN:O	8:a:421:ASP:HB2	2.18	0.44
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.44
7:1:171:ARG:HA	7:1:174:MET:HE3	2.00	0.44
8:a:565:ARG:HD2	25:a:845:LHG:HC61	2.00	0.44
9:b:466:GLN:NE2	22:b:835:CLA:OBD	2.34	0.44
22:b:835:CLA:H12	22:b:836:CLA:O1A	2.18	0.44
10:d:20:TRP:HB2	10:d:24:ALA:HB3	1.99	0.44
29:f:804:BCR:H341	29:f:804:BCR:H11C	1.73	0.44
27:j:105:LMG:H122	27:j:105:LMG:H151	1.56	0.44
19:c:25:VAL:HG21	19:c:48:CYS:HA	2.00	0.44
20:5:301:XAT:H35	20:5:301:XAT:H401	1.77	0.44
25:9:307:LHG:H352	14:i:16:LEU:HD22	1.99	0.44
4:4:59:PHE:HE1	22:4:306:CLA:HBC3	1.83	0.44
5:3:189:GLU:HB2	22:3:313:CLA:C1B	2.47	0.44
8:a:282:LEU:HD21	8:a:367:MET:HB3	1.98	0.44
29:a:850:BCR:H11C	29:a:850:BCR:H341	1.88	0.44
9:b:26:ALA:HB1	26:b:848:DGD:O1B	2.17	0.44
9:b:172:ARG:HD2	22:b:824:CLA:OBD	2.18	0.44
9:b:605:GLN:HE21	9:b:734:LYS:HB3	1.82	0.44
12:f:79:ARG:O	12:f:83:SER:HB2	2.17	0.44
15:j:30:ASN:ND2	22:j:102:CLA:O1A	2.47	0.44
19:c:59:PRO:HD2	30:c:102:SF4:S2	2.58	0.44
22:9:314:CLA:H2A	22:9:314:CLA:O2D	2.17	0.44
22:2:307:CLA:H3A	22:2:307:CLA:HBA2	1.76	0.44
7:1:141:ARG:HD3	7:1:149:TRP:HB3	1.99	0.44
7:1:152:VAL:HG11	7:1:159:TRP:CD1	2.53	0.44
8:a:532:HIS:CE1	8:a:599:VAL:HA	2.53	0.44
8:a:673:TRP:O	8:a:676:SER:OG	2.32	0.44
22:a:820:CLA:CAD	22:a:830:CLA:H41	2.48	0.44
22:a:854:CLA:H142	22:a:854:CLA:H111	1.80	0.44
13:h:72:PRO:CG	24:h:204:A1L1F:C56	2.96	0.44
13:h:112:ILE:O	13:h:113:SER:C	2.60	0.44
22:4:310:CLA:H162	22:4:310:CLA:H141	1.70	0.44
6:2:118:LEU:HB2	6:2:123:TYR:HD2	1.83	0.44
8:a:517:MET:HE2	8:a:611:VAL:HA	2.00	0.44
22:a:829:CLA:H91	22:a:831:CLA:H192	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:844:CLA:C1C	25:a:846:LHG:HC31	2.48	0.44
9:b:302:ILE:HD13	22:b:822:CLA:HMD2	1.99	0.44
9:b:343:THR:HG23	9:b:377:ALA:HB2	1.99	0.44
9:b:529:LEU:HD23	9:b:588:THR:HG21	2.00	0.44
22:b:839:CLA:HBA1	22:b:839:CLA:H3A	1.59	0.44
10:d:81:ASN:H	10:d:81:ASN:ND2	2.16	0.44
20:8:301:XAT:H382	22:8:312:CLA:HAC2	1.99	0.43
22:2:316:CLA:C1C	27:2:317:LMG:H111	2.46	0.43
8:a:84:MET:SD	22:a:829:CLA:HED1	2.58	0.43
8:a:442:GLY:HA3	22:b:804:CLA:O1A	2.18	0.43
22:a:827:CLA:HBA2	22:a:827:CLA:H3A	1.79	0.43
22:a:833:CLA:H72	22:l:203:CLA:H12	2.00	0.43
22:b:836:CLA:H62	22:b:836:CLA:H102	1.77	0.43
20:9:305:XAT:H11	20:9:305:XAT:H191	1.60	0.43
20:8:302:XAT:H11	20:8:302:XAT:H191	1.71	0.43
22:4:310:CLA:C1A	22:4:310:CLA:CGA	2.96	0.43
8:a:367:MET:HG2	8:a:500:SER:HB2	1.99	0.43
9:b:647:VAL:HG21	22:b:809:CLA:HAC1	2.00	0.43
22:b:838:CLA:H62	22:b:838:CLA:H41	1.70	0.43
20:j:101:XAT:H15	20:j:101:XAT:H201	1.82	0.43
22:j:103:CLA:O1D	22:j:103:CLA:H2A	2.18	0.43
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.43
2:9:120:TRP:CD1	2:9:121:VAL:HG13	2.53	0.43
24:9:302:A1L1F:C42	22:9:311:CLA:O1A	2.66	0.43
4:7:112:HIS:O	4:7:116:VAL:HG13	2.18	0.43
8:a:143:ALA:HB2	8:a:371:PRO:HD2	2.00	0.43
8:a:364:MET:HE1	22:a:830:CLA:CAD	2.49	0.43
8:a:701:LEU:HD12	22:a:841:CLA:HMA2	2.00	0.43
22:a:807:CLA:H102	22:a:807:CLA:H161	2.00	0.43
22:b:818:CLA:H3A	22:b:818:CLA:HBA2	1.37	0.43
12:f:160:TRP:CG	12:f:161:PRO:HD3	2.52	0.43
22:9:318:CLA:HMC2	14:i:17:VAL:HG21	2.01	0.43
8:a:194:HIS:HE1	22:a:826:CLA:H72	1.84	0.43
22:a:822:CLA:OBD	22:a:824:CLA:HMD3	2.19	0.43
20:a:852:XAT:H201	20:a:852:XAT:H15	1.67	0.43
20:5:301:XAT:H31	20:5:301:XAT:H391	1.88	0.43
2:9:153:PHE:CE2	16:l:155:LEU:HD22	2.53	0.43
22:9:316:CLA:H112	22:9:318:CLA:HAB	1.99	0.43
8:a:683:GLY:HA3	9:b:571:ASP:HB2	1.99	0.43
22:a:806:CLA:H162	22:a:806:CLA:H141	1.59	0.43
22:a:810:CLA:HBB1	29:j:104:BCR:H23C	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:430:PHE:O	9:b:434:HIS:ND1	2.41	0.43
22:5:307:CLA:HBC1	20:4:301:XAT:H383	2.01	0.43
2:9:198:VAL:HG12	20:9:304:XAT:H34	2.01	0.43
20:9:305:XAT:H35	20:9:305:XAT:H401	1.74	0.43
3:8:47:PRO:HG2	3:8:50:LEU:HG	2.00	0.43
20:4:302:XAT:H35	20:4:302:XAT:H401	1.76	0.43
5:3:51:LEU:HD23	5:3:51:LEU:HA	1.87	0.43
4:7:142:MET:C	4:7:144:GLU:H	2.26	0.43
20:7:303:XAT:H35	20:7:303:XAT:H401	1.76	0.43
8:a:75:ALA:HB2	8:a:166:MET:HB2	2.01	0.43
8:a:651:VAL:O	8:a:654:SER:OG	2.29	0.43
28:a:843:PQN:H302	28:a:843:PQN:H261	1.75	0.43
9:b:274:HIS:HB2	22:b:817:CLA:CHB	2.48	0.43
22:b:805:CLA:H162	22:b:805:CLA:H141	1.67	0.43
22:b:838:CLA:H161	16:l:92:LEU:HD21	1.99	0.43
19:c:54:CYS:SG	19:c:55:GLU:N	2.91	0.43
3:8:172:LYS:HD3	22:8:313:CLA:HAA2	2.01	0.43
8:a:52:PHE:CD2	22:a:806:CLA:HMC2	2.53	0.43
22:a:841:CLA:HED3	22:a:841:CLA:H2A	2.01	0.43
9:b:83:LYS:HE3	9:b:83:LYS:HB3	1.85	0.43
9:b:345:LEU:CD1	22:b:826:CLA:HAA1	2.49	0.43
22:b:833:CLA:H3A	22:b:833:CLA:HBA2	1.52	0.43
22:5:309:CLA:H92	22:5:309:CLA:H61	1.77	0.43
20:8:301:XAT:H401	20:8:301:XAT:H35	1.77	0.43
4:4:183:LEU:HD11	22:4:308:CLA:HAC1	2.00	0.43
20:4:303:XAT:H15	20:4:303:XAT:H201	1.82	0.43
7:1:151:TRP:CH2	16:l:20:PRO:HA	2.54	0.43
7:1:171:ARG:HA	7:1:174:MET:CE	2.49	0.43
22:b:816:CLA:C9	13:h:105:LEU:HG	2.49	0.43
16:l:96:LEU:HG	29:l:205:BCR:H24C	2.01	0.43
20:4:304:XAT:H31	20:4:304:XAT:H391	1.92	0.43
5:3:56:ASN:HB3	5:3:82:LEU:HD22	2.01	0.43
20:2:302:XAT:H31	20:2:302:XAT:H391	1.84	0.43
9:b:526:ALA:HB2	22:b:836:CLA:HMA1	2.00	0.43
22:b:802:CLA:H41	22:b:802:CLA:H61	1.78	0.43
22:b:807:CLA:H161	22:b:807:CLA:H102	2.01	0.43
10:d:32:ILE:HG21	10:d:70:LEU:HD23	2.00	0.43
13:h:107:SER:O	13:h:110:THR:OG1	2.32	0.43
3:8:138:LEU:HB2	22:8:311:CLA:HMA1	1.99	0.43
20:3:303:XAT:H11	20:3:303:XAT:H191	1.89	0.43
20:2:303:XAT:H35	20:2:303:XAT:H401	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:87:ALA:HB1	20:7:303:XAT:H161	2.01	0.43
4:7:185:PHE:CE1	20:7:303:XAT:H162	2.53	0.43
8:a:525:ASP:HA	8:a:528:VAL:HG12	2.01	0.43
22:a:806:CLA:H202	22:a:806:CLA:H161	1.70	0.43
22:a:819:CLA:HBA2	22:a:819:CLA:H3A	1.53	0.43
29:j:104:BCR:H24C	29:j:104:BCR:H371	1.85	0.43
2:9:91:GLY:HA3	20:9:303:XAT:O4	2.19	0.42
2:9:204:VAL:HG22	22:9:308:CLA:H203	2.01	0.42
20:7:303:XAT:C36	22:7:308:CLA:H2	2.49	0.42
7:1:82:LEU:HD11	22:1:311:CLA:HBC1	2.01	0.42
7:1:128:GLU:HG3	20:1:302:XAT:H372	2.01	0.42
7:1:168:ASN:HA	7:1:171:ARG:HD2	2.01	0.42
8:a:361:ALA:HB2	8:a:387:HIS:HB2	2.01	0.42
22:a:807:CLA:H161	22:a:807:CLA:H192	1.83	0.42
22:a:823:CLA:CHD	20:a:852:XAT:H183	2.49	0.42
22:a:840:CLA:H72	29:a:850:BCR:H373	2.00	0.42
9:b:207:TRP:HE1	22:b:814:CLA:H11	1.84	0.42
9:b:699:PRO:O	19:c:81:TYR:OH	2.34	0.42
22:b:801:CLA:H51	22:b:838:CLA:H102	2.01	0.42
29:b:845:BCR:H20C	29:b:845:BCR:H361	1.86	0.42
2:9:138:ALA:O	2:9:142:ILE:HG12	2.20	0.42
3:8:38:SER:OG	3:8:41:LEU:O	2.36	0.42
20:7:303:XAT:H201	20:7:303:XAT:H15	1.78	0.42
8:a:684:ARG:NH1	8:a:711:ALA:O	2.52	0.42
29:b:842:BCR:H351	29:b:842:BCR:H15C	1.73	0.42
25:9:317:LHG:H321	25:9:317:LHG:H291	1.65	0.42
3:8:42:PRO:HB2	4:7:154:LYS:HB2	2.01	0.42
22:4:306:CLA:CHA	22:4:306:CLA:HBA1	2.48	0.42
6:2:109:TRP:CE3	20:2:303:XAT:H22	2.54	0.42
6:2:205:PHE:CD2	20:2:303:XAT:H12	2.54	0.42
4:7:174:GLU:HB2	22:7:313:CLA:C1B	2.50	0.42
8:a:692:GLU:CD	9:b:547:LYS:HB2	2.44	0.42
8:a:741:ILE:HD12	8:a:741:ILE:HA	1.93	0.42
22:a:834:CLA:H142	29:b:846:BCR:H17C	2.01	0.42
9:b:518:ASP:OD2	9:b:595:TYR:OH	2.23	0.42
9:b:682:TRP:NE1	16:l:15:GLY:O	2.43	0.42
22:b:809:CLA:H142	22:b:809:CLA:H111	1.70	0.42
12:f:114:PHE:HB2	29:f:801:BCR:C32	2.49	0.42
3:8:140:GLN:HE21	3:8:140:GLN:HB3	1.72	0.42
3:8:184:ILE:HG21	20:8:302:XAT:H12	2.01	0.42
20:4:303:XAT:H35	20:4:303:XAT:H401	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:81:CYS:SG	4:7:175:LEU:HD23	2.59	0.42
8:a:567:PRO:HB3	8:a:714:ILE:HB	2.01	0.42
1:5:98:PHE:HE1	22:5:305:CLA:HBC3	1.84	0.42
2:9:217:ILE:HG21	22:9:314:CLA:HHB	2.01	0.42
20:4:302:XAT:H11	20:4:302:XAT:H191	1.89	0.42
5:3:172:PRO:HD2	20:3:305:XAT:H242	2.00	0.42
20:3:303:XAT:H15	20:3:303:XAT:H201	1.79	0.42
20:2:302:XAT:H401	20:2:302:XAT:H35	1.71	0.42
21:7:302:A1L1G:O9	22:7:311:CLA:O1A	2.37	0.42
8:a:73:GLN:HG2	22:a:806:CLA:H3A	2.00	0.42
8:a:440:PHE:CE2	22:a:839:CLA:HAB	2.55	0.42
22:a:809:CLA:H3A	22:a:809:CLA:HBA2	1.67	0.42
9:b:220:LEU:HD21	29:b:842:BCR:H391	2.01	0.42
22:b:816:CLA:CHD	22:b:817:CLA:HBB2	2.49	0.42
29:b:842:BCR:H341	29:b:842:BCR:H11C	1.74	0.42
11:e:16:TYR:CD2	11:e:44:ASN:HA	2.54	0.42
14:i:29:TYR:HE1	17:m:30:ASN:HD21	1.67	0.42
19:c:32:ASP:OD1	19:c:32:ASP:N	2.53	0.42
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.42
2:9:222:ASP:OD1	2:9:227:GLY:HA2	2.19	0.42
3:8:153:ASP:OD1	20:8:303:XAT:O3	2.28	0.42
5:3:103:ILE:HD11	20:3:304:XAT:H363	2.01	0.42
5:3:205:LEU:HD12	5:3:205:LEU:HA	1.86	0.42
20:3:301:XAT:H35	20:3:301:XAT:H401	1.81	0.42
8:a:427:ARG:NH2	10:d:46:THR:O	2.53	0.42
22:a:831:CLA:H93	22:a:842:CLA:HED3	2.01	0.42
20:a:852:XAT:H31	20:a:852:XAT:H391	1.82	0.42
9:b:347:ALA:HB3	9:b:374:GLN:HE21	1.85	0.42
9:b:381:MET:HE1	29:b:845:BCR:H352	2.02	0.42
9:b:500:LEU:HA	9:b:503:ILE:HG22	2.02	0.42
20:9:303:XAT:H7	22:9:309:CLA:HAB	2.01	0.42
20:9:304:XAT:H35	20:9:304:XAT:H401	1.86	0.42
22:8:308:CLA:HBA1	22:8:308:CLA:H11	1.78	0.42
20:3:304:XAT:H12	22:3:309:CLA:HAB	2.01	0.42
8:a:67:PHE:HE2	8:a:173:HIS:CG	2.38	0.42
22:a:831:CLA:H62	22:a:831:CLA:H41	1.76	0.42
9:b:424:LEU:HG	22:b:837:CLA:CBB	2.49	0.42
9:b:702:LEU:HD22	9:b:706:GLN:NE2	2.35	0.42
22:b:820:CLA:HBA2	22:b:820:CLA:H3A	1.33	0.42
15:j:14:LEU:CD2	27:j:105:LMG:H141	2.49	0.42
20:9:303:XAT:H35	20:9:303:XAT:H401	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:8:303:XAT:C34	22:8:313:CLA:HBB1	2.49	0.42
22:4:309:CLA:H3A	22:4:309:CLA:HBA1	1.77	0.42
20:3:304:XAT:H11	20:3:304:XAT:H191	1.88	0.42
4:7:59:PHE:HE1	22:7:306:CLA:HBC3	1.85	0.42
20:7:303:XAT:H362	22:7:308:CLA:H2	2.01	0.42
9:b:56:ILE:HD11	29:m:101:BCR:HC7	2.02	0.42
9:b:597:HIS:CE1	9:b:727:VAL:HG23	2.54	0.42
1:5:115:ALA:O	1:5:119:ASN:ND2	2.42	0.42
2:9:120:TRP:HB3	9:b:94:PRO:HA	2.02	0.42
7:1:147:GLY:HA2	7:1:149:TRP:CZ3	2.55	0.42
8:a:272:LYS:HG2	8:a:496:LEU:HD12	2.02	0.42
8:a:356:LEU:HB2	22:a:828:CLA:H41	2.02	0.42
22:a:804:CLA:C4D	15:j:12:PRO:HG3	2.50	0.42
9:b:140:LEU:HD23	9:b:143:LEU:HD12	2.01	0.42
22:b:802:CLA:HMA1	22:b:803:CLA:H161	2.02	0.42
22:b:835:CLA:HBB1	22:b:835:CLA:HMB1	2.02	0.42
29:b:844:BCR:H351	29:b:844:BCR:H15C	1.78	0.42
20:4:304:XAT:H30	22:4:313:CLA:H71	2.02	0.42
8:a:680:LEU:HB3	9:b:667:ILE:HG12	2.02	0.42
8:a:727:LEU:HD22	22:a:842:CLA:HMA3	2.01	0.42
22:a:835:CLA:H141	22:a:835:CLA:H161	1.84	0.42
9:b:197:ILE:HB	9:b:198:PRO:HD3	2.02	0.42
29:l:201:BCR:H352	22:l:203:CLA:HAB	2.01	0.42
20:4:301:XAT:H401	20:4:301:XAT:H35	1.66	0.41
6:2:203:LEU:HD13	20:2:301:XAT:C10	2.50	0.41
4:7:71:SER:HB3	4:7:142:MET:CE	2.49	0.41
20:7:304:XAT:H30	22:7:313:CLA:H71	2.01	0.41
22:7:306:CLA:HBA2	22:7:306:CLA:H3A	1.58	0.41
22:a:816:CLA:C4B	20:a:852:XAT:H242	2.50	0.41
9:b:440:VAL:HG12	22:j:102:CLA:HAC1	2.01	0.41
22:b:814:CLA:CHA	22:b:814:CLA:HBA1	2.49	0.41
11:e:51:ASN:ND2	19:c:61:ASP:HB2	2.35	0.41
20:9:305:XAT:H31	20:9:305:XAT:H391	1.83	0.41
3:8:47:PRO:HG3	3:8:61:ASP:HB3	2.01	0.41
4:4:85:MET:HE3	4:4:177:ASN:HB3	2.00	0.41
20:3:305:XAT:H15	20:3:305:XAT:H201	1.84	0.41
22:7:308:CLA:H142	22:7:308:CLA:H111	1.77	0.41
22:1:306:CLA:H3A	22:1:306:CLA:O2A	2.20	0.41
8:a:271:PHE:HE2	8:a:495:ALA:HB2	1.84	0.41
22:a:806:CLA:H62	22:a:806:CLA:H2	1.67	0.41
22:a:818:CLA:OBD	22:a:837:CLA:HED2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:839:CLA:H161	22:a:839:CLA:H141	1.68	0.41
29:a:849:BCR:H15C	29:a:849:BCR:H351	1.79	0.41
20:a:852:XAT:H11	20:a:852:XAT:H191	1.91	0.41
9:b:629:ASN:HA	9:b:734:LYS:HE2	2.02	0.41
28:b:841:PQN:H243	28:b:841:PQN:H262	1.84	0.41
10:d:88:TYR:HB3	10:d:89:PRO:HD2	2.01	0.41
2:9:120:TRP:CH2	22:9:318:CLA:H43	2.56	0.41
2:9:217:ILE:HB	22:9:314:CLA:H3A	2.02	0.41
25:9:317:LHG:HC81	25:9:317:LHG:HC5	1.98	0.41
22:7:307:CLA:C3D	22:7:314:CLA:HMA3	2.51	0.41
7:1:71:GLU:HG2	7:1:142:PRO:O	2.20	0.41
8:a:226:SER:HG	8:a:229:GLU:HG2	1.86	0.41
8:a:290:HIS:O	8:a:294:ILE:HG12	2.20	0.41
22:a:803:CLA:O1A	22:a:803:CLA:H3A	2.19	0.41
22:b:816:CLA:CBB	29:h:202:BCR:H14C	2.50	0.41
22:b:821:CLA:H12	22:b:822:CLA:H52	2.03	0.41
22:b:824:CLA:H141	22:b:824:CLA:H161	1.83	0.41
16:l:53:THR:HG22	22:l:202:CLA:C1B	2.49	0.41
29:m:101:BCR:H20C	29:m:101:BCR:H361	1.84	0.41
2:9:91:GLY:CA	20:9:303:XAT:H173	2.51	0.41
22:9:314:CLA:H51	22:9:314:CLA:C1C	2.50	0.41
3:8:77:ALA:HB2	3:8:147:PRO:HB2	2.02	0.41
20:3:305:XAT:H31	20:3:305:XAT:H391	1.91	0.41
6:2:57:PHE:CZ	20:2:305:XAT:H172	2.56	0.41
7:1:162:TYR:CE2	22:a:844:CLA:HBD	2.55	0.41
22:a:806:CLA:H72	29:a:848:BCR:C8	2.50	0.41
22:b:826:CLA:HED1	29:b:845:BCR:H21C	2.02	0.41
10:d:70:LEU:O	10:d:74:LEU:HG	2.19	0.41
29:j:104:BCR:H341	29:j:104:BCR:H11C	1.72	0.41
1:5:117:LEU:HD23	1:5:117:LEU:HA	1.92	0.41
20:4:301:XAT:H11	20:4:301:XAT:H191	1.86	0.41
20:4:305:XAT:H391	20:4:305:XAT:H31	1.62	0.41
7:1:54:PRO:HD2	20:1:303:XAT:H242	2.02	0.41
7:1:87:TRP:CG	7:1:180:LEU:HD13	2.56	0.41
8:a:293:ALA:HB1	22:a:818:CLA:HBC2	2.03	0.41
22:a:829:CLA:H3A	22:a:829:CLA:HBA2	1.83	0.41
22:b:809:CLA:C4A	22:b:809:CLA:HBA2	2.50	0.41
22:b:813:CLA:H192	22:b:813:CLA:H161	1.76	0.41
22:b:824:CLA:H52	22:b:824:CLA:H12	1.85	0.41
22:b:827:CLA:H143	22:b:827:CLA:H161	1.78	0.41
10:d:107:VAL:HG21	19:c:38:GLN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:94:LEU:HD12	13:h:94:LEU:HA	1.94	0.41
29:i:101:BCR:H11C	29:i:101:BCR:H341	1.86	0.41
6:2:205:PHE:HE1	20:2:303:XAT:H162	1.85	0.41
8:a:342:TRP:HB3	22:a:806:CLA:HAC1	2.02	0.41
8:a:452:ASN:HD22	8:a:634:ILE:HB	1.85	0.41
9:b:181:PHE:CE2	22:b:819:CLA:HAB	2.56	0.41
9:b:273:HIS:HB3	22:b:817:CLA:HMB1	2.03	0.41
15:j:12:PRO:HB2	20:j:101:XAT:H21	2.01	0.41
20:9:304:XAT:H31	20:9:304:XAT:H391	1.97	0.41
20:3:301:XAT:H15	20:3:301:XAT:H201	1.79	0.41
20:3:304:XAT:H35	20:3:304:XAT:H401	1.68	0.41
20:2:302:XAT:H11	20:2:302:XAT:H191	1.93	0.41
8:a:357:SER:HB2	22:a:830:CLA:HMC2	2.01	0.41
8:a:434:LEU:HG	8:a:541:LEU:HB2	2.03	0.41
8:a:675:PHE:HZ	22:a:842:CLA:HBC2	1.86	0.41
22:a:826:CLA:H141	22:a:826:CLA:H161	1.81	0.41
9:b:547:LYS:HE2	12:f:180:ILE:HD11	2.03	0.41
29:b:846:BCR:H15C	29:b:846:BCR:H351	1.85	0.41
29:i:101:BCR:H15C	29:i:101:BCR:H351	1.85	0.41
20:4:301:XAT:H373	20:4:301:XAT:H23	1.87	0.41
22:1:311:CLA:H72	16:l:21:ILE:HG12	2.02	0.41
8:a:555:LEU:HD11	9:b:674:GLN:HB3	2.01	0.41
22:a:806:CLA:H52	29:a:848:BCR:HC8	2.03	0.41
22:a:841:CLA:HAA2	22:b:831:CLA:HMB1	2.02	0.41
29:a:849:BCR:H11C	29:a:849:BCR:H341	1.84	0.41
9:b:278:ILE:HD13	9:b:278:ILE:HA	1.93	0.41
9:b:346:THR:HG21	22:b:828:CLA:HHD	2.03	0.41
9:b:709:LEU:CD1	26:b:848:DGD:HB41	2.51	0.41
10:d:27:GLU:O	10:d:89:PRO:HD3	2.21	0.41
29:f:801:BCR:H20C	29:f:801:BCR:H361	1.85	0.41
1:5:98:PHE:CD2	22:5:305:CLA:HMD2	2.56	0.41
1:5:149:VAL:HG22	20:5:304:XAT:H182	2.02	0.41
24:9:302:A1L1F:C28	22:9:310:CLA:HMC1	2.51	0.41
20:8:302:XAT:H403	22:8:307:CLA:H202	2.02	0.41
20:4:304:XAT:H401	20:4:304:XAT:H35	1.81	0.41
22:4:307:CLA:HBD	22:4:314:CLA:OBD	2.20	0.41
7:1:58:ALA:HB1	7:1:66:LEU:HD21	2.01	0.41
8:a:318:ILE:O	8:a:322:HIS:ND1	2.54	0.41
8:a:601:PHE:CZ	22:a:801:CLA:HED3	2.55	0.41
9:b:518:ASP:O	9:b:522:HIS:ND1	2.38	0.41
9:b:585:MET:O	9:b:589:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:807:CLA:H201	22:b:827:CLA:H143	2.03	0.41
22:b:827:CLA:H13	22:b:829:CLA:H141	2.02	0.41
22:b:828:CLA:H3A	22:b:828:CLA:HBA2	1.76	0.41
22:b:828:CLA:H61	22:b:828:CLA:H41	1.75	0.41
22:b:834:CLA:H62	22:b:834:CLA:H41	1.86	0.41
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.41
2:9:201:LEU:HD13	22:9:308:CLA:HBC1	2.03	0.41
25:9:317:LHG:H312	17:m:22:ILE:HD12	2.02	0.41
20:4:303:XAT:H163	22:4:308:CLA:H2	2.02	0.41
4:7:39:ALA:HB2	4:7:57:VAL:HG23	2.03	0.41
20:7:301:XAT:H15	20:7:301:XAT:H201	1.81	0.41
22:7:307:CLA:CAD	22:7:314:CLA:HMA3	2.51	0.41
20:1:302:XAT:H15	20:1:302:XAT:H201	1.87	0.41
22:1:308:CLA:H192	22:1:308:CLA:H161	1.87	0.41
9:b:301:LEU:HB3	13:h:46:THR:HG21	2.02	0.41
9:b:314:GLY:HA3	9:b:412:ARG:HD2	2.02	0.41
9:b:412:ARG:NE	22:b:830:CLA:OBD	2.47	0.41
9:b:431:LEU:HD11	22:b:836:CLA:HMB1	2.03	0.41
9:b:499:TRP:CD1	22:b:833:CLA:HED2	2.57	0.41
9:b:523:HIS:CE1	29:b:849:BCR:H322	2.56	0.41
29:b:845:BCR:H24C	29:b:845:BCR:H371	1.83	0.41
2:9:218:LEU:HD23	2:9:218:LEU:HA	1.84	0.40
22:3:312:CLA:HBA1	22:3:312:CLA:H3A	1.93	0.40
22:2:309:CLA:HAC2	22:2:314:CLA:HAB	2.03	0.40
23:1:315:SQD:H132	23:1:315:SQD:H161	1.72	0.40
8:a:399:ALA:HB1	8:a:543:LEU:HB3	2.02	0.40
8:a:632:SER:O	8:a:638:GLY:HA3	2.21	0.40
22:a:828:CLA:H2	22:a:828:CLA:H61	1.78	0.40
22:a:828:CLA:H152	22:a:840:CLA:H191	2.03	0.40
22:a:834:CLA:H162	22:a:834:CLA:H202	1.79	0.40
9:b:86:PRO:HB3	9:b:119:TYR:CD2	2.56	0.40
9:b:668:SER:OG	9:b:673:TRP:NE1	2.52	0.40
22:f:802:CLA:H11	22:j:102:CLA:H122	2.03	0.40
16:l:56:TYR:CD2	16:l:161:ALA:HB2	2.56	0.40
29:l:205:BCR:H20C	29:l:205:BCR:H361	1.90	0.40
20:4:303:XAT:H383	22:4:310:CLA:C2B	2.51	0.40
20:2:305:XAT:H15	20:2:305:XAT:H201	1.78	0.40
8:a:209:HIS:HB2	22:a:815:CLA:C1C	2.52	0.40
8:a:232:LEU:HD23	8:a:232:LEU:HA	1.92	0.40
8:a:586:PHE:CE1	8:a:722:VAL:HB	2.57	0.40
8:a:685:GLY:N	9:b:570:CYS:O	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:193:VAL:O	9:b:198:PRO:HD3	2.20	0.40
9:b:461:PHE:HB2	22:b:836:CLA:CAD	2.52	0.40
22:b:805:CLA:HHC	22:b:807:CLA:OBD	2.22	0.40
10:d:89:PRO:HB2	10:d:90:PRO:HD3	2.03	0.40
13:h:104:VAL:HG22	29:h:202:BCR:H383	2.02	0.40
20:j:101:XAT:H31	20:j:101:XAT:H391	1.92	0.40
16:l:54:HIS:O	16:l:58:LEU:HB2	2.22	0.40
19:c:64:SER:HB2	30:c:102:SF4:S3	2.62	0.40
20:4:304:XAT:H11	20:4:304:XAT:H191	1.90	0.40
5:3:106:VAL:HG11	22:3:311:CLA:HED1	2.03	0.40
8:a:426:HIS:HA	10:d:17:THR:OG1	2.22	0.40
8:a:570:GLY:O	8:a:576:THR:OG1	2.32	0.40
22:a:803:CLA:HBB1	22:a:803:CLA:HMB3	2.04	0.40
22:a:826:CLA:H143	22:a:826:CLA:HMD2	2.02	0.40
22:b:804:CLA:HBC2	22:b:804:CLA:HHD	2.03	0.40
22:b:818:CLA:H91	22:b:818:CLA:H111	1.85	0.40
22:b:839:CLA:H121	22:b:839:CLA:H8	1.92	0.40
12:f:114:PHE:HB2	29:f:801:BCR:H321	2.02	0.40
29:h:201:BCR:H15C	29:h:201:BCR:H351	1.83	0.40
2:9:86:ARG:NE	2:9:192:GLU:OE2	2.36	0.40
20:4:302:XAT:H14	22:4:310:CLA:C1	2.49	0.40
20:3:305:XAT:H11	20:3:305:XAT:H191	1.99	0.40
4:7:79:LYS:HE3	4:7:79:LYS:HB2	1.79	0.40
20:7:305:XAT:H191	20:7:305:XAT:H11	1.84	0.40
7:1:131:GLN:O	7:1:135:LYS:HG3	2.21	0.40
7:1:186:ILE:HG13	7:1:187:THR:N	2.37	0.40
8:a:406:PHE:HE2	8:a:424:ILE:HD11	1.86	0.40
9:b:339:LEU:HD11	22:b:806:CLA:H51	2.04	0.40
9:b:585:MET:HE3	9:b:585:MET:HB3	1.83	0.40
9:b:633:LEU:HD21	9:b:652:PHE:CG	2.57	0.40
22:b:813:CLA:H161	22:b:813:CLA:H141	1.77	0.40
22:b:825:CLA:H3A	22:b:825:CLA:HBA2	1.72	0.40
22:b:840:CLA:H192	22:b:840:CLA:H161	1.82	0.40
16:l:4:PHE:HB3	16:l:20:PRO:HG3	2.03	0.40
22:5:305:CLA:HAB	4:4:153:PHE:O	2.21	0.40
3:8:44:LEU:HD22	4:7:137:ILE:HG22	2.03	0.40
20:8:302:XAT:H401	20:8:302:XAT:H35	1.76	0.40
5:3:97:MET:HG3	5:3:193:GLY:HA2	2.03	0.40
5:3:188:LYS:O	5:3:192:ASN:ND2	2.45	0.40
6:2:92:ARG:NH2	22:2:308:CLA:HED3	2.36	0.40
22:2:308:CLA:H51	22:2:309:CLA:H3A	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:303:XAT:H15	20:1:303:XAT:H201	1.85	0.40
20:1:303:XAT:H31	20:1:303:XAT:H391	1.93	0.40
22:a:842:CLA:H12	28:a:843:PQN:H301	2.02	0.40
9:b:433:PHE:CZ	29:f:801:BCR:H372	2.56	0.40
22:b:809:CLA:H143	22:b:809:CLA:H161	1.83	0.40
12:f:132:VAL:O	12:f:135:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	24	49
3	8	162/200 (81%)	157 (97%)	5 (3%)	0	100	100
4	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	21	45
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	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	7	21
7	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
8	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	72
9	b	633/737 (86%)	606 (96%)	27 (4%)	0	100	100
10	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
11	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
12	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
13	h	83/128 (65%)	76 (92%)	6 (7%)	1 (1%)	10	28
14	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	j	39/41 (95%)	39 (100%)	0	0	100	100
16	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	10	28
17	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
19	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3520/4098 (86%)	3297 (94%)	214 (6%)	9 (0%)	37	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	9	32	THR
6	2	45	LYS
16	l	120	VAL
6	2	127	ASN
6	2	213	VAL
8	a	580	SER
16	l	131	ILE
4	4	146	SER
13	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	91/167 (54%)	91 (100%)	0	100	100
3	8	84/160 (52%)	83 (99%)	1 (1%)	63	79
4	4	133/159 (84%)	133 (100%)	0	100	100
4	7	121/159 (76%)	120 (99%)	1 (1%)	73	85
5	3	17/164 (10%)	17 (100%)	0	100	100
6	2	36/172 (21%)	36 (100%)	0	100	100
7	1	128/165 (78%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	a	607/613 (99%)	603 (99%)	4 (1%)	76	87
9	b	599/602 (100%)	599 (100%)	0	100	100
10	d	107/113 (95%)	107 (100%)	0	100	100
11	e	56/62 (90%)	56 (100%)	0	100	100
12	f	138/162 (85%)	138 (100%)	0	100	100
13	h	71/107 (66%)	70 (99%)	1 (1%)	59	77
14	i	32/43 (74%)	32 (100%)	0	100	100
15	j	36/36 (100%)	36 (100%)	0	100	100
16	l	130/141 (92%)	130 (100%)	0	100	100
17	m	21/24 (88%)	21 (100%)	0	100	100
19	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2607/3299 (79%)	2600 (100%)	7 (0%)	84	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	8	175	LYS
4	7	95	ASP
8	a	428	ASP
8	a	448	LEU
8	a	579	VAL
8	a	580	SER
13	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
3	8	156	ASN
7	1	119	GLN
7	1	132	ASN
7	1	194	GLN
8	a	127	ASN
8	a	186	ASN
8	a	415	ASN
8	a	435	ASN
9	b	80	ASN

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Mol	Chain	Res	Type
9	b	112	ASN
9	b	169	ASN
9	b	326	ASN
9	b	373	HIS
9	b	605	GLN
9	b	629	ASN
10	d	7	GLN
12	f	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

257 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$
20	XAT	3	303	-	41,47,47	0.89	2 (4%)	54,74,74	2.60	20 (37%)
20	XAT	a	852	-	41,47,47	0.92	2 (4%)	54,74,74	2.71	18 (33%)
22	CLA	7	310	-	50,54,73	1.37	7 (14%)	59,90,113	1.40	4 (6%)
22	CLA	b	806	-	69,73,73	1.16	6 (8%)	82,113,113	1.30	6 (7%)
22	CLA	l	202	-	46,50,73	1.40	8 (17%)	53,85,113	1.44	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	b	842	-	41,41,41	0.64	0	56,56,56	2.31	21 (37%)
20	XAT	9	303	-	41,47,47	0.95	2 (4%)	54,74,74	2.62	20 (37%)
20	XAT	2	301	-	41,47,47	0.92	2 (4%)	54,74,74	2.72	18 (33%)
22	CLA	7	313	-	58,62,73	1.29	7 (12%)	68,99,113	1.35	6 (8%)
22	CLA	a	838	-	55,59,73	1.31	8 (14%)	64,96,113	1.40	6 (9%)
22	CLA	b	817	-	63,67,73	1.23	8 (12%)	74,105,113	1.36	9 (12%)
22	CLA	b	838	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	f	802	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
22	CLA	a	816	-	54,58,73	1.32	8 (14%)	64,95,113	1.41	7 (10%)
22	CLA	a	827	-	69,73,73	1.16	7 (10%)	82,113,113	1.31	7 (8%)
20	XAT	8	301	-	41,47,47	0.92	2 (4%)	54,74,74	2.55	18 (33%)
22	CLA	9	309	2	50,54,73	1.36	8 (16%)	59,90,113	1.36	5 (8%)
22	CLA	1	310	7	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
22	CLA	a	840	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
29	BCR	a	849	-	41,41,41	0.67	0	56,56,56	2.19	22 (39%)
21	A1L1G	1	301	-	40,47,47	1.14	5 (12%)	49,71,71	1.46	10 (20%)
26	DGD	b	848	-	58,58,67	1.13	4 (6%)	72,72,81	1.50	10 (13%)
22	CLA	4	312	-	50,54,73	1.37	8 (16%)	59,90,113	1.37	4 (6%)
29	BCR	l	201	-	41,41,41	0.68	0	56,56,56	1.98	17 (30%)
22	CLA	a	842	-	69,73,73	1.19	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	3	312	5	63,67,73	1.23	8 (12%)	74,105,113	1.29	4 (5%)
22	CLA	a	804	-	59,63,73	1.27	7 (11%)	70,101,113	1.40	8 (11%)
22	CLA	2	316	6	50,54,73	1.37	8 (16%)	59,90,113	1.40	4 (6%)
22	CLA	a	810	8	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
29	BCR	m	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	6 (10%)
22	CLA	b	822	-	64,68,73	1.21	7 (10%)	76,107,113	1.26	5 (6%)
20	XAT	5	302	-	41,47,47	0.95	2 (4%)	54,74,74	2.59	19 (35%)
22	CLA	a	813	-	58,62,73	1.28	8 (13%)	68,99,113	1.31	5 (7%)
22	CLA	a	854	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
29	BCR	l	205	-	41,41,41	0.66	0	56,56,56	2.04	15 (26%)
22	CLA	2	312	-	51,55,73	1.36	8 (15%)	60,91,113	1.41	5 (8%)
20	XAT	5	304	-	41,47,47	0.86	2 (4%)	54,74,74	2.85	20 (37%)
22	CLA	7	307	-	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
22	CLA	7	306	4	52,56,73	1.36	7 (13%)	61,92,113	1.36	5 (8%)
22	CLA	a	830	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	XAT	4	301	-	41,47,47	0.97	2 (4%)	54,74,74	2.63	19 (35%)
20	XAT	7	305	-	41,47,47	0.87	2 (4%)	54,74,74	2.66	19 (35%)
29	BCR	j	104	-	41,41,41	0.68	0	56,56,56	2.09	17 (30%)
22	CLA	5	314	-	56,60,73	1.30	6 (10%)	65,97,113	1.40	5 (7%)
29	BCR	f	804	-	41,41,41	0.69	0	56,56,56	2.05	14 (25%)
22	CLA	b	809	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
22	CLA	5	307	1	64,68,73	1.20	6 (9%)	76,107,113	1.28	6 (7%)
20	XAT	3	305	-	41,47,47	0.89	2 (4%)	54,74,74	2.58	18 (33%)
20	XAT	7	301	-	41,47,47	0.93	2 (4%)	54,74,74	2.64	19 (35%)
22	CLA	a	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
22	CLA	b	810	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)
22	CLA	1	312	7	56,60,73	1.32	7 (12%)	65,97,113	1.36	5 (7%)
20	XAT	4	303	-	41,47,47	0.92	2 (4%)	54,74,74	2.58	17 (31%)
20	XAT	8	302	-	41,47,47	0.94	2 (4%)	54,74,74	2.66	18 (33%)
22	CLA	b	820	-	54,58,73	1.32	7 (12%)	64,95,113	1.44	7 (10%)
22	CLA	b	837	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	6 (7%)
22	CLA	l	203	-	64,68,73	1.21	9 (14%)	76,107,113	1.35	5 (6%)
22	CLA	4	311	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	5 (8%)
22	CLA	b	832	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	b	839	-	69,73,73	1.18	6 (8%)	82,113,113	1.31	6 (7%)
29	BCR	b	845	-	41,41,41	0.65	0	56,56,56	2.22	22 (39%)
20	XAT	8	303	-	41,47,47	0.87	2 (4%)	54,74,74	2.66	18 (33%)
22	CLA	a	802	-	62,66,73	1.22	8 (12%)	73,104,113	1.35	7 (9%)
22	CLA	j	102	-	62,66,73	1.24	6 (9%)	73,104,113	1.30	5 (6%)
22	CLA	4	313	-	57,61,73	1.29	7 (12%)	67,98,113	1.31	7 (10%)
21	A1L1G	9	306	-	40,47,47	1.14	4 (10%)	49,71,71	1.44	7 (14%)
22	CLA	8	310	-	50,54,73	1.38	8 (16%)	59,90,113	1.38	5 (8%)
22	CLA	a	819	-	58,62,73	1.28	8 (13%)	68,99,113	1.33	5 (7%)
22	CLA	3	314	5	51,55,73	1.36	7 (13%)	60,91,113	1.40	4 (6%)
22	CLA	b	801	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	b	831	-	53,57,73	1.32	6 (11%)	61,93,113	1.39	5 (8%)
22	CLA	8	314	-	45,49,73	1.43	7 (15%)	54,84,113	1.47	5 (9%)
22	CLA	a	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	9	310	-	50,54,73	1.37	7 (14%)	59,90,113	1.48	4 (6%)
22	CLA	4	307	-	60,64,73	1.27	6 (10%)	71,102,113	1.32	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
22	CLA	8	307	3	69,73,73	1.17	6 (8%)	82,113,113	1.25	5 (6%)
22	CLA	8	309	-	61,65,73	1.25	7 (11%)	72,103,113	1.33	6 (8%)
25	LHG	a	846	22	26,26,48	1.30	5 (19%)	29,32,54	1.18	2 (6%)
22	CLA	5	305	1	50,54,73	1.37	7 (14%)	59,90,113	1.39	4 (6%)
22	CLA	a	805	22	59,63,73	1.26	7 (11%)	70,101,113	1.35	6 (8%)
22	CLA	3	315	5	50,54,73	1.38	7 (14%)	59,90,113	1.38	4 (6%)
20	XAT	2	303	-	41,47,47	1.01	2 (4%)	54,74,74	2.63	17 (31%)
22	CLA	b	802	-	69,73,73	1.17	7 (10%)	82,113,113	1.18	5 (6%)
24	A1L1F	1	304	-	52,59,59	1.41	6 (11%)	63,85,85	2.26	18 (28%)
22	CLA	j	103	15	46,50,73	1.40	7 (15%)	53,85,113	1.48	4 (7%)
24	A1L1F	h	204	-	52,59,59	1.47	6 (11%)	63,85,85	2.59	22 (34%)
20	XAT	j	101	-	41,47,47	0.87	2 (4%)	54,74,74	2.73	18 (33%)
20	XAT	7	303	-	41,47,47	1.00	2 (4%)	54,74,74	2.60	18 (33%)
22	CLA	4	306	4	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
24	A1L1F	9	302	-	52,59,59	1.48	6 (11%)	63,85,85	2.55	20 (31%)
22	CLA	b	823	-	57,61,73	1.29	7 (12%)	67,98,113	1.35	6 (8%)
22	CLA	7	311	-	50,54,73	1.38	8 (16%)	59,90,113	1.40	5 (8%)
29	BCR	b	846	-	41,41,41	0.69	0	56,56,56	1.81	14 (25%)
21	A1L1G	5	303	-	40,47,47	1.15	3 (7%)	49,71,71	1.38	7 (14%)
22	CLA	1	204	-	50,54,73	1.37	9 (18%)	59,90,113	1.40	4 (6%)
22	CLA	5	308	-	59,63,73	1.28	7 (11%)	70,101,113	1.35	6 (8%)
27	LMG	j	105	-	32,32,55	1.13	2 (6%)	40,40,63	1.15	4 (10%)
22	CLA	9	311	-	50,54,73	1.36	7 (14%)	59,90,113	1.45	5 (8%)
22	CLA	1	307	-	58,62,73	1.28	8 (13%)	68,99,113	1.35	6 (8%)
22	CLA	a	835	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
22	CLA	a	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
21	A1L1G	3	306	-	40,47,47	1.18	4 (10%)	49,71,71	1.41	8 (16%)
22	CLA	4	317	-	59,63,73	1.28	8 (13%)	70,101,113	1.35	5 (7%)
22	CLA	1	305	-	65,69,73	1.21	6 (9%)	77,108,113	1.29	5 (6%)
22	CLA	2	306	-	45,50,73	1.42	6 (13%)	52,85,113	1.40	4 (7%)
22	CLA	5	309	1	69,73,73	1.17	7 (10%)	82,113,113	1.25	4 (4%)
24	A1L1F	8	304	-	52,59,59	1.41	5 (9%)	63,85,85	2.75	22 (34%)
22	CLA	2	314	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	4 (5%)
22	CLA	a	831	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	7	312	-	52,56,73	1.35	7 (13%)	61,92,113	1.39	5 (8%)
23	SQD	1	315	-	43,45,54	1.22	3 (6%)	53,56,65	1.12	2 (3%)
22	CLA	b	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	8 (9%)
22	CLA	4	309	-	54,58,73	1.31	6 (11%)	64,95,113	1.40	5 (7%)
22	CLA	5	306	23	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
22	CLA	a	808	-	55,59,73	1.32	8 (14%)	64,96,113	1.37	5 (7%)
22	CLA	8	308	-	59,63,73	1.28	8 (13%)	70,101,113	1.36	8 (11%)
22	CLA	b	808	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
22	CLA	b	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.25	7 (8%)
22	CLA	a	825	-	59,63,73	1.26	6 (10%)	70,101,113	1.32	5 (7%)
22	CLA	b	816	-	59,63,73	1.26	6 (10%)	70,101,113	1.33	6 (8%)
22	CLA	b	833	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)
26	DGD	8	315	22	41,41,67	1.06	2 (4%)	55,55,81	1.12	5 (9%)
22	CLA	8	312	3	56,60,73	1.29	8 (14%)	65,97,113	1.38	5 (7%)
23	SQD	5	316	22	33,35,54	1.39	3 (9%)	43,46,65	1.30	5 (11%)
22	CLA	5	312	-	56,60,73	1.30	8 (14%)	65,97,113	1.39	6 (9%)
25	LHG	a	845	-	47,47,48	1.15	6 (12%)	50,53,54	0.98	2 (4%)
20	XAT	3	304	-	41,47,47	0.93	2 (4%)	54,74,74	2.63	17 (31%)
22	CLA	b	813	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
27	LMG	a	853	-	34,34,55	1.14	2 (5%)	42,42,63	1.17	3 (7%)
27	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.31	4 (9%)
22	CLA	a	820	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
22	CLA	2	311	-	62,66,73	1.25	9 (14%)	73,104,113	1.27	5 (6%)
22	CLA	f	803	12	56,60,73	1.30	8 (14%)	65,97,113	1.38	5 (7%)
22	CLA	b	814	-	59,63,73	1.27	6 (10%)	70,101,113	1.40	8 (11%)
22	CLA	b	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
30	SF4	a	851	-	0,12,12	-	-	-	-	-
22	CLA	2	309	-	50,54,73	1.37	7 (14%)	59,90,113	1.39	4 (6%)
22	CLA	9	313	2	50,54,73	1.36	6 (12%)	59,90,113	1.47	4 (6%)
22	CLA	2	313	6	45,49,73	1.43	7 (15%)	54,84,113	1.51	5 (9%)
29	BCR	f	801	-	41,41,41	0.66	0	56,56,56	2.16	16 (28%)
28	PQN	a	843	-	34,34,34	1.62	2 (5%)	43,45,45	1.16	4 (9%)
22	CLA	b	805	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	5	310	-	50,54,73	1.36	7 (14%)	59,90,113	1.41	4 (6%)
22	CLA	3	309	5	60,64,73	1.25	7 (11%)	71,102,113	1.30	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	9	308	2	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
29	BCR	h	201	-	41,41,41	0.66	0	56,56,56	1.99	21 (37%)
22	CLA	5	313	1	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	b	811	-	58,62,73	1.35	9 (15%)	71,100,113	1.34	8 (11%)
29	BCR	a	850	-	41,41,41	0.70	0	56,56,56	2.17	14 (25%)
21	A1L1G	7	302	-	40,47,47	1.14	3 (7%)	49,71,71	1.41	8 (16%)
21	A1L1G	9	301	-	40,47,47	1.16	5 (12%)	49,71,71	1.48	9 (18%)
25	LHG	9	307	-	35,35,48	1.27	6 (17%)	38,41,54	0.92	2 (5%)
22	CLA	1	306	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
22	CLA	4	314	4	49,53,73	1.40	9 (18%)	58,89,113	1.42	4 (6%)
22	CLA	b	815	-	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	a	829	-	66,70,73	1.20	6 (9%)	78,109,113	1.24	7 (8%)
29	BCR	a	848	-	41,41,41	0.68	0	56,56,56	1.95	18 (32%)
22	CLA	a	812	22	66,70,73	1.19	7 (10%)	78,109,113	1.30	5 (6%)
22	CLA	b	812	-	57,61,73	1.29	8 (14%)	67,98,113	1.35	5 (7%)
20	XAT	1	302	-	41,47,47	0.90	2 (4%)	54,74,74	2.61	18 (33%)
22	CLA	a	815	-	49,53,73	1.39	6 (12%)	58,89,113	1.42	4 (6%)
22	CLA	7	314	-	49,53,73	1.40	8 (16%)	58,89,113	1.50	5 (8%)
29	BCR	i	101	-	41,41,41	0.72	0	56,56,56	2.15	13 (23%)
22	CLA	a	803	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	6 (7%)
20	XAT	1	303	-	41,47,47	0.90	2 (4%)	54,74,74	2.53	19 (35%)
22	CLA	9	314	-	59,63,73	1.26	6 (10%)	70,101,113	1.34	6 (8%)
22	CLA	b	824	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
22	CLA	7	309	-	50,55,73	1.36	7 (14%)	58,91,113	1.35	5 (8%)
29	BCR	h	202	-	41,41,41	0.67	0	56,56,56	1.90	17 (30%)
22	CLA	9	312	-	50,54,73	1.36	7 (14%)	59,90,113	1.49	6 (10%)
22	CLA	1	311	-	57,61,73	1.28	8 (14%)	67,98,113	1.36	7 (10%)
22	CLA	b	819	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
28	PQN	b	841	-	34,34,34	1.58	2 (5%)	43,45,45	1.24	5 (11%)
22	CLA	8	305	3	47,51,73	1.40	7 (14%)	55,86,113	1.45	6 (10%)
22	CLA	9	315	2	46,50,73	1.41	6 (13%)	53,85,113	1.42	4 (7%)
22	CLA	b	830	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	6 (11%)
29	BCR	b	844	-	41,41,41	0.66	0	56,56,56	2.09	16 (28%)
22	CLA	4	315	4	45,49,73	1.43	7 (15%)	54,84,113	1.49	5 (9%)
29	BCR	b	843	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	XAT	9	305	-	41,47,47	1.03	3 (7%)	54,74,74	2.33	17 (31%)
22	CLA	a	826	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
22	CLA	1	313	-	45,49,73	1.41	7 (15%)	54,84,113	1.47	5 (9%)
25	LHG	9	317	-	45,45,48	1.19	6 (13%)	48,51,54	0.96	2 (4%)
29	BCR	a	847	-	41,41,41	0.68	0	56,56,56	1.95	17 (30%)
22	CLA	7	315	4	45,49,73	1.43	8 (17%)	54,84,113	1.49	5 (9%)
29	BCR	b	849	-	41,41,41	0.70	0	56,56,56	2.06	13 (23%)
20	XAT	2	304	-	41,47,47	0.89	2 (4%)	54,74,74	2.55	20 (37%)
22	CLA	4	308	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	7 (8%)
22	CLA	2	310	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
22	CLA	a	818	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	7 (9%)
22	CLA	3	308	-	51,55,73	1.36	8 (15%)	60,91,113	1.43	6 (10%)
20	XAT	5	301	-	41,47,47	0.93	2 (4%)	54,74,74	2.59	19 (35%)
22	CLA	a	841	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	6 (7%)
22	CLA	1	308	7	69,73,73	1.16	6 (8%)	82,113,113	1.29	6 (7%)
22	CLA	a	814	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	a	839	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
22	CLA	7	317	-	49,53,73	1.40	7 (14%)	58,89,113	1.45	4 (6%)
22	CLA	b	827	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
20	XAT	4	302	-	41,47,47	0.89	2 (4%)	54,74,74	2.59	19 (35%)
25	LHG	b	847	22	30,30,48	1.38	6 (20%)	33,36,54	1.17	2 (6%)
22	CLA	a	834	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	3	307	5	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
22	CLA	b	826	-	69,73,73	1.17	7 (10%)	82,113,113	1.24	5 (6%)
26	DGD	4	318	-	41,41,67	1.07	2 (4%)	55,55,81	1.79	6 (10%)
22	CLA	a	809	8	69,73,73	1.16	7 (10%)	82,113,113	1.29	8 (9%)
30	SF4	c	101	-	0,12,12	-	-	-	-	-
22	CLA	8	306	26	50,54,73	1.36	8 (16%)	59,90,113	1.40	4 (6%)
22	CLA	b	835	-	62,66,73	1.24	7 (11%)	73,104,113	1.37	8 (10%)
20	XAT	2	302	-	41,47,47	0.93	2 (4%)	54,74,74	2.52	18 (33%)
22	CLA	5	311	-	55,59,73	1.30	8 (14%)	64,96,113	1.36	7 (10%)
20	XAT	4	304	-	41,47,47	0.91	2 (4%)	54,74,74	2.57	18 (33%)
22	CLA	4	316	-	50,54,73	1.36	6 (12%)	59,90,113	1.43	4 (6%)
22	CLA	7	308	-	64,68,73	1.22	6 (9%)	76,107,113	1.27	6 (7%)
22	CLA	a	806	-	69,73,73	1.21	10 (14%)	82,113,113	1.55	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	XAT	3	301	-	41,47,47	0.91	2 (4%)	54,74,74	2.56	19 (35%)
22	CLA	b	836	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
20	XAT	4	305	-	41,47,47	0.91	2 (4%)	54,74,74	2.76	18 (33%)
22	CLA	4	310	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	5 (6%)
22	CLA	9	318	-	66,70,73	1.21	8 (12%)	78,109,113	1.27	6 (7%)
22	CLA	8	313	-	50,54,73	1.38	9 (18%)	59,90,113	1.40	4 (6%)
22	CLA	a	837	8	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	7	316	-	55,59,73	1.31	7 (12%)	64,96,113	1.45	7 (10%)
22	CLA	a	832	-	54,58,73	1.32	8 (14%)	64,95,113	1.39	6 (9%)
20	XAT	9	304	-	41,47,47	0.96	2 (4%)	54,74,74	2.43	18 (33%)
22	CLA	b	825	-	68,72,73	1.17	8 (11%)	80,111,113	1.30	8 (10%)
22	CLA	2	307	-	51,55,73	1.36	8 (15%)	60,91,113	1.45	8 (13%)
20	XAT	7	304	-	41,47,47	0.94	2 (4%)	54,74,74	2.67	17 (31%)
22	CLA	h	205	-	59,63,73	1.27	8 (13%)	70,101,113	1.34	7 (10%)
22	CLA	a	823	-	53,57,73	1.32	7 (13%)	61,93,113	1.43	6 (9%)
22	CLA	b	818	-	64,68,73	1.22	7 (10%)	76,107,113	1.27	5 (6%)
22	CLA	b	840	25	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
22	CLA	a	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.28	5 (6%)
22	CLA	a	821	-	49,53,73	1.39	7 (14%)	58,89,113	1.46	4 (6%)
20	XAT	2	305	-	41,47,47	0.94	2 (4%)	54,74,74	2.43	18 (33%)
22	CLA	2	315	-	46,50,73	1.42	8 (17%)	53,85,113	1.38	4 (7%)
22	CLA	a	824	-	50,54,73	1.37	8 (16%)	59,90,113	1.35	4 (6%)
22	CLA	3	310	-	60,64,73	1.26	6 (10%)	71,102,113	1.30	5 (7%)
22	CLA	3	311	-	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
22	CLA	a	811	-	60,64,73	1.26	6 (10%)	71,102,113	1.34	6 (8%)
22	CLA	a	844	25	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
22	CLA	8	311	-	60,64,73	1.24	7 (11%)	71,102,113	1.33	8 (11%)
22	CLA	3	313	-	56,60,73	1.30	8 (14%)	65,97,113	1.38	6 (9%)
22	CLA	b	834	-	57,61,73	1.30	8 (14%)	67,98,113	1.36	5 (7%)
21	A1L1G	3	302	-	40,47,47	1.16	5 (12%)	49,71,71	1.33	7 (14%)
22	CLA	1	309	7	50,54,73	1.37	8 (16%)	59,90,113	1.35	4 (6%)
22	CLA	a	836	-	54,58,73	1.32	7 (12%)	64,95,113	1.38	6 (9%)
22	CLA	h	203	-	69,73,73	1.18	6 (8%)	82,113,113	1.33	6 (7%)
22	CLA	5	315	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
22	CLA	1	314	-	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	817	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
22	CLA	b	829	-	69,73,73	1.20	8 (11%)	82,113,113	1.31	9 (10%)
30	SF4	c	102	-	0,12,12	-	-	-	-	-
22	CLA	b	821	-	55,59,73	1.31	7 (12%)	64,96,113	1.41	7 (10%)
22	CLA	a	833	-	59,63,73	1.25	7 (11%)	70,101,113	1.40	8 (11%)
22	CLA	2	308	6	58,62,73	1.28	7 (12%)	68,99,113	1.29	6 (8%)
22	CLA	9	316	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	8 (9%)

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
20	XAT	3	303	-	-	3/31/93/93	0/4/4/4
20	XAT	a	852	-	-	7/31/93/93	0/4/4/4
22	CLA	7	310	-	1/1/11/20	6/17/93/115	-
22	CLA	b	806	-	1/1/15/20	13/39/115/115	-
22	CLA	1	202	-	1/1/10/20	0/12/88/115	-
29	BCR	b	842	-	-	2/29/63/63	0/2/2/2
20	XAT	9	303	-	-	4/31/93/93	0/4/4/4
20	XAT	2	301	-	-	3/31/93/93	0/4/4/4
22	CLA	7	313	-	1/1/12/20	5/26/102/115	-
22	CLA	a	838	-	1/1/12/20	6/23/99/115	-
22	CLA	b	817	-	1/1/13/20	11/32/108/115	-
22	CLA	b	838	-	1/1/15/20	15/39/115/115	-
22	CLA	f	802	-	1/1/15/20	13/39/115/115	-
22	CLA	a	816	-	1/1/12/20	4/21/97/115	-
22	CLA	a	827	-	1/1/15/20	6/39/115/115	-
20	XAT	8	301	-	-	3/31/93/93	0/4/4/4
22	CLA	9	309	2	1/1/11/20	5/17/93/115	-
22	CLA	1	310	7	1/1/15/20	17/39/115/115	-
22	CLA	a	840	-	1/1/15/20	8/39/115/115	-
29	BCR	a	849	-	-	0/29/63/63	0/2/2/2
21	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
26	DGD	b	848	-	-	20/46/86/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	312	-	1/1/11/20	6/17/93/115	-
29	BCR	1	201	-	-	4/29/63/63	0/2/2/2
22	CLA	a	842	-	1/1/15/20	8/39/115/115	-
22	CLA	3	312	5	1/1/13/20	10/32/108/115	-
22	CLA	a	804	-	1/1/13/20	9/27/103/115	-
22	CLA	2	316	6	1/1/11/20	6/17/93/115	-
22	CLA	a	810	8	1/1/15/20	15/39/115/115	-
29	BCR	m	101	-	-	8/29/63/63	0/2/2/2
22	CLA	b	822	-	1/1/14/20	7/33/109/115	-
22	CLA	a	854	-	1/1/15/20	14/39/115/115	-
22	CLA	a	813	-	1/1/12/20	9/26/102/115	-
20	XAT	5	302	-	-	3/31/93/93	0/4/4/4
29	BCR	1	205	-	-	8/29/63/63	0/2/2/2
22	CLA	2	312	-	1/1/11/20	4/18/94/115	-
22	CLA	7	307	-	1/1/11/20	6/15/91/115	-
20	XAT	5	304	-	-	1/31/93/93	0/4/4/4
22	CLA	7	306	4	1/1/11/20	10/19/95/115	-
22	CLA	a	830	-	1/1/15/20	13/39/115/115	-
20	XAT	4	301	-	-	4/31/93/93	0/4/4/4
20	XAT	7	305	-	-	2/31/93/93	0/4/4/4
29	BCR	j	104	-	-	2/29/63/63	0/2/2/2
22	CLA	5	314	-	1/1/12/20	4/24/100/115	-
29	BCR	f	804	-	-	4/29/63/63	0/2/2/2
22	CLA	b	809	-	1/1/15/20	13/39/115/115	-
22	CLA	5	307	1	1/1/14/20	5/33/109/115	-
20	XAT	3	305	-	-	0/31/93/93	0/4/4/4
22	CLA	a	807	-	1/1/15/20	18/39/115/115	-
20	XAT	7	301	-	-	6/31/93/93	0/4/4/4
22	CLA	b	810	-	1/1/15/20	14/39/115/115	-
22	CLA	1	312	7	1/1/12/20	3/24/100/115	-
20	XAT	4	303	-	-	3/31/93/93	0/4/4/4
22	CLA	b	837	-	1/1/15/20	9/39/115/115	-
22	CLA	b	820	-	1/1/12/20	5/21/97/115	-
20	XAT	8	302	-	-	4/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	l	203	-	1/1/14/20	4/33/109/115	-
22	CLA	4	311	-	1/1/11/20	9/17/93/115	-
22	CLA	b	832	-	1/1/15/20	13/39/115/115	-
22	CLA	b	839	-	1/1/15/20	15/39/115/115	-
29	BCR	b	845	-	-	0/29/63/63	0/2/2/2
20	XAT	8	303	-	-	0/31/93/93	0/4/4/4
22	CLA	a	802	-	1/1/13/20	5/31/107/115	-
22	CLA	j	102	-	1/1/13/20	18/31/107/115	-
22	CLA	4	313	-	1/1/12/20	4/25/101/115	-
22	CLA	a	819	-	1/1/12/20	6/26/102/115	-
22	CLA	8	310	-	1/1/11/20	6/17/93/115	-
21	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
22	CLA	3	314	5	1/1/11/20	8/18/94/115	-
22	CLA	b	801	-	1/1/15/20	20/39/115/115	-
22	CLA	b	831	-	1/1/11/20	5/20/96/115	-
22	CLA	8	314	-	1/1/10/20	6/10/86/115	-
22	CLA	a	822	-	1/1/15/20	5/39/115/115	-
22	CLA	9	310	-	1/1/11/20	6/17/93/115	-
22	CLA	4	307	-	1/1/13/20	9/29/105/115	-
22	CLA	b	807	-	1/1/15/20	18/39/115/115	-
22	CLA	8	307	3	1/1/15/20	11/39/115/115	-
22	CLA	8	309	-	1/1/13/20	7/30/106/115	-
25	LHG	a	846	22	-	15/31/31/53	-
22	CLA	5	305	1	1/1/11/20	6/17/93/115	-
22	CLA	a	805	22	1/1/13/20	6/27/103/115	-
22	CLA	3	315	5	1/1/11/20	9/17/93/115	-
20	XAT	2	303	-	-	6/31/93/93	0/4/4/4
22	CLA	b	802	-	1/1/15/20	15/39/115/115	-
24	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
22	CLA	j	103	15	1/1/10/20	7/12/88/115	-
24	A1L1F	h	204	-	-	11/43/99/99	1/3/3/3
20	XAT	j	101	-	-	5/31/93/93	0/4/4/4
20	XAT	7	303	-	-	7/31/93/93	0/4/4/4
22	CLA	4	306	4	1/1/11/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
22	CLA	b	823	-	1/1/12/20	6/25/101/115	-
22	CLA	7	311	-	1/1/11/20	4/17/93/115	-
29	BCR	b	846	-	-	2/29/63/63	0/2/2/2
22	CLA	1	204	-	1/1/11/20	3/17/93/115	-
21	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
22	CLA	5	308	-	1/1/13/20	6/27/103/115	-
27	LMG	j	105	-	-	11/27/47/70	0/1/1/1
22	CLA	9	311	-	1/1/11/20	6/17/93/115	-
22	CLA	1	307	-	1/1/12/20	5/26/102/115	-
22	CLA	a	835	-	1/1/15/20	11/39/115/115	-
22	CLA	a	828	-	1/1/15/20	8/39/115/115	-
21	A1L1G	3	306	-	-	19/29/85/85	0/3/3/3
22	CLA	4	317	-	1/1/13/20	9/27/103/115	-
22	CLA	1	305	-	1/1/14/20	9/35/111/115	-
22	CLA	2	306	-	1/1/10/20	4/11/87/115	-
22	CLA	5	309	1	1/1/15/20	10/39/115/115	-
24	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
22	CLA	2	314	-	1/1/13/20	14/29/105/115	-
22	CLA	a	831	-	1/1/15/20	11/39/115/115	-
22	CLA	7	312	-	1/1/11/20	3/19/95/115	-
23	SQD	1	315	-	-	19/40/60/69	0/1/1/1
22	CLA	b	804	-	1/1/15/20	7/39/115/115	-
22	CLA	4	309	-	1/1/12/20	4/21/97/115	-
22	CLA	5	306	23	1/1/11/20	8/15/91/115	-
22	CLA	a	808	-	1/1/12/20	4/23/99/115	-
22	CLA	8	308	-	1/1/13/20	7/27/103/115	-
22	CLA	b	808	-	1/1/15/20	11/39/115/115	-
22	CLA	b	803	-	1/1/15/20	17/39/115/115	-
22	CLA	a	825	-	1/1/13/20	8/27/103/115	-
22	CLA	b	816	-	1/1/13/20	3/27/103/115	-
22	CLA	b	833	-	1/1/15/20	13/39/115/115	-
26	DGD	8	315	22	-	10/29/69/95	0/2/2/2
22	CLA	8	312	3	1/1/12/20	2/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	SQD	5	316	22	-	11/30/50/69	0/1/1/1
22	CLA	5	312	-	1/1/12/20	0/24/100/115	-
25	LHG	a	845	-	-	26/52/52/53	-
22	CLA	b	813	-	1/1/15/20	13/39/115/115	-
20	XAT	3	304	-	-	3/31/93/93	0/4/4/4
27	LMG	a	853	-	-	13/29/49/70	0/1/1/1
27	LMG	2	317	-	-	11/30/50/70	0/1/1/1
22	CLA	a	820	-	1/1/15/20	13/39/115/115	-
22	CLA	2	311	-	1/1/13/20	5/31/107/115	-
22	CLA	f	803	12	1/1/12/20	5/24/100/115	-
22	CLA	b	814	-	1/1/13/20	10/27/103/115	-
22	CLA	b	828	-	1/1/15/20	13/39/115/115	-
30	SF4	a	851	-	-	-	0/6/5/5
22	CLA	2	309	-	1/1/11/20	3/17/93/115	-
22	CLA	9	313	2	1/1/11/20	12/17/93/115	-
22	CLA	2	313	6	1/1/10/20	2/10/86/115	-
29	BCR	f	801	-	-	3/29/63/63	0/2/2/2
28	PQN	a	843	-	-	5/23/43/43	0/2/2/2
22	CLA	b	805	-	1/1/15/20	11/39/115/115	-
22	CLA	5	310	-	1/1/11/20	8/17/93/115	-
22	CLA	3	309	5	1/1/13/20	3/29/105/115	-
22	CLA	9	308	2	1/1/15/20	14/39/115/115	-
29	BCR	h	201	-	-	0/29/63/63	0/2/2/2
22	CLA	5	313	1	1/1/11/20	6/15/91/115	-
22	CLA	b	811	-	1/1/13/20	4/25/101/115	-
29	BCR	a	850	-	-	4/29/63/63	0/2/2/2
21	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
21	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
25	LHG	9	307	-	-	20/40/40/53	-
22	CLA	1	306	-	1/1/15/20	15/39/115/115	-
22	CLA	4	314	4	1/1/11/20	6/15/91/115	-
22	CLA	b	815	-	1/1/11/20	3/15/91/115	-
22	CLA	a	829	-	1/1/14/20	13/36/112/115	-
29	BCR	a	848	-	-	0/29/63/63	0/2/2/2
22	CLA	a	812	22	1/1/14/20	9/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	812	-	1/1/12/20	5/25/101/115	-
20	XAT	1	302	-	-	0/31/93/93	0/4/4/4
22	CLA	a	815	-	1/1/11/20	0/15/91/115	-
22	CLA	7	314	-	1/1/11/20	5/15/91/115	-
29	BCR	i	101	-	-	3/29/63/63	0/2/2/2
22	CLA	a	803	-	1/1/15/20	3/39/115/115	-
20	XAT	1	303	-	-	0/31/93/93	0/4/4/4
22	CLA	9	314	-	1/1/13/20	10/27/103/115	-
22	CLA	b	824	-	1/1/15/20	15/39/115/115	-
22	CLA	7	309	-	1/1/11/20	5/17/93/115	-
29	BCR	h	202	-	-	0/29/63/63	0/2/2/2
22	CLA	9	312	-	1/1/11/20	7/17/93/115	-
22	CLA	1	311	-	1/1/12/20	4/25/101/115	-
22	CLA	b	819	-	1/1/13/20	5/27/103/115	-
28	PQN	b	841	-	-	1/23/43/43	0/2/2/2
22	CLA	8	305	3	1/1/10/20	2/13/89/115	-
22	CLA	9	315	2	1/1/10/20	5/12/88/115	-
22	CLA	b	830	-	1/1/10/20	2/10/86/115	-
29	BCR	b	844	-	-	6/29/63/63	0/2/2/2
22	CLA	4	315	4	1/1/10/20	6/10/86/115	-
29	BCR	b	843	-	-	2/29/63/63	0/2/2/2
20	XAT	9	305	-	-	3/31/93/93	0/4/4/4
22	CLA	a	826	-	1/1/15/20	8/39/115/115	-
22	CLA	1	313	-	1/1/10/20	6/10/86/115	-
25	LHG	9	317	-	-	28/50/50/53	-
29	BCR	a	847	-	-	0/29/63/63	0/2/2/2
22	CLA	7	315	4	1/1/10/20	4/10/86/115	-
29	BCR	b	849	-	-	4/29/63/63	0/2/2/2
20	XAT	2	304	-	-	3/31/93/93	0/4/4/4
22	CLA	4	308	-	1/1/15/20	13/39/115/115	-
22	CLA	2	310	-	1/1/15/20	14/39/115/115	-
22	CLA	a	818	-	1/1/13/20	11/29/105/115	-
22	CLA	3	308	-	1/1/11/20	7/18/94/115	-
22	CLA	a	841	-	1/1/15/20	15/39/115/115	-
20	XAT	5	301	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	308	7	1/1/15/20	13/39/115/115	-
22	CLA	a	814	-	1/1/15/20	19/39/115/115	-
22	CLA	a	839	-	1/1/15/20	14/39/115/115	-
22	CLA	7	317	-	1/1/11/20	7/15/91/115	-
22	CLA	b	827	-	1/1/15/20	14/39/115/115	-
20	XAT	4	302	-	-	0/31/93/93	0/4/4/4
25	LHG	b	847	22	-	20/35/35/53	-
22	CLA	a	834	-	1/1/15/20	9/39/115/115	-
22	CLA	3	307	5	1/1/11/20	2/15/91/115	-
22	CLA	b	826	-	1/1/15/20	3/39/115/115	-
26	DGD	4	318	-	-	10/29/69/95	0/2/2/2
22	CLA	a	809	8	1/1/15/20	15/39/115/115	-
30	SF4	c	101	-	-	-	0/6/5/5
22	CLA	8	306	26	1/1/11/20	4/17/93/115	-
22	CLA	b	835	-	1/1/13/20	10/31/107/115	-
22	CLA	5	311	-	1/1/12/20	7/23/99/115	-
22	CLA	4	316	-	1/1/11/20	7/17/93/115	-
22	CLA	7	308	-	1/1/14/20	12/33/109/115	-
22	CLA	a	806	-	1/1/15/20	11/39/115/115	-
20	XAT	4	304	-	-	0/31/93/93	0/4/4/4
20	XAT	2	302	-	-	0/31/93/93	0/4/4/4
20	XAT	3	301	-	-	3/31/93/93	0/4/4/4
22	CLA	b	836	-	1/1/15/20	7/39/115/115	-
20	XAT	4	305	-	-	4/31/93/93	0/4/4/4
22	CLA	4	310	-	1/1/15/20	15/39/115/115	-
22	CLA	9	318	-	1/1/14/20	11/36/112/115	-
22	CLA	8	313	-	1/1/11/20	5/17/93/115	-
22	CLA	a	837	8	1/1/11/20	4/15/91/115	-
22	CLA	7	316	-	1/1/12/20	10/23/99/115	-
22	CLA	a	832	-	1/1/12/20	7/21/97/115	-
20	XAT	9	304	-	-	1/31/93/93	0/4/4/4
22	CLA	b	825	-	1/1/14/20	4/38/114/115	-
22	CLA	2	307	-	1/1/11/20	7/18/94/115	-
22	CLA	h	205	-	1/1/13/20	9/27/103/115	-
20	XAT	7	304	-	-	6/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	823	-	1/1/11/20	7/20/96/115	-
22	CLA	b	818	-	1/1/14/20	15/33/109/115	-
22	CLA	b	840	25	1/1/15/20	11/39/115/115	-
22	CLA	a	801	-	1/1/15/20	22/39/115/115	-
22	CLA	a	821	-	1/1/11/20	1/15/91/115	-
20	XAT	2	305	-	-	2/31/93/93	0/4/4/4
22	CLA	2	315	-	1/1/10/20	3/12/88/115	-
22	CLA	a	824	-	1/1/11/20	5/17/93/115	-
22	CLA	3	310	-	1/1/13/20	3/29/105/115	-
22	CLA	3	311	-	1/1/12/20	4/21/97/115	-
22	CLA	a	811	-	1/1/13/20	6/29/105/115	-
22	CLA	a	844	25	1/1/15/20	15/39/115/115	-
22	CLA	8	311	-	1/1/13/20	7/29/105/115	-
22	CLA	3	313	-	1/1/12/20	1/24/100/115	-
22	CLA	b	834	-	1/1/12/20	9/25/101/115	-
21	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
22	CLA	1	309	7	1/1/11/20	7/17/93/115	-
22	CLA	a	836	-	1/1/12/20	8/21/97/115	-
22	CLA	h	203	-	1/1/15/20	9/39/115/115	-
22	CLA	5	315	-	1/1/11/20	5/17/93/115	-
22	CLA	1	314	-	1/1/11/20	7/15/91/115	-
22	CLA	a	817	-	1/1/11/20	8/15/91/115	-
22	CLA	b	829	-	1/1/15/20	11/39/115/115	-
30	SF4	c	102	-	-	-	0/6/5/5
22	CLA	b	821	-	1/1/12/20	4/23/99/115	-
22	CLA	a	833	-	1/1/13/20	2/27/103/115	-
22	CLA	2	308	6	1/1/12/20	3/26/102/115	-
22	CLA	9	316	-	1/1/15/20	16/39/115/115	-

All (1485) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	843	PQN	C3-C2	7.72	1.49	1.35
28	b	841	PQN	C3-C2	7.50	1.48	1.35
28	a	843	PQN	C10-C5	4.93	1.48	1.40
28	b	841	PQN	C10-C5	4.92	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	h	204	A1L1F	O7-C54	4.68	1.45	1.35
24	9	302	A1L1F	O7-C54	4.66	1.45	1.35
24	8	304	A1L1F	O7-C54	4.65	1.45	1.35
24	1	304	A1L1F	O7-C54	4.55	1.45	1.35
23	5	316	SQD	O8-S	4.46	1.64	1.47
23	1	315	SQD	O8-S	4.43	1.63	1.47
24	9	302	A1L1F	C57-C1	-4.39	1.25	1.30
24	h	204	A1L1F	C57-C1	-4.34	1.25	1.30
24	8	304	A1L1F	C57-C1	-4.33	1.25	1.30
23	1	315	SQD	O48-C23	4.30	1.45	1.33
26	8	315	DGD	O1G-C1A	4.28	1.45	1.33
24	1	304	A1L1F	O13-C45	4.24	1.45	1.33
23	5	316	SQD	O48-C23	4.24	1.45	1.33
27	a	853	LMG	O8-C28	4.22	1.45	1.33
24	1	304	A1L1F	C57-C1	-4.22	1.25	1.30
23	1	315	SQD	O47-C7	4.20	1.46	1.34
24	h	204	A1L1F	O13-C45	4.16	1.45	1.33
27	a	853	LMG	O7-C10	4.14	1.46	1.34
27	j	105	LMG	O8-C28	4.11	1.45	1.33
23	5	316	SQD	O47-C7	4.11	1.45	1.34
24	8	304	A1L1F	O13-C45	4.10	1.45	1.33
27	2	317	LMG	O8-C28	4.06	1.45	1.33
26	4	318	DGD	O1G-C1A	4.03	1.45	1.33
26	b	848	DGD	O2G-C1B	4.01	1.45	1.34
29	m	101	BCR	C1-C6	-3.97	1.48	1.53
26	b	848	DGD	O1G-C1A	3.97	1.44	1.33
27	2	317	LMG	O7-C10	3.96	1.45	1.34
24	h	204	A1L1F	C57-C2	-3.93	1.25	1.31
24	9	302	A1L1F	O13-C45	3.93	1.44	1.33
24	8	304	A1L1F	C57-C2	-3.90	1.25	1.31
26	4	318	DGD	O2G-C1B	3.87	1.45	1.34
24	9	302	A1L1F	C57-C2	-3.87	1.25	1.31
27	j	105	LMG	O7-C10	3.86	1.45	1.34
26	8	315	DGD	O2G-C1B	3.77	1.44	1.34
22	2	313	CLA	C1D-ND	3.68	1.42	1.37
24	1	304	A1L1F	C57-C2	-3.67	1.25	1.31
22	h	203	CLA	C1D-ND	3.67	1.42	1.37
22	a	804	CLA	C1D-ND	3.65	1.42	1.37
22	7	306	CLA	C1D-ND	3.64	1.42	1.37
22	8	314	CLA	C1D-ND	3.63	1.42	1.37
22	1	312	CLA	C1D-ND	3.63	1.42	1.37
22	3	308	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	837	CLA	C1D-ND	3.63	1.42	1.37
22	3	314	CLA	C1D-ND	3.63	1.42	1.37
22	8	308	CLA	C1D-ND	3.63	1.42	1.37
22	8	313	CLA	C1D-ND	3.62	1.42	1.37
22	a	828	CLA	C1D-ND	3.62	1.42	1.37
22	5	308	CLA	C1D-ND	3.60	1.42	1.37
22	9	312	CLA	C1D-ND	3.60	1.42	1.37
22	8	310	CLA	C1D-ND	3.60	1.42	1.37
22	9	313	CLA	C1D-ND	3.59	1.42	1.37
22	9	310	CLA	C1D-ND	3.59	1.42	1.37
22	4	307	CLA	C1D-ND	3.59	1.42	1.37
22	9	315	CLA	C1D-ND	3.58	1.42	1.37
22	7	315	CLA	C1D-ND	3.58	1.42	1.37
22	7	307	CLA	C1D-ND	3.58	1.42	1.37
22	2	311	CLA	C1D-ND	3.58	1.42	1.37
22	b	820	CLA	C1D-ND	3.57	1.42	1.37
22	2	315	CLA	C1D-ND	3.57	1.42	1.37
22	a	840	CLA	C1D-ND	3.57	1.42	1.37
22	4	306	CLA	C1D-ND	3.57	1.42	1.37
22	a	814	CLA	C1D-ND	3.57	1.42	1.37
22	l	204	CLA	C1D-ND	3.56	1.42	1.37
22	b	840	CLA	C1D-ND	3.56	1.42	1.37
22	4	316	CLA	C1D-ND	3.56	1.42	1.37
22	2	307	CLA	C1D-ND	3.56	1.42	1.37
22	7	308	CLA	C1D-ND	3.56	1.42	1.37
22	a	811	CLA	C1D-ND	3.56	1.42	1.37
22	b	818	CLA	C1D-ND	3.56	1.42	1.37
22	j	103	CLA	C1D-ND	3.55	1.42	1.37
22	3	315	CLA	C1D-ND	3.55	1.42	1.37
22	3	311	CLA	C1D-ND	3.55	1.42	1.37
22	2	306	CLA	C1D-ND	3.55	1.42	1.37
22	a	815	CLA	C1D-ND	3.55	1.42	1.37
22	b	814	CLA	C1D-ND	3.55	1.42	1.37
22	9	314	CLA	C1D-ND	3.54	1.42	1.37
22	7	317	CLA	C1D-ND	3.54	1.42	1.37
22	8	305	CLA	C1D-ND	3.54	1.42	1.37
22	5	311	CLA	C1D-ND	3.54	1.42	1.37
22	5	314	CLA	C1D-ND	3.54	1.42	1.37
22	a	835	CLA	C1D-ND	3.54	1.42	1.37
22	5	313	CLA	C1D-ND	3.54	1.42	1.37
22	b	839	CLA	C1D-ND	3.53	1.42	1.37
22	7	311	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	314	CLA	C1D-ND	3.53	1.42	1.37
22	8	309	CLA	C1D-ND	3.53	1.42	1.37
22	a	839	CLA	C1D-ND	3.53	1.42	1.37
22	b	824	CLA	C1D-ND	3.53	1.42	1.37
22	3	310	CLA	C1D-ND	3.53	1.42	1.37
22	1	310	CLA	C1D-ND	3.53	1.42	1.37
22	b	833	CLA	C1D-ND	3.53	1.42	1.37
22	4	315	CLA	C1D-ND	3.53	1.42	1.37
22	7	310	CLA	C1D-ND	3.53	1.42	1.37
22	a	817	CLA	C1D-ND	3.53	1.42	1.37
22	5	306	CLA	C1D-ND	3.52	1.42	1.37
22	4	314	CLA	C1D-ND	3.52	1.42	1.37
22	a	829	CLA	C1D-ND	3.52	1.42	1.37
22	7	316	CLA	C1D-ND	3.52	1.42	1.37
22	b	807	CLA	C1D-ND	3.52	1.42	1.37
22	j	102	CLA	C1D-ND	3.52	1.42	1.37
22	5	305	CLA	C1D-ND	3.52	1.42	1.37
22	5	309	CLA	C1D-ND	3.52	1.42	1.37
22	b	819	CLA	C1D-ND	3.52	1.42	1.37
22	a	838	CLA	C1D-ND	3.51	1.42	1.37
22	5	310	CLA	C1D-ND	3.51	1.42	1.37
22	1	311	CLA	C1D-ND	3.51	1.42	1.37
22	b	817	CLA	C1D-ND	3.51	1.42	1.37
22	a	822	CLA	C1D-ND	3.51	1.42	1.37
22	b	826	CLA	C1D-ND	3.51	1.42	1.37
22	f	802	CLA	C1D-ND	3.51	1.42	1.37
22	7	313	CLA	C1D-ND	3.51	1.42	1.37
22	a	834	CLA	C1D-ND	3.51	1.42	1.37
22	a	821	CLA	C1D-ND	3.51	1.42	1.37
22	7	314	CLA	C1D-ND	3.50	1.42	1.37
22	1	314	CLA	C1D-ND	3.50	1.42	1.37
22	a	819	CLA	C1D-ND	3.50	1.42	1.37
22	a	825	CLA	C1D-ND	3.50	1.42	1.37
22	2	309	CLA	C1D-ND	3.50	1.42	1.37
22	h	205	CLA	C1D-ND	3.50	1.42	1.37
22	8	306	CLA	C1D-ND	3.50	1.42	1.37
22	a	809	CLA	C1D-ND	3.50	1.42	1.37
22	b	837	CLA	C1D-ND	3.49	1.42	1.37
22	1	306	CLA	C1D-ND	3.49	1.42	1.37
22	b	805	CLA	C1D-ND	3.49	1.42	1.37
22	3	313	CLA	C1D-ND	3.49	1.42	1.37
22	b	835	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	813	CLA	C1D-ND	3.49	1.42	1.37
22	a	820	CLA	C1D-ND	3.49	1.42	1.37
22	a	826	CLA	C1D-ND	3.49	1.42	1.37
22	b	834	CLA	C1D-ND	3.49	1.42	1.37
22	2	312	CLA	C1D-ND	3.48	1.42	1.37
22	a	807	CLA	C1D-ND	3.48	1.42	1.37
22	b	838	CLA	C1D-ND	3.48	1.42	1.37
22	9	318	CLA	C1D-ND	3.48	1.42	1.37
22	b	816	CLA	C1D-ND	3.48	1.42	1.37
22	4	309	CLA	C1D-ND	3.48	1.42	1.37
22	3	309	CLA	C1D-ND	3.48	1.42	1.37
22	4	310	CLA	C1D-ND	3.48	1.42	1.37
22	7	312	CLA	C1D-ND	3.48	1.42	1.37
22	1	309	CLA	C1D-ND	3.48	1.42	1.37
22	8	307	CLA	C1D-ND	3.47	1.42	1.37
22	3	312	CLA	C1D-ND	3.47	1.42	1.37
22	a	836	CLA	C1D-ND	3.47	1.42	1.37
22	b	829	CLA	C1D-ND	3.47	1.42	1.37
22	7	309	CLA	C1D-ND	3.47	1.42	1.37
22	4	317	CLA	C1D-ND	3.47	1.42	1.37
22	1	308	CLA	C1D-ND	3.47	1.42	1.37
22	5	312	CLA	C1D-ND	3.46	1.42	1.37
22	9	316	CLA	C1D-ND	3.46	1.42	1.37
22	1	307	CLA	C1D-ND	3.46	1.42	1.37
22	a	816	CLA	C1D-ND	3.46	1.42	1.37
22	5	315	CLA	C1D-ND	3.46	1.42	1.37
22	a	841	CLA	C1D-ND	3.45	1.42	1.37
22	b	812	CLA	C1D-ND	3.45	1.42	1.37
22	b	831	CLA	C1D-ND	3.45	1.42	1.37
22	4	312	CLA	C1D-ND	3.45	1.42	1.37
22	a	844	CLA	C1D-ND	3.45	1.42	1.37
22	b	821	CLA	C1D-ND	3.45	1.42	1.37
22	a	813	CLA	C1D-ND	3.44	1.42	1.37
22	a	818	CLA	C1D-ND	3.44	1.42	1.37
22	b	808	CLA	C1D-ND	3.44	1.42	1.37
22	a	823	CLA	C1D-ND	3.44	1.42	1.37
22	a	854	CLA	C1D-ND	3.44	1.42	1.37
22	a	805	CLA	C1D-ND	3.44	1.42	1.37
22	a	808	CLA	C1D-ND	3.44	1.42	1.37
22	1	202	CLA	C1D-ND	3.44	1.42	1.37
22	2	308	CLA	C1D-ND	3.43	1.42	1.37
22	b	801	CLA	C1D-ND	3.43	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	305	CLA	C1D-ND	3.43	1.42	1.37
22	4	308	CLA	C1D-ND	3.43	1.42	1.37
22	a	803	CLA	C1D-ND	3.43	1.42	1.37
22	f	803	CLA	C1D-ND	3.43	1.42	1.37
22	b	815	CLA	C1D-ND	3.42	1.42	1.37
22	a	810	CLA	C1D-ND	3.42	1.42	1.37
22	9	308	CLA	C1D-ND	3.42	1.42	1.37
22	a	842	CLA	C1D-ND	3.42	1.42	1.37
22	b	828	CLA	C1D-ND	3.42	1.42	1.37
22	4	311	CLA	C1D-ND	3.42	1.42	1.37
22	b	825	CLA	C1D-ND	3.42	1.42	1.37
22	a	832	CLA	C1D-ND	3.41	1.42	1.37
22	b	822	CLA	C1D-ND	3.41	1.42	1.37
22	8	311	CLA	C1D-ND	3.41	1.42	1.37
22	a	824	CLA	C1D-ND	3.41	1.42	1.37
22	a	831	CLA	C1D-ND	3.41	1.42	1.37
22	a	812	CLA	C1D-ND	3.40	1.42	1.37
22	b	809	CLA	C1D-ND	3.39	1.42	1.37
22	9	311	CLA	C1D-ND	3.39	1.42	1.37
22	l	203	CLA	C1D-ND	3.39	1.42	1.37
22	3	307	CLA	C1D-ND	3.39	1.42	1.37
22	b	810	CLA	C1D-ND	3.39	1.42	1.37
22	4	313	CLA	C1D-ND	3.39	1.42	1.37
22	b	806	CLA	C1D-ND	3.39	1.42	1.37
22	1	313	CLA	C1D-ND	3.39	1.42	1.37
22	a	830	CLA	C1D-ND	3.38	1.42	1.37
29	m	101	BCR	C30-C25	-3.38	1.49	1.53
22	2	316	CLA	C1D-ND	3.38	1.42	1.37
22	b	836	CLA	C1D-ND	3.37	1.42	1.37
22	b	827	CLA	C1D-ND	3.37	1.42	1.37
22	b	823	CLA	C1D-ND	3.36	1.42	1.37
22	5	307	CLA	C1D-ND	3.36	1.42	1.37
22	1	312	CLA	C4B-NB	3.36	1.42	1.37
22	8	312	CLA	C1D-ND	3.35	1.42	1.37
22	a	827	CLA	C1D-ND	3.34	1.42	1.37
22	2	310	CLA	C1D-ND	3.34	1.42	1.37
22	b	832	CLA	C1D-ND	3.34	1.42	1.37
22	b	802	CLA	C1D-ND	3.33	1.42	1.37
22	b	811	CLA	C1D-ND	3.31	1.42	1.37
22	9	309	CLA	C1D-ND	3.29	1.42	1.37
22	2	315	CLA	C4B-NB	3.28	1.42	1.37
22	a	842	CLA	C4B-NB	3.27	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	830	CLA	C1D-ND	3.26	1.42	1.37
22	b	803	CLA	C1D-ND	3.25	1.42	1.37
25	a	845	LHG	C26-C25	-3.25	1.35	1.51
22	a	801	CLA	C1D-ND	3.25	1.42	1.37
22	a	802	CLA	C1D-ND	3.25	1.42	1.37
25	9	317	LHG	C26-C25	-3.24	1.35	1.51
22	3	315	CLA	C4B-NB	3.21	1.42	1.37
22	4	315	CLA	C4B-NB	3.21	1.42	1.37
22	a	840	CLA	C4B-NB	3.20	1.42	1.37
22	a	818	CLA	C4B-NB	3.20	1.42	1.37
25	b	847	LHG	C26-C25	-3.20	1.35	1.51
22	4	312	CLA	C4B-NB	3.20	1.42	1.37
25	9	307	LHG	C26-C25	-3.20	1.35	1.51
22	b	837	CLA	C4B-NB	3.20	1.42	1.37
22	b	820	CLA	C4B-NB	3.19	1.42	1.37
22	5	313	CLA	C4B-NB	3.19	1.42	1.37
22	1	309	CLA	C4B-NB	3.19	1.42	1.37
22	h	203	CLA	C4B-NB	3.19	1.42	1.37
22	a	833	CLA	C1D-ND	3.18	1.42	1.37
22	4	314	CLA	C4B-NB	3.18	1.42	1.37
22	a	813	CLA	C4B-NB	3.17	1.42	1.37
22	2	311	CLA	C4B-NB	3.16	1.42	1.37
22	1	305	CLA	C4B-NB	3.15	1.42	1.37
22	7	311	CLA	C4B-NB	3.15	1.42	1.37
22	4	306	CLA	C4B-NB	3.15	1.42	1.37
22	a	824	CLA	C4B-NB	3.15	1.42	1.37
22	1	314	CLA	C4B-NB	3.14	1.42	1.37
22	2	309	CLA	C4B-NB	3.14	1.42	1.37
22	9	314	CLA	C4B-NB	3.14	1.42	1.37
22	8	313	CLA	C4B-NB	3.14	1.42	1.37
22	5	305	CLA	C4B-NB	3.14	1.42	1.37
22	2	308	CLA	C4B-NB	3.13	1.42	1.37
22	b	802	CLA	C4B-NB	3.13	1.42	1.37
22	a	831	CLA	C4B-NB	3.13	1.42	1.37
22	j	102	CLA	C4B-NB	3.13	1.42	1.37
22	b	811	CLA	CAB-C3B	-3.12	1.44	1.50
22	5	310	CLA	C4B-NB	3.12	1.42	1.37
22	a	808	CLA	C4B-NB	3.12	1.42	1.37
22	b	834	CLA	C4B-NB	3.12	1.42	1.37
22	b	840	CLA	C4B-NB	3.12	1.42	1.37
22	7	315	CLA	C4B-NB	3.12	1.42	1.37
22	7	313	CLA	C4B-NB	3.12	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	829	CLA	C4B-NB	3.12	1.42	1.37
22	2	313	CLA	C4B-NB	3.11	1.42	1.37
22	4	317	CLA	C4B-NB	3.11	1.41	1.37
22	7	307	CLA	C4B-NB	3.11	1.41	1.37
22	3	311	CLA	C4B-NB	3.11	1.41	1.37
22	a	825	CLA	C4B-NB	3.11	1.41	1.37
22	1	313	CLA	C4B-NB	3.11	1.41	1.37
22	2	312	CLA	C4B-NB	3.11	1.41	1.37
22	4	311	CLA	C4B-NB	3.10	1.41	1.37
22	9	318	CLA	C4B-NB	3.09	1.41	1.37
22	8	309	CLA	C4B-NB	3.09	1.41	1.37
22	4	309	CLA	C4B-NB	3.09	1.41	1.37
22	4	313	CLA	C4B-NB	3.09	1.41	1.37
22	a	817	CLA	C4B-NB	3.09	1.41	1.37
22	9	309	CLA	C4B-NB	3.09	1.41	1.37
22	7	317	CLA	C4B-NB	3.08	1.41	1.37
22	b	801	CLA	C4B-NB	3.08	1.41	1.37
22	b	828	CLA	C4B-NB	3.08	1.41	1.37
22	b	826	CLA	C4B-NB	3.08	1.41	1.37
22	2	316	CLA	C4B-NB	3.08	1.41	1.37
22	2	310	CLA	C4B-NB	3.08	1.41	1.37
22	2	314	CLA	C4B-NB	3.08	1.41	1.37
22	b	818	CLA	C4B-NB	3.07	1.41	1.37
22	a	804	CLA	C4B-NB	3.07	1.41	1.37
22	4	316	CLA	C4B-NB	3.07	1.41	1.37
22	4	307	CLA	C4B-NB	3.07	1.41	1.37
22	4	310	CLA	C4B-NB	3.06	1.41	1.37
22	2	306	CLA	C4B-NB	3.06	1.41	1.37
22	a	841	CLA	C4B-NB	3.06	1.41	1.37
22	b	839	CLA	C4B-NB	3.06	1.41	1.37
22	b	822	CLA	C4B-NB	3.06	1.41	1.37
22	3	307	CLA	C4B-NB	3.06	1.41	1.37
22	b	831	CLA	C4B-NB	3.05	1.41	1.37
22	a	810	CLA	C4B-NB	3.05	1.41	1.37
22	a	822	CLA	C4B-NB	3.05	1.41	1.37
22	a	834	CLA	C4B-NB	3.05	1.41	1.37
22	1	202	CLA	C4B-NB	3.05	1.41	1.37
22	3	312	CLA	C4B-NB	3.05	1.41	1.37
22	3	308	CLA	C4B-NB	3.05	1.41	1.37
22	8	312	CLA	C4B-NB	3.04	1.41	1.37
22	1	307	CLA	C4B-NB	3.04	1.41	1.37
22	5	306	CLA	C4B-NB	3.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	805	CLA	C4B-NB	3.04	1.41	1.37
22	3	310	CLA	C4B-NB	3.04	1.41	1.37
22	8	308	CLA	C4B-NB	3.03	1.41	1.37
22	a	837	CLA	C4B-NB	3.03	1.41	1.37
22	a	854	CLA	C4B-NB	3.03	1.41	1.37
22	b	809	CLA	C4B-NB	3.03	1.41	1.37
22	8	314	CLA	C4B-NB	3.03	1.41	1.37
22	8	306	CLA	C4B-NB	3.03	1.41	1.37
22	a	816	CLA	C4B-NB	3.03	1.41	1.37
22	f	803	CLA	C4B-NB	3.03	1.41	1.37
22	b	816	CLA	C4B-NB	3.03	1.41	1.37
22	9	310	CLA	C4B-NB	3.02	1.41	1.37
22	b	814	CLA	C4B-NB	3.02	1.41	1.37
22	8	310	CLA	C4B-NB	3.02	1.41	1.37
22	b	808	CLA	C4B-NB	3.02	1.41	1.37
22	a	805	CLA	C4B-NB	3.02	1.41	1.37
22	5	315	CLA	C4B-NB	3.02	1.41	1.37
22	a	820	CLA	C4B-NB	3.01	1.41	1.37
22	a	829	CLA	C4B-NB	3.01	1.41	1.37
22	7	314	CLA	C4B-NB	3.01	1.41	1.37
22	b	838	CLA	C4B-NB	3.01	1.41	1.37
22	b	804	CLA	C1D-ND	3.01	1.41	1.37
22	j	103	CLA	C4B-NB	3.01	1.41	1.37
22	7	308	CLA	C4B-NB	3.01	1.41	1.37
22	1	310	CLA	C4B-NB	3.01	1.41	1.37
22	9	308	CLA	C4B-NB	3.01	1.41	1.37
22	9	313	CLA	C4B-NB	3.01	1.41	1.37
22	7	306	CLA	C4B-NB	3.01	1.41	1.37
22	b	804	CLA	C4B-NB	3.01	1.41	1.37
22	9	315	CLA	C4B-NB	3.00	1.41	1.37
22	b	827	CLA	C4B-NB	3.00	1.41	1.37
22	a	812	CLA	C4B-NB	3.00	1.41	1.37
22	a	815	CLA	C4B-NB	3.00	1.41	1.37
22	8	305	CLA	C4B-NB	3.00	1.41	1.37
22	a	823	CLA	C4B-NB	3.00	1.41	1.37
22	3	313	CLA	C4B-NB	3.00	1.41	1.37
22	b	824	CLA	C4B-NB	2.99	1.41	1.37
22	5	308	CLA	C4B-NB	2.99	1.41	1.37
22	1	308	CLA	C4B-NB	2.99	1.41	1.37
22	a	827	CLA	C4B-NB	2.99	1.41	1.37
22	7	310	CLA	C4B-NB	2.99	1.41	1.37
22	5	309	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	811	CLA	C4B-NB	2.99	1.41	1.37
22	b	836	CLA	C4B-NB	2.99	1.41	1.37
22	a	826	CLA	C4B-NB	2.99	1.41	1.37
22	3	309	CLA	C4B-NB	2.98	1.41	1.37
22	7	312	CLA	C4B-NB	2.98	1.41	1.37
24	h	204	A1L1F	O15-C20	-2.98	1.42	1.46
22	7	309	CLA	C4B-NB	2.98	1.41	1.37
22	a	836	CLA	C4B-NB	2.98	1.41	1.37
22	a	821	CLA	C4B-NB	2.97	1.41	1.37
22	a	811	CLA	C4B-NB	2.97	1.41	1.37
22	b	819	CLA	C4B-NB	2.97	1.41	1.37
22	b	832	CLA	C4B-NB	2.97	1.41	1.37
22	b	833	CLA	C4B-NB	2.96	1.41	1.37
22	l	203	CLA	C4B-NB	2.96	1.41	1.37
22	a	839	CLA	C4B-NB	2.96	1.41	1.37
22	l	204	CLA	C4B-NB	2.96	1.41	1.37
22	b	813	CLA	C4B-NB	2.96	1.41	1.37
22	l	306	CLA	C4B-NB	2.96	1.41	1.37
22	a	830	CLA	C4B-NB	2.95	1.41	1.37
22	b	803	CLA	C1B-C2B	2.95	1.50	1.43
22	9	311	CLA	C4B-NB	2.95	1.41	1.37
22	a	802	CLA	C4B-NB	2.95	1.41	1.37
22	a	832	CLA	C4B-NB	2.95	1.41	1.37
22	b	817	CLA	C4B-NB	2.95	1.41	1.37
22	b	803	CLA	C4B-NB	2.94	1.41	1.37
22	b	806	CLA	C4B-NB	2.94	1.41	1.37
22	a	819	CLA	C4B-NB	2.94	1.41	1.37
22	f	802	CLA	C4B-NB	2.94	1.41	1.37
24	9	302	A1L1F	C6-C1	-2.94	1.49	1.54
22	a	833	CLA	C4B-NB	2.94	1.41	1.37
22	8	307	CLA	C4B-NB	2.94	1.41	1.37
22	5	314	CLA	C4B-NB	2.94	1.41	1.37
22	5	312	CLA	C4B-NB	2.94	1.41	1.37
22	a	835	CLA	C4B-NB	2.93	1.41	1.37
22	5	307	CLA	C4B-NB	2.93	1.41	1.37
22	a	844	CLA	C4B-NB	2.93	1.41	1.37
22	3	314	CLA	C4B-NB	2.93	1.41	1.37
22	b	823	CLA	C4B-NB	2.93	1.41	1.37
22	a	814	CLA	C4B-NB	2.92	1.41	1.37
22	b	810	CLA	C4B-NB	2.92	1.41	1.37
22	b	815	CLA	C4B-NB	2.92	1.41	1.37
22	h	205	CLA	C4B-NB	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	812	CLA	C4B-NB	2.91	1.41	1.37
22	8	311	CLA	C4B-NB	2.91	1.41	1.37
22	9	312	CLA	C4B-NB	2.91	1.41	1.37
22	5	311	CLA	C4B-NB	2.91	1.41	1.37
22	b	807	CLA	C4B-NB	2.91	1.41	1.37
22	a	803	CLA	C4B-NB	2.90	1.41	1.37
22	b	825	CLA	C4B-NB	2.90	1.41	1.37
22	a	838	CLA	C4B-NB	2.90	1.41	1.37
22	2	307	CLA	C4B-NB	2.89	1.41	1.37
22	b	821	CLA	C4B-NB	2.89	1.41	1.37
22	a	801	CLA	C4B-NB	2.89	1.41	1.37
22	b	835	CLA	C4B-NB	2.88	1.41	1.37
22	b	839	CLA	C1B-C2B	2.88	1.49	1.43
22	1	311	CLA	C4B-NB	2.87	1.41	1.37
22	4	308	CLA	C4B-NB	2.86	1.41	1.37
22	9	316	CLA	C4B-NB	2.86	1.41	1.37
22	b	830	CLA	C4B-NB	2.86	1.41	1.37
22	a	807	CLA	C4B-NB	2.84	1.41	1.37
22	a	823	CLA	C1B-C2B	2.82	1.49	1.43
22	b	827	CLA	C1B-C2B	2.82	1.49	1.43
22	7	308	CLA	C1B-C2B	2.81	1.49	1.43
22	1	305	CLA	C1B-C2B	2.81	1.49	1.43
22	7	316	CLA	C4B-NB	2.81	1.41	1.37
22	9	316	CLA	C1B-C2B	2.81	1.49	1.43
22	3	308	CLA	C1B-C2B	2.80	1.49	1.43
22	a	809	CLA	C4B-NB	2.80	1.41	1.37
22	a	828	CLA	C4B-NB	2.80	1.41	1.37
22	a	821	CLA	C1B-C2B	2.80	1.49	1.43
22	2	316	CLA	C1B-C2B	2.79	1.49	1.43
22	b	821	CLA	C1B-C2B	2.79	1.49	1.43
22	a	810	CLA	C1B-C2B	2.78	1.49	1.43
22	3	311	CLA	C1B-C2B	2.78	1.49	1.43
21	9	301	A1L1G	C33-C34	-2.78	1.40	1.46
22	b	820	CLA	C1B-C2B	2.78	1.49	1.43
22	4	310	CLA	C1B-C2B	2.78	1.49	1.43
22	a	806	CLA	MG-NB	-2.78	2.00	2.05
22	b	807	CLA	C1B-C2B	2.78	1.49	1.43
22	b	823	CLA	C1B-C2B	2.78	1.49	1.43
22	b	808	CLA	C1B-C2B	2.78	1.49	1.43
22	j	103	CLA	C1B-C2B	2.78	1.49	1.43
22	8	305	CLA	C1B-C2B	2.78	1.49	1.43
22	7	317	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	834	CLA	C1B-C2B	2.77	1.49	1.43
22	7	306	CLA	C1B-C2B	2.77	1.49	1.43
22	j	102	CLA	C1B-C2B	2.77	1.49	1.43
22	7	315	CLA	C1B-C2B	2.77	1.49	1.43
22	1	306	CLA	C1B-C2B	2.77	1.49	1.43
22	7	316	CLA	C1B-C2B	2.77	1.49	1.43
22	1	311	CLA	C1B-C2B	2.77	1.49	1.43
22	3	310	CLA	C1B-C2B	2.77	1.49	1.43
22	a	842	CLA	C1B-C2B	2.77	1.49	1.43
22	f	802	CLA	C1B-C2B	2.76	1.49	1.43
22	7	312	CLA	C1B-C2B	2.76	1.49	1.43
22	2	313	CLA	C1B-C2B	2.76	1.49	1.43
22	b	833	CLA	C1B-C2B	2.76	1.49	1.43
22	a	844	CLA	C1B-C2B	2.76	1.49	1.43
22	8	306	CLA	C1B-C2B	2.75	1.49	1.43
22	3	309	CLA	C1B-C2B	2.75	1.49	1.43
22	a	838	CLA	C1B-C2B	2.75	1.49	1.43
22	5	315	CLA	C1B-C2B	2.75	1.49	1.43
22	a	828	CLA	C1B-C2B	2.75	1.49	1.43
22	a	817	CLA	C1B-C2B	2.75	1.49	1.43
22	b	832	CLA	C1B-C2B	2.75	1.49	1.43
22	9	318	CLA	C1B-C2B	2.75	1.49	1.43
22	4	316	CLA	C1B-C2B	2.75	1.49	1.43
22	2	315	CLA	C1B-C2B	2.75	1.49	1.43
22	8	309	CLA	C1B-C2B	2.75	1.49	1.43
22	7	309	CLA	C1B-C2B	2.75	1.49	1.43
22	5	311	CLA	C1B-C2B	2.74	1.49	1.43
22	b	812	CLA	C1B-C2B	2.74	1.49	1.43
22	4	312	CLA	C1B-C2B	2.74	1.49	1.43
22	a	830	CLA	C1B-C2B	2.74	1.49	1.43
22	4	314	CLA	C1B-C2B	2.74	1.49	1.43
22	3	313	CLA	C1B-C2B	2.74	1.49	1.43
22	9	313	CLA	C1B-C2B	2.74	1.49	1.43
22	7	310	CLA	C1B-C2B	2.73	1.49	1.43
22	3	314	CLA	C1B-C2B	2.73	1.49	1.43
22	a	812	CLA	C1B-C2B	2.73	1.49	1.43
22	9	310	CLA	C1B-C2B	2.73	1.49	1.43
22	8	307	CLA	C1B-C2B	2.73	1.49	1.43
22	b	805	CLA	C1B-C2B	2.73	1.49	1.43
22	a	840	CLA	C1B-C2B	2.73	1.49	1.43
22	h	205	CLA	C1B-C2B	2.73	1.49	1.43
22	1	308	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	l	204	CLA	C1B-C2B	2.73	1.49	1.43
22	8	314	CLA	C1B-C2B	2.73	1.49	1.43
22	a	835	CLA	C1B-C2B	2.73	1.49	1.43
22	b	822	CLA	C1B-C2B	2.73	1.49	1.43
22	b	836	CLA	C1B-C2B	2.73	1.49	1.43
22	2	306	CLA	C1B-C2B	2.73	1.49	1.43
22	1	309	CLA	C1B-C2B	2.73	1.49	1.43
22	9	312	CLA	C1B-C2B	2.73	1.49	1.43
22	b	811	CLA	C4B-C3B	2.73	1.49	1.43
22	a	809	CLA	C1B-C2B	2.72	1.49	1.43
22	b	826	CLA	C1B-C2B	2.72	1.49	1.43
22	2	311	CLA	C1B-C2B	2.72	1.49	1.43
22	4	317	CLA	C1B-C2B	2.72	1.49	1.43
22	5	309	CLA	C1B-C2B	2.72	1.49	1.43
22	2	309	CLA	C1B-C2B	2.72	1.49	1.43
22	b	837	CLA	C1B-C2B	2.72	1.49	1.43
22	1	313	CLA	C1B-C2B	2.72	1.49	1.43
22	a	825	CLA	C1B-C2B	2.72	1.49	1.43
22	9	311	CLA	C1B-C2B	2.72	1.49	1.43
22	9	315	CLA	C1B-C2B	2.72	1.49	1.43
22	f	803	CLA	C1B-C2B	2.72	1.49	1.43
22	7	307	CLA	C1B-C2B	2.71	1.49	1.43
22	4	308	CLA	C1B-C2B	2.71	1.49	1.43
22	9	308	CLA	C1B-C2B	2.71	1.49	1.43
22	2	312	CLA	C1B-C2B	2.71	1.49	1.43
22	a	824	CLA	C1B-C2B	2.71	1.49	1.43
22	b	806	CLA	C1B-C2B	2.71	1.49	1.43
22	5	310	CLA	C1B-C2B	2.71	1.49	1.43
22	2	308	CLA	C1B-C2B	2.71	1.49	1.43
22	1	202	CLA	C1B-C2B	2.71	1.49	1.43
20	9	303	XAT	O4-C5	-2.71	1.42	1.46
22	5	305	CLA	C1B-C2B	2.71	1.49	1.43
22	a	811	CLA	C1B-C2B	2.71	1.49	1.43
22	a	829	CLA	C1B-C2B	2.71	1.49	1.43
22	7	314	CLA	C1B-C2B	2.71	1.49	1.43
22	4	306	CLA	C1B-C2B	2.70	1.49	1.43
22	1	314	CLA	C1B-C2B	2.70	1.49	1.43
22	b	801	CLA	C1B-C2B	2.70	1.49	1.43
22	4	307	CLA	C1B-C2B	2.70	1.49	1.43
22	a	818	CLA	C3B-C4B	2.70	1.50	1.42
22	8	308	CLA	C1B-C2B	2.70	1.49	1.43
22	a	807	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	311	CLA	C1B-C2B	2.70	1.49	1.43
22	a	814	CLA	C1B-C2B	2.70	1.49	1.43
22	8	313	CLA	C1B-C2B	2.70	1.49	1.43
22	1	312	CLA	C3B-C4B	2.69	1.50	1.42
22	a	816	CLA	C1B-C2B	2.69	1.49	1.43
22	5	306	CLA	C1B-C2B	2.69	1.49	1.43
22	4	311	CLA	C1B-C2B	2.69	1.49	1.43
22	a	805	CLA	C1B-C2B	2.69	1.49	1.43
22	5	307	CLA	C1B-C2B	2.69	1.49	1.43
22	3	307	CLA	C1B-C2B	2.69	1.49	1.43
22	3	312	CLA	C1B-C2B	2.69	1.49	1.43
22	a	836	CLA	C1B-C2B	2.68	1.49	1.43
22	b	802	CLA	C1B-C2B	2.68	1.49	1.43
22	b	831	CLA	C1B-C2B	2.68	1.49	1.43
22	a	813	CLA	C1B-C2B	2.68	1.49	1.43
22	a	839	CLA	C1B-C2B	2.68	1.49	1.43
22	b	813	CLA	C1B-C2B	2.68	1.49	1.43
22	4	315	CLA	C1B-C2B	2.68	1.49	1.43
21	5	303	A1L1G	C33-C34	-2.68	1.40	1.46
22	a	804	CLA	C1B-C2B	2.68	1.49	1.43
22	5	313	CLA	C1B-C2B	2.68	1.49	1.43
22	b	840	CLA	C1B-C2B	2.67	1.49	1.43
22	5	312	CLA	C1B-C2B	2.67	1.49	1.43
22	b	811	CLA	C1B-C2B	2.67	1.49	1.43
22	5	314	CLA	C1B-C2B	2.67	1.49	1.43
22	2	310	CLA	C1B-C2B	2.67	1.49	1.43
22	b	809	CLA	C1B-C2B	2.67	1.49	1.43
22	a	826	CLA	C1B-C2B	2.66	1.49	1.43
22	1	307	CLA	C1B-C2B	2.66	1.49	1.43
22	a	801	CLA	C1B-C2B	2.66	1.49	1.43
22	8	312	CLA	C1B-C2B	2.66	1.49	1.43
22	a	854	CLA	C1B-C2B	2.66	1.49	1.43
22	b	829	CLA	CMB-C2B	-2.66	1.45	1.50
22	b	835	CLA	C1B-C2B	2.66	1.49	1.43
22	b	816	CLA	C1B-C2B	2.66	1.49	1.43
22	a	832	CLA	C1B-C2B	2.66	1.49	1.43
24	h	204	A1L1F	C6-C1	-2.66	1.50	1.54
22	a	837	CLA	C1B-C2B	2.66	1.49	1.43
22	a	808	CLA	C1B-C2B	2.66	1.49	1.43
22	3	315	CLA	C1B-C2B	2.65	1.49	1.43
22	b	815	CLA	C1B-C2B	2.65	1.49	1.43
22	4	309	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	819	CLA	C1B-C2B	2.65	1.49	1.43
22	a	815	CLA	C1B-C2B	2.65	1.49	1.43
24	9	302	A1L1F	O15-C20	-2.64	1.42	1.46
22	h	203	CLA	C1B-C2B	2.64	1.49	1.43
22	a	827	CLA	C1B-C2B	2.64	1.49	1.43
22	b	814	CLA	C1B-C2B	2.63	1.49	1.43
22	2	314	CLA	C1B-C2B	2.63	1.49	1.43
22	l	203	CLA	C1B-C2B	2.63	1.49	1.43
22	9	314	CLA	C1B-C2B	2.63	1.49	1.43
22	b	810	CLA	C1B-C2B	2.63	1.49	1.43
21	3	306	A1L1G	C40-C39	-2.62	1.40	1.46
22	1	312	CLA	C1B-C2B	2.62	1.49	1.43
22	b	818	CLA	C1B-C2B	2.62	1.49	1.43
21	3	306	A1L1G	C33-C34	-2.62	1.40	1.46
22	8	310	CLA	C1B-C2B	2.62	1.49	1.43
22	1	310	CLA	C1B-C2B	2.62	1.49	1.43
22	5	308	CLA	C1B-C2B	2.61	1.49	1.43
22	b	828	CLA	C1B-C2B	2.61	1.49	1.43
22	7	311	CLA	C1B-C2B	2.61	1.49	1.43
22	a	833	CLA	C1B-C2B	2.61	1.49	1.43
22	a	831	CLA	CMB-C2B	-2.61	1.45	1.50
22	b	824	CLA	C1B-C2B	2.60	1.49	1.43
22	b	838	CLA	C1B-C2B	2.60	1.49	1.43
22	b	825	CLA	C1B-C2B	2.60	1.49	1.43
22	7	313	CLA	C1B-C2B	2.59	1.49	1.43
22	a	822	CLA	C1B-C2B	2.59	1.49	1.43
22	b	819	CLA	C1B-C2B	2.57	1.49	1.43
22	b	834	CLA	C1B-C2B	2.57	1.49	1.43
22	a	841	CLA	C1B-C2B	2.57	1.49	1.43
22	9	309	CLA	C1B-C2B	2.56	1.49	1.43
21	7	302	A1L1G	C33-C34	-2.56	1.40	1.46
21	3	302	A1L1G	C33-C34	-2.54	1.40	1.46
22	4	313	CLA	C3B-C4B	2.54	1.50	1.42
22	9	314	CLA	C3B-C4B	2.54	1.50	1.42
21	9	306	A1L1G	C33-C34	-2.54	1.40	1.46
22	b	830	CLA	C1B-C2B	2.53	1.49	1.43
22	a	806	CLA	CMD-C2D	-2.52	1.45	1.50
22	a	818	CLA	C1B-C2B	2.52	1.49	1.43
22	a	831	CLA	C1B-C2B	2.51	1.49	1.43
22	b	829	CLA	CMD-C2D	-2.50	1.45	1.50
22	3	315	CLA	C3B-C4B	2.49	1.50	1.42
22	4	313	CLA	CHC-C1C	2.49	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	315	CLA	C3B-C4B	2.49	1.50	1.42
21	5	303	A1L1G	C40-C39	-2.48	1.40	1.46
22	4	313	CLA	C1B-C2B	2.48	1.48	1.43
22	b	814	CLA	C3B-C4B	2.47	1.49	1.42
24	1	304	A1L1F	O15-C20	-2.47	1.43	1.46
21	9	306	A1L1G	C40-C39	-2.47	1.40	1.46
22	a	806	CLA	CMC-C2C	-2.46	1.45	1.50
22	a	820	CLA	C1B-C2B	2.46	1.48	1.43
22	a	830	CLA	CMC-C2C	-2.46	1.45	1.50
22	5	313	CLA	C3B-C4B	2.46	1.49	1.42
22	a	841	CLA	C3B-C4B	2.46	1.49	1.42
22	a	813	CLA	C3B-C4B	2.46	1.49	1.42
22	a	802	CLA	C1B-C2B	2.46	1.48	1.43
22	7	313	CLA	C3B-C4B	2.46	1.49	1.42
22	a	801	CLA	CMD-C2D	-2.46	1.45	1.50
22	b	829	CLA	C1B-C2B	2.45	1.48	1.43
22	9	311	CLA	C3B-C4B	2.45	1.49	1.42
22	a	803	CLA	C1B-C2B	2.45	1.48	1.43
22	2	307	CLA	C1B-C2B	2.45	1.48	1.43
22	b	804	CLA	C3B-C4B	2.45	1.49	1.42
21	3	302	A1L1G	C40-C39	-2.44	1.40	1.46
22	a	827	CLA	C3B-C4B	2.44	1.49	1.42
22	a	842	CLA	C3B-C4B	2.44	1.49	1.42
22	2	314	CLA	C3B-C4B	2.44	1.49	1.42
22	a	822	CLA	C3B-C4B	2.44	1.49	1.42
21	7	302	A1L1G	C40-C39	-2.43	1.40	1.46
21	1	301	A1L1G	C33-C34	-2.43	1.40	1.46
22	4	307	CLA	C3B-C4B	2.43	1.49	1.42
22	a	829	CLA	C3B-C4B	2.43	1.49	1.42
22	5	306	CLA	C3B-C4B	2.43	1.49	1.42
22	2	311	CLA	C3B-C4B	2.43	1.49	1.42
22	b	806	CLA	C3B-C4B	2.43	1.49	1.42
22	b	809	CLA	C3B-C4B	2.43	1.49	1.42
20	4	301	XAT	O24-C25	-2.43	1.43	1.46
22	9	318	CLA	C3B-C4B	2.42	1.49	1.42
22	b	816	CLA	C3B-C4B	2.42	1.49	1.42
25	a	846	LHG	O8-C6	-2.42	1.39	1.45
22	b	813	CLA	C3B-C4B	2.42	1.49	1.42
22	a	840	CLA	C3B-C4B	2.42	1.49	1.42
22	a	802	CLA	CHC-C1C	2.42	1.43	1.38
22	b	838	CLA	CHC-C1C	2.42	1.43	1.38
22	a	819	CLA	C3B-C4B	2.42	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	f	803	CLA	C3B-C4B	2.41	1.49	1.42
20	3	305	XAT	O4-C5	-2.41	1.43	1.46
22	a	814	CLA	C3B-C4B	2.41	1.49	1.42
22	b	837	CLA	C3B-C4B	2.41	1.49	1.42
22	b	835	CLA	C3B-C4B	2.41	1.49	1.42
22	b	834	CLA	C3B-C4B	2.41	1.49	1.42
22	a	802	CLA	C3B-C4B	2.41	1.49	1.42
22	b	817	CLA	C1B-C2B	2.41	1.48	1.43
22	a	817	CLA	C3B-C4B	2.41	1.49	1.42
25	b	847	LHG	O8-C6	-2.40	1.39	1.45
22	7	313	CLA	CHC-C1C	2.40	1.43	1.38
22	5	312	CLA	C3B-C4B	2.40	1.49	1.42
22	a	816	CLA	C3B-C4B	2.40	1.49	1.42
22	2	308	CLA	C3B-C4B	2.40	1.49	1.42
22	b	828	CLA	C3B-C4B	2.40	1.49	1.42
22	a	804	CLA	C3B-C4B	2.40	1.49	1.42
25	a	846	LHG	O7-C5	-2.40	1.41	1.46
22	b	816	CLA	CHC-C1C	2.40	1.43	1.38
22	8	313	CLA	C3B-C4B	2.40	1.49	1.42
22	9	309	CLA	C3B-C4B	2.40	1.49	1.42
22	2	315	CLA	C3B-C4B	2.39	1.49	1.42
25	a	845	LHG	O8-C6	-2.39	1.39	1.45
22	4	312	CLA	CHC-C1C	2.39	1.43	1.38
22	a	828	CLA	C3B-C4B	2.39	1.49	1.42
22	2	308	CLA	CHC-C1C	2.39	1.43	1.38
22	5	305	CLA	C3B-C4B	2.39	1.49	1.42
22	a	833	CLA	C3B-C4B	2.39	1.49	1.42
22	a	808	CLA	C3B-C4B	2.39	1.49	1.42
22	4	306	CLA	C3B-C4B	2.39	1.49	1.42
25	9	317	LHG	O8-C6	-2.39	1.39	1.45
22	8	311	CLA	CHC-C1C	2.39	1.43	1.38
22	b	802	CLA	C3B-C4B	2.39	1.49	1.42
22	b	836	CLA	CHC-C1C	2.39	1.43	1.38
22	j	103	CLA	C3B-C4B	2.39	1.49	1.42
22	4	316	CLA	C3B-C4B	2.38	1.49	1.42
22	a	837	CLA	C3B-C4B	2.38	1.49	1.42
22	a	809	CLA	C3B-C4B	2.38	1.49	1.42
22	b	831	CLA	C3B-C4B	2.38	1.49	1.42
22	a	805	CLA	C3B-C4B	2.38	1.49	1.42
22	b	821	CLA	C3B-C4B	2.38	1.49	1.42
22	b	804	CLA	C1B-C2B	2.38	1.48	1.43
22	a	844	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	315	CLA	C3B-C4B	2.38	1.49	1.42
22	4	308	CLA	C3B-C4B	2.38	1.49	1.42
22	b	833	CLA	C3B-C4B	2.38	1.49	1.42
22	7	317	CLA	C3B-C4B	2.38	1.49	1.42
22	b	825	CLA	C3B-C4B	2.38	1.49	1.42
22	8	312	CLA	C3B-C4B	2.38	1.49	1.42
22	2	316	CLA	C3B-C4B	2.38	1.49	1.42
22	1	309	CLA	C3B-C4B	2.38	1.49	1.42
22	a	801	CLA	CMB-C2B	-2.38	1.45	1.50
22	8	311	CLA	C3B-C4B	2.38	1.49	1.42
22	b	814	CLA	CHC-C1C	2.38	1.43	1.38
22	9	310	CLA	C3B-C4B	2.37	1.49	1.42
25	b	847	LHG	O7-C5	-2.37	1.41	1.46
22	4	312	CLA	C3B-C4B	2.37	1.49	1.42
22	7	306	CLA	C3B-C4B	2.37	1.49	1.42
22	8	312	CLA	CHC-C1C	2.37	1.43	1.38
22	8	314	CLA	C3B-C4B	2.37	1.49	1.42
22	a	826	CLA	C3B-C4B	2.37	1.49	1.42
22	a	818	CLA	CHC-C1C	2.37	1.43	1.38
22	5	307	CLA	C3B-C4B	2.37	1.49	1.42
22	7	311	CLA	CHC-C1C	2.37	1.43	1.38
22	a	806	CLA	CMB-C2B	-2.37	1.45	1.50
22	2	306	CLA	C3B-C4B	2.37	1.49	1.42
22	a	822	CLA	CHC-C1C	2.37	1.43	1.38
22	7	312	CLA	C3B-C4B	2.37	1.49	1.42
22	b	805	CLA	C3B-C4B	2.37	1.49	1.42
22	a	825	CLA	C3B-C4B	2.37	1.49	1.42
22	5	311	CLA	C3B-C4B	2.37	1.49	1.42
22	a	813	CLA	CHC-C1C	2.37	1.43	1.38
22	5	309	CLA	C3B-C4B	2.37	1.49	1.42
22	7	311	CLA	C3B-C4B	2.37	1.49	1.42
22	5	314	CLA	C3B-C4B	2.37	1.49	1.42
22	b	838	CLA	C3B-C4B	2.37	1.49	1.42
22	2	313	CLA	C3B-C4B	2.37	1.49	1.42
22	9	308	CLA	C3B-C4B	2.36	1.49	1.42
22	h	205	CLA	C3B-C4B	2.36	1.49	1.42
22	a	829	CLA	CHC-C1C	2.36	1.43	1.38
22	a	854	CLA	C3B-C4B	2.36	1.49	1.42
22	a	811	CLA	C3B-C4B	2.36	1.49	1.42
22	h	203	CLA	C3B-C4B	2.36	1.49	1.42
22	a	819	CLA	CHC-C1C	2.36	1.43	1.38
22	f	802	CLA	C3B-C4B	2.36	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	l	203	CLA	C3B-C4B	2.36	1.49	1.42
22	a	835	CLA	C3B-C4B	2.36	1.49	1.42
25	9	307	LHG	O8-C6	-2.36	1.39	1.45
22	7	307	CLA	C3B-C4B	2.36	1.49	1.42
22	b	815	CLA	C3B-C4B	2.36	1.49	1.42
22	3	313	CLA	C3B-C4B	2.36	1.49	1.42
22	2	309	CLA	C3B-C4B	2.36	1.49	1.42
22	l	204	CLA	C3B-C4B	2.36	1.49	1.42
22	9	308	CLA	CHC-C1C	2.36	1.43	1.38
22	a	824	CLA	C3B-C4B	2.36	1.49	1.42
20	5	302	XAT	O4-C5	-2.36	1.43	1.46
21	3	302	A1L1G	C29-C30	-2.36	1.40	1.45
22	a	820	CLA	C3B-C4B	2.36	1.49	1.42
22	3	312	CLA	C3B-C4B	2.36	1.49	1.42
22	4	314	CLA	C3B-C4B	2.36	1.49	1.42
22	3	315	CLA	CHC-C1C	2.36	1.43	1.38
22	a	839	CLA	C3B-C4B	2.36	1.49	1.42
22	b	836	CLA	C3B-C4B	2.36	1.49	1.42
22	4	311	CLA	CMD-C2D	-2.36	1.45	1.50
22	5	308	CLA	C3B-C4B	2.36	1.49	1.42
22	j	102	CLA	C3B-C4B	2.35	1.49	1.42
22	b	811	CLA	CHC-C1C	2.35	1.43	1.38
22	4	311	CLA	C3B-C4B	2.35	1.49	1.42
22	4	317	CLA	C3B-C4B	2.35	1.49	1.42
22	8	305	CLA	C3B-C4B	2.35	1.49	1.42
22	a	823	CLA	C3B-C4B	2.35	1.49	1.42
22	5	310	CLA	C3B-C4B	2.35	1.49	1.42
22	b	817	CLA	C3B-C4B	2.35	1.49	1.42
22	b	807	CLA	C3B-C4B	2.35	1.49	1.42
22	b	832	CLA	C3B-C4B	2.35	1.49	1.42
22	8	307	CLA	C3B-C4B	2.35	1.49	1.42
20	4	304	XAT	O24-C25	-2.35	1.43	1.46
22	a	841	CLA	CHC-C1C	2.35	1.43	1.38
22	b	824	CLA	C3B-C4B	2.35	1.49	1.42
22	l	314	CLA	C3B-C4B	2.35	1.49	1.42
22	a	815	CLA	C3B-C4B	2.35	1.49	1.42
25	9	317	LHG	O8-C23	2.35	1.40	1.33
22	f	803	CLA	CHC-C1C	2.35	1.43	1.38
22	7	308	CLA	CHC-C1C	2.35	1.43	1.38
22	2	307	CLA	C3B-C4B	2.34	1.49	1.42
22	9	318	CLA	CHC-C1C	2.34	1.43	1.38
22	3	307	CLA	C3B-C4B	2.34	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	835	CLA	CHC-C1C	2.34	1.43	1.38
22	b	813	CLA	CHC-C1C	2.34	1.43	1.38
22	8	308	CLA	C3B-C4B	2.34	1.49	1.42
22	1	310	CLA	C3B-C4B	2.34	1.49	1.42
22	1	313	CLA	C3B-C4B	2.34	1.49	1.42
22	b	828	CLA	CHC-C1C	2.34	1.43	1.38
22	a	837	CLA	CHC-C1C	2.34	1.43	1.38
22	b	806	CLA	CHC-C1C	2.34	1.43	1.38
22	8	310	CLA	C3B-C4B	2.34	1.49	1.42
22	7	308	CLA	C3B-C4B	2.34	1.49	1.42
20	9	305	XAT	O4-C5	-2.34	1.43	1.46
22	b	802	CLA	CHC-C1C	2.34	1.43	1.38
22	5	312	CLA	CHC-C1C	2.34	1.43	1.38
20	1	302	XAT	O4-C5	-2.34	1.43	1.46
22	9	311	CLA	CHC-C1C	2.34	1.43	1.38
22	8	313	CLA	CHC-C1C	2.34	1.43	1.38
22	3	309	CLA	C3B-C4B	2.34	1.49	1.42
22	b	831	CLA	CHC-C1C	2.34	1.43	1.38
22	8	309	CLA	C3B-C4B	2.34	1.49	1.42
22	a	804	CLA	CHC-C1C	2.34	1.43	1.38
22	a	820	CLA	CHC-C1C	2.34	1.43	1.38
22	a	809	CLA	CHC-C1C	2.33	1.43	1.38
22	7	310	CLA	C3B-C4B	2.33	1.49	1.42
20	7	301	XAT	O24-C25	-2.33	1.43	1.46
22	7	306	CLA	CHC-C1C	2.33	1.43	1.38
22	9	312	CLA	C3B-C4B	2.33	1.49	1.42
22	5	314	CLA	CHC-C1C	2.33	1.43	1.38
22	5	315	CLA	CHC-C1C	2.33	1.43	1.38
22	3	311	CLA	C3B-C4B	2.33	1.49	1.42
22	1	311	CLA	CHC-C1C	2.33	1.43	1.38
22	1	308	CLA	C3B-C4B	2.33	1.49	1.42
22	9	315	CLA	C3B-C4B	2.33	1.49	1.42
22	4	310	CLA	C3B-C4B	2.33	1.49	1.42
22	b	822	CLA	C3B-C4B	2.33	1.49	1.42
22	1	314	CLA	CHC-C1C	2.33	1.43	1.38
22	2	309	CLA	CHC-C1C	2.33	1.43	1.38
22	b	839	CLA	C3B-C4B	2.33	1.49	1.42
22	a	836	CLA	C3B-C4B	2.33	1.49	1.42
22	a	832	CLA	CHC-C1C	2.33	1.43	1.38
25	b	847	LHG	O8-C23	2.33	1.40	1.33
22	3	308	CLA	C3B-C4B	2.33	1.49	1.42
22	3	310	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	307	LHG	O8-C23	2.32	1.40	1.33
22	b	832	CLA	CHC-C1C	2.32	1.43	1.38
22	9	308	CLA	CMC-C2C	-2.32	1.46	1.50
22	8	305	CLA	CHC-C1C	2.32	1.43	1.38
22	a	834	CLA	C3B-C4B	2.32	1.49	1.42
22	b	805	CLA	CHC-C1C	2.32	1.43	1.38
22	b	815	CLA	CHC-C1C	2.32	1.43	1.38
22	1	308	CLA	CHC-C1C	2.32	1.43	1.38
22	1	311	CLA	C3B-C4B	2.32	1.49	1.42
22	2	312	CLA	C3B-C4B	2.32	1.49	1.42
24	8	304	A1L1F	O15-C20	-2.32	1.43	1.46
22	a	806	CLA	C1D-ND	2.32	1.40	1.37
22	a	812	CLA	C3B-C4B	2.32	1.49	1.42
25	9	307	LHG	O7-C7	2.32	1.40	1.34
22	b	801	CLA	C3B-C4B	2.32	1.49	1.42
22	b	833	CLA	CHC-C1C	2.32	1.43	1.38
25	a	845	LHG	O7-C5	-2.32	1.41	1.46
22	5	311	CLA	CHC-C1C	2.31	1.43	1.38
22	1	202	CLA	C3B-C4B	2.31	1.49	1.42
22	2	315	CLA	CHC-C1C	2.31	1.43	1.38
22	7	312	CLA	CHC-C1C	2.31	1.43	1.38
25	9	317	LHG	O7-C5	-2.31	1.41	1.46
22	2	310	CLA	C3B-C4B	2.31	1.49	1.42
20	2	302	XAT	O4-C5	-2.31	1.43	1.46
20	2	303	XAT	O4-C5	-2.31	1.43	1.46
22	b	834	CLA	CHC-C1C	2.31	1.43	1.38
21	1	301	A1L1G	C40-C39	-2.31	1.41	1.46
22	b	817	CLA	CHC-C1C	2.31	1.43	1.38
22	4	309	CLA	C3B-C4B	2.31	1.49	1.42
22	1	312	CLA	CHC-C1C	2.31	1.43	1.38
25	a	845	LHG	O7-C7	2.31	1.40	1.34
22	a	832	CLA	C3B-C4B	2.31	1.49	1.42
22	1	310	CLA	CHC-C1C	2.31	1.43	1.38
22	1	307	CLA	C3B-C4B	2.31	1.49	1.42
22	a	821	CLA	C3B-C4B	2.31	1.49	1.42
22	7	314	CLA	CHC-C1C	2.31	1.43	1.38
22	7	314	CLA	C3B-C4B	2.31	1.49	1.42
22	5	313	CLA	CHC-C1C	2.31	1.43	1.38
22	8	309	CLA	CHC-C1C	2.30	1.43	1.38
20	3	304	XAT	O4-C5	-2.30	1.43	1.46
22	a	808	CLA	CHC-C1C	2.30	1.43	1.38
22	a	826	CLA	CHC-C1C	2.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	830	CLA	C3B-C4B	2.30	1.49	1.42
22	b	809	CLA	CMD-C2D	-2.30	1.46	1.50
22	a	824	CLA	CHC-C1C	2.30	1.43	1.38
22	a	833	CLA	CHC-C1C	2.30	1.43	1.38
20	a	852	XAT	O4-C5	-2.30	1.43	1.46
22	7	315	CLA	C3B-C4B	2.30	1.49	1.42
22	9	313	CLA	C3B-C4B	2.30	1.49	1.42
22	a	827	CLA	CHC-C1C	2.30	1.43	1.38
22	a	842	CLA	CHC-C1C	2.30	1.43	1.38
22	2	313	CLA	CHC-C1C	2.30	1.43	1.38
22	8	306	CLA	CHC-C1C	2.30	1.43	1.38
22	8	314	CLA	CHC-C1C	2.30	1.43	1.38
22	2	311	CLA	CHC-C1C	2.30	1.43	1.38
22	a	844	CLA	CHC-C1C	2.30	1.43	1.38
22	8	306	CLA	C3B-C4B	2.30	1.49	1.42
22	b	822	CLA	CMD-C2D	-2.29	1.46	1.50
22	4	314	CLA	CHC-C1C	2.29	1.43	1.38
22	b	825	CLA	CHC-C1C	2.29	1.43	1.38
22	b	809	CLA	CHC-C1C	2.29	1.43	1.38
22	b	830	CLA	C3B-C4B	2.29	1.49	1.42
22	h	205	CLA	CHC-C1C	2.29	1.43	1.38
22	b	817	CLA	MG-NB	-2.29	2.01	2.05
20	5	301	XAT	O4-C5	-2.29	1.43	1.46
22	b	812	CLA	C3B-C4B	2.29	1.49	1.42
22	f	802	CLA	CHC-C1C	2.29	1.43	1.38
25	9	307	LHG	O7-C5	-2.29	1.41	1.46
22	b	827	CLA	CHC-C1C	2.29	1.43	1.38
20	9	304	XAT	O4-C5	-2.29	1.43	1.46
20	8	303	XAT	O4-C5	-2.29	1.43	1.46
22	a	854	CLA	CHC-C1C	2.29	1.43	1.38
22	1	306	CLA	C3B-C4B	2.29	1.49	1.42
22	9	312	CLA	CHC-C1C	2.29	1.43	1.38
22	2	310	CLA	CHC-C1C	2.29	1.43	1.38
25	9	317	LHG	O7-C7	2.29	1.40	1.34
22	3	312	CLA	CHC-C1C	2.28	1.43	1.38
22	a	811	CLA	CHC-C1C	2.28	1.43	1.38
22	b	823	CLA	CHC-C1C	2.28	1.43	1.38
22	5	306	CLA	CHC-C1C	2.28	1.43	1.38
22	4	315	CLA	CHC-C1C	2.28	1.43	1.38
22	a	803	CLA	CHC-C1C	2.28	1.43	1.38
22	b	807	CLA	CHC-C1C	2.28	1.43	1.38
22	b	820	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	827	CLA	C3B-C4B	2.28	1.49	1.42
22	7	310	CLA	CHC-C1C	2.28	1.43	1.38
22	3	314	CLA	C3B-C4B	2.28	1.49	1.42
20	7	305	XAT	O4-C5	-2.28	1.43	1.46
22	a	838	CLA	C3B-C4B	2.28	1.49	1.42
25	a	846	LHG	O7-C7	2.28	1.40	1.34
22	9	314	CLA	CHC-C1C	2.28	1.43	1.38
22	a	828	CLA	CHC-C1C	2.28	1.43	1.38
22	b	812	CLA	CHC-C1C	2.28	1.43	1.38
22	a	823	CLA	CHC-C1C	2.28	1.43	1.38
22	3	311	CLA	CHC-C1C	2.28	1.43	1.38
22	b	819	CLA	CMB-C2B	-2.28	1.46	1.50
22	9	316	CLA	C3B-C4B	2.28	1.49	1.42
22	8	310	CLA	CHC-C1C	2.28	1.43	1.38
22	2	316	CLA	CHC-C1C	2.28	1.43	1.38
22	a	814	CLA	CHC-C1C	2.28	1.43	1.38
22	a	816	CLA	CHC-C1C	2.28	1.43	1.38
25	a	845	LHG	O8-C23	2.28	1.40	1.33
22	b	818	CLA	C3B-C4B	2.28	1.49	1.42
22	b	819	CLA	C3B-C4B	2.28	1.49	1.42
20	3	301	XAT	O24-C25	-2.27	1.43	1.46
22	1	309	CLA	CHC-C1C	2.27	1.43	1.38
22	9	309	CLA	CHC-C1C	2.27	1.43	1.38
22	3	309	CLA	CHC-C1C	2.27	1.43	1.38
22	1	202	CLA	CHC-C1C	2.27	1.43	1.38
22	5	309	CLA	CHC-C1C	2.27	1.43	1.38
22	4	310	CLA	CHC-C1C	2.27	1.43	1.38
22	7	309	CLA	C3B-C4B	2.27	1.49	1.42
22	2	312	CLA	CHC-C1C	2.27	1.43	1.38
22	7	315	CLA	CHC-C1C	2.27	1.43	1.38
20	4	305	XAT	O4-C5	-2.27	1.43	1.46
20	7	303	XAT	O4-C5	-2.27	1.43	1.46
22	4	309	CLA	CHC-C1C	2.27	1.43	1.38
22	3	313	CLA	CHC-C1C	2.27	1.43	1.38
22	b	830	CLA	MG-NB	-2.27	2.01	2.05
22	b	830	CLA	CMD-C2D	-2.27	1.46	1.50
20	1	303	XAT	O4-C5	-2.27	1.43	1.46
22	7	316	CLA	C3B-C4B	2.27	1.49	1.42
22	b	808	CLA	C3B-C4B	2.27	1.49	1.42
22	5	307	CLA	CHC-C1C	2.27	1.43	1.38
22	9	310	CLA	CHC-C1C	2.27	1.43	1.38
22	4	308	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	305	CLA	CHC-C1C	2.27	1.43	1.38
22	a	810	CLA	C3B-C4B	2.27	1.49	1.42
22	b	822	CLA	CHC-C1C	2.27	1.43	1.38
20	2	305	XAT	O4-C5	-2.26	1.43	1.46
22	b	826	CLA	C3B-C4B	2.26	1.49	1.42
20	3	304	XAT	O24-C25	-2.26	1.43	1.46
22	a	805	CLA	CHC-C1C	2.26	1.43	1.38
22	a	840	CLA	CHC-C1C	2.26	1.43	1.38
22	b	837	CLA	CHC-C1C	2.26	1.43	1.38
20	4	301	XAT	O4-C5	-2.26	1.43	1.46
22	l	204	CLA	CHC-C1C	2.26	1.43	1.38
22	a	830	CLA	CHC-C1C	2.26	1.43	1.38
22	1	305	CLA	C3B-C4B	2.26	1.49	1.42
22	l	203	CLA	CHC-C1C	2.26	1.43	1.38
22	9	313	CLA	CHC-C1C	2.26	1.43	1.38
22	7	309	CLA	CHC-C1C	2.26	1.43	1.38
22	a	836	CLA	CHC-C1C	2.26	1.43	1.38
22	9	315	CLA	CHC-C1C	2.26	1.43	1.38
22	2	307	CLA	CMB-C2B	-2.26	1.46	1.50
22	7	307	CLA	CHC-C1C	2.26	1.43	1.38
25	a	846	LHG	O8-C23	2.26	1.39	1.33
22	b	830	CLA	CHC-C1C	2.26	1.43	1.38
22	5	310	CLA	CHC-C1C	2.25	1.43	1.38
22	a	834	CLA	CHC-C1C	2.25	1.43	1.38
22	b	810	CLA	CMB-C2B	-2.25	1.46	1.50
21	9	301	A1L1G	C40-C39	-2.25	1.41	1.46
22	b	801	CLA	CMB-C2B	-2.25	1.46	1.50
24	1	304	A1L1F	C6-C1	-2.25	1.50	1.54
22	b	804	CLA	CHC-C1C	2.25	1.43	1.38
22	1	307	CLA	CHC-C1C	2.25	1.43	1.38
22	b	823	CLA	CMD-C2D	-2.25	1.46	1.50
22	j	102	CLA	CHC-C1C	2.25	1.43	1.38
22	4	317	CLA	CHC-C1C	2.25	1.43	1.38
20	a	852	XAT	O24-C25	-2.25	1.43	1.46
22	4	307	CLA	CHC-C1C	2.25	1.43	1.38
22	a	815	CLA	CHC-C1C	2.25	1.43	1.38
22	a	830	CLA	CMD-C2D	-2.25	1.46	1.50
20	5	302	XAT	O24-C25	-2.25	1.43	1.46
20	j	101	XAT	O4-C5	-2.25	1.43	1.46
22	b	840	CLA	CHC-C1C	2.25	1.43	1.38
22	a	817	CLA	CHC-C1C	2.24	1.43	1.38
22	b	824	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	821	CLA	CHC-C1C	2.24	1.43	1.38
20	2	301	XAT	O4-C5	-2.24	1.43	1.46
22	a	839	CLA	CHC-C1C	2.24	1.43	1.38
22	4	311	CLA	CHC-C1C	2.24	1.43	1.38
20	3	303	XAT	O4-C5	-2.24	1.43	1.46
22	3	307	CLA	CHC-C1C	2.24	1.43	1.38
22	a	812	CLA	CHC-C1C	2.24	1.43	1.38
25	b	847	LHG	O7-C7	2.24	1.40	1.34
22	2	314	CLA	CHC-C1C	2.24	1.43	1.38
22	b	803	CLA	C3B-C4B	2.24	1.49	1.42
22	1	313	CLA	CHC-C1C	2.24	1.43	1.38
22	2	310	CLA	MG-NB	-2.24	2.01	2.05
22	3	307	CLA	CMD-C2D	-2.24	1.46	1.50
22	a	807	CLA	C3B-C4B	2.24	1.49	1.42
20	7	304	XAT	O4-C5	-2.24	1.43	1.46
22	a	801	CLA	CMC-C2C	-2.23	1.46	1.50
22	a	838	CLA	CHC-C1C	2.23	1.43	1.38
20	4	304	XAT	O4-C5	-2.23	1.43	1.46
22	a	803	CLA	C3B-C4B	2.23	1.49	1.42
22	b	823	CLA	C3B-C4B	2.23	1.49	1.42
22	5	308	CLA	CHC-C1C	2.23	1.43	1.38
20	8	301	XAT	O4-C5	-2.23	1.43	1.46
22	a	833	CLA	MG-NB	-2.23	2.01	2.05
22	a	835	CLA	CHC-C1C	2.23	1.42	1.38
20	8	302	XAT	O4-C5	-2.23	1.43	1.46
20	4	303	XAT	O4-C5	-2.23	1.43	1.46
22	b	839	CLA	CMB-C2B	-2.23	1.46	1.50
21	1	301	A1L1G	C38-C39	2.23	1.40	1.35
22	5	305	CLA	CMD-C2D	-2.23	1.46	1.50
22	a	824	CLA	CMD-C2D	-2.23	1.46	1.50
22	3	310	CLA	CHC-C1C	2.22	1.42	1.38
22	a	831	CLA	C3B-C4B	2.22	1.49	1.42
20	2	304	XAT	O4-C5	-2.22	1.43	1.46
22	b	820	CLA	CHC-C1C	2.22	1.42	1.38
21	9	301	A1L1G	C29-C30	-2.22	1.40	1.45
20	3	301	XAT	O4-C5	-2.22	1.43	1.46
20	7	304	XAT	O24-C25	-2.22	1.43	1.46
22	b	803	CLA	CHC-C1C	2.22	1.42	1.38
22	a	828	CLA	CMC-C2C	-2.22	1.46	1.50
22	a	810	CLA	CMD-C2D	-2.22	1.46	1.50
22	7	317	CLA	CHC-C1C	2.22	1.42	1.38
22	2	306	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	810	CLA	CHC-C1C	2.22	1.42	1.38
22	1	306	CLA	CHC-C1C	2.22	1.42	1.38
22	a	836	CLA	CMB-C2B	-2.22	1.46	1.50
22	7	314	CLA	CMD-C2D	-2.22	1.46	1.50
22	a	832	CLA	MG-NB	-2.21	2.01	2.05
22	h	203	CLA	CHC-C1C	2.21	1.42	1.38
22	b	840	CLA	C3B-C4B	2.21	1.49	1.42
22	b	803	CLA	CMD-C2D	-2.21	1.46	1.50
20	9	305	XAT	O24-C25	-2.21	1.43	1.46
22	4	311	CLA	CMB-C2B	-2.21	1.46	1.50
22	8	308	CLA	CHC-C1C	2.21	1.42	1.38
22	8	307	CLA	CHC-C1C	2.21	1.42	1.38
22	a	821	CLA	CHC-C1C	2.20	1.42	1.38
22	5	305	CLA	CHC-C1C	2.20	1.42	1.38
22	3	314	CLA	CHC-C1C	2.20	1.42	1.38
22	7	316	CLA	CMD-C2D	-2.20	1.46	1.50
22	b	810	CLA	C3B-C4B	2.20	1.49	1.42
22	b	829	CLA	C3B-C4B	2.20	1.49	1.42
22	a	832	CLA	CMB-C2B	-2.20	1.46	1.50
22	b	801	CLA	CHC-C1C	2.20	1.42	1.38
20	2	302	XAT	O24-C25	-2.20	1.43	1.46
22	9	309	CLA	CMD-C2D	-2.20	1.46	1.50
22	2	310	CLA	CMB-C2B	-2.20	1.46	1.50
22	b	801	CLA	CMD-C2D	-2.20	1.46	1.50
22	b	830	CLA	CMB-C2B	-2.20	1.46	1.50
21	3	306	A1L1G	C29-C30	-2.19	1.40	1.45
22	b	819	CLA	CHC-C1C	2.19	1.42	1.38
22	a	806	CLA	CAA-C2A	-2.19	1.50	1.54
20	4	302	XAT	O24-C25	-2.19	1.43	1.46
20	4	303	XAT	O24-C25	-2.19	1.43	1.46
22	3	308	CLA	CHC-C1C	2.19	1.42	1.38
22	8	310	CLA	CMB-C2B	-2.19	1.46	1.50
22	a	820	CLA	CMB-C2B	-2.19	1.46	1.50
22	a	825	CLA	CHC-C1C	2.19	1.42	1.38
20	8	303	XAT	O24-C25	-2.19	1.43	1.46
22	b	838	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	811	CLA	CMD-C2D	-2.18	1.46	1.50
22	2	310	CLA	CMD-C2D	-2.18	1.46	1.50
22	b	823	CLA	MG-NB	-2.18	2.01	2.05
22	j	103	CLA	CHC-C1C	2.18	1.42	1.38
22	b	808	CLA	CHC-C1C	2.18	1.42	1.38
22	4	306	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	316	CLA	CHC-C1C	2.18	1.42	1.38
20	2	304	XAT	O24-C25	-2.18	1.43	1.46
20	5	304	XAT	O24-C25	-2.18	1.43	1.46
22	b	826	CLA	CHC-C1C	2.18	1.42	1.38
22	a	801	CLA	CHC-C1C	2.18	1.42	1.38
22	a	801	CLA	C3B-C4B	2.18	1.49	1.42
20	3	303	XAT	O24-C25	-2.17	1.43	1.46
22	9	309	CLA	MG-NB	-2.17	2.01	2.05
20	5	301	XAT	O24-C25	-2.17	1.43	1.46
22	9	316	CLA	CHC-C1C	2.17	1.42	1.38
22	a	807	CLA	CHC-C1C	2.17	1.42	1.38
21	1	301	A1L1G	C29-C30	-2.17	1.40	1.45
20	j	101	XAT	O24-C25	-2.17	1.43	1.46
20	8	302	XAT	O24-C25	-2.17	1.43	1.46
22	a	803	CLA	MG-NB	-2.17	2.01	2.05
22	b	804	CLA	MG-NB	-2.17	2.01	2.05
22	b	837	CLA	CMD-C2D	-2.16	1.46	1.50
22	b	819	CLA	MG-NB	-2.16	2.01	2.05
22	2	307	CLA	CHC-C1C	2.16	1.42	1.38
21	5	303	A1L1G	C29-C30	-2.16	1.40	1.45
22	b	814	CLA	CMD-C2D	-2.16	1.46	1.50
20	2	305	XAT	O24-C25	-2.16	1.43	1.46
22	a	831	CLA	MG-NB	-2.16	2.01	2.05
22	a	820	CLA	MG-NB	-2.16	2.01	2.05
22	a	806	CLA	C1B-NB	-2.15	1.35	1.37
22	7	316	CLA	CHC-C1C	2.15	1.42	1.38
22	a	807	CLA	CMD-C2D	-2.15	1.46	1.50
22	a	806	CLA	C4B-NB	2.15	1.40	1.37
20	5	304	XAT	O4-C5	-2.15	1.43	1.46
22	a	804	CLA	CMC-C2C	-2.15	1.46	1.50
22	b	824	CLA	MG-NB	-2.15	2.01	2.05
22	2	307	CLA	MG-NB	-2.15	2.01	2.05
22	b	817	CLA	CMB-C2B	-2.15	1.46	1.50
22	a	812	CLA	CMD-C2D	-2.15	1.46	1.50
20	1	302	XAT	O24-C25	-2.15	1.43	1.46
21	7	302	A1L1G	C38-C39	2.15	1.40	1.35
22	a	802	CLA	CMB-C2B	-2.15	1.46	1.50
22	b	829	CLA	MG-NB	-2.14	2.01	2.05
22	b	835	CLA	MG-NB	-2.14	2.01	2.05
22	8	310	CLA	MG-NB	-2.14	2.01	2.05
21	9	301	A1L1G	C38-C39	2.14	1.40	1.35
22	2	309	CLA	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	307	CLA	MG-NB	-2.14	2.01	2.05
22	5	312	CLA	MG-NB	-2.14	2.01	2.05
22	7	309	CLA	MG-NB	-2.14	2.01	2.05
22	a	842	CLA	CMD-C2D	-2.14	1.46	1.50
20	2	301	XAT	O24-C25	-2.14	1.43	1.46
22	b	834	CLA	CMB-C2B	-2.13	1.46	1.50
22	a	807	CLA	MG-NB	-2.13	2.01	2.05
22	b	822	CLA	MG-NB	-2.13	2.01	2.05
22	a	816	CLA	CMD-C2D	-2.13	1.46	1.50
21	9	306	A1L1G	C29-C30	-2.13	1.40	1.45
22	8	306	CLA	MG-NB	-2.13	2.01	2.05
22	b	828	CLA	CMD-C2D	-2.13	1.46	1.50
22	3	307	CLA	MG-NB	-2.13	2.01	2.05
22	a	832	CLA	CMD-C2D	-2.13	1.46	1.50
22	8	312	CLA	MG-NB	-2.13	2.01	2.05
22	9	312	CLA	CMD-C2D	-2.13	1.46	1.50
22	3	307	CLA	CMB-C2B	-2.13	1.46	1.50
22	a	801	CLA	MG-NB	-2.13	2.01	2.05
22	7	311	CLA	CMB-C2B	-2.13	1.46	1.50
20	8	301	XAT	O24-C25	-2.13	1.43	1.46
22	a	821	CLA	CMD-C2D	-2.13	1.46	1.50
22	b	818	CLA	CHC-C1C	2.13	1.42	1.38
21	1	301	A1L1G	C35-C34	2.13	1.40	1.35
22	a	824	CLA	CMB-C2B	-2.13	1.46	1.50
22	a	802	CLA	MG-NB	-2.13	2.01	2.05
20	9	304	XAT	O24-C25	-2.13	1.43	1.46
22	a	808	CLA	CMB-C2B	-2.13	1.46	1.50
22	a	822	CLA	MG-NB	-2.13	2.01	2.05
22	b	818	CLA	CMB-C2B	-2.13	1.46	1.50
22	9	309	CLA	CMB-C2B	-2.12	1.46	1.50
22	a	822	CLA	CMB-C2B	-2.12	1.46	1.50
22	a	816	CLA	MG-NB	-2.12	2.01	2.05
22	b	828	CLA	CMB-C2B	-2.12	1.46	1.50
20	2	303	XAT	O24-C25	-2.12	1.43	1.46
22	b	813	CLA	MG-NB	-2.12	2.01	2.05
25	9	317	LHG	P-O6	2.12	1.67	1.59
20	1	303	XAT	O24-C25	-2.12	1.43	1.46
22	b	825	CLA	CMD-C2D	-2.12	1.46	1.50
22	a	828	CLA	MG-NB	-2.12	2.01	2.05
22	8	308	CLA	MG-NB	-2.12	2.01	2.05
25	9	307	LHG	P-O6	2.12	1.67	1.59
20	9	303	XAT	O24-C25	-2.12	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	803	CLA	CMB-C2B	-2.12	1.46	1.50
25	a	845	LHG	P-O6	2.11	1.67	1.59
22	2	316	CLA	CMD-C2D	-2.11	1.46	1.50
20	7	303	XAT	O24-C25	-2.11	1.43	1.46
22	4	308	CLA	CMD-C2D	-2.11	1.46	1.50
22	3	309	CLA	CMD-C2D	-2.11	1.46	1.50
22	4	308	CLA	MG-NB	-2.11	2.01	2.05
22	8	313	CLA	CMD-C2D	-2.11	1.46	1.50
22	3	309	CLA	MG-NB	-2.11	2.01	2.05
20	4	302	XAT	O4-C5	-2.11	1.43	1.46
22	a	810	CLA	MG-NB	-2.11	2.01	2.05
22	4	309	CLA	MG-NB	-2.11	2.01	2.05
22	a	837	CLA	CMB-C2B	-2.11	1.46	1.50
22	b	809	CLA	CMC-C2C	-2.11	1.46	1.50
22	a	838	CLA	MG-NB	-2.11	2.01	2.05
22	b	832	CLA	MG-NB	-2.11	2.01	2.05
22	b	816	CLA	MG-NB	-2.11	2.01	2.05
22	1	313	CLA	MG-NB	-2.11	2.01	2.05
22	b	810	CLA	MG-NB	-2.11	2.01	2.05
22	7	310	CLA	MG-NB	-2.10	2.01	2.05
22	b	827	CLA	CMD-C2D	-2.10	1.46	1.50
25	b	847	LHG	P-O6	2.10	1.67	1.59
22	1	309	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	825	CLA	MG-NB	-2.10	2.01	2.05
22	b	838	CLA	MG-NB	-2.10	2.01	2.05
20	7	301	XAT	O4-C5	-2.10	1.43	1.46
22	7	311	CLA	CMD-C2D	-2.10	1.46	1.50
22	9	315	CLA	MG-NB	-2.10	2.01	2.05
22	b	826	CLA	MG-NB	-2.10	2.01	2.05
22	1	310	CLA	MG-NB	-2.10	2.01	2.05
22	2	306	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	810	CLA	CHC-C1C	2.10	1.42	1.38
22	b	820	CLA	CMD-C2D	-2.10	1.46	1.50
22	7	312	CLA	CMD-C2D	-2.10	1.46	1.50
22	5	308	CLA	MG-NB	-2.10	2.01	2.05
22	b	834	CLA	CMD-C2D	-2.09	1.46	1.50
22	j	102	CLA	CMD-C2D	-2.09	1.46	1.50
22	3	310	CLA	MG-NB	-2.09	2.01	2.05
22	b	815	CLA	CMC-C2C	-2.09	1.46	1.50
22	5	307	CLA	MG-NB	-2.09	2.01	2.05
22	3	315	CLA	CMD-C2D	-2.09	1.46	1.50
22	a	827	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	301	A1L1G	C35-C34	2.09	1.40	1.35
22	2	314	CLA	CMD-C2D	-2.09	1.46	1.50
22	b	802	CLA	CMD-C2D	-2.09	1.46	1.50
22	b	808	CLA	MG-NB	-2.09	2.01	2.05
20	9	305	XAT	C26-C27	2.09	1.54	1.50
22	a	826	CLA	CMD-C2D	-2.09	1.46	1.50
22	b	828	CLA	MG-NB	-2.09	2.01	2.05
22	4	317	CLA	CMB-C2B	-2.09	1.46	1.50
22	l	203	CLA	CMB-C2B	-2.09	1.46	1.50
22	7	316	CLA	MG-NB	-2.09	2.01	2.05
22	a	824	CLA	MG-NB	-2.09	2.01	2.05
22	3	314	CLA	CMD-C2D	-2.09	1.46	1.50
22	8	305	CLA	MG-NB	-2.08	2.01	2.05
22	5	308	CLA	CMD-C2D	-2.08	1.46	1.50
22	4	314	CLA	MG-NB	-2.08	2.01	2.05
22	a	834	CLA	CMD-C2D	-2.08	1.46	1.50
22	a	826	CLA	MG-NB	-2.08	2.01	2.05
22	b	827	CLA	MG-NB	-2.08	2.01	2.05
22	2	307	CLA	CMD-C2D	-2.08	1.46	1.50
22	1	313	CLA	CMD-C2D	-2.08	1.46	1.50
22	a	837	CLA	CMD-C2D	-2.08	1.46	1.50
22	l	202	CLA	MG-NB	-2.08	2.01	2.05
22	2	312	CLA	CMD-C2D	-2.08	1.46	1.50
21	9	306	A1L1G	C35-C34	2.08	1.40	1.35
22	a	823	CLA	MG-NB	-2.08	2.01	2.05
22	l	204	CLA	CMC-C2C	-2.08	1.46	1.50
22	a	818	CLA	CMB-C2B	-2.08	1.46	1.50
22	b	807	CLA	MG-NB	-2.08	2.01	2.05
22	9	308	CLA	MG-NB	-2.08	2.01	2.05
22	7	312	CLA	MG-NB	-2.08	2.01	2.05
22	2	312	CLA	MG-NB	-2.08	2.01	2.05
22	a	827	CLA	MG-NB	-2.08	2.01	2.05
22	8	307	CLA	MG-NB	-2.08	2.01	2.05
22	8	311	CLA	MG-NB	-2.08	2.01	2.05
22	9	313	CLA	MG-NB	-2.08	2.01	2.05
22	2	314	CLA	CMC-C2C	-2.08	1.46	1.50
22	9	318	CLA	CMD-C2D	-2.07	1.46	1.50
22	b	833	CLA	CMD-C2D	-2.07	1.46	1.50
22	b	811	CLA	MG-NB	-2.07	2.01	2.05
22	4	313	CLA	CMB-C2B	-2.07	1.46	1.50
22	8	310	CLA	CMD-C2D	-2.07	1.46	1.50
22	a	819	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	830	CLA	MG-NB	-2.07	2.01	2.05
22	4	311	CLA	MG-NB	-2.07	2.01	2.05
22	8	309	CLA	MG-NB	-2.07	2.01	2.05
22	1	309	CLA	CMB-C2B	-2.07	1.46	1.50
22	b	834	CLA	MG-NB	-2.07	2.01	2.05
22	4	306	CLA	CMD-C2D	-2.07	1.46	1.50
22	b	803	CLA	CMC-C2C	-2.07	1.46	1.50
22	1	203	CLA	MG-NB	-2.07	2.01	2.05
22	b	809	CLA	CMB-C2B	-2.07	1.46	1.50
21	3	302	A1L1G	C35-C34	2.07	1.40	1.35
22	b	840	CLA	MG-NB	-2.07	2.01	2.05
22	b	825	CLA	CMB-C2B	-2.07	1.46	1.50
22	1	307	CLA	CMB-C2B	-2.07	1.46	1.50
20	7	305	XAT	O24-C25	-2.07	1.43	1.46
26	b	848	DGD	C1E-C2E	2.07	1.58	1.52
22	5	310	CLA	CMD-C2D	-2.07	1.46	1.50
22	2	308	CLA	MG-NB	-2.07	2.01	2.05
22	a	811	CLA	MG-NB	-2.07	2.01	2.05
22	7	311	CLA	MG-NB	-2.06	2.01	2.05
22	a	803	CLA	CMD-C2D	-2.06	1.46	1.50
22	b	826	CLA	CMD-C2D	-2.06	1.46	1.50
22	h	203	CLA	CMD-C2D	-2.06	1.46	1.50
22	4	312	CLA	MG-NB	-2.06	2.01	2.05
22	3	313	CLA	MG-NB	-2.06	2.01	2.05
22	4	312	CLA	CMD-C2D	-2.06	1.46	1.50
22	a	835	CLA	MG-NB	-2.06	2.01	2.05
22	9	310	CLA	MG-NB	-2.06	2.01	2.05
22	b	805	CLA	CMD-C2D	-2.06	1.46	1.50
22	b	820	CLA	MG-NB	-2.06	2.01	2.05
22	9	314	CLA	CMD-C2D	-2.06	1.46	1.50
22	7	306	CLA	CMD-C2D	-2.06	1.46	1.50
22	b	807	CLA	CMD-C2D	-2.06	1.46	1.50
22	a	814	CLA	CMD-C2D	-2.06	1.46	1.50
22	5	311	CLA	MG-NB	-2.06	2.01	2.05
22	1	202	CLA	CMB-C2B	-2.06	1.46	1.50
22	b	832	CLA	CMD-C2D	-2.06	1.46	1.50
22	8	305	CLA	CMD-C2D	-2.06	1.46	1.50
22	7	315	CLA	CMD-C2D	-2.06	1.46	1.50
22	b	837	CLA	MG-NB	-2.06	2.01	2.05
22	1	204	CLA	MG-NB	-2.06	2.01	2.05
22	1	309	CLA	MG-NB	-2.06	2.01	2.05
22	b	804	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	310	CLA	CMD-C2D	-2.06	1.46	1.50
22	a	829	CLA	CMD-C2D	-2.06	1.46	1.50
22	l	203	CLA	CMC-C2C	-2.06	1.46	1.50
22	b	813	CLA	CMD-C2D	-2.06	1.46	1.50
22	5	312	CLA	CMB-C2B	-2.05	1.46	1.50
22	b	811	CLA	CMB-C2B	-2.05	1.46	1.50
22	b	812	CLA	CMD-C2D	-2.05	1.46	1.50
22	2	311	CLA	CMC-C2C	-2.05	1.46	1.50
22	7	307	CLA	CMB-C2B	-2.05	1.46	1.50
22	a	831	CLA	CHC-C1C	2.05	1.42	1.38
22	a	810	CLA	CMB-C2B	-2.05	1.46	1.50
22	b	838	CLA	CMB-C2B	-2.05	1.46	1.50
22	5	305	CLA	MG-NB	-2.05	2.01	2.05
22	2	311	CLA	CMD-C2D	-2.05	1.46	1.50
22	3	314	CLA	MG-NB	-2.05	2.01	2.05
22	a	825	CLA	MG-NB	-2.05	2.01	2.05
22	7	308	CLA	MG-NB	-2.05	2.01	2.05
22	a	806	CLA	MG-ND	-2.05	2.01	2.05
22	a	814	CLA	MG-NB	-2.05	2.01	2.05
22	4	310	CLA	CMD-C2D	-2.05	1.46	1.50
22	1	305	CLA	MG-NB	-2.05	2.01	2.05
22	b	815	CLA	CMD-C2D	-2.05	1.46	1.50
22	a	802	CLA	CMD-C2D	-2.05	1.46	1.50
22	7	315	CLA	MG-NB	-2.05	2.01	2.05
22	3	311	CLA	MG-NB	-2.05	2.01	2.05
22	b	815	CLA	MG-NB	-2.05	2.01	2.05
20	4	305	XAT	O24-C25	-2.05	1.43	1.46
22	a	841	CLA	CMC-C2C	-2.05	1.46	1.50
22	a	842	CLA	CMB-C2B	-2.05	1.46	1.50
22	b	819	CLA	CMD-C2D	-2.05	1.46	1.50
22	b	821	CLA	MG-NB	-2.05	2.01	2.05
25	a	846	LHG	P-O6	2.05	1.67	1.59
22	9	316	CLA	MG-NB	-2.05	2.01	2.05
22	7	313	CLA	MG-NB	-2.05	2.01	2.05
22	a	842	CLA	MG-NB	-2.05	2.01	2.05
20	3	305	XAT	O24-C25	-2.05	1.43	1.46
22	b	812	CLA	MG-NB	-2.04	2.01	2.05
22	b	831	CLA	MG-NB	-2.04	2.01	2.05
22	9	318	CLA	MG-NB	-2.04	2.01	2.05
22	b	806	CLA	MG-NB	-2.04	2.01	2.05
22	4	315	CLA	CMD-C2D	-2.04	1.46	1.50
22	3	312	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	805	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	835	CLA	CMD-C2D	-2.04	1.46	1.50
22	j	103	CLA	CMB-C2B	-2.04	1.46	1.50
22	a	854	CLA	MG-NB	-2.04	2.01	2.05
22	l	204	CLA	CMB-C2B	-2.04	1.46	1.50
22	1	306	CLA	MG-NB	-2.04	2.01	2.05
22	a	817	CLA	CMD-C2D	-2.04	1.46	1.50
22	1	314	CLA	CMB-C2B	-2.04	1.46	1.50
22	1	314	CLA	CMD-C2D	-2.04	1.46	1.50
22	4	314	CLA	CMD-C2D	-2.04	1.46	1.50
22	4	317	CLA	CMD-C2D	-2.04	1.46	1.50
22	3	311	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	804	CLA	CMC-C2C	-2.04	1.46	1.50
22	a	812	CLA	MG-NB	-2.04	2.01	2.05
22	8	308	CLA	CMB-C2B	-2.04	1.46	1.50
22	8	312	CLA	CMD-C2D	-2.04	1.46	1.50
22	7	309	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	819	CLA	CMC-C2C	-2.04	1.46	1.50
22	a	821	CLA	MG-NB	-2.04	2.01	2.05
22	2	309	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	823	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	828	CLA	CMD-C2D	-2.04	1.46	1.50
22	5	315	CLA	MG-NB	-2.04	2.01	2.05
22	2	315	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	812	CLA	CMB-C2B	-2.04	1.46	1.50
22	a	818	CLA	CMC-C2C	-2.04	1.46	1.50
21	3	306	A1L1G	C38-C39	2.04	1.40	1.35
22	a	835	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	835	CLA	CMD-C2D	-2.04	1.46	1.50
22	l	202	CLA	CMD-C2D	-2.04	1.46	1.50
22	4	314	CLA	CMB-C2B	-2.04	1.46	1.50
22	a	844	CLA	CMD-C2D	-2.04	1.46	1.50
22	8	308	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	808	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	844	CLA	MG-NB	-2.04	2.01	2.05
22	1	312	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	816	CLA	CMC-C2C	-2.04	1.46	1.50
22	f	803	CLA	CMB-C2B	-2.04	1.46	1.50
22	8	314	CLA	CMD-C2D	-2.03	1.46	1.50
22	a	817	CLA	CMB-C2B	-2.03	1.46	1.50
22	9	312	CLA	MG-NB	-2.03	2.01	2.05
22	7	314	CLA	MG-NB	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	818	CLA	MG-NB	-2.03	2.01	2.05
22	3	313	CLA	CMB-C2B	-2.03	1.46	1.50
22	f	802	CLA	CMD-C2D	-2.03	1.46	1.50
22	7	313	CLA	CMD-C2D	-2.03	1.46	1.50
22	7	317	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	836	CLA	MG-NB	-2.03	2.01	2.05
22	h	205	CLA	CMC-C2C	-2.03	1.46	1.50
22	a	834	CLA	CMB-C2B	-2.03	1.46	1.50
22	a	806	CLA	CHC-C1C	2.03	1.42	1.38
22	b	809	CLA	MG-NB	-2.03	2.01	2.05
22	3	308	CLA	CMD-C2D	-2.03	1.46	1.50
22	2	311	CLA	CMB-C2B	-2.03	1.46	1.50
22	1	310	CLA	CMB-C2B	-2.03	1.46	1.50
22	a	831	CLA	CMC-C2C	-2.03	1.46	1.50
22	b	810	CLA	CMD-C2D	-2.03	1.46	1.50
22	5	311	CLA	CMD-C2D	-2.03	1.46	1.50
22	2	315	CLA	CMB-C2B	-2.03	1.46	1.50
22	a	813	CLA	CMD-C2D	-2.03	1.46	1.50
22	a	839	CLA	CMD-C2D	-2.03	1.46	1.50
22	a	819	CLA	MG-NB	-2.03	2.01	2.05
22	9	316	CLA	CMD-C2D	-2.03	1.46	1.50
22	7	317	CLA	CMB-C2B	-2.03	1.46	1.50
22	f	802	CLA	MG-NB	-2.03	2.01	2.05
22	a	839	CLA	MG-NB	-2.03	2.01	2.05
22	a	822	CLA	CMD-C2D	-2.03	1.46	1.50
22	3	308	CLA	MG-NB	-2.03	2.01	2.05
22	3	308	CLA	CMB-C2B	-2.03	1.46	1.50
22	2	316	CLA	CMC-C2C	-2.03	1.46	1.50
22	a	838	CLA	CMD-C2D	-2.03	1.46	1.50
22	a	854	CLA	CMB-C2B	-2.03	1.46	1.50
22	5	313	CLA	CMC-C2C	-2.03	1.46	1.50
22	2	308	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	813	CLA	CMC-C2C	-2.03	1.46	1.50
22	l	203	CLA	CMD-C2D	-2.03	1.46	1.50
22	4	310	CLA	MG-NB	-2.03	2.01	2.05
22	j	103	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	824	CLA	CMD-C2D	-2.03	1.46	1.50
22	1	311	CLA	MG-NB	-2.03	2.01	2.05
22	a	808	CLA	MG-NB	-2.03	2.01	2.05
22	9	308	CLA	CMB-C2B	-2.03	1.46	1.50
21	3	302	A1L1G	C38-C39	2.03	1.40	1.35
22	5	309	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	313	CLA	CMB-C2B	-2.02	1.46	1.50
22	2	314	CLA	CMB-C2B	-2.02	1.46	1.50
22	1	307	CLA	CMD-C2D	-2.02	1.46	1.50
22	a	815	CLA	MG-NB	-2.02	2.01	2.05
22	8	313	CLA	CMC-C2C	-2.02	1.46	1.50
22	4	315	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	829	CLA	CHC-C1C	2.02	1.42	1.38
22	9	310	CLA	CMD-C2D	-2.02	1.46	1.50
22	4	316	CLA	CMD-C2D	-2.02	1.46	1.50
22	7	314	CLA	CMB-C2B	-2.02	1.46	1.50
22	5	312	CLA	CMD-C2D	-2.02	1.46	1.50
22	a	833	CLA	CMC-C2C	-2.02	1.46	1.50
22	3	312	CLA	CMB-C2B	-2.02	1.46	1.50
22	h	205	CLA	CMD-C2D	-2.02	1.46	1.50
22	5	313	CLA	CMD-C2D	-2.02	1.46	1.50
22	b	839	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	316	CLA	MG-NB	-2.02	2.01	2.05
22	b	802	CLA	MG-NB	-2.02	2.01	2.05
22	9	308	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	313	CLA	MG-NB	-2.02	2.01	2.05
22	9	318	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	824	CLA	CMB-C2B	-2.02	1.46	1.50
22	7	315	CLA	CMB-C2B	-2.02	1.46	1.50
22	8	309	CLA	CMD-C2D	-2.02	1.46	1.50
22	4	307	CLA	CMD-C2D	-2.02	1.46	1.50
22	b	821	CLA	CMD-C2D	-2.02	1.46	1.50
22	7	307	CLA	MG-NB	-2.02	2.01	2.05
22	a	808	CLA	CMD-C2D	-2.02	1.46	1.50
22	a	813	CLA	CMB-C2B	-2.02	1.46	1.50
22	l	204	CLA	CMD-C2D	-2.02	1.46	1.50
22	8	312	CLA	CMB-C2B	-2.02	1.46	1.50
22	b	840	CLA	CMB-C2B	-2.02	1.46	1.50
22	a	804	CLA	MG-NB	-2.02	2.01	2.05
22	1	308	CLA	CMD-C2D	-2.02	1.46	1.50
22	f	803	CLA	CMD-C2D	-2.02	1.46	1.50
22	7	307	CLA	CMD-C2D	-2.01	1.46	1.50
22	3	315	CLA	CMC-C2C	-2.01	1.46	1.50
22	4	317	CLA	MG-NB	-2.01	2.01	2.05
22	b	805	CLA	MG-NB	-2.01	2.01	2.05
22	b	833	CLA	MG-NB	-2.01	2.01	2.05
26	b	848	DGD	O3D-C3D	-2.01	1.38	1.43
22	1	306	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	312	CLA	CMB-C2B	-2.01	1.46	1.50
22	a	836	CLA	MG-NB	-2.01	2.01	2.05
22	b	801	CLA	MG-NB	-2.01	2.01	2.05
22	a	838	CLA	CMB-C2B	-2.01	1.46	1.50
22	2	312	CLA	CMC-C2C	-2.01	1.46	1.50
22	9	311	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	817	CLA	CMD-C2D	-2.01	1.46	1.50
22	1	310	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	833	CLA	CMB-C2B	-2.01	1.46	1.50
22	4	306	CLA	MG-NB	-2.01	2.01	2.05
22	2	311	CLA	MG-NB	-2.01	2.01	2.05
22	5	310	CLA	CMB-C2B	-2.01	1.46	1.50
22	8	311	CLA	CMD-C2D	-2.01	1.46	1.50
22	8	313	CLA	MG-NB	-2.01	2.01	2.05
22	2	315	CLA	MG-NB	-2.01	2.01	2.05
22	f	803	CLA	MG-NB	-2.01	2.01	2.05
22	h	205	CLA	MG-NB	-2.01	2.01	2.05
22	5	306	CLA	MG-NB	-2.01	2.01	2.05
22	a	813	CLA	MG-NB	-2.01	2.01	2.05
22	b	803	CLA	MG-NB	-2.01	2.01	2.05
22	8	306	CLA	CMB-C2B	-2.01	1.46	1.50
22	1	311	CLA	CMB-C2B	-2.01	1.46	1.50
22	5	306	CLA	CMB-C2B	-2.01	1.46	1.50
22	a	817	CLA	MG-NB	-2.01	2.01	2.05
22	5	315	CLA	CMD-C2D	-2.01	1.46	1.50
22	8	314	CLA	CMB-C2B	-2.01	1.46	1.50
22	4	314	CLA	CMC-C2C	-2.01	1.46	1.50
22	a	809	CLA	CMD-C2D	-2.01	1.46	1.50
22	a	831	CLA	CMD-C2D	-2.01	1.46	1.50
22	3	312	CLA	MG-NB	-2.01	2.01	2.05
22	a	805	CLA	MG-NB	-2.01	2.01	2.05
22	4	312	CLA	CMB-C2B	-2.01	1.46	1.50
22	1	311	CLA	CMD-C2D	-2.01	1.46	1.50
22	2	313	CLA	CMD-C2D	-2.01	1.46	1.50
22	a	841	CLA	CMD-C2D	-2.01	1.46	1.50
22	5	311	CLA	CMC-C2C	-2.01	1.46	1.50
22	a	840	CLA	MG-NB	-2.01	2.01	2.05
22	a	840	CLA	CMD-C2D	-2.00	1.46	1.50
22	b	827	CLA	CMC-C2C	-2.00	1.46	1.50
22	a	818	CLA	CMD-C2D	-2.00	1.46	1.50
22	a	854	CLA	CMD-C2D	-2.00	1.46	1.50
22	9	311	CLA	MG-NB	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	313	CLA	CMD-C2D	-2.00	1.46	1.50
22	b	836	CLA	CMD-C2D	-2.00	1.46	1.50
22	a	809	CLA	MG-NB	-2.00	2.01	2.05
22	5	314	CLA	MG-NB	-2.00	2.01	2.05
22	5	309	CLA	CMD-C2D	-2.00	1.46	1.50
22	4	313	CLA	MG-NB	-2.00	2.01	2.05
22	5	306	CLA	CMD-C2D	-2.00	1.46	1.50
22	8	306	CLA	CMD-C2D	-2.00	1.46	1.50
22	a	814	CLA	CMC-C2C	-2.00	1.46	1.50
22	f	802	CLA	CMB-C2B	-2.00	1.46	1.50
22	7	306	CLA	MG-NB	-2.00	2.01	2.05

All (2072) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	302	A1L1F	O15-C20-C21	10.50	123.33	113.49
26	4	318	DGD	C6E-C5E-C4E	-8.98	90.97	113.02
24	9	302	A1L1F	C17-C20-C25	-8.66	108.05	122.30
24	h	204	A1L1F	C17-C20-C25	-8.53	108.27	122.30
24	8	304	A1L1F	C17-C20-C25	-8.39	108.49	122.30
24	1	304	A1L1F	C17-C20-C25	-8.27	108.68	122.30
24	8	304	A1L1F	C37-C38-C39	-7.99	116.07	127.28
22	7	314	CLA	C4A-NA-C1A	7.35	110.03	106.68
20	9	303	XAT	C38-C25-C24	7.27	122.41	114.24
20	3	305	XAT	C38-C25-C24	7.27	122.41	114.24
22	9	310	CLA	C4A-NA-C1A	7.27	110.00	106.68
22	9	313	CLA	C4A-NA-C1A	7.27	110.00	106.68
20	4	305	XAT	C38-C25-C24	7.25	122.38	114.24
20	5	304	XAT	C38-C25-C24	7.23	122.37	114.24
20	a	852	XAT	C15-C14-C13	-7.22	117.15	127.28
20	7	304	XAT	C38-C25-C24	7.21	122.34	114.24
20	1	303	XAT	C38-C25-C24	7.21	122.34	114.24
22	l	203	CLA	C4A-NA-C1A	7.20	109.97	106.68
22	a	806	CLA	C4A-NA-C1A	7.18	109.95	106.68
22	b	839	CLA	C4A-NA-C1A	7.18	109.95	106.68
22	b	803	CLA	C4A-NA-C1A	7.16	109.95	106.68
20	7	305	XAT	C38-C25-C24	7.14	122.27	114.24
29	f	801	BCR	C24-C23-C22	-7.14	115.67	126.23
20	j	101	XAT	C38-C25-C24	7.10	122.22	114.24
20	9	304	XAT	C38-C25-C24	7.07	122.19	114.24
20	5	304	XAT	C18-C5-C4	7.07	122.18	114.24
22	a	833	CLA	C4A-NA-C1A	7.05	109.89	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	304	XAT	C38-C25-C24	7.03	122.14	114.24
20	4	304	XAT	C38-C25-C24	7.03	122.14	114.24
22	a	823	CLA	C4A-NA-C1A	7.03	109.89	106.68
20	5	301	XAT	C38-C25-C26	-7.03	110.73	122.30
20	2	301	XAT	C18-C5-C6	-7.03	110.74	122.30
22	b	809	CLA	C4A-NA-C1A	7.01	109.88	106.68
22	a	821	CLA	C4A-NA-C1A	6.99	109.87	106.68
22	b	820	CLA	C4A-NA-C1A	6.98	109.86	106.68
20	4	305	XAT	C38-C25-C26	-6.98	110.82	122.30
22	4	310	CLA	C4A-NA-C1A	6.98	109.86	106.68
22	9	308	CLA	C4A-NA-C1A	6.96	109.86	106.68
20	3	304	XAT	C38-C25-C26	-6.95	110.86	122.30
22	a	835	CLA	C4A-NA-C1A	6.94	109.84	106.68
20	9	303	XAT	C38-C25-C26	-6.94	110.89	122.30
20	1	302	XAT	C38-C25-C24	6.93	122.02	114.24
20	8	301	XAT	C38-C25-C24	6.91	122.01	114.24
22	7	317	CLA	C4A-NA-C1A	6.91	109.83	106.68
20	8	301	XAT	C38-C25-C26	-6.91	110.94	122.30
20	8	303	XAT	C18-C5-C6	-6.90	110.94	122.30
22	j	103	CLA	C4A-NA-C1A	6.89	109.82	106.68
22	4	317	CLA	C4A-NA-C1A	6.88	109.82	106.68
22	a	826	CLA	C4A-NA-C1A	6.87	109.81	106.68
22	b	801	CLA	C4A-NA-C1A	6.87	109.81	106.68
22	a	810	CLA	C4A-NA-C1A	6.85	109.81	106.68
22	a	828	CLA	C4A-NA-C1A	6.85	109.80	106.68
20	4	303	XAT	C38-C25-C24	6.84	121.92	114.24
22	4	316	CLA	C4A-NA-C1A	6.83	109.80	106.68
22	3	308	CLA	C4A-NA-C1A	6.83	109.80	106.68
22	f	802	CLA	C4A-NA-C1A	6.83	109.80	106.68
20	8	303	XAT	C38-C25-C24	6.83	121.91	114.24
20	5	304	XAT	C6-C7-C8	-6.83	111.55	125.99
20	2	304	XAT	C38-C25-C24	6.82	121.91	114.24
20	9	304	XAT	C38-C25-C26	-6.82	111.07	122.30
20	5	304	XAT	C18-C5-C6	-6.82	111.08	122.30
22	5	310	CLA	C4A-NA-C1A	6.82	109.79	106.68
20	7	304	XAT	C18-C5-C6	-6.82	111.08	122.30
20	7	301	XAT	C18-C5-C6	-6.81	111.09	122.30
20	a	852	XAT	C38-C25-C24	6.79	121.87	114.24
22	b	827	CLA	C4A-NA-C1A	6.79	109.78	106.68
22	7	316	CLA	C4A-NA-C1A	6.78	109.77	106.68
20	3	304	XAT	C18-C5-C6	-6.78	111.15	122.30
22	a	801	CLA	C4A-NA-C1A	6.77	109.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	i	101	BCR	C24-C23-C22	-6.77	116.22	126.23
20	j	101	XAT	C38-C25-C26	-6.76	111.18	122.30
22	a	807	CLA	C4A-NA-C1A	6.76	109.76	106.68
22	h	203	CLA	C4A-NA-C1A	6.75	109.76	106.68
20	8	302	XAT	C38-C25-C24	6.75	121.82	114.24
22	b	836	CLA	C4A-NA-C1A	6.74	109.75	106.68
20	7	303	XAT	C38-C25-C26	-6.74	111.21	122.30
22	a	809	CLA	C4A-NA-C1A	6.74	109.75	106.68
20	7	304	XAT	C38-C25-C26	-6.73	111.22	122.30
22	b	821	CLA	C4A-NA-C1A	6.73	109.75	106.68
24	8	304	A1L1F	O15-C20-C21	6.73	119.79	113.49
22	1	305	CLA	C4A-NA-C1A	6.72	109.75	106.68
22	1	308	CLA	C4A-NA-C1A	6.72	109.75	106.68
20	4	302	XAT	C38-C25-C24	6.72	121.79	114.24
20	5	302	XAT	C18-C5-C6	-6.71	111.25	122.30
22	3	313	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	b	824	CLA	C4A-NA-C1A	6.71	109.74	106.68
20	3	303	XAT	C38-C25-C24	6.71	121.78	114.24
20	2	301	XAT	C18-C5-C4	6.71	121.78	114.24
22	9	316	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	a	817	CLA	C4A-NA-C1A	6.71	109.74	106.68
20	8	302	XAT	C18-C5-C6	-6.71	111.27	122.30
22	b	806	CLA	C4A-NA-C1A	6.70	109.74	106.68
20	8	302	XAT	C38-C25-C26	-6.70	111.27	122.30
20	2	303	XAT	C18-C5-C6	-6.69	111.28	122.30
22	4	315	CLA	C4A-NA-C1A	6.69	109.73	106.68
22	1	306	CLA	C4A-NA-C1A	6.69	109.73	106.68
20	3	305	XAT	C38-C25-C26	-6.69	111.29	122.30
22	a	805	CLA	C4A-NA-C1A	6.69	109.73	106.68
20	7	301	XAT	C18-C5-C4	6.69	121.75	114.24
22	2	316	CLA	C4A-NA-C1A	6.69	109.73	106.68
22	2	312	CLA	C4A-NA-C1A	6.68	109.73	106.68
20	2	304	XAT	C18-C5-C4	6.68	121.75	114.24
22	7	315	CLA	C4A-NA-C1A	6.68	109.73	106.68
22	b	814	CLA	C4A-NA-C1A	6.68	109.72	106.68
20	4	303	XAT	C18-C5-C6	-6.67	111.32	122.30
20	4	301	XAT	C31-C30-C29	-6.67	117.92	127.28
22	a	841	CLA	C4A-NA-C1A	6.67	109.72	106.68
22	b	812	CLA	C4A-NA-C1A	6.67	109.72	106.68
20	5	304	XAT	C38-C25-C26	-6.67	111.33	122.30
22	a	840	CLA	C4A-NA-C1A	6.67	109.72	106.68
20	7	305	XAT	C38-C25-C26	-6.66	111.33	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	834	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	b	810	CLA	C4A-NA-C1A	6.66	109.72	106.68
22	a	831	CLA	C4A-NA-C1A	6.66	109.72	106.68
20	4	301	XAT	C18-C5-C6	-6.66	111.34	122.30
22	b	805	CLA	C4A-NA-C1A	6.66	109.72	106.68
20	3	301	XAT	C18-C5-C4	6.65	121.71	114.24
22	4	306	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	4	311	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	3	314	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	5	314	CLA	C4A-NA-C1A	6.64	109.71	106.68
22	4	314	CLA	C4A-NA-C1A	6.64	109.71	106.68
22	3	312	CLA	C4A-NA-C1A	6.64	109.71	106.68
20	7	303	XAT	C18-C5-C6	-6.64	111.38	122.30
20	2	305	XAT	C18-C5-C6	-6.63	111.39	122.30
22	a	842	CLA	C4A-NA-C1A	6.63	109.70	106.68
20	4	303	XAT	C38-C25-C26	-6.62	111.40	122.30
20	5	301	XAT	C38-C25-C24	6.62	121.68	114.24
29	a	850	BCR	C24-C23-C22	-6.62	116.44	126.23
22	5	306	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	8	312	CLA	C4A-NA-C1A	6.62	109.70	106.68
24	h	204	AI1L1F	O15-C20-C21	6.61	119.69	113.49
22	8	313	CLA	C4A-NA-C1A	6.61	109.69	106.68
20	4	301	XAT	C18-C5-C4	6.61	121.66	114.24
20	2	303	XAT	C38-C25-C26	-6.60	111.44	122.30
22	l	202	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	l	204	CLA	C4A-NA-C1A	6.60	109.69	106.68
22	7	310	CLA	C4A-NA-C1A	6.59	109.69	106.68
22	b	832	CLA	C4A-NA-C1A	6.59	109.69	106.68
22	f	803	CLA	C4A-NA-C1A	6.59	109.69	106.68
20	2	304	XAT	C38-C25-C26	-6.59	111.45	122.30
22	9	314	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	a	825	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	a	829	CLA	C4A-NA-C1A	6.58	109.68	106.68
22	b	822	CLA	C4A-NA-C1A	6.58	109.68	106.68
20	7	303	XAT	C38-C25-C24	6.57	121.62	114.24
22	4	307	CLA	C4A-NA-C1A	6.57	109.68	106.68
20	3	303	XAT	C18-C5-C6	-6.57	111.48	122.30
22	8	309	CLA	C4A-NA-C1A	6.57	109.68	106.68
22	a	837	CLA	C4A-NA-C1A	6.57	109.68	106.68
20	2	304	XAT	C18-C5-C6	-6.57	111.49	122.30
22	7	307	CLA	C4A-NA-C1A	6.57	109.67	106.68
22	8	305	CLA	C4A-NA-C1A	6.56	109.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	839	CLA	C4A-NA-C1A	6.56	109.67	106.68
22	a	811	CLA	C4A-NA-C1A	6.56	109.67	106.68
20	4	302	XAT	C18-C5-C4	6.56	121.61	114.24
22	2	311	CLA	C4A-NA-C1A	6.56	109.67	106.68
20	8	303	XAT	C18-C5-C4	6.55	121.60	114.24
22	5	311	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	5	308	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	5	313	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	2	313	CLA	C4A-NA-C1A	6.55	109.67	106.68
22	a	838	CLA	C4A-NA-C1A	6.55	109.67	106.68
20	1	302	XAT	C38-C25-C26	-6.54	111.54	122.30
22	a	804	CLA	C4A-NA-C1A	6.54	109.66	106.68
22	a	830	CLA	C4A-NA-C1A	6.54	109.66	106.68
20	3	301	XAT	C18-C5-C6	-6.53	111.55	122.30
20	7	305	XAT	C18-C5-C6	-6.53	111.55	122.30
22	a	812	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	b	807	CLA	C4A-NA-C1A	6.53	109.66	106.68
22	8	307	CLA	C4A-NA-C1A	6.52	109.65	106.68
22	b	818	CLA	C4A-NA-C1A	6.52	109.65	106.68
22	4	308	CLA	C4A-NA-C1A	6.52	109.65	106.68
22	b	831	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	b	826	CLA	C4A-NA-C1A	6.51	109.65	106.68
20	3	303	XAT	C38-C25-C26	-6.51	111.59	122.30
22	j	102	CLA	C4A-NA-C1A	6.51	109.65	106.68
20	j	101	XAT	C18-C5-C6	-6.50	111.60	122.30
22	3	311	CLA	C4A-NA-C1A	6.50	109.64	106.68
22	a	818	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	b	808	CLA	C4A-NA-C1A	6.49	109.64	106.68
20	9	303	XAT	C18-C5-C6	-6.49	111.61	122.30
22	5	312	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	a	844	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	a	836	CLA	C4A-NA-C1A	6.48	109.64	106.68
20	4	302	XAT	C18-C5-C6	-6.48	111.63	122.30
20	4	304	XAT	C18-C5-C6	-6.48	111.63	122.30
22	3	309	CLA	C4A-NA-C1A	6.48	109.64	106.68
22	b	823	CLA	C4A-NA-C1A	6.48	109.64	106.68
22	8	306	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	1	307	CLA	C4A-NA-C1A	6.47	109.63	106.68
22	2	306	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	a	815	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	7	312	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	a	854	CLA	C4A-NA-C1A	6.46	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	822	CLA	C4A-NA-C1A	6.46	109.62	106.68
20	1	302	XAT	C18-C5-C6	-6.45	111.68	122.30
22	8	314	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	4	309	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	b	833	CLA	C4A-NA-C1A	6.45	109.62	106.68
20	4	305	XAT	C18-C5-C6	-6.45	111.68	122.30
22	5	309	CLA	C4A-NA-C1A	6.44	109.62	106.68
22	a	816	CLA	C4A-NA-C1A	6.44	109.61	106.68
22	3	310	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	2	309	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	b	838	CLA	C4A-NA-C1A	6.43	109.61	106.68
20	2	302	XAT	C18-C5-C6	-6.43	111.72	122.30
22	1	313	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	2	315	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	3	315	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	b	815	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	b	835	CLA	C4A-NA-C1A	6.42	109.61	106.68
20	3	305	XAT	C18-C5-C6	-6.42	111.74	122.30
20	3	301	XAT	C38-C25-C26	-6.42	111.74	122.30
22	8	308	CLA	C4A-NA-C1A	6.42	109.61	106.68
20	8	303	XAT	C38-C25-C26	-6.41	111.75	122.30
20	4	302	XAT	C38-C25-C26	-6.41	111.75	122.30
20	4	304	XAT	C38-C25-C26	-6.41	111.75	122.30
20	4	305	XAT	C31-C30-C29	-6.41	118.29	127.28
20	2	303	XAT	C38-C25-C24	6.41	121.44	114.24
22	5	315	CLA	C4A-NA-C1A	6.41	109.60	106.68
20	5	302	XAT	C26-C27-C28	-6.40	112.45	125.99
22	1	312	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	a	808	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	8	311	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	2	307	CLA	C4A-NA-C1A	6.39	109.60	106.68
22	2	314	CLA	C4A-NA-C1A	6.39	109.60	106.68
22	7	308	CLA	C4A-NA-C1A	6.39	109.60	106.68
20	8	301	XAT	C18-C5-C6	-6.39	111.78	122.30
22	9	312	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	b	813	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	a	832	CLA	C4A-NA-C1A	6.38	109.59	106.68
20	1	303	XAT	C18-C5-C6	-6.38	111.81	122.30
20	1	302	XAT	C18-C5-C4	6.38	121.40	114.24
22	5	307	CLA	C4A-NA-C1A	6.37	109.59	106.68
20	2	302	XAT	C38-C25-C24	6.37	121.40	114.24
22	a	827	CLA	C4A-NA-C1A	6.36	109.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	852	XAT	C38-C25-C26	-6.36	111.83	122.30
20	1	303	XAT	C38-C25-C26	-6.36	111.84	122.30
20	5	301	XAT	C18-C5-C6	-6.36	111.84	122.30
20	9	305	XAT	C18-C5-C6	-6.35	111.84	122.30
20	3	303	XAT	C18-C5-C4	6.35	121.37	114.24
20	7	305	XAT	C18-C5-C4	6.35	121.37	114.24
22	b	834	CLA	C4A-NA-C1A	6.35	109.57	106.68
20	j	101	XAT	C18-C5-C4	6.34	121.36	114.24
22	9	318	CLA	C4A-NA-C1A	6.34	109.57	106.68
22	7	311	CLA	C4A-NA-C1A	6.34	109.57	106.68
20	8	302	XAT	C11-C10-C9	-6.34	118.39	127.28
29	i	101	BCR	C20-C21-C22	-6.34	118.39	127.28
20	3	305	XAT	C18-C5-C4	6.34	121.36	114.24
20	2	302	XAT	C38-C25-C26	-6.34	111.87	122.30
22	9	311	CLA	C4A-NA-C1A	6.33	109.57	106.68
22	1	311	CLA	C4A-NA-C1A	6.33	109.57	106.68
22	b	819	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	3	307	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	1	314	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	a	819	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	h	205	CLA	C4A-NA-C1A	6.30	109.56	106.68
20	9	305	XAT	C11-C10-C9	-6.30	118.44	127.28
22	1	309	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	a	814	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	a	802	CLA	C4A-NA-C1A	6.30	109.55	106.68
24	8	304	A1L1F	O15-C20-C17	6.28	122.07	115.05
20	3	304	XAT	C18-C5-C4	6.28	121.30	114.24
20	2	301	XAT	C38-C25-C24	6.28	121.30	114.24
22	4	312	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	7	306	CLA	C4A-NA-C1A	6.28	109.55	106.68
22	7	309	CLA	C4A-NA-C1A	6.28	109.55	106.68
20	4	303	XAT	C18-C5-C4	6.28	121.30	114.24
22	b	825	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	5	305	CLA	C4A-NA-C1A	6.26	109.53	106.68
22	9	315	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	2	310	CLA	C4A-NA-C1A	6.25	109.53	106.68
22	a	824	CLA	C4A-NA-C1A	6.24	109.52	106.68
22	a	813	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	b	829	CLA	C4A-NA-C1A	6.23	109.52	106.68
20	4	304	XAT	C18-C5-C4	6.23	121.24	114.24
22	b	840	CLA	C4A-NA-C1A	6.22	109.52	106.68
20	2	301	XAT	C38-C25-C26	-6.21	112.07	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	313	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	3	301	XAT	C38-C25-C24	6.21	121.22	114.24
22	1	310	CLA	C4A-NA-C1A	6.21	109.51	106.68
20	5	302	XAT	C38-C25-C24	6.21	121.22	114.24
22	b	804	CLA	C4A-NA-C1A	6.19	109.50	106.68
22	a	820	CLA	C4A-NA-C1A	6.18	109.50	106.68
22	b	837	CLA	C4A-NA-C1A	6.18	109.50	106.68
20	1	303	XAT	C18-C5-C4	6.15	121.15	114.24
20	2	301	XAT	C31-C30-C29	-6.15	118.66	127.28
22	b	811	CLA	C4A-NA-C1A	6.14	109.48	106.68
20	2	305	XAT	C18-C5-C4	6.12	121.11	114.24
20	4	305	XAT	C18-C5-C4	6.11	121.10	114.24
22	2	308	CLA	C4A-NA-C1A	6.10	109.46	106.68
22	b	828	CLA	C4A-NA-C1A	6.09	109.46	106.68
29	b	842	BCR	C7-C8-C9	-6.09	117.23	126.23
20	a	852	XAT	C26-C27-C28	-6.08	113.14	125.99
20	7	304	XAT	C18-C5-C4	6.07	121.06	114.24
22	b	816	CLA	C4A-NA-C1A	6.07	109.45	106.68
22	9	309	CLA	C4A-NA-C1A	6.06	109.44	106.68
24	1	304	A1L1F	O15-C20-C17	6.05	121.81	115.05
20	2	302	XAT	C18-C5-C4	6.03	121.01	114.24
22	b	830	CLA	C4A-NA-C1A	5.98	109.41	106.68
20	5	302	XAT	C18-C5-C4	5.96	120.94	114.24
24	h	204	A1L1F	C37-C38-C39	-5.96	118.92	127.28
20	5	304	XAT	C26-C27-C28	-5.95	113.41	125.99
22	b	817	CLA	C4A-NA-C1A	5.95	109.39	106.68
20	5	302	XAT	C38-C25-C26	-5.94	112.52	122.30
20	8	301	XAT	C18-C5-C4	5.94	120.92	114.24
20	8	302	XAT	C18-C5-C4	5.94	120.92	114.24
20	7	301	XAT	C38-C25-C24	5.94	120.91	114.24
22	b	802	CLA	C4A-NA-C1A	5.93	109.39	106.68
20	7	301	XAT	C38-C25-C26	-5.92	112.55	122.30
29	b	849	BCR	C16-C17-C18	-5.92	118.97	127.28
20	7	303	XAT	C18-C5-C4	5.92	120.89	114.24
20	7	301	XAT	C31-C30-C29	-5.90	119.00	127.28
22	4	313	CLA	C4A-NA-C1A	5.90	109.37	106.68
22	8	310	CLA	C4A-NA-C1A	5.89	109.37	106.68
20	5	301	XAT	C18-C5-C4	5.89	120.86	114.24
24	h	204	A1L1F	O15-C20-C17	5.89	121.63	115.05
20	j	101	XAT	C6-C7-C8	-5.85	113.63	125.99
20	9	303	XAT	C18-C5-C4	5.84	120.80	114.24
20	2	303	XAT	C18-C5-C4	5.81	120.77	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	301	XAT	C35-C34-C33	-5.80	119.14	127.28
29	a	850	BCR	C20-C21-C22	-5.77	119.19	127.28
29	b	844	BCR	C24-C23-C22	-5.77	117.71	126.23
20	5	302	XAT	C11-C10-C9	-5.75	119.22	127.28
29	f	801	BCR	C16-C17-C18	-5.72	119.25	127.28
24	1	304	A1L1F	O15-C20-C21	5.71	118.84	113.49
29	b	842	BCR	C11-C10-C9	-5.70	119.28	127.28
20	4	301	XAT	C38-C25-C24	5.68	120.62	114.24
20	9	304	XAT	C26-C27-C28	-5.67	114.01	125.99
29	b	844	BCR	C7-C8-C9	-5.65	117.88	126.23
20	7	305	XAT	C15-C14-C13	-5.60	119.42	127.28
29	b	845	BCR	C16-C17-C18	-5.53	119.52	127.28
20	9	303	XAT	C15-C14-C13	-5.50	119.57	127.28
20	8	303	XAT	C26-C27-C28	-5.48	114.40	125.99
29	f	801	BCR	C20-C21-C22	-5.48	119.60	127.28
29	f	804	BCR	C15-C14-C13	-5.47	119.60	127.28
29	j	104	BCR	C28-C27-C26	-5.47	104.30	114.06
20	a	852	XAT	C18-C5-C6	-5.46	113.32	122.30
20	3	304	XAT	C35-C34-C33	-5.46	119.62	127.28
20	4	301	XAT	C38-C25-C26	-5.45	113.33	122.30
20	2	303	XAT	C35-C34-C33	-5.44	119.64	127.28
20	3	301	XAT	C6-C7-C8	-5.44	114.48	125.99
29	b	844	BCR	C33-C5-C6	-5.44	118.55	124.48
22	a	803	CLA	C4A-NA-C1A	5.43	109.16	106.68
20	2	303	XAT	C31-C30-C29	-5.40	119.71	127.28
29	l	201	BCR	C7-C8-C9	-5.38	118.28	126.23
29	b	842	BCR	C15-C14-C13	-5.36	119.76	127.28
24	8	304	A1L1F	O7-C54-C56	5.33	120.59	111.09
20	4	305	XAT	C15-C14-C13	-5.32	119.81	127.28
20	2	302	XAT	C35-C34-C33	-5.31	119.83	127.28
20	7	304	XAT	C11-C10-C9	-5.31	119.83	127.28
29	b	842	BCR	C3-C4-C5	-5.31	104.59	114.06
20	2	303	XAT	C11-C10-C9	-5.30	119.84	127.28
20	2	305	XAT	C31-C30-C29	-5.30	119.84	127.28
20	a	852	XAT	C18-C5-C4	5.30	120.19	114.24
29	a	849	BCR	C3-C4-C5	-5.29	104.63	114.06
26	b	848	DGD	O2G-C1B-C2B	5.28	122.91	111.48
24	8	304	A1L1F	C41-C42-C44	-5.28	119.87	127.28
20	4	303	XAT	C26-C27-C28	-5.27	114.84	125.99
20	7	301	XAT	C35-C34-C33	-5.27	119.89	127.28
20	2	301	XAT	C35-C34-C33	-5.27	119.89	127.28
20	4	304	XAT	C26-C27-C28	-5.24	114.91	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	852	XAT	C6-C7-C8	-5.24	114.92	125.99
29	l	205	BCR	C24-C23-C22	-5.23	118.50	126.23
20	9	305	XAT	C18-C5-C4	5.23	120.11	114.24
20	2	304	XAT	C6-C7-C8	-5.21	114.98	125.99
20	8	303	XAT	C15-C14-C13	-5.19	119.99	127.28
20	9	303	XAT	C26-C27-C28	-5.19	115.02	125.99
20	j	101	XAT	C26-C27-C28	-5.18	115.05	125.99
20	2	305	XAT	C35-C34-C33	-5.12	120.10	127.28
20	1	302	XAT	C35-C34-C33	-5.12	120.10	127.28
29	h	201	BCR	C3-C4-C5	-5.10	104.96	114.06
29	a	847	BCR	C16-C17-C18	-5.09	120.14	127.28
29	b	849	BCR	C11-C10-C9	-5.05	120.19	127.28
20	7	305	XAT	C26-C27-C28	-5.04	115.34	125.99
20	8	303	XAT	C6-C7-C8	-5.04	115.34	125.99
20	3	305	XAT	C26-C27-C28	-5.03	115.36	125.99
29	f	804	BCR	C11-C10-C9	-5.02	120.24	127.28
20	5	301	XAT	C26-C27-C28	-5.02	115.38	125.99
29	b	849	BCR	C20-C21-C22	-5.02	120.24	127.28
29	a	850	BCR	C16-C17-C18	-5.01	120.25	127.28
20	2	301	XAT	C15-C14-C13	-4.99	120.28	127.28
20	4	304	XAT	C6-C7-C8	-4.98	115.46	125.99
29	a	849	BCR	C16-C17-C18	-4.98	120.30	127.28
20	1	302	XAT	C26-C27-C28	-4.98	115.47	125.99
20	7	303	XAT	C31-C30-C29	-4.95	120.33	127.28
20	3	305	XAT	C6-C7-C8	-4.95	115.53	125.99
20	j	101	XAT	C11-C10-C9	-4.90	120.41	127.28
29	b	849	BCR	C38-C26-C25	-4.89	119.14	124.48
20	7	304	XAT	C26-C27-C28	-4.89	115.66	125.99
20	1	303	XAT	C6-C7-C8	-4.89	115.66	125.99
20	5	302	XAT	C15-C14-C13	-4.89	120.42	127.28
29	j	104	BCR	C11-C10-C9	-4.87	120.44	127.28
20	4	303	XAT	C11-C10-C9	-4.87	120.45	127.28
20	2	305	XAT	C6-C7-C8	-4.86	115.71	125.99
20	9	305	XAT	C35-C34-C33	-4.84	120.49	127.28
20	5	304	XAT	C15-C14-C13	-4.83	120.50	127.28
29	i	101	BCR	C16-C17-C18	-4.83	120.51	127.28
29	l	205	BCR	C15-C14-C13	-4.83	120.51	127.28
20	2	301	XAT	C6-C7-C8	-4.82	115.80	125.99
29	h	202	BCR	C16-C17-C18	-4.81	120.53	127.28
20	1	302	XAT	C6-C7-C8	-4.80	115.84	125.99
20	7	304	XAT	C35-C34-C33	-4.78	120.57	127.28
29	b	849	BCR	C7-C8-C9	-4.78	119.17	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	304	XAT	C15-C14-C13	-4.77	120.59	127.28
20	7	301	XAT	C6-C7-C8	-4.77	115.91	125.99
20	9	304	XAT	C15-C14-C13	-4.76	120.60	127.28
20	4	302	XAT	C26-C27-C28	-4.73	115.99	125.99
20	8	301	XAT	C26-C27-C28	-4.72	116.00	125.99
24	9	302	A1L1F	O7-C54-C56	4.71	119.49	111.09
20	4	302	XAT	C6-C7-C8	-4.69	116.07	125.99
20	7	305	XAT	C6-C7-C8	-4.68	116.10	125.99
20	7	303	XAT	C11-C10-C9	-4.67	120.72	127.28
20	8	302	XAT	C15-C14-C13	-4.67	120.73	127.28
29	b	846	BCR	C16-C17-C18	-4.67	120.73	127.28
20	9	305	XAT	C38-C25-C24	4.67	119.48	114.24
20	3	303	XAT	C26-C27-C28	-4.66	116.14	125.99
20	5	301	XAT	C35-C34-C33	-4.65	120.75	127.28
29	b	843	BCR	C7-C8-C9	-4.64	119.37	126.23
24	h	204	A1L1F	O7-C54-C56	4.63	119.34	111.09
20	4	302	XAT	C35-C34-C33	-4.63	120.79	127.28
29	b	843	BCR	C11-C10-C9	-4.62	120.80	127.28
20	3	304	XAT	C6-C7-C8	-4.60	116.26	125.99
20	2	305	XAT	C15-C14-C13	-4.60	120.83	127.28
20	7	301	XAT	C27-C28-C29	-4.57	118.44	125.53
20	8	302	XAT	C35-C34-C33	-4.57	120.87	127.28
20	4	305	XAT	C26-C27-C28	-4.56	116.35	125.99
20	7	303	XAT	C35-C34-C33	-4.53	120.93	127.28
20	8	302	XAT	C26-C27-C28	-4.52	116.44	125.99
29	a	848	BCR	C16-C17-C18	-4.51	120.95	127.28
20	3	303	XAT	C6-C7-C8	-4.51	116.45	125.99
20	3	305	XAT	C35-C34-C33	-4.50	120.97	127.28
20	2	304	XAT	C26-C27-C28	-4.49	116.50	125.99
29	a	848	BCR	C15-C14-C13	-4.49	120.99	127.28
20	7	303	XAT	C26-C27-C28	-4.48	116.51	125.99
20	2	302	XAT	C6-C7-C8	-4.48	116.52	125.99
24	9	302	A1L1F	C36-C35-C34	-4.47	121.01	127.28
24	h	204	A1L1F	O15-C25-C14	-4.46	104.11	116.88
29	a	850	BCR	C15-C14-C13	-4.43	121.06	127.28
29	a	849	BCR	C15-C14-C13	-4.43	121.07	127.28
29	j	104	BCR	C15-C14-C13	-4.42	121.08	127.28
29	b	846	BCR	C33-C5-C6	-4.41	119.67	124.48
20	3	303	XAT	C35-C34-C33	-4.39	121.12	127.28
29	b	842	BCR	C16-C17-C18	-4.39	121.12	127.28
29	b	844	BCR	C16-C17-C18	-4.38	121.13	127.28
20	j	101	XAT	C35-C34-C33	-4.38	121.14	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	301	XAT	C35-C34-C33	-4.37	121.14	127.28
26	4	318	DGD	O6E-C5E-C6E	4.37	117.27	106.44
20	3	303	XAT	C15-C14-C13	-4.36	121.16	127.28
24	h	204	A1L1F	C25-C14-C29	-4.36	116.78	125.99
24	9	302	A1L1F	C14-C29-C30	-4.36	118.06	125.47
27	2	317	LMG	O7-C10-C11	4.35	120.89	111.48
20	3	304	XAT	C31-C30-C29	-4.35	121.18	127.28
20	5	304	XAT	C35-C34-C33	-4.34	121.19	127.28
29	j	104	BCR	C16-C17-C18	-4.34	121.19	127.28
29	b	843	BCR	C15-C14-C13	-4.32	121.21	127.28
24	1	304	A1L1F	O7-C54-C56	4.31	118.78	111.09
29	f	804	BCR	C24-C23-C22	-4.30	119.88	126.23
20	3	301	XAT	C15-C14-C13	-4.29	121.27	127.28
20	4	301	XAT	C6-C7-C8	-4.28	116.94	125.99
29	j	104	BCR	C7-C8-C9	-4.28	119.90	126.23
20	2	305	XAT	C38-C25-C24	4.28	119.05	114.24
29	h	202	BCR	C33-C5-C6	-4.28	119.82	124.48
20	9	304	XAT	C18-C5-C4	4.27	119.03	114.24
20	4	304	XAT	C35-C34-C33	-4.27	121.30	127.28
20	4	305	XAT	C35-C34-C33	-4.26	121.30	127.28
29	b	844	BCR	C15-C14-C13	-4.26	121.30	127.28
20	7	303	XAT	C15-C14-C13	-4.26	121.30	127.28
24	h	204	A1L1F	C41-C42-C44	-4.25	121.31	127.28
24	1	304	A1L1F	C37-C38-C39	-4.24	121.33	127.28
29	b	845	BCR	C24-C23-C22	-4.23	119.97	126.23
29	l	201	BCR	C15-C14-C13	-4.23	121.34	127.28
29	a	850	BCR	C38-C26-C25	-4.23	119.87	124.48
24	8	304	A1L1F	C41-C40-C39	-4.23	114.76	126.36
29	l	201	BCR	C33-C5-C6	-4.23	119.87	124.48
26	4	318	DGD	O2G-C1B-C2B	4.23	120.63	111.48
29	l	205	BCR	C20-C21-C22	-4.21	121.37	127.28
21	9	301	A1L1G	C37-C36-C35	4.21	132.13	123.52
24	8	304	A1L1F	C32-C31-C30	-4.19	121.39	127.23
25	a	845	LHG	O7-C7-C8	4.19	120.54	111.48
20	7	305	XAT	C11-C10-C9	-4.19	121.41	127.28
24	1	304	A1L1F	C17-C20-C21	4.18	118.94	114.24
20	3	304	XAT	C15-C14-C13	-4.18	121.42	127.28
29	f	804	BCR	C7-C8-C9	-4.17	120.07	126.23
29	h	201	BCR	C16-C17-C18	-4.16	121.44	127.28
29	b	845	BCR	C7-C8-C9	-4.16	120.08	126.23
29	b	845	BCR	C20-C21-C22	-4.15	121.45	127.28
25	b	847	LHG	O7-C7-C8	4.11	120.38	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	205	BCR	C38-C26-C25	-4.11	120.00	124.48
20	5	301	XAT	C11-C10-C9	-4.10	121.52	127.28
20	4	301	XAT	C15-C14-C13	-4.10	121.53	127.28
29	a	848	BCR	C11-C10-C9	-4.10	121.53	127.28
29	a	847	BCR	C38-C26-C25	-4.09	120.02	124.48
29	f	801	BCR	C3-C4-C5	-4.09	106.77	114.06
28	b	841	PQN	C11-C12-C13	-4.08	119.80	126.83
27	a	853	LMG	O7-C10-C11	4.08	120.31	111.48
29	b	845	BCR	C16-C15-C14	-4.06	115.21	123.52
20	9	304	XAT	C18-C5-C6	-4.06	115.62	122.30
29	b	842	BCR	C28-C27-C26	-4.06	106.82	114.06
20	3	301	XAT	C35-C34-C33	-4.05	121.60	127.28
29	f	804	BCR	C33-C5-C6	-4.04	120.08	124.48
20	7	303	XAT	C6-C7-C8	-4.02	117.50	125.99
20	a	852	XAT	C31-C30-C29	-4.02	121.65	127.28
29	i	101	BCR	C7-C8-C9	-4.01	120.30	126.23
29	l	201	BCR	C11-C10-C9	-4.01	121.65	127.28
20	4	305	XAT	C11-C10-C9	-4.01	121.66	127.28
20	4	305	XAT	C6-C7-C8	-4.00	117.53	125.99
24	9	302	A1L1F	O15-C20-C17	4.00	119.52	115.05
25	9	317	LHG	O7-C7-C8	3.98	120.10	111.48
24	8	304	A1L1F	C37-C36-C35	-3.98	115.37	123.52
29	b	845	BCR	C28-C27-C26	-3.98	106.96	114.06
29	b	845	BCR	C15-C14-C13	-3.97	121.72	127.28
20	4	303	XAT	C15-C14-C13	-3.96	121.72	127.28
29	f	804	BCR	C38-C26-C25	-3.96	120.17	124.48
20	2	302	XAT	C31-C30-C29	-3.95	121.73	127.28
25	a	846	LHG	O7-C7-C8	3.95	120.03	111.48
27	j	105	LMG	O7-C10-C11	3.94	120.01	111.48
20	2	303	XAT	C15-C14-C13	-3.94	121.75	127.28
20	1	303	XAT	C26-C27-C28	-3.93	117.68	125.99
20	j	101	XAT	C15-C14-C13	-3.92	121.78	127.28
22	b	804	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
20	2	302	XAT	C15-C14-C13	-3.91	121.79	127.28
29	f	804	BCR	C20-C21-C22	-3.91	121.79	127.28
29	a	847	BCR	C20-C21-C22	-3.91	121.80	127.28
29	l	205	BCR	C33-C5-C6	-3.89	120.24	124.48
29	l	201	BCR	C16-C17-C18	-3.89	121.82	127.28
20	7	301	XAT	C15-C14-C13	-3.87	121.85	127.28
20	2	305	XAT	C27-C28-C29	-3.86	119.53	125.53
20	2	302	XAT	C26-C27-C28	-3.86	117.82	125.99
29	l	205	BCR	C16-C17-C18	-3.86	121.86	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	315	DGD	O2G-C1B-C2B	3.84	119.78	111.48
29	b	846	BCR	C15-C14-C13	-3.83	121.90	127.28
21	1	301	A1L1G	C37-C36-C35	3.83	131.35	123.52
29	f	804	BCR	C16-C17-C18	-3.82	121.92	127.28
20	5	301	XAT	C15-C14-C13	-3.82	121.92	127.28
21	3	306	A1L1G	C36-C37-C38	3.82	131.34	123.52
29	j	104	BCR	C20-C21-C22	-3.81	121.93	127.28
24	h	204	A1L1F	C36-C35-C34	-3.80	121.94	127.28
20	1	303	XAT	C35-C34-C33	-3.79	121.96	127.28
26	b	848	DGD	O5D-C6D-C5D	-3.79	100.88	109.42
20	8	301	XAT	C15-C14-C13	-3.79	121.97	127.28
29	f	801	BCR	C16-C15-C14	-3.79	115.77	123.52
29	a	849	BCR	C28-C27-C26	-3.78	107.31	114.06
20	9	305	XAT	C15-C14-C13	-3.78	121.98	127.28
29	a	850	BCR	C33-C5-C6	-3.77	120.37	124.48
29	h	201	BCR	C15-C14-C13	-3.76	122.00	127.28
23	1	315	SQD	O47-C7-C8	3.76	119.61	111.48
22	a	806	CLA	O2D-CGD-O1D	-3.76	116.54	123.85
21	5	303	A1L1G	C36-C37-C38	3.75	131.20	123.52
20	3	301	XAT	C31-C30-C29	-3.73	122.05	127.28
20	a	852	XAT	C35-C34-C33	-3.72	122.06	127.28
20	2	303	XAT	C26-C27-C28	-3.71	118.14	125.99
29	h	202	BCR	C7-C8-C9	-3.71	120.75	126.23
20	3	301	XAT	C26-C27-C28	-3.70	118.17	125.99
29	a	849	BCR	C4-C5-C6	-3.70	117.71	122.70
29	a	849	BCR	C20-C21-C22	-3.70	122.09	127.28
24	9	302	A1L1F	C32-C31-C30	-3.69	122.09	127.23
29	b	843	BCR	C3-C4-C5	-3.69	107.47	114.06
20	2	301	XAT	C27-C28-C29	-3.69	119.81	125.53
21	9	306	A1L1G	C37-C36-C35	3.68	131.04	123.52
20	8	301	XAT	C11-C10-C9	-3.67	122.13	127.28
20	2	303	XAT	C6-C7-C8	-3.67	118.24	125.99
20	7	304	XAT	C6-C7-C8	-3.66	118.25	125.99
20	9	305	XAT	C31-C30-C29	-3.65	122.17	127.28
29	a	847	BCR	C33-C5-C6	-3.64	120.51	124.48
21	7	302	A1L1G	C37-C36-C35	3.64	130.97	123.52
20	4	302	XAT	C35-C15-C14	-3.64	116.08	123.52
29	i	101	BCR	C33-C5-C6	-3.64	120.52	124.48
20	8	303	XAT	C30-C31-C32	-3.63	112.69	123.20
20	8	301	XAT	C6-C7-C8	-3.62	118.33	125.99
20	1	302	XAT	C11-C10-C9	-3.62	122.20	127.28
29	b	843	BCR	C33-C5-C6	-3.62	120.54	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	845	BCR	C3-C4-C5	-3.61	107.62	114.06
29	b	845	BCR	C10-C11-C12	-3.60	112.75	123.20
22	a	806	CLA	CAA-CBA-CGA	-3.60	102.98	113.21
29	a	849	BCR	C11-C10-C9	-3.60	122.23	127.28
29	a	847	BCR	C7-C8-C9	-3.60	120.91	126.23
20	9	303	XAT	C11-C10-C9	-3.59	122.24	127.28
29	h	202	BCR	C38-C26-C25	-3.59	120.56	124.48
20	j	101	XAT	C10-C11-C12	-3.59	112.81	123.20
24	8	304	A1L1F	C31-C32-C33	-3.59	112.81	123.20
29	l	205	BCR	C11-C10-C9	-3.58	122.26	127.28
20	2	305	XAT	C24-C23-C22	-3.58	104.10	110.79
20	4	303	XAT	C35-C34-C33	-3.57	122.27	127.28
29	a	847	BCR	C15-C14-C13	-3.57	122.28	127.28
29	h	201	BCR	C24-C23-C22	-3.57	120.96	126.23
29	a	848	BCR	C24-C23-C22	-3.56	120.96	126.23
20	8	303	XAT	C15-C35-C34	-3.56	116.24	123.52
20	1	303	XAT	C15-C14-C13	-3.54	122.32	127.28
22	9	312	CLA	CAA-C2A-C3A	-3.54	103.44	113.00
29	l	205	BCR	C3-C4-C5	-3.54	107.75	114.06
20	8	302	XAT	C31-C30-C29	-3.53	122.33	127.28
24	1	304	A1L1F	C8-O7-C54	-3.52	111.62	117.85
20	9	303	XAT	C35-C34-C33	-3.52	122.34	127.28
21	9	301	A1L1G	C36-C37-C38	3.52	130.72	123.52
21	9	306	A1L1G	C36-C37-C38	3.50	130.69	123.52
20	4	302	XAT	C11-C10-C9	-3.50	122.38	127.28
29	a	847	BCR	C24-C23-C22	-3.49	121.07	126.23
29	a	849	BCR	C7-C8-C9	-3.49	121.08	126.23
24	h	204	A1L1F	C31-C32-C33	-3.48	113.11	123.20
23	5	316	SQD	O47-C7-C8	3.48	119.01	111.48
21	7	302	A1L1G	C36-C37-C38	3.48	130.64	123.52
29	i	101	BCR	C28-C27-C26	-3.48	107.86	114.06
20	2	304	XAT	C11-C10-C9	-3.47	122.42	127.28
20	3	305	XAT	C15-C14-C13	-3.47	122.42	127.28
22	b	804	CLA	CHB-C4A-NA	3.47	129.40	124.40
29	a	849	BCR	C24-C23-C22	-3.46	121.11	126.23
29	a	848	BCR	C20-C21-C22	-3.46	122.43	127.28
20	3	303	XAT	C11-C10-C9	-3.45	122.43	127.28
20	a	852	XAT	C10-C11-C12	-3.45	113.19	123.20
20	2	304	XAT	C31-C30-C29	-3.45	122.44	127.28
22	9	314	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
21	3	302	A1L1G	C36-C37-C38	3.45	130.57	123.52
29	a	847	BCR	C11-C10-C9	-3.44	122.45	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	304	XAT	C31-C30-C29	-3.44	122.45	127.28
22	a	806	CLA	C3B-C4B-NB	-3.44	107.46	110.53
21	3	302	A1L1G	C37-C36-C35	3.44	130.55	123.52
24	8	304	A1L1F	C14-C29-C30	-3.44	119.62	125.47
24	9	302	A1L1F	C37-C38-C39	-3.43	122.47	127.28
20	1	303	XAT	C24-C23-C22	-3.42	104.39	110.79
20	5	302	XAT	C6-C7-C8	-3.41	118.78	125.99
20	5	304	XAT	C24-C23-C22	-3.40	104.43	110.79
20	9	304	XAT	C35-C34-C33	-3.39	122.52	127.28
26	b	848	DGD	C2G-O2G-C1B	-3.39	109.68	117.80
20	9	305	XAT	C38-C25-C26	-3.38	116.74	122.30
20	5	301	XAT	C24-C23-C22	-3.38	104.47	110.79
29	j	104	BCR	C24-C23-C22	-3.37	121.24	126.23
29	h	202	BCR	C11-C10-C9	-3.37	122.55	127.28
20	5	304	XAT	C4-C3-C2	-3.37	104.49	110.79
29	b	846	BCR	C10-C11-C12	-3.37	113.45	123.20
21	5	303	A1L1G	C37-C36-C35	3.36	130.38	123.52
20	5	301	XAT	C7-C8-C9	-3.35	120.33	125.53
20	1	303	XAT	C31-C30-C29	-3.35	122.58	127.28
22	5	312	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
29	i	101	BCR	C15-C14-C13	-3.34	122.60	127.28
24	1	304	A1L1F	C14-C29-C30	-3.33	119.80	125.47
22	b	804	CLA	C3B-C4B-NB	-3.33	107.56	110.53
29	a	847	BCR	C3-C4-C5	-3.32	108.14	114.06
20	4	301	XAT	C11-C10-C9	-3.32	122.63	127.28
20	5	301	XAT	C6-C7-C8	-3.31	118.98	125.99
24	8	304	A1L1F	C26-C30-C31	-3.31	120.77	124.97
20	4	303	XAT	C6-C7-C8	-3.31	119.00	125.99
29	a	850	BCR	C7-C8-C9	-3.31	121.34	126.23
29	i	101	BCR	C11-C10-C9	-3.30	122.65	127.28
22	9	311	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
24	9	302	A1L1F	C25-C14-C29	-3.29	119.04	125.99
21	1	301	A1L1G	C36-C37-C38	3.28	130.23	123.52
20	9	304	XAT	C24-C23-C22	-3.27	104.67	110.79
24	h	204	A1L1F	C17-C20-C21	3.27	117.92	114.24
24	9	302	A1L1F	C42-C41-C40	-3.27	113.72	123.20
20	9	304	XAT	C11-C10-C9	-3.27	122.69	127.28
29	b	849	BCR	C24-C23-C22	-3.26	121.41	126.23
21	9	301	A1L1G	C33-C34-C35	3.26	124.14	119.01
20	4	304	XAT	C24-C23-C22	-3.26	104.69	110.79
20	9	305	XAT	C24-C23-C22	-3.26	104.69	110.79
22	j	103	CLA	O2D-CGD-O1D	-3.26	117.50	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	809	CLA	O2A-CGA-O1A	-3.26	115.48	123.63
20	4	303	XAT	C24-C23-C22	-3.25	104.70	110.79
20	9	303	XAT	C24-C23-C22	-3.25	104.71	110.79
24	9	302	A1L1F	O15-C25-C14	-3.25	107.58	116.88
20	3	303	XAT	C24-C23-C22	-3.24	104.72	110.79
29	a	848	BCR	C33-C5-C6	-3.24	120.95	124.48
29	a	848	BCR	C38-C26-C25	-3.24	120.95	124.48
29	b	849	BCR	C33-C5-C6	-3.24	120.95	124.48
29	l	201	BCR	C38-C26-C25	-3.24	120.95	124.48
20	1	302	XAT	C15-C14-C13	-3.24	122.74	127.28
20	a	852	XAT	C11-C10-C9	-3.24	122.74	127.28
28	a	843	PQN	C14-C13-C15	3.23	120.84	115.23
29	h	201	BCR	C20-C21-C22	-3.23	122.75	127.28
20	4	304	XAT	C15-C14-C13	-3.23	122.75	127.28
22	b	830	CLA	C3B-C4B-NB	-3.22	107.66	110.53
29	l	201	BCR	C24-C23-C22	-3.22	121.47	126.23
22	b	820	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
26	4	318	DGD	O1G-C1A-C2A	3.21	121.63	111.83
20	3	304	XAT	C11-C10-C9	-3.21	122.77	127.28
20	8	301	XAT	C24-C23-C22	-3.21	104.78	110.79
24	h	204	A1L1F	C37-C36-C35	-3.20	116.96	123.52
22	a	835	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
20	3	304	XAT	C26-C27-C28	-3.20	119.23	125.99
29	a	849	BCR	C38-C26-C25	-3.20	121.00	124.48
20	7	304	XAT	C24-C23-C22	-3.19	104.82	110.79
20	7	305	XAT	C35-C34-C33	-3.19	122.81	127.28
29	a	850	BCR	C11-C10-C9	-3.19	122.81	127.28
20	2	301	XAT	C11-C10-C9	-3.18	122.81	127.28
29	b	843	BCR	C16-C17-C18	-3.18	122.82	127.28
20	3	304	XAT	C4-C3-C2	-3.17	104.85	110.79
22	7	316	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
22	a	804	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
22	b	817	CLA	C3B-C4B-NB	-3.17	107.70	110.53
26	8	315	DGD	O1G-C1A-C2A	3.17	121.49	111.83
22	1	313	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
20	9	303	XAT	C6-C7-C8	-3.16	119.32	125.99
22	a	818	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
21	3	306	A1L1G	C37-C36-C35	3.15	129.97	123.52
20	4	303	XAT	C30-C31-C32	-3.15	114.07	123.20
29	a	848	BCR	C3-C4-C5	-3.14	108.45	114.06
24	8	304	A1L1F	C36-C35-C34	-3.14	122.88	127.28
29	b	845	BCR	C11-C10-C9	-3.13	122.88	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	l	205	BCR	C8-C7-C6	-3.13	118.63	127.00
20	4	305	XAT	C24-C23-C22	-3.12	104.95	110.79
20	8	302	XAT	C24-C23-C22	-3.12	104.95	110.79
21	9	306	A1L1G	C33-C34-C35	3.12	123.92	119.01
20	2	301	XAT	C26-C27-C28	-3.12	119.39	125.99
22	b	832	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
22	b	809	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
20	3	305	XAT	C4-C3-C2	-3.12	104.96	110.79
29	h	201	BCR	C38-C26-C25	-3.12	121.08	124.48
22	a	819	CLA	C3B-C4B-NB	-3.12	107.75	110.53
29	f	801	BCR	C8-C7-C6	-3.12	118.67	127.00
22	4	316	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
24	9	302	A1L1F	C26-C30-C31	-3.11	121.02	124.97
20	a	852	XAT	C35-C15-C14	-3.11	117.17	123.52
29	a	848	BCR	C8-C7-C6	-3.10	118.71	127.00
29	b	842	BCR	C20-C21-C22	-3.10	122.93	127.28
22	3	308	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
24	8	304	A1L1F	O15-C25-C14	-3.10	108.00	116.88
20	4	304	XAT	C35-C15-C14	-3.09	117.19	123.52
20	8	303	XAT	C24-C23-C22	-3.09	105.00	110.79
20	a	852	XAT	C31-C32-C33	-3.08	117.91	126.36
22	4	311	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
20	1	302	XAT	C31-C30-C29	-3.08	122.96	127.28
20	7	305	XAT	C4-C3-C2	-3.08	105.03	110.79
20	5	301	XAT	C31-C30-C29	-3.07	122.97	127.28
22	a	832	CLA	C3B-C4B-NB	-3.07	107.79	110.53
22	a	854	CLA	C3B-C4B-NB	-3.07	107.79	110.53
21	1	301	A1L1G	C33-C34-C35	3.07	123.84	119.01
24	8	304	A1L1F	C25-C14-C29	-3.07	119.51	125.99
22	a	809	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
21	5	303	A1L1G	C40-C39-C38	3.06	123.83	119.01
22	a	802	CLA	C3B-C4B-NB	-3.06	107.80	110.53
25	a	846	LHG	O8-C23-C24	3.06	120.44	111.15
22	4	307	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
20	9	305	XAT	C8-C9-C10	3.06	123.82	119.01
22	b	816	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
20	3	305	XAT	C24-C23-C22	-3.05	105.08	110.79
22	8	308	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
22	a	807	CLA	C3B-C4B-NB	-3.05	107.81	110.53
22	4	312	CLA	C3B-C4B-NB	-3.05	107.81	110.53
20	8	303	XAT	C4-C3-C2	-3.05	105.09	110.79
22	9	313	CLA	O2D-CGD-O1D	-3.04	117.92	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	202	BCR	C15-C14-C13	-3.04	123.01	127.28
22	9	311	CLA	C3B-C4B-NB	-3.04	107.82	110.53
29	h	201	BCR	C8-C7-C6	-3.04	118.88	127.00
29	h	201	BCR	C4-C5-C6	-3.03	118.61	122.70
22	a	831	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
20	4	304	XAT	C4-C3-C2	-3.03	105.12	110.79
22	a	813	CLA	C3B-C4B-NB	-3.03	107.82	110.53
29	b	846	BCR	C8-C7-C6	-3.03	118.90	127.00
22	9	310	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
29	h	202	BCR	C16-C15-C14	-3.03	117.32	123.52
22	7	314	CLA	C3B-C4B-NB	-3.03	107.83	110.53
21	9	301	A1L1G	C27-C34-C35	-3.03	117.91	122.82
22	4	315	CLA	C3B-C4B-NB	-3.03	107.83	110.53
22	3	315	CLA	C3B-C4B-NB	-3.02	107.83	110.53
20	7	305	XAT	C24-C23-C22	-3.02	105.14	110.79
29	b	846	BCR	C21-C20-C19	-3.02	114.45	123.20
22	a	841	CLA	C3B-C4B-NB	-3.02	107.84	110.53
20	7	301	XAT	C4-C3-C2	-3.02	105.15	110.79
22	b	811	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
24	h	204	A1L1F	C12-C6-C1	-3.01	107.78	110.47
20	5	302	XAT	C24-C23-C22	-3.01	105.16	110.79
20	3	301	XAT	C4-C3-C2	-3.01	105.16	110.79
22	b	808	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
22	9	314	CLA	O2D-CGD-CBD	3.01	116.49	111.23
28	b	841	PQN	C16-C15-C13	-3.01	106.14	113.47
20	3	305	XAT	C31-C30-C29	-3.01	123.06	127.28
20	4	301	XAT	C31-C32-C33	-3.01	118.12	126.36
20	4	302	XAT	C24-C23-C22	-3.01	105.17	110.79
20	1	302	XAT	C4-C3-C2	-3.00	105.17	110.79
20	2	303	XAT	C4-C3-C2	-3.00	105.18	110.79
20	2	304	XAT	C24-C23-C22	-3.00	105.18	110.79
22	3	307	CLA	C3B-C4B-NB	-3.00	107.85	110.53
21	1	301	A1L1G	C40-C39-C38	3.00	123.72	119.01
29	b	843	BCR	C38-C26-C25	-3.00	121.22	124.48
22	1	314	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
22	9	318	CLA	C3B-C4B-NB	-3.00	107.86	110.53
20	9	305	XAT	C27-C28-C29	-2.99	120.88	125.53
22	b	809	CLA	C3B-C4B-NB	-2.99	107.86	110.53
22	b	814	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
29	b	849	BCR	C16-C15-C14	-2.99	117.40	123.52
21	3	302	A1L1G	C33-C34-C35	2.99	123.71	119.01
21	3	306	A1L1G	C40-C39-C38	2.99	123.71	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	302	XAT	C35-C15-C14	-2.99	117.40	123.52
20	8	302	XAT	C6-C7-C8	-2.99	119.68	125.99
21	7	302	A1L1G	C40-C39-C38	2.99	123.71	119.01
22	a	830	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
20	9	304	XAT	C30-C31-C32	-2.98	114.56	123.20
21	7	302	A1L1G	C33-C34-C35	2.98	123.70	119.01
22	b	836	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
20	1	302	XAT	C24-C23-C22	-2.98	105.22	110.79
21	9	306	A1L1G	C40-C39-C38	2.98	123.69	119.01
22	7	313	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
22	2	309	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	a	822	CLA	C3B-C4B-NB	-2.97	107.88	110.53
29	b	843	BCR	C21-C20-C19	-2.97	114.59	123.20
22	2	313	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
22	a	820	CLA	C1-C2-C3	-2.97	121.33	126.20
22	b	834	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	b	845	BCR	C33-C5-C6	-2.97	121.25	124.48
20	3	303	XAT	C4-C3-C2	-2.97	105.24	110.79
20	3	301	XAT	C10-C11-C12	-2.97	114.61	123.20
22	4	308	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
22	4	309	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
29	b	844	BCR	C38-C26-C25	-2.96	121.25	124.48
22	a	839	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
22	8	314	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	b	805	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
20	a	852	XAT	C24-C23-C22	-2.96	105.25	110.79
22	7	308	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	2	316	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	a	812	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
22	a	808	CLA	C3B-C4B-NB	-2.95	107.89	110.53
22	h	203	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
22	7	314	CLA	CHB-C4A-NA	2.95	128.66	124.40
29	a	849	BCR	C2-C1-C6	2.95	114.72	110.44
29	a	850	BCR	C28-C27-C26	-2.95	108.80	114.06
22	b	839	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
22	b	824	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
29	h	202	BCR	C23-C24-C25	-2.94	119.14	127.00
20	4	302	XAT	C4-C3-C2	-2.94	105.29	110.79
22	9	309	CLA	C3B-C4B-NB	-2.94	107.91	110.53
22	1	311	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	8	313	CLA	C3B-C4B-NB	-2.94	107.91	110.53
24	1	304	A1L1F	C26-O13-C45	2.94	121.80	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	309	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	1	312	CLA	C3B-C4B-NB	-2.94	107.91	110.53
21	7	302	A1L1G	C27-C34-C35	-2.93	118.06	122.82
22	b	829	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	j	102	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	b	818	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	a	817	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	7	317	CLA	C3B-C4B-NB	-2.93	107.92	110.53
20	2	304	XAT	C4-C3-C2	-2.93	105.31	110.79
22	h	203	CLA	C1-C2-C3	-2.93	121.40	126.20
22	8	310	CLA	C3B-C4B-NB	-2.93	107.92	110.53
22	f	803	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	5	302	XAT	C35-C34-C33	-2.92	123.18	127.28
22	b	817	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	2	309	CLA	C3B-C4B-NB	-2.92	107.92	110.53
22	a	818	CLA	C3B-C4B-NB	-2.92	107.92	110.53
22	5	315	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
26	b	848	DGD	O3E-C3E-C2E	-2.92	103.49	110.38
21	9	301	A1L1G	C40-C39-C38	2.92	123.60	119.01
22	b	814	CLA	CHB-C4A-NA	2.92	128.61	124.40
22	4	317	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	j	101	XAT	C4-C3-C2	-2.92	105.33	110.79
29	f	801	BCR	C20-C19-C18	-2.92	118.36	126.36
22	b	826	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	a	840	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
22	5	306	CLA	C3B-C4B-NB	-2.92	107.93	110.53
22	b	816	CLA	C3B-C4B-NB	-2.91	107.93	110.53
20	1	303	XAT	C4-C3-C2	-2.91	105.34	110.79
22	3	307	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
21	9	306	A1L1G	C28-C39-C38	-2.91	118.10	122.82
22	a	842	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	a	833	CLA	C3B-C4B-NB	-2.91	107.93	110.53
20	4	301	XAT	C4-C3-C2	-2.91	105.35	110.79
20	9	304	XAT	C4-C3-C2	-2.91	105.35	110.79
22	2	310	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
29	f	801	BCR	C33-C5-C6	-2.90	121.31	124.48
29	b	842	BCR	C4-C5-C6	-2.90	118.78	122.70
20	3	304	XAT	C24-C23-C22	-2.90	105.36	110.79
21	5	303	A1L1G	C28-C39-C38	-2.90	118.11	122.82
22	4	312	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
22	b	838	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	5	312	CLA	O2D-CGD-CBD	2.90	116.30	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	304	XAT	C19-C9-C8	2.90	122.52	118.09
22	a	837	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	3	306	A1L1G	C27-C34-C35	-2.90	118.12	122.82
21	1	301	A1L1G	C28-C39-C38	-2.90	118.12	122.82
20	2	301	XAT	C4-C3-C2	-2.90	105.37	110.79
29	a	848	BCR	C7-C8-C9	-2.90	121.95	126.23
21	7	302	A1L1G	C28-C39-C38	-2.90	118.12	122.82
22	1	202	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
22	7	315	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	a	828	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	b	846	BCR	C15-C16-C17	-2.89	117.60	123.52
22	7	307	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	8	311	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
21	5	303	A1L1G	C33-C34-C35	2.89	123.56	119.01
20	1	303	XAT	C10-C11-C12	-2.89	114.82	123.20
20	8	303	XAT	C11-C10-C9	-2.89	123.22	127.28
22	b	806	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
22	a	813	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
22	a	820	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
22	1	310	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	8	306	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
21	3	306	A1L1G	C33-C34-C35	2.89	123.55	119.01
22	4	314	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	7	315	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
22	5	307	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
21	1	301	A1L1G	C27-C34-C35	-2.89	118.14	122.82
22	a	804	CLA	C1-C2-C3	-2.89	121.47	126.20
22	7	312	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
21	9	306	A1L1G	C27-C34-C35	-2.88	118.14	122.82
22	2	316	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
26	b	848	DGD	O1G-C1A-C2A	2.88	120.63	111.83
22	b	819	CLA	C3B-C4B-NB	-2.88	107.96	110.53
22	b	834	CLA	C3B-C4B-NB	-2.88	107.96	110.53
21	3	302	A1L1G	C40-C39-C38	2.88	123.54	119.01
22	2	314	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	1	307	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
24	8	304	A1L1F	C11-C1-C6	2.88	122.55	119.70
29	h	201	BCR	C10-C11-C12	-2.88	114.86	123.20
20	2	305	XAT	C11-C10-C9	-2.88	123.24	127.28
22	8	310	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	2	307	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
22	a	823	CLA	O2D-CGD-O1D	-2.87	118.25	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	304	A1L1F	C17-C20-C21	2.87	117.47	114.24
20	9	304	XAT	C15-C35-C34	-2.87	117.64	123.52
22	a	825	CLA	C3B-C4B-NB	-2.87	107.97	110.53
20	2	301	XAT	C24-C23-C22	-2.87	105.42	110.79
22	7	311	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	1	314	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	a	811	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
21	9	301	A1L1G	C28-C39-C38	-2.87	118.17	122.82
22	b	838	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
22	3	311	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
20	4	305	XAT	C4-C3-C2	-2.86	105.44	110.79
27	2	317	LMG	O8-C28-C29	2.86	120.56	111.83
22	8	312	CLA	C3B-C4B-NB	-2.86	107.97	110.53
22	b	837	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	3	302	A1L1G	C28-C39-C38	-2.86	118.18	122.82
22	1	312	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	8	305	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
26	4	318	DGD	O5E-C6E-C5E	-2.86	101.60	111.33
20	2	305	XAT	C38-C25-C26	-2.86	117.60	122.30
20	5	304	XAT	C10-C11-C12	-2.86	114.92	123.20
22	5	309	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
22	5	310	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
24	h	204	A1L1F	C26-C30-C31	-2.86	121.35	124.97
22	a	836	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	a	816	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
22	4	307	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	3	313	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
29	b	842	BCR	C2-C1-C6	2.85	114.58	110.44
22	9	312	CLA	CHB-C4A-NA	2.85	128.51	124.40
22	a	817	CLA	C3B-C4B-NB	-2.85	107.99	110.53
22	7	312	CLA	C3B-C4B-NB	-2.85	107.99	110.53
22	5	305	CLA	C3B-C4B-NB	-2.85	107.99	110.53
22	2	307	CLA	C3B-C4B-NB	-2.84	107.99	110.53
22	9	315	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
22	j	103	CLA	C3B-C4B-NB	-2.84	107.99	110.53
22	a	805	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	8	303	XAT	C39-C29-C28	2.84	122.43	118.09
22	8	309	CLA	C3B-C4B-NB	-2.84	107.99	110.53
22	a	834	CLA	C3B-C4B-NB	-2.84	108.00	110.53
22	b	823	CLA	C3B-C4B-NB	-2.84	108.00	110.53
22	2	307	CLA	CHB-C4A-NA	2.84	128.50	124.40
22	8	313	CLA	O2D-CGD-O1D	-2.84	118.32	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	314	CLA	C3B-C4B-NB	-2.84	108.00	110.53
27	a	853	LMG	O8-C28-C29	2.84	120.49	111.83
28	a	843	PQN	C11-C3-C2	-2.84	120.03	124.89
22	4	316	CLA	C3B-C4B-NB	-2.84	108.00	110.53
22	1	305	CLA	C3B-C4B-NB	-2.84	108.00	110.53
29	i	101	BCR	C29-C30-C25	2.83	114.56	110.44
22	a	825	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
21	5	303	A1L1G	C27-C34-C35	-2.83	118.22	122.82
21	3	302	A1L1G	C27-C34-C35	-2.83	118.22	122.82
22	2	310	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	a	826	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
22	7	315	CLA	CAA-C2A-C3A	-2.83	109.73	116.23
22	7	306	CLA	C3B-C4B-NB	-2.83	108.00	110.53
22	8	312	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	2	305	XAT	C4-C3-C2	-2.83	105.50	110.79
22	4	311	CLA	C3B-C4B-NB	-2.83	108.01	110.53
22	1	203	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
22	3	312	CLA	C3B-C4B-NB	-2.83	108.01	110.53
22	7	310	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
24	8	304	A1L1F	O7-C54-O55	-2.82	117.54	122.99
21	3	306	A1L1G	C28-C39-C38	-2.82	118.24	122.82
22	5	308	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
22	9	313	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	j	102	CLA	C3B-C4B-NB	-2.82	108.01	110.53
24	8	304	A1L1F	O13-C45-C47	2.82	120.44	111.83
22	8	307	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	a	844	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
22	8	306	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	a	815	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	9	302	A1L1F	O13-C45-C47	2.82	120.43	111.83
20	7	305	XAT	C15-C35-C34	-2.82	117.75	123.52
22	4	306	CLA	C3B-C4B-NB	-2.82	108.02	110.53
22	1	313	CLA	C3B-C4B-NB	-2.82	108.02	110.53
22	a	831	CLA	CMB-C2B-C1B	-2.82	121.13	125.42
22	5	313	CLA	C3B-C4B-NB	-2.82	108.02	110.53
24	h	204	A1L1F	O13-C45-C47	2.82	120.42	111.83
22	7	307	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
22	b	828	CLA	C3B-C4B-NB	-2.81	108.02	110.53
22	a	833	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
22	5	309	CLA	C3B-C4B-NB	-2.81	108.02	110.53
29	f	801	BCR	C10-C11-C12	-2.81	115.05	123.20
29	h	202	BCR	C21-C20-C19	-2.81	115.05	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	204	A1L1F	C8-O7-C54	-2.81	112.88	117.85
22	a	836	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	a	803	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	b	827	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	7	306	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
29	h	201	BCR	C33-C5-C4	2.81	119.58	113.60
22	4	313	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	a	827	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
20	9	303	XAT	C30-C31-C32	-2.81	115.07	123.20
22	a	824	CLA	C3B-C4B-NB	-2.81	108.03	110.53
29	b	844	BCR	C20-C21-C22	-2.81	123.34	127.28
23	1	315	SQD	O48-C23-C24	2.81	120.39	111.83
22	b	831	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
22	a	832	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
20	9	303	XAT	C15-C35-C34	-2.80	117.78	123.52
24	1	304	A1L1F	C36-C35-C34	-2.80	123.35	127.28
22	a	802	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
29	b	842	BCR	C38-C26-C25	-2.80	121.43	124.48
22	1	310	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
22	5	310	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	2	308	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	b	840	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	3	314	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
20	4	304	XAT	C11-C10-C9	-2.80	123.36	127.28
22	a	811	CLA	C3B-C4B-NB	-2.80	108.03	110.53
20	j	101	XAT	C24-C23-C22	-2.80	105.56	110.79
22	1	305	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
29	m	101	BCR	C27-C26-C25	2.79	126.48	122.70
22	9	310	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	5	315	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	b	813	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	b	821	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	9	308	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	b	801	CLA	C3B-C4B-NB	-2.79	108.04	110.53
22	a	821	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	8	314	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	b	801	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	b	823	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	9	308	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
29	j	104	BCR	C23-C24-C25	-2.79	119.55	127.00
22	8	309	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	1	308	CLA	O2D-CGD-O1D	-2.79	118.42	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	841	CLA	CHB-C4A-NA	2.79	128.42	124.40
20	2	302	XAT	C24-C23-C22	-2.78	105.58	110.79
22	a	841	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
29	a	849	BCR	C33-C5-C4	2.78	119.53	113.60
22	b	828	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
22	b	812	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	h	205	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	b	832	CLA	C3B-C4B-NB	-2.78	108.05	110.53
20	3	301	XAT	C19-C9-C8	2.78	122.33	118.09
22	b	815	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	a	837	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	h	205	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
22	7	317	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
22	b	815	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	4	302	XAT	C31-C30-C29	-2.77	123.39	127.28
20	7	301	XAT	C11-C10-C9	-2.77	123.39	127.28
22	4	310	CLA	C3B-C4B-NB	-2.77	108.05	110.53
22	4	313	CLA	C3B-C4B-NB	-2.77	108.05	110.53
22	l	203	CLA	C3B-C4B-NB	-2.77	108.05	110.53
29	h	201	BCR	C2-C1-C6	2.77	114.47	110.44
22	1	308	CLA	C1-C2-C3	-2.77	121.65	126.20
22	1	306	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
22	9	311	CLA	CHB-C4A-NA	2.77	128.40	124.40
22	3	315	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
29	b	845	BCR	C35-C13-C12	2.77	122.32	118.09
22	2	306	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	9	317	LHG	O8-C23-C24	2.77	120.28	111.83
22	a	819	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
29	i	101	BCR	C20-C19-C18	-2.77	118.77	126.36
22	9	312	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
20	3	303	XAT	C31-C30-C29	-2.77	123.39	127.28
22	b	805	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	5	313	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
22	9	316	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
22	a	839	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	3	312	CLA	CHB-C4A-NA	2.77	128.39	124.40
29	h	201	BCR	C7-C8-C9	-2.77	122.14	126.23
22	b	830	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
23	5	316	SQD	O48-C23-C24	2.76	120.25	111.83
20	5	302	XAT	C4-C3-C2	-2.76	105.63	110.79
22	5	308	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	b	840	CLA	C3B-C4B-NB	-2.76	108.07	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	806	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	b	836	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	4	306	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
22	2	313	CLA	CAA-C2A-C3A	-2.76	109.90	116.23
20	4	301	XAT	C26-C27-C28	-2.76	120.16	125.99
22	2	315	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
22	3	311	CLA	C3B-C4B-NB	-2.76	108.07	110.53
22	l	204	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
22	a	807	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
22	b	835	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
22	a	828	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
22	b	812	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
20	9	304	XAT	C7-C8-C9	-2.75	121.26	125.53
29	h	202	BCR	C24-C23-C22	-2.75	122.17	126.23
22	3	314	CLA	C3B-C4B-NB	-2.75	108.08	110.53
22	5	314	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
22	a	838	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
22	a	824	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
29	b	842	BCR	C23-C24-C25	-2.75	119.66	127.00
29	b	849	BCR	C20-C19-C18	-2.75	118.83	126.36
22	5	305	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
20	2	301	XAT	C31-C32-C33	-2.75	118.83	126.36
22	9	315	CLA	C3B-C4B-NB	-2.75	108.08	110.53
22	f	802	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
22	f	803	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
22	a	820	CLA	C3B-C4B-NB	-2.74	108.08	110.53
22	b	810	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
22	b	819	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
22	b	825	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
22	a	827	CLA	C3B-C4B-NB	-2.74	108.08	110.53
22	b	817	CLA	CMB-C2B-C1B	-2.74	121.25	125.42
20	3	305	XAT	C35-C15-C14	-2.74	117.92	123.52
22	3	313	CLA	C3B-C4B-NB	-2.74	108.09	110.53
20	4	303	XAT	C39-C29-C28	2.74	122.27	118.09
22	a	801	CLA	C3B-C4B-NB	-2.74	108.09	110.53
22	2	313	CLA	C3B-C4B-NB	-2.74	108.09	110.53
20	3	301	XAT	C24-C23-C22	-2.74	105.67	110.79
22	2	312	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
22	5	314	CLA	C3B-C4B-NB	-2.73	108.09	110.53
29	b	842	BCR	C24-C23-C22	-2.73	122.19	126.23
22	b	829	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
20	4	303	XAT	C4-C3-C2	-2.73	105.68	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	314	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
22	1	309	CLA	C3B-C4B-NB	-2.73	108.09	110.53
20	j	101	XAT	C15-C35-C34	-2.73	117.94	123.52
21	1	301	A1L1G	C43-C44-C42	-2.73	118.40	122.82
22	b	831	CLA	C3B-C4B-NB	-2.73	108.10	110.53
22	a	815	CLA	C3B-C4B-NB	-2.72	108.10	110.53
20	8	302	XAT	C4-C3-C2	-2.72	105.70	110.79
20	j	101	XAT	C31-C32-C33	-2.72	118.90	126.36
20	2	302	XAT	C35-C15-C14	-2.72	117.95	123.52
22	9	310	CLA	CHB-C4A-NA	2.72	128.32	124.40
22	7	311	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
22	a	816	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	9	309	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	a	808	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	b	822	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
22	b	830	CLA	CAA-C2A-C3A	-2.71	110.02	116.23
22	4	315	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
20	7	303	XAT	C4-C3-C2	-2.70	105.73	110.79
20	7	303	XAT	C24-C23-C22	-2.70	105.73	110.79
20	7	304	XAT	C4-C3-C2	-2.70	105.73	110.79
22	7	309	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	b	824	CLA	C3B-C4B-NB	-2.70	108.12	110.53
20	8	301	XAT	C7-C8-C9	-2.70	121.34	125.53
20	4	302	XAT	C15-C14-C13	-2.70	123.49	127.28
22	a	814	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	b	847	LHG	O8-C23-C24	2.70	120.06	111.83
22	a	802	CLA	C1-C2-C3	-2.70	121.78	126.20
22	3	312	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
22	7	313	CLA	C3B-C4B-NB	-2.69	108.12	110.53
22	a	812	CLA	C3B-C4B-NB	-2.69	108.12	110.53
29	h	202	BCR	C20-C21-C22	-2.69	123.50	127.28
25	9	307	LHG	O8-C23-C24	2.69	120.05	111.83
24	1	304	A1L1F	O15-C25-C14	-2.69	109.16	116.88
22	a	814	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
20	4	305	XAT	C31-C32-C33	-2.69	118.98	126.36
24	1	304	A1L1F	C26-C30-C31	-2.69	121.55	124.97
22	4	309	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	4	315	CLA	CHB-C4A-NA	2.69	128.28	124.40
22	7	317	CLA	CHB-C4A-NA	2.69	128.28	124.40
20	8	301	XAT	C4-C3-C2	-2.69	105.76	110.79
22	a	822	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
22	a	810	CLA	C3B-C4B-NB	-2.69	108.13	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	j	101	XAT	C31-C30-C29	-2.68	123.51	127.28
27	j	105	LMG	O8-C28-C29	2.68	120.02	111.83
22	2	311	CLA	C3B-C4B-NB	-2.68	108.13	110.53
22	5	307	CLA	C3B-C4B-NB	-2.68	108.14	110.53
29	m	101	BCR	C33-C5-C6	-2.68	121.56	124.48
22	a	841	CLA	C1-C2-C3	-2.68	121.81	126.20
22	b	814	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	5	312	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	2	315	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	b	825	CLA	C3B-C4B-NB	-2.68	108.14	110.53
29	b	846	BCR	C24-C23-C22	-2.68	122.27	126.23
22	l	203	CLA	CHB-C4A-NA	2.68	128.26	124.40
20	2	304	XAT	C15-C14-C13	-2.68	123.53	127.28
29	a	847	BCR	C16-C15-C14	-2.68	118.05	123.52
22	b	837	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	l	202	CLA	C3B-C4B-NB	-2.68	108.14	110.53
29	b	844	BCR	C11-C10-C9	-2.67	123.53	127.28
22	4	310	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
20	5	304	XAT	C31-C30-C29	-2.67	123.53	127.28
24	1	304	A1L1F	O13-C45-C47	2.67	119.98	111.83
22	4	315	CLA	CAA-C2A-C3A	-2.67	110.11	116.23
22	5	306	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
23	5	316	SQD	C44-O6-C1	-2.66	108.08	113.80
20	8	303	XAT	C35-C34-C33	-2.66	123.54	127.28
25	a	845	LHG	O8-C23-C24	2.66	119.96	111.83
22	a	834	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
22	8	307	CLA	C3B-C4B-NB	-2.66	108.16	110.53
20	3	301	XAT	C27-C28-C29	-2.66	121.41	125.53
22	5	314	CLA	CHB-C4A-NA	2.66	128.24	124.40
22	a	805	CLA	CHB-C4A-NA	2.66	128.24	124.40
29	f	801	BCR	C2-C1-C6	2.66	114.30	110.44
22	b	807	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
20	4	304	XAT	C31-C30-C29	-2.66	123.55	127.28
28	b	841	PQN	C2M-C2-C3	-2.65	120.09	124.45
26	b	848	DGD	C1E-O6E-C5E	2.65	118.90	113.72
20	5	304	XAT	C30-C31-C32	-2.65	115.52	123.20
22	1	308	CLA	C3B-C4B-NB	-2.65	108.17	110.53
20	5	301	XAT	C35-C15-C14	-2.65	118.10	123.52
20	2	305	XAT	C31-C32-C33	-2.65	119.10	126.36
22	4	317	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
29	j	104	BCR	C27-C26-C25	-2.65	119.13	122.70
20	4	305	XAT	C7-C8-C9	-2.64	121.43	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	824	CLA	CHB-C4A-NA	2.64	128.22	124.40
22	a	810	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
22	b	802	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
20	4	301	XAT	C27-C28-C29	-2.64	121.44	125.53
22	b	833	CLA	C3B-C4B-NB	-2.64	108.18	110.53
22	5	311	CLA	C3B-C4B-NB	-2.63	108.18	110.53
20	9	303	XAT	C4-C3-C2	-2.63	105.86	110.79
22	7	310	CLA	C3B-C4B-NB	-2.63	108.18	110.53
22	a	826	CLA	CHB-C4A-NA	2.63	128.20	124.40
22	a	829	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
22	8	314	CLA	CAA-C2A-C3A	-2.63	110.20	116.23
20	2	302	XAT	C4-C3-C2	-2.63	105.87	110.79
22	a	821	CLA	CHB-C4A-NA	2.63	128.19	124.40
22	h	203	CLA	CHB-C4A-NA	2.63	128.19	124.40
29	a	849	BCR	C23-C24-C25	-2.62	119.99	127.00
22	1	309	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
29	b	845	BCR	C8-C7-C6	-2.62	120.00	127.00
22	3	308	CLA	C3B-C4B-NB	-2.62	108.19	110.53
22	a	844	CLA	C3B-C4B-NB	-2.62	108.19	110.53
29	a	849	BCR	C16-C15-C14	-2.62	118.16	123.52
22	9	318	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
22	a	810	CLA	C1-C2-C3	-2.61	121.91	126.20
29	h	201	BCR	C21-C20-C19	-2.61	115.63	123.20
22	8	311	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	a	804	CLA	C3B-C4B-NB	-2.61	108.20	110.53
29	l	201	BCR	C21-C20-C19	-2.61	115.63	123.20
22	b	833	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
29	h	202	BCR	C28-C27-C26	-2.61	109.40	114.06
22	3	309	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	a	835	CLA	CHB-C4A-NA	2.61	128.17	124.40
22	a	838	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	b	813	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
20	2	304	XAT	C35-C15-C14	-2.61	118.18	123.52
29	m	101	BCR	C15-C16-C17	-2.61	118.18	123.52
22	a	840	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	1	307	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	l	204	CLA	C3B-C4B-NB	-2.61	108.20	110.53
29	b	845	BCR	C38-C26-C25	-2.61	121.64	124.48
22	b	801	CLA	CHB-C4A-NA	2.61	128.16	124.40
22	a	842	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
22	3	310	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
29	b	846	BCR	C34-C9-C8	2.60	122.06	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	311	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
27	a	853	LMG	C8-O7-C10	-2.60	111.57	117.80
22	b	803	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	a	854	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
22	b	822	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	a	835	CLA	C3B-C4B-NB	-2.60	108.21	110.53
20	8	302	XAT	C11-C12-C13	-2.60	119.24	126.36
29	b	849	BCR	C15-C14-C13	-2.60	123.64	127.28
22	9	316	CLA	CHB-C4A-NA	2.59	128.14	124.40
21	9	306	A1L1G	C43-C44-C42	-2.59	118.62	122.82
22	b	806	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	7	309	CLA	O2D-CGD-O1D	-2.59	118.20	124.08
22	9	313	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	a	833	CLA	CHB-C4A-NA	2.59	128.14	124.40
29	j	104	BCR	C33-C5-C6	-2.59	121.66	124.48
22	b	820	CLA	C1-C2-C3	-2.58	122.58	126.76
22	4	317	CLA	CHB-C4A-NA	2.58	128.13	124.40
22	7	316	CLA	CHB-C4A-NA	2.58	128.12	124.40
22	a	814	CLA	CHB-C4A-NA	2.58	128.12	124.40
22	b	821	CLA	C3B-C4B-NB	-2.58	108.23	110.53
29	l	201	BCR	C20-C21-C22	-2.58	123.66	127.28
29	b	842	BCR	C29-C30-C25	2.58	114.19	110.44
22	2	311	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
22	j	103	CLA	CHB-C4A-NA	2.58	128.12	124.40
29	b	842	BCR	C21-C20-C19	-2.58	115.73	123.20
22	b	808	CLA	C3B-C4B-NB	-2.58	108.23	110.53
29	b	843	BCR	C24-C23-C22	-2.58	122.42	126.23
20	3	305	XAT	C10-C11-C12	-2.58	115.74	123.20
22	a	821	CLA	C3B-C4B-NB	-2.58	108.23	110.53
22	a	832	CLA	C1-C2-C3	-2.57	122.60	126.76
22	4	311	CLA	CHB-C4A-NA	2.57	128.12	124.40
29	l	205	BCR	C28-C27-C26	-2.57	109.47	114.06
22	3	315	CLA	CHB-C4A-NA	2.57	128.11	124.40
20	2	303	XAT	C19-C9-C10	-2.57	118.65	122.82
22	b	807	CLA	C3B-C4B-NB	-2.57	108.24	110.53
22	a	809	CLA	CHB-C4A-NA	2.57	128.10	124.40
20	4	302	XAT	C10-C11-C12	-2.57	115.77	123.20
29	a	850	BCR	C10-C11-C12	-2.57	115.77	123.20
24	h	204	A1L1F	C29-C30-C31	-2.57	115.01	119.00
22	a	801	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
22	b	809	CLA	CHB-C4A-NA	2.56	128.10	124.40
22	a	807	CLA	CHB-C4A-NA	2.56	128.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	314	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	h	204	A1L1F	C27-C34-C33	2.56	122.00	118.09
21	7	302	A1L1G	C43-C44-C42	-2.56	118.67	122.82
22	1	311	CLA	C3B-C4B-NB	-2.56	108.24	110.53
20	5	304	XAT	C15-C35-C34	-2.56	118.28	123.52
20	8	301	XAT	C31-C30-C29	-2.56	123.69	127.28
22	a	830	CLA	C1-C2-C3	-2.56	122.00	126.20
26	b	848	DGD	O2G-C1B-O1B	-2.56	117.73	123.70
20	2	302	XAT	C11-C10-C9	-2.56	123.69	127.28
22	a	819	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	3	308	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	4	306	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	2	306	CLA	O2D-CGD-O1D	-2.55	118.28	124.08
22	a	805	CLA	C3B-C4B-NB	-2.55	108.25	110.53
20	5	304	XAT	C8-C9-C10	-2.55	115.00	119.01
22	5	313	CLA	CHB-C4A-NA	2.55	128.08	124.40
20	5	304	XAT	C39-C29-C28	2.55	121.98	118.09
20	3	303	XAT	C30-C31-C32	-2.55	115.82	123.20
22	b	807	CLA	C1-C2-C3	-2.54	122.03	126.20
22	4	310	CLA	CHB-C4A-NA	2.54	128.07	124.40
22	1	306	CLA	CHB-C4A-NA	2.54	128.07	124.40
25	9	307	LHG	O7-C7-C8	2.54	120.26	110.93
22	2	312	CLA	C3B-C4B-NB	-2.54	108.27	110.53
20	1	303	XAT	C35-C15-C14	-2.54	118.33	123.52
29	b	846	BCR	C20-C21-C22	-2.54	123.72	127.28
22	8	308	CLA	CHB-C4A-NA	2.54	128.06	124.40
22	a	828	CLA	C1-C2-C3	-2.53	122.05	126.20
29	f	804	BCR	C15-C16-C17	-2.53	118.34	123.52
20	5	301	XAT	C4-C3-C2	-2.53	106.06	110.79
22	b	835	CLA	CHB-C4A-NA	2.53	128.05	124.40
22	a	804	CLA	CHB-C4A-NA	2.53	128.05	124.40
22	b	803	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
29	h	202	BCR	C10-C11-C12	-2.53	115.88	123.20
22	8	311	CLA	CHB-C4A-NA	2.52	128.04	124.40
21	3	306	A1L1G	C43-C44-C42	-2.52	118.73	122.82
22	8	305	CLA	C3B-C4B-NB	-2.52	108.28	110.53
22	5	312	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	2	313	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	a	832	CLA	CHB-C4A-NA	2.52	128.04	124.40
20	4	302	XAT	C30-C31-C32	-2.52	115.89	123.20
20	8	301	XAT	C35-C15-C14	-2.52	118.36	123.52
22	a	836	CLA	CHB-C4A-NA	2.52	128.04	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	812	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	b	817	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	3	314	CLA	CHB-C4A-NA	2.52	128.04	124.40
29	l	205	BCR	C15-C16-C17	-2.52	118.36	123.52
22	a	806	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	b	813	CLA	CHB-C4A-NA	2.52	128.04	124.40
22	4	314	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	5	306	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	2	312	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	b	820	CLA	O2D-CGD-CBD	2.52	115.63	111.23
22	1	306	CLA	C3B-C4B-NB	-2.51	108.29	110.53
20	9	303	XAT	C7-C8-C9	-2.51	121.63	125.53
22	8	307	CLA	CHB-C4A-NA	2.51	128.03	124.40
22	a	840	CLA	CHB-C4A-NA	2.51	128.03	124.40
29	j	104	BCR	C38-C26-C27	2.51	118.95	113.60
22	5	308	CLA	CHB-C4A-NA	2.51	128.03	124.40
22	a	838	CLA	CHB-C4A-NA	2.51	128.02	124.40
22	f	802	CLA	CHB-C4A-NA	2.51	128.02	124.40
22	a	806	CLA	C6-C5-C3	-2.51	107.35	113.47
22	a	816	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	1	304	AI1L1F	C31-C32-C33	-2.51	115.94	123.20
29	b	842	BCR	C33-C5-C4	2.50	118.94	113.60
22	5	310	CLA	CHB-C4A-NA	2.50	128.01	124.40
29	b	846	BCR	C38-C26-C25	-2.50	121.75	124.48
22	8	313	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	l	204	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	1	312	CLA	CHB-C4A-NA	2.50	128.01	124.40
29	b	845	BCR	C39-C30-C25	-2.50	106.32	110.24
29	l	201	BCR	C28-C27-C26	-2.50	109.60	114.06
22	b	831	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	7	307	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	f	803	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	a	802	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
29	a	848	BCR	C10-C11-C12	-2.50	115.97	123.20
22	b	833	CLA	CHB-C4A-NA	2.50	128.00	124.40
20	9	305	XAT	C19-C9-C10	-2.50	118.77	122.82
22	a	806	CLA	O1D-CGD-CBD	2.50	129.44	124.52
22	a	825	CLA	CHB-C4A-NA	2.50	128.00	124.40
22	1	307	CLA	CHB-C4A-NA	2.49	128.00	124.40
24	h	204	AI1L1F	C23-C22-C21	-2.49	106.13	110.79
22	b	820	CLA	C3B-C4B-NB	-2.49	108.30	110.53
20	4	301	XAT	C35-C15-C14	-2.49	118.42	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	823	CLA	CHB-C4A-NA	2.49	128.00	124.40
21	3	306	A1L1G	C17-C20-C21	2.49	117.04	114.24
20	7	304	XAT	C11-C12-C13	-2.49	119.53	126.36
22	4	307	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	a	827	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	b	820	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	8	309	CLA	C1-C2-C3	-2.49	122.12	126.20
22	7	315	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	8	309	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	b	836	CLA	CHB-C4A-NA	2.49	127.99	124.40
29	a	850	BCR	C38-C26-C27	2.49	118.90	113.60
20	2	303	XAT	C24-C23-C22	-2.49	106.14	110.79
20	7	301	XAT	C35-C15-C14	-2.48	118.44	123.52
22	9	312	CLA	C3B-C4B-NB	-2.48	108.31	110.53
22	8	312	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	1	308	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	a	817	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	a	822	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	3	307	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	5	303	A1L1G	C43-C44-C42	-2.48	118.80	122.82
24	9	302	A1L1F	C36-C37-C38	-2.48	118.44	123.52
29	b	843	BCR	C15-C16-C17	-2.48	118.44	123.52
24	1	304	A1L1F	C27-C34-C33	2.48	121.88	118.09
20	2	301	XAT	C10-C11-C12	-2.48	116.02	123.20
22	a	815	CLA	CHB-C4A-NA	2.48	127.98	124.40
22	1	313	CLA	CAA-C2A-C3A	-2.48	110.55	116.23
26	b	848	DGD	C6D-O5D-C1E	2.48	119.11	113.80
22	a	837	CLA	CHB-C4A-NA	2.48	127.97	124.40
22	4	316	CLA	CHB-C4A-NA	2.48	127.97	124.40
20	9	304	XAT	C39-C29-C28	2.48	121.87	118.09
29	b	842	BCR	C15-C16-C17	-2.47	118.45	123.52
29	j	104	BCR	C15-C16-C17	-2.47	118.45	123.52
22	3	313	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	7	313	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	5	305	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	8	305	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	9	314	CLA	C3B-C4B-NB	-2.47	108.32	110.53
22	2	308	CLA	C3B-C4B-NB	-2.47	108.32	110.53
22	b	811	CLA	CMB-C2B-C3B	2.47	130.10	123.53
22	a	811	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	2	306	CLA	CHB-C4A-NA	2.47	127.97	124.40
24	h	204	A1L1F	C41-C40-C39	-2.47	119.59	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	807	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	4	308	CLA	C3B-C4B-NB	-2.47	108.33	110.53
22	a	826	CLA	C3B-C4B-NB	-2.47	108.33	110.53
22	a	802	CLA	CHB-C4A-NA	2.47	127.96	124.40
22	a	804	CLA	O2D-CGD-CBD	2.47	115.54	111.23
22	5	315	CLA	CHB-C4A-NA	2.47	127.96	124.40
22	b	835	CLA	C3B-C4B-NB	-2.46	108.33	110.53
22	a	835	CLA	O2D-CGD-CBD	2.46	115.53	111.23
29	h	201	BCR	C33-C5-C6	-2.46	121.80	124.48
24	8	304	A1L1F	C12-C6-C1	-2.46	108.27	110.47
22	b	839	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	7	305	XAT	C31-C30-C29	-2.46	123.83	127.28
22	b	821	CLA	C1-C2-C3	-2.46	122.17	126.20
22	f	802	CLA	C3B-C4B-NB	-2.46	108.33	110.53
20	5	302	XAT	C31-C30-C29	-2.46	123.83	127.28
20	8	303	XAT	C28-C29-C30	-2.46	115.14	119.01
20	2	302	XAT	C10-C11-C12	-2.46	116.08	123.20
22	a	810	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	8	304	A1L1F	C23-C22-C21	-2.46	106.20	110.79
22	7	310	CLA	CHB-C4A-NA	2.46	127.94	124.40
22	a	808	CLA	CHB-C4A-NA	2.46	127.94	124.40
29	a	850	BCR	C8-C7-C6	-2.45	120.44	127.00
20	9	305	XAT	C35-C15-C14	-2.45	118.50	123.52
22	a	830	CLA	C3B-C4B-NB	-2.45	108.34	110.53
22	9	308	CLA	CHB-C4A-NA	2.45	127.94	124.40
22	b	819	CLA	CHB-C4A-NA	2.45	127.94	124.40
22	l	202	CLA	CHB-C4A-NA	2.45	127.94	124.40
22	9	311	CLA	O2D-CGD-CBD	2.45	115.51	111.23
22	a	829	CLA	C3B-C4B-NB	-2.45	108.34	110.53
22	8	308	CLA	C1-C2-C3	-2.45	122.19	126.20
22	2	316	CLA	CHB-C4A-NA	2.45	127.93	124.40
22	7	308	CLA	C3B-C4B-NB	-2.45	108.35	110.53
22	a	809	CLA	C3B-C4B-NB	-2.45	108.35	110.53
22	b	839	CLA	C3B-C4B-NB	-2.44	108.35	110.53
22	8	314	CLA	CHB-C4A-NA	2.44	127.93	124.40
22	2	314	CLA	CHB-C4A-NA	2.44	127.93	124.40
28	b	841	PQN	C11-C3-C2	-2.44	120.70	124.89
22	b	805	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	b	838	CLA	CHB-C4A-NA	2.44	127.92	124.40
20	3	304	XAT	C31-C32-C33	-2.44	119.67	126.36
22	7	306	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	b	834	CLA	CHB-C4A-NA	2.44	127.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	818	CLA	CHB-C4A-NA	2.44	127.92	124.40
22	7	316	CLA	C3B-C4B-NB	-2.43	108.36	110.53
21	9	301	A1L1G	C43-C44-C42	-2.43	118.87	122.82
22	2	309	CLA	CHB-C4A-NA	2.43	127.91	124.40
29	h	202	BCR	C8-C7-C6	-2.43	120.50	127.00
22	a	828	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	8	303	XAT	C40-C33-C32	2.43	121.80	118.09
27	j	105	LMG	C8-O7-C10	-2.43	111.98	117.80
22	a	812	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	b	815	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	7	303	XAT	C19-C9-C10	-2.43	118.88	122.82
22	1	310	CLA	CHB-C4A-NA	2.43	127.90	124.40
22	4	309	CLA	CHB-C4A-NA	2.42	127.90	124.40
29	b	845	BCR	C21-C20-C19	-2.42	116.18	123.20
26	8	315	DGD	C2G-O2G-C1B	-2.42	112.00	117.80
22	a	839	CLA	CHB-C4A-NA	2.42	127.90	124.40
22	b	810	CLA	C1-C2-C3	-2.42	122.23	126.20
22	7	311	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	h	205	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	9	315	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	3	309	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	a	820	CLA	CHB-C4A-NA	2.42	127.89	124.40
22	b	827	CLA	C3B-C4B-NB	-2.42	108.37	110.53
22	b	827	CLA	CHB-C4A-NA	2.41	127.89	124.40
22	b	821	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	a	833	CLA	C1-C2-C3	-2.41	122.25	126.20
22	9	309	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	h	204	A1L1F	O7-C54-O55	-2.41	118.34	122.99
28	b	841	PQN	C14-C13-C15	2.41	119.41	115.23
20	8	301	XAT	C30-C31-C32	-2.41	116.22	123.20
24	9	302	A1L1F	O7-C54-O55	-2.41	118.34	122.99
22	b	811	CLA	CAB-C3B-C2B	2.41	129.93	123.53
29	a	848	BCR	C21-C20-C19	-2.41	116.22	123.20
22	4	308	CLA	CHB-C4A-NA	2.41	127.88	124.40
22	b	813	CLA	C1-C2-C3	-2.41	122.25	126.20
29	a	850	BCR	C16-C15-C14	-2.41	118.59	123.52
22	b	808	CLA	CHB-C4A-NA	2.41	127.87	124.40
22	7	308	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	3	311	CLA	C1-C2-C3	-2.40	122.87	126.76
22	3	311	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	9	302	A1L1F	C26-O13-C45	2.40	120.67	115.64
22	5	309	CLA	CHB-C4A-NA	2.40	127.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	804	BCR	C28-C27-C26	-2.40	109.78	114.06
22	7	314	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
22	b	822	CLA	CHB-C4A-NA	2.40	127.86	124.40
22	a	842	CLA	CHB-C4A-NA	2.40	127.86	124.40
21	7	302	A1L1G	C17-C20-C21	2.40	116.93	114.24
22	2	311	CLA	CHB-C4A-NA	2.39	127.86	124.40
29	j	104	BCR	C38-C26-C25	-2.39	121.87	124.48
20	9	303	XAT	C39-C29-C28	2.39	121.74	118.09
20	9	303	XAT	O24-C25-C38	2.39	117.72	115.05
22	1	311	CLA	CHB-C4A-NA	2.39	127.85	124.40
29	b	844	BCR	C28-C27-C26	-2.39	109.79	114.06
22	a	834	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	9	314	CLA	CHB-C4A-NA	2.39	127.85	124.40
29	a	847	BCR	C23-C24-C25	-2.39	120.62	127.00
29	f	801	BCR	C33-C5-C4	2.38	118.68	113.60
20	8	302	XAT	C7-C8-C9	-2.38	121.83	125.53
22	a	823	CLA	C3B-C4B-NB	-2.38	108.40	110.53
22	8	310	CLA	CHB-C4A-NA	2.38	127.84	124.40
29	a	848	BCR	C15-C16-C17	-2.38	118.64	123.52
22	b	811	CLA	CHB-C4A-NA	2.38	127.84	124.40
22	7	312	CLA	CHB-C4A-NA	2.38	127.84	124.40
29	h	201	BCR	C16-C15-C14	-2.38	118.65	123.52
22	b	818	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	a	834	CLA	C1-C2-C3	-2.38	122.31	126.20
22	8	306	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	b	810	CLA	C3B-C4B-NB	-2.37	108.41	110.53
22	a	813	CLA	CHB-C4A-NA	2.37	127.83	124.40
22	4	312	CLA	CHB-C4A-NA	2.37	127.82	124.40
22	a	803	CLA	C3B-C4B-NB	-2.37	108.41	110.53
22	7	316	CLA	O2D-CGD-CBD	2.37	115.37	111.23
21	3	302	A1L1G	C43-C44-C42	-2.37	118.98	122.82
22	b	816	CLA	CHB-C4A-NA	2.37	127.82	124.40
29	b	843	BCR	C23-C24-C25	-2.37	120.67	127.00
20	j	101	XAT	C39-C29-C28	2.37	121.70	118.09
22	9	318	CLA	CHB-C4A-NA	2.37	127.81	124.40
22	b	825	CLA	CHB-C4A-NA	2.37	127.81	124.40
22	b	835	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
29	b	844	BCR	C34-C9-C10	-2.36	118.98	122.82
29	l	201	BCR	C15-C16-C17	-2.36	118.68	123.52
22	7	314	CLA	C2A-C1A-CHA	2.36	127.97	123.87
24	9	302	A1L1F	C31-C32-C33	-2.36	116.36	123.20
22	1	313	CLA	CHB-C4A-NA	2.36	127.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	849	BCR	C21-C20-C19	-2.36	116.36	123.20
22	5	311	CLA	CHB-C4A-NA	2.36	127.81	124.40
22	a	854	CLA	CHB-C4A-NA	2.36	127.81	124.40
22	5	307	CLA	CHB-C4A-NA	2.36	127.80	124.40
22	2	307	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
20	8	301	XAT	O24-C25-C38	2.36	117.68	115.05
20	3	303	XAT	O24-C25-C38	2.36	117.68	115.05
29	f	804	BCR	C11-C12-C13	-2.35	119.91	126.36
20	5	301	XAT	C30-C31-C32	-2.35	116.38	123.20
20	4	303	XAT	O24-C25-C38	2.35	117.68	115.05
22	h	203	CLA	C3B-C4B-NB	-2.35	108.43	110.53
20	a	852	XAT	C19-C9-C8	2.35	121.68	118.09
29	b	843	BCR	C28-C27-C26	-2.35	109.86	114.06
20	7	305	XAT	C30-C31-C32	-2.35	116.39	123.20
22	4	313	CLA	CHB-C4A-NA	2.35	127.79	124.40
22	b	810	CLA	CHB-C4A-NA	2.35	127.79	124.40
29	b	842	BCR	C11-C12-C13	-2.35	119.92	126.36
22	a	841	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
22	a	831	CLA	CHB-C4A-NA	2.35	127.79	124.40
22	1	305	CLA	CHB-C4A-NA	2.35	127.79	124.40
22	b	837	CLA	C1-C2-C3	-2.35	122.35	126.20
20	7	301	XAT	C31-C32-C33	-2.35	119.93	126.36
20	5	301	XAT	O24-C25-C38	2.35	117.67	115.05
22	2	315	CLA	CHB-C4A-NA	2.35	127.78	124.40
22	3	310	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	j	102	CLA	CHB-C4A-NA	2.34	127.78	124.40
29	m	101	BCR	C8-C7-C6	-2.34	120.74	127.00
20	4	305	XAT	O24-C25-C38	2.34	117.66	115.05
20	7	304	XAT	O24-C25-C38	2.34	117.66	115.05
22	b	811	CLA	C3B-C4B-NB	-2.34	107.90	110.33
22	b	832	CLA	CHB-C4A-NA	2.33	127.77	124.40
29	b	844	BCR	C7-C6-C5	-2.33	116.18	121.56
22	b	835	CLA	C1-C2-C3	-2.33	122.38	126.20
24	1	304	A1L1F	O7-C54-O55	-2.33	118.50	122.99
22	b	830	CLA	CHB-C4A-NA	2.33	127.76	124.40
20	5	302	XAT	C15-C35-C34	-2.33	118.76	123.52
20	3	304	XAT	O4-C5-C18	2.33	117.65	115.05
22	9	316	CLA	C3B-C4B-NB	-2.33	108.45	110.53
29	b	849	BCR	C23-C24-C25	-2.32	120.79	127.00
22	7	309	CLA	CHB-C4A-NA	2.32	127.75	124.40
22	b	816	CLA	C1-C2-C3	-2.32	122.39	126.20
22	b	839	CLA	C1-C2-C3	-2.32	122.39	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	840	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	l	201	BCR	C29-C30-C25	2.32	113.81	110.44
22	1	309	CLA	CHB-C4A-NA	2.32	127.75	124.40
29	b	845	BCR	C34-C9-C8	2.32	121.63	118.09
22	b	829	CLA	C1-C2-C3	-2.32	122.40	126.20
29	i	101	BCR	C16-C15-C14	-2.32	118.78	123.52
24	1	304	A1L1F	C37-C36-C35	-2.32	118.78	123.52
20	2	303	XAT	C8-C9-C10	2.31	122.65	119.01
22	5	314	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
20	2	304	XAT	C35-C34-C33	-2.31	124.04	127.28
22	1	306	CLA	C1-C2-C3	-2.31	122.41	126.20
20	3	301	XAT	C15-C35-C34	-2.31	118.79	123.52
20	8	303	XAT	O4-C5-C18	2.31	117.63	115.05
29	f	804	BCR	C3-C4-C5	-2.31	109.94	114.06
21	1	301	A1L1G	C14-C29-C30	-2.31	121.54	125.47
29	b	844	BCR	C37-C22-C21	-2.31	119.08	122.82
20	8	302	XAT	O24-C25-C38	2.31	117.63	115.05
22	a	833	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
21	1	301	A1L1G	C17-C20-C21	2.31	116.83	114.24
29	f	801	BCR	C34-C9-C8	2.31	121.61	118.09
22	7	313	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
20	5	304	XAT	O24-C25-C38	2.31	117.63	115.05
22	b	809	CLA	O2D-CGD-CBD	2.31	115.26	111.23
22	a	836	CLA	C1-C2-C3	-2.31	123.03	126.76
20	j	101	XAT	O24-C25-C38	2.31	117.62	115.05
23	5	316	SQD	C45-O47-C7	-2.30	112.28	117.80
20	7	301	XAT	C24-C23-C22	-2.30	106.48	110.79
22	a	844	CLA	C1-C2-C3	-2.30	122.42	126.20
22	b	818	CLA	C3B-C4B-NB	-2.30	108.47	110.53
22	a	816	CLA	C1-C2-C3	-2.30	123.04	126.76
22	a	805	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
29	l	201	BCR	C23-C24-C25	-2.30	120.85	127.00
20	2	304	XAT	O24-C25-C38	2.30	117.62	115.05
20	9	304	XAT	O24-C25-C38	2.30	117.62	115.05
20	7	305	XAT	O4-C5-C18	2.30	117.62	115.05
22	a	810	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
29	a	848	BCR	C16-C15-C14	-2.30	118.82	123.52
22	4	313	CLA	CMB-C2B-C1B	-2.29	121.92	125.42
29	m	101	BCR	C24-C23-C22	-2.29	122.84	126.23
22	b	821	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
20	2	305	XAT	C19-C9-C8	2.29	121.59	118.09
22	b	823	CLA	CHB-C4A-NA	2.29	127.71	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	308	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
22	a	824	CLA	CHB-C4A-NA	2.29	127.71	124.40
20	9	304	XAT	C10-C11-C12	-2.29	116.56	123.20
20	5	302	XAT	O4-C5-C18	2.29	117.61	115.05
20	a	852	XAT	O24-C25-C38	2.29	117.61	115.05
22	a	844	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
20	2	303	XAT	O4-C5-C18	2.29	117.61	115.05
24	h	204	A1L1F	C26-O13-C45	2.29	120.44	115.64
22	b	803	CLA	CHB-C4A-NA	2.29	127.70	124.40
29	a	849	BCR	C10-C11-C12	-2.29	116.58	123.20
22	b	823	CLA	C1-C2-C3	-2.29	122.45	126.20
22	3	310	CLA	C3B-C4B-NB	-2.29	108.49	110.53
20	7	305	XAT	O24-C25-C38	2.29	117.60	115.05
29	b	845	BCR	C33-C5-C4	2.29	118.47	113.60
22	b	804	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
29	b	845	BCR	C29-C30-C25	2.28	113.76	110.44
20	2	304	XAT	C20-C13-C12	2.28	121.58	118.09
22	b	834	CLA	C1-C2-C3	-2.28	122.45	126.20
21	9	301	A1L1G	C14-C29-C30	-2.28	121.59	125.47
29	i	101	BCR	C10-C11-C12	-2.28	116.59	123.20
20	1	303	XAT	C27-C28-C29	-2.28	121.99	125.53
20	7	303	XAT	C8-C9-C10	2.28	122.59	119.01
22	a	818	CLA	O2D-CGD-CBD	2.28	115.21	111.23
22	a	844	CLA	CHB-C4A-NA	2.28	127.68	124.40
29	h	202	BCR	C37-C22-C23	2.27	121.56	118.09
22	7	313	CLA	C1-C2-C3	-2.27	122.47	126.20
22	b	825	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
20	4	305	XAT	C15-C35-C34	-2.27	118.87	123.52
22	9	308	CLA	C1-C2-C3	-2.27	122.47	126.20
22	b	837	CLA	CHB-C4A-NA	2.27	127.68	124.40
20	7	301	XAT	C26-C27-C28	-2.27	121.19	125.99
22	b	817	CLA	CMB-C2B-C3B	2.27	131.89	126.55
20	3	303	XAT	C10-C11-C12	-2.27	116.63	123.20
28	a	843	PQN	C11-C12-C13	-2.27	122.92	126.83
20	7	301	XAT	C10-C11-C12	-2.27	116.63	123.20
20	2	304	XAT	C10-C11-C12	-2.27	116.63	123.20
22	4	310	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
20	5	302	XAT	C11-C12-C13	-2.26	120.16	126.36
22	f	803	CLA	C1-C2-C3	-2.26	122.49	126.20
22	a	826	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
22	f	802	CLA	C1-C2-C3	-2.26	122.49	126.20
20	3	301	XAT	O4-C5-C18	2.26	117.57	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	304	XAT	C27-C28-C29	-2.26	122.03	125.53
22	a	840	CLA	C1-C2-C3	-2.26	122.50	126.20
22	b	836	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
20	2	305	XAT	O4-C5-C18	2.26	117.57	115.05
29	l	205	BCR	C38-C26-C27	2.26	118.41	113.60
29	l	205	BCR	C33-C5-C4	2.26	118.41	113.60
20	2	301	XAT	O24-C25-C38	2.26	117.57	115.05
24	9	302	A1L1F	C23-C22-C21	-2.26	106.57	110.79
20	4	304	XAT	O4-C5-C18	2.25	117.57	115.05
20	8	301	XAT	O4-C5-C18	2.25	117.57	115.05
20	7	305	XAT	C39-C29-C28	2.25	121.53	118.09
22	a	806	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
22	8	305	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
29	h	201	BCR	C11-C10-C9	-2.25	124.12	127.28
22	b	826	CLA	CHB-C4A-NA	2.25	127.65	124.40
20	7	303	XAT	O24-C25-C38	2.25	117.56	115.05
22	8	308	CLA	C3B-C4B-NB	-2.25	108.52	110.53
22	a	827	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
22	7	308	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
22	a	809	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
20	2	302	XAT	O24-C25-C38	2.25	117.56	115.05
29	b	846	BCR	C35-C13-C12	2.25	121.52	118.09
22	2	311	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
29	f	801	BCR	C35-C13-C12	2.25	121.52	118.09
29	a	850	BCR	C20-C19-C18	-2.25	120.21	126.36
20	1	302	XAT	O24-C25-C38	2.25	117.56	115.05
22	2	310	CLA	CHB-C4A-NA	2.24	127.64	124.40
20	5	304	XAT	O4-C5-C18	2.24	117.56	115.05
20	1	303	XAT	C19-C9-C8	2.24	121.51	118.09
22	3	313	CLA	C1-C2-C3	-2.24	122.53	126.20
20	3	303	XAT	O4-C5-C18	2.24	117.55	115.05
29	f	801	BCR	C28-C27-C26	-2.24	110.06	114.06
22	3	310	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
22	b	804	CLA	O1D-CGD-CBD	2.24	128.93	124.52
22	b	814	CLA	C1-C2-C3	-2.24	122.53	126.20
29	f	801	BCR	C15-C14-C13	-2.24	124.14	127.28
20	4	301	XAT	C39-C29-C30	-2.24	119.19	122.82
20	3	305	XAT	C19-C9-C8	2.23	121.50	118.09
29	b	843	BCR	C37-C22-C23	2.23	121.50	118.09
22	a	820	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
22	a	811	CLA	C1-C2-C3	-2.23	122.54	126.20
20	5	302	XAT	C30-C31-C32	-2.23	116.73	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	829	CLA	CHB-C4A-NA	2.23	127.62	124.40
22	b	829	CLA	CHB-C4A-NA	2.23	127.62	124.40
22	5	311	CLA	C1-C2-C3	-2.23	122.54	126.20
22	a	829	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
22	1	312	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
22	5	307	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
29	b	845	BCR	C23-C24-C25	-2.23	121.05	127.00
20	1	303	XAT	O24-C25-C38	2.22	117.53	115.05
22	a	820	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
29	h	201	BCR	C34-C9-C8	2.22	121.48	118.09
29	h	202	BCR	C35-C13-C12	2.22	121.48	118.09
20	3	303	XAT	C15-C35-C34	-2.22	118.97	123.52
22	a	823	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
20	2	304	XAT	O4-C5-C18	2.22	117.53	115.05
22	a	838	CLA	C1-C2-C3	-2.22	122.56	126.20
22	b	817	CLA	C1-C2-C3	-2.22	122.56	126.20
20	4	303	XAT	O4-C5-C18	2.22	117.53	115.05
20	3	304	XAT	O24-C25-C38	2.22	117.53	115.05
22	8	311	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
29	b	846	BCR	C37-C22-C23	2.21	121.47	118.09
29	b	843	BCR	C36-C18-C19	2.21	121.47	118.09
22	b	805	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
22	h	205	CLA	C1-C2-C3	-2.21	122.58	126.20
22	a	819	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
22	8	312	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
20	4	302	XAT	C39-C29-C28	2.21	121.46	118.09
20	4	305	XAT	C39-C29-C30	-2.21	119.24	122.82
22	3	311	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
20	a	852	XAT	C40-C33-C32	2.20	121.45	118.09
22	a	831	CLA	O2D-CGD-CBD	2.20	115.08	111.23
22	8	308	CLA	O2D-CGD-CBD	2.20	115.08	111.23
20	3	305	XAT	O24-C25-C38	2.20	117.51	115.05
20	2	303	XAT	O24-C25-C38	2.20	117.51	115.05
20	2	303	XAT	C31-C32-C33	-2.20	120.33	126.36
20	3	301	XAT	O24-C25-C38	2.20	117.51	115.05
20	3	303	XAT	C39-C29-C28	2.20	121.45	118.09
20	2	305	XAT	C15-C35-C34	-2.20	119.02	123.52
29	j	104	BCR	C29-C30-C25	2.20	113.63	110.44
20	8	303	XAT	O24-C25-C38	2.20	117.50	115.05
29	a	848	BCR	C23-C24-C25	-2.20	121.13	127.00
22	b	835	CLA	CAC-C3C-C4C	2.20	127.65	124.79
22	9	316	CLA	C1-C2-C3	-2.20	122.60	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	827	CLA	C1-C2-C3	-2.20	122.60	126.20
20	8	302	XAT	O4-C5-C18	2.19	117.50	115.05
29	b	843	BCR	C11-C12-C13	-2.19	120.35	126.36
22	2	308	CLA	CHB-C4A-NA	2.19	127.56	124.40
22	b	814	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
29	a	848	BCR	C33-C5-C4	2.19	118.27	113.60
22	a	830	CLA	CHB-C4A-NA	2.19	127.56	124.40
22	5	308	CLA	C1-C2-C3	-2.19	122.61	126.20
20	5	301	XAT	O4-C5-C18	2.19	117.50	115.05
22	a	804	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
22	a	806	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
27	2	317	LMG	C8-O7-C10	-2.19	112.56	117.80
20	4	302	XAT	O24-C25-C38	2.18	117.49	115.05
20	7	304	XAT	O4-C5-C18	2.18	117.49	115.05
20	1	302	XAT	O4-C5-C18	2.18	117.49	115.05
22	5	311	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
29	h	202	BCR	C33-C5-C4	2.18	118.25	113.60
29	l	201	BCR	C39-C30-C25	-2.18	106.82	110.24
29	a	849	BCR	C8-C7-C6	-2.18	121.17	127.00
20	3	303	XAT	C35-C15-C14	-2.18	119.06	123.52
20	4	305	XAT	O4-C5-C18	2.18	117.48	115.05
22	a	831	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
22	b	840	CLA	C1-C2-C3	-2.18	122.63	126.20
22	1	308	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
22	5	312	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
20	4	302	XAT	O4-C5-C18	2.17	117.48	115.05
20	2	304	XAT	C30-C31-C32	-2.17	116.90	123.20
22	7	316	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
20	4	302	XAT	C20-C13-C12	2.17	121.40	118.09
20	2	305	XAT	C10-C11-C12	-2.17	116.91	123.20
29	f	804	BCR	C21-C20-C19	-2.17	116.91	123.20
20	7	301	XAT	O4-C5-C18	2.17	117.47	115.05
22	a	806	CLA	C5-C3-C2	-2.17	116.30	121.17
29	h	201	BCR	C23-C24-C25	-2.17	121.21	127.00
22	4	307	CLA	O2D-CGD-CBD	2.17	115.02	111.23
20	4	304	XAT	O24-C25-C38	2.17	117.47	115.05
20	4	303	XAT	C7-C8-C9	-2.17	122.17	125.53
22	a	816	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
20	1	303	XAT	O4-C5-C18	2.16	117.47	115.05
22	a	834	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
20	3	305	XAT	O4-C5-C18	2.16	117.46	115.05
29	b	845	BCR	C2-C1-C6	2.16	113.58	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	801	CLA	CHB-C4A-NA	2.16	127.52	124.40
22	3	313	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
29	a	847	BCR	C8-C7-C6	-2.16	121.23	127.00
22	a	839	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
22	b	830	CLA	CMA-C3A-C2A	-2.16	111.28	116.23
22	b	818	CLA	C1-C2-C3	-2.16	122.66	126.20
26	8	315	DGD	O2G-C1B-O1B	-2.16	118.67	123.70
29	j	104	BCR	C21-C20-C19	-2.15	116.96	123.20
20	3	301	XAT	C8-C9-C10	-2.15	115.62	119.01
20	4	301	XAT	O4-C5-C18	2.15	117.45	115.05
22	f	802	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
22	a	812	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
22	a	838	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
22	4	308	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
22	4	308	CLA	O2D-CGD-CBD	2.15	114.99	111.23
28	a	843	PQN	C2M-C2-C3	-2.15	120.91	124.45
22	7	312	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
20	7	301	XAT	O24-C25-C38	2.15	117.45	115.05
22	9	318	CLA	C1-C2-C3	-2.15	122.67	126.20
22	9	318	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	b	826	CLA	C1-C2-C3	-2.15	122.68	126.20
22	8	308	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
22	b	828	CLA	CHB-C4A-NA	2.15	127.50	124.40
22	b	832	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
29	m	101	BCR	C15-C14-C13	-2.15	124.27	127.28
22	9	314	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
22	a	803	CLA	CMB-C2B-C3B	2.14	131.59	126.55
20	j	101	XAT	O4-C5-C18	2.14	117.44	115.05
20	7	303	XAT	O4-C5-C18	2.14	117.44	115.05
20	9	304	XAT	C40-C33-C32	2.14	121.36	118.09
20	9	305	XAT	C31-C32-C33	-2.14	120.49	126.36
22	b	822	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	4	311	CLA	O2D-CGD-CBD	2.14	114.97	111.23
22	4	313	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	b	807	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
21	9	301	A1L1G	C29-C30-C31	2.14	122.32	119.00
22	8	309	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	b	823	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
20	8	302	XAT	C19-C9-C10	-2.14	119.35	122.82
22	b	829	CLA	CHB-C1B-NB	2.14	127.25	124.05
29	b	844	BCR	C1-C6-C7	2.14	121.44	115.65
29	a	849	BCR	C15-C16-C17	-2.13	119.15	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	316	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
29	l	201	BCR	C37-C22-C23	2.13	121.35	118.09
29	b	849	BCR	C32-C1-C6	-2.13	106.90	110.24
29	b	846	BCR	C23-C24-C25	-2.13	121.30	127.00
22	b	820	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
29	j	104	BCR	C16-C15-C14	-2.13	119.16	123.52
20	9	303	XAT	C11-C12-C13	-2.13	120.52	126.36
20	2	302	XAT	O4-C5-C18	2.13	117.43	115.05
29	l	201	BCR	C34-C9-C10	-2.13	119.37	122.82
23	5	316	SQD	O7-S-C6	2.13	109.93	106.76
22	b	802	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
29	h	201	BCR	C15-C16-C17	-2.13	119.17	123.52
22	b	829	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
22	a	842	CLA	C1-C2-C3	-2.13	122.72	126.20
22	9	316	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
22	9	308	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
22	a	829	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
24	8	304	A1L1F	C27-C34-C33	2.12	121.33	118.09
20	8	302	XAT	C8-C9-C10	2.12	122.35	119.01
29	a	848	BCR	C34-C9-C8	2.12	121.33	118.09
20	1	302	XAT	C30-C31-C32	-2.12	117.05	123.20
22	8	311	CLA	C1-C2-C3	-2.12	122.72	126.20
29	l	201	BCR	C3-C4-C5	-2.12	110.27	114.06
22	a	807	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	a	836	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	b	801	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	3	309	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
26	b	848	DGD	O3D-C3D-C4D	-2.12	105.38	110.38
22	b	812	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
20	5	302	XAT	O24-C25-C26	-2.12	57.25	58.93
22	a	827	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
22	a	802	CLA	CMB-C2B-C3B	2.12	131.53	126.55
22	2	308	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
20	5	304	XAT	C35-C15-C14	-2.12	119.19	123.52
20	1	302	XAT	C10-C11-C12	-2.11	117.08	123.20
22	b	825	CLA	C1-C2-C3	-2.11	122.73	126.20
20	4	303	XAT	C35-C15-C14	-2.11	119.19	123.52
29	a	849	BCR	C37-C22-C23	2.11	121.32	118.09
29	b	842	BCR	C38-C26-C27	2.11	118.10	113.60
22	a	803	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
22	b	838	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
29	b	843	BCR	C33-C5-C4	2.11	118.09	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	h	205	CLA	O2D-CGD-CBD	2.11	114.92	111.23
22	a	831	CLA	C3B-C4B-NB	-2.11	108.65	110.53
22	a	818	CLA	C1-C2-C3	-2.11	122.74	126.20
22	b	808	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
29	b	842	BCR	C37-C22-C23	2.11	121.31	118.09
22	a	801	CLA	O1D-CGD-CBD	2.11	128.68	124.52
22	a	826	CLA	C1-C2-C3	-2.11	122.74	126.20
22	a	826	CLA	CMB-C2B-C3B	2.11	131.51	126.55
20	5	301	XAT	C39-C29-C28	2.11	121.31	118.09
22	b	805	CLA	C1-C2-C3	-2.11	122.75	126.20
22	a	827	CLA	C1-C2-C3	-2.11	122.75	126.20
22	b	816	CLA	O2D-CGD-CBD	2.10	114.91	111.23
22	b	829	CLA	C3B-C4B-NB	-2.10	108.65	110.53
22	2	308	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
22	b	803	CLA	O2D-CGD-CBD	2.10	114.91	111.23
22	b	831	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
22	9	309	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
20	2	302	XAT	C19-C9-C8	2.10	121.30	118.09
20	3	304	XAT	C35-C15-C14	-2.10	119.22	123.52
20	7	301	XAT	C19-C9-C8	2.10	121.30	118.09
22	a	809	CLA	O2D-CGD-CBD	2.10	114.90	111.23
29	j	104	BCR	C3-C4-C5	-2.10	110.31	114.06
22	b	819	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
20	a	852	XAT	C39-C29-C28	2.10	121.30	118.09
22	b	827	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
29	a	847	BCR	C33-C5-C4	2.10	118.07	113.60
20	7	303	XAT	C15-C35-C34	-2.10	119.22	123.52
22	a	804	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
20	9	305	XAT	C11-C12-C13	-2.10	120.61	126.36
22	1	306	CLA	CAC-C3C-C4C	2.10	127.52	124.79
29	i	101	BCR	C23-C22-C21	2.10	122.31	119.01
22	1	307	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
22	a	825	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
20	4	304	XAT	C30-C31-C32	-2.09	117.13	123.20
22	1	310	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
22	b	819	CLA	C1-C2-C3	-2.09	122.77	126.20
22	4	309	CLA	C1-C2-C3	-2.09	123.38	126.76
22	9	316	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
22	b	835	CLA	CMB-C2B-C3B	2.09	131.47	126.55
20	9	305	XAT	O4-C5-C18	2.09	117.39	115.05
22	5	307	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
20	2	304	XAT	C40-C33-C32	2.09	121.28	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	j	102	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	a	854	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
24	9	302	A1L1F	C17-C20-C21	2.09	116.59	114.24
22	a	844	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
20	5	302	XAT	C19-C9-C10	-2.09	119.44	122.82
22	b	808	CLA	O2D-CGD-CBD	2.09	114.88	111.23
22	b	839	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
29	a	847	BCR	C28-C27-C26	-2.08	110.34	114.06
27	2	317	LMG	C4-C3-C2	-2.08	107.17	110.83
20	5	302	XAT	O24-C25-C38	2.08	117.38	115.05
22	8	311	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
20	9	303	XAT	O4-C5-C18	2.08	117.37	115.05
22	5	308	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	4	317	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	3	308	CLA	O2D-CGD-CBD	2.08	114.87	111.23
22	b	840	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	a	822	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
22	b	838	CLA	C1-C2-C3	-2.08	122.79	126.20
22	a	814	CLA	C1-C2-C3	-2.08	122.80	126.20
29	b	844	BCR	C16-C15-C14	-2.08	119.27	123.52
22	a	818	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	b	837	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
20	4	304	XAT	C19-C9-C8	2.07	121.25	118.09
22	2	312	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	h	203	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
22	h	205	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	a	806	CLA	C6-C7-C8	-2.07	109.08	115.97
22	b	804	CLA	O2D-CGD-CBD	2.07	114.85	111.23
22	2	310	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
22	3	308	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
22	a	808	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
20	1	303	XAT	C20-C13-C12	2.07	121.25	118.09
20	7	304	XAT	C19-C9-C10	-2.07	119.47	122.82
22	1	311	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
22	a	814	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
26	b	848	DGD	O5E-C6E-C5E	-2.07	104.30	111.33
22	5	311	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
22	4	307	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
22	b	817	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
22	b	829	CLA	O2D-CGD-CBD	2.06	114.84	111.23
22	a	829	CLA	CMB-C2B-C3B	2.06	131.40	126.55
21	1	301	A1L1G	C29-C30-C31	2.06	122.20	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	304	XAT	C31-C32-C33	-2.06	120.71	126.36
20	7	305	XAT	C11-C12-C13	-2.06	120.71	126.36
22	1	306	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
22	a	832	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
20	2	302	XAT	C27-C28-C29	-2.06	122.33	125.53
22	2	307	CLA	CMB-C2B-C3B	2.06	131.39	126.55
20	2	304	XAT	C15-C35-C34	-2.06	119.31	123.52
22	8	307	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
29	f	804	BCR	C8-C7-C6	-2.06	121.50	127.00
20	8	301	XAT	C39-C29-C28	2.06	121.23	118.09
20	4	301	XAT	C10-C11-C12	-2.06	117.24	123.20
22	b	821	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
22	a	806	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
20	3	303	XAT	C19-C9-C8	2.05	121.22	118.09
22	a	823	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
29	h	201	BCR	C35-C13-C12	2.05	121.22	118.09
22	1	307	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
22	1	311	CLA	O2D-CGD-CBD	2.05	114.81	111.23
29	a	847	BCR	C20-C19-C18	-2.05	120.75	126.36
22	7	311	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
22	b	806	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
22	2	307	CLA	C2A-C1A-CHA	2.05	127.42	123.87
22	a	830	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	a	839	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
29	b	849	BCR	C38-C26-C27	2.04	117.95	113.60
20	3	305	XAT	C20-C13-C12	2.04	121.21	118.09
20	9	304	XAT	C31-C30-C29	-2.04	124.41	127.28
20	1	303	XAT	C11-C10-C9	-2.04	124.41	127.28
29	b	844	BCR	C21-C20-C19	-2.04	117.28	123.20
20	1	302	XAT	C39-C29-C28	2.04	121.21	118.09
29	a	849	BCR	C38-C26-C27	2.04	117.95	113.60
20	4	301	XAT	C24-C23-C22	-2.04	106.97	110.79
22	b	824	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
20	9	303	XAT	C19-C9-C8	2.04	121.21	118.09
20	7	305	XAT	C7-C8-C9	-2.04	122.36	125.53
22	a	842	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
20	2	301	XAT	O4-C5-C18	2.04	117.33	115.05
22	a	809	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	b	810	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
29	b	842	BCR	C33-C5-C6	-2.04	122.26	124.48
29	b	845	BCR	C38-C26-C27	2.04	117.94	113.60
22	b	809	CLA	C1-C2-C3	-2.04	122.86	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	805	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
29	b	842	BCR	C16-C15-C14	-2.04	119.35	123.52
22	b	803	CLA	C1-C2-C3	-2.04	122.86	126.20
22	b	826	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
20	2	301	XAT	C19-C9-C8	2.04	121.20	118.09
22	9	316	CLA	CMB-C2B-C3B	2.04	131.34	126.55
22	a	809	CLA	CMB-C2B-C3B	2.04	131.34	126.55
22	8	305	CLA	CMB-C2B-C3B	2.03	131.34	126.55
22	a	854	CLA	C1-C2-C3	-2.03	122.86	126.20
29	a	849	BCR	C29-C30-C25	2.03	113.39	110.44
22	b	836	CLA	O2D-CGD-CBD	2.03	114.78	111.23
22	a	833	CLA	CMB-C2B-C3B	2.03	131.33	126.55
29	l	205	BCR	C10-C11-C12	-2.03	117.31	123.20
22	7	308	CLA	CMB-C2B-C3B	2.03	131.33	126.55
22	l	203	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
29	a	849	BCR	C35-C13-C12	2.03	121.19	118.09
22	b	814	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
22	b	802	CLA	C3B-C4B-NB	-2.03	108.72	110.53
22	1	311	CLA	C1-C2-C3	-2.03	122.87	126.20
22	b	810	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
20	9	305	XAT	O4-C5-C4	2.03	115.39	113.49
22	b	817	CLA	CHB-C1B-NB	2.03	127.09	124.05
22	b	811	CLA	C1-C2-C3	-2.03	122.88	126.20
22	b	825	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
22	a	844	CLA	CMB-C2B-C3B	2.02	131.31	126.55
20	3	305	XAT	C39-C29-C28	2.02	121.18	118.09
29	b	844	BCR	C10-C11-C12	-2.02	117.34	123.20
29	l	205	BCR	C7-C8-C9	-2.02	123.25	126.23
22	a	816	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
22	2	307	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
29	a	847	BCR	C10-C11-C12	-2.02	117.35	123.20
22	b	804	CLA	CAC-C3C-C4C	2.02	127.42	124.79
22	b	802	CLA	C1-C2-C3	-2.02	122.89	126.20
20	2	305	XAT	O24-C25-C38	2.02	117.30	115.05
20	4	304	XAT	C39-C29-C28	2.02	121.17	118.09
20	7	303	XAT	C31-C32-C33	-2.02	120.83	126.36
22	a	835	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
26	8	315	DGD	C4D-C3D-C2D	-2.01	107.29	110.83
22	b	811	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
22	b	803	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
22	b	828	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
29	h	201	BCR	C28-C27-C26	-2.01	110.46	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	811	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
22	a	813	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
22	b	807	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
24	1	304	A1L1F	C25-C14-C29	-2.01	121.74	125.99
22	4	313	CLA	CMB-C2B-C3B	2.01	131.28	126.55
22	4	308	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
29	a	847	BCR	C2-C1-C6	2.01	113.36	110.44
22	b	806	CLA	C1-C2-C3	-2.01	122.91	126.20
27	j	105	LMG	O7-C10-O9	-2.01	119.01	123.70
20	9	303	XAT	C40-C33-C32	2.01	121.16	118.09
20	4	301	XAT	C28-C29-C30	2.01	122.17	119.01
24	9	302	A1L1F	O13-C45-O46	-2.01	118.61	123.63
22	a	831	CLA	CHB-C1B-NB	2.01	127.06	124.05
22	a	833	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
20	5	301	XAT	C10-C11-C12	-2.01	117.39	123.20
22	8	311	CLA	CMB-C2B-C3B	2.01	131.27	126.55
20	3	301	XAT	C30-C31-C32	-2.00	117.39	123.20
29	f	801	BCR	C4-C5-C6	-2.00	120.00	122.70
29	a	848	BCR	C28-C27-C26	-2.00	110.48	114.06
22	7	306	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
22	7	309	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
26	4	318	DGD	C4D-C3D-C2D	-2.00	107.31	110.83
22	2	310	CLA	C1-C2-C3	-2.00	122.92	126.20
22	8	310	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
22	b	825	CLA	CMB-C2B-C3B	2.00	131.26	126.55
22	1	305	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
22	b	814	CLA	CMB-C2B-C3B	2.00	131.26	126.55
22	a	803	CLA	CHB-C4A-NA	2.00	127.29	124.40
22	9	312	CLA	CMB-C2B-C1B	-2.00	122.37	125.42

All (178) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	5	305	CLA	ND
22	5	306	CLA	ND
22	5	307	CLA	ND
22	5	308	CLA	ND
22	5	309	CLA	ND
22	5	310	CLA	ND
22	5	311	CLA	ND
22	5	312	CLA	ND
22	5	313	CLA	ND

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Mol	Chain	Res	Type	Atom
22	5	314	CLA	ND
22	5	315	CLA	ND
22	9	308	CLA	ND
22	9	309	CLA	ND
22	9	310	CLA	ND
22	9	311	CLA	ND
22	9	312	CLA	ND
22	9	313	CLA	ND
22	9	314	CLA	ND
22	9	315	CLA	ND
22	9	316	CLA	ND
22	9	318	CLA	ND
22	8	305	CLA	ND
22	8	306	CLA	ND
22	8	307	CLA	ND
22	8	308	CLA	ND
22	8	309	CLA	ND
22	8	310	CLA	ND
22	8	311	CLA	ND
22	8	312	CLA	ND
22	8	313	CLA	ND
22	8	314	CLA	ND
22	4	306	CLA	ND
22	4	307	CLA	ND
22	4	308	CLA	ND
22	4	309	CLA	ND
22	4	310	CLA	ND
22	4	311	CLA	ND
22	4	312	CLA	ND
22	4	313	CLA	ND
22	4	314	CLA	ND
22	4	315	CLA	ND
22	4	316	CLA	ND
22	4	317	CLA	ND
22	3	307	CLA	ND
22	3	308	CLA	ND
22	3	309	CLA	ND
22	3	310	CLA	ND
22	3	311	CLA	ND
22	3	312	CLA	ND
22	3	313	CLA	ND
22	3	314	CLA	ND

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Mol	Chain	Res	Type	Atom
22	3	315	CLA	ND
22	2	306	CLA	ND
22	2	307	CLA	ND
22	2	308	CLA	ND
22	2	309	CLA	ND
22	2	310	CLA	ND
22	2	311	CLA	ND
22	2	312	CLA	ND
22	2	313	CLA	ND
22	2	314	CLA	ND
22	2	315	CLA	ND
22	2	316	CLA	ND
22	7	306	CLA	ND
22	7	307	CLA	ND
22	7	308	CLA	ND
22	7	309	CLA	ND
22	7	310	CLA	ND
22	7	311	CLA	ND
22	7	312	CLA	ND
22	7	313	CLA	ND
22	7	314	CLA	ND
22	7	315	CLA	ND
22	7	316	CLA	ND
22	7	317	CLA	ND
22	1	305	CLA	ND
22	1	306	CLA	ND
22	1	307	CLA	ND
22	1	308	CLA	ND
22	1	309	CLA	ND
22	1	310	CLA	ND
22	1	311	CLA	ND
22	1	312	CLA	ND
22	1	313	CLA	ND
22	1	314	CLA	ND
22	a	801	CLA	ND
22	a	802	CLA	ND
22	a	803	CLA	ND
22	a	804	CLA	ND
22	a	805	CLA	ND
22	a	806	CLA	ND
22	a	807	CLA	ND
22	a	808	CLA	ND

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Mol	Chain	Res	Type	Atom
22	a	809	CLA	ND
22	a	810	CLA	ND
22	a	811	CLA	ND
22	a	812	CLA	ND
22	a	813	CLA	ND
22	a	814	CLA	ND
22	a	815	CLA	ND
22	a	816	CLA	ND
22	a	817	CLA	ND
22	a	818	CLA	ND
22	a	819	CLA	ND
22	a	820	CLA	ND
22	a	821	CLA	ND
22	a	822	CLA	ND
22	a	823	CLA	ND
22	a	824	CLA	ND
22	a	825	CLA	ND
22	a	826	CLA	ND
22	a	827	CLA	ND
22	a	828	CLA	ND
22	a	829	CLA	ND
22	a	830	CLA	ND
22	a	831	CLA	ND
22	a	832	CLA	ND
22	a	833	CLA	ND
22	a	834	CLA	ND
22	a	835	CLA	ND
22	a	836	CLA	ND
22	a	837	CLA	ND
22	a	838	CLA	ND
22	a	839	CLA	ND
22	a	840	CLA	ND
22	a	841	CLA	ND
22	a	842	CLA	ND
22	a	844	CLA	ND
22	a	854	CLA	ND
22	b	801	CLA	ND
22	b	802	CLA	ND
22	b	803	CLA	ND
22	b	804	CLA	ND
22	b	805	CLA	ND
22	b	806	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	807	CLA	ND
22	b	808	CLA	ND
22	b	809	CLA	ND
22	b	810	CLA	ND
22	b	811	CLA	ND
22	b	812	CLA	ND
22	b	813	CLA	ND
22	b	814	CLA	ND
22	b	815	CLA	ND
22	b	816	CLA	ND
22	b	817	CLA	ND
22	b	818	CLA	ND
22	b	819	CLA	ND
22	b	820	CLA	ND
22	b	821	CLA	ND
22	b	822	CLA	ND
22	b	823	CLA	ND
22	b	824	CLA	ND
22	b	825	CLA	ND
22	b	826	CLA	ND
22	b	827	CLA	ND
22	b	828	CLA	ND
22	b	829	CLA	ND
22	b	830	CLA	ND
22	b	831	CLA	ND
22	b	832	CLA	ND
22	b	833	CLA	ND
22	b	834	CLA	ND
22	b	835	CLA	ND
22	b	836	CLA	ND
22	b	837	CLA	ND
22	b	838	CLA	ND
22	b	839	CLA	ND
22	b	840	CLA	ND
22	f	802	CLA	ND
22	f	803	CLA	ND
22	h	203	CLA	ND
22	h	205	CLA	ND
22	j	102	CLA	ND
22	j	103	CLA	ND
22	l	202	CLA	ND
22	l	203	CLA	ND

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Mol	Chain	Res	Type	Atom
22	1	204	CLA	ND

All (1966) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	5	302	XAT	O4-C6-C7-C8
20	5	302	XAT	C7-C8-C9-C10
20	5	302	XAT	C7-C8-C9-C19
20	9	303	XAT	O4-C6-C7-C8
20	9	304	XAT	O24-C26-C27-C28
20	9	305	XAT	O4-C6-C7-C8
20	9	305	XAT	C7-C8-C9-C10
20	9	305	XAT	C7-C8-C9-C19
20	8	302	XAT	O4-C6-C7-C8
20	8	302	XAT	C7-C8-C9-C10
20	8	302	XAT	C7-C8-C9-C19
20	4	301	XAT	C27-C28-C29-C30
20	4	301	XAT	C27-C28-C29-C39
20	4	303	XAT	O4-C6-C7-C8
20	4	303	XAT	C7-C8-C9-C10
20	4	303	XAT	C7-C8-C9-C19
20	4	305	XAT	O24-C26-C27-C28
20	3	301	XAT	O4-C6-C7-C8
20	3	301	XAT	C27-C28-C29-C30
20	3	301	XAT	C27-C28-C29-C39
20	3	303	XAT	C27-C28-C29-C30
20	3	304	XAT	O24-C26-C27-C28
20	3	304	XAT	C27-C28-C29-C30
20	3	304	XAT	C27-C28-C29-C39
20	2	303	XAT	O4-C6-C7-C8
20	2	303	XAT	O24-C26-C27-C28
20	2	303	XAT	C27-C28-C29-C30
20	2	303	XAT	C27-C28-C29-C39
20	2	305	XAT	C25-C26-C27-C28
20	7	301	XAT	O4-C6-C7-C8
20	7	301	XAT	C27-C28-C29-C30
20	7	301	XAT	C27-C28-C29-C39
20	7	303	XAT	O4-C6-C7-C8
20	7	303	XAT	O24-C26-C27-C28
20	7	303	XAT	C27-C28-C29-C30
20	7	303	XAT	C27-C28-C29-C39
20	7	304	XAT	O4-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	7	304	XAT	C11-C12-C13-C14
20	7	304	XAT	C11-C12-C13-C20
20	a	852	XAT	C7-C8-C9-C10
20	a	852	XAT	C7-C8-C9-C19
20	a	852	XAT	C11-C12-C13-C14
20	a	852	XAT	C27-C28-C29-C30
20	j	101	XAT	O4-C6-C7-C8
20	j	101	XAT	C7-C8-C9-C10
20	j	101	XAT	O24-C26-C27-C28
21	5	303	A1L1G	C26-C30-C31-C32
21	5	303	A1L1G	C31-C32-C33-C34
21	5	303	A1L1G	C32-C33-C34-C27
21	5	303	A1L1G	C32-C33-C34-C35
21	5	303	A1L1G	C41-C42-C44-C2
21	5	303	A1L1G	C41-C42-C44-C43
21	9	301	A1L1G	O13-C26-C30-C29
21	9	301	A1L1G	C26-C30-C31-C32
21	9	301	A1L1G	C31-C32-C33-C34
21	9	301	A1L1G	C38-C39-C40-C41
21	9	301	A1L1G	C39-C40-C41-C42
21	9	306	A1L1G	C45-C2-C44-C42
21	9	306	A1L1G	C45-C2-C44-C43
21	9	306	A1L1G	C29-C14-C25-C24
21	9	306	A1L1G	C25-C14-C29-C30
21	9	306	A1L1G	C35-C36-C37-C38
21	9	306	A1L1G	C37-C38-C39-C28
21	9	306	A1L1G	C37-C38-C39-C40
21	3	302	A1L1G	C25-C14-C29-C30
21	3	302	A1L1G	C14-C29-C30-C26
21	3	302	A1L1G	C26-C30-C31-C32
21	3	302	A1L1G	C29-C30-C31-C32
21	3	302	A1L1G	C41-C42-C44-C2
21	3	302	A1L1G	C41-C42-C44-C43
21	3	306	A1L1G	C45-C2-C44-C42
21	3	306	A1L1G	C45-C2-C44-C43
21	3	306	A1L1G	O13-C26-C30-C29
21	3	306	A1L1G	C37-C38-C39-C28
21	3	306	A1L1G	C37-C38-C39-C40
21	3	306	A1L1G	C39-C40-C41-C42
21	3	306	A1L1G	C41-C42-C44-C2
21	3	306	A1L1G	C41-C42-C44-C43
21	7	302	A1L1G	C45-C2-C44-C42

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Mol	Chain	Res	Type	Atoms
21	7	302	A1L1G	C29-C14-C25-C24
21	7	302	A1L1G	C35-C36-C37-C38
21	7	302	A1L1G	C37-C38-C39-C28
21	7	302	A1L1G	C37-C38-C39-C40
21	7	302	A1L1G	C39-C40-C41-C42
21	7	302	A1L1G	C41-C42-C44-C2
21	7	302	A1L1G	C41-C42-C44-C43
21	1	301	A1L1G	C45-C2-C44-C42
21	1	301	A1L1G	C45-C2-C44-C43
21	1	301	A1L1G	O13-C26-C30-C29
21	1	301	A1L1G	C27-C34-C35-C36
21	1	301	A1L1G	C33-C34-C35-C36
21	1	301	A1L1G	C35-C36-C37-C38
21	1	301	A1L1G	C38-C39-C40-C41
21	1	301	A1L1G	C39-C40-C41-C42
22	5	308	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	CAD-CBD-CGD-O1D
22	5	309	CLA	CAD-CBD-CGD-O2D
22	5	310	CLA	CBD-CGD-O2D-CED
22	5	314	CLA	C1A-C2A-CAA-CBA
22	5	314	CLA	C3A-C2A-CAA-CBA
22	5	315	CLA	CBD-CGD-O2D-CED
22	5	315	CLA	O1D-CGD-O2D-CED
22	9	308	CLA	CBD-CGD-O2D-CED
22	9	310	CLA	CHA-CBD-CGD-O1D
22	9	310	CLA	CHA-CBD-CGD-O2D
22	9	311	CLA	CBD-CGD-O2D-CED
22	9	311	CLA	O1D-CGD-O2D-CED
22	9	314	CLA	CHA-CBD-CGD-O1D
22	9	314	CLA	CHA-CBD-CGD-O2D
22	9	315	CLA	CAD-CBD-CGD-O2D
22	9	315	CLA	CBD-CGD-O2D-CED
22	9	316	CLA	C1A-C2A-CAA-CBA
22	9	316	CLA	CAD-CBD-CGD-O1D
22	9	316	CLA	CAD-CBD-CGD-O2D
22	8	308	CLA	CHA-CBD-CGD-O1D
22	8	308	CLA	CHA-CBD-CGD-O2D
22	4	306	CLA	C1A-C2A-CAA-CBA
22	4	307	CLA	CHA-CBD-CGD-O1D
22	4	307	CLA	CHA-CBD-CGD-O2D
22	4	309	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	4	311	CLA	CBA-CGA-O2A-C1
22	4	311	CLA	CBD-CGD-O2D-CED
22	4	312	CLA	C1A-C2A-CAA-CBA
22	4	312	CLA	C3A-C2A-CAA-CBA
22	4	315	CLA	CAD-CBD-CGD-O2D
22	4	316	CLA	CBD-CGD-O2D-CED
22	4	317	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CHA-CBD-CGD-O1D
22	3	308	CLA	CHA-CBD-CGD-O2D
22	3	312	CLA	C1A-C2A-CAA-CBA
22	3	315	CLA	C1A-C2A-CAA-CBA
22	2	307	CLA	CHA-CBD-CGD-O2D
22	2	307	CLA	CBD-CGD-O2D-CED
22	2	309	CLA	CBD-CGD-O2D-CED
22	2	310	CLA	CHA-CBD-CGD-O1D
22	2	310	CLA	CHA-CBD-CGD-O2D
22	2	312	CLA	CBD-CGD-O2D-CED
22	2	313	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	C3A-C2A-CAA-CBA
22	7	306	CLA	CBD-CGD-O2D-CED
22	7	307	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBA-CGA-O2A-C1
22	7	311	CLA	CBA-CGA-O2A-C1
22	7	314	CLA	CBD-CGD-O2D-CED
22	7	315	CLA	C4B-C3B-CAB-CBB
22	7	315	CLA	CBD-CGD-O2D-CED
22	7	316	CLA	C1A-C2A-CAA-CBA
22	7	316	CLA	C3A-C2A-CAA-CBA
22	7	316	CLA	CHA-CBD-CGD-O1D
22	7	316	CLA	CHA-CBD-CGD-O2D
22	1	305	CLA	C11-C10-C8-C9
22	1	310	CLA	CBD-CGD-O2D-CED
22	1	313	CLA	CBD-CGD-O2D-CED
22	1	314	CLA	C1A-C2A-CAA-CBA
22	1	314	CLA	C3A-C2A-CAA-CBA
22	a	801	CLA	CBD-CGD-O2D-CED
22	a	804	CLA	CHA-CBD-CGD-O1D
22	a	804	CLA	CHA-CBD-CGD-O2D
22	a	805	CLA	C1A-C2A-CAA-CBA
22	a	805	CLA	C3A-C2A-CAA-CBA
22	a	806	CLA	CAD-CBD-CGD-O2D
22	a	809	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	a	809	CLA	C3A-C2A-CAA-CBA
22	a	809	CLA	CHA-CBD-CGD-O1D
22	a	809	CLA	CHA-CBD-CGD-O2D
22	a	811	CLA	CBD-CGD-O2D-CED
22	a	817	CLA	CHA-CBD-CGD-O1D
22	a	817	CLA	CHA-CBD-CGD-O2D
22	a	818	CLA	C1A-C2A-CAA-CBA
22	a	818	CLA	C3A-C2A-CAA-CBA
22	a	818	CLA	CHA-CBD-CGD-O1D
22	a	818	CLA	CHA-CBD-CGD-O2D
22	a	819	CLA	C3A-C2A-CAA-CBA
22	a	820	CLA	C1A-C2A-CAA-CBA
22	a	820	CLA	C3A-C2A-CAA-CBA
22	a	823	CLA	C1A-C2A-CAA-CBA
22	a	823	CLA	C3A-C2A-CAA-CBA
22	a	823	CLA	CHA-CBD-CGD-O1D
22	a	823	CLA	CHA-CBD-CGD-O2D
22	a	829	CLA	C1A-C2A-CAA-CBA
22	a	829	CLA	CBD-CGD-O2D-CED
22	a	831	CLA	CHA-CBD-CGD-O1D
22	a	831	CLA	CHA-CBD-CGD-O2D
22	a	832	CLA	C1A-C2A-CAA-CBA
22	a	832	CLA	C3A-C2A-CAA-CBA
22	a	834	CLA	C2B-C3B-CAB-CBB
22	a	834	CLA	C4B-C3B-CAB-CBB
22	a	838	CLA	C1A-C2A-CAA-CBA
22	a	838	CLA	C2-C3-C5-C6
22	a	838	CLA	C4-C3-C5-C6
22	a	854	CLA	C1A-C2A-CAA-CBA
22	a	854	CLA	C2B-C3B-CAB-CBB
22	a	854	CLA	C4B-C3B-CAB-CBB
22	b	803	CLA	CBD-CGD-O2D-CED
22	b	804	CLA	CBD-CGD-O2D-CED
22	b	805	CLA	CHA-CBD-CGD-O1D
22	b	805	CLA	CHA-CBD-CGD-O2D
22	b	806	CLA	C1A-C2A-CAA-CBA
22	b	806	CLA	C3A-C2A-CAA-CBA
22	b	806	CLA	CAD-CBD-CGD-O1D
22	b	806	CLA	CAD-CBD-CGD-O2D
22	b	809	CLA	CHA-CBD-CGD-O1D
22	b	809	CLA	CHA-CBD-CGD-O2D
22	b	810	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	b	812	CLA	C1A-C2A-CAA-CBA
22	b	812	CLA	C2-C3-C5-C6
22	b	812	CLA	C4-C3-C5-C6
22	b	814	CLA	C1A-C2A-CAA-CBA
22	b	814	CLA	CBD-CGD-O2D-CED
22	b	815	CLA	CHA-CBD-CGD-O1D
22	b	815	CLA	CHA-CBD-CGD-O2D
22	b	817	CLA	C3A-C2A-CAA-CBA
22	b	818	CLA	C1A-C2A-CAA-CBA
22	b	818	CLA	C3A-C2A-CAA-CBA
22	b	819	CLA	C4B-C3B-CAB-CBB
22	b	820	CLA	C1A-C2A-CAA-CBA
22	b	820	CLA	C3A-C2A-CAA-CBA
22	b	821	CLA	CHA-CBD-CGD-O2D
22	b	824	CLA	CHA-CBD-CGD-O1D
22	b	824	CLA	CHA-CBD-CGD-O2D
22	b	828	CLA	C1A-C2A-CAA-CBA
22	b	828	CLA	C3A-C2A-CAA-CBA
22	b	829	CLA	CHA-CBD-CGD-O1D
22	b	829	CLA	CHA-CBD-CGD-O2D
22	b	832	CLA	C1A-C2A-CAA-CBA
22	b	832	CLA	C3A-C2A-CAA-CBA
22	b	833	CLA	C1A-C2A-CAA-CBA
22	b	833	CLA	C3A-C2A-CAA-CBA
22	b	833	CLA	C11-C12-C13-C14
22	b	834	CLA	CHA-CBD-CGD-O1D
22	b	834	CLA	CHA-CBD-CGD-O2D
22	b	834	CLA	CBD-CGD-O2D-CED
22	b	838	CLA	C4B-C3B-CAB-CBB
22	b	839	CLA	C1A-C2A-CAA-CBA
22	b	839	CLA	C3A-C2A-CAA-CBA
22	b	839	CLA	CAD-CBD-CGD-O1D
22	b	839	CLA	CAD-CBD-CGD-O2D
22	b	839	CLA	CBD-CGD-O2D-CED
22	h	203	CLA	C1A-C2A-CAA-CBA
22	j	102	CLA	C1A-C2A-CAA-CBA
22	j	103	CLA	CAD-CBD-CGD-O1D
22	j	103	CLA	CAD-CBD-CGD-O2D
22	j	103	CLA	CBD-CGD-O2D-CED
22	l	203	CLA	C6-C7-C8-C9
23	5	316	SQD	O49-C7-O47-C45
23	5	316	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
23	5	316	SQD	C5-C6-S-O7
23	5	316	SQD	C5-C6-S-O8
23	5	316	SQD	C5-C6-S-O9
23	1	315	SQD	O5-C5-C6-S
23	1	315	SQD	C5-C6-S-O7
23	1	315	SQD	C5-C6-S-O8
23	1	315	SQD	C5-C6-S-O9
24	9	302	A1L1F	O13-C26-C30-C31
24	9	302	A1L1F	C56-C54-O7-C8
24	8	304	A1L1F	C32-C33-C34-C35
24	8	304	A1L1F	C56-C54-O7-C8
24	8	304	A1L1F	O55-C54-O7-C8
24	1	304	A1L1F	C32-C33-C34-C35
24	1	304	A1L1F	C38-C39-C40-C41
24	h	204	A1L1F	C56-C54-O7-C8
24	h	204	A1L1F	O55-C54-O7-C8
25	9	307	LHG	C3-O3-P-O4
25	9	307	LHG	C3-O3-P-O5
25	9	307	LHG	C3-O3-P-O6
25	9	307	LHG	O9-C7-O7-C5
25	9	307	LHG	C8-C7-O7-C5
25	9	317	LHG	C1-C2-C3-O3
25	9	317	LHG	C3-O3-P-O4
25	9	317	LHG	O9-C7-O7-C5
25	9	317	LHG	C8-C7-O7-C5
25	a	845	LHG	O1-C1-C2-C3
25	a	845	LHG	C3-O3-P-O4
25	a	845	LHG	C3-O3-P-O6
25	a	845	LHG	C4-O6-P-O3
25	a	845	LHG	C4-O6-P-O5
25	a	845	LHG	O6-C4-C5-O7
25	a	845	LHG	O7-C5-C6-O8
25	a	846	LHG	O1-C1-C2-C3
25	a	846	LHG	O6-C4-C5-O7
25	b	847	LHG	O1-C1-C2-C3
25	b	847	LHG	C1-C2-C3-O3
25	b	847	LHG	O2-C2-C3-O3
25	b	847	LHG	C3-O3-P-O5
25	b	847	LHG	C3-O3-P-O6
25	b	847	LHG	C4-O6-P-O3
25	b	847	LHG	C4-O6-P-O4
25	b	847	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
26	8	315	DGD	C2B-C1B-O2G-C2G
26	4	318	DGD	C2B-C1B-O2G-C2G
26	4	318	DGD	O1B-C1B-O2G-C2G
27	2	317	LMG	O1-C7-C8-O7
27	a	853	LMG	C11-C10-O7-C8
27	j	105	LMG	O9-C10-O7-C8
27	j	105	LMG	C11-C10-O7-C8
29	a	850	BCR	C23-C24-C25-C26
29	b	842	BCR	C7-C8-C9-C10
29	b	842	BCR	C7-C8-C9-C34
29	b	844	BCR	C1-C6-C7-C8
29	b	844	BCR	C5-C6-C7-C8
29	i	101	BCR	C21-C22-C23-C24
29	i	101	BCR	C37-C22-C23-C24
29	j	104	BCR	C7-C8-C9-C10
29	j	104	BCR	C7-C8-C9-C34
29	m	101	BCR	C21-C22-C23-C24
29	m	101	BCR	C37-C22-C23-C24
22	5	310	CLA	O1D-CGD-O2D-CED
22	9	315	CLA	O1D-CGD-O2D-CED
22	4	309	CLA	O1D-CGD-O2D-CED
22	2	314	CLA	O1D-CGD-O2D-CED
22	7	314	CLA	O1D-CGD-O2D-CED
24	9	302	A1L1F	O55-C54-O7-C8
22	9	308	CLA	O1D-CGD-O2D-CED
22	2	307	CLA	O1D-CGD-O2D-CED
22	2	309	CLA	O1D-CGD-O2D-CED
22	2	313	CLA	O1D-CGD-O2D-CED
22	7	307	CLA	O1D-CGD-O2D-CED
22	1	313	CLA	O1D-CGD-O2D-CED
22	a	812	CLA	O1D-CGD-O2D-CED
22	b	803	CLA	O1D-CGD-O2D-CED
22	b	834	CLA	O1D-CGD-O2D-CED
22	5	313	CLA	CBD-CGD-O2D-CED
22	9	318	CLA	CBD-CGD-O2D-CED
22	8	306	CLA	CBD-CGD-O2D-CED
22	4	306	CLA	CBD-CGD-O2D-CED
22	2	314	CLA	CBD-CGD-O2D-CED
22	1	309	CLA	CBD-CGD-O2D-CED
22	a	812	CLA	CBD-CGD-O2D-CED
22	8	308	CLA	O1A-CGA-O2A-C1
22	1	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	a	806	CLA	O1A-CGA-O2A-C1
22	b	814	CLA	O1A-CGA-O2A-C1
25	9	317	LHG	O10-C23-O8-C6
27	2	317	LMG	O10-C28-O8-C9
22	7	310	CLA	O1A-CGA-O2A-C1
22	4	316	CLA	O1D-CGD-O2D-CED
22	7	315	CLA	O1D-CGD-O2D-CED
22	b	804	CLA	O1D-CGD-O2D-CED
24	9	302	A1L1F	C4-C8-O7-C54
22	a	801	CLA	O1D-CGD-O2D-CED
22	8	308	CLA	CBA-CGA-O2A-C1
22	1	307	CLA	CBA-CGA-O2A-C1
22	a	806	CLA	CBA-CGA-O2A-C1
22	b	814	CLA	CBA-CGA-O2A-C1
25	9	317	LHG	C24-C23-O8-C6
22	4	310	CLA	O1A-CGA-O2A-C1
22	2	310	CLA	O1A-CGA-O2A-C1
22	2	311	CLA	O1A-CGA-O2A-C1
22	7	312	CLA	O1A-CGA-O2A-C1
22	a	805	CLA	O1A-CGA-O2A-C1
22	a	818	CLA	O1A-CGA-O2A-C1
22	b	821	CLA	O1A-CGA-O2A-C1
22	f	802	CLA	O1A-CGA-O2A-C1
25	b	847	LHG	O10-C23-O8-C6
26	8	315	DGD	O1A-C1A-O1G-C1G
27	a	853	LMG	O10-C28-O8-C9
22	4	311	CLA	O1A-CGA-O2A-C1
22	7	311	CLA	O1A-CGA-O2A-C1
22	2	312	CLA	O1D-CGD-O2D-CED
22	b	814	CLA	O1D-CGD-O2D-CED
22	5	308	CLA	O1D-CGD-O2D-CED
22	4	317	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	O1D-CGD-O2D-CED
22	1	310	CLA	O1D-CGD-O2D-CED
22	a	811	CLA	O1D-CGD-O2D-CED
22	a	829	CLA	O1D-CGD-O2D-CED
22	b	839	CLA	O1D-CGD-O2D-CED
22	j	103	CLA	O1D-CGD-O2D-CED
26	8	315	DGD	O1B-C1B-O2G-C2G
27	a	853	LMG	O9-C10-O7-C8
22	1	309	CLA	CBA-CGA-O2A-C1
22	1	309	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	1	204	CLA	O1A-CGA-O2A-C1
22	3	312	CLA	C3-C5-C6-C7
22	2	310	CLA	C3-C5-C6-C7
22	2	311	CLA	C3-C5-C6-C7
22	2	314	CLA	C3-C5-C6-C7
22	7	308	CLA	C3-C5-C6-C7
22	a	810	CLA	C3-C5-C6-C7
22	b	802	CLA	C3-C5-C6-C7
22	b	805	CLA	C3-C5-C6-C7
22	b	807	CLA	C3-C5-C6-C7
22	b	809	CLA	C3-C5-C6-C7
22	2	310	CLA	CBA-CGA-O2A-C1
22	2	311	CLA	CBA-CGA-O2A-C1
22	7	312	CLA	CBA-CGA-O2A-C1
22	a	805	CLA	CBA-CGA-O2A-C1
22	a	818	CLA	CBA-CGA-O2A-C1
22	a	836	CLA	CBA-CGA-O2A-C1
22	b	821	CLA	CBA-CGA-O2A-C1
22	b	823	CLA	CBA-CGA-O2A-C1
22	f	802	CLA	CBA-CGA-O2A-C1
27	2	317	LMG	C29-C28-O8-C9
27	a	853	LMG	C29-C28-O8-C9
24	1	304	A1L1F	C56-C54-O7-C8
24	1	304	A1L1F	O55-C54-O7-C8
22	5	305	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	CBD-CGD-O2D-CED
22	9	312	CLA	CBD-CGD-O2D-CED
22	9	314	CLA	CBD-CGD-O2D-CED
22	8	309	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CBD-CGD-O2D-CED
22	2	316	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBD-CGD-O2D-CED
22	a	804	CLA	CBD-CGD-O2D-CED
22	a	814	CLA	CBD-CGD-O2D-CED
22	b	806	CLA	CBD-CGD-O2D-CED
22	b	819	CLA	CBD-CGD-O2D-CED
22	b	835	CLA	CBD-CGD-O2D-CED
22	h	205	CLA	CBD-CGD-O2D-CED
22	4	311	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	O1A-CGA-O2A-C1
22	1	309	CLA	O1D-CGD-O2D-CED
22	8	311	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	3	310	CLA	C4-C3-C5-C6
22	a	825	CLA	C4-C3-C5-C6
22	a	831	CLA	C4-C3-C5-C6
22	a	839	CLA	C4-C3-C5-C6
22	j	102	CLA	C4-C3-C5-C6
22	8	311	CLA	C2-C3-C5-C6
22	3	310	CLA	C2-C3-C5-C6
22	a	831	CLA	C2-C3-C5-C6
22	a	839	CLA	C2-C3-C5-C6
22	j	102	CLA	C2-C3-C5-C6
22	9	309	CLA	CBA-CGA-O2A-C1
22	l	204	CLA	CBA-CGA-O2A-C1
22	5	306	CLA	CBD-CGD-O2D-CED
22	b	810	CLA	C2A-CAA-CBA-CGA
22	9	308	CLA	C3-C5-C6-C7
22	8	308	CLA	C3-C5-C6-C7
22	1	307	CLA	C3-C5-C6-C7
22	1	310	CLA	C3-C5-C6-C7
22	b	818	CLA	C3-C5-C6-C7
22	9	316	CLA	CBA-CGA-O2A-C1
22	4	310	CLA	CBA-CGA-O2A-C1
22	1	305	CLA	CBA-CGA-O2A-C1
22	a	807	CLA	CBA-CGA-O2A-C1
22	a	811	CLA	CBA-CGA-O2A-C1
22	b	806	CLA	CBA-CGA-O2A-C1
22	b	818	CLA	CBA-CGA-O2A-C1
25	9	307	LHG	C24-C23-O8-C6
25	b	847	LHG	C24-C23-O8-C6
26	8	315	DGD	C2A-C1A-O1G-C1G
27	j	105	LMG	C29-C28-O8-C9
27	j	105	LMG	C4-C5-C6-O5
21	9	301	A1L1G	C30-C31-C32-C33
21	9	301	A1L1G	C40-C41-C42-C44
21	3	302	A1L1G	C30-C31-C32-C33
21	7	302	A1L1G	C30-C31-C32-C33
24	8	304	A1L1F	C30-C31-C32-C33
22	5	311	CLA	O1A-CGA-O2A-C1
22	1	305	CLA	O1A-CGA-O2A-C1
22	a	811	CLA	O1A-CGA-O2A-C1
22	a	812	CLA	O1A-CGA-O2A-C1
22	a	820	CLA	O1A-CGA-O2A-C1
22	b	806	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	b	818	CLA	O1A-CGA-O2A-C1
27	j	105	LMG	O10-C28-O8-C9
22	4	307	CLA	CBD-CGD-O2D-CED
22	7	308	CLA	CBD-CGD-O2D-CED
22	a	818	CLA	CBD-CGD-O2D-CED
22	a	837	CLA	CBD-CGD-O2D-CED
27	j	105	LMG	C12-C13-C14-C15
25	9	307	LHG	O2-C2-C3-O3
25	9	317	LHG	O2-C2-C3-O3
25	a	845	LHG	O2-C2-C3-O3
22	7	306	CLA	CBA-CGA-O2A-C1
22	a	812	CLA	CBA-CGA-O2A-C1
22	b	839	CLA	CBA-CGA-O2A-C1
22	a	836	CLA	O1A-CGA-O2A-C1
22	b	823	CLA	O1A-CGA-O2A-C1
25	9	307	LHG	O10-C23-O8-C6
22	9	316	CLA	CBD-CGD-O2D-CED
22	3	309	CLA	CBD-CGD-O2D-CED
22	3	315	CLA	CBD-CGD-O2D-CED
22	9	312	CLA	CBA-CGA-O2A-C1
22	b	839	CLA	O1A-CGA-O2A-C1
22	9	318	CLA	O1D-CGD-O2D-CED
22	8	306	CLA	O1D-CGD-O2D-CED
22	5	309	CLA	C3-C5-C6-C7
22	a	807	CLA	C3-C5-C6-C7
22	a	835	CLA	C3-C5-C6-C7
22	b	823	CLA	CBD-CGD-O2D-CED
22	b	827	CLA	CBD-CGD-O2D-CED
26	b	848	DGD	O6E-C5E-C6E-O5E
22	4	306	CLA	O1D-CGD-O2D-CED
22	5	311	CLA	CBA-CGA-O2A-C1
22	a	820	CLA	CBA-CGA-O2A-C1
22	a	813	CLA	C4-C3-C5-C6
22	b	828	CLA	C4-C3-C5-C6
22	a	825	CLA	C2-C3-C5-C6
22	9	316	CLA	O1A-CGA-O2A-C1
22	a	807	CLA	O1A-CGA-O2A-C1
22	8	313	CLA	CBA-CGA-O2A-C1
22	7	317	CLA	CBD-CGD-O2D-CED
22	a	835	CLA	CBD-CGD-O2D-CED
22	a	841	CLA	CBD-CGD-O2D-CED
22	1	312	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	a	817	CLA	C2A-CAA-CBA-CGA
26	8	315	DGD	O6E-C1E-O5D-C6D
26	4	318	DGD	O6E-C1E-O5D-C6D
22	7	316	CLA	CBA-CGA-O2A-C1
22	4	308	CLA	CBD-CGD-O2D-CED
22	a	807	CLA	CBD-CGD-O2D-CED
22	a	810	CLA	CBD-CGD-O2D-CED
22	a	834	CLA	CBD-CGD-O2D-CED
22	b	840	CLA	CBD-CGD-O2D-CED
25	a	845	LHG	C23-C24-C25-C26
22	9	312	CLA	O1A-CGA-O2A-C1
27	a	853	LMG	O6-C5-C6-O5
27	j	105	LMG	O6-C5-C6-O5
22	5	313	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	C12-C13-C14-C15
22	9	309	CLA	O1A-CGA-O2A-C1
21	5	303	A1L1G	C40-C41-C42-C44
24	8	304	A1L1F	C40-C41-C42-C44
25	9	307	LHG	C1-C2-C3-O3
25	a	845	LHG	C1-C2-C3-O3
22	5	308	CLA	CBA-CGA-O2A-C1
22	8	311	CLA	CBA-CGA-O2A-C1
22	3	311	CLA	CBA-CGA-O2A-C1
22	a	809	CLA	CBA-CGA-O2A-C1
22	a	839	CLA	CBA-CGA-O2A-C1
22	a	854	CLA	CBA-CGA-O2A-C1
22	b	820	CLA	CBA-CGA-O2A-C1
22	b	826	CLA	CBA-CGA-O2A-C1
22	b	833	CLA	CBA-CGA-O2A-C1
22	h	203	CLA	CBA-CGA-O2A-C1
22	5	311	CLA	CBD-CGD-O2D-CED
27	a	853	LMG	C4-C5-C6-O5
24	9	302	A1L1F	C47-C48-C49-C50
22	a	804	CLA	O1D-CGD-O2D-CED
22	b	806	CLA	O1D-CGD-O2D-CED
22	a	854	CLA	O1A-CGA-O2A-C1
25	a	845	LHG	C28-C29-C30-C31
22	a	813	CLA	C2-C3-C5-C6
22	b	822	CLA	CBD-CGD-O2D-CED
22	9	318	CLA	C11-C10-C8-C9
22	9	318	CLA	C11-C12-C13-C14
22	8	307	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	8	311	CLA	C6-C7-C8-C9
22	2	310	CLA	C11-C12-C13-C14
22	1	306	CLA	C6-C7-C8-C9
22	1	306	CLA	C11-C12-C13-C14
22	1	310	CLA	C14-C13-C15-C16
22	a	829	CLA	C11-C10-C8-C9
22	b	801	CLA	C11-C10-C8-C9
22	b	801	CLA	C14-C13-C15-C16
22	b	805	CLA	C11-C10-C8-C9
22	b	818	CLA	C11-C10-C8-C9
22	b	824	CLA	C6-C7-C8-C9
22	b	829	CLA	C14-C13-C15-C16
22	b	838	CLA	C6-C7-C8-C9
22	f	802	CLA	C11-C12-C13-C14
27	2	317	LMG	C29-C30-C31-C32
22	9	312	CLA	O1D-CGD-O2D-CED
22	9	314	CLA	O1D-CGD-O2D-CED
22	7	310	CLA	O1D-CGD-O2D-CED
26	8	315	DGD	C2E-C1E-O5D-C6D
26	4	318	DGD	C2E-C1E-O5D-C6D
25	a	846	LHG	O2-C2-C3-O3
22	8	309	CLA	O1D-CGD-O2D-CED
22	b	835	CLA	O1D-CGD-O2D-CED
22	8	311	CLA	O1A-CGA-O2A-C1
22	a	809	CLA	O1A-CGA-O2A-C1
22	h	205	CLA	O1D-CGD-O2D-CED
20	8	301	XAT	C7-C8-C9-C19
20	3	303	XAT	C27-C28-C29-C39
20	2	301	XAT	C27-C28-C29-C39
20	a	852	XAT	C11-C12-C13-C20
20	a	852	XAT	C27-C28-C29-C39
20	j	101	XAT	C7-C8-C9-C19
21	9	301	A1L1G	C28-C39-C40-C41
21	3	306	A1L1G	C28-C39-C40-C41
21	1	301	A1L1G	C28-C39-C40-C41
24	8	304	A1L1F	C32-C33-C34-C27
24	8	304	A1L1F	C28-C39-C40-C41
24	1	304	A1L1F	C32-C33-C34-C27
24	1	304	A1L1F	C28-C39-C40-C41
29	b	849	BCR	C7-C8-C9-C34
29	l	205	BCR	C7-C8-C9-C34
29	l	205	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	m	101	BCR	C7-C8-C9-C34
20	2	301	XAT	C27-C28-C29-C30
21	3	306	A1L1G	C38-C39-C40-C41
29	b	849	BCR	C7-C8-C9-C10
29	l	205	BCR	C7-C8-C9-C10
29	l	205	BCR	C21-C22-C23-C24
22	5	310	CLA	C2A-CAA-CBA-CGA
22	9	313	CLA	C2A-CAA-CBA-CGA
22	4	311	CLA	C2A-CAA-CBA-CGA
22	4	316	CLA	C2A-CAA-CBA-CGA
22	b	805	CLA	C2A-CAA-CBA-CGA
22	b	826	CLA	C2A-CAA-CBA-CGA
27	a	853	LMG	C28-C29-C30-C31
22	5	305	CLA	O1D-CGD-O2D-CED
22	3	311	CLA	O1A-CGA-O2A-C1
22	b	820	CLA	O1A-CGA-O2A-C1
22	h	203	CLA	O1A-CGA-O2A-C1
22	9	313	CLA	CBA-CGA-O2A-C1
22	4	316	CLA	CBA-CGA-O2A-C1
22	2	312	CLA	CBA-CGA-O2A-C1
22	b	838	CLA	CBA-CGA-O2A-C1
22	a	810	CLA	C13-C15-C16-C17
22	b	826	CLA	O1A-CGA-O2A-C1
22	2	316	CLA	O1D-CGD-O2D-CED
21	3	302	A1L1G	C35-C36-C37-C38
22	9	318	CLA	C8-C10-C11-C12
22	8	307	CLA	C5-C6-C7-C8
22	a	807	CLA	C5-C6-C7-C8
22	b	809	CLA	C5-C6-C7-C8
22	a	814	CLA	O1D-CGD-O2D-CED
22	b	823	CLA	C3-C5-C6-C7
22	5	308	CLA	O1A-CGA-O2A-C1
22	b	807	CLA	C15-C16-C17-C18
22	4	315	CLA	CBD-CGD-O2D-CED
22	b	807	CLA	CBD-CGD-O2D-CED
22	h	203	CLA	CBD-CGD-O2D-CED
22	1	310	CLA	C11-C10-C8-C7
22	a	801	CLA	C12-C13-C15-C16
22	a	809	CLA	C12-C13-C15-C16
22	a	828	CLA	C12-C13-C15-C16
22	a	844	CLA	C12-C13-C15-C16
22	b	808	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	833	CLA	C13-C15-C16-C17
26	b	848	DGD	C1A-C2A-C3A-C4A
22	5	309	CLA	O1D-CGD-O2D-CED
25	b	847	LHG	C7-C8-C9-C10
22	a	839	CLA	O1A-CGA-O2A-C1
22	b	833	CLA	O1A-CGA-O2A-C1
22	b	827	CLA	CBA-CGA-O2A-C1
22	2	310	CLA	C15-C16-C17-C18
22	a	809	CLA	C5-C6-C7-C8
22	b	801	CLA	C15-C16-C17-C18
22	9	311	CLA	C2A-CAA-CBA-CGA
22	9	312	CLA	C2A-CAA-CBA-CGA
22	7	317	CLA	C2A-CAA-CBA-CGA
22	a	825	CLA	C2A-CAA-CBA-CGA
22	a	830	CLA	C2A-CAA-CBA-CGA
22	a	842	CLA	C2A-CAA-CBA-CGA
22	b	820	CLA	C2A-CAA-CBA-CGA
22	b	833	CLA	C2A-CAA-CBA-CGA
22	b	838	CLA	C2A-CAA-CBA-CGA
21	9	306	A1L1G	C39-C40-C41-C42
21	3	302	A1L1G	C39-C40-C41-C42
22	9	308	CLA	C5-C6-C7-C8
22	9	318	CLA	C10-C11-C12-C13
22	4	308	CLA	C10-C11-C12-C13
22	a	802	CLA	C5-C6-C7-C8
22	a	814	CLA	C13-C15-C16-C17
22	a	834	CLA	C15-C16-C17-C18
22	b	832	CLA	C13-C15-C16-C17
22	b	840	CLA	C13-C15-C16-C17
24	1	304	A1L1F	C45-C47-C48-C49
25	a	846	LHG	C7-C8-C9-C10
27	a	853	LMG	C10-C11-C12-C13
22	a	801	CLA	C3-C5-C6-C7
24	1	304	A1L1F	C49-C50-C51-C52
22	3	308	CLA	O1D-CGD-O2D-CED
22	b	819	CLA	O1D-CGD-O2D-CED
22	5	309	CLA	C13-C15-C16-C17
22	1	306	CLA	C5-C6-C7-C8
22	1	306	CLA	C8-C10-C11-C12
22	a	809	CLA	C8-C10-C11-C12
22	a	830	CLA	C13-C15-C16-C17
22	a	831	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	b	809	CLA	C8-C10-C11-C12
22	b	813	CLA	C15-C16-C17-C18
22	b	829	CLA	C8-C10-C11-C12
22	l	203	CLA	C10-C11-C12-C13
22	8	310	CLA	CBD-CGD-O2D-CED
22	7	316	CLA	O1A-CGA-O2A-C1
22	a	807	CLA	C15-C16-C17-C18
22	a	841	CLA	C5-C6-C7-C8
22	b	814	CLA	C5-C6-C7-C8
22	b	836	CLA	C5-C6-C7-C8
22	a	837	CLA	O1D-CGD-O2D-CED
22	5	305	CLA	CBA-CGA-O2A-C1
22	5	306	CLA	O1D-CGD-O2D-CED
22	7	308	CLA	O1D-CGD-O2D-CED
22	9	308	CLA	C8-C10-C11-C12
22	f	802	CLA	CBD-CGD-O2D-CED
22	7	308	CLA	C4-C3-C5-C6
22	2	312	CLA	O1A-CGA-O2A-C1
22	1	306	CLA	C15-C16-C17-C18
22	a	841	CLA	C15-C16-C17-C18
22	4	317	CLA	CBA-CGA-O2A-C1
22	a	816	CLA	CBA-CGA-O2A-C1
22	b	802	CLA	CBA-CGA-O2A-C1
22	b	831	CLA	CBA-CGA-O2A-C1
26	b	848	DGD	C4E-C5E-C6E-O5E
22	7	306	CLA	O2A-C1-C2-C3
22	b	802	CLA	CBD-CGD-O2D-CED
22	a	818	CLA	O1D-CGD-O2D-CED
22	b	840	CLA	C10-C11-C12-C13
22	4	313	CLA	C3-C5-C6-C7
22	7	313	CLA	C3-C5-C6-C7
21	9	306	A1L1G	C40-C41-C42-C44
22	b	801	CLA	C2A-CAA-CBA-CGA
22	4	307	CLA	O1D-CGD-O2D-CED
22	a	814	CLA	CBA-CGA-O2A-C1
22	a	838	CLA	CBA-CGA-O2A-C1
22	a	801	CLA	C8-C10-C11-C12
22	a	828	CLA	C13-C15-C16-C17
22	a	828	CLA	C15-C16-C17-C18
22	f	802	CLA	C13-C15-C16-C17
22	h	205	CLA	C5-C6-C7-C8
28	b	841	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
22	a	826	CLA	CBD-CGD-O2D-CED
22	3	315	CLA	O1D-CGD-O2D-CED
22	7	308	CLA	C10-C11-C12-C13
22	b	836	CLA	C8-C10-C11-C12
22	f	802	CLA	C5-C6-C7-C8
22	7	316	CLA	C2C-C3C-CAC-CBC
22	8	313	CLA	O1A-CGA-O2A-C1
22	a	831	CLA	C15-C16-C17-C18
22	a	839	CLA	C13-C15-C16-C17
22	b	802	CLA	C8-C10-C11-C12
22	b	827	CLA	C13-C15-C16-C17
22	a	833	CLA	CBA-CGA-O2A-C1
22	a	844	CLA	CBA-CGA-O2A-C1
23	1	315	SQD	C24-C23-O48-C46
26	4	318	DGD	C3B-C4B-C5B-C6B
22	b	828	CLA	C2-C3-C5-C6
22	b	801	CLA	C8-C10-C11-C12
22	b	801	CLA	C13-C15-C16-C17
22	1	203	CLA	C8-C10-C11-C12
23	1	315	SQD	C8-C7-O47-C45
22	9	316	CLA	O1D-CGD-O2D-CED
23	1	315	SQD	O49-C7-O47-C45
22	7	309	CLA	O2A-C1-C2-C3
22	9	310	CLA	CBA-CGA-O2A-C1
22	a	824	CLA	CBA-CGA-O2A-C1
22	9	316	CLA	C16-C17-C18-C20
22	a	801	CLA	C16-C17-C18-C20
22	b	833	CLA	C16-C17-C18-C19
22	b	838	CLA	O1A-CGA-O2A-C1
21	9	306	A1L1G	C14-C29-C30-C31
21	3	302	A1L1G	C14-C29-C30-C31
21	9	301	A1L1G	C41-C42-C44-C43
21	9	306	A1L1G	C41-C42-C44-C43
21	3	302	A1L1G	C37-C38-C39-C28
21	3	306	A1L1G	C27-C34-C35-C36
20	9	303	XAT	C7-C8-C9-C19
20	2	303	XAT	C7-C8-C9-C19
20	2	304	XAT	C7-C8-C9-C19
21	9	301	A1L1G	C32-C33-C34-C27
21	3	302	A1L1G	C32-C33-C34-C27
21	7	302	A1L1G	C32-C33-C34-C27
29	a	850	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
29	f	801	BCR	C37-C22-C23-C24
20	9	303	XAT	C7-C8-C9-C10
20	8	301	XAT	C7-C8-C9-C10
20	2	303	XAT	C7-C8-C9-C10
20	7	304	XAT	C7-C8-C9-C10
21	9	301	A1L1G	C32-C33-C34-C35
21	3	302	A1L1G	C32-C33-C34-C35
24	8	304	A1L1F	C38-C39-C40-C41
29	a	850	BCR	C21-C22-C23-C24
29	f	801	BCR	C21-C22-C23-C24
22	4	317	CLA	O1A-CGA-O2A-C1
22	a	816	CLA	O1A-CGA-O2A-C1
22	b	802	CLA	O1A-CGA-O2A-C1
22	2	310	CLA	C2A-CAA-CBA-CGA
22	7	310	CLA	C2A-CAA-CBA-CGA
22	b	831	CLA	C2A-CAA-CBA-CGA
22	h	205	CLA	C2A-CAA-CBA-CGA
22	b	829	CLA	C10-C11-C12-C13
22	b	839	CLA	C5-C6-C7-C8
22	3	309	CLA	O1D-CGD-O2D-CED
22	a	806	CLA	O2A-C1-C2-C3
21	5	303	A1L1G	C29-C30-C31-C32
21	9	301	A1L1G	C29-C30-C31-C32
21	9	306	A1L1G	C29-C30-C31-C32
22	b	840	CLA	C16-C17-C18-C20
22	a	841	CLA	O1D-CGD-O2D-CED
22	b	823	CLA	O1D-CGD-O2D-CED
22	a	814	CLA	O1A-CGA-O2A-C1
22	b	827	CLA	O1A-CGA-O2A-C1
22	5	315	CLA	C2C-C3C-CAC-CBC
21	9	301	A1L1G	C41-C42-C44-C2
21	9	306	A1L1G	C41-C42-C44-C2
21	3	302	A1L1G	C37-C38-C39-C40
21	3	306	A1L1G	C33-C34-C35-C36
22	a	835	CLA	O1D-CGD-O2D-CED
22	b	824	CLA	C5-C6-C7-C8
22	7	317	CLA	O1D-CGD-O2D-CED
22	a	834	CLA	O1D-CGD-O2D-CED
22	b	827	CLA	O1D-CGD-O2D-CED
22	a	818	CLA	C2-C1-O2A-CGA
22	9	316	CLA	C16-C17-C18-C19
22	4	308	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	a	854	CLA	C5-C6-C7-C8
26	b	848	DGD	C9B-CAB-CBB-CCB
22	a	836	CLA	CBD-CGD-O2D-CED
21	9	301	A1L1G	C35-C36-C37-C38
21	3	306	A1L1G	C35-C36-C37-C38
29	m	101	BCR	C14-C15-C16-C17
25	a	845	LHG	C11-C10-C9-C8
22	b	827	CLA	C8-C10-C11-C12
28	a	843	PQN	C25-C26-C27-C28
22	b	831	CLA	O1A-CGA-O2A-C1
22	b	816	CLA	CBA-CGA-O2A-C1
25	9	307	LHG	C31-C32-C33-C34
25	9	307	LHG	C34-C35-C36-C37
25	a	845	LHG	O1-C1-C2-O2
25	a	846	LHG	O1-C1-C2-O2
25	b	847	LHG	O1-C1-C2-O2
25	9	307	LHG	C28-C29-C30-C31
25	a	845	LHG	C27-C28-C29-C30
22	8	310	CLA	C4B-C3B-CAB-CBB
22	8	314	CLA	C4B-C3B-CAB-CBB
22	4	312	CLA	C4B-C3B-CAB-CBB
22	2	307	CLA	C4B-C3B-CAB-CBB
22	7	307	CLA	C4B-C3B-CAB-CBB
22	a	841	CLA	C4B-C3B-CAB-CBB
22	b	840	CLA	C4B-C3B-CAB-CBB
24	9	302	A1L1F	C45-C47-C48-C49
25	9	317	LHG	C9-C10-C11-C12
22	b	811	CLA	C6-C7-C8-C9
22	f	802	CLA	C16-C17-C18-C19
22	f	802	CLA	C16-C17-C18-C20
22	1	314	CLA	C2A-CAA-CBA-CGA
22	b	828	CLA	C2A-CAA-CBA-CGA
22	a	814	CLA	C10-C11-C12-C13
22	a	827	CLA	C8-C10-C11-C12
22	a	841	CLA	C8-C10-C11-C12
22	b	806	CLA	C15-C16-C17-C18
22	b	835	CLA	C5-C6-C7-C8
22	1	308	CLA	C11-C10-C8-C7
25	a	845	LHG	C13-C14-C15-C16
27	2	317	LMG	C28-C29-C30-C31
22	b	840	CLA	O1D-CGD-O2D-CED
22	9	308	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	b	809	CLA	C10-C11-C12-C13
25	9	307	LHG	C27-C28-C29-C30
22	9	310	CLA	C3A-C2A-CAA-CBA
22	9	313	CLA	C3A-C2A-CAA-CBA
22	4	310	CLA	C3A-C2A-CAA-CBA
22	3	312	CLA	C3A-C2A-CAA-CBA
22	3	314	CLA	C3A-C2A-CAA-CBA
22	2	306	CLA	C3A-C2A-CAA-CBA
22	7	311	CLA	C3A-C2A-CAA-CBA
22	a	807	CLA	C3A-C2A-CAA-CBA
22	a	838	CLA	C3A-C2A-CAA-CBA
22	a	854	CLA	C3A-C2A-CAA-CBA
22	b	810	CLA	C3A-C2A-CAA-CBA
22	b	812	CLA	C3A-C2A-CAA-CBA
22	b	814	CLA	C3A-C2A-CAA-CBA
22	f	803	CLA	C3A-C2A-CAA-CBA
22	h	203	CLA	C3A-C2A-CAA-CBA
22	h	203	CLA	C10-C11-C12-C13
22	b	811	CLA	C6-C7-C8-C10
22	b	833	CLA	C16-C17-C18-C20
22	a	833	CLA	O1A-CGA-O2A-C1
22	a	838	CLA	O1A-CGA-O2A-C1
22	a	844	CLA	O1A-CGA-O2A-C1
23	1	315	SQD	O10-C23-O48-C46
25	9	317	LHG	C28-C29-C30-C31
22	a	814	CLA	C5-C6-C7-C8
22	a	823	CLA	CBA-CGA-O2A-C1
22	b	807	CLA	CBA-CGA-O2A-C1
22	b	835	CLA	CBA-CGA-O2A-C1
24	8	304	A1L1F	C45-C47-C48-C49
23	1	315	SQD	C11-C10-C9-C8
25	9	317	LHG	C14-C15-C16-C17
26	4	318	DGD	C2B-C3B-C4B-C5B
22	a	807	CLA	O1D-CGD-O2D-CED
26	b	848	DGD	C4A-C5A-C6A-C7A
22	b	801	CLA	C16-C17-C18-C20
22	8	314	CLA	C2B-C3B-CAB-CBB
22	4	311	CLA	C2B-C3B-CAB-CBB
22	4	312	CLA	C2B-C3B-CAB-CBB
22	4	314	CLA	C2B-C3B-CAB-CBB
22	2	307	CLA	C2B-C3B-CAB-CBB
22	7	307	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	7	315	CLA	C2B-C3B-CAB-CBB
22	a	808	CLA	C2B-C3B-CAB-CBB
22	a	836	CLA	C2B-C3B-CAB-CBB
22	b	819	CLA	C2B-C3B-CAB-CBB
22	b	838	CLA	C2B-C3B-CAB-CBB
29	a	850	BCR	C23-C24-C25-C30
29	l	205	BCR	C23-C24-C25-C26
29	l	205	BCR	C23-C24-C25-C30
22	3	314	CLA	CBD-CGD-O2D-CED
22	4	308	CLA	O1D-CGD-O2D-CED
22	a	810	CLA	O1D-CGD-O2D-CED
22	b	824	CLA	CBA-CGA-O2A-C1
22	b	808	CLA	C5-C6-C7-C8
22	b	808	CLA	C3-C5-C6-C7
22	5	306	CLA	C2A-CAA-CBA-CGA
22	a	814	CLA	C2A-CAA-CBA-CGA
25	9	317	LHG	C11-C12-C13-C14
26	b	848	DGD	C4B-C5B-C6B-C7B
22	9	308	CLA	O1A-CGA-O2A-C1
22	j	102	CLA	CBD-CGD-O2D-CED
22	a	811	CLA	C11-C10-C8-C7
22	1	308	CLA	C4-C3-C5-C6
22	1	310	CLA	C4-C3-C5-C6
21	5	303	A1L1G	C39-C40-C41-C42
21	7	302	A1L1G	C31-C32-C33-C34
22	7	308	CLA	C2-C3-C5-C6
26	b	848	DGD	C2B-C3B-C4B-C5B
26	b	848	DGD	C3B-C4B-C5B-C6B
22	a	825	CLA	CBA-CGA-O2A-C1
22	b	825	CLA	C11-C10-C8-C9
22	9	313	CLA	O1A-CGA-O2A-C1
22	4	316	CLA	O1A-CGA-O2A-C1
26	4	318	DGD	O6D-C1D-O3G-C3G
22	b	816	CLA	O1A-CGA-O2A-C1
22	a	840	CLA	C13-C15-C16-C17
24	h	204	A1L1F	C40-C41-C42-C44
25	a	846	LHG	C8-C7-O7-C5
26	b	848	DGD	C2B-C1B-O2G-C2G
22	b	838	CLA	C15-C16-C17-C18
22	a	809	CLA	C13-C15-C16-C17
20	7	304	XAT	C7-C8-C9-C19
25	9	307	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
22	b	804	CLA	C2C-C3C-CAC-CBC
24	9	302	A1L1F	C48-C49-C50-C51
22	a	810	CLA	C2A-CAA-CBA-CGA
22	b	832	CLA	C2A-CAA-CBA-CGA
22	2	314	CLA	C11-C10-C8-C9
22	b	801	CLA	C16-C17-C18-C19
22	4	310	CLA	C4-C3-C5-C6
22	b	834	CLA	C4-C3-C5-C6
22	b	839	CLA	C4-C3-C5-C6
22	1	308	CLA	C2-C3-C5-C6
24	1	304	A1L1F	C47-C48-C49-C50
22	8	307	CLA	C15-C16-C17-C18
22	b	829	CLA	C15-C16-C17-C18
22	j	102	CLA	C8-C10-C11-C12
24	h	204	A1L1F	C47-C48-C49-C50
25	a	845	LHG	C26-C27-C28-C29
22	a	823	CLA	O1A-CGA-O2A-C1
22	b	807	CLA	O1A-CGA-O2A-C1
22	4	307	CLA	C3-C5-C6-C7
22	b	805	CLA	C13-C15-C16-C17
22	b	810	CLA	C5-C6-C7-C8
27	2	317	LMG	C10-C11-C12-C13
25	b	847	LHG	O6-C4-C5-O7
22	b	832	CLA	C15-C16-C17-C18
22	a	806	CLA	C16-C17-C18-C19
22	b	840	CLA	C16-C17-C18-C19
22	b	835	CLA	O1A-CGA-O2A-C1
23	1	315	SQD	C7-C8-C9-C10
22	4	308	CLA	C15-C16-C17-C18
22	a	806	CLA	C13-C15-C16-C17
22	2	308	CLA	C3-C5-C6-C7
26	4	318	DGD	O1G-C1G-C2G-O2G
22	8	310	CLA	CBA-CGA-O2A-C1
22	3	315	CLA	CBA-CGA-O2A-C1
22	a	801	CLA	C16-C17-C18-C19
22	a	820	CLA	C16-C17-C18-C20
22	4	308	CLA	C13-C15-C16-C17
22	b	824	CLA	O1A-CGA-O2A-C1
22	4	310	CLA	C2-C3-C5-C6
22	b	839	CLA	C2-C3-C5-C6
25	a	846	LHG	O9-C7-O7-C5
22	b	810	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	a	822	CLA	C2A-CAA-CBA-CGA
22	9	313	CLA	CBD-CGD-O2D-CED
22	a	808	CLA	CBD-CGD-O2D-CED
22	5	305	CLA	O1A-CGA-O2A-C1
22	1	305	CLA	C8-C10-C11-C12
22	a	844	CLA	C10-C11-C12-C13
22	5	311	CLA	O1D-CGD-O2D-CED
22	5	306	CLA	C1A-C2A-CAA-CBA
22	9	310	CLA	C1A-C2A-CAA-CBA
22	9	313	CLA	C1A-C2A-CAA-CBA
22	4	313	CLA	C1A-C2A-CAA-CBA
22	3	314	CLA	C1A-C2A-CAA-CBA
22	2	306	CLA	C1A-C2A-CAA-CBA
22	7	306	CLA	C1A-C2A-CAA-CBA
22	7	311	CLA	C1A-C2A-CAA-CBA
22	7	313	CLA	C1A-C2A-CAA-CBA
22	1	306	CLA	C1A-C2A-CAA-CBA
22	a	807	CLA	C1A-C2A-CAA-CBA
22	a	817	CLA	C1A-C2A-CAA-CBA
22	a	819	CLA	C1A-C2A-CAA-CBA
22	a	825	CLA	C1A-C2A-CAA-CBA
22	b	816	CLA	C1A-C2A-CAA-CBA
22	b	817	CLA	C1A-C2A-CAA-CBA
22	b	837	CLA	C1A-C2A-CAA-CBA
22	f	803	CLA	C1A-C2A-CAA-CBA
22	b	809	CLA	C15-C16-C17-C18
25	a	845	LHG	O6-C4-C5-C6
22	a	839	CLA	C3-C5-C6-C7
22	b	801	CLA	C3-C5-C6-C7
22	b	813	CLA	C3-C5-C6-C7
22	9	316	CLA	C11-C12-C13-C15
22	a	807	CLA	C12-C13-C15-C16
22	a	810	CLA	C12-C13-C15-C16
22	a	822	CLA	C6-C7-C8-C10
22	a	830	CLA	C12-C13-C15-C16
22	a	841	CLA	C11-C10-C8-C7
22	a	844	CLA	C11-C12-C13-C15
22	b	807	CLA	C11-C10-C8-C7
22	b	807	CLA	C12-C13-C15-C16
22	b	818	CLA	C6-C7-C8-C10
22	b	822	CLA	C6-C7-C8-C10
22	b	824	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	b	825	CLA	C6-C7-C8-C10
22	b	827	CLA	C6-C7-C8-C10
22	b	833	CLA	C11-C12-C13-C15
22	b	838	CLA	C6-C7-C8-C10
22	f	802	CLA	C11-C12-C13-C15
22	b	814	CLA	C6-C7-C8-C10
22	9	316	CLA	C2-C3-C5-C6
26	b	848	DGD	CAB-CBB-CCB-CDB
22	7	316	CLA	C4C-C3C-CAC-CBC
22	b	829	CLA	C13-C15-C16-C17
22	b	835	CLA	C2C-C3C-CAC-CBC
25	b	847	LHG	C8-C7-O7-C5
22	8	308	CLA	C2A-CAA-CBA-CGA
22	a	806	CLA	C2A-CAA-CBA-CGA
22	4	308	CLA	C11-C12-C13-C14
22	2	310	CLA	C14-C13-C15-C16
22	1	308	CLA	C11-C10-C8-C9
22	a	807	CLA	C11-C12-C13-C14
22	a	809	CLA	C14-C13-C15-C16
22	a	814	CLA	C11-C10-C8-C9
22	a	822	CLA	C6-C7-C8-C9
22	a	827	CLA	C11-C10-C8-C9
22	a	842	CLA	C11-C12-C13-C14
22	a	844	CLA	C11-C10-C8-C9
22	a	844	CLA	C14-C13-C15-C16
22	b	801	CLA	C11-C12-C13-C14
22	b	803	CLA	C11-C10-C8-C9
22	b	807	CLA	C14-C13-C15-C16
22	b	808	CLA	C11-C10-C8-C9
22	b	822	CLA	C6-C7-C8-C9
22	b	824	CLA	C11-C10-C8-C9
22	b	825	CLA	C6-C7-C8-C9
22	b	836	CLA	C14-C13-C15-C16
26	b	848	DGD	CBB-CCB-CDB-CEB
24	h	204	A1L1F	C4-C8-O7-C54
22	8	307	CLA	CBA-CGA-O2A-C1
22	a	812	CLA	C10-C11-C12-C13
25	a	845	LHG	C4-C5-C6-O8
25	b	847	LHG	C4-C5-C6-O8
26	4	318	DGD	O1G-C1G-C2G-C3G
22	5	315	CLA	C4C-C3C-CAC-CBC
26	8	315	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
26	b	848	DGD	C6A-C7A-C8A-C9A
22	b	807	CLA	O1D-CGD-O2D-CED
22	b	822	CLA	O1D-CGD-O2D-CED
22	a	835	CLA	CBA-CGA-O2A-C1
22	a	844	CLA	C16-C17-C18-C19
25	9	317	LHG	C29-C30-C31-C32
22	a	825	CLA	O1A-CGA-O2A-C1
22	4	315	CLA	O1D-CGD-O2D-CED
22	a	829	CLA	C10-C11-C12-C13
22	b	838	CLA	C4-C3-C5-C6
22	a	820	CLA	C8-C10-C11-C12
22	a	854	CLA	C10-C11-C12-C13
28	a	843	PQN	C23-C25-C26-C27
20	7	303	XAT	C7-C8-C9-C19
22	b	814	CLA	C6-C7-C8-C9
22	b	818	CLA	C11-C12-C13-C14
20	4	305	XAT	C27-C28-C29-C30
22	1	308	CLA	C13-C15-C16-C17
22	b	839	CLA	C13-C15-C16-C17
25	9	317	LHG	C11-C10-C9-C8
22	h	203	CLA	O1D-CGD-O2D-CED
22	4	307	CLA	CBA-CGA-O2A-C1
22	a	841	CLA	CBA-CGA-O2A-C1
22	1	310	CLA	C5-C6-C7-C8
22	7	313	CLA	C5-C6-C7-C8
24	9	302	A1L1F	C49-C50-C51-C52
22	a	844	CLA	C16-C17-C18-C20
22	9	314	CLA	C3-C5-C6-C7
22	b	836	CLA	C2C-C3C-CAC-CBC
22	b	804	CLA	C15-C16-C17-C18
22	8	310	CLA	O1D-CGD-O2D-CED
26	b	848	DGD	C2A-C1A-O1G-C1G
22	8	307	CLA	O1A-CGA-O2A-C1
24	h	204	A1L1F	C48-C49-C50-C51
22	9	316	CLA	C4-C3-C5-C6
22	b	802	CLA	C4-C3-C5-C6
25	9	317	LHG	C12-C13-C14-C15
22	b	805	CLA	C16-C17-C18-C20
24	1	304	A1L1F	C50-C51-C52-C53
27	a	853	LMG	C14-C15-C16-C17
24	h	204	A1L1F	C3-C8-O7-C54
22	5	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	j	105	LMG	C13-C14-C15-C16
26	b	848	DGD	C3A-C4A-C5A-C6A
22	b	827	CLA	C15-C16-C17-C18
22	3	314	CLA	CBA-CGA-O2A-C1
22	1	306	CLA	CBA-CGA-O2A-C1
22	1	310	CLA	CBA-CGA-O2A-C1
22	b	828	CLA	CBA-CGA-O2A-C1
22	1	311	CLA	CBD-CGD-O2D-CED
22	4	317	CLA	C3-C5-C6-C7
22	b	833	CLA	C3-C5-C6-C7
22	a	829	CLA	C8-C10-C11-C12
22	b	802	CLA	O1D-CGD-O2D-CED
22	f	802	CLA	O1D-CGD-O2D-CED
22	a	811	CLA	C11-C10-C8-C9
22	a	805	CLA	C6-C7-C8-C9
22	8	314	CLA	CBD-CGD-O2D-CED
22	9	310	CLA	O1A-CGA-O2A-C1
22	a	824	CLA	O1A-CGA-O2A-C1
22	a	801	CLA	C4-C3-C5-C6
22	a	804	CLA	C2-C3-C5-C6
22	b	803	CLA	C2-C3-C5-C6
22	a	831	CLA	CBA-CGA-O2A-C1
22	b	811	CLA	CBA-CGA-O2A-C1
22	9	316	CLA	C11-C12-C13-C14
22	4	310	CLA	C11-C10-C8-C9
22	7	308	CLA	C11-C10-C8-C9
22	a	807	CLA	C14-C13-C15-C16
22	a	810	CLA	C14-C13-C15-C16
22	a	814	CLA	C11-C12-C13-C14
22	a	830	CLA	C14-C13-C15-C16
22	a	835	CLA	C6-C7-C8-C9
22	a	841	CLA	C11-C10-C8-C9
22	a	844	CLA	C11-C12-C13-C14
22	b	803	CLA	C6-C7-C8-C9
22	b	810	CLA	C6-C7-C8-C9
22	b	818	CLA	C6-C7-C8-C9
22	b	828	CLA	C11-C12-C13-C14
22	b	832	CLA	C14-C13-C15-C16
22	b	837	CLA	C14-C13-C15-C16
22	j	102	CLA	C6-C7-C8-C9
22	1	308	CLA	C15-C16-C17-C18
22	a	810	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	a	826	CLA	C15-C16-C17-C18
25	9	317	LHG	C2-C3-O3-P
22	5	308	CLA	C4B-C3B-CAB-CBB
22	4	311	CLA	C4B-C3B-CAB-CBB
22	4	314	CLA	C4B-C3B-CAB-CBB
22	3	307	CLA	C4B-C3B-CAB-CBB
22	3	308	CLA	C4B-C3B-CAB-CBB
22	7	314	CLA	C4B-C3B-CAB-CBB
22	7	317	CLA	C4B-C3B-CAB-CBB
22	1	305	CLA	C4B-C3B-CAB-CBB
22	1	309	CLA	C4B-C3B-CAB-CBB
22	1	313	CLA	C4B-C3B-CAB-CBB
22	1	314	CLA	C4B-C3B-CAB-CBB
22	a	801	CLA	C4B-C3B-CAB-CBB
22	a	808	CLA	C4B-C3B-CAB-CBB
22	a	825	CLA	C4B-C3B-CAB-CBB
22	a	836	CLA	C4B-C3B-CAB-CBB
22	a	837	CLA	C4B-C3B-CAB-CBB
22	b	817	CLA	C4B-C3B-CAB-CBB
22	b	818	CLA	C4B-C3B-CAB-CBB
22	j	102	CLA	C4B-C3B-CAB-CBB
22	3	315	CLA	CAA-CBA-CGA-O2A
22	a	844	CLA	C15-C16-C17-C18
22	b	807	CLA	C10-C11-C12-C13
26	b	848	DGD	CCB-CDB-CEB-CFB
22	a	819	CLA	C2A-CAA-CBA-CGA
26	4	318	DGD	C2D-C1D-O3G-C3G
22	b	832	CLA	C3-C5-C6-C7
22	h	205	CLA	C3-C5-C6-C7
25	a	845	LHG	C7-C8-C9-C10
25	b	847	LHG	O6-C4-C5-C6
21	9	306	A1L1G	C26-C30-C31-C32
25	b	847	LHG	C9-C10-C11-C12
22	8	307	CLA	C11-C10-C8-C7
22	4	308	CLA	C12-C13-C15-C16
22	4	310	CLA	C11-C10-C8-C7
22	1	308	CLA	C11-C12-C13-C15
22	a	807	CLA	C11-C12-C13-C15
22	a	809	CLA	C6-C7-C8-C10
22	a	812	CLA	C6-C7-C8-C10
22	a	814	CLA	C11-C12-C13-C15
22	a	827	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	a	829	CLA	C6-C7-C8-C10
22	a	835	CLA	C6-C7-C8-C10
22	a	842	CLA	C11-C12-C13-C15
22	a	844	CLA	C11-C10-C8-C7
22	b	801	CLA	C11-C12-C13-C15
22	b	803	CLA	C6-C7-C8-C10
22	b	803	CLA	C11-C10-C8-C7
22	b	803	CLA	C12-C13-C15-C16
22	b	808	CLA	C11-C10-C8-C7
22	b	810	CLA	C6-C7-C8-C10
22	b	828	CLA	C12-C13-C15-C16
22	b	829	CLA	C12-C13-C15-C16
22	b	836	CLA	C12-C13-C15-C16
22	b	837	CLA	C12-C13-C15-C16
22	b	838	CLA	C12-C13-C15-C16
22	j	102	CLA	C6-C7-C8-C10
22	a	812	CLA	C8-C10-C11-C12
22	4	311	CLA	C3A-C2A-CAA-CBA
22	3	315	CLA	C3A-C2A-CAA-CBA
22	2	314	CLA	C3A-C2A-CAA-CBA
22	a	804	CLA	C4-C3-C5-C6
22	a	820	CLA	C4-C3-C5-C6
22	a	829	CLA	C3A-C2A-CAA-CBA
22	a	840	CLA	C4-C3-C5-C6
22	b	803	CLA	C4-C3-C5-C6
22	b	813	CLA	C4-C3-C5-C6
22	j	102	CLA	C3A-C2A-CAA-CBA
22	b	801	CLA	C5-C6-C7-C8
22	a	828	CLA	C2-C3-C5-C6
22	a	835	CLA	O1A-CGA-O2A-C1
27	j	105	LMG	C28-C29-C30-C31
22	9	314	CLA	CBA-CGA-O2A-C1
25	9	307	LHG	C25-C26-C27-C28
21	9	306	A1L1G	C30-C31-C32-C33
21	3	306	A1L1G	C40-C41-C42-C44
21	7	302	A1L1G	C34-C35-C36-C37
20	5	301	XAT	C7-C8-C9-C19
20	4	305	XAT	C27-C28-C29-C39
21	9	306	A1L1G	C32-C33-C34-C27
22	4	307	CLA	O1A-CGA-O2A-C1
22	a	826	CLA	O1D-CGD-O2D-CED
20	7	303	XAT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	7	314	CLA	C2A-CAA-CBA-CGA
22	a	809	CLA	C2A-CAA-CBA-CGA
23	1	315	SQD	O6-C44-C45-C46
25	a	846	LHG	C4-C5-C6-O8
27	2	317	LMG	O1-C7-C8-C9
22	b	812	CLA	C5-C6-C7-C8
22	b	835	CLA	C3-C5-C6-C7
22	a	805	CLA	C6-C7-C8-C10
22	b	818	CLA	C11-C12-C13-C15
22	j	102	CLA	C5-C6-C7-C8
22	a	828	CLA	C4-C3-C5-C6
22	a	801	CLA	C2-C3-C5-C6
22	b	807	CLA	C2-C3-C5-C6
22	a	827	CLA	C3-C5-C6-C7
22	a	836	CLA	O1D-CGD-O2D-CED
22	4	308	CLA	C16-C17-C18-C19
22	1	310	CLA	C16-C17-C18-C20
22	a	806	CLA	C16-C17-C18-C20
26	b	848	DGD	O1B-C1B-O2G-C2G
22	3	307	CLA	C2B-C3B-CAB-CBB
22	7	317	CLA	C2B-C3B-CAB-CBB
22	1	309	CLA	C2B-C3B-CAB-CBB
22	a	825	CLA	C2B-C3B-CAB-CBB
22	a	837	CLA	C2B-C3B-CAB-CBB
22	a	841	CLA	C2B-C3B-CAB-CBB
22	b	817	CLA	C2B-C3B-CAB-CBB
22	j	102	CLA	C2B-C3B-CAB-CBB
29	b	843	BCR	C1-C6-C7-C8
29	m	101	BCR	C1-C6-C7-C8
22	a	830	CLA	C5-C6-C7-C8
25	9	307	LHG	C33-C34-C35-C36
25	a	845	LHG	C34-C35-C36-C37
22	b	822	CLA	C10-C11-C12-C13
22	b	807	CLA	C4-C3-C5-C6
21	9	306	A1L1G	C31-C32-C33-C34
22	5	309	CLA	C5-C6-C7-C8
22	a	820	CLA	C2-C3-C5-C6
22	b	813	CLA	C2-C3-C5-C6
22	a	820	CLA	C16-C17-C18-C19
22	4	317	CLA	C5-C6-C7-C8
22	a	803	CLA	C15-C16-C17-C18
22	1	308	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	1	310	CLA	C6-C7-C8-C9
22	1	310	CLA	C11-C10-C8-C9
22	a	829	CLA	C6-C7-C8-C9
22	b	802	CLA	C11-C10-C8-C9
22	b	824	CLA	C11-C12-C13-C14
22	3	314	CLA	O1D-CGD-O2D-CED
26	b	848	DGD	C7A-C8A-C9A-CAA
22	a	841	CLA	O1A-CGA-O2A-C1
22	9	308	CLA	C16-C17-C18-C19
22	a	806	CLA	CBD-CGD-O2D-CED
22	b	806	CLA	C10-C11-C12-C13
22	2	315	CLA	C1A-C2A-CAA-CBA
22	j	103	CLA	C1A-C2A-CAA-CBA
22	b	803	CLA	C13-C15-C16-C17
20	2	304	XAT	C33-C34-C35-C15
24	1	304	A1L1F	C14-C29-C30-C31
22	b	811	CLA	O1A-CGA-O2A-C1
22	4	313	CLA	CBA-CGA-O2A-C1
25	9	317	LHG	O6-C4-C5-C6
25	a	846	LHG	O6-C4-C5-C6
22	b	827	CLA	C16-C17-C18-C20
22	a	854	CLA	C8-C10-C11-C12
21	3	306	A1L1G	C32-C33-C34-C27
24	h	204	A1L1F	C28-C39-C40-C41
22	9	308	CLA	C11-C12-C13-C15
22	9	318	CLA	C11-C10-C8-C7
22	8	309	CLA	C11-C10-C8-C7
22	1	306	CLA	C6-C7-C8-C10
22	a	801	CLA	C6-C7-C8-C10
22	a	802	CLA	C6-C7-C8-C10
22	a	814	CLA	C6-C7-C8-C10
22	a	820	CLA	C11-C12-C13-C15
22	a	829	CLA	C11-C10-C8-C7
22	b	813	CLA	C11-C10-C8-C7
22	b	824	CLA	C6-C7-C8-C10
22	b	832	CLA	C12-C13-C15-C16
22	4	310	CLA	C15-C16-C17-C18
22	b	838	CLA	C13-C15-C16-C17
21	7	302	A1L1G	C32-C33-C34-C35
26	b	848	DGD	O1A-C1A-O1G-C1G
25	b	847	LHG	O9-C7-O7-C5
22	a	807	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	b	810	CLA	CAA-CBA-CGA-O2A
22	3	314	CLA	O1A-CGA-O2A-C1
22	1	310	CLA	C2-C3-C5-C6
22	a	840	CLA	C2-C3-C5-C6
27	a	853	LMG	C12-C13-C14-C15
22	9	313	CLA	O1D-CGD-O2D-CED
22	b	807	CLA	C5-C6-C7-C8
22	b	828	CLA	C5-C6-C7-C8
27	a	853	LMG	C9-C8-O7-C10
22	a	831	CLA	O1A-CGA-O2A-C1
22	b	828	CLA	O1A-CGA-O2A-C1
25	9	307	LHG	C32-C33-C34-C35
22	9	308	CLA	C16-C17-C18-C20
22	1	306	CLA	C16-C17-C18-C20
22	9	314	CLA	O1A-CGA-O2A-C1
22	1	306	CLA	O1A-CGA-O2A-C1
22	1	310	CLA	O1A-CGA-O2A-C1
22	9	318	CLA	CBA-CGA-O2A-C1
23	1	315	SQD	C9-C10-C11-C12
22	a	842	CLA	C8-C10-C11-C12
26	8	315	DGD	C1G-C2G-C3G-O3G
22	a	827	CLA	C5-C6-C7-C8
22	2	310	CLA	C16-C17-C18-C20
22	1	310	CLA	C16-C17-C18-C19
22	b	805	CLA	C16-C17-C18-C19
22	2	314	CLA	C2A-CAA-CBA-CGA
22	b	834	CLA	C2-C3-C5-C6
21	7	302	A1L1G	C45-C2-C44-C43
24	8	304	A1L1F	C57-C2-C44-C43
22	4	313	CLA	O1A-CGA-O2A-C1
22	1	306	CLA	C3-C5-C6-C7
27	2	317	LMG	C31-C32-C33-C34
26	8	315	DGD	O2G-C2G-C3G-O3G
22	9	308	CLA	C11-C10-C8-C9
22	9	308	CLA	C11-C12-C13-C14
22	8	309	CLA	C11-C10-C8-C9
22	1	306	CLA	C11-C10-C8-C9
22	a	801	CLA	C6-C7-C8-C9
22	a	802	CLA	C6-C7-C8-C9
22	a	820	CLA	C11-C12-C13-C14
22	a	840	CLA	C11-C10-C8-C9
22	b	802	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	802	CLA	C11-C12-C13-C14
22	b	804	CLA	C6-C7-C8-C9
22	b	806	CLA	C6-C7-C8-C9
22	b	813	CLA	C11-C10-C8-C9
22	b	838	CLA	C11-C12-C13-C14
22	b	838	CLA	C14-C13-C15-C16
25	a	845	LHG	C9-C10-C11-C12
22	a	841	CLA	C13-C15-C16-C17
22	a	808	CLA	O1D-CGD-O2D-CED
22	2	310	CLA	C16-C17-C18-C19
22	b	808	CLA	C16-C17-C18-C20
22	2	314	CLA	C4-C3-C5-C6
22	2	307	CLA	C2A-CAA-CBA-CGA
22	b	810	CLA	C16-C17-C18-C19
22	b	817	CLA	C10-C11-C12-C13
27	2	317	LMG	C33-C34-C35-C36
22	8	311	CLA	C3-C5-C6-C7
22	5	305	CLA	C4B-C3B-CAB-CBB
22	5	306	CLA	C4B-C3B-CAB-CBB
22	5	310	CLA	C4B-C3B-CAB-CBB
22	9	311	CLA	C4B-C3B-CAB-CBB
22	9	318	CLA	C4B-C3B-CAB-CBB
22	8	313	CLA	C4B-C3B-CAB-CBB
22	4	306	CLA	C4B-C3B-CAB-CBB
22	4	307	CLA	C4B-C3B-CAB-CBB
22	4	315	CLA	C4B-C3B-CAB-CBB
22	4	317	CLA	C4B-C3B-CAB-CBB
22	3	311	CLA	C1A-C2A-CAA-CBA
22	3	312	CLA	C4B-C3B-CAB-CBB
22	2	306	CLA	C4B-C3B-CAB-CBB
22	2	311	CLA	C4B-C3B-CAB-CBB
22	2	314	CLA	C1A-C2A-CAA-CBA
22	2	314	CLA	C4B-C3B-CAB-CBB
22	2	315	CLA	C4B-C3B-CAB-CBB
22	2	316	CLA	C4B-C3B-CAB-CBB
22	a	807	CLA	C4B-C3B-CAB-CBB
22	a	813	CLA	C4B-C3B-CAB-CBB
22	a	817	CLA	C4B-C3B-CAB-CBB
22	a	819	CLA	C4B-C3B-CAB-CBB
22	a	824	CLA	C1A-C2A-CAA-CBA
22	a	824	CLA	C4B-C3B-CAB-CBB
22	b	801	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	b	809	CLA	C4B-C3B-CAB-CBB
22	b	813	CLA	C1A-C2A-CAA-CBA
22	b	823	CLA	C1A-C2A-CAA-CBA
22	b	828	CLA	C4B-C3B-CAB-CBB
22	b	834	CLA	C4B-C3B-CAB-CBB
22	b	837	CLA	C4B-C3B-CAB-CBB
22	f	803	CLA	C4B-C3B-CAB-CBB
22	j	103	CLA	C4B-C3B-CAB-CBB
22	j	102	CLA	O1D-CGD-O2D-CED
20	5	301	XAT	C7-C8-C9-C10
24	h	204	A1L1F	C38-C39-C40-C41
22	b	802	CLA	C2A-CAA-CBA-CGA
22	b	808	CLA	C2A-CAA-CBA-CGA
22	b	818	CLA	C8-C10-C11-C12
22	7	313	CLA	CBD-CGD-O2D-CED
22	5	311	CLA	C2-C3-C5-C6
22	5	307	CLA	C11-C10-C8-C7
22	8	307	CLA	C6-C7-C8-C10
22	2	310	CLA	C11-C12-C13-C15
22	a	842	CLA	C12-C13-C15-C16
22	b	801	CLA	C11-C10-C8-C7
22	b	801	CLA	C12-C13-C15-C16
22	b	806	CLA	C11-C12-C13-C15
22	b	827	CLA	C11-C10-C8-C7
22	b	829	CLA	C11-C12-C13-C15
28	a	843	PQN	C22-C23-C25-C26
27	a	853	LMG	C31-C32-C33-C34
22	1	307	CLA	C5-C6-C7-C8
22	9	316	CLA	C3A-C2A-CAA-CBA
25	9	317	LHG	O6-C4-C5-O7
22	3	311	CLA	C2A-CAA-CBA-CGA
22	4	308	CLA	C14-C13-C15-C16
22	a	809	CLA	C6-C7-C8-C9
22	a	814	CLA	C6-C7-C8-C9
23	1	315	SQD	C13-C14-C15-C16
22	a	830	CLA	C8-C10-C11-C12
20	4	301	XAT	C29-C30-C31-C32
21	3	302	A1L1G	C36-C37-C38-C39
29	m	101	BCR	C13-C14-C15-C16
22	4	312	CLA	CBA-CGA-O2A-C1
22	8	314	CLA	O1D-CGD-O2D-CED
22	a	806	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	8	304	A1L1F	C47-C48-C49-C50
22	a	823	CLA	C1-C2-C3-C4
22	b	831	CLA	C1-C2-C3-C4
22	3	315	CLA	O1A-CGA-O2A-C1
22	b	814	CLA	C3-C5-C6-C7
22	9	318	CLA	O1A-CGA-O2A-C1
23	5	316	SQD	O47-C45-C46-O48
23	1	315	SQD	O6-C44-C45-O47
25	a	846	LHG	O7-C5-C6-O8
25	b	847	LHG	O7-C5-C6-O8
22	7	312	CLA	O2A-C1-C2-C3
22	9	308	CLA	C10-C11-C12-C13
22	b	840	CLA	C15-C16-C17-C18
23	5	316	SQD	C44-C45-C46-O48
22	a	809	CLA	C10-C11-C12-C13
22	8	310	CLA	O1A-CGA-O2A-C1
21	9	301	A1L1G	O13-C26-C30-C31
22	9	313	CLA	CAD-CBD-CGD-O2D
22	8	309	CLA	CAD-CBD-CGD-O2D
22	8	314	CLA	CAD-CBD-CGD-O2D
22	1	313	CLA	CAD-CBD-CGD-O2D
22	a	814	CLA	CAD-CBD-CGD-O2D
22	a	839	CLA	CAD-CBD-CGD-O2D
22	a	844	CLA	CAD-CBD-CGD-O2D
22	b	832	CLA	CAD-CBD-CGD-O2D
22	b	836	CLA	CAD-CBD-CGD-O2D
22	1	311	CLA	CBA-CGA-O2A-C1
22	8	309	CLA	C2A-CAA-CBA-CGA
22	b	824	CLA	C2A-CAA-CBA-CGA
25	a	846	LHG	C10-C11-C12-C13
22	b	805	CLA	CBA-CGA-O2A-C1
20	7	301	XAT	C29-C30-C31-C32
20	j	101	XAT	C9-C10-C11-C12
21	3	302	A1L1G	C40-C41-C42-C44
21	1	301	A1L1G	C37-C38-C39-C28
22	5	313	CLA	CHA-CBD-CGD-O1D
22	5	313	CLA	CHA-CBD-CGD-O2D
22	9	313	CLA	CAD-CBD-CGD-O1D
22	9	315	CLA	CAD-CBD-CGD-O1D
22	8	309	CLA	CAD-CBD-CGD-O1D
22	8	314	CLA	CAD-CBD-CGD-O1D
22	4	314	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	4	314	CLA	CHA-CBD-CGD-O2D
22	4	315	CLA	CAD-CBD-CGD-O1D
22	2	307	CLA	CHA-CBD-CGD-O1D
22	7	309	CLA	CHA-CBD-CGD-O2D
22	7	309	CLA	CAD-CBD-CGD-O2D
22	1	313	CLA	CAD-CBD-CGD-O1D
22	a	806	CLA	CAD-CBD-CGD-O1D
22	a	814	CLA	CAD-CBD-CGD-O1D
22	a	828	CLA	CAD-CBD-CGD-O1D
22	a	839	CLA	CAD-CBD-CGD-O1D
22	a	844	CLA	CAD-CBD-CGD-O1D
22	b	821	CLA	CHA-CBD-CGD-O1D
22	b	832	CLA	CAD-CBD-CGD-O1D
22	b	835	CLA	CAD-CBD-CGD-O1D
22	b	836	CLA	CAD-CBD-CGD-O1D
22	f	802	CLA	CAD-CBD-CGD-O1D
22	f	803	CLA	CHA-CBD-CGD-O2D
22	j	102	CLA	CHA-CBD-CGD-O1D
22	j	102	CLA	CHA-CBD-CGD-O2D
25	9	317	LHG	C3-O3-P-O5
25	9	317	LHG	C3-O3-P-O6
25	9	317	LHG	C4-O6-P-O3
25	9	317	LHG	C4-O6-P-O5
25	a	845	LHG	C3-O3-P-O5
25	a	846	LHG	C3-O3-P-O5
25	a	846	LHG	C4-O6-P-O3
25	a	846	LHG	C4-O6-P-O5
22	b	822	CLA	C3-C5-C6-C7
22	a	841	CLA	C4-C3-C5-C6
22	h	205	CLA	C4-C3-C5-C6
22	5	306	CLA	C2B-C3B-CAB-CBB
22	5	310	CLA	C2B-C3B-CAB-CBB
22	9	318	CLA	C2B-C3B-CAB-CBB
22	8	310	CLA	C2B-C3B-CAB-CBB
22	8	313	CLA	C2B-C3B-CAB-CBB
22	4	317	CLA	C2B-C3B-CAB-CBB
22	2	311	CLA	C2B-C3B-CAB-CBB
22	2	315	CLA	C2B-C3B-CAB-CBB
22	2	316	CLA	C2B-C3B-CAB-CBB
22	1	314	CLA	C2B-C3B-CAB-CBB
22	a	819	CLA	C2B-C3B-CAB-CBB
22	b	801	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	b	834	CLA	C2B-C3B-CAB-CBB
22	b	837	CLA	C2B-C3B-CAB-CBB
22	b	840	CLA	C2B-C3B-CAB-CBB
22	f	803	CLA	C2B-C3B-CAB-CBB
29	l	201	BCR	C1-C6-C7-C8
22	a	807	CLA	C2-C3-C5-C6
22	b	838	CLA	C2-C3-C5-C6
22	a	834	CLA	C5-C6-C7-C8
22	b	824	CLA	C8-C10-C11-C12
25	9	307	LHG	C2-C3-O3-P
22	1	308	CLA	CBD-CGD-O2D-CED
22	1	308	CLA	C16-C17-C18-C19
22	b	808	CLA	C16-C17-C18-C19
22	b	839	CLA	C2C-C3C-CAC-CBC
22	2	308	CLA	C6-C7-C8-C9
22	b	803	CLA	C3-C5-C6-C7
23	1	315	SQD	C46-C45-O47-C7
25	9	317	LHG	C10-C11-C12-C13
21	3	306	A1L1G	C30-C31-C32-C33
22	a	830	CLA	C16-C17-C18-C19
22	5	309	CLA	C6-C7-C8-C9
22	3	312	CLA	C6-C7-C8-C9
22	a	807	CLA	C6-C7-C8-C9
22	a	812	CLA	C6-C7-C8-C9
22	a	842	CLA	C14-C13-C15-C16
22	b	803	CLA	C14-C13-C15-C16
22	b	804	CLA	C11-C12-C13-C14
22	b	807	CLA	C11-C12-C13-C14
22	b	810	CLA	C11-C10-C8-C9
22	b	828	CLA	C14-C13-C15-C16
22	3	312	CLA	C6-C7-C8-C10
22	b	802	CLA	C11-C12-C13-C15
22	b	807	CLA	C11-C12-C13-C15
22	b	810	CLA	C11-C10-C8-C7
22	a	839	CLA	C15-C16-C17-C18
22	a	821	CLA	C2A-CAA-CBA-CGA
22	1	311	CLA	O1A-CGA-O2A-C1
22	b	805	CLA	O1A-CGA-O2A-C1
25	9	317	LHG	C13-C14-C15-C16
22	7	308	CLA	C8-C10-C11-C12
22	b	827	CLA	C10-C11-C12-C13
22	b	817	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	b	817	CLA	CBA-CGA-O2A-C1
22	b	832	CLA	C2C-C3C-CAC-CBC
22	8	307	CLA	C16-C17-C18-C20
22	3	308	CLA	CAA-CBA-CGA-O2A
22	1	305	CLA	C2A-CAA-CBA-CGA
22	1	308	CLA	C2A-CAA-CBA-CGA
22	a	854	CLA	CBD-CGD-O2D-CED
22	a	802	CLA	C4-C3-C5-C6
22	b	827	CLA	C16-C17-C18-C19
22	2	314	CLA	C2-C3-C5-C6
22	b	802	CLA	C2-C3-C5-C6
22	a	801	CLA	CAA-CBA-CGA-O2A
22	1	311	CLA	O1D-CGD-O2D-CED
22	b	801	CLA	O1A-CGA-O2A-C1
25	b	847	LHG	C25-C26-C27-C28
21	9	306	A1L1G	C32-C33-C34-C35
22	4	317	CLA	C2A-CAA-CBA-CGA
22	a	813	CLA	C2A-CAA-CBA-CGA
22	b	827	CLA	C2A-CAA-CBA-CGA
21	1	301	A1L1G	C40-C41-C42-C44
23	5	316	SQD	C7-C8-C9-C10
22	a	841	CLA	C2-C3-C5-C6
22	b	801	CLA	CBA-CGA-O2A-C1
22	1	308	CLA	O1D-CGD-O2D-CED
22	b	803	CLA	C16-C17-C18-C20
22	a	801	CLA	C14-C13-C15-C16
22	a	826	CLA	C11-C10-C8-C9
22	b	827	CLA	C11-C10-C8-C9
28	a	843	PQN	C24-C23-C25-C26
22	9	309	CLA	C4B-C3B-CAB-CBB
22	3	314	CLA	C4B-C3B-CAB-CBB
22	a	832	CLA	C4B-C3B-CAB-CBB
22	b	830	CLA	C4B-C3B-CAB-CBB
22	a	813	CLA	O1A-CGA-O2A-C1
22	5	307	CLA	C8-C10-C11-C12
22	a	830	CLA	C15-C16-C17-C18
22	h	203	CLA	C13-C15-C16-C17
22	a	813	CLA	CBA-CGA-O2A-C1
22	a	854	CLA	C15-C16-C17-C18
22	2	309	CLA	C2A-CAA-CBA-CGA
22	5	315	CLA	CAA-CBA-CGA-O2A
22	a	802	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	9	301	A1L1G	C34-C35-C36-C37
21	7	302	A1L1G	C36-C37-C38-C39
22	a	830	CLA	C16-C17-C18-C20
22	a	826	CLA	C11-C10-C8-C7
22	a	831	CLA	C11-C10-C8-C7
22	b	802	CLA	C12-C13-C15-C16
22	f	802	CLA	C6-C7-C8-C10
22	3	312	CLA	CBA-CGA-O2A-C1
22	8	307	CLA	C16-C17-C18-C19
22	1	308	CLA	C16-C17-C18-C20
22	5	310	CLA	CAA-CBA-CGA-O1A
26	b	848	DGD	O2G-C2G-C3G-O3G
22	2	310	CLA	C3A-C2A-CAA-CBA
22	a	830	CLA	C4-C3-C5-C6
22	b	813	CLA	C3A-C2A-CAA-CBA
22	b	831	CLA	C3A-C2A-CAA-CBA
29	b	844	BCR	C11-C10-C9-C34
29	b	844	BCR	C20-C21-C22-C37
29	f	804	BCR	C35-C13-C14-C15
29	l	201	BCR	C11-C10-C9-C34
22	a	812	CLA	C3-C5-C6-C7
22	a	820	CLA	C13-C15-C16-C17
24	9	302	A1L1F	C3-C8-O7-C54
22	5	306	CLA	CAA-CBA-CGA-O1A
22	7	308	CLA	C2-C1-O2A-CGA
24	h	204	A1L1F	C36-C37-C38-C39
22	b	839	CLA	C16-C17-C18-C20
20	7	303	XAT	C11-C12-C13-C20
22	5	311	CLA	C4-C3-C5-C6
22	b	813	CLA	C10-C11-C12-C13
21	3	306	A1L1G	C32-C33-C34-C35
22	a	854	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	C25-C26-C27-C28
22	5	307	CLA	C11-C10-C8-C9
22	1	310	CLA	C11-C12-C13-C14
22	a	822	CLA	C11-C10-C8-C9
22	a	829	CLA	C11-C12-C13-C14
22	a	831	CLA	C6-C7-C8-C9
22	a	831	CLA	C11-C10-C8-C9
22	a	844	CLA	C6-C7-C8-C9
22	a	854	CLA	C11-C10-C8-C9
22	b	808	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	8	312	CLA	CBD-CGD-O2D-CED
22	7	313	CLA	O1D-CGD-O2D-CED
22	a	832	CLA	CBD-CGD-O2D-CED
22	a	839	CLA	C16-C17-C18-C20
22	8	305	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	CBD-CGD-O2D-CED
22	3	312	CLA	O1A-CGA-O2A-C1
22	5	309	CLA	C2A-CAA-CBA-CGA
22	9	314	CLA	C2A-CAA-CBA-CGA
22	9	316	CLA	C2A-CAA-CBA-CGA
22	8	307	CLA	C2A-CAA-CBA-CGA
22	a	803	CLA	C2A-CAA-CBA-CGA
22	3	315	CLA	CAA-CBA-CGA-O1A
22	4	311	CLA	C1A-C2A-CAA-CBA
22	4	316	CLA	C1A-C2A-CAA-CBA
22	2	310	CLA	C1A-C2A-CAA-CBA
22	2	316	CLA	C1A-C2A-CAA-CBA
22	b	815	CLA	C1A-C2A-CAA-CBA
22	b	822	CLA	C1A-C2A-CAA-CBA
22	b	834	CLA	C1A-C2A-CAA-CBA
29	b	844	BCR	C11-C10-C9-C8
29	b	844	BCR	C20-C21-C22-C23
29	f	804	BCR	C12-C13-C14-C15
29	l	201	BCR	C11-C10-C9-C8
22	4	314	CLA	CAA-CBA-CGA-O1A
22	4	314	CLA	CAA-CBA-CGA-O2A
22	5	305	CLA	C2B-C3B-CAB-CBB
22	5	308	CLA	C2B-C3B-CAB-CBB
22	9	313	CLA	C2B-C3B-CAB-CBB
22	4	306	CLA	C2B-C3B-CAB-CBB
22	4	307	CLA	C2B-C3B-CAB-CBB
22	4	315	CLA	C2B-C3B-CAB-CBB
22	3	308	CLA	C2B-C3B-CAB-CBB
22	3	312	CLA	C2B-C3B-CAB-CBB
22	3	314	CLA	C2B-C3B-CAB-CBB
22	2	306	CLA	C2B-C3B-CAB-CBB
22	2	314	CLA	C2B-C3B-CAB-CBB
22	7	314	CLA	C2B-C3B-CAB-CBB
22	1	305	CLA	C2B-C3B-CAB-CBB
22	1	313	CLA	C2B-C3B-CAB-CBB
22	a	801	CLA	C2B-C3B-CAB-CBB
22	a	807	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	a	810	CLA	C2B-C3B-CAB-CBB
22	a	813	CLA	C2B-C3B-CAB-CBB
22	a	817	CLA	C2B-C3B-CAB-CBB
22	a	824	CLA	C2B-C3B-CAB-CBB
22	a	832	CLA	C2B-C3B-CAB-CBB
22	b	809	CLA	C2B-C3B-CAB-CBB
22	b	828	CLA	C2B-C3B-CAB-CBB
22	b	830	CLA	C2B-C3B-CAB-CBB
22	j	103	CLA	C2B-C3B-CAB-CBB
29	b	843	BCR	C5-C6-C7-C8
29	b	849	BCR	C23-C24-C25-C30
29	l	205	BCR	C1-C6-C7-C8
29	m	101	BCR	C5-C6-C7-C8
22	5	306	CLA	CAA-CBA-CGA-O2A
22	a	801	CLA	CBA-CGA-O2A-C1
22	b	840	CLA	CBA-CGA-O2A-C1
22	a	801	CLA	O1A-CGA-O2A-C1
22	b	840	CLA	O1A-CGA-O2A-C1
22	b	808	CLA	C4-C3-C5-C6
22	a	830	CLA	C2-C3-C5-C6
27	2	317	LMG	O9-C10-O7-C8
22	7	306	CLA	C2A-CAA-CBA-CGA
22	b	809	CLA	C2A-CAA-CBA-CGA
22	a	832	CLA	O1D-CGD-O2D-CED
22	5	313	CLA	CAA-CBA-CGA-O1A
22	a	817	CLA	CAA-CBA-CGA-O1A
25	a	845	LHG	C14-C15-C16-C17
27	2	317	LMG	C11-C10-O7-C8
22	1	305	CLA	C3-C5-C6-C7
25	a	846	LHG	C1-C2-C3-O3
25	9	317	LHG	C15-C16-C17-C18
22	2	314	CLA	C11-C10-C8-C7
22	h	203	CLA	C8-C10-C11-C12
20	7	301	XAT	C7-C8-C9-C19
22	7	307	CLA	CAA-CBA-CGA-O2A
22	a	817	CLA	CAA-CBA-CGA-O2A
22	b	808	CLA	C2-C3-C5-C6
22	8	312	CLA	O1D-CGD-O2D-CED
22	1	307	CLA	C6-C7-C8-C9
22	8	305	CLA	O1D-CGD-O2D-CED
22	5	313	CLA	CAA-CBA-CGA-O2A
22	b	837	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	a	853	LMG	C11-C12-C13-C14
20	8	302	XAT	C9-C10-C11-C12
22	7	317	CLA	CAA-CBA-CGA-O2A
22	4	310	CLA	C13-C15-C16-C17
22	b	839	CLA	C4C-C3C-CAC-CBC
22	a	835	CLA	C4-C3-C5-C6
22	7	307	CLA	CAA-CBA-CGA-O1A
22	a	835	CLA	C2-C3-C5-C6
22	b	817	CLA	CBD-CGD-O2D-CED
22	4	306	CLA	C2A-CAA-CBA-CGA
22	4	310	CLA	O1D-CGD-O2D-CED
23	1	315	SQD	C15-C16-C17-C18
22	a	826	CLA	C13-C15-C16-C17
22	5	314	CLA	C4-C3-C5-C6
22	b	833	CLA	C4-C3-C5-C6
22	a	819	CLA	CAA-CBA-CGA-O2A
22	9	313	CLA	C4B-C3B-CAB-CBB
22	8	306	CLA	C4B-C3B-CAB-CBB
22	4	310	CLA	C4B-C3B-CAB-CBB
22	a	810	CLA	C4B-C3B-CAB-CBB
22	a	842	CLA	O1A-CGA-O2A-C1
22	9	312	CLA	CAA-CBA-CGA-O2A
22	a	804	CLA	O1A-CGA-O2A-C1
22	5	310	CLA	CBA-CGA-O2A-C1
22	1	314	CLA	CAA-CBA-CGA-O2A
22	1	306	CLA	C16-C17-C18-C19
22	b	813	CLA	C16-C17-C18-C19
22	a	830	CLA	O1A-CGA-O2A-C1
22	5	307	CLA	C11-C12-C13-C14
22	8	311	CLA	C6-C7-C8-C10
22	1	314	CLA	CAA-CBA-CGA-O1A
22	b	802	CLA	C10-C11-C12-C13
20	7	304	XAT	C9-C10-C11-C12
22	b	817	CLA	O1D-CGD-O2D-CED
22	a	813	CLA	C6-C7-C8-C9
22	7	317	CLA	CAA-CBA-CGA-O1A
22	a	828	CLA	C14-C13-C15-C16
22	a	839	CLA	C6-C7-C8-C9
22	a	840	CLA	C14-C13-C15-C16
22	b	806	CLA	C11-C12-C13-C14
22	b	829	CLA	C11-C12-C13-C14
22	5	307	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	a	839	CLA	C2A-CAA-CBA-CGA
22	a	830	CLA	CBA-CGA-O2A-C1
22	a	842	CLA	CBA-CGA-O2A-C1
22	9	311	CLA	C3A-C2A-CAA-CBA
22	4	306	CLA	C3A-C2A-CAA-CBA
22	2	316	CLA	C3A-C2A-CAA-CBA
22	1	310	CLA	C3A-C2A-CAA-CBA
22	b	809	CLA	C3A-C2A-CAA-CBA
22	2	314	CLA	O1A-CGA-O2A-C1
25	9	317	LHG	O1-C1-C2-C3
22	b	813	CLA	C13-C15-C16-C17
22	l	204	CLA	CAA-CBA-CGA-O2A
26	b	848	DGD	C1B-C2B-C3B-C4B
22	b	813	CLA	C5-C6-C7-C8
22	a	804	CLA	CBA-CGA-O2A-C1
28	a	843	PQN	C18-C20-C21-C22
20	5	301	XAT	O4-C6-C7-C8
20	5	304	XAT	O24-C26-C27-C28
20	9	303	XAT	O24-C26-C27-C28
20	8	301	XAT	O24-C26-C27-C28
20	4	301	XAT	O4-C6-C7-C8
20	4	305	XAT	O4-C6-C7-C8
20	3	303	XAT	O4-C6-C7-C8
20	2	301	XAT	O4-C6-C7-C8
20	2	305	XAT	O24-C26-C27-C28
20	7	305	XAT	O4-C6-C7-C8
20	7	305	XAT	O24-C26-C27-C28
21	3	302	A1L1G	C29-C14-C25-O15
27	j	105	LMG	C11-C12-C13-C14
22	9	316	CLA	C8-C10-C11-C12
22	b	833	CLA	C15-C16-C17-C18
22	a	804	CLA	C6-C7-C8-C9
22	9	313	CLA	CAA-CBA-CGA-O2A
22	4	308	CLA	C3-C5-C6-C7
22	h	205	CLA	C2-C3-C5-C6
25	9	317	LHG	C35-C36-C37-C38
22	4	306	CLA	CAA-CBA-CGA-O2A
22	b	803	CLA	C10-C11-C12-C13
25	9	307	LHG	O7-C5-C6-O8
22	8	307	CLA	C6-C7-C8-C9
22	4	308	CLA	C6-C7-C8-C9
22	4	312	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	4	309	CLA	CAA-CBA-CGA-O2A
22	b	803	CLA	CAA-CBA-CGA-O2A
20	2	304	XAT	C7-C8-C9-C10
20	a	852	XAT	C31-C32-C33-C34
22	a	829	CLA	CAA-CBA-CGA-O2A
22	9	308	CLA	C2A-CAA-CBA-CGA
22	b	818	CLA	C2A-CAA-CBA-CGA
22	1	305	CLA	C11-C10-C8-C7
22	1	310	CLA	C12-C13-C15-C16
22	a	801	CLA	C11-C10-C8-C7
22	a	835	CLA	C11-C12-C13-C15
22	a	839	CLA	C6-C7-C8-C10
22	a	840	CLA	C12-C13-C15-C16
22	b	837	CLA	C11-C12-C13-C15
22	9	309	CLA	C2B-C3B-CAB-CBB
22	8	306	CLA	C2B-C3B-CAB-CBB
22	b	818	CLA	C2B-C3B-CAB-CBB
29	b	846	BCR	C1-C6-C7-C8
29	b	846	BCR	C5-C6-C7-C8
29	b	849	BCR	C23-C24-C25-C26
29	f	804	BCR	C23-C24-C25-C26
29	f	804	BCR	C23-C24-C25-C30
29	l	201	BCR	C5-C6-C7-C8
29	l	205	BCR	C5-C6-C7-C8
22	b	837	CLA	CAA-CBA-CGA-O2A
22	5	311	CLA	C2-C1-O2A-CGA
22	7	306	CLA	C2-C1-O2A-CGA
22	a	814	CLA	C2-C1-O2A-CGA
22	a	822	CLA	C2-C1-O2A-CGA
22	b	810	CLA	C2-C1-O2A-CGA
22	b	824	CLA	C10-C11-C12-C13
22	1	306	CLA	CAA-CBA-CGA-O2A
22	1	309	CLA	CAA-CBA-CGA-O2A
24	9	302	A1L1F	O13-C26-C30-C29
24	9	302	A1L1F	C50-C51-C52-C53
22	a	818	CLA	CAA-CBA-CGA-O2A
22	b	801	CLA	CAA-CBA-CGA-O2A
22	a	827	CLA	C10-C11-C12-C13
22	4	308	CLA	C2A-CAA-CBA-CGA
22	2	308	CLA	C2A-CAA-CBA-CGA
22	b	835	CLA	C4C-C3C-CAC-CBC
22	j	102	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	2	314	CLA	CBA-CGA-O2A-C1
23	1	315	SQD	O47-C7-C8-C9
23	5	316	SQD	C4-C5-C6-S
24	h	204	A1L1F	C14-C29-C30-C31
22	3	313	CLA	C4-C3-C5-C6
22	4	306	CLA	CAA-CBA-CGA-O1A
22	b	807	CLA	CAA-CBA-CGA-O2A
22	a	801	CLA	C11-C10-C8-C9
22	b	803	CLA	C5-C6-C7-C8
27	j	105	LMG	C7-C8-C9-O8
22	9	311	CLA	C1A-C2A-CAA-CBA
22	4	316	CLA	C4B-C3B-CAB-CBB
22	3	315	CLA	C4B-C3B-CAB-CBB
22	a	803	CLA	C1A-C2A-CAA-CBA
22	a	814	CLA	C1A-C2A-CAA-CBA
22	a	840	CLA	C4B-C3B-CAB-CBB
22	b	803	CLA	C4B-C3B-CAB-CBB
22	b	825	CLA	C1A-C2A-CAA-CBA
22	8	308	CLA	C4-C3-C5-C6
22	b	810	CLA	CAA-CBA-CGA-O1A
26	8	315	DGD	O6D-C1D-O3G-C3G
29	m	101	BCR	C22-C23-C24-C25
22	a	810	CLA	CAA-CBA-CGA-O2A
29	f	801	BCR	C17-C18-C19-C20
22	b	807	CLA	C16-C17-C18-C19
24	8	304	A1L1F	C3-C8-O7-C54
22	a	836	CLA	CAA-CBA-CGA-O2A
22	b	817	CLA	CAA-CBA-CGA-O2A
22	h	205	CLA	CAA-CBA-CGA-O2A
22	a	829	CLA	C2A-CAA-CBA-CGA
22	a	841	CLA	C2A-CAA-CBA-CGA
25	9	317	LHG	C27-C28-C29-C30
22	b	838	CLA	C3-C5-C6-C7
22	b	819	CLA	C6-C7-C8-C9
22	b	809	CLA	CAA-CBA-CGA-O2A
22	7	316	CLA	C2-C3-C5-C6
22	a	810	CLA	C2-C1-O2A-CGA
22	1	312	CLA	CAA-CBA-CGA-O2A
22	b	832	CLA	CAA-CBA-CGA-O2A
22	a	801	CLA	C11-C12-C13-C15
22	a	834	CLA	C11-C12-C13-C15
22	b	805	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	b	818	CLA	C11-C10-C8-C7
22	l	203	CLA	C6-C7-C8-C10
22	a	826	CLA	C10-C11-C12-C13
22	b	810	CLA	C16-C17-C18-C20
25	9	307	LHG	C6-C5-O7-C7
22	j	102	CLA	C10-C11-C12-C13
22	a	834	CLA	C10-C11-C12-C13
22	j	102	CLA	CAA-CBA-CGA-O2A
25	a	845	LHG	O8-C23-C24-C25
25	9	317	LHG	C30-C31-C32-C33
22	9	315	CLA	C2C-C3C-CAC-CBC
22	4	310	CLA	C8-C10-C11-C12
22	a	801	CLA	C5-C6-C7-C8
22	b	837	CLA	CAA-CBA-CGA-O1A
22	5	309	CLA	C15-C16-C17-C18
22	9	312	CLA	C3A-C2A-CAA-CBA
22	1	306	CLA	C3A-C2A-CAA-CBA
22	a	814	CLA	C3A-C2A-CAA-CBA
22	a	810	CLA	C16-C17-C18-C20
22	a	814	CLA	C16-C17-C18-C19
21	3	306	A1L1G	C14-C29-C30-C31
22	a	818	CLA	CAA-CBA-CGA-O1A
22	b	817	CLA	CAA-CBA-CGA-O1A
22	4	309	CLA	CAA-CBA-CGA-O1A
22	b	801	CLA	CAA-CBA-CGA-O1A
22	a	801	CLA	C11-C12-C13-C14
22	a	834	CLA	C11-C12-C13-C14
22	f	802	CLA	C6-C7-C8-C9
22	3	312	CLA	CAA-CBA-CGA-O2A
23	1	315	SQD	O49-C7-C8-C9
22	9	314	CLA	C4-C3-C5-C6
23	5	316	SQD	O5-C5-C6-S
24	1	304	A1L1F	C29-C14-C25-C24
22	7	309	CLA	O1A-CGA-O2A-C1
24	9	302	A1L1F	O46-C45-O13-C26
22	b	807	CLA	CAA-CBA-CGA-O1A
20	7	301	XAT	C7-C8-C9-C10
29	i	101	BCR	C17-C18-C19-C20
22	b	824	CLA	C15-C16-C17-C18
22	3	309	CLA	C2A-CAA-CBA-CGA
22	7	308	CLA	C2A-CAA-CBA-CGA
22	b	813	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	5	316	SQD	C10-C11-C12-C13
22	b	809	CLA	CAA-CBA-CGA-O1A
22	b	832	CLA	CAA-CBA-CGA-O1A
22	b	824	CLA	C4-C3-C5-C6
22	9	314	CLA	CAA-CBA-CGA-O2A
22	a	813	CLA	CAA-CBA-CGA-O2A
22	1	312	CLA	CAA-CBA-CGA-O1A
22	a	836	CLA	CAA-CBA-CGA-O1A
22	h	205	CLA	CAA-CBA-CGA-O1A
21	3	306	A1L1G	O13-C26-C30-C31
22	5	314	CLA	CAD-CBD-CGD-O2D
22	9	309	CLA	CAD-CBD-CGD-O2D
22	8	313	CLA	CAD-CBD-CGD-O2D
22	4	310	CLA	CAD-CBD-CGD-O2D
22	3	310	CLA	CAD-CBD-CGD-O2D
22	7	306	CLA	CAD-CBD-CGD-O2D
22	a	810	CLA	CAD-CBD-CGD-O2D
22	a	816	CLA	CAD-CBD-CGD-O2D
22	a	828	CLA	CAD-CBD-CGD-O2D
22	a	832	CLA	CAD-CBD-CGD-O2D
22	a	854	CLA	CAD-CBD-CGD-O2D
22	b	835	CLA	CAD-CBD-CGD-O2D
22	7	309	CLA	CBA-CGA-O2A-C1
22	a	816	CLA	C2-C1-O2A-CGA
22	a	839	CLA	C2-C1-O2A-CGA
22	7	308	CLA	CAA-CBA-CGA-O2A
22	a	826	CLA	C8-C10-C11-C12
22	7	316	CLA	CAA-CBA-CGA-O2A
22	b	804	CLA	CAA-CBA-CGA-O2A
22	7	308	CLA	C5-C6-C7-C8
22	a	840	CLA	C16-C17-C18-C19
22	j	102	CLA	CAA-CBA-CGA-O1A
23	1	315	SQD	C12-C13-C14-C15
22	a	820	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CAA-CBA-CGA-O2A
22	a	835	CLA	CAA-CBA-CGA-O2A
24	9	302	A1L1F	C47-C45-O13-C26
22	b	829	CLA	O1A-CGA-O2A-C1
22	a	810	CLA	CAA-CBA-CGA-O1A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	h	204	A1L1F	C1-C11-C3-C4-C6-C8

217 monomers are involved in 660 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	303	XAT	3	0
20	a	852	XAT	6	0
22	b	806	CLA	3	0
22	l	202	CLA	1	0
29	b	842	BCR	4	0
20	9	303	XAT	7	0
20	2	301	XAT	3	0
22	7	313	CLA	4	0
22	a	838	CLA	1	0
22	b	817	CLA	8	0
22	b	838	CLA	6	0
22	f	802	CLA	2	0
22	a	816	CLA	2	0
22	a	827	CLA	3	0
20	8	301	XAT	2	0
22	9	309	CLA	1	0
22	l	310	CLA	1	0
22	a	840	CLA	6	0
29	a	849	BCR	3	0
21	1	301	A1L1G	1	0
26	b	848	DGD	6	0
22	4	312	CLA	1	0
29	l	201	BCR	3	0
22	a	842	CLA	4	0
22	3	312	CLA	2	0
22	a	804	CLA	4	0
22	2	316	CLA	2	0
22	a	810	CLA	4	0
29	m	101	BCR	2	0
22	b	822	CLA	7	0
20	5	302	XAT	6	0
22	a	854	CLA	3	0
29	l	205	BCR	11	0
20	5	304	XAT	3	0
22	7	307	CLA	2	0
22	7	306	CLA	3	0
22	a	830	CLA	5	0
20	4	301	XAT	6	0
20	7	305	XAT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	j	104	BCR	9	0
22	5	314	CLA	1	0
29	f	804	BCR	5	0
22	b	809	CLA	4	0
22	5	307	CLA	7	0
20	3	305	XAT	6	0
20	7	301	XAT	3	0
22	a	807	CLA	4	0
22	1	312	CLA	2	0
20	4	303	XAT	11	0
20	8	302	XAT	6	0
22	b	820	CLA	3	0
22	b	837	CLA	5	0
22	l	203	CLA	2	0
22	4	311	CLA	1	0
22	b	832	CLA	3	0
22	b	839	CLA	4	0
29	b	845	BCR	7	0
20	8	303	XAT	4	0
22	a	802	CLA	5	0
22	j	102	CLA	7	0
22	4	313	CLA	4	0
21	9	306	A1L1G	1	0
22	a	819	CLA	5	0
22	b	801	CLA	3	0
22	b	831	CLA	2	0
22	a	822	CLA	5	0
22	9	310	CLA	2	0
22	4	307	CLA	1	0
22	b	807	CLA	7	0
22	8	307	CLA	4	0
25	a	846	LHG	3	0
22	5	305	CLA	3	0
20	2	303	XAT	12	0
22	b	802	CLA	3	0
24	1	304	A1L1F	2	0
22	j	103	CLA	2	0
24	h	204	A1L1F	4	0
20	j	101	XAT	7	0
20	7	303	XAT	12	0
22	4	306	CLA	2	0
24	9	302	A1L1F	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	823	CLA	6	0
22	7	311	CLA	3	0
29	b	846	BCR	3	0
21	5	303	A1L1G	1	0
22	5	308	CLA	1	0
27	j	105	LMG	7	0
22	9	311	CLA	2	0
22	a	835	CLA	5	0
22	a	828	CLA	5	0
22	4	317	CLA	6	0
22	5	309	CLA	4	0
24	8	304	A1L1F	2	0
22	2	314	CLA	2	0
22	a	831	CLA	6	0
22	7	312	CLA	1	0
23	1	315	SQD	2	0
22	b	804	CLA	5	0
22	4	309	CLA	3	0
22	a	808	CLA	1	0
22	8	308	CLA	2	0
22	b	808	CLA	1	0
22	b	803	CLA	2	0
22	a	825	CLA	4	0
22	b	816	CLA	6	0
22	b	833	CLA	4	0
26	8	315	DGD	2	0
22	8	312	CLA	2	0
23	5	316	SQD	1	0
22	5	312	CLA	3	0
25	a	845	LHG	3	0
20	3	304	XAT	6	0
22	b	813	CLA	7	0
27	a	853	LMG	10	0
27	2	317	LMG	3	0
22	a	820	CLA	6	0
22	b	814	CLA	2	0
22	b	828	CLA	4	0
22	2	309	CLA	2	0
22	9	313	CLA	2	0
29	f	801	BCR	9	0
28	a	843	PQN	4	0
22	b	805	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	310	CLA	1	0
22	3	309	CLA	1	0
22	9	308	CLA	5	0
29	h	201	BCR	2	0
22	b	811	CLA	3	0
29	a	850	BCR	2	0
21	7	302	A1L1G	2	0
21	9	301	A1L1G	2	0
25	9	307	LHG	2	0
22	1	306	CLA	6	0
22	4	314	CLA	1	0
22	a	829	CLA	6	0
29	a	848	BCR	7	0
22	b	812	CLA	4	0
20	1	302	XAT	3	0
22	a	815	CLA	1	0
22	7	314	CLA	3	0
29	i	101	BCR	3	0
22	a	803	CLA	5	0
20	1	303	XAT	4	0
22	9	314	CLA	7	0
22	b	824	CLA	6	0
29	h	202	BCR	4	0
22	9	312	CLA	4	0
22	1	311	CLA	2	0
22	b	819	CLA	2	0
28	b	841	PQN	3	0
22	8	305	CLA	5	0
22	9	315	CLA	1	0
22	b	830	CLA	6	0
29	b	844	BCR	5	0
22	4	315	CLA	1	0
20	9	305	XAT	3	0
22	a	826	CLA	7	0
25	9	317	LHG	3	0
29	a	847	BCR	1	0
22	7	315	CLA	2	0
29	b	849	BCR	5	0
22	4	308	CLA	6	0
22	2	310	CLA	3	0
22	a	818	CLA	10	0
22	3	308	CLA	2	0

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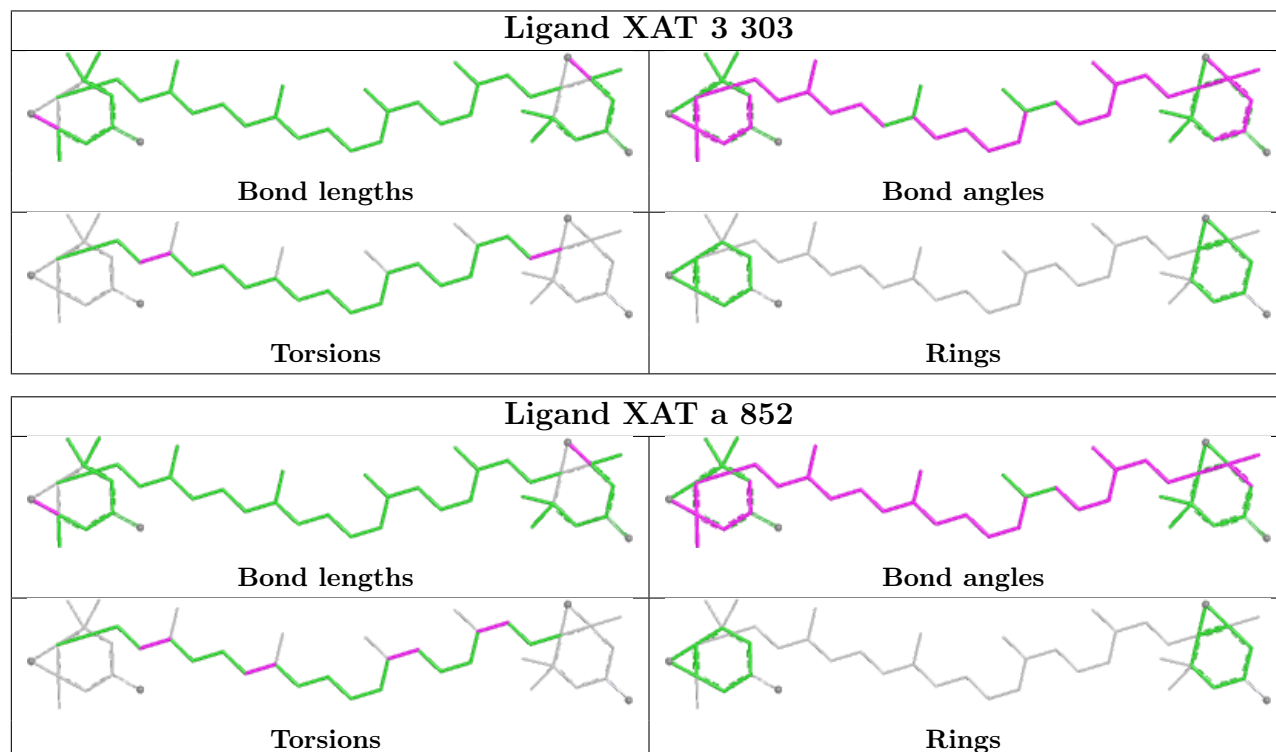
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	a	841	CLA	7	0
22	1	308	CLA	4	0
22	a	814	CLA	3	0
22	a	839	CLA	4	0
22	b	827	CLA	5	0
20	4	302	XAT	6	0
22	a	834	CLA	6	0
22	b	826	CLA	3	0
26	4	318	DGD	11	0
22	a	809	CLA	3	0
22	8	306	CLA	1	0
22	b	835	CLA	4	0
20	2	302	XAT	3	0
22	5	311	CLA	1	0
20	4	304	XAT	5	0
22	4	316	CLA	1	0
22	7	308	CLA	6	0
22	a	806	CLA	10	0
20	3	301	XAT	4	0
22	b	836	CLA	7	0
20	4	305	XAT	3	0
22	4	310	CLA	7	0
22	9	318	CLA	6	0
22	8	313	CLA	3	0
22	a	837	CLA	1	0
22	7	316	CLA	1	0
22	a	832	CLA	2	0
20	9	304	XAT	7	0
22	b	825	CLA	3	0
22	2	307	CLA	1	0
20	7	304	XAT	8	0
22	h	205	CLA	2	0
22	a	823	CLA	3	0
22	b	818	CLA	4	0
22	b	840	CLA	5	0
22	a	801	CLA	5	0
20	2	305	XAT	2	0
22	a	824	CLA	1	0
22	3	311	CLA	1	0
22	a	844	CLA	5	0
22	8	311	CLA	3	0

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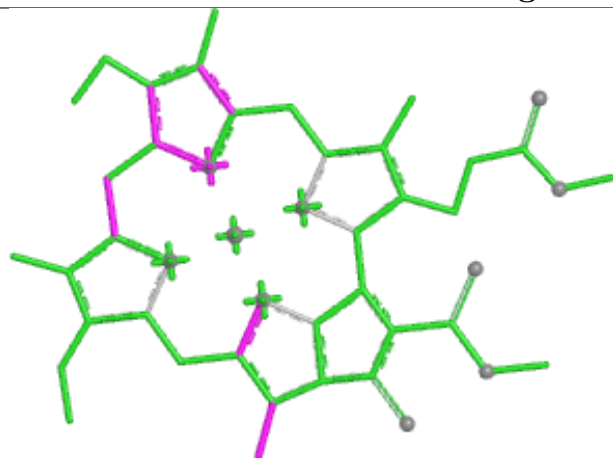
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	313	CLA	3	0
22	b	834	CLA	1	0
22	h	203	CLA	4	0
22	5	315	CLA	1	0
22	b	829	CLA	4	0
30	c	102	SF4	3	0
22	b	821	CLA	3	0
22	a	833	CLA	2	0
22	2	308	CLA	5	0
22	9	316	CLA	5	0

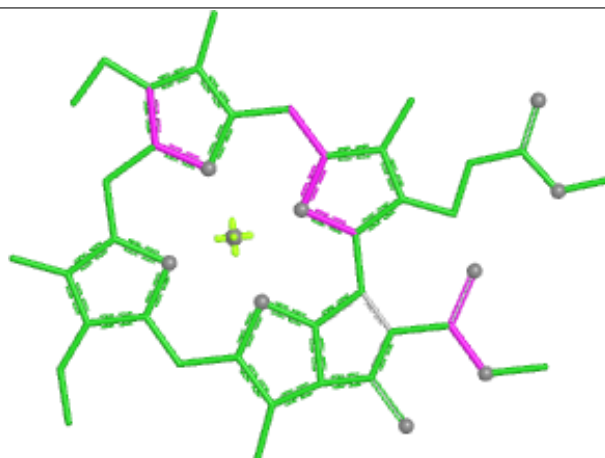
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



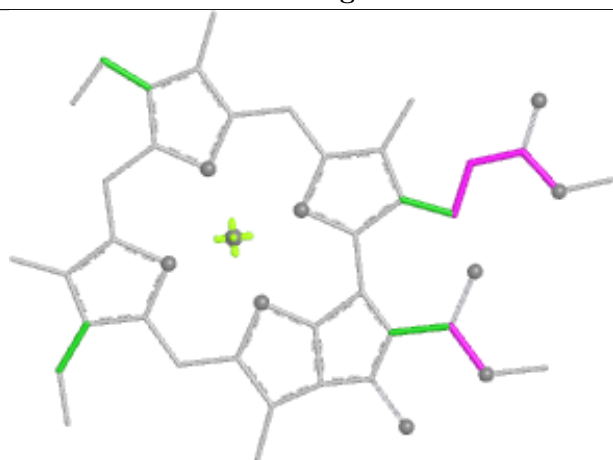
Ligand CLA 7 310



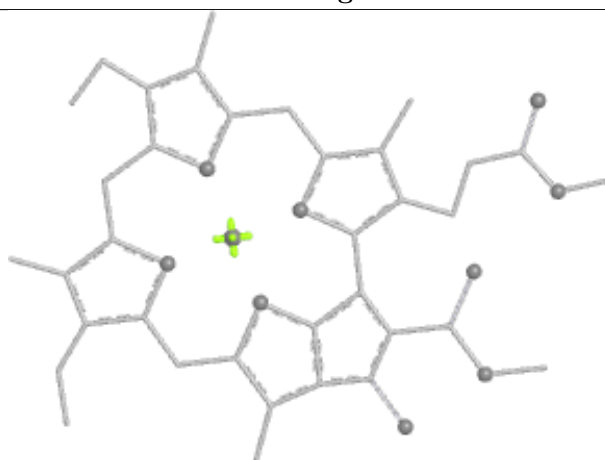
Bond lengths



Bond angles

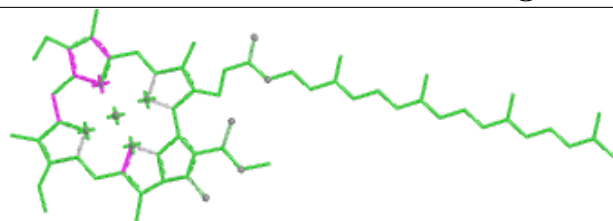


Torsions

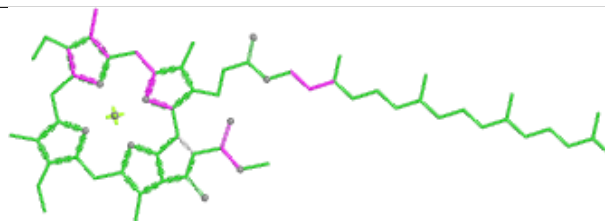


Rings

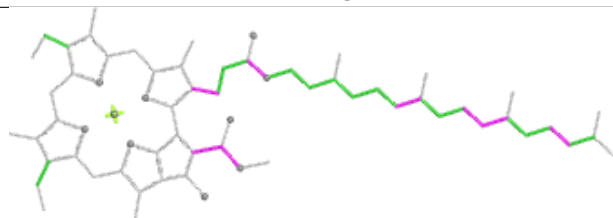
Ligand CLA b 806



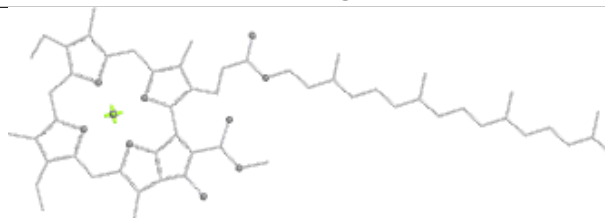
Bond lengths



Bond angles

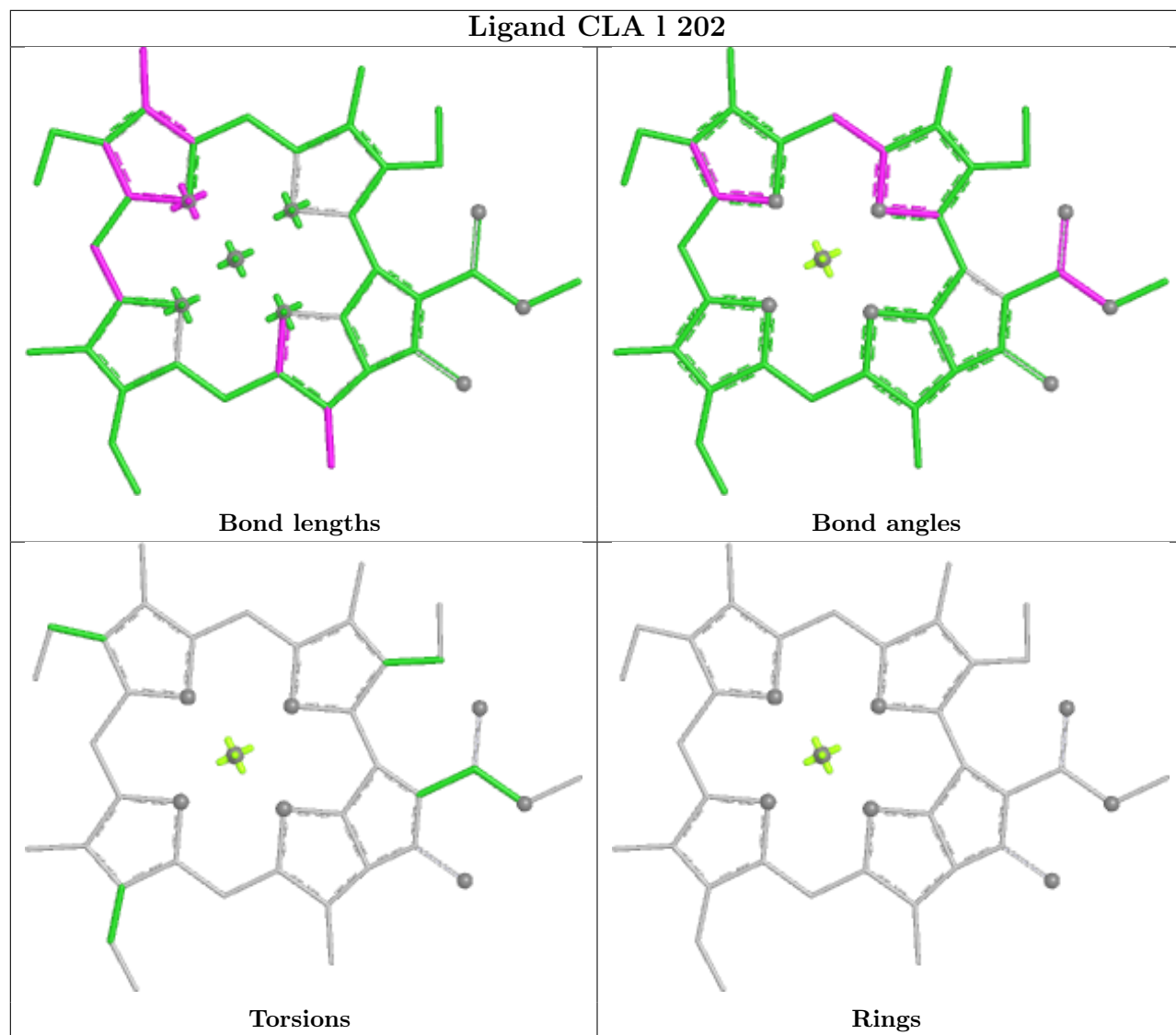


Torsions

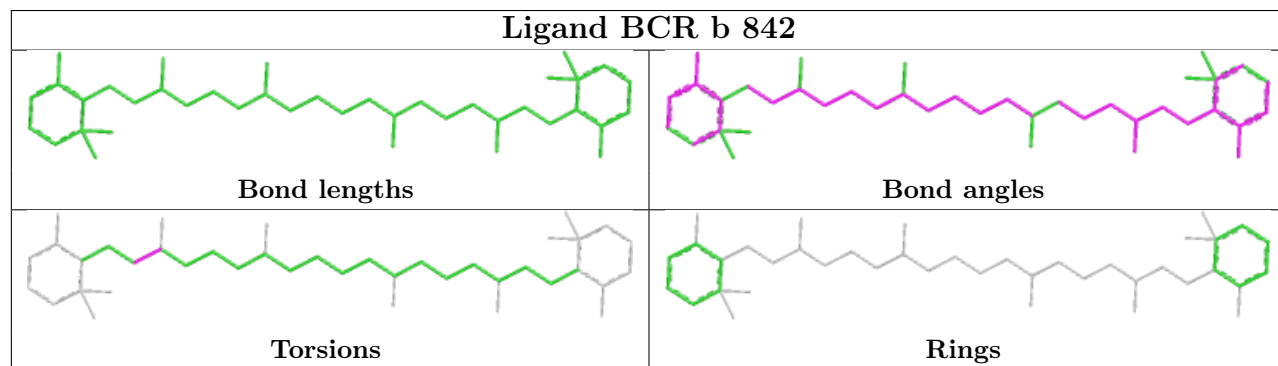


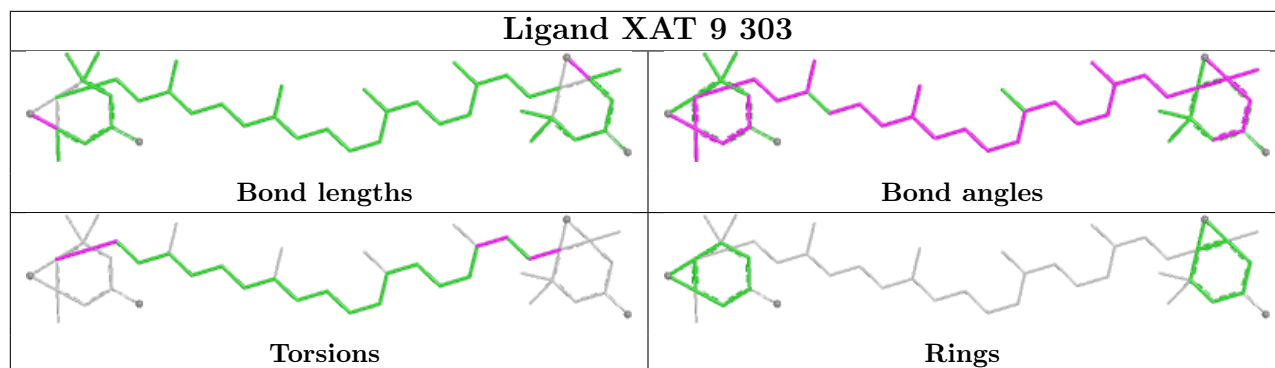
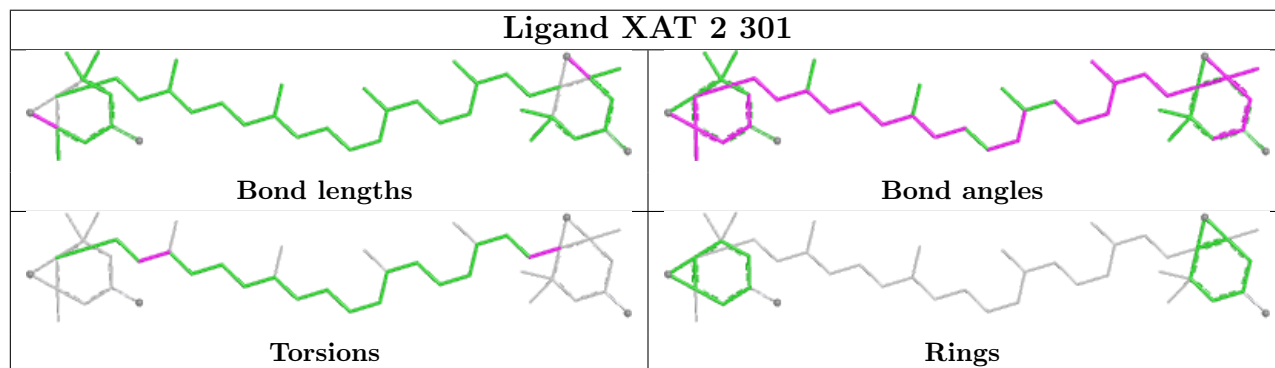
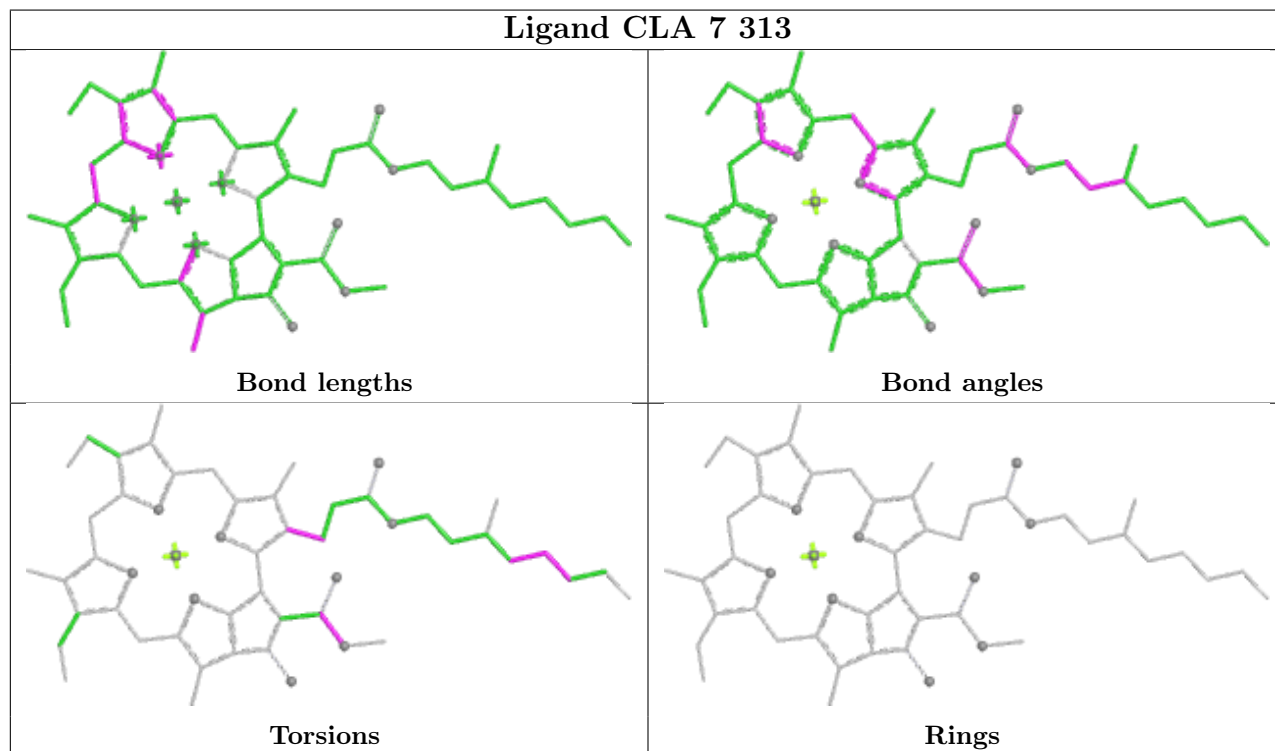
Rings

Ligand CLA 1 202

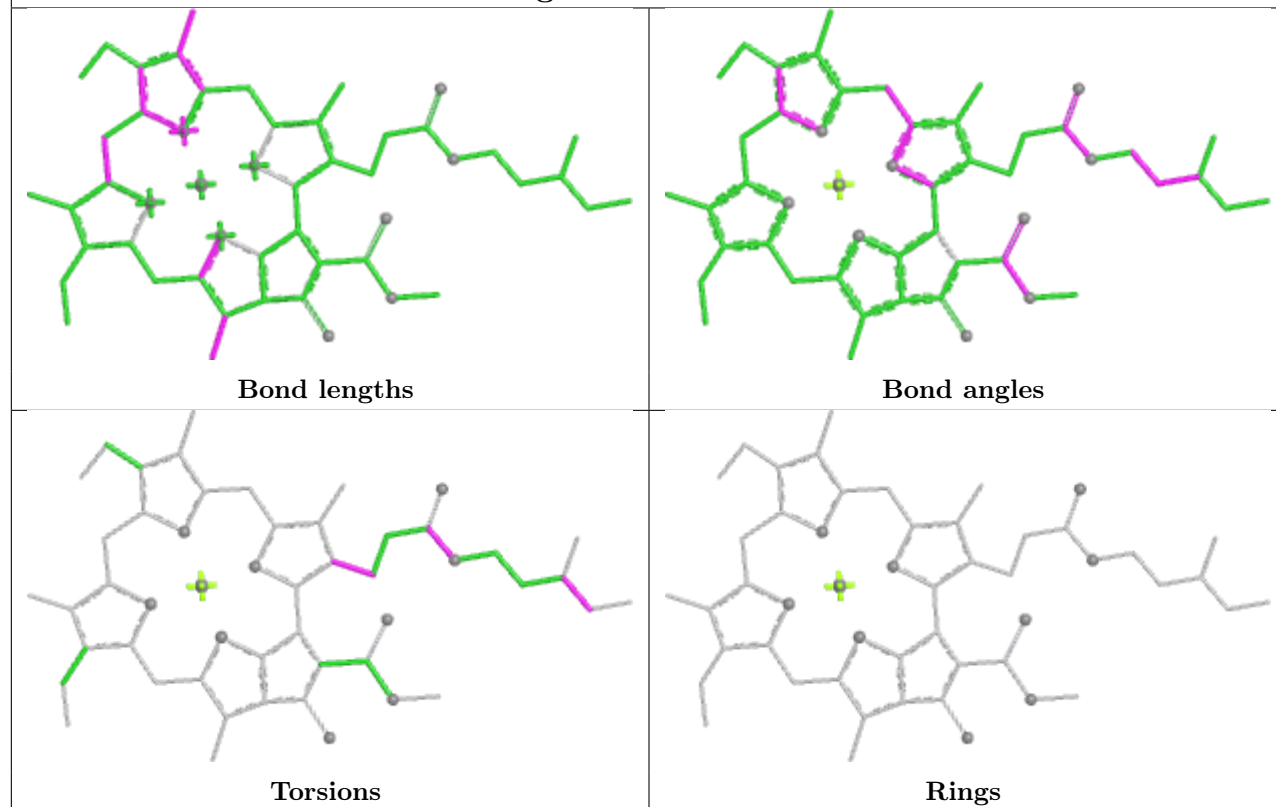


Ligand BCR b 842

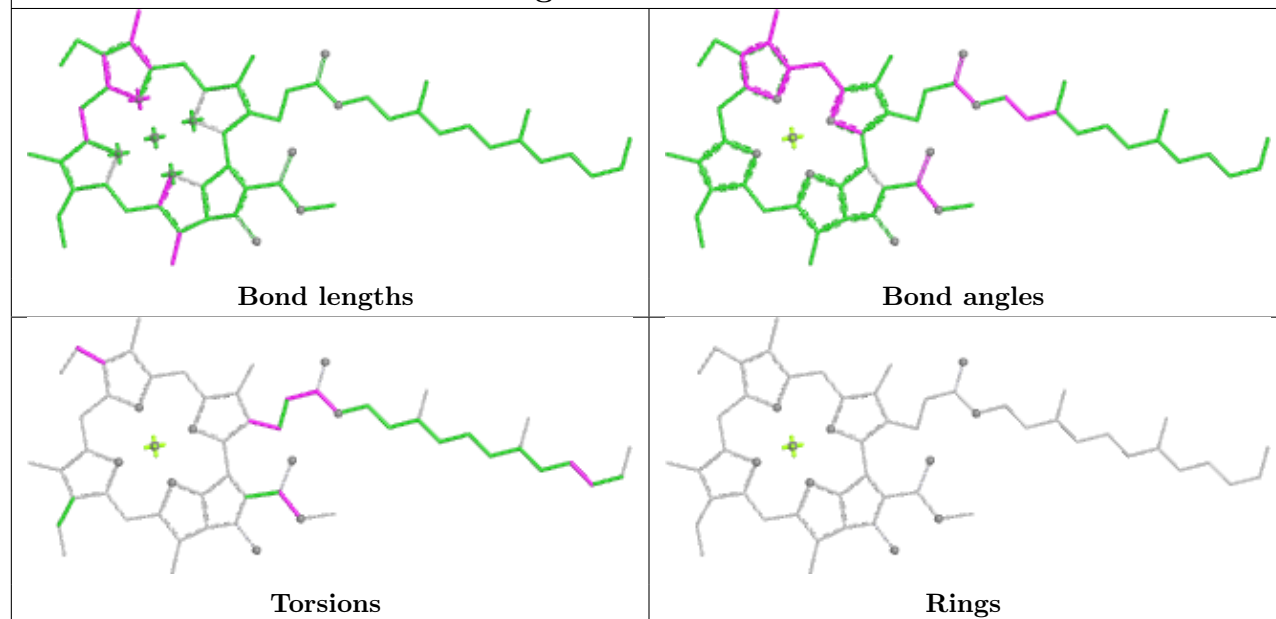


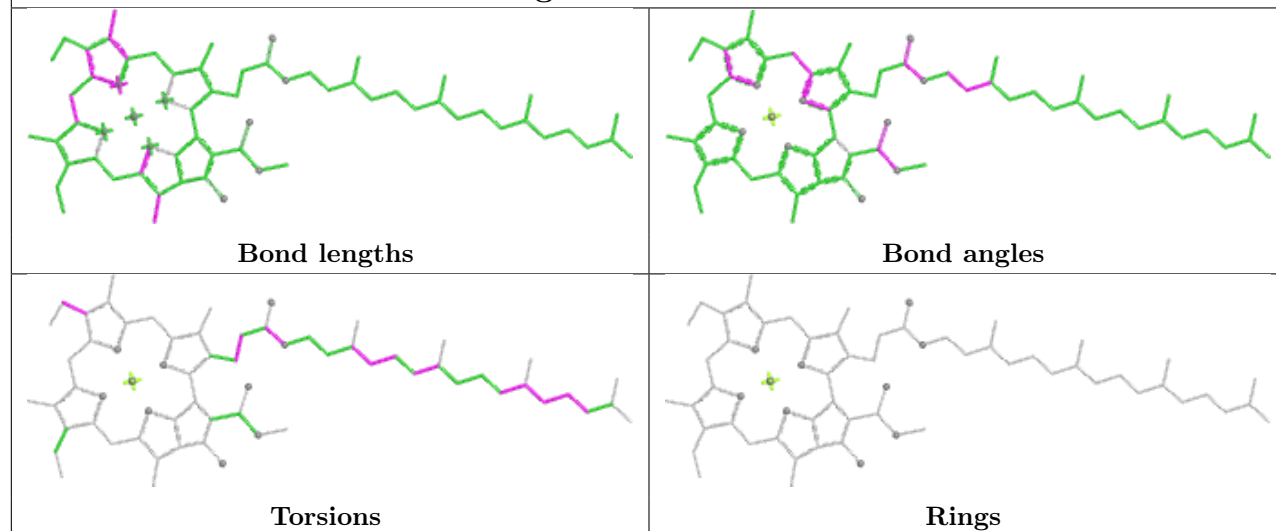
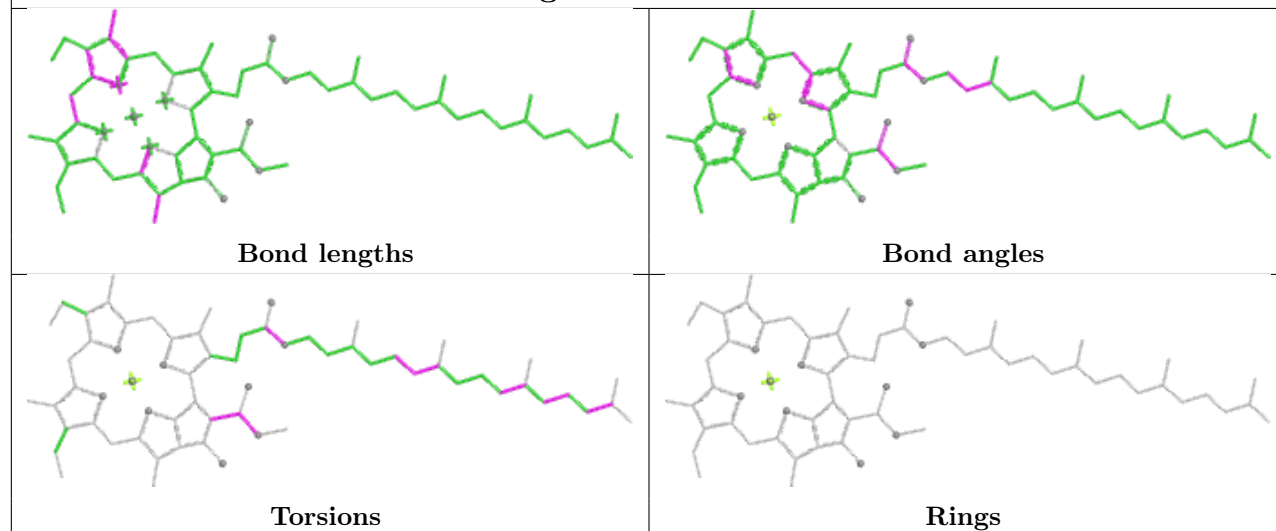
Ligand XAT 9 303**Ligand XAT 2 301****Ligand CLA 7 313**

Ligand CLA a 838

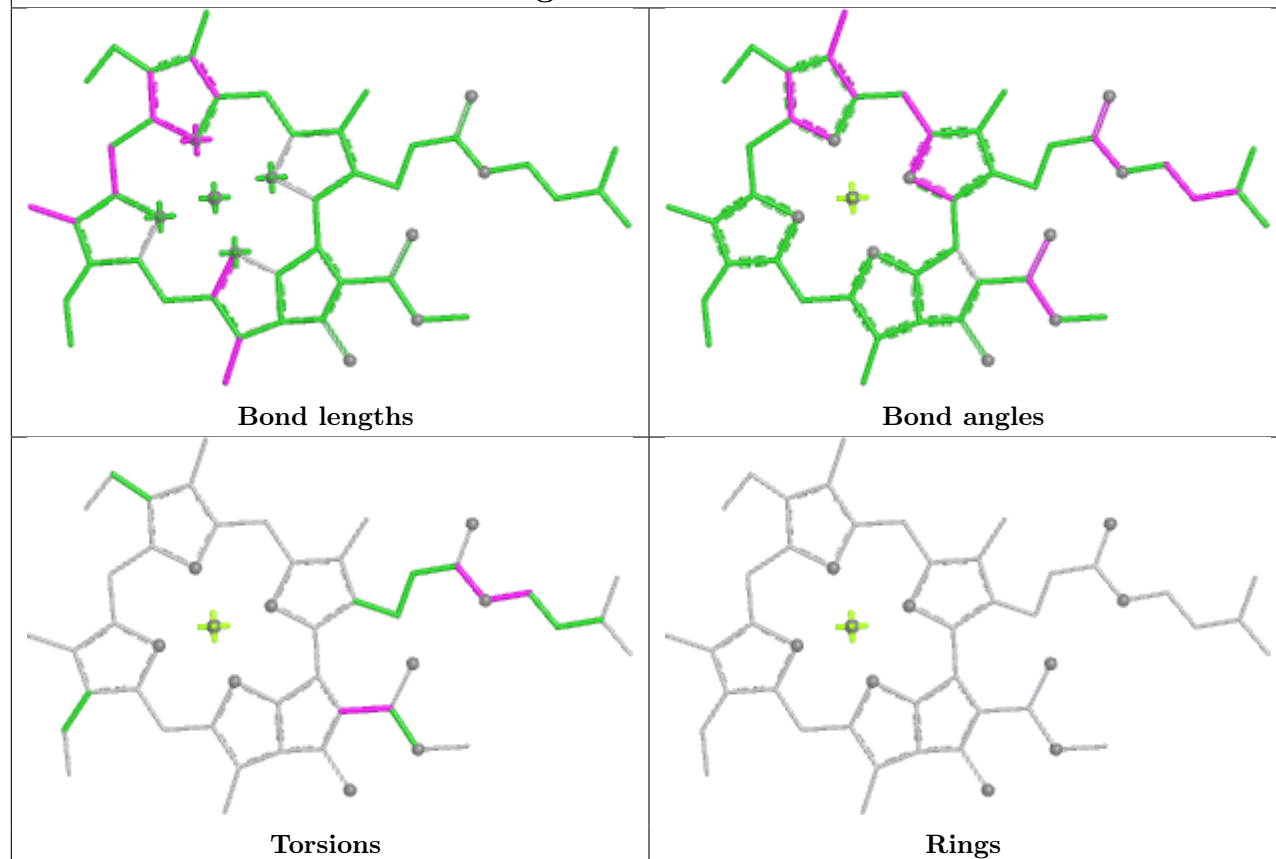


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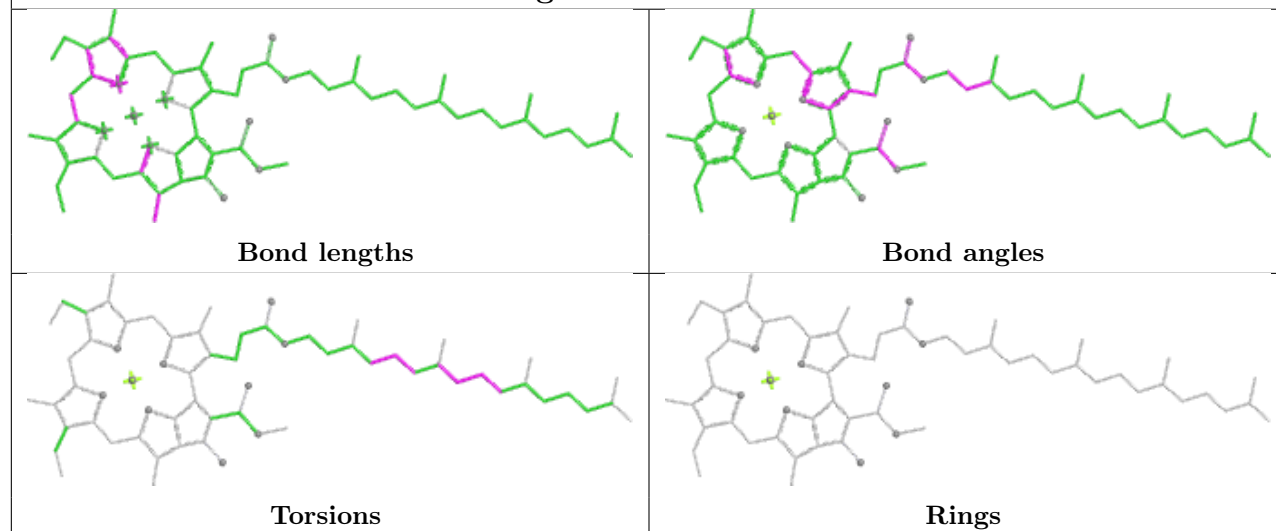


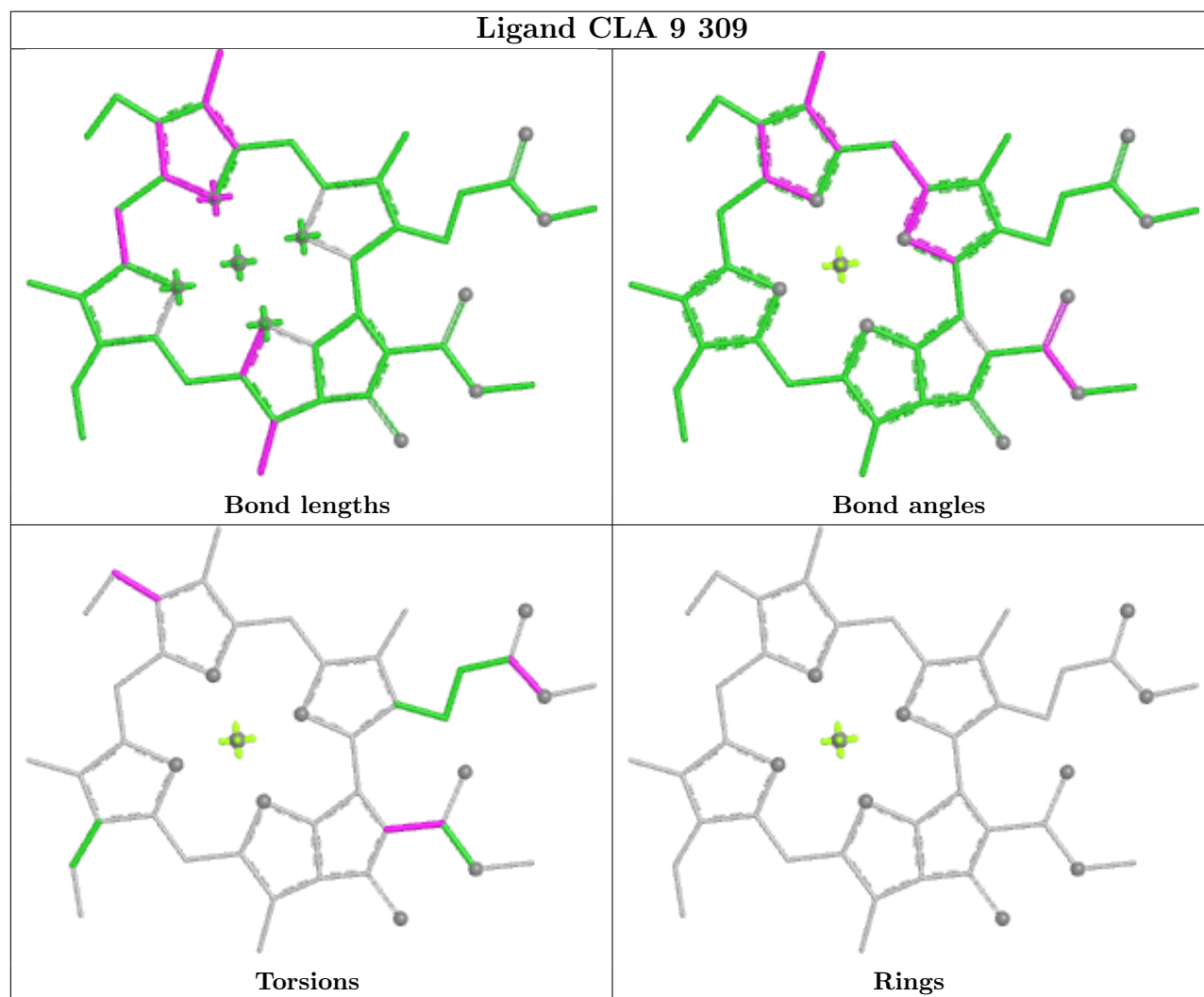
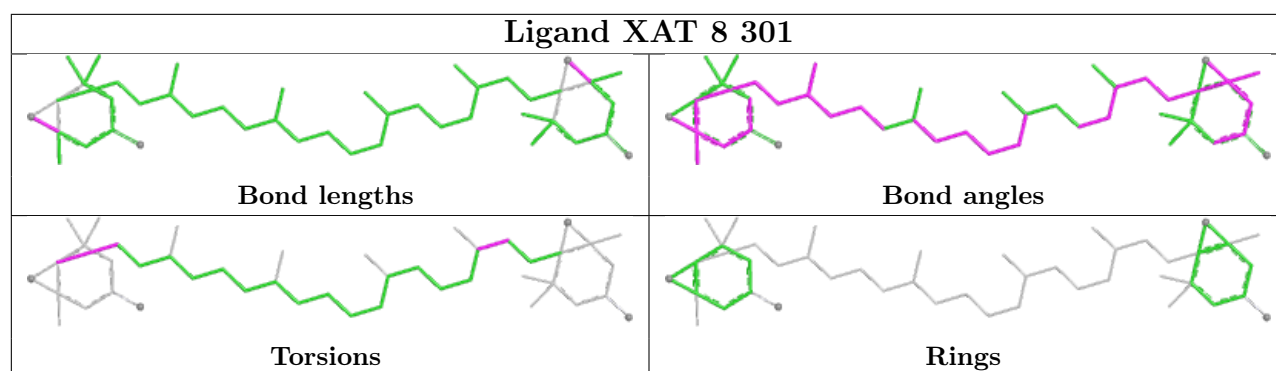
Ligand CLA b 838**Ligand CLA f 802**

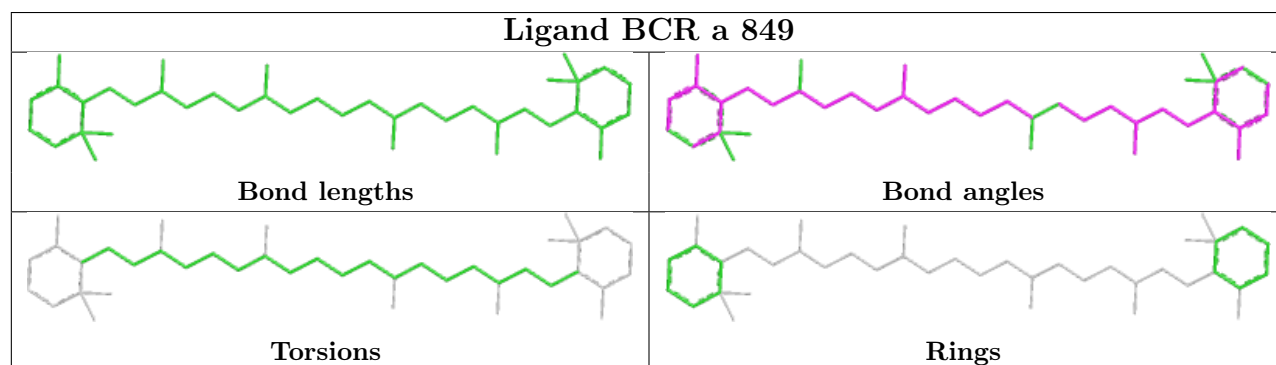
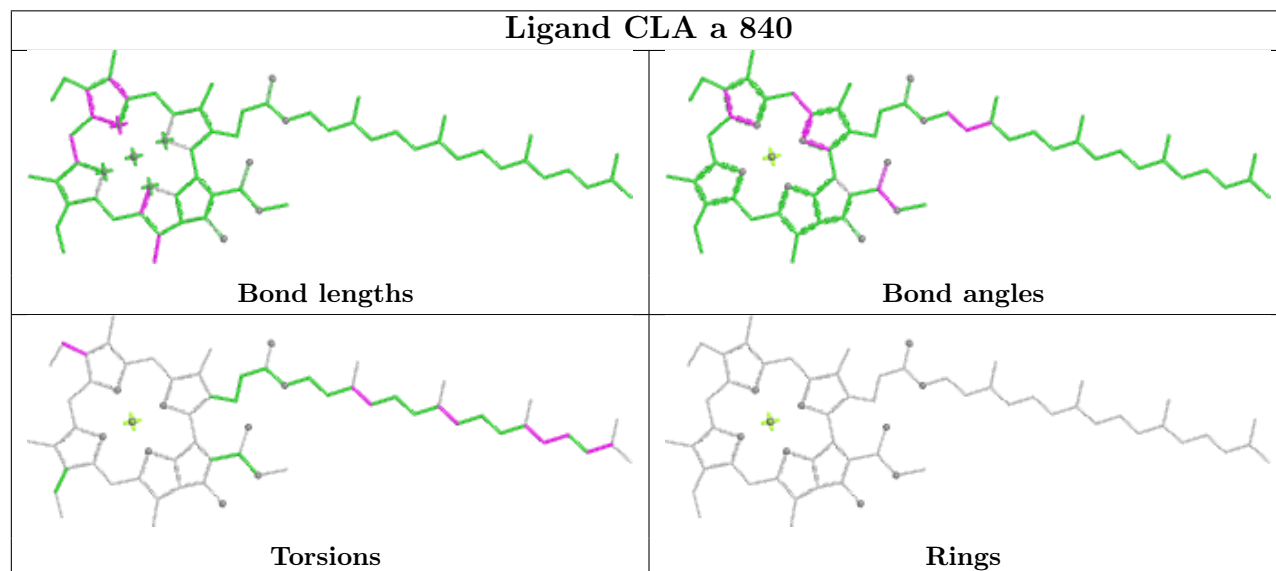
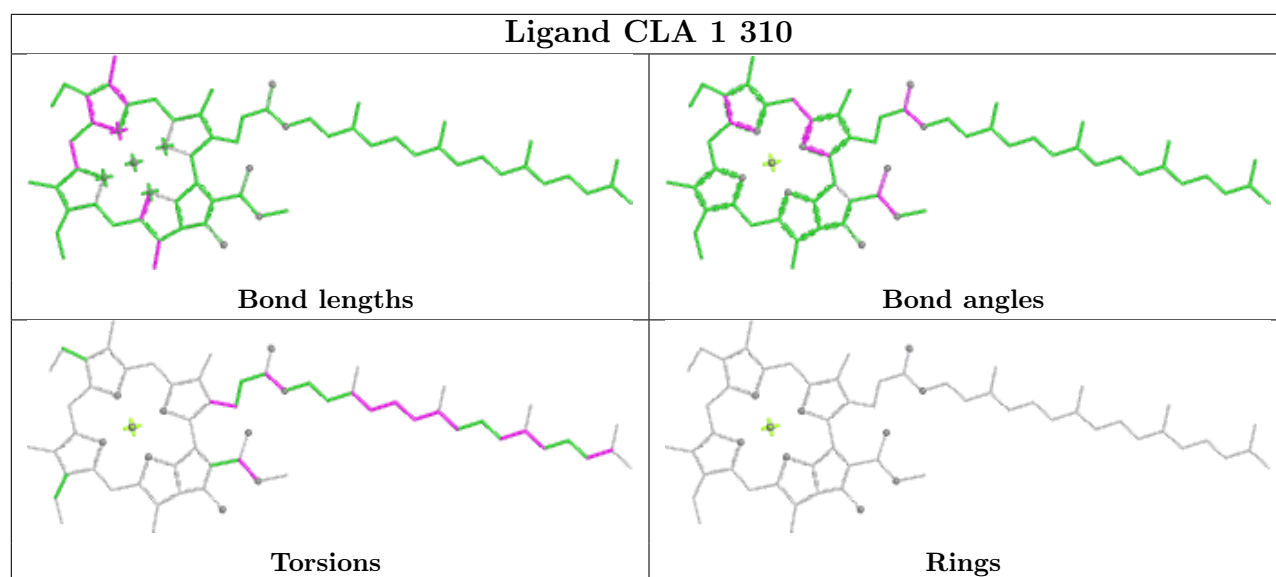
Ligand CLA a 816

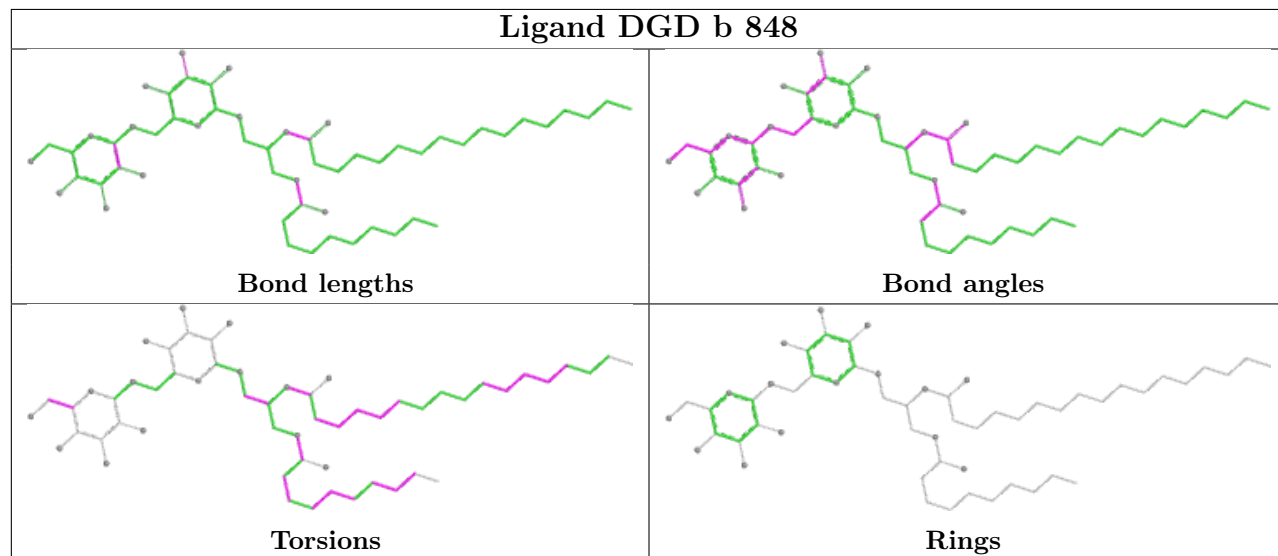
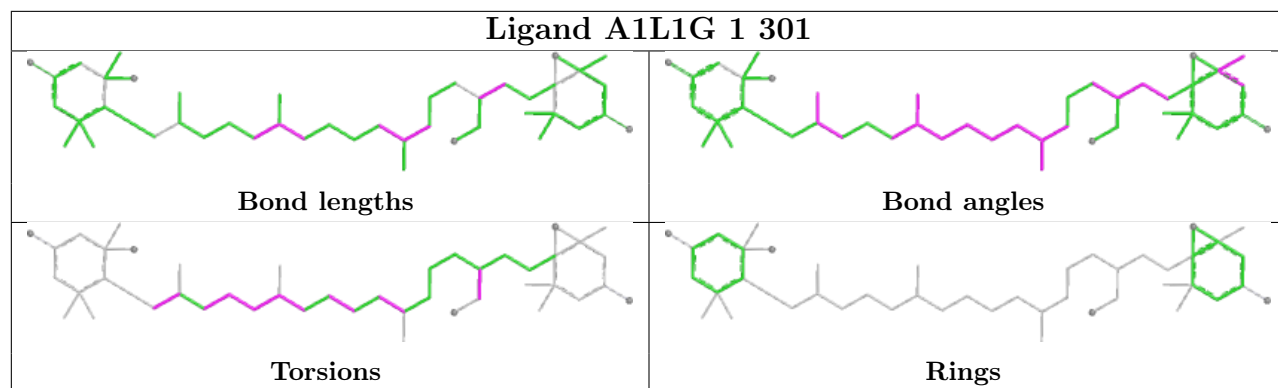


Ligand CLA a 827

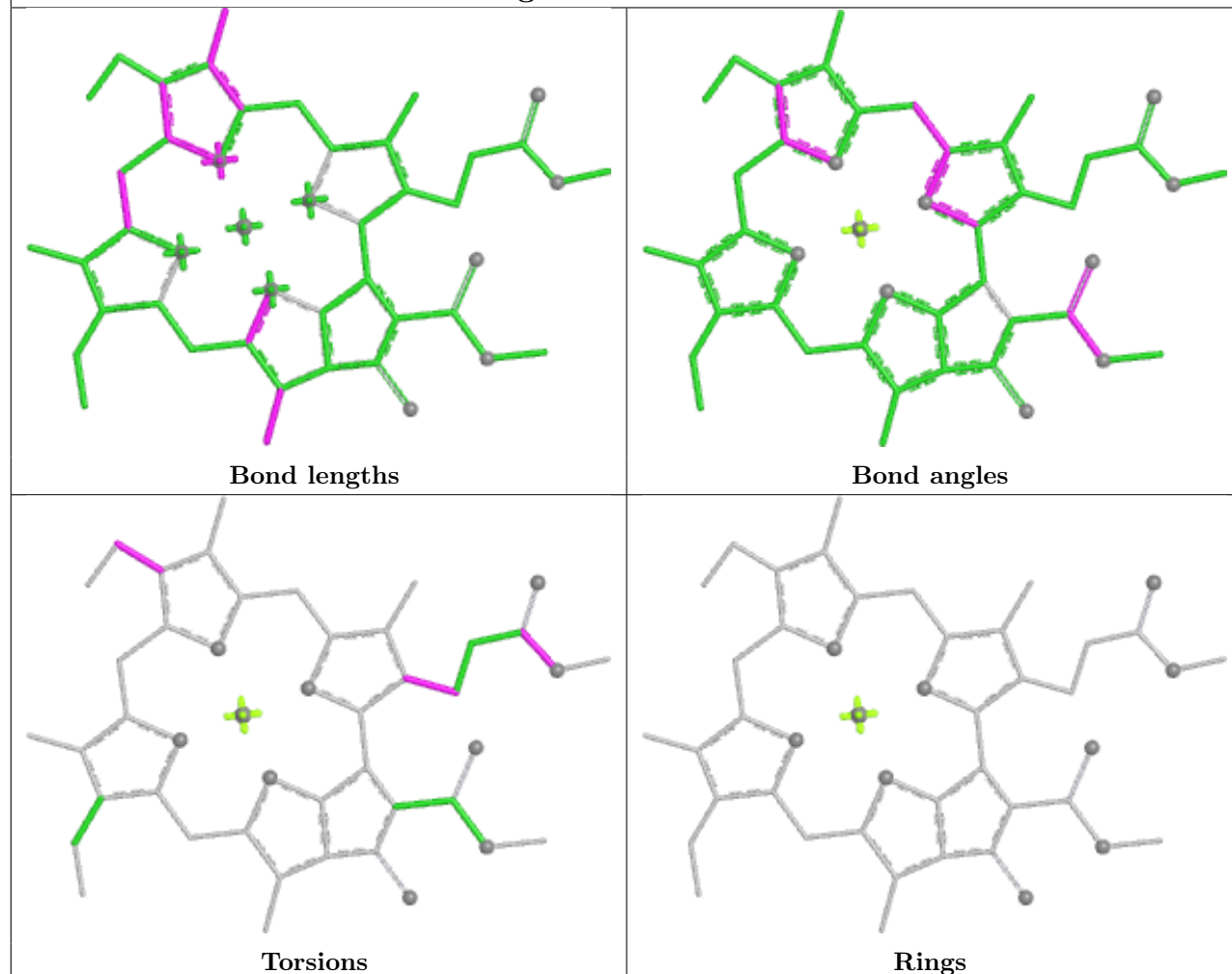




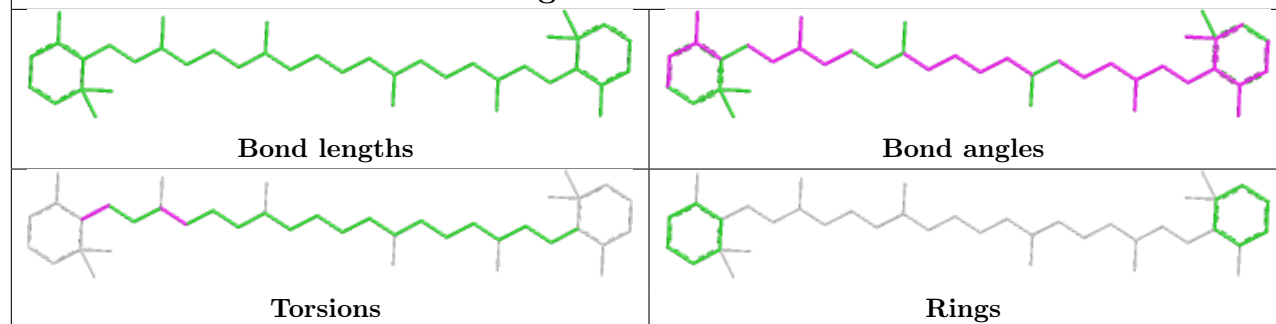


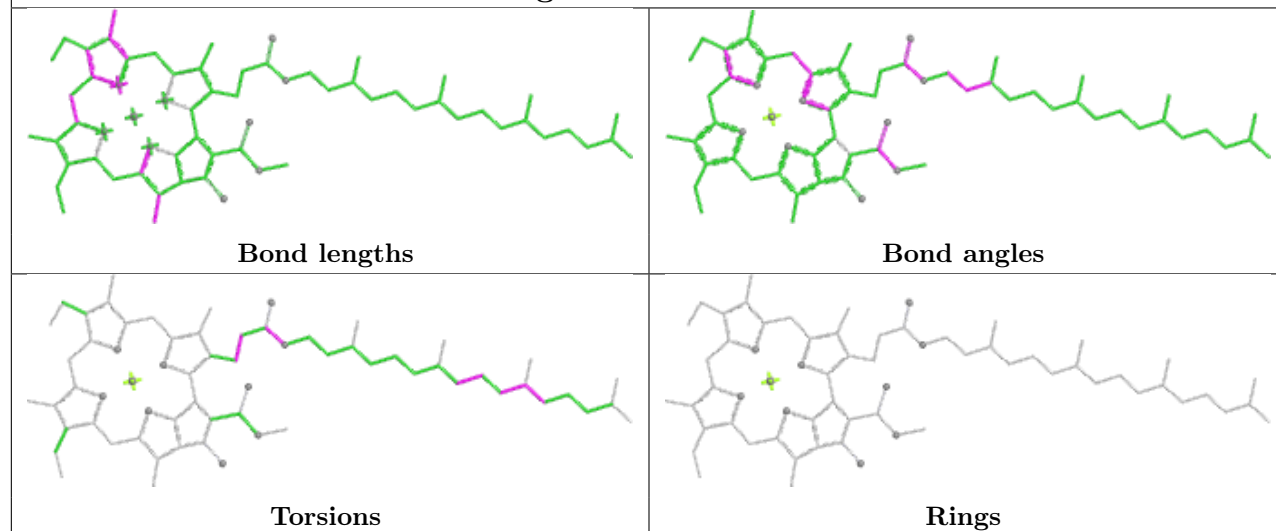
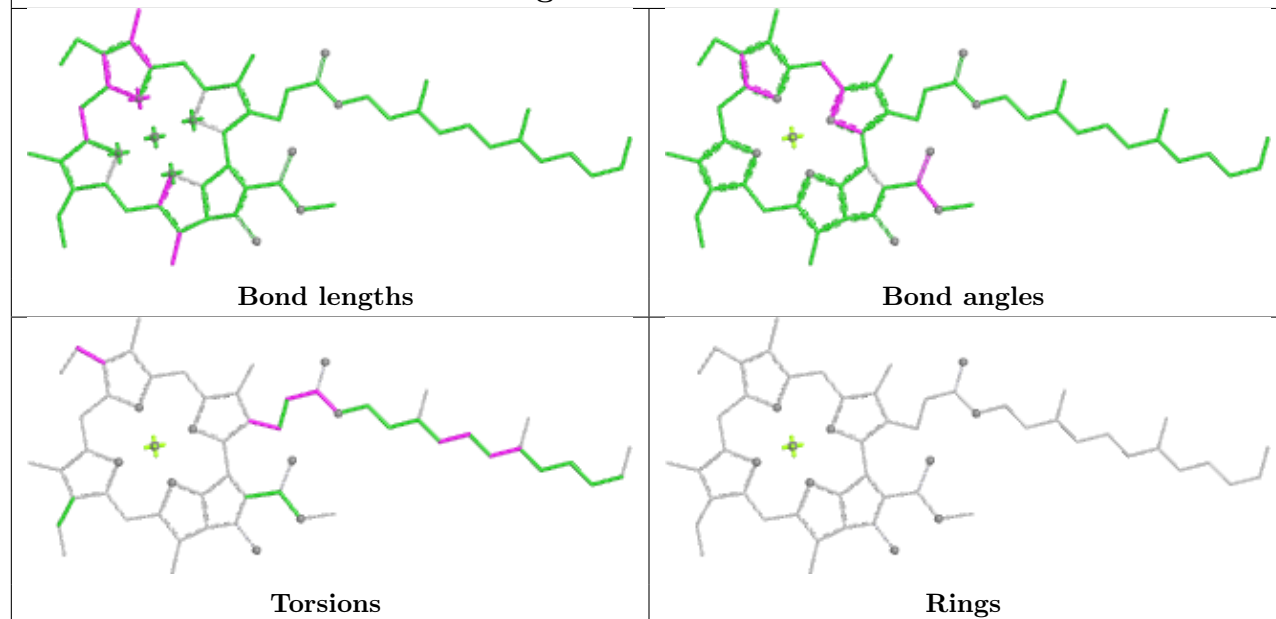


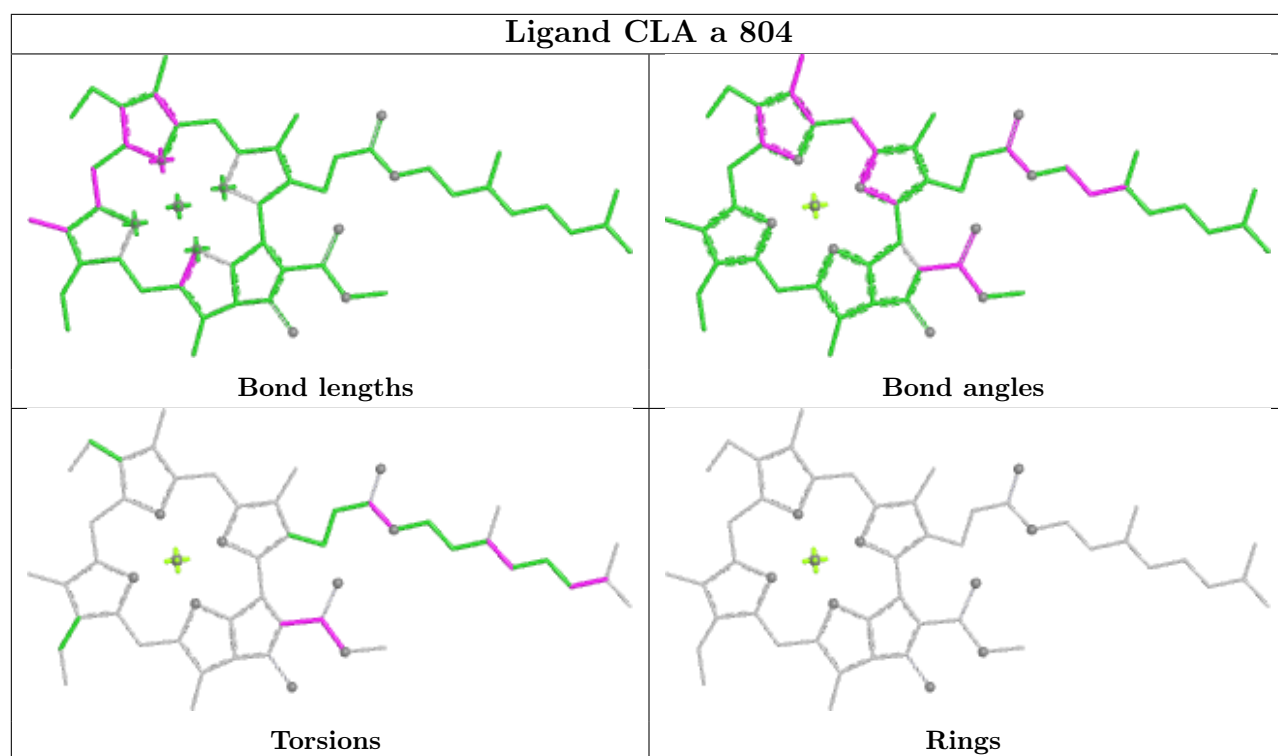
Ligand CLA 4 312



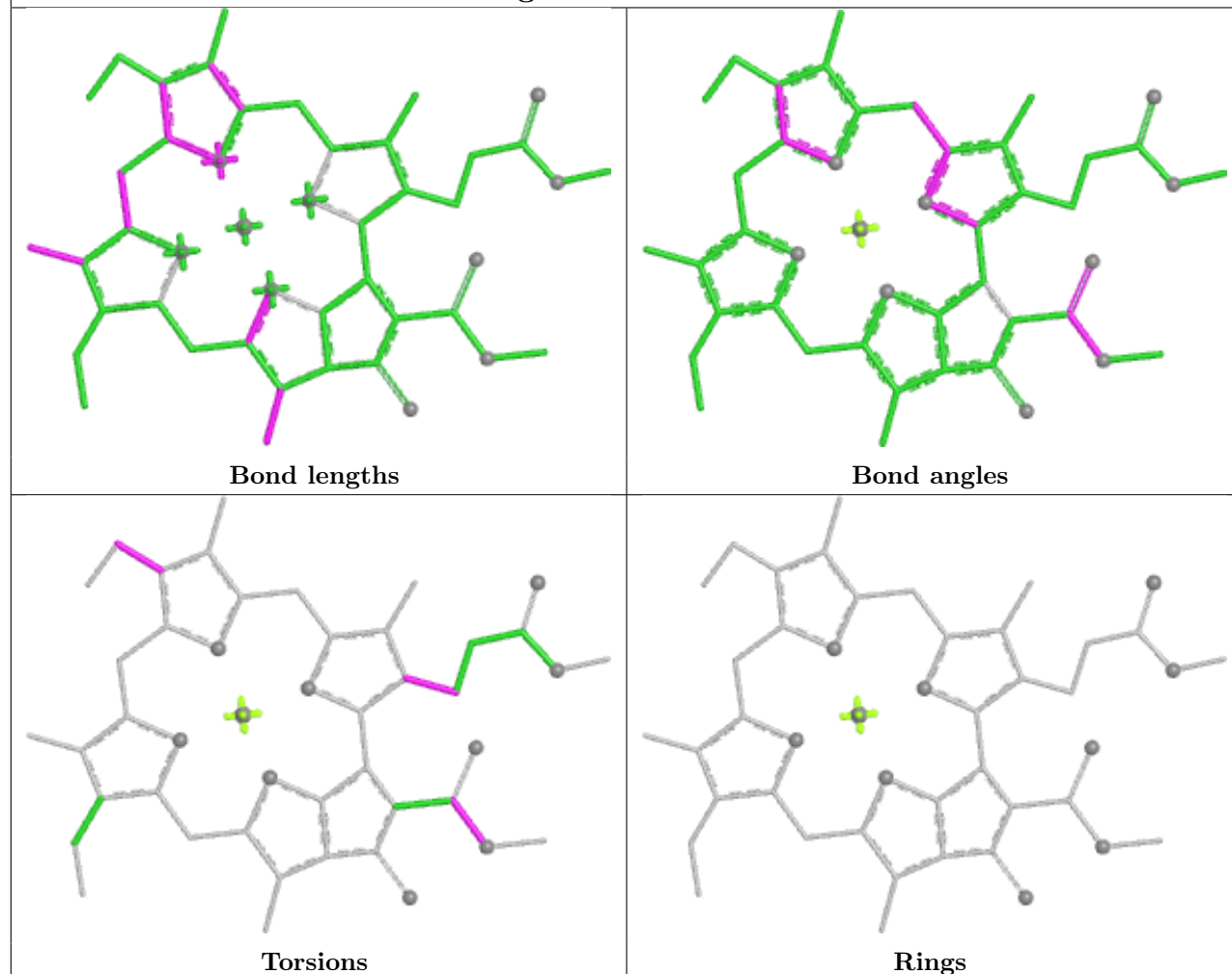
Ligand BCR 1 201



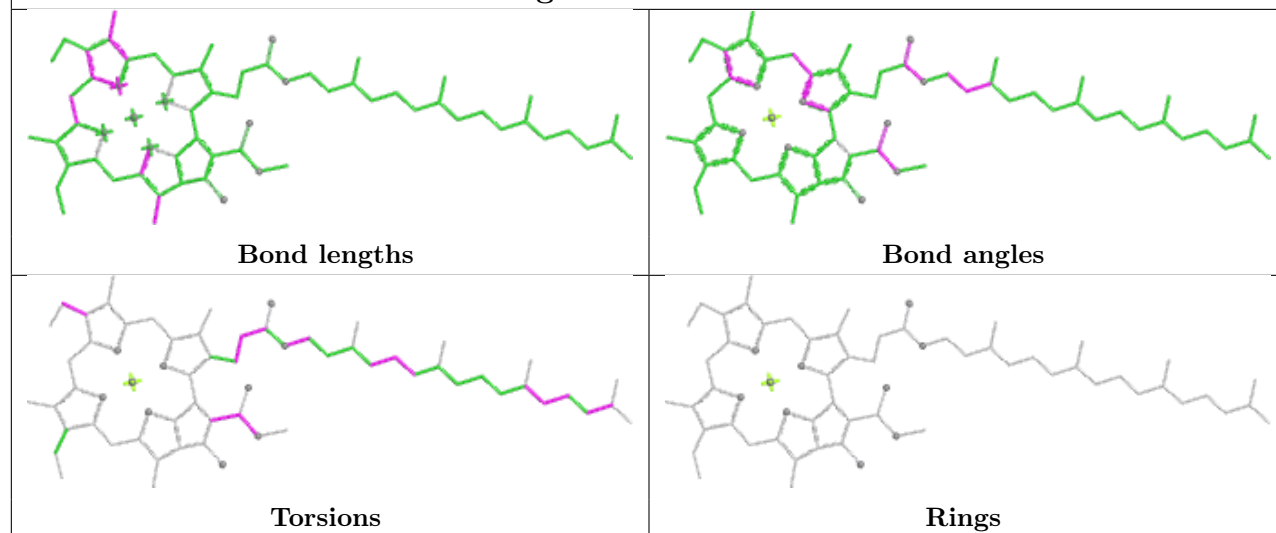
Ligand CLA a 842**Ligand CLA 3 312**

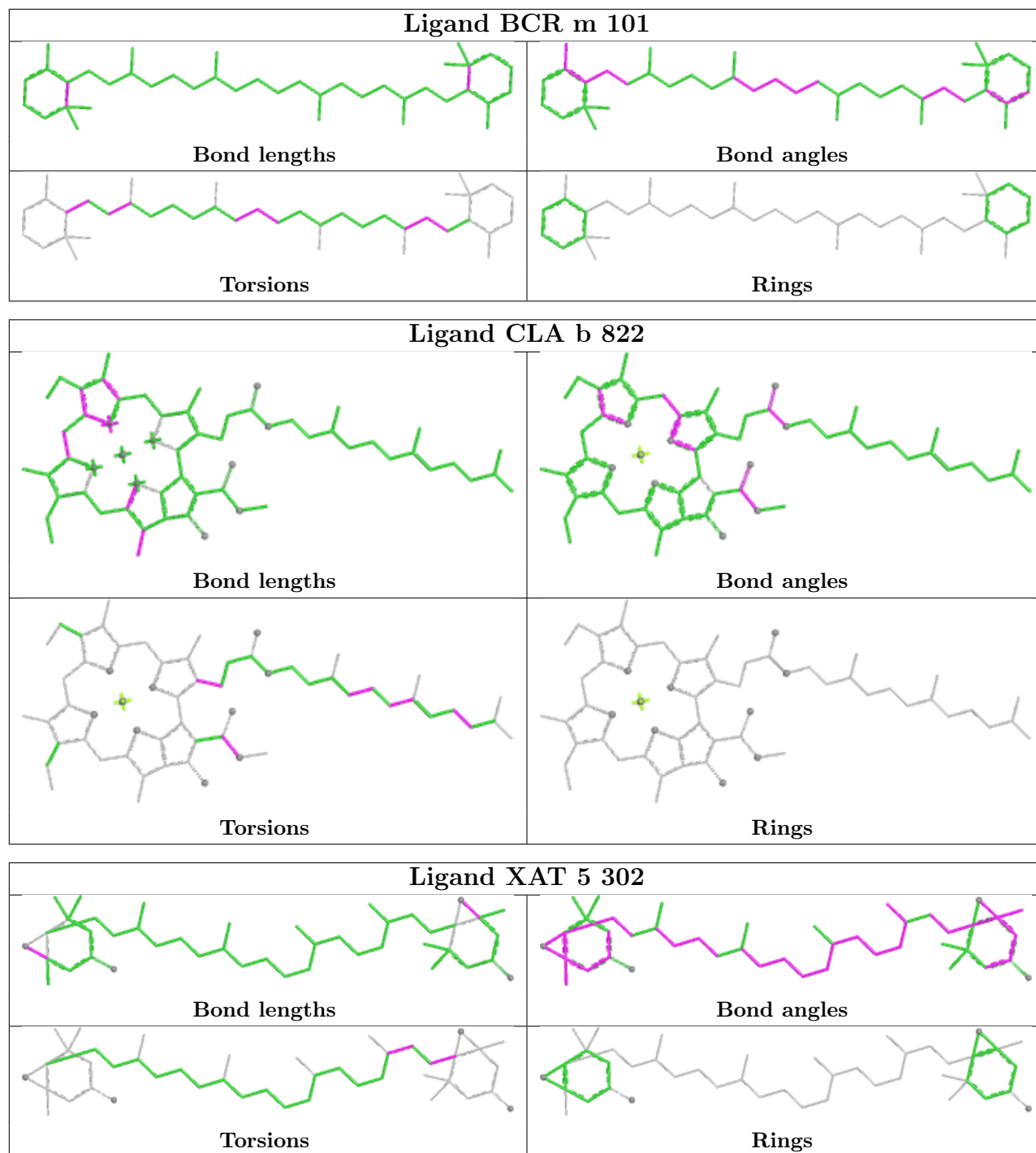


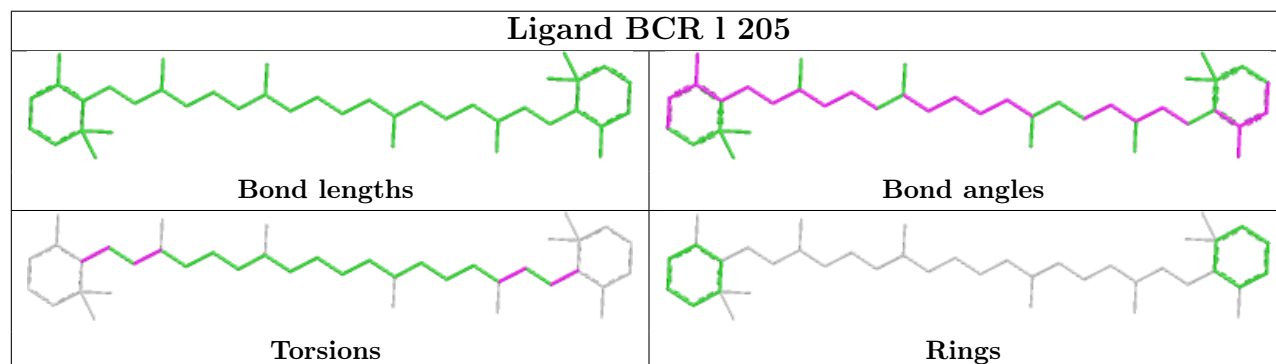
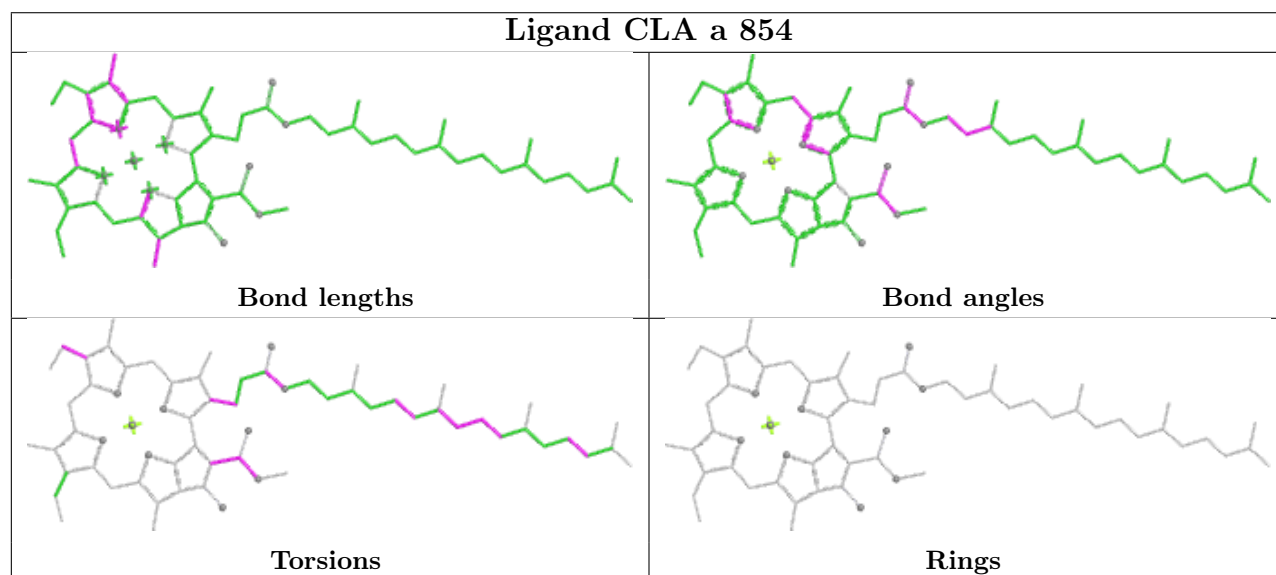
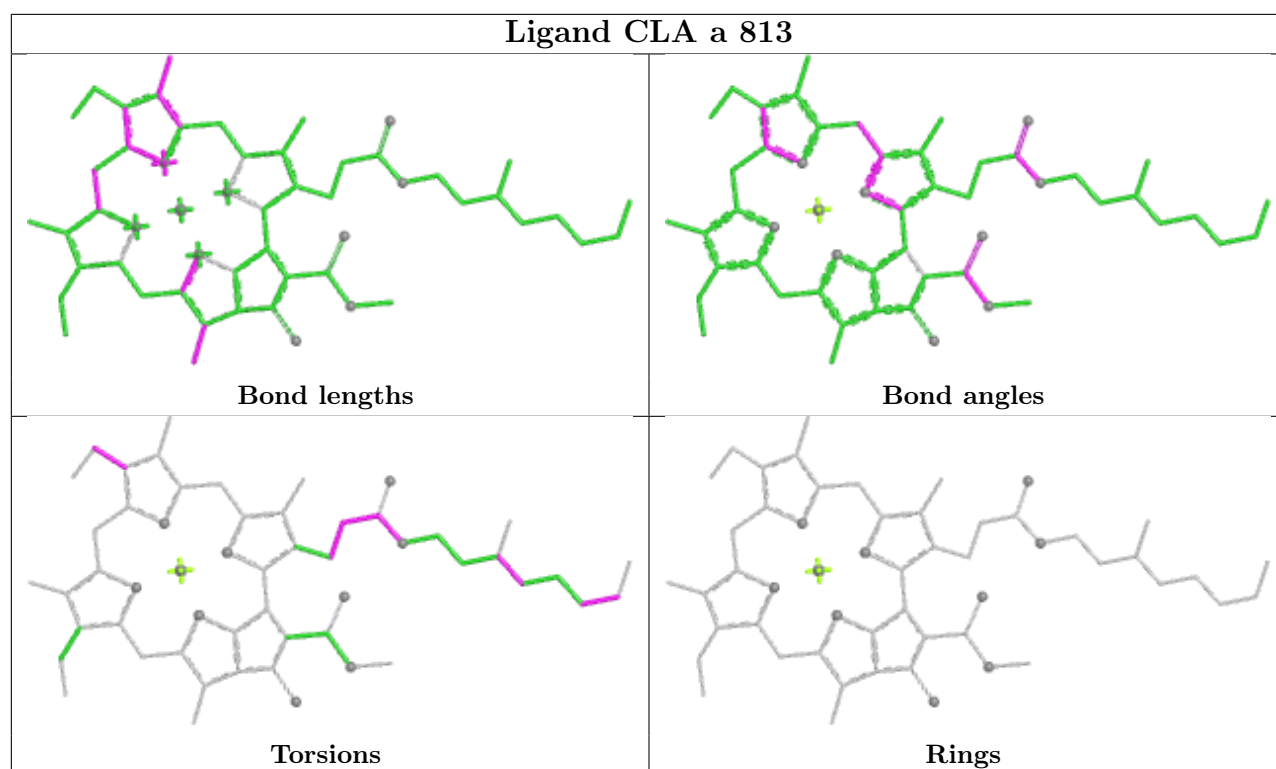
Ligand CLA 2 316



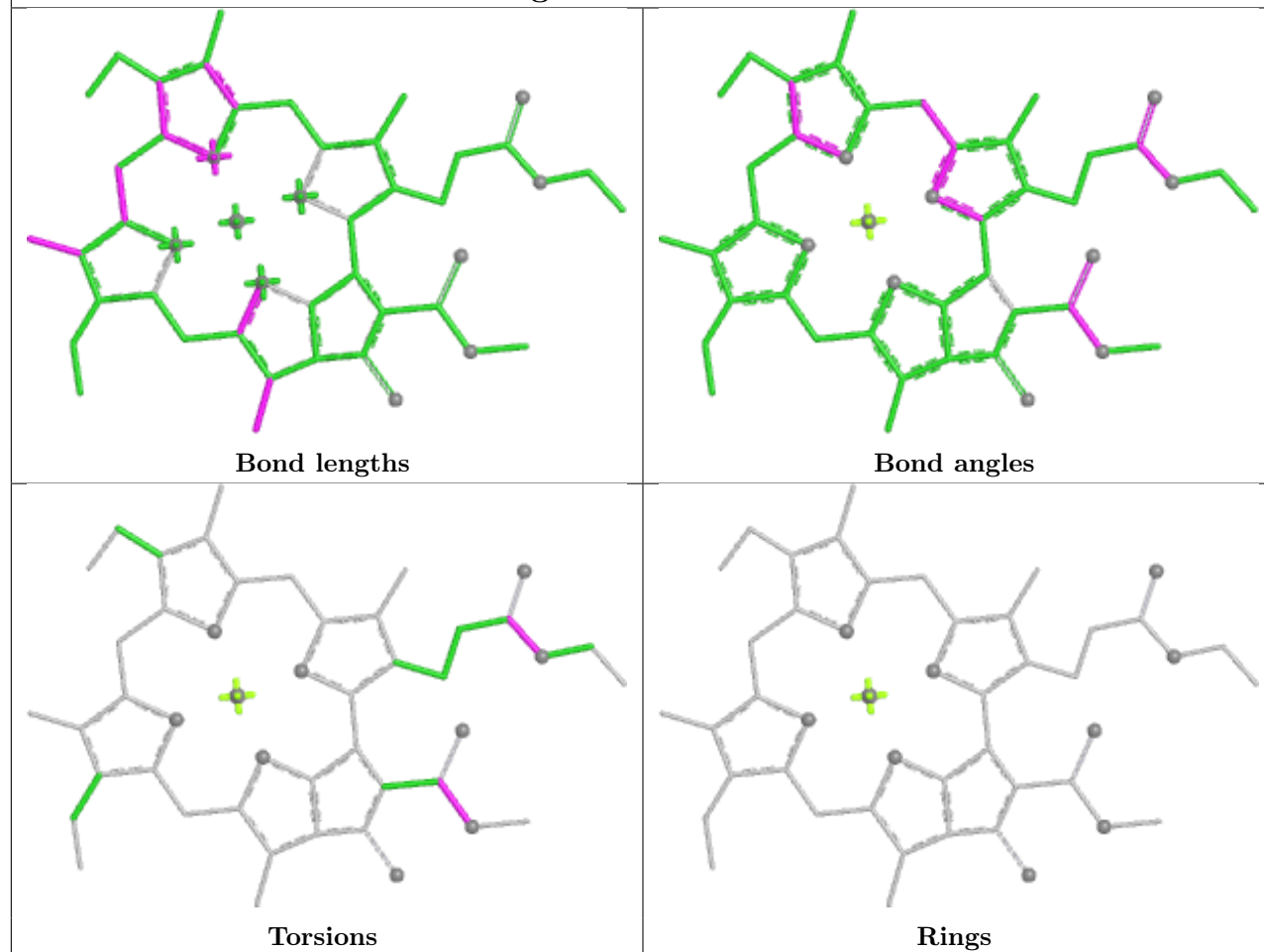
Ligand CLA a 810



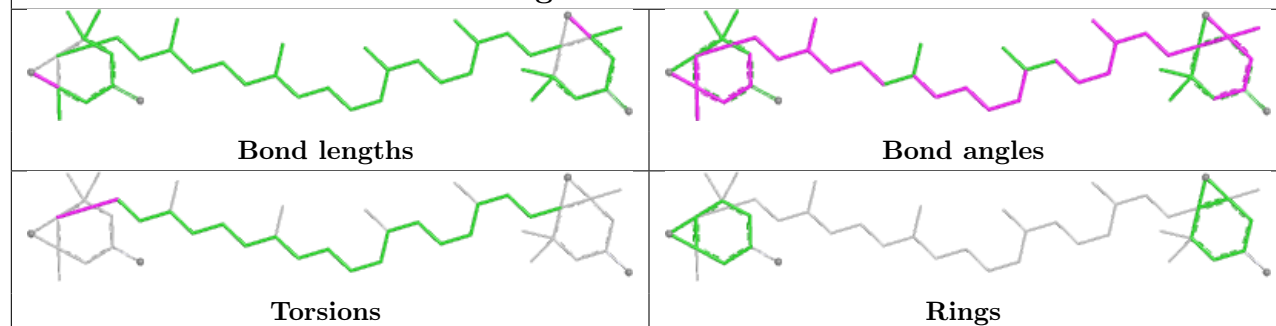




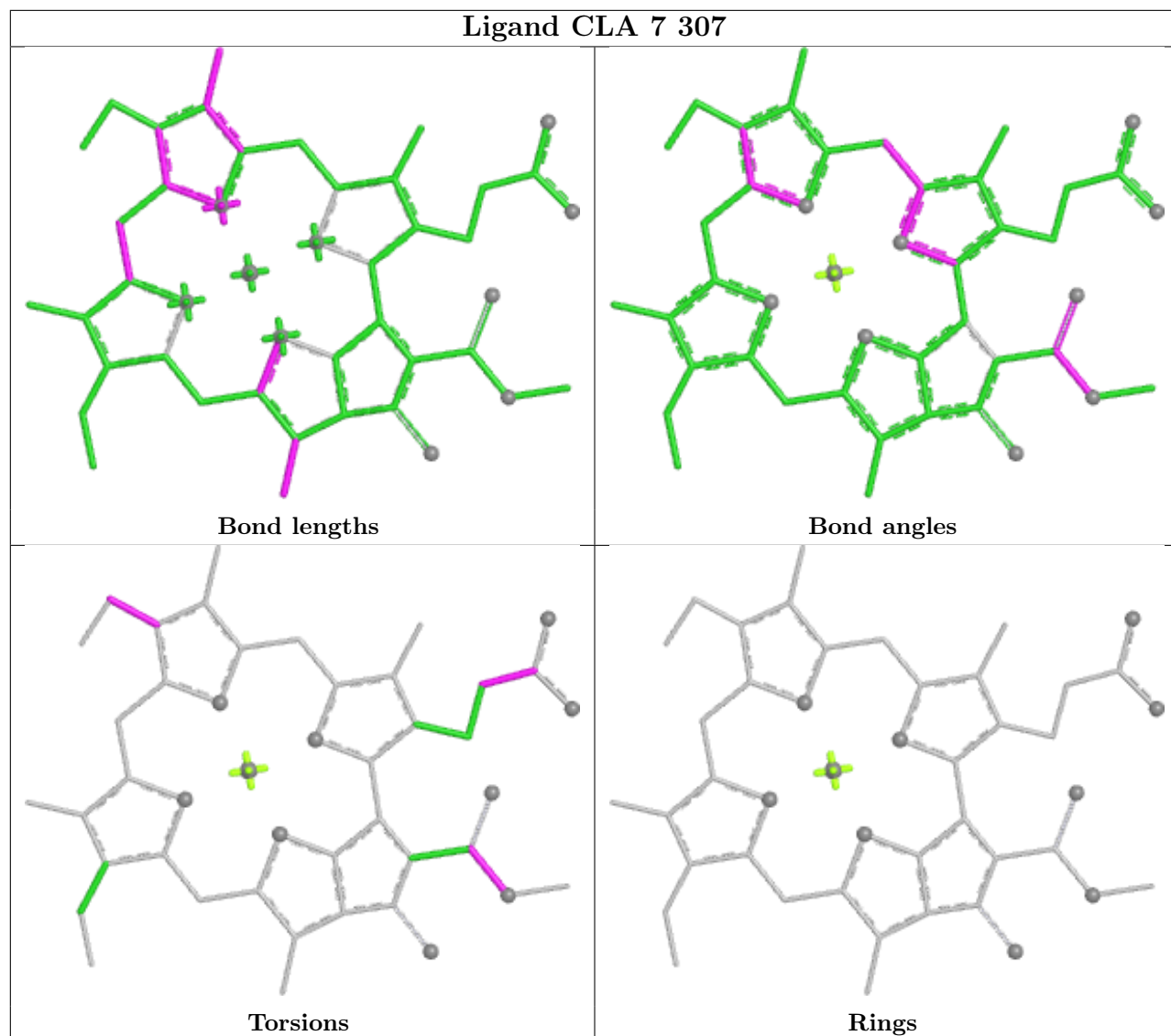
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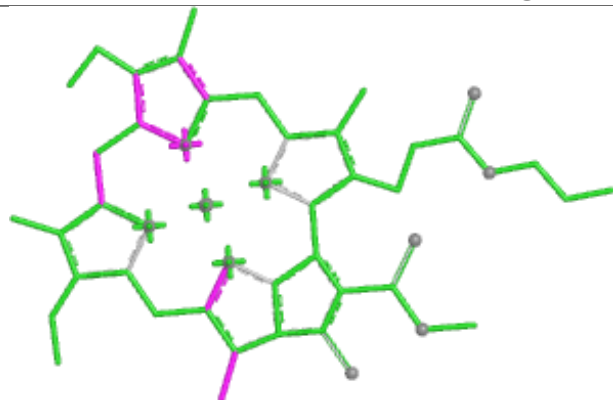
Ligand XAT 5 304



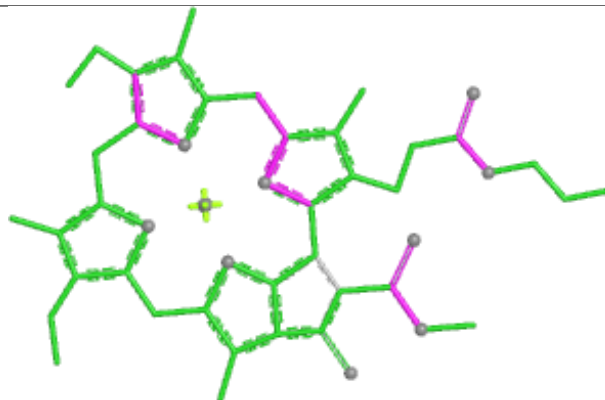
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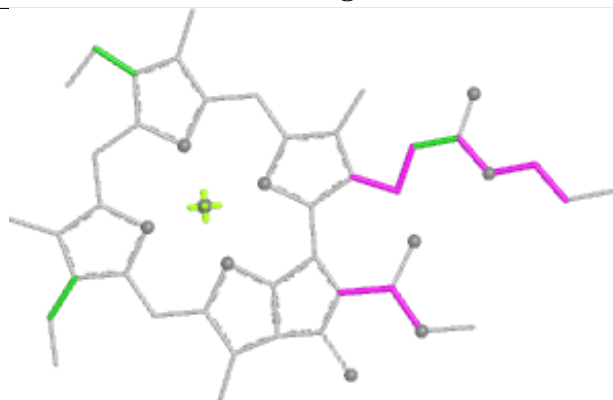
Ligand CLA 7 306



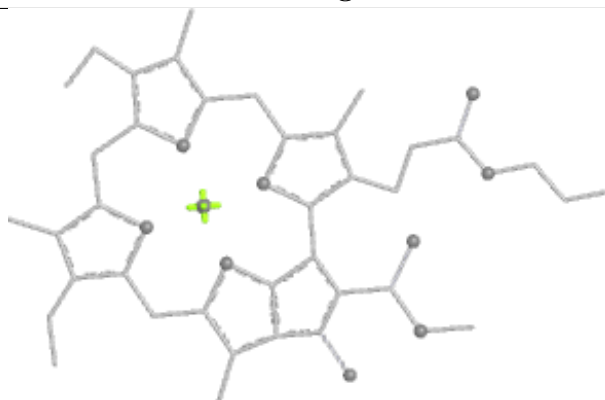
Bond lengths



Bond angles

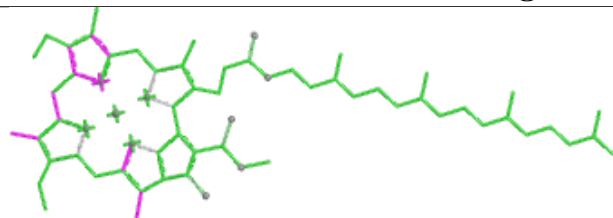


Torsions

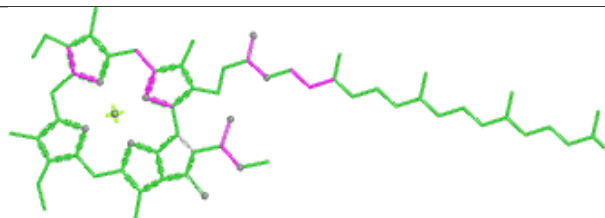


Rings

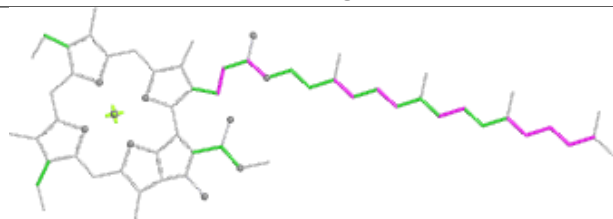
Ligand CLA a 830



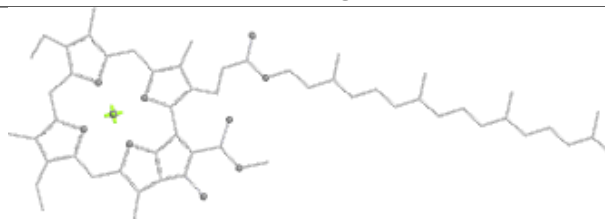
Bond lengths



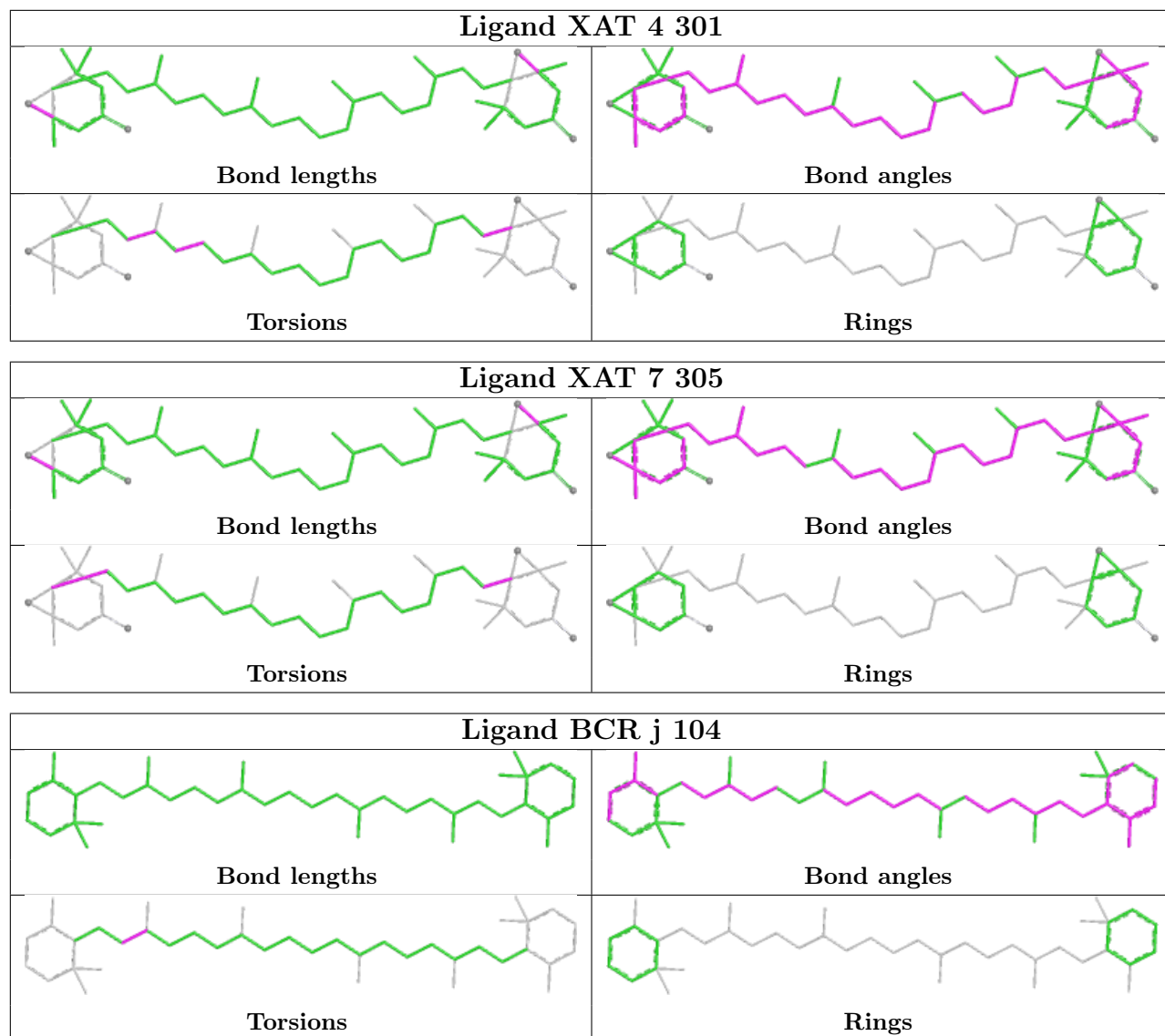
Bond angles

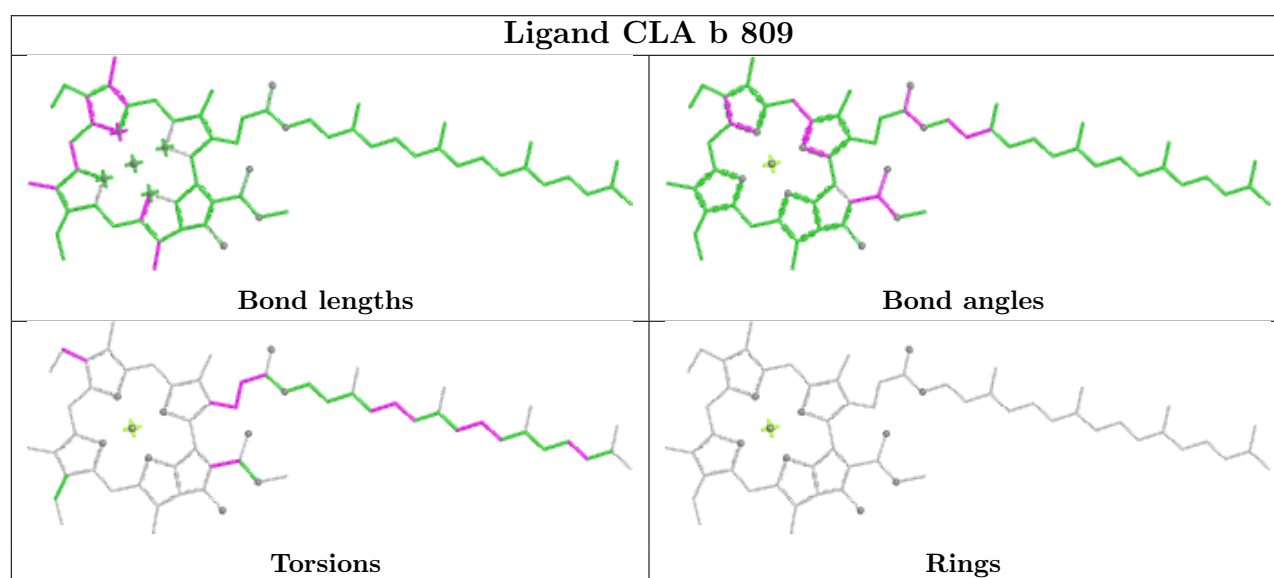
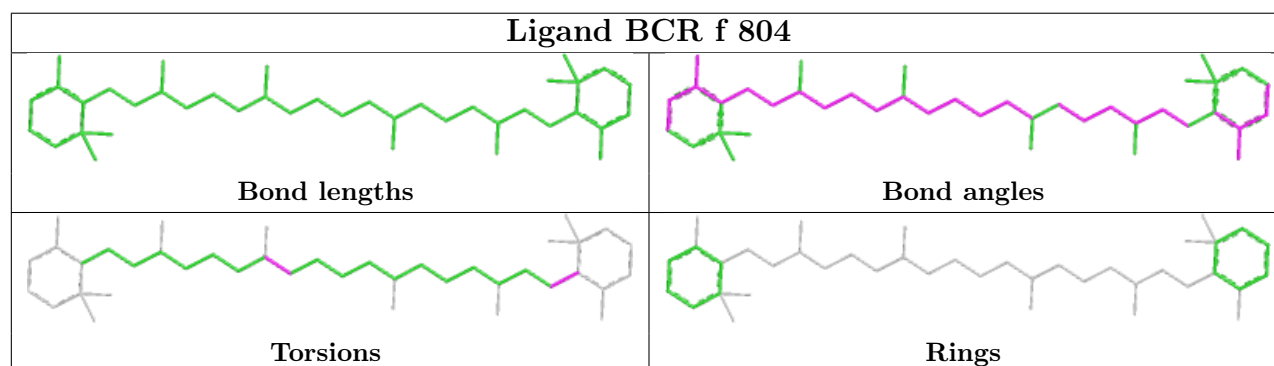
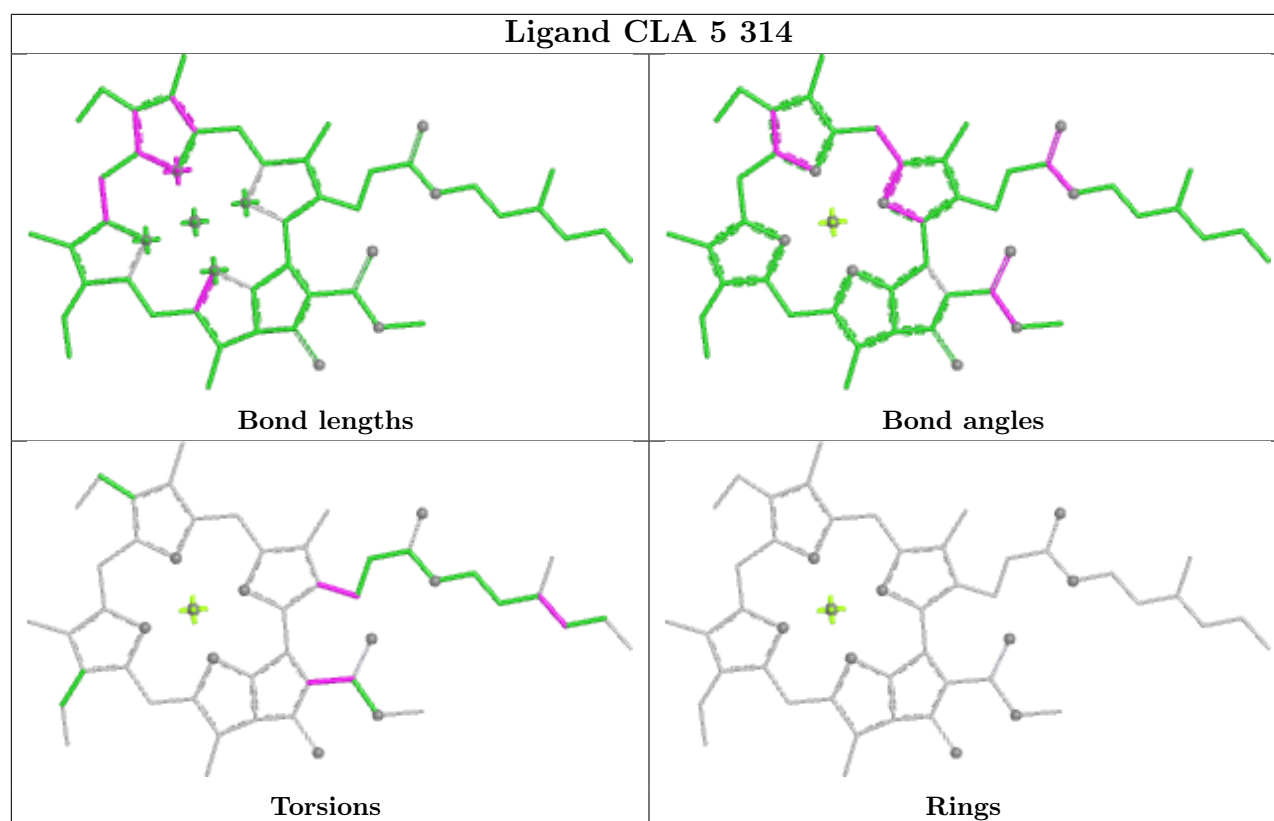


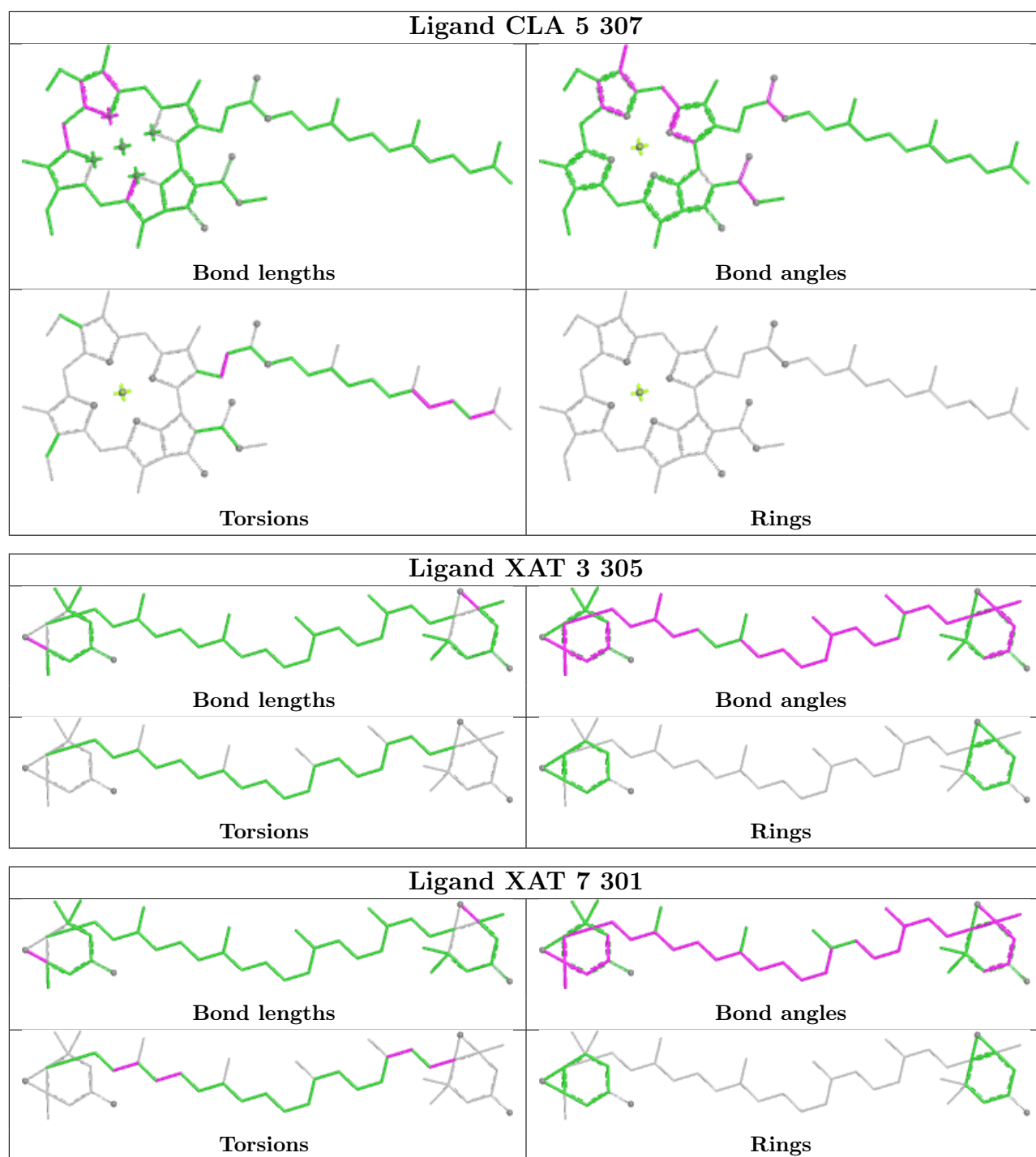
Torsions

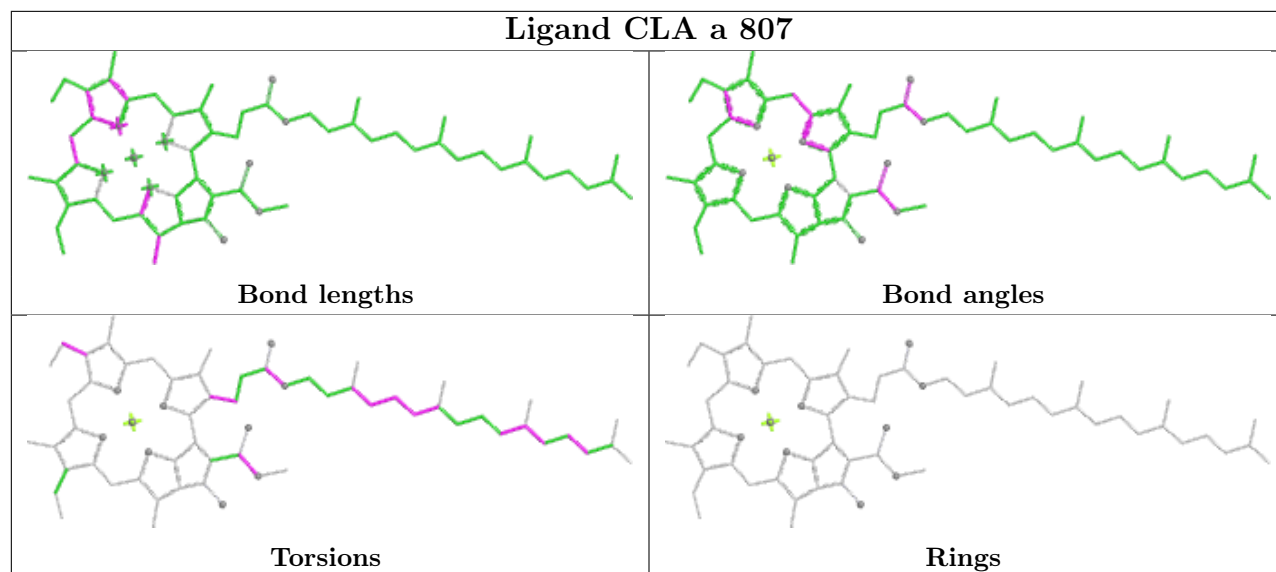
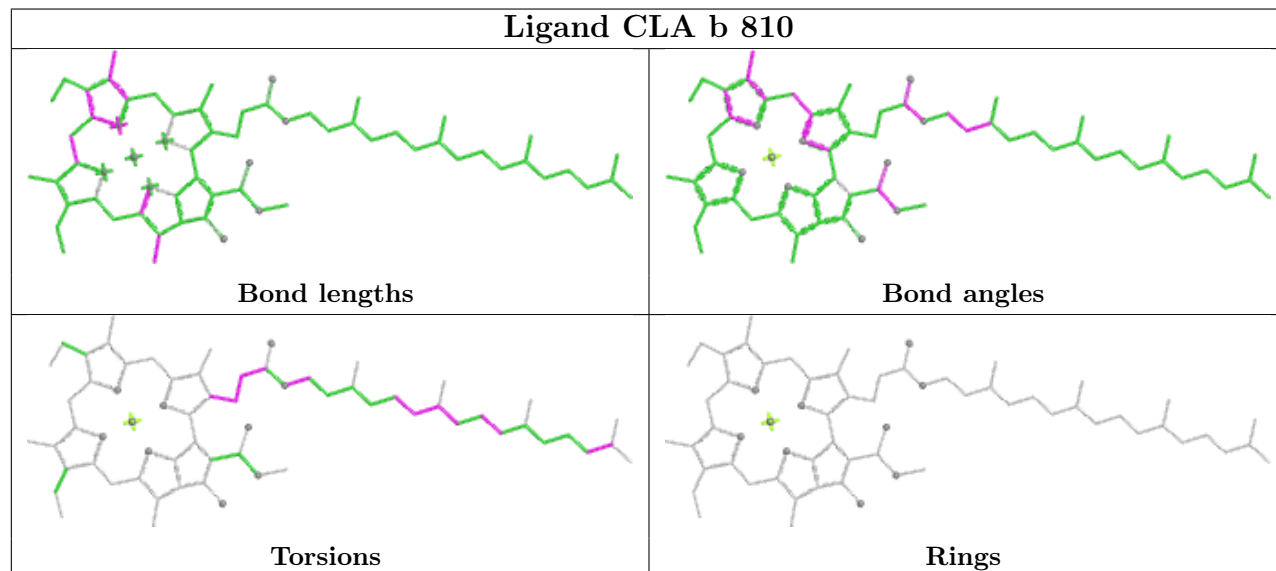


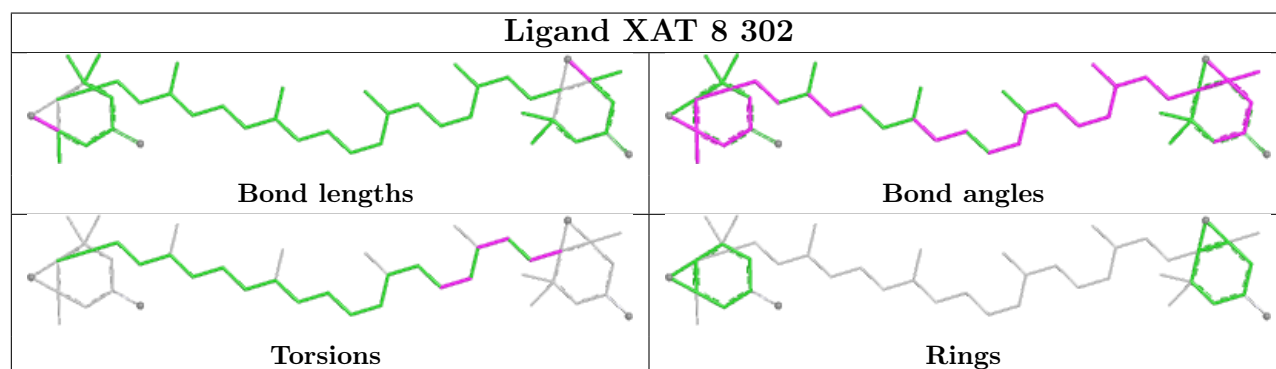
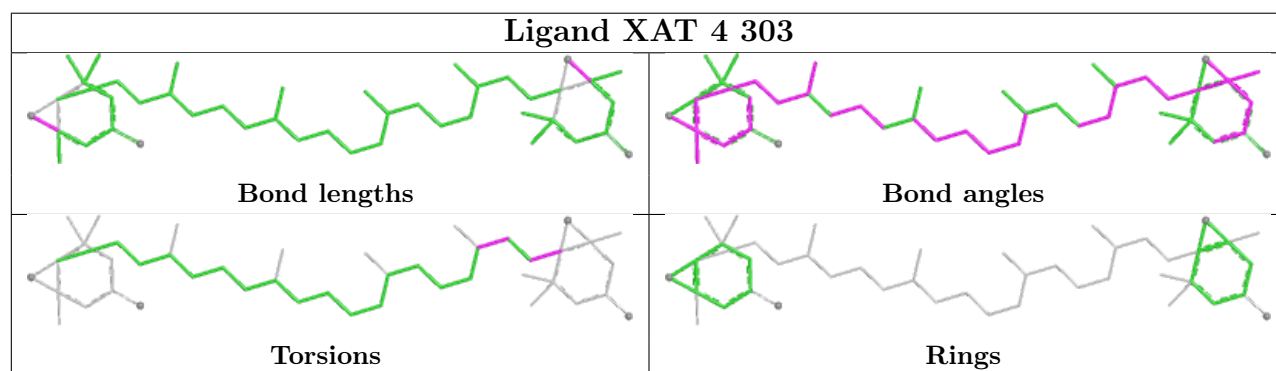
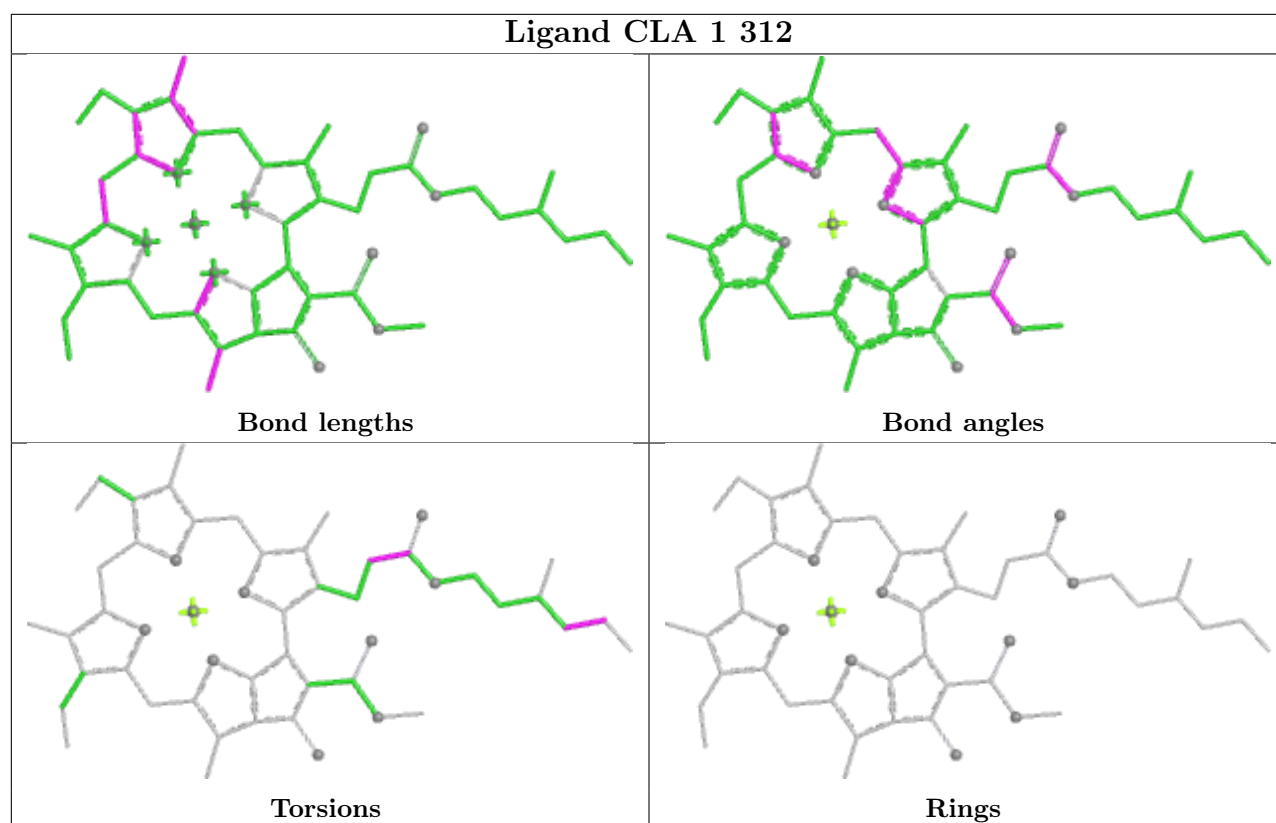
Rings



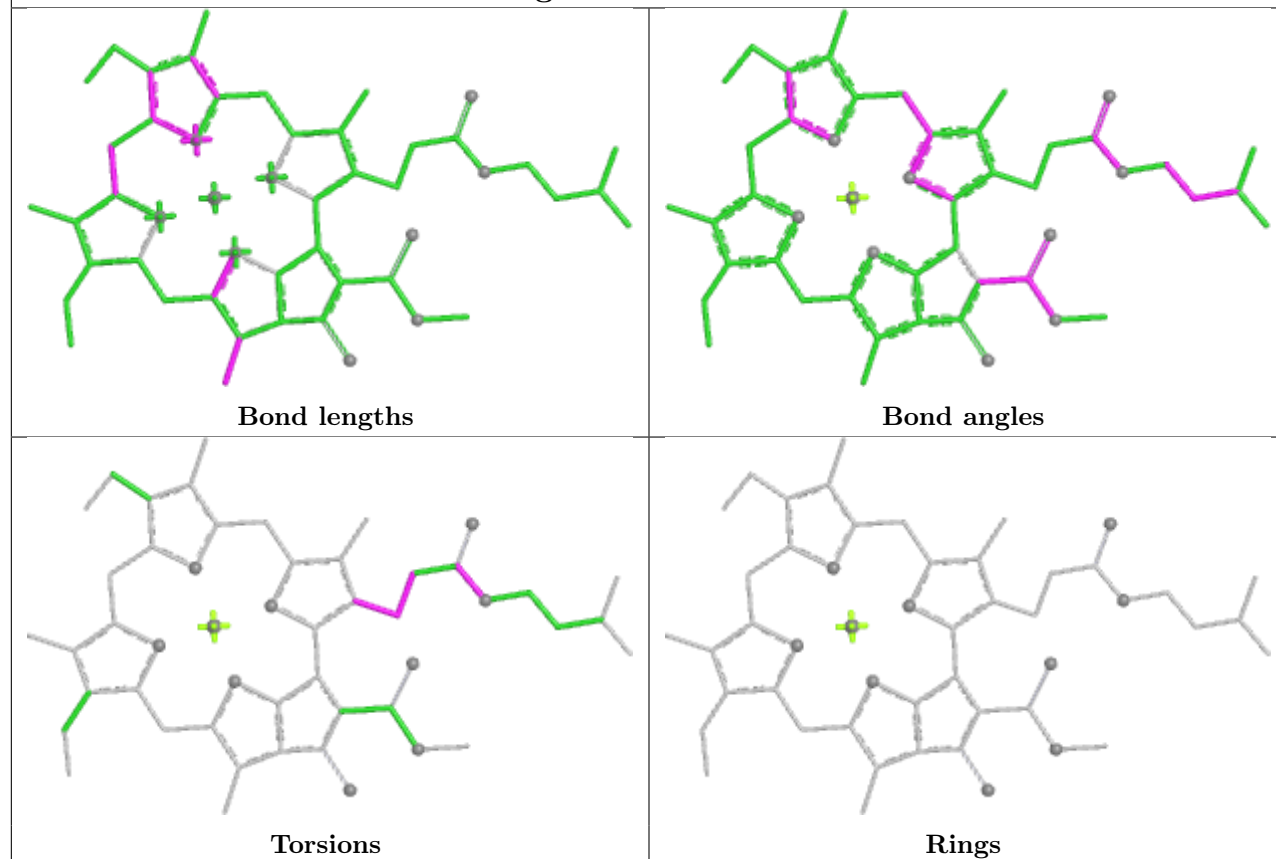




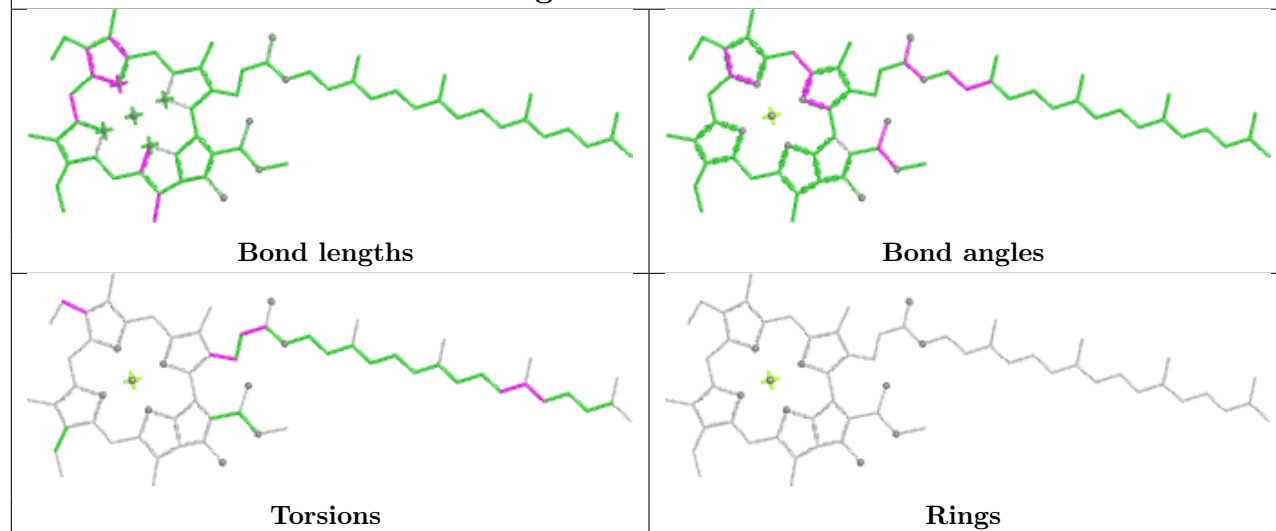
Ligand CLA a 807**Ligand CLA b 810**



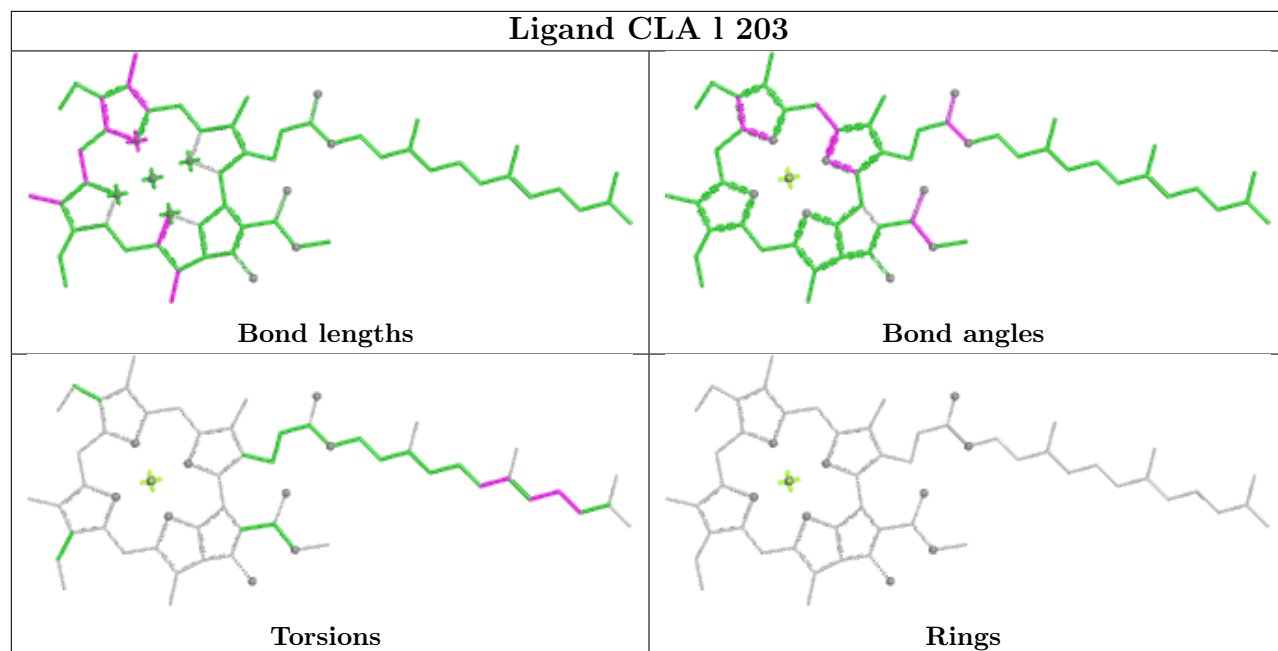
Ligand CLA b 820



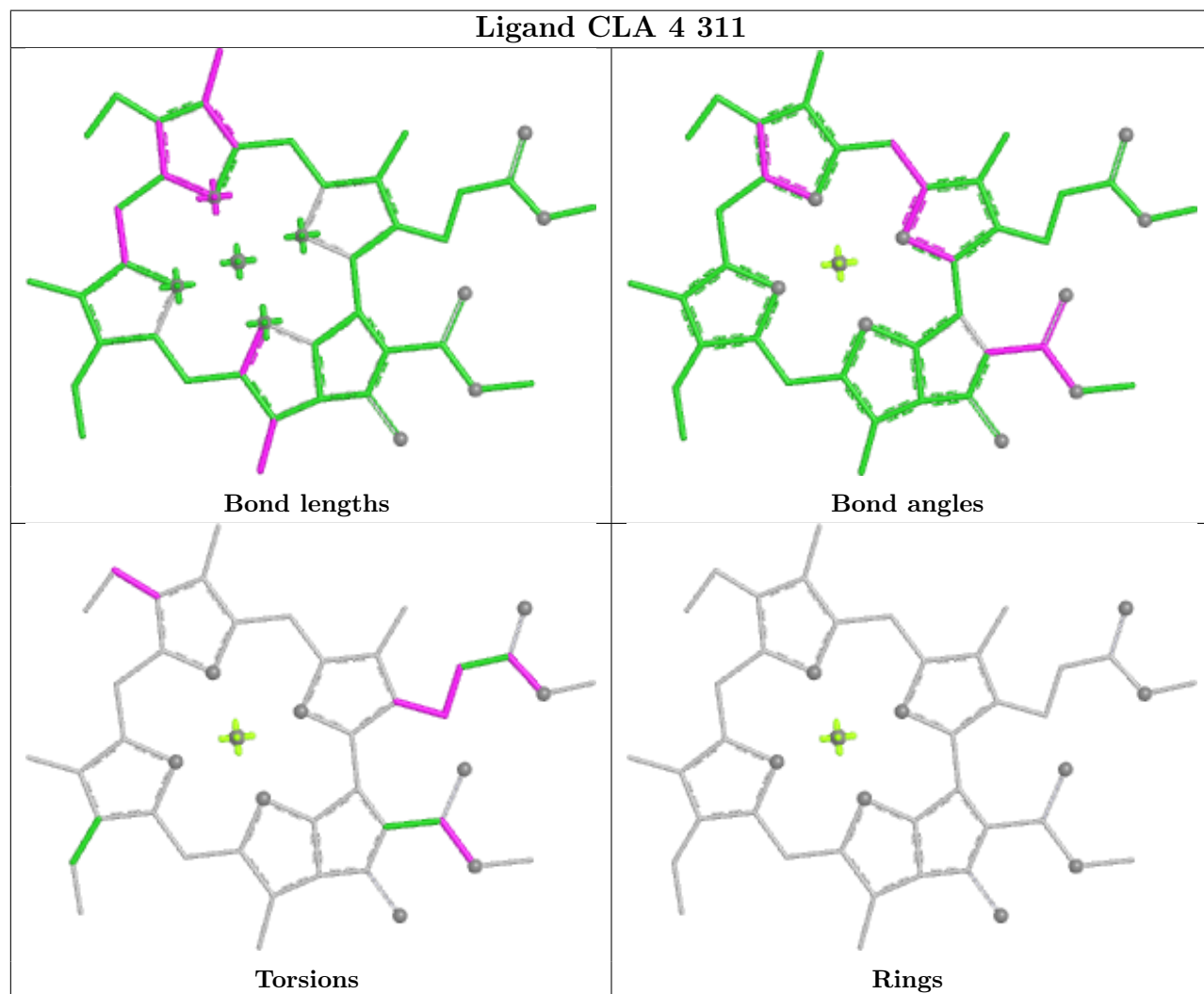
Ligand CLA b 837

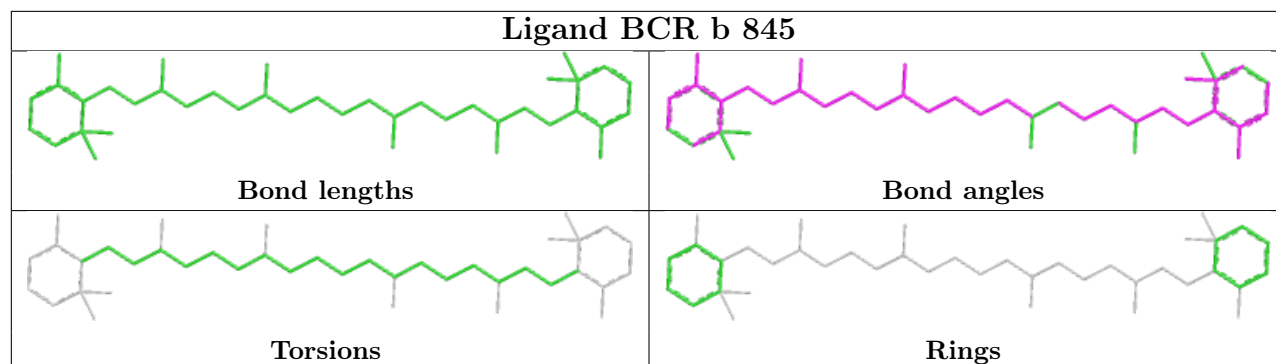
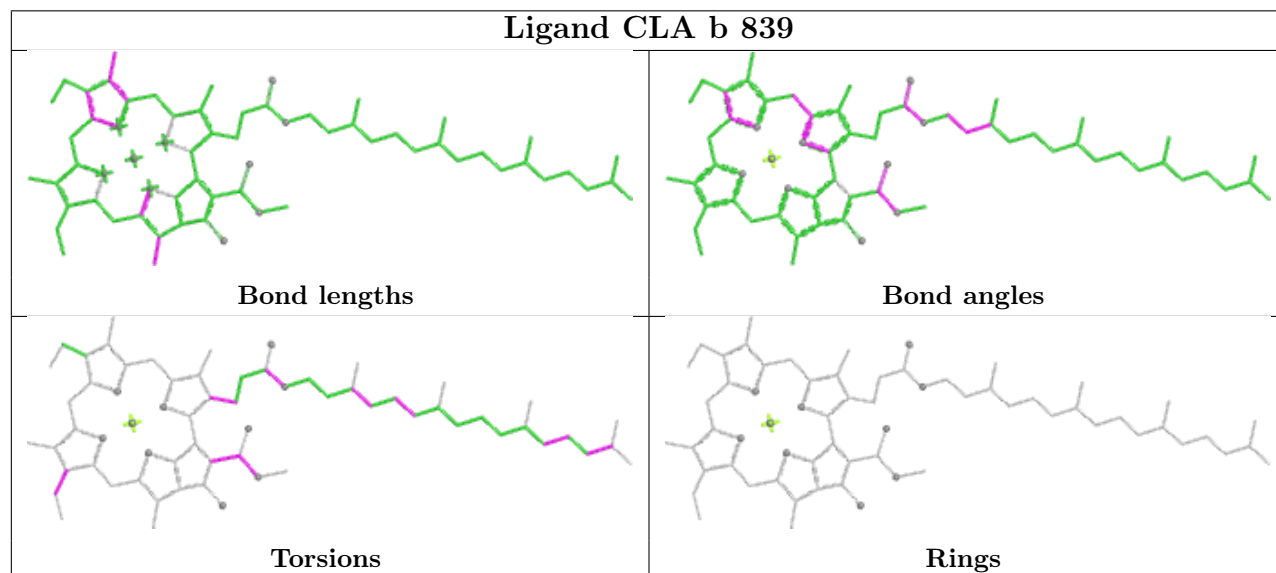
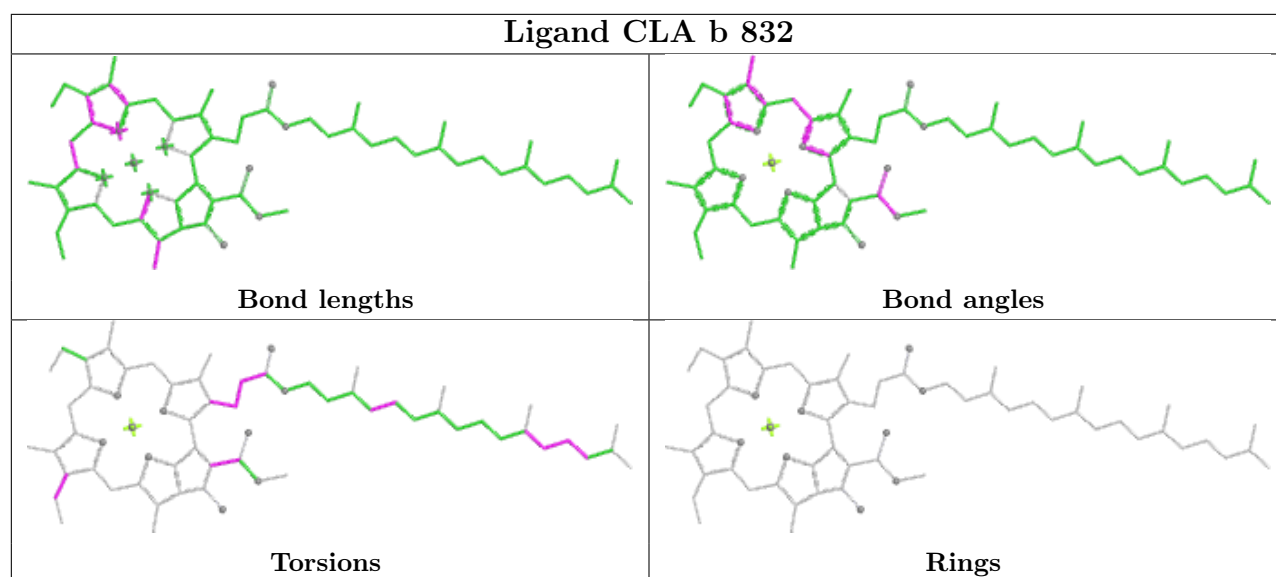


Ligand CLA 1 203

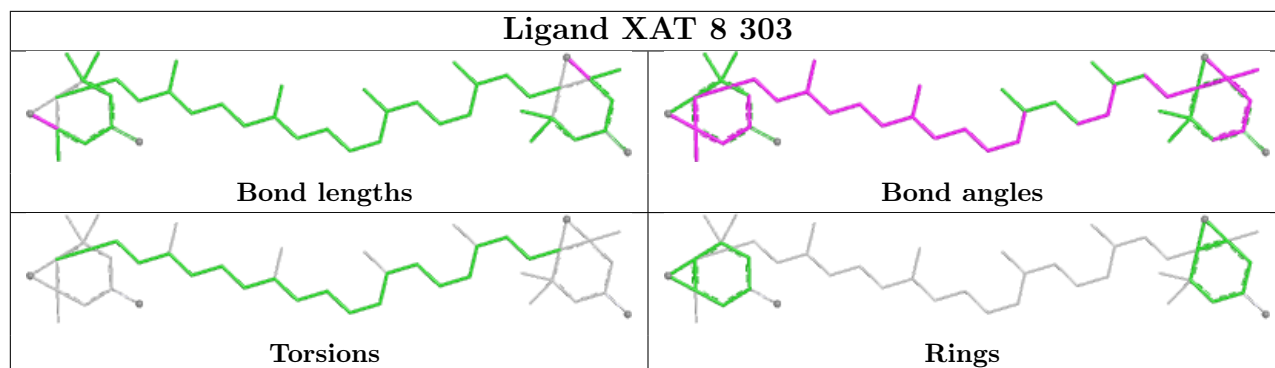


Ligand CLA 4 311

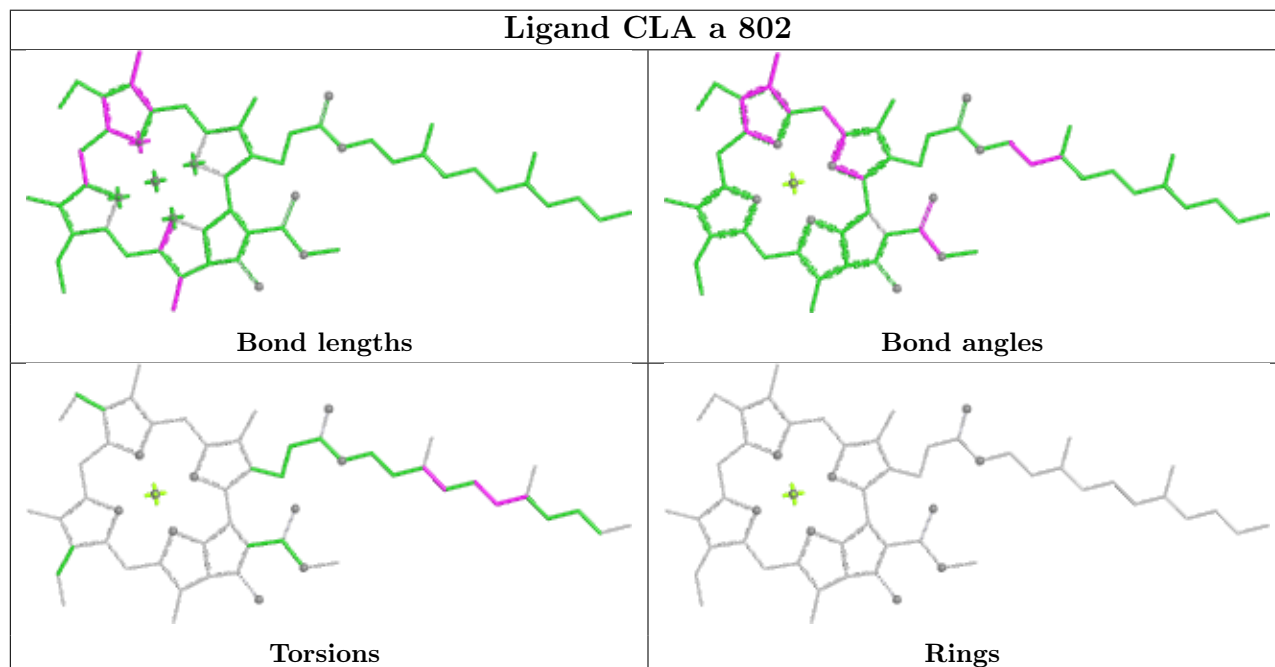




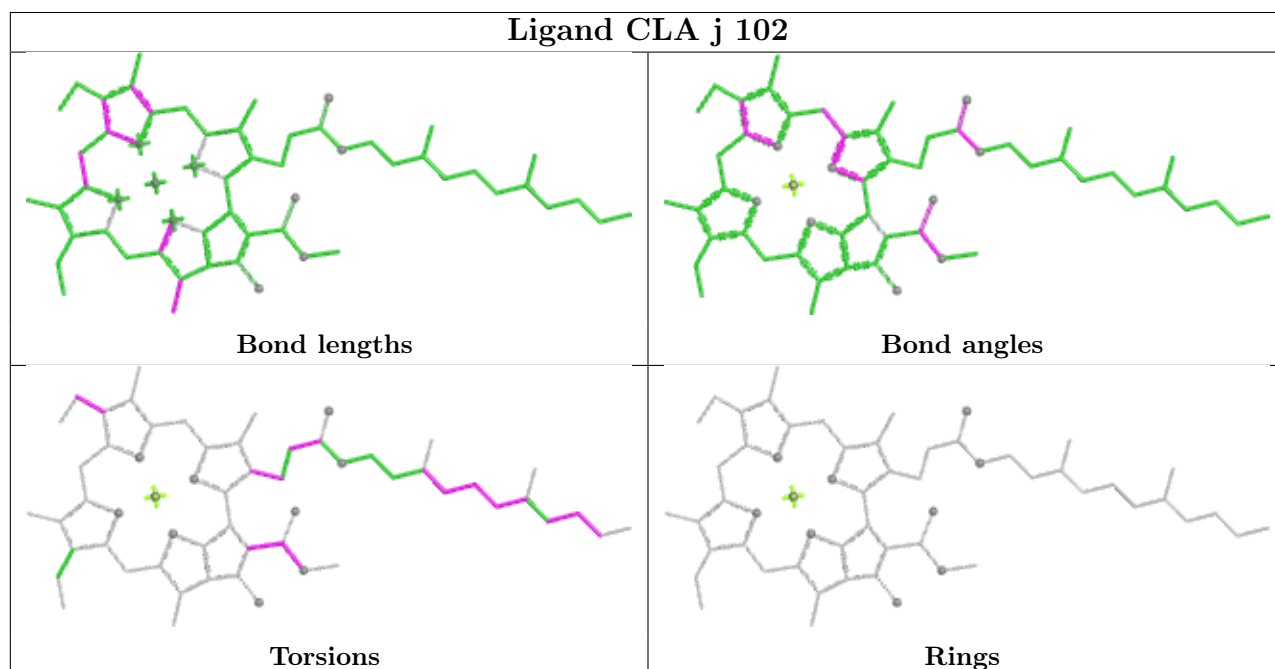
Ligand XAT 8 303



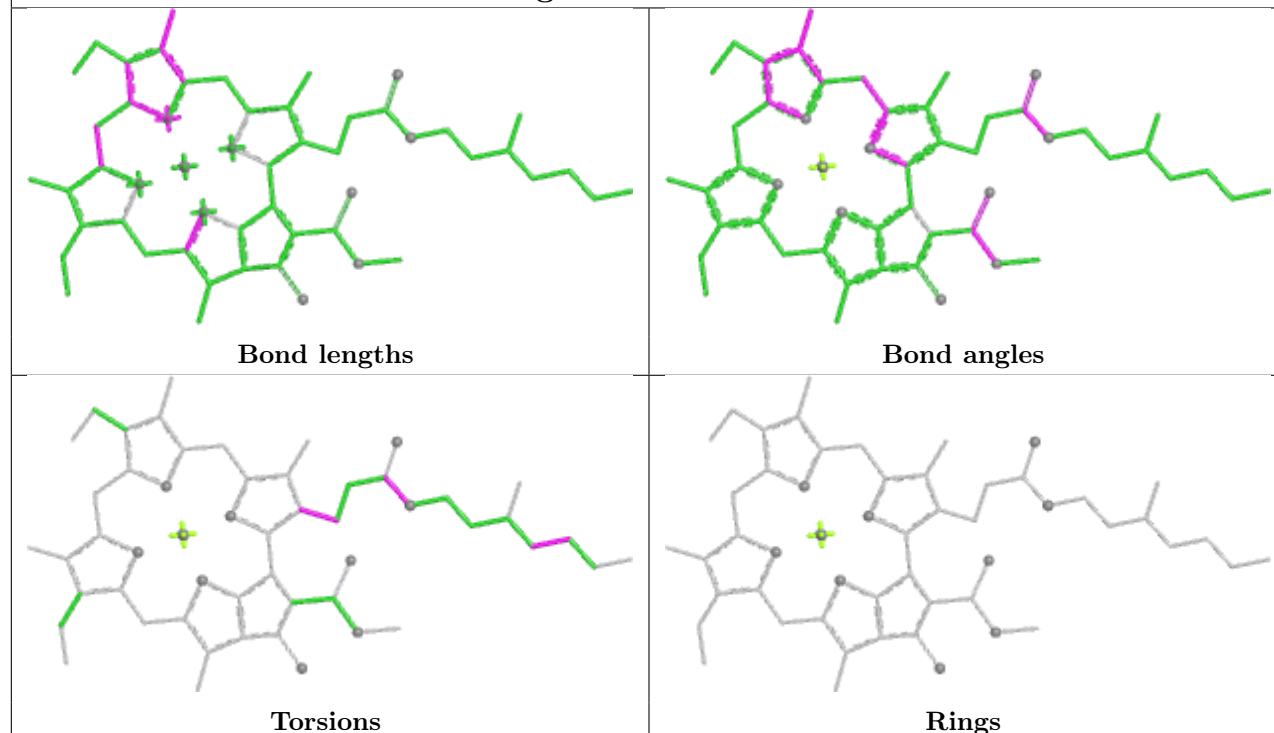
Ligand CLA a 802



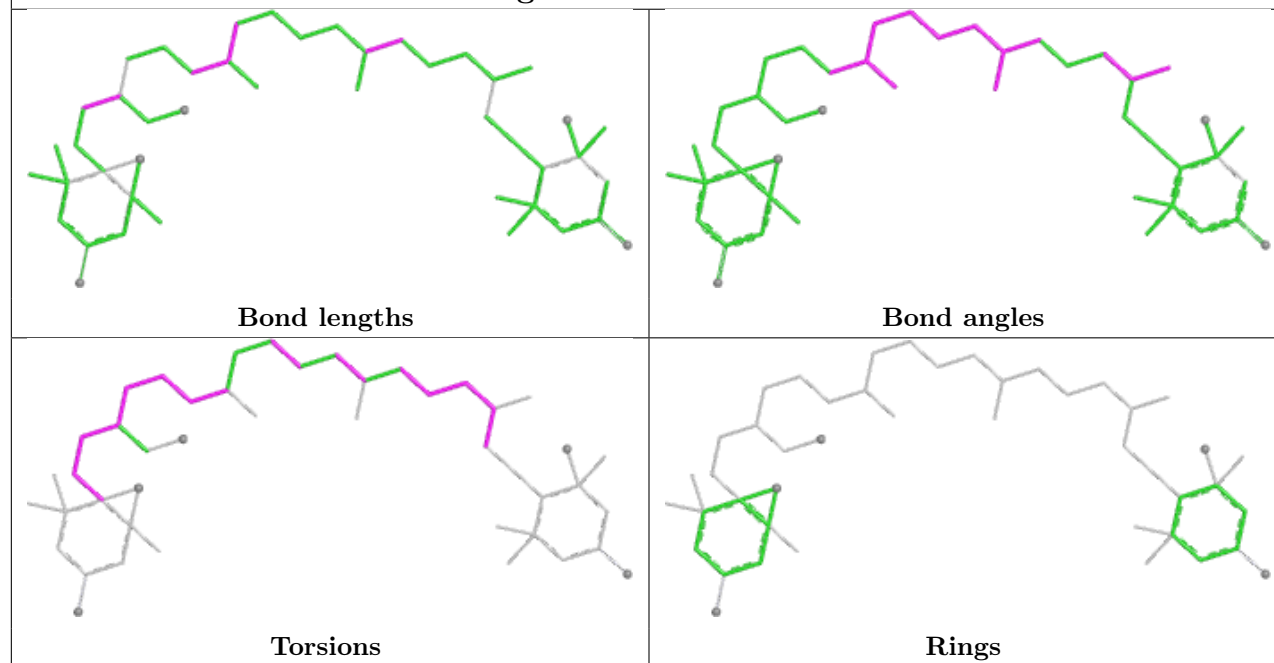
Ligand CLA j 102



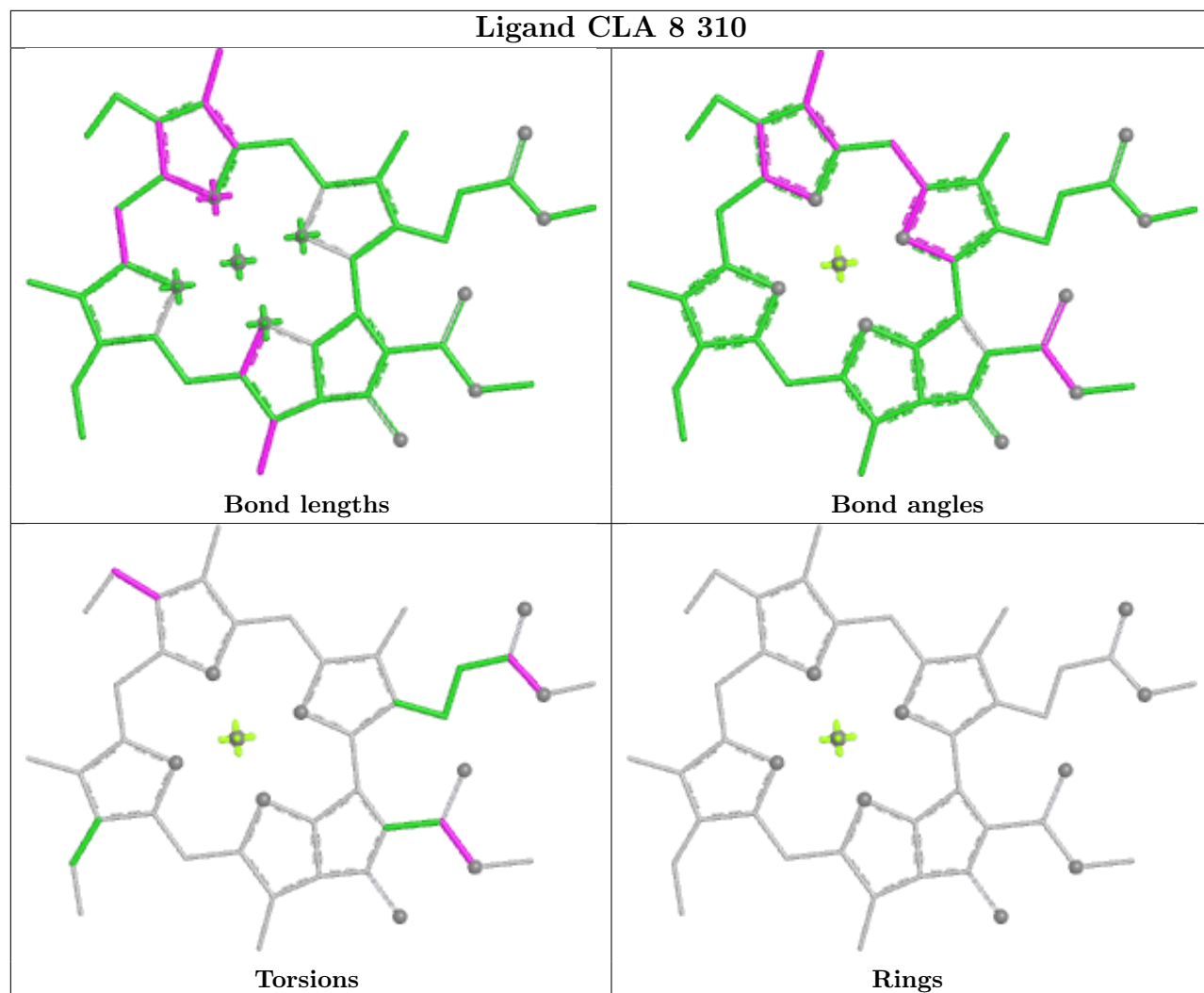
Ligand CLA 4 313



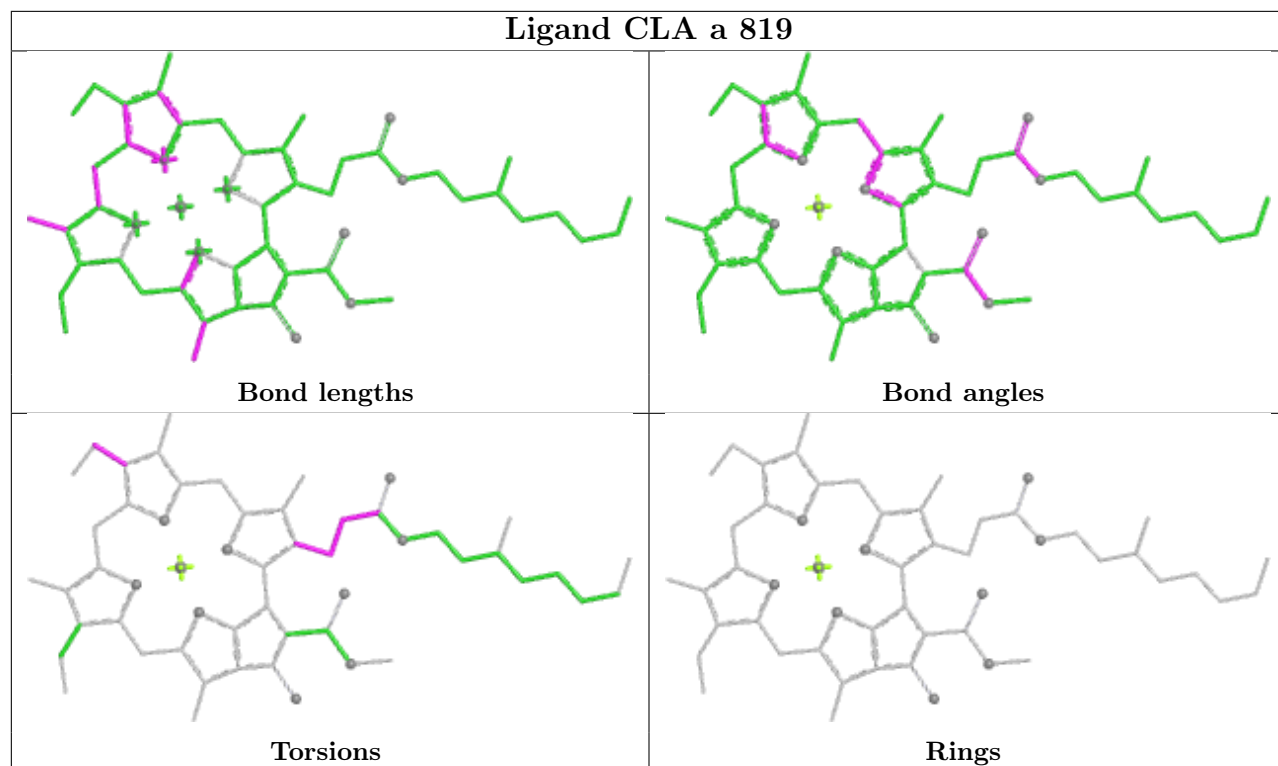
Ligand A1L1G 9 306



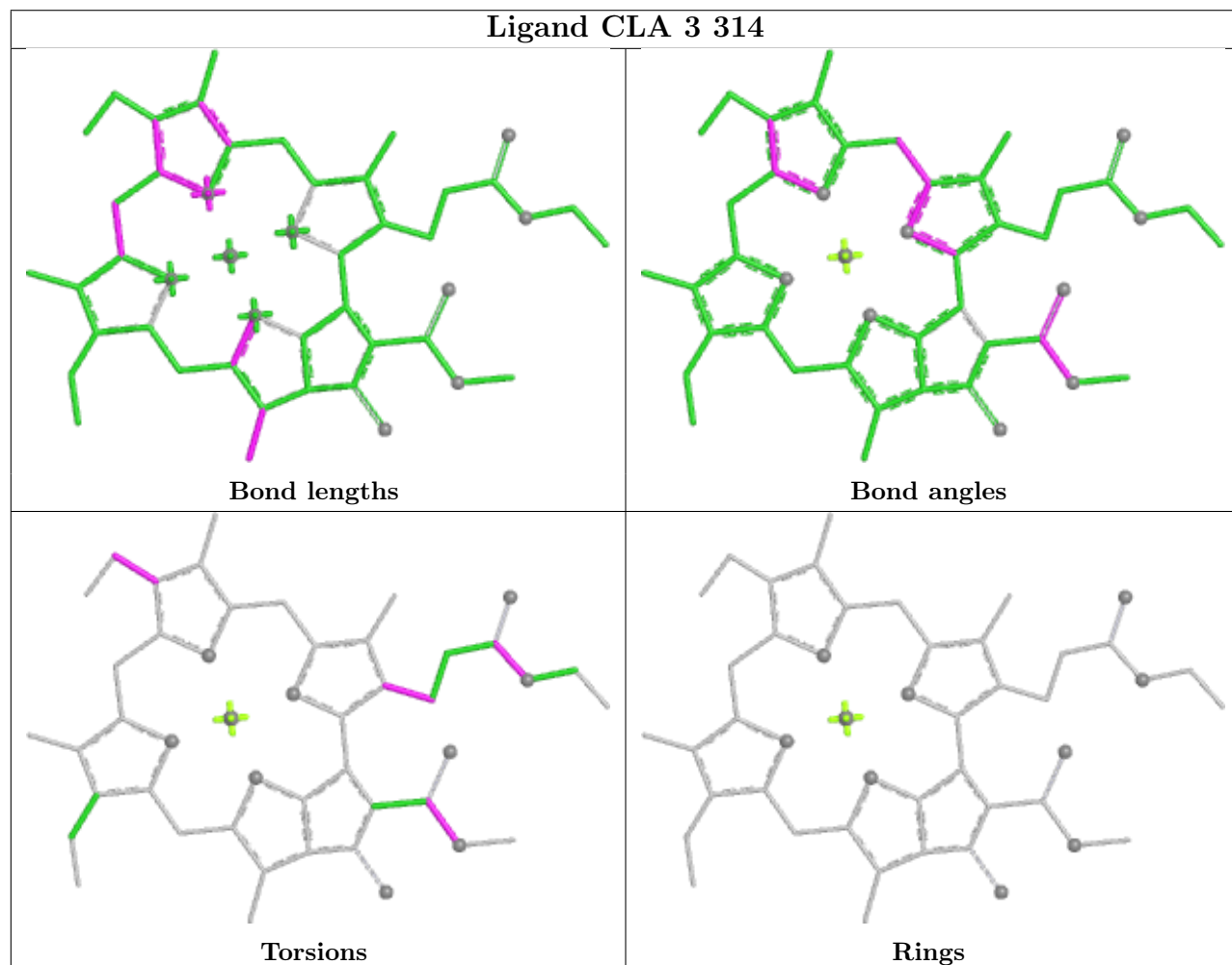
Ligand CLA 8 310



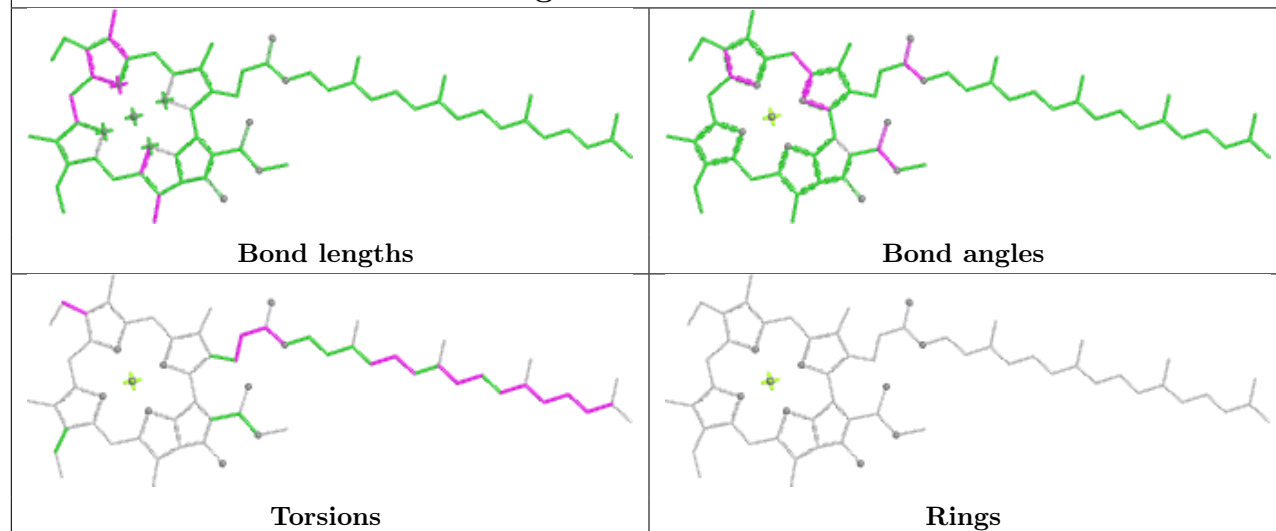
Ligand CLA a 819



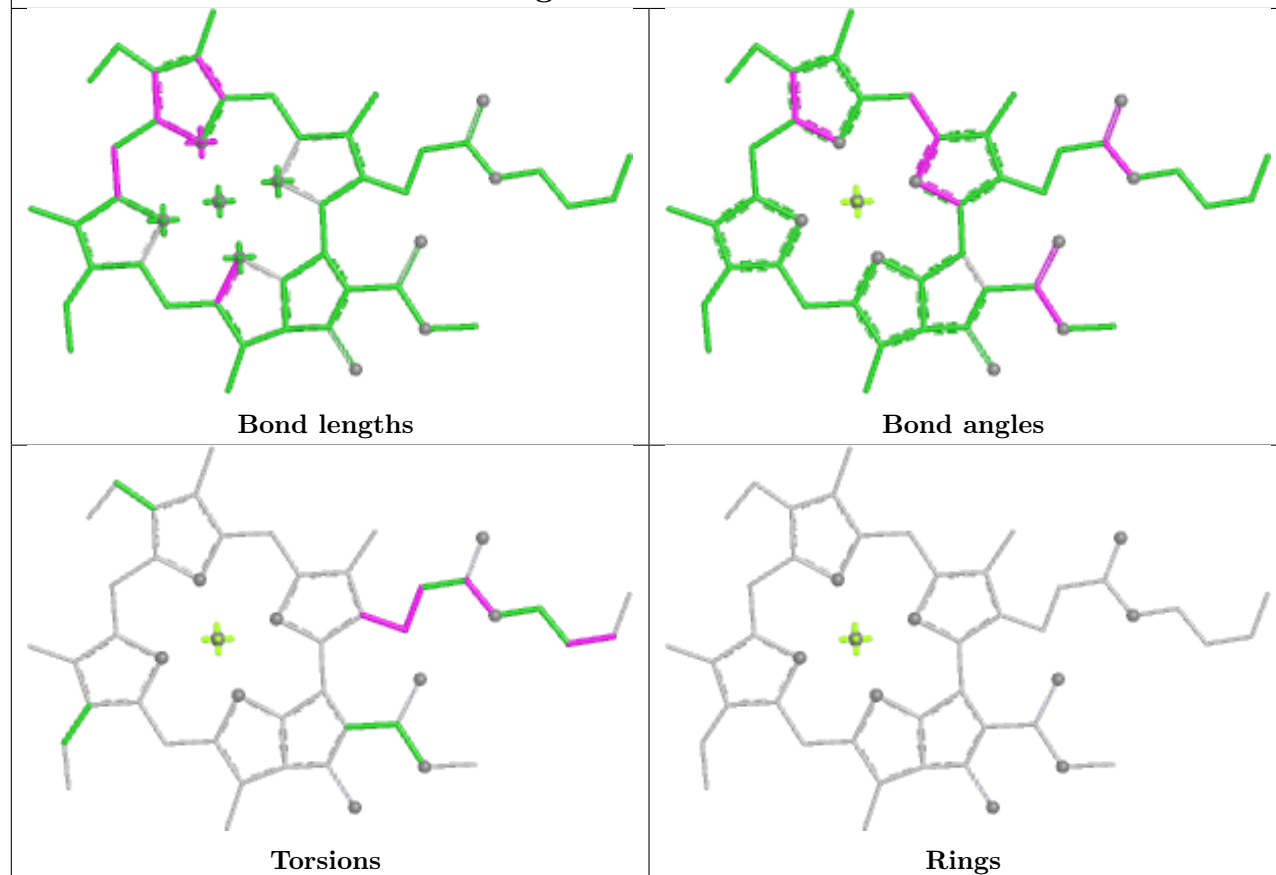
Ligand CLA 3 314



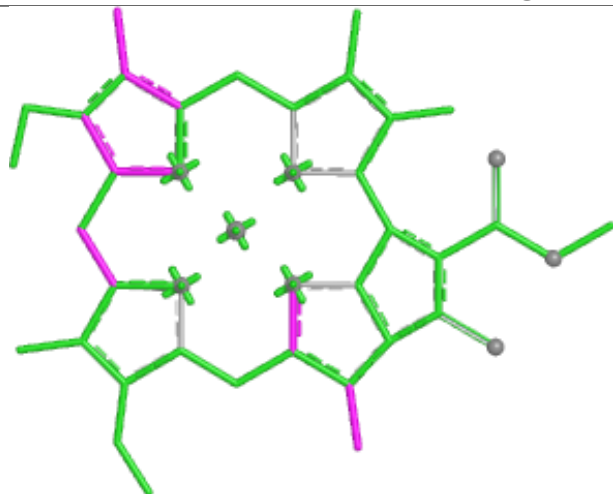
Ligand CLA b 801



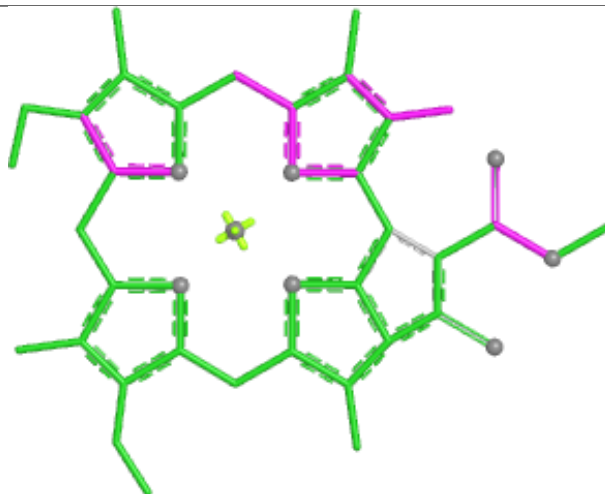
Ligand CLA b 831



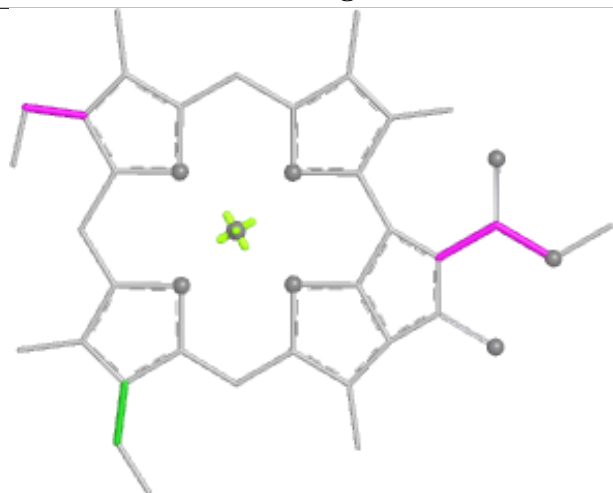
Ligand CLA 8 314



Bond lengths



Bond angles

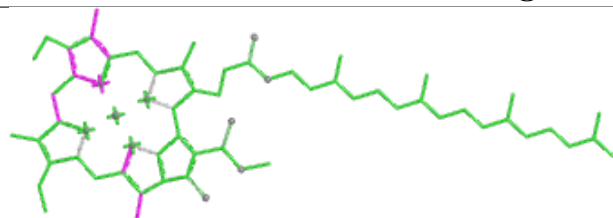


Torsions

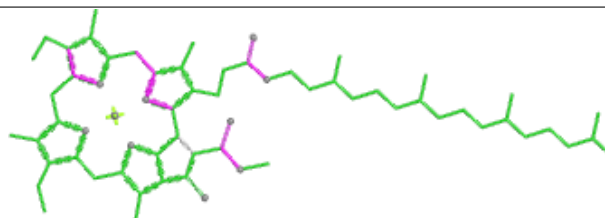


Rings

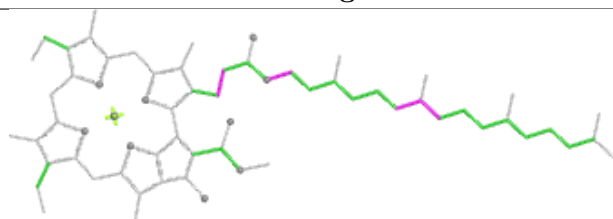
Ligand CLA a 822



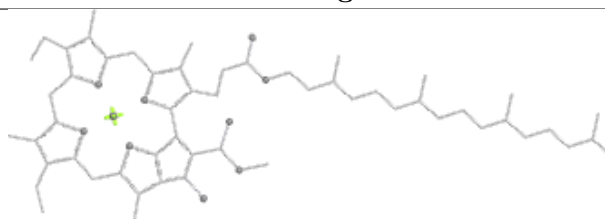
Bond lengths



Bond angles

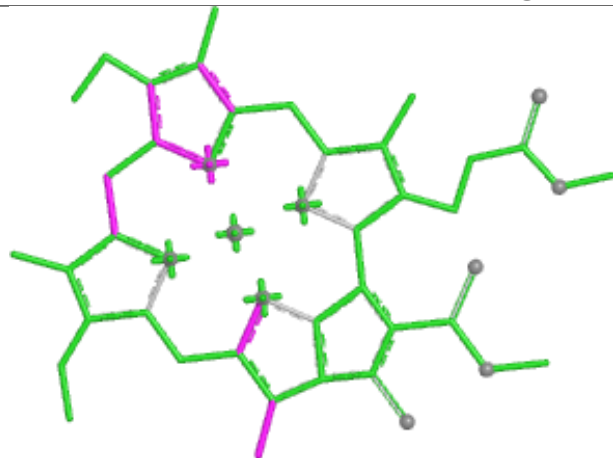


Torsions

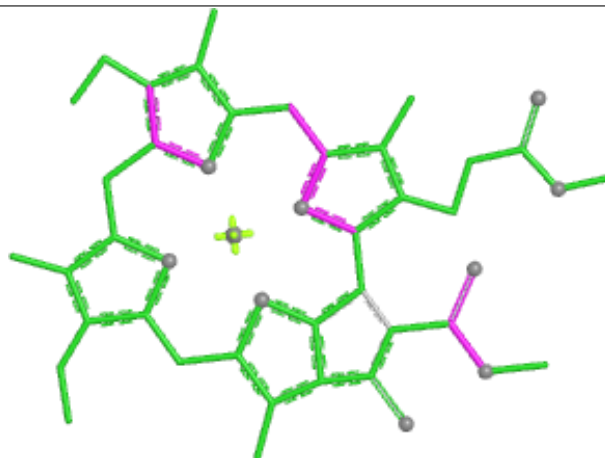


Rings

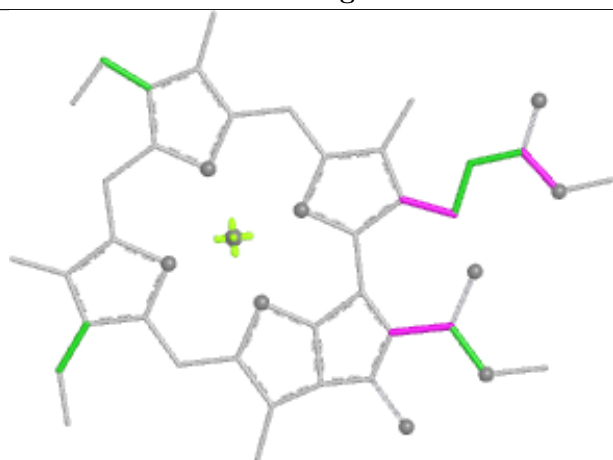
Ligand CLA 9 310



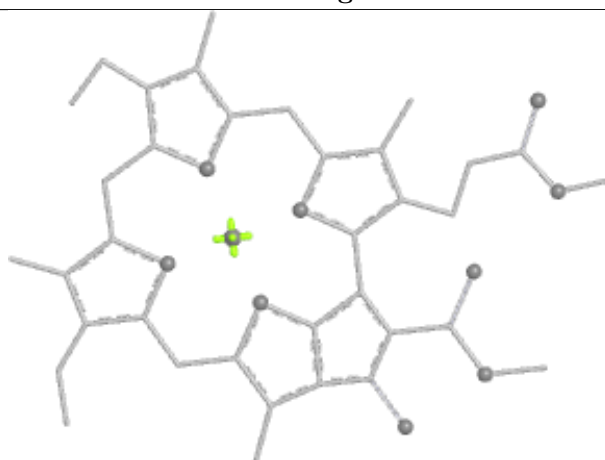
Bond lengths



Bond angles

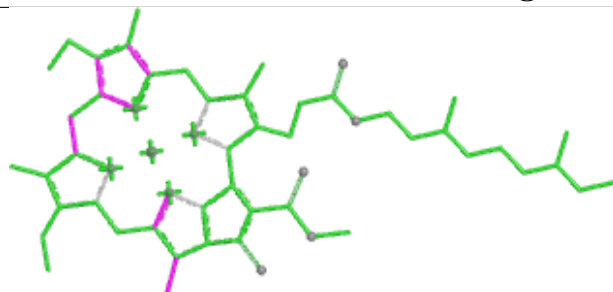


Torsions

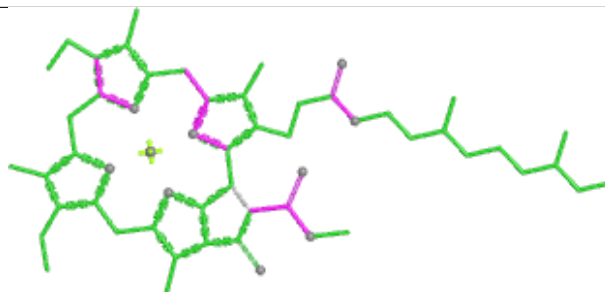


Rings

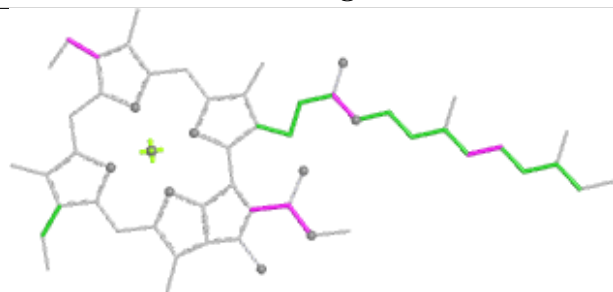
Ligand CLA 4 307



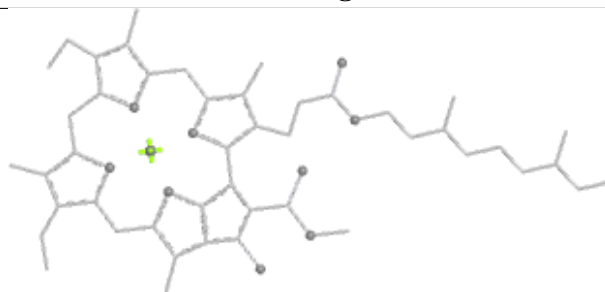
Bond lengths



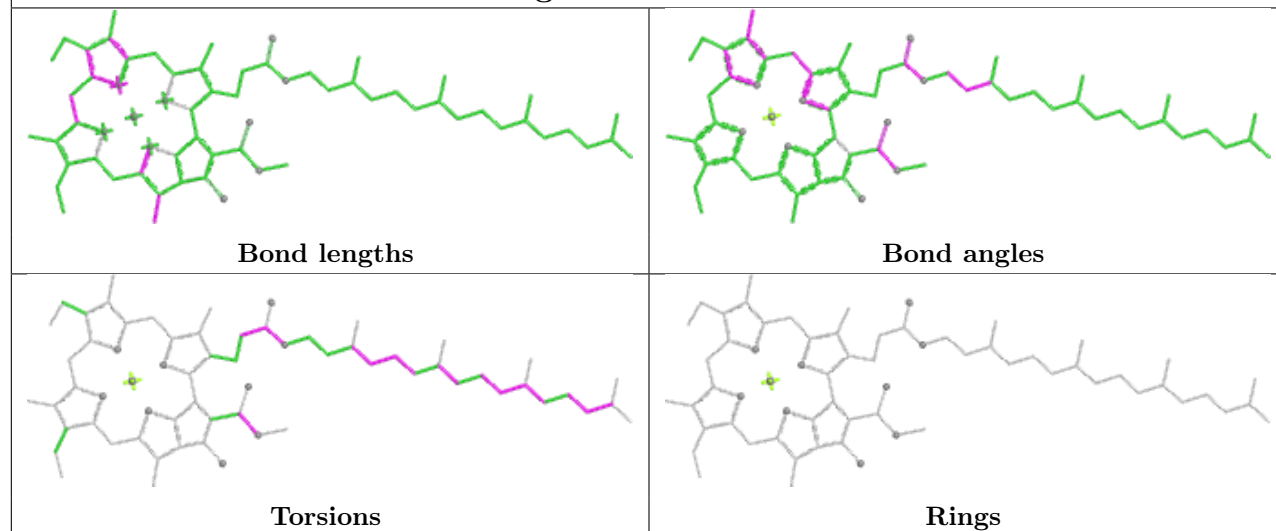
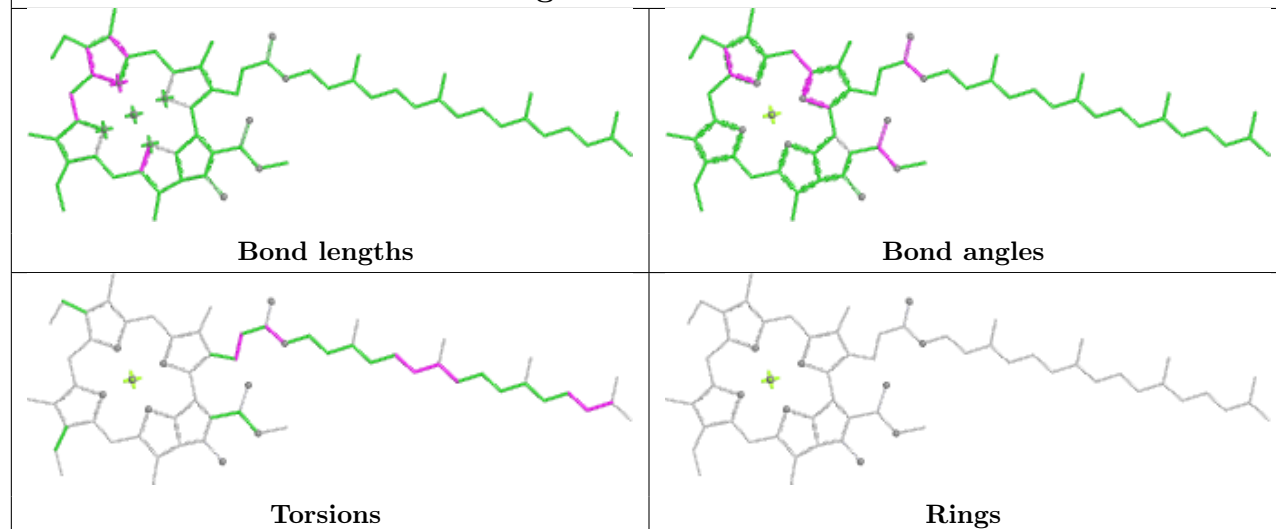
Bond angles



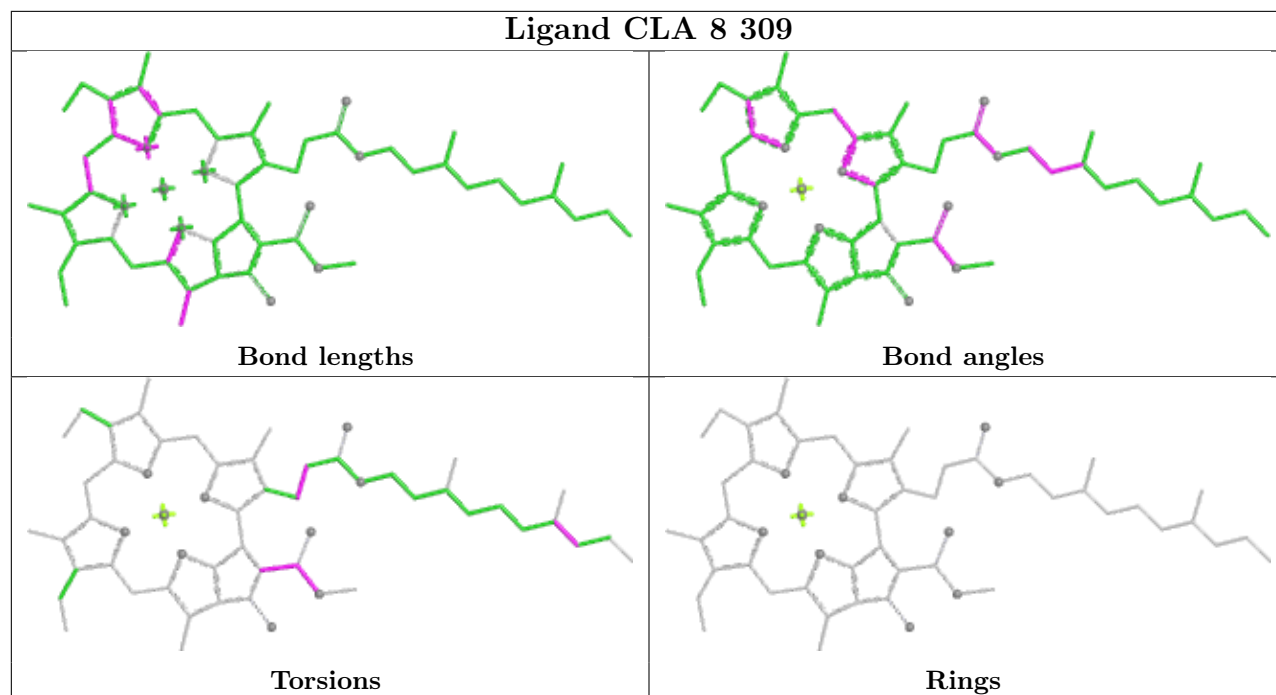
Torsions



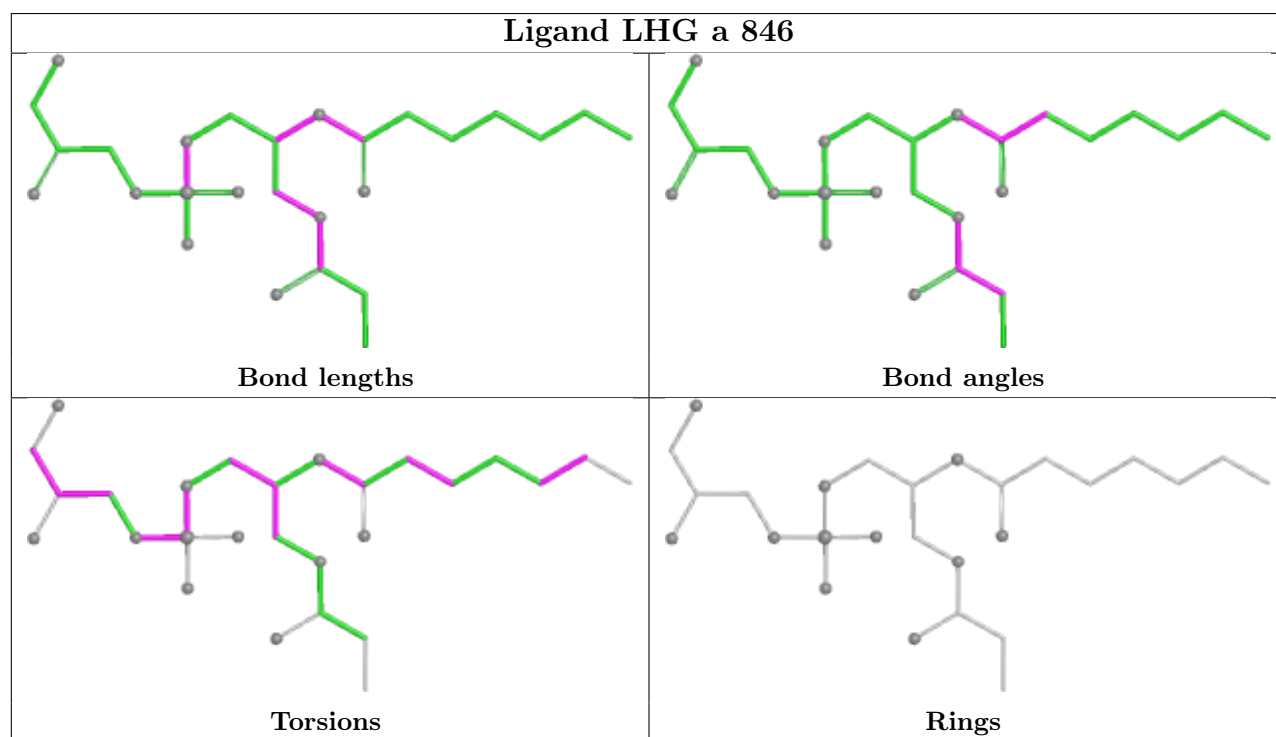
Rings

Ligand CLA b 807**Ligand CLA 8 307**

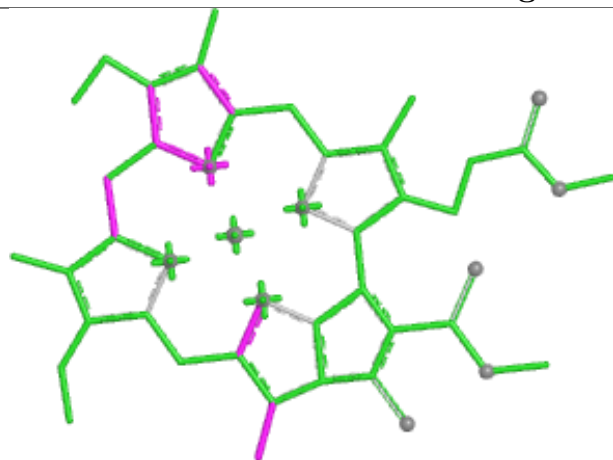
Ligand CLA 8 309



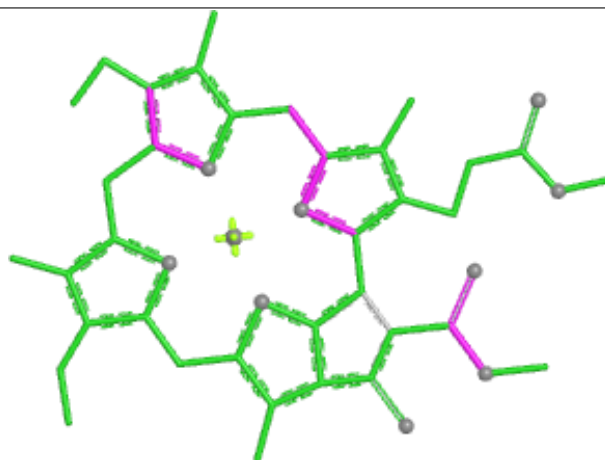
Ligand LHG a 846



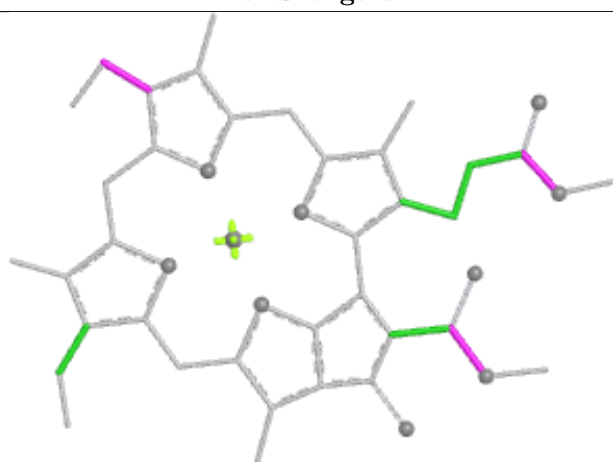
Ligand CLA 5 305



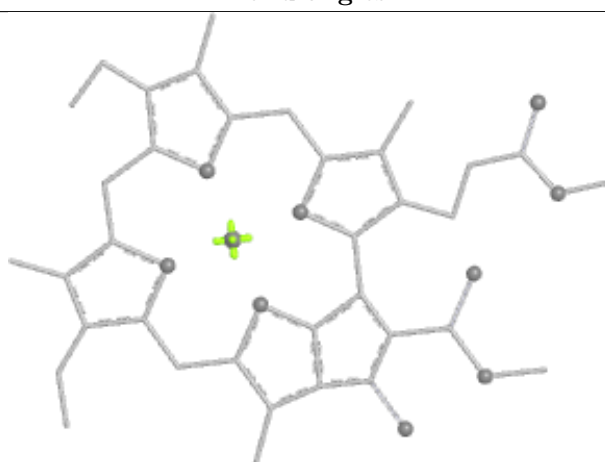
Bond lengths



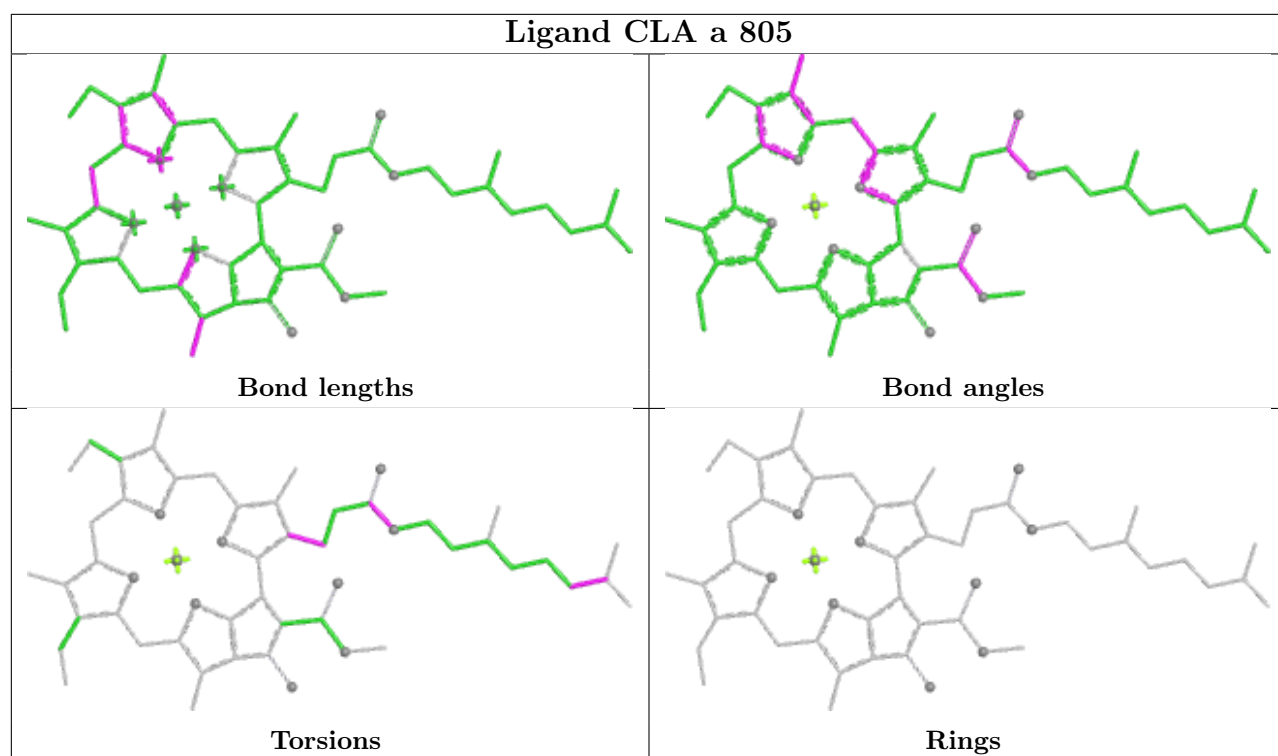
Bond angles



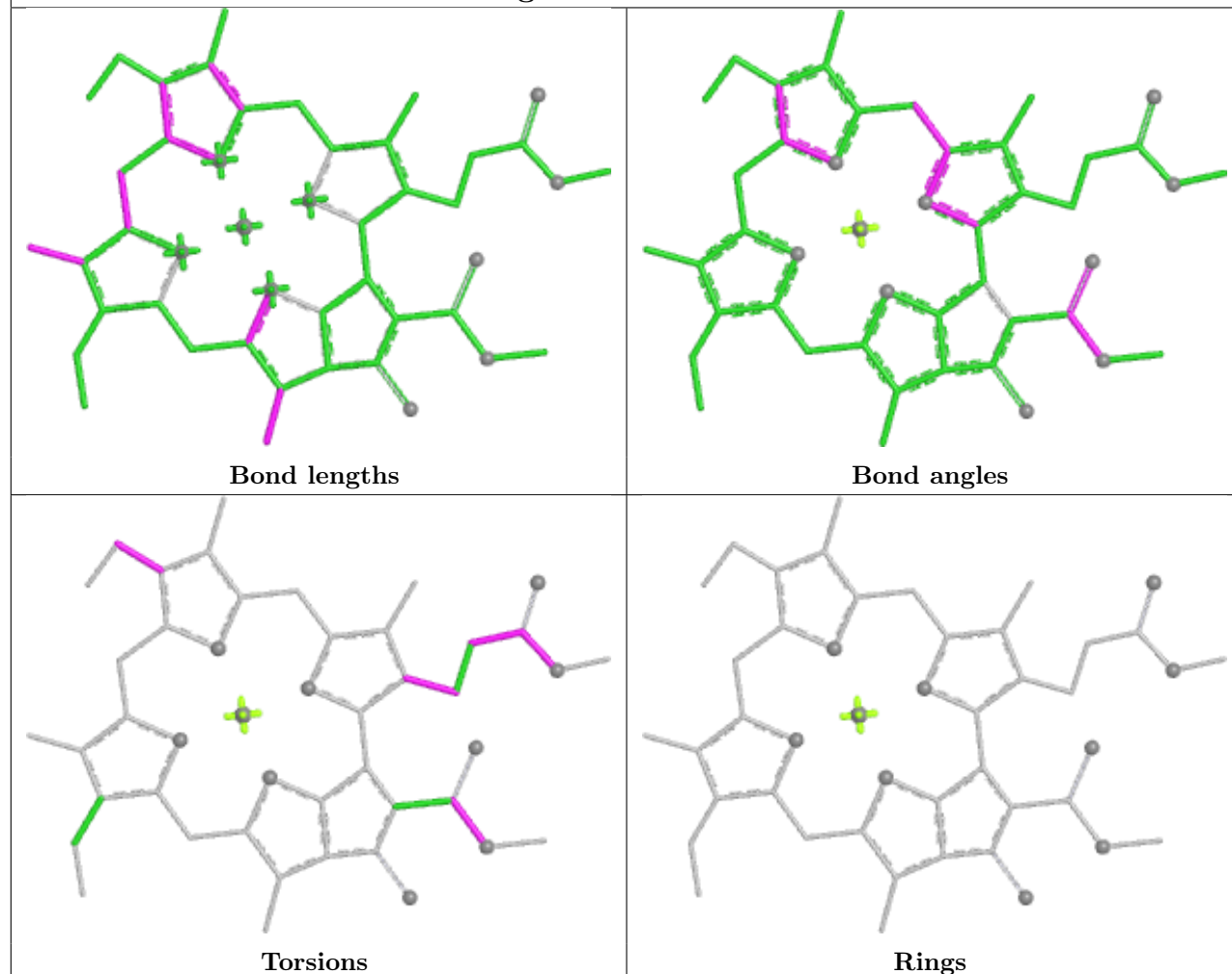
Torsions



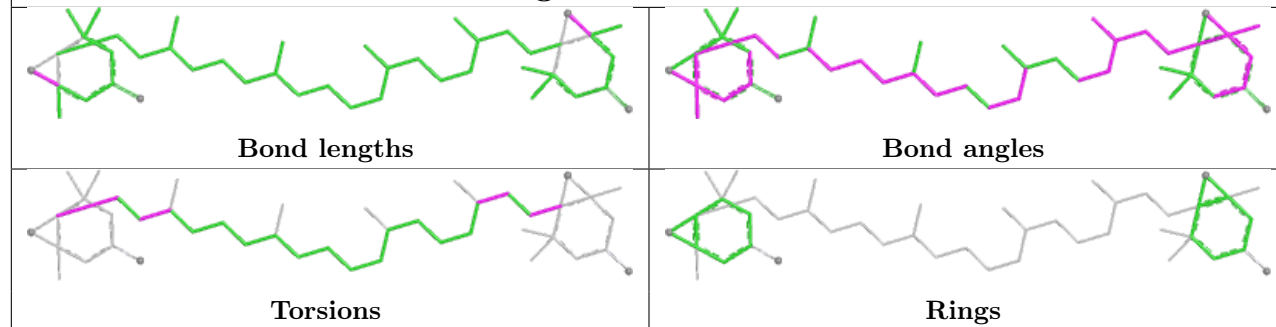
Rings

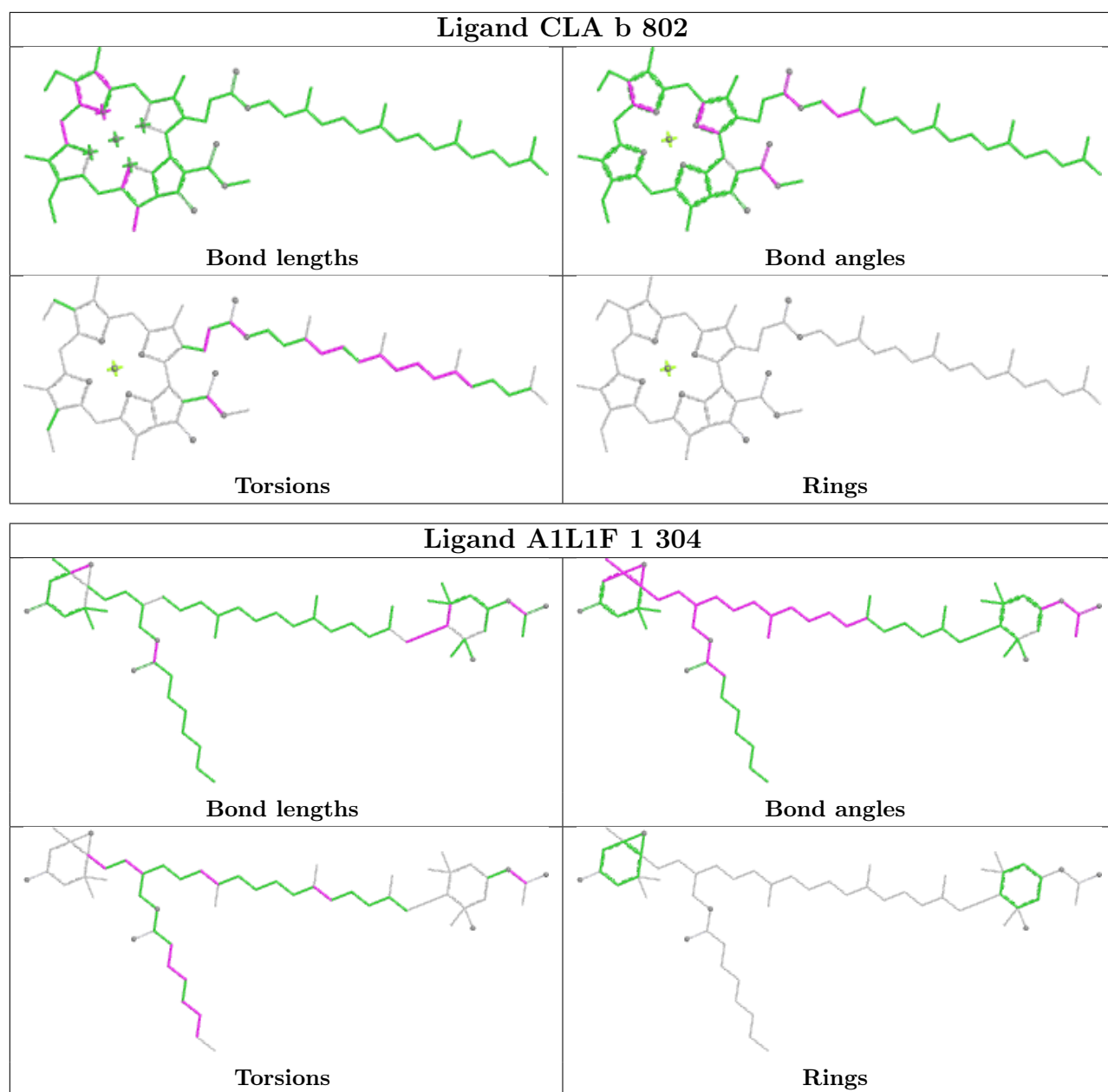


Ligand CLA 3 315

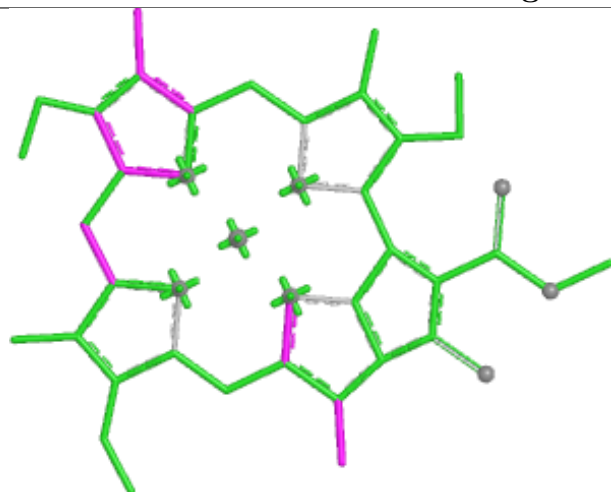


Ligand XAT 2 303

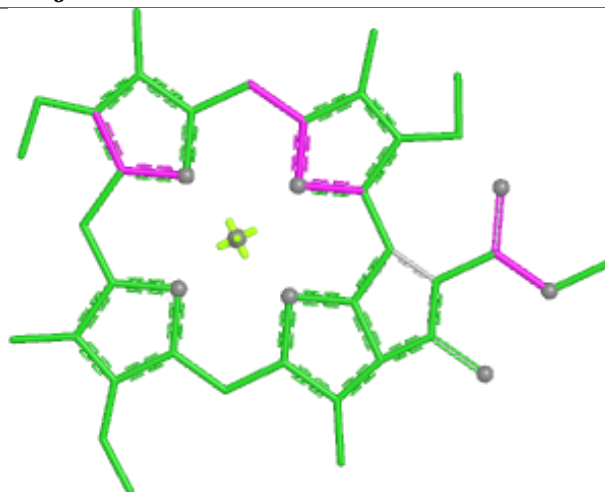




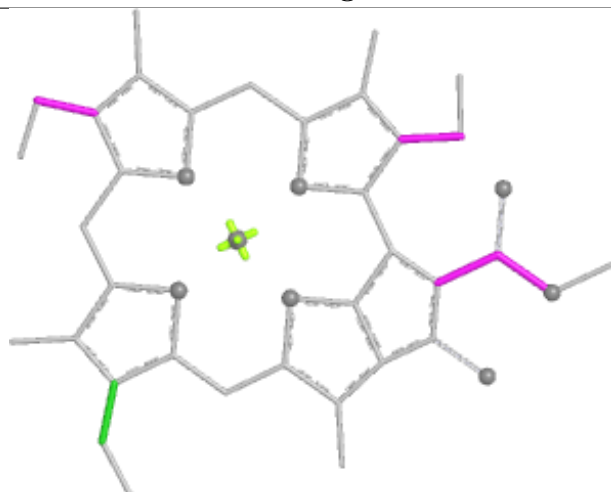
Ligand CLA j 103



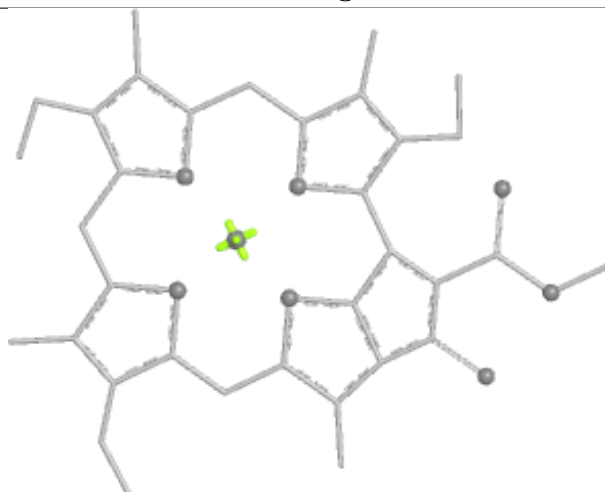
Bond lengths



Bond angles

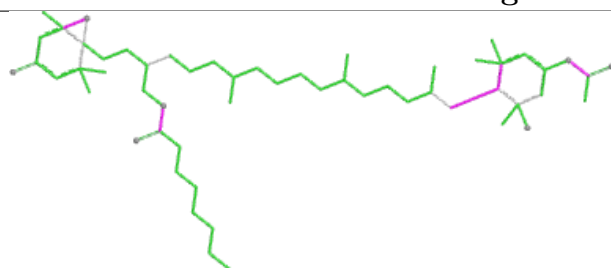


Torsions

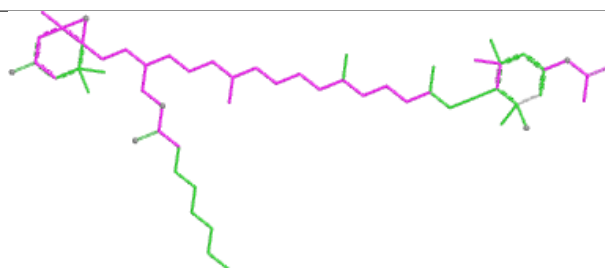


Rings

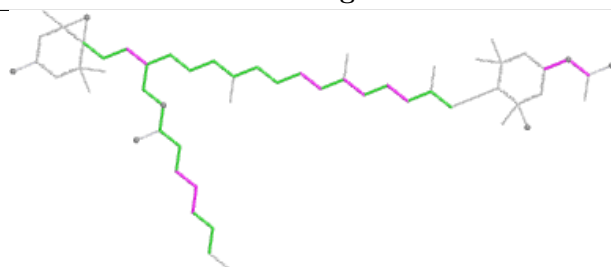
Ligand A1L1F h 204



Bond lengths



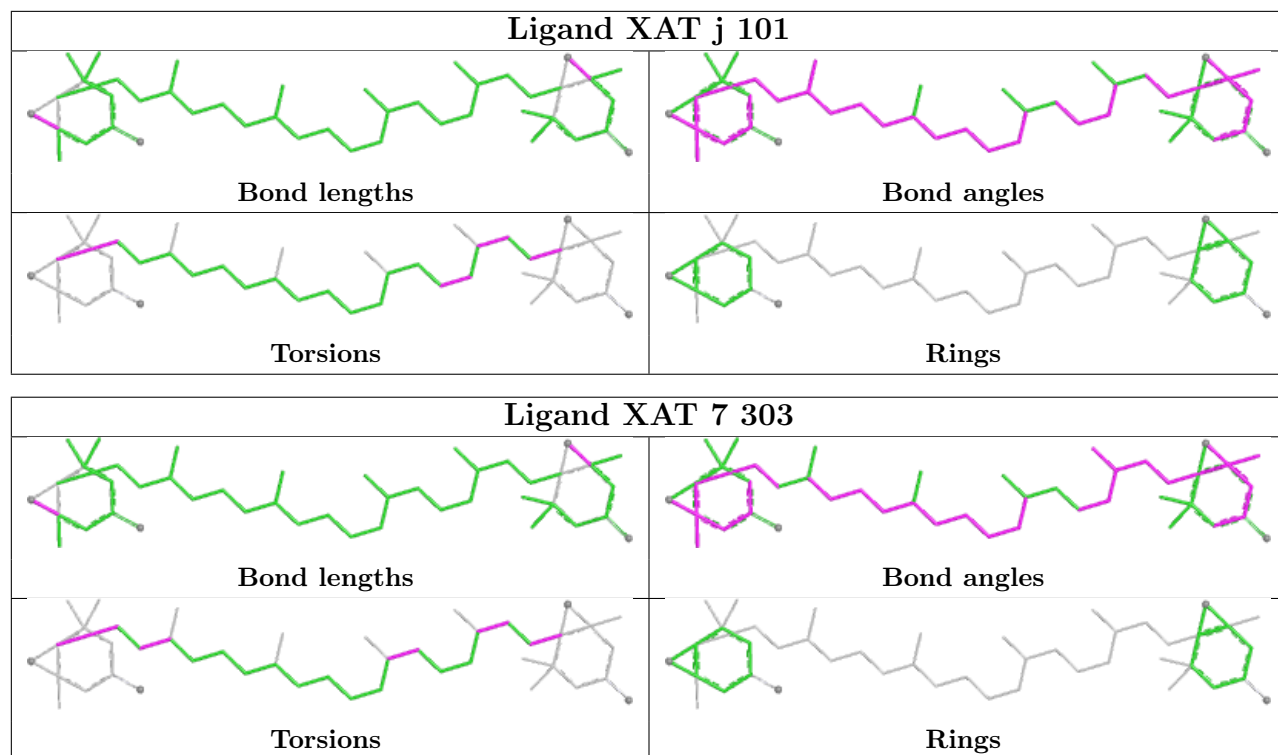
Bond angles



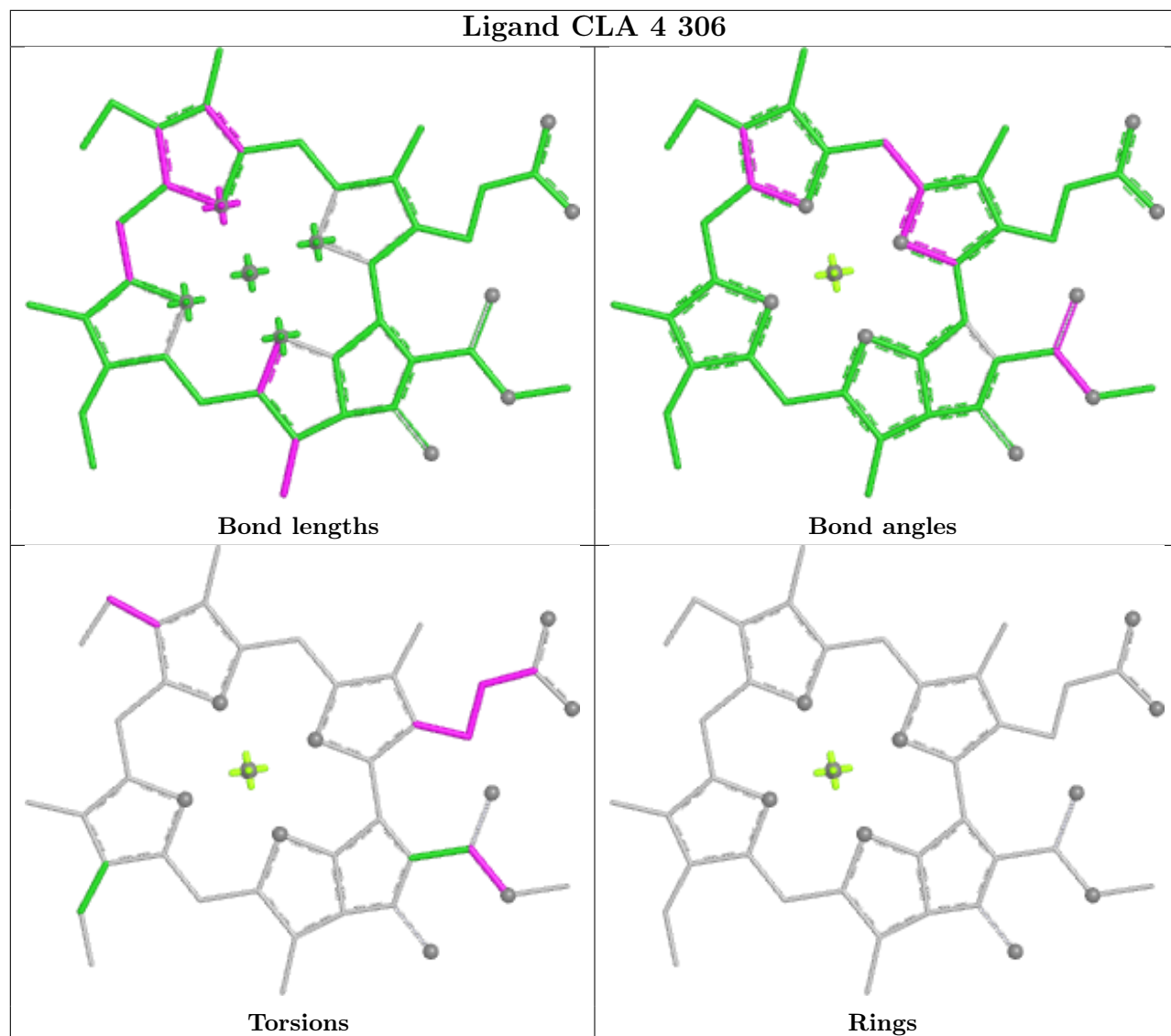
Torsions



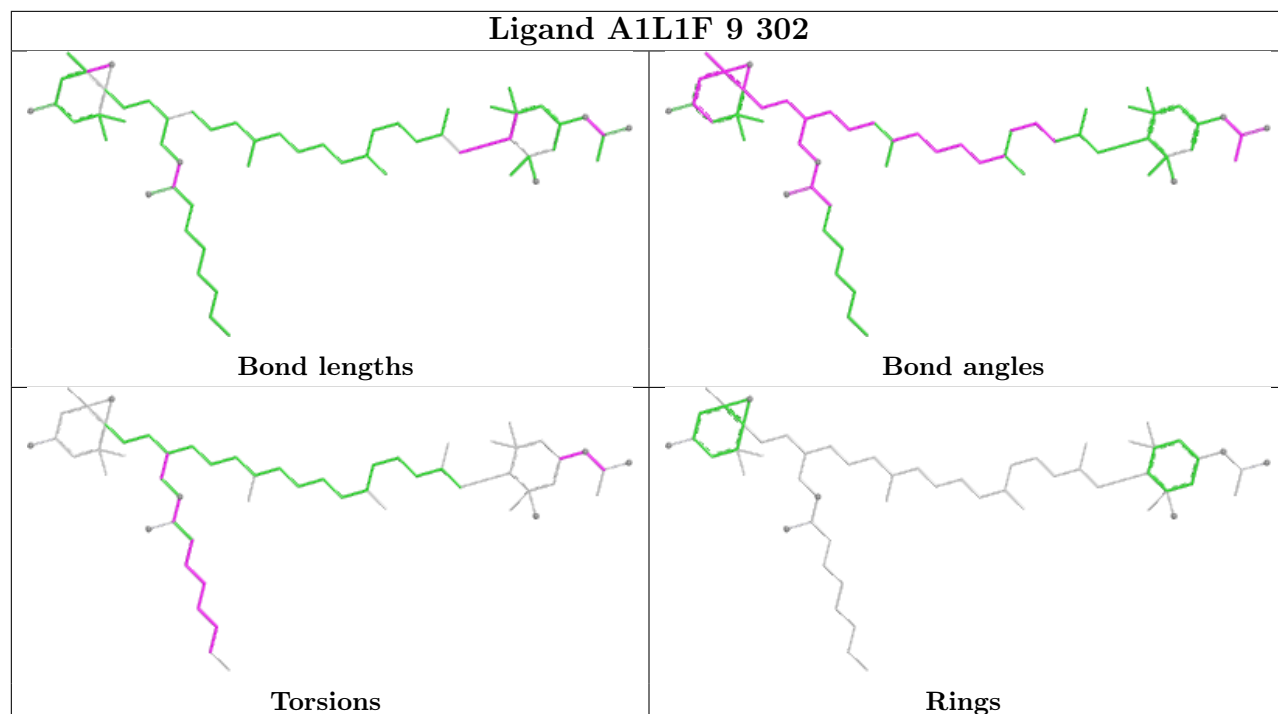
Rings



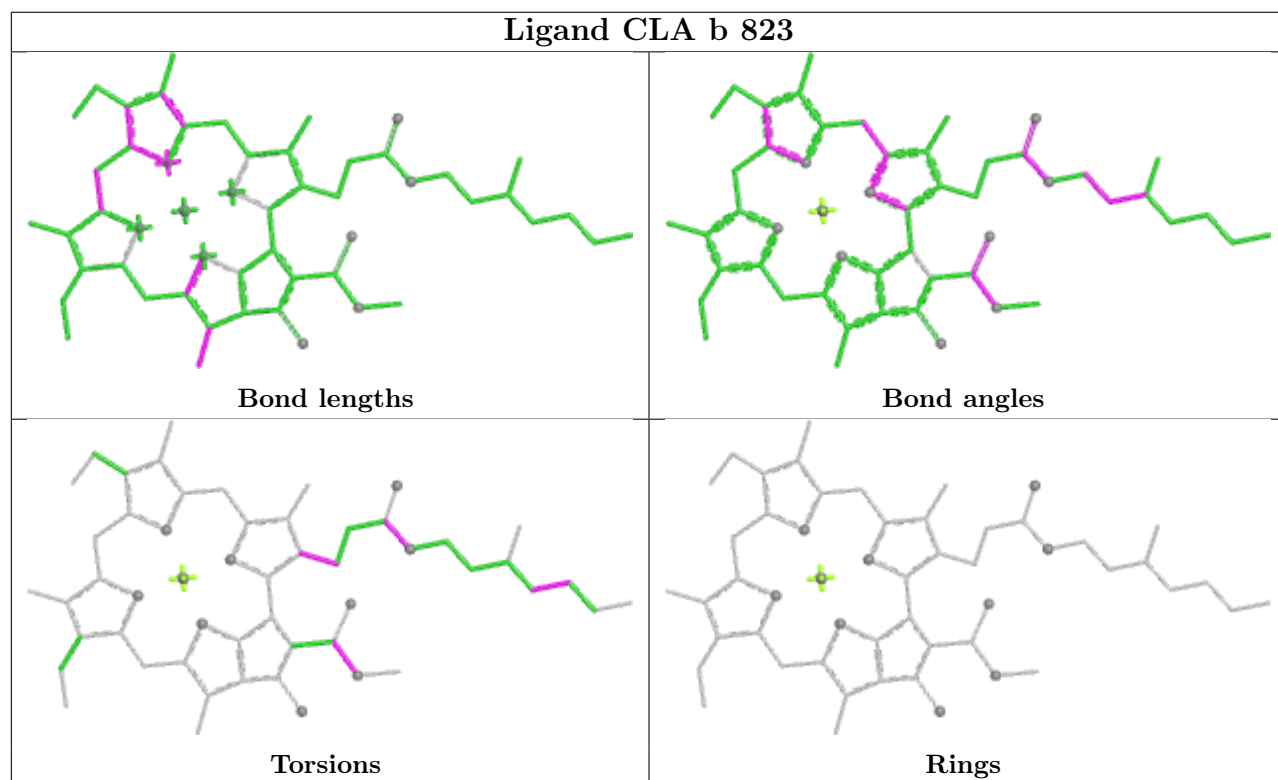
Ligand CLA 4 306



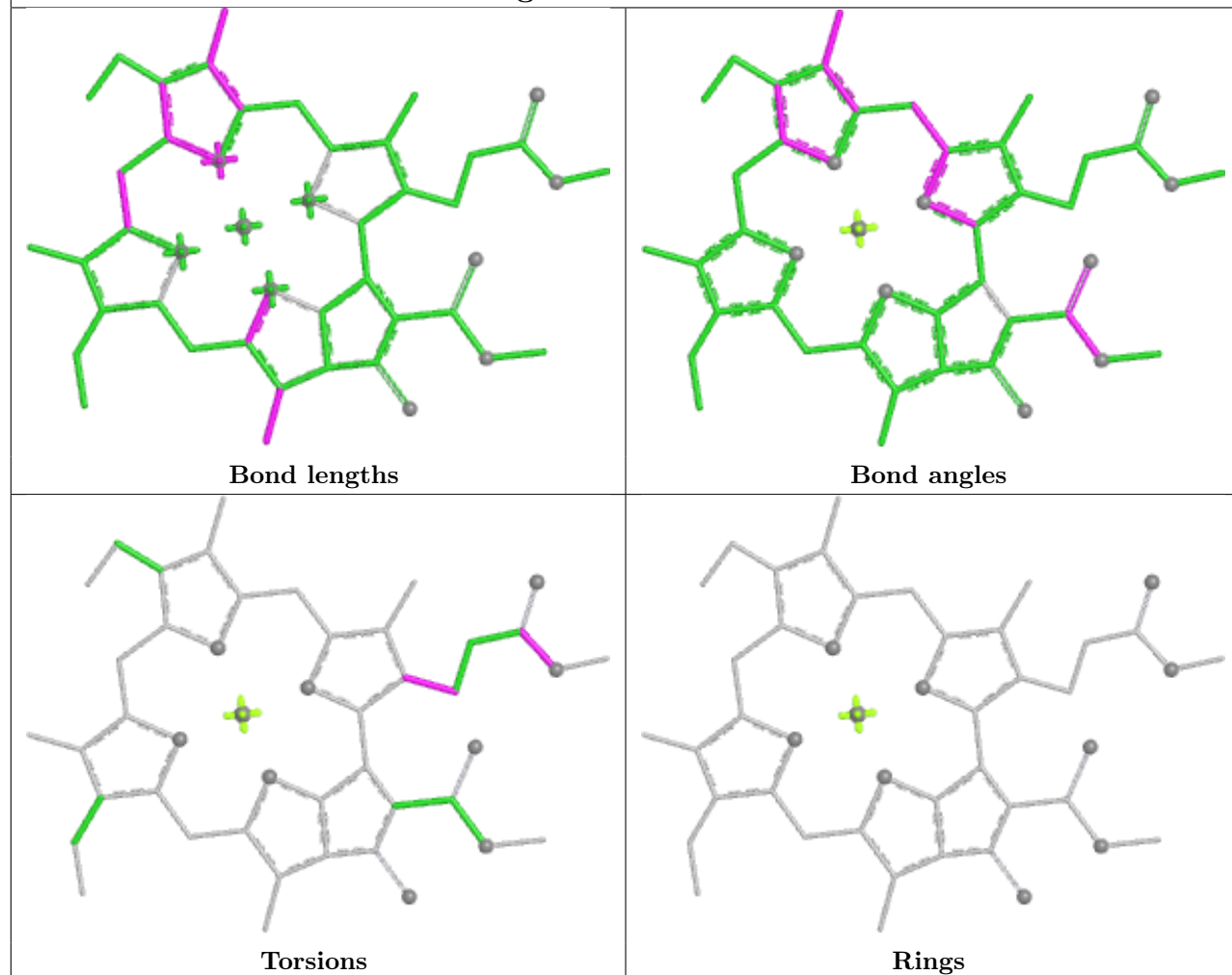
Ligand A1L1F 9 302



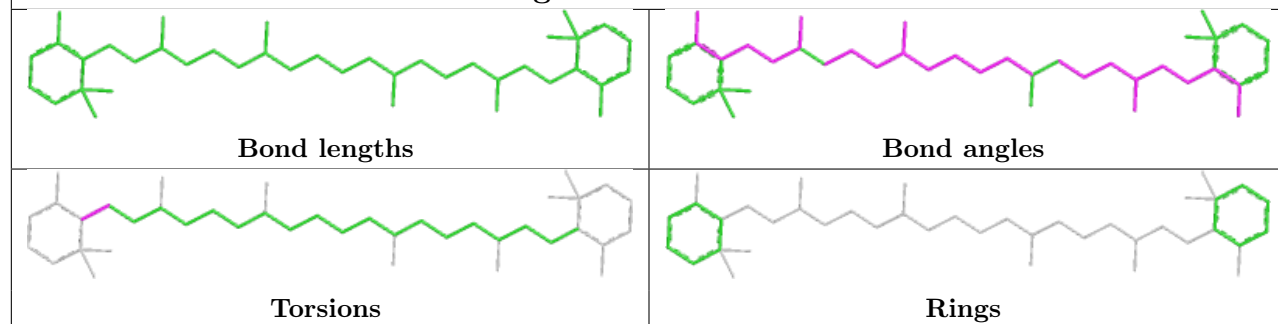
Ligand CLA b 823



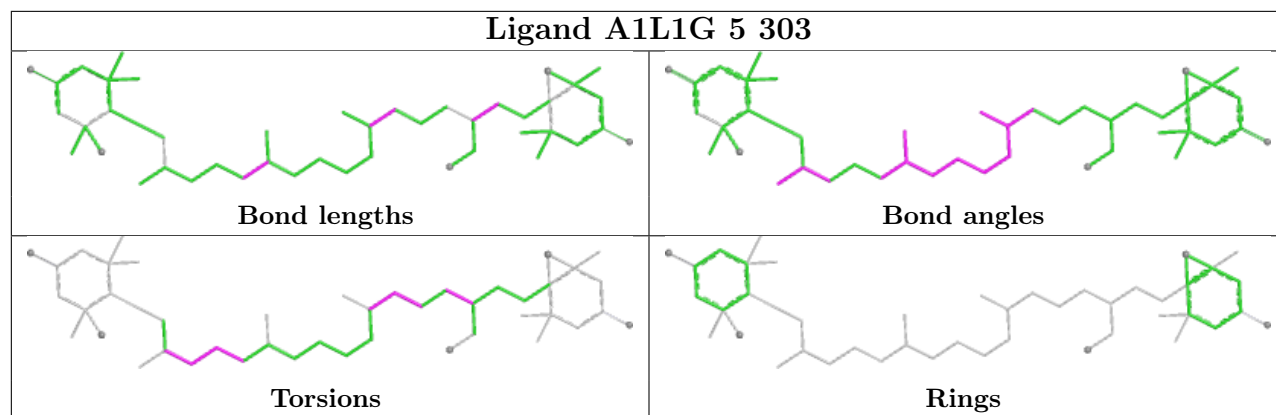
Ligand CLA 7 311



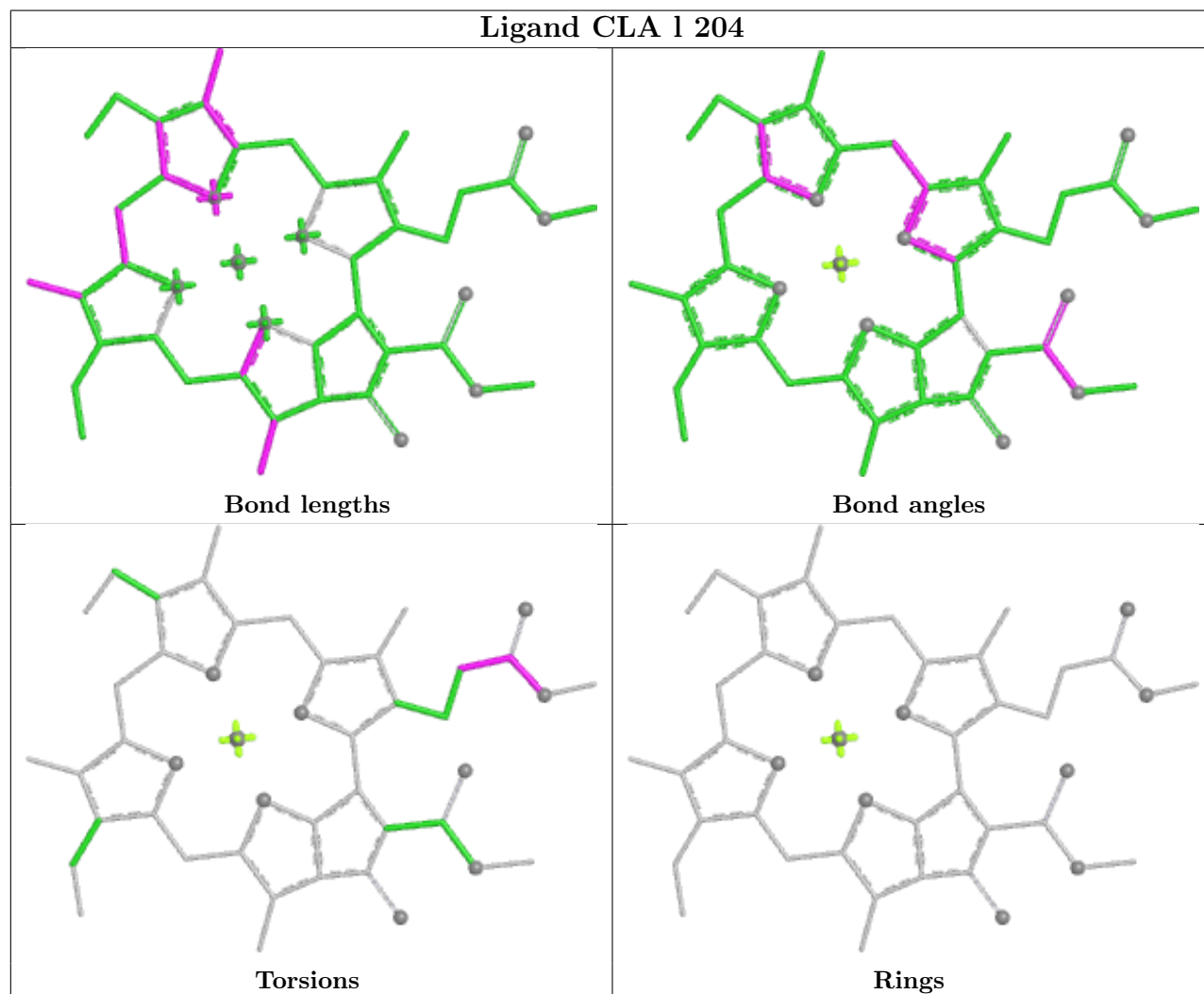
Ligand BCR b 846



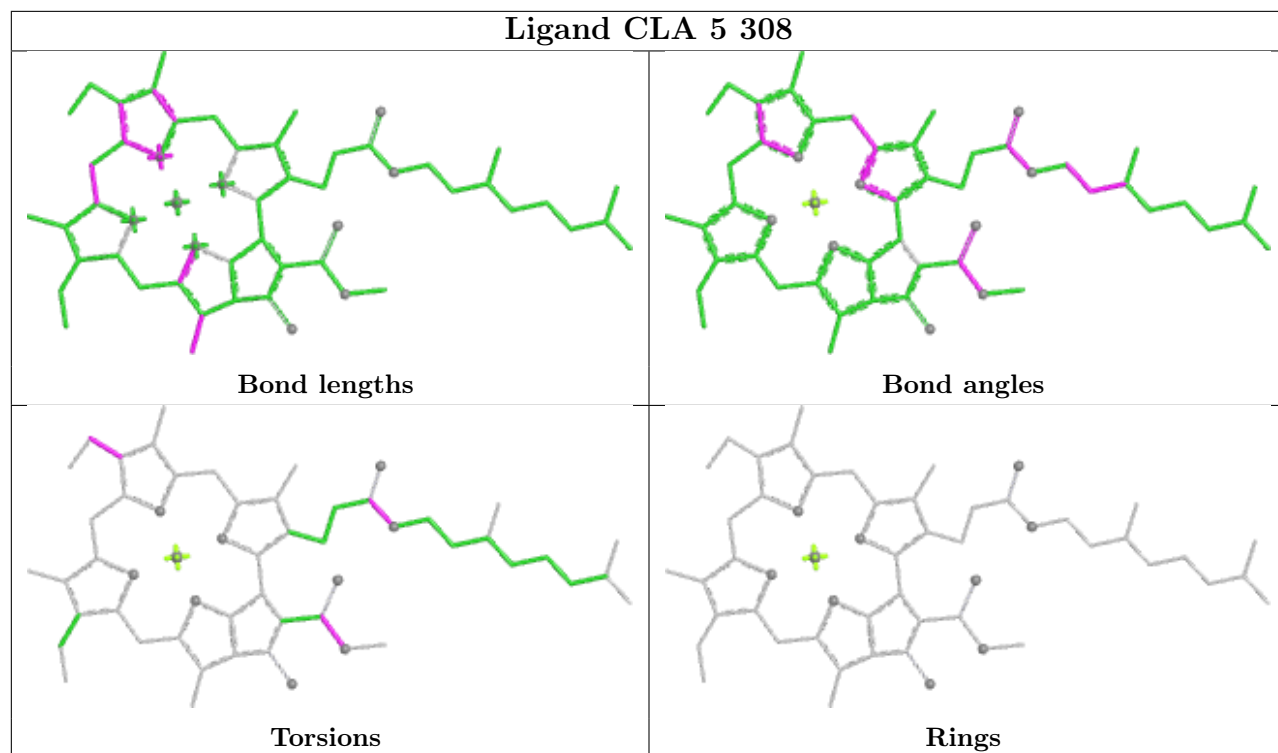
Ligand A1L1G 5 303



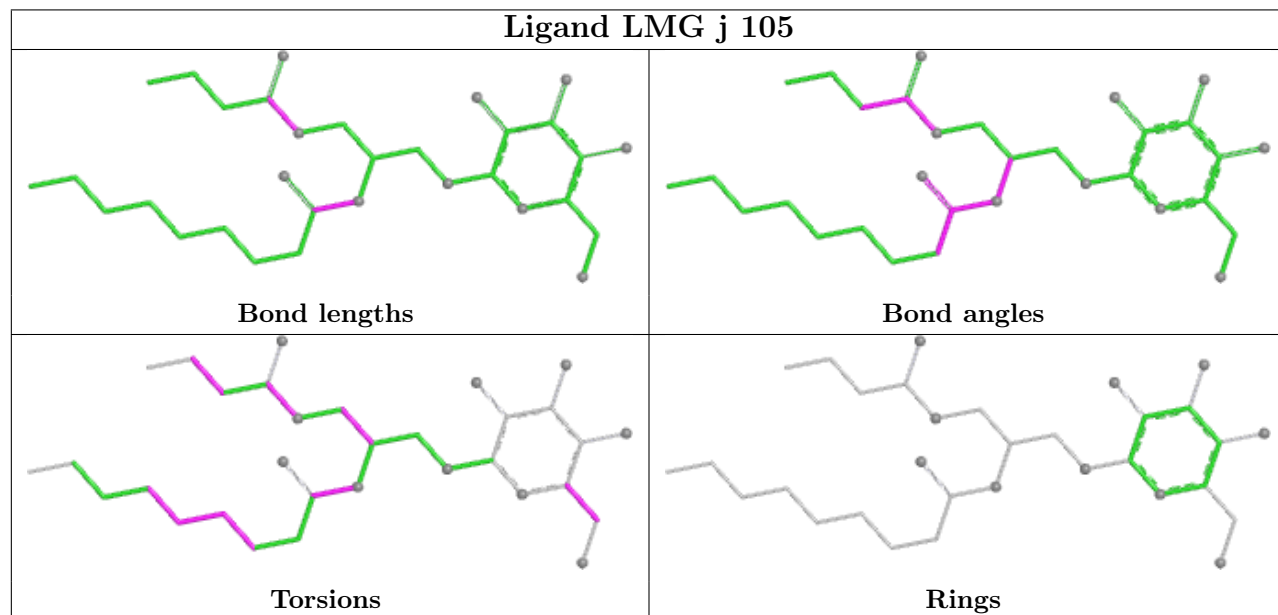
Ligand CLA 1 204



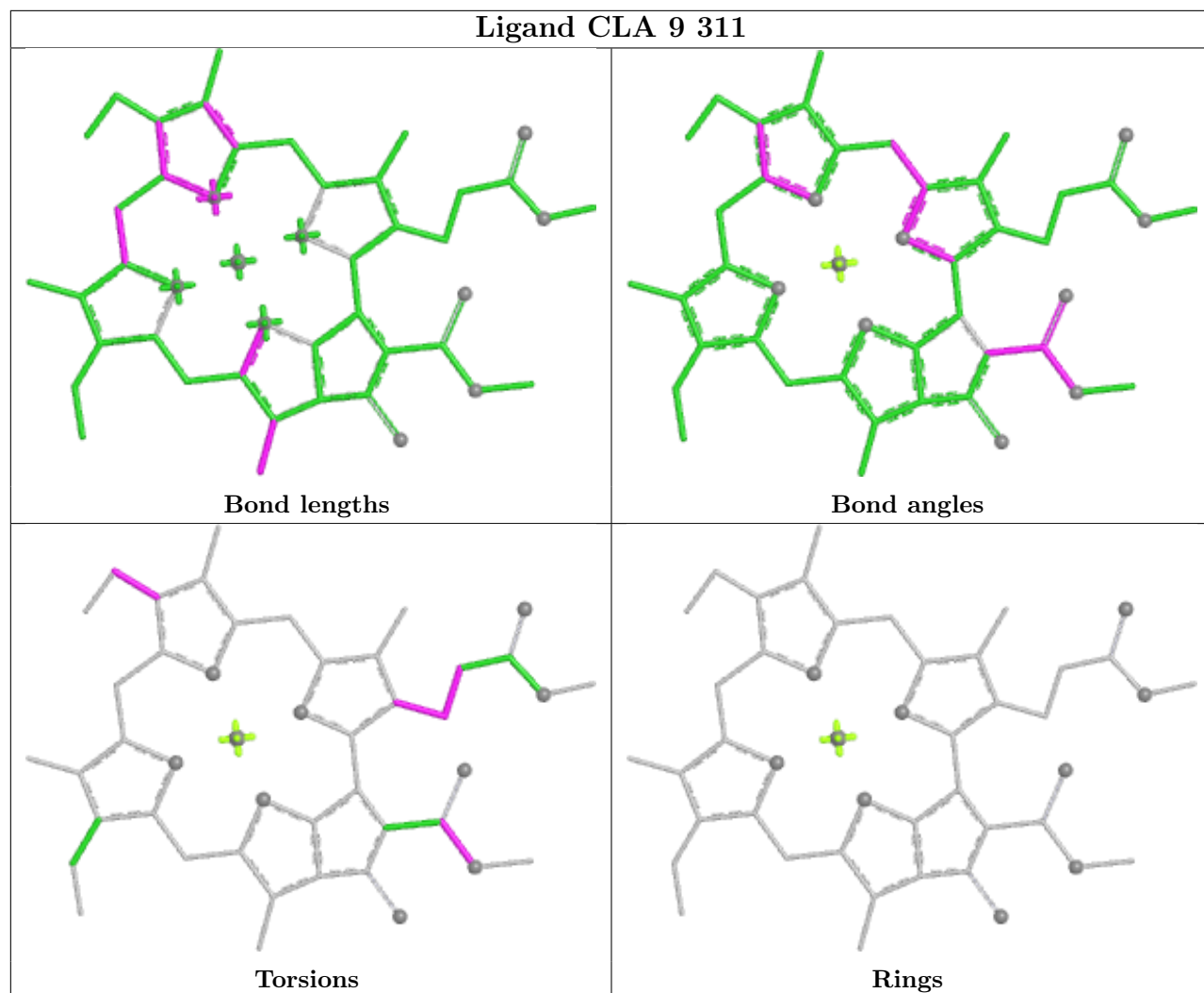
Ligand CLA 5 308



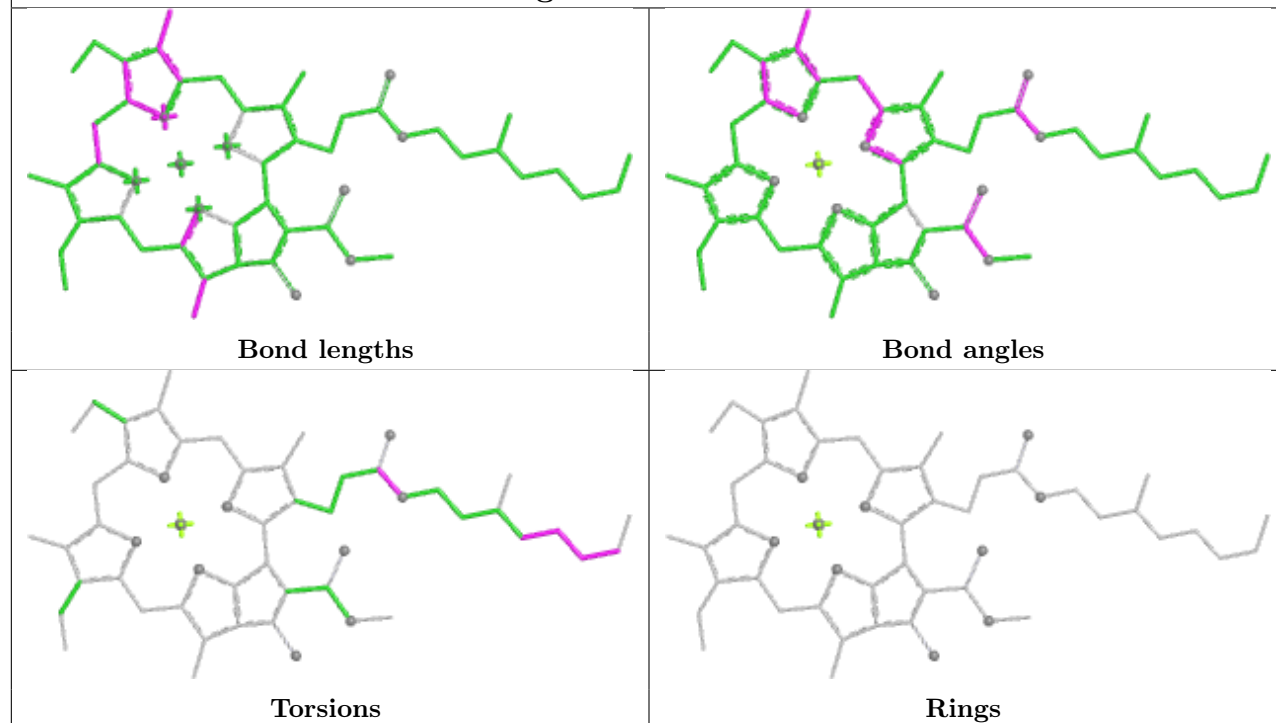
Ligand LMG j 105



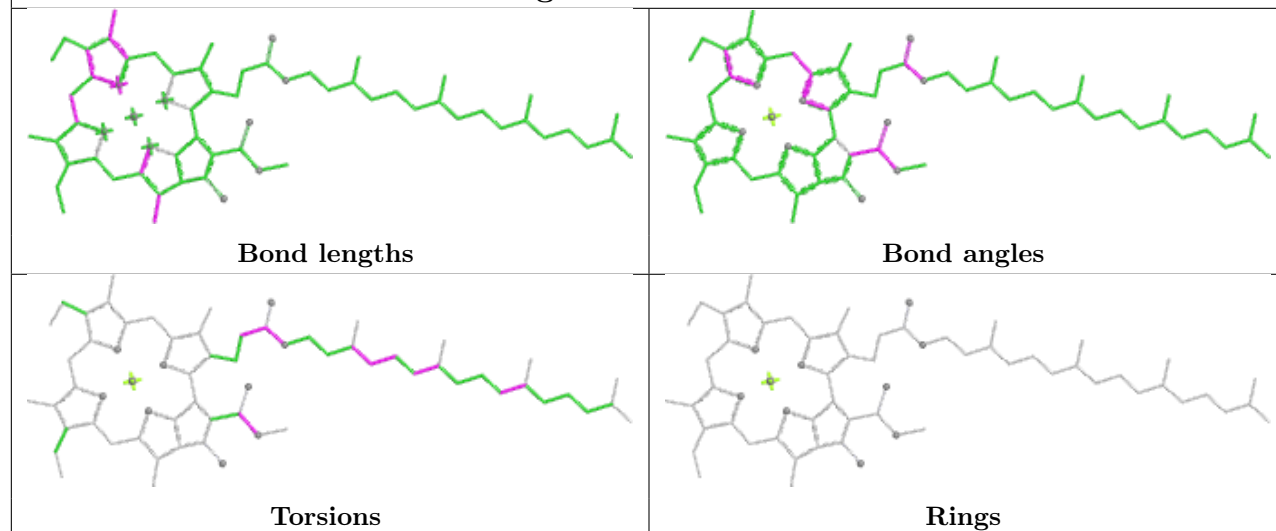
Ligand CLA 9 311

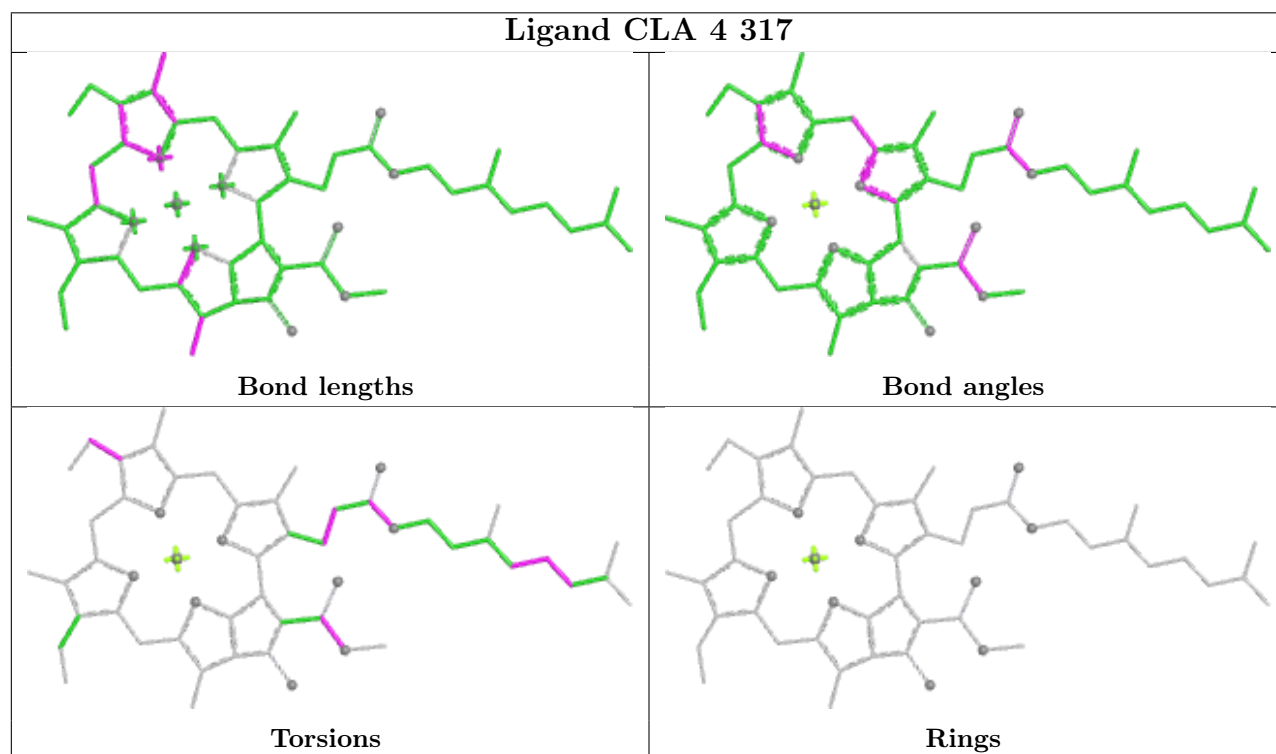
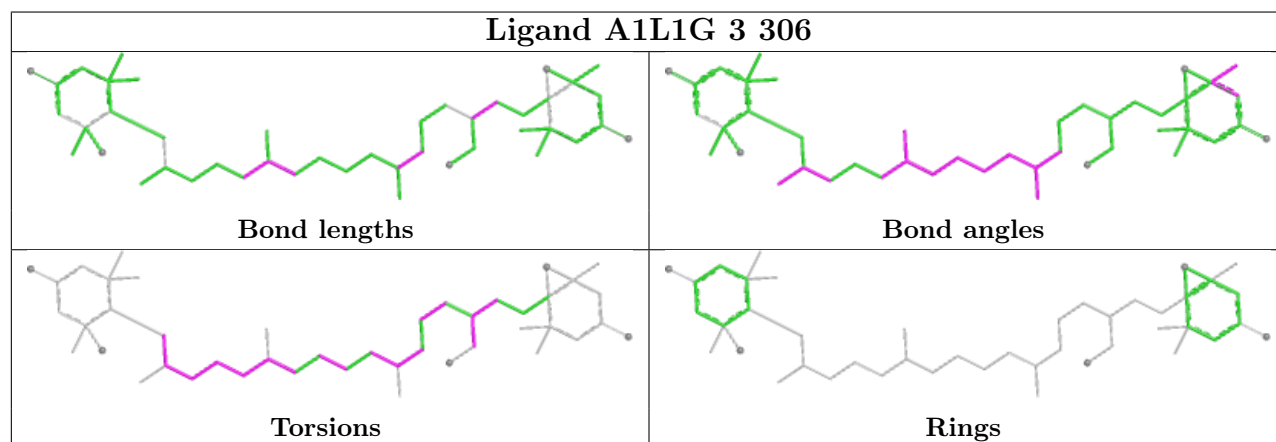
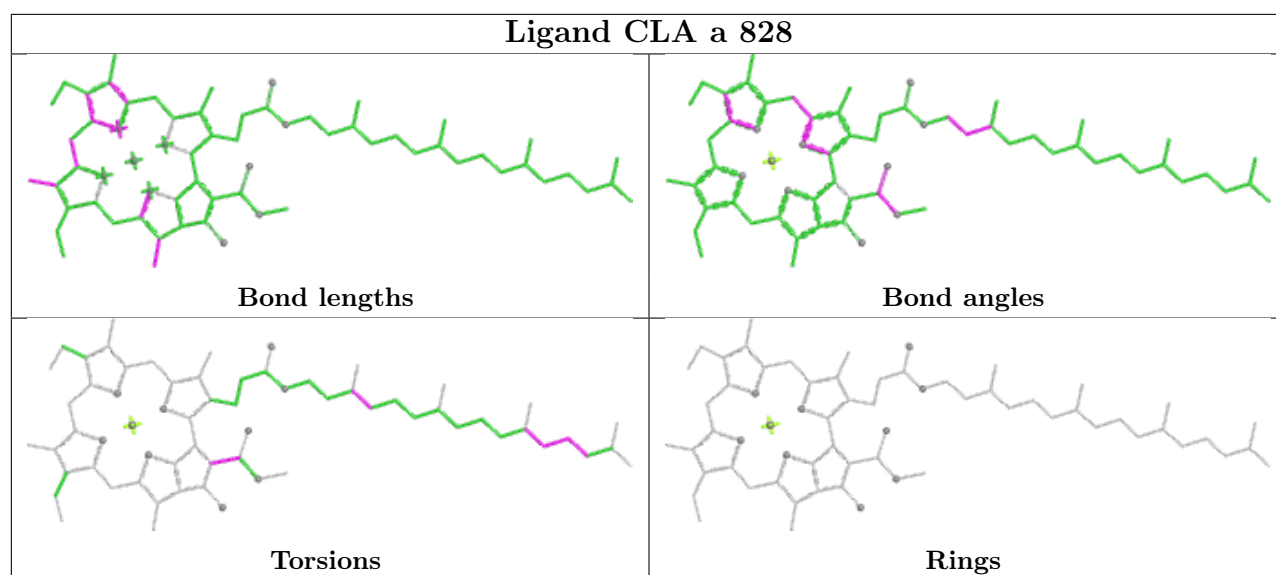


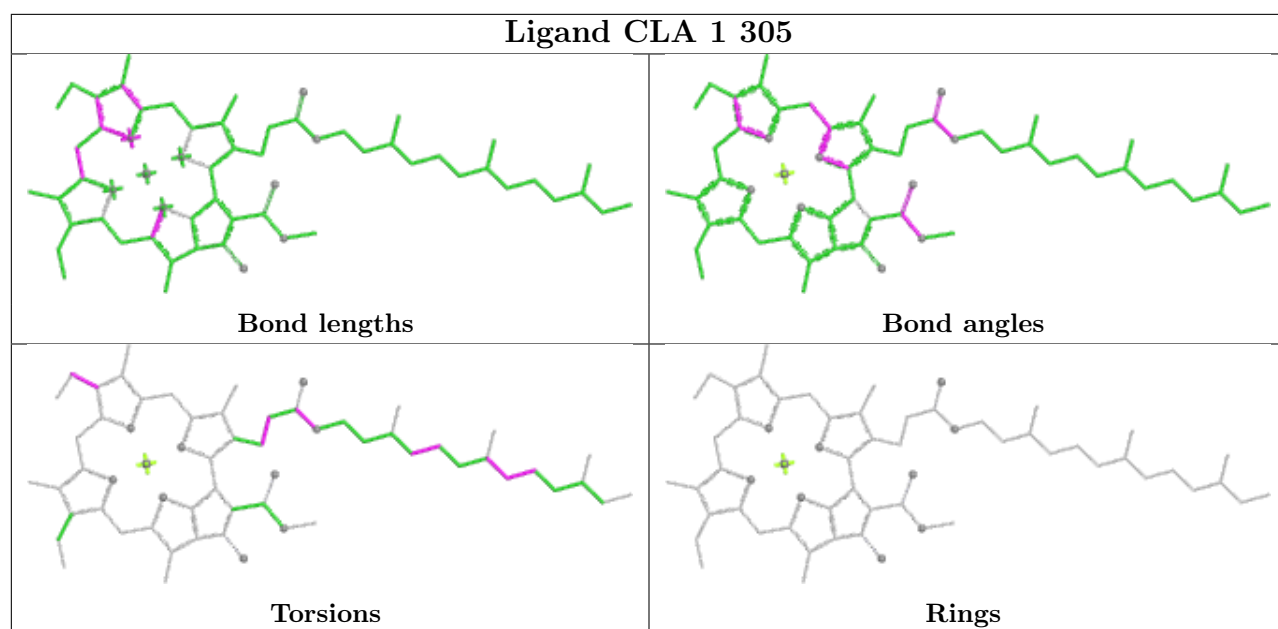
Ligand CLA 1 307



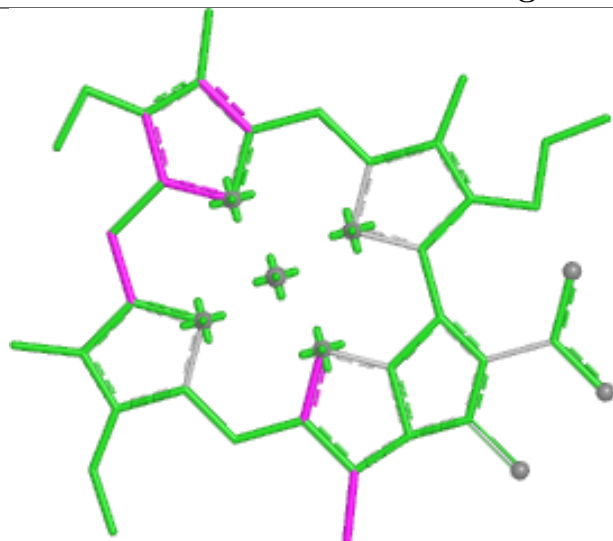
Ligand CLA a 835



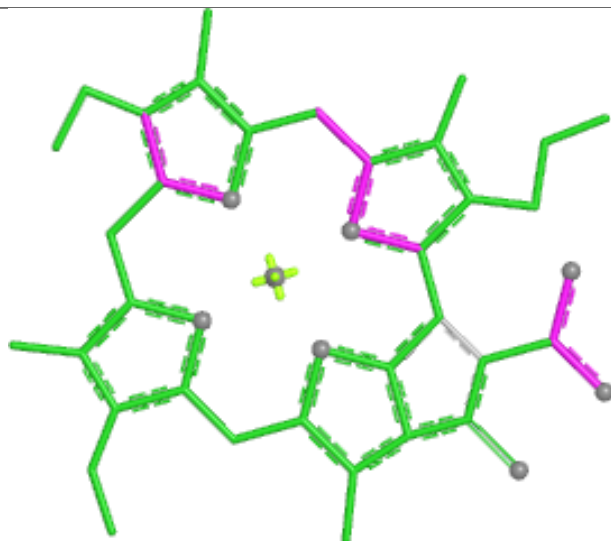




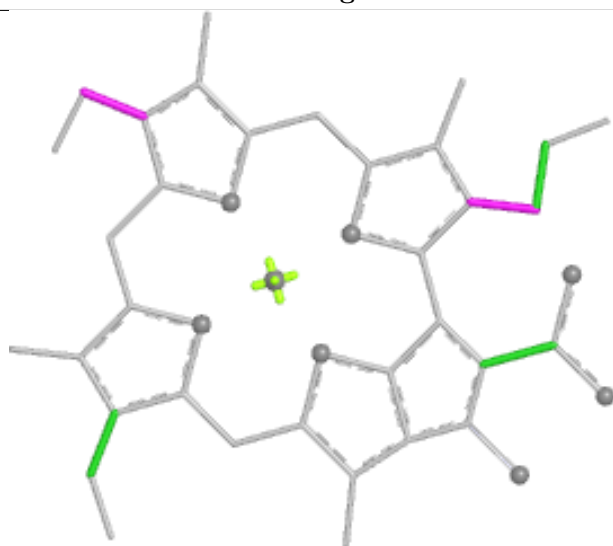
Ligand CLA 2 306



Bond lengths



Bond angles

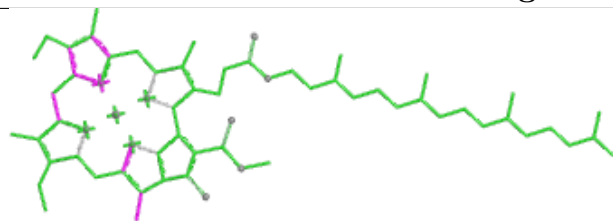


Torsions

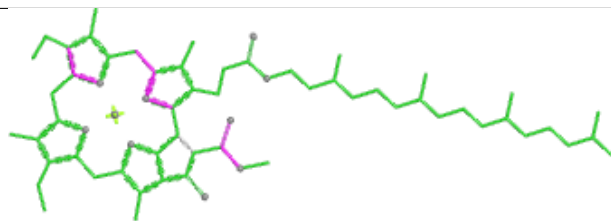


Rings

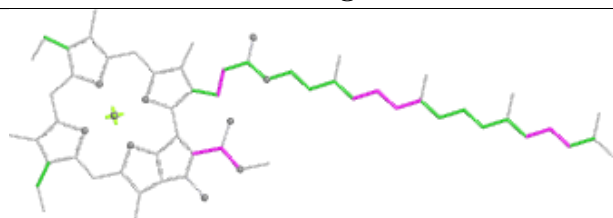
Ligand CLA 5 309



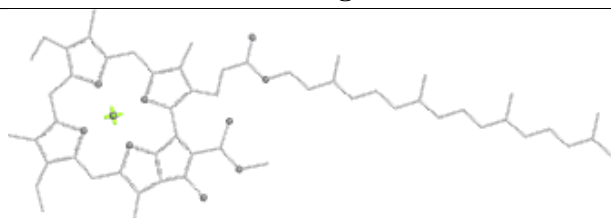
Bond lengths



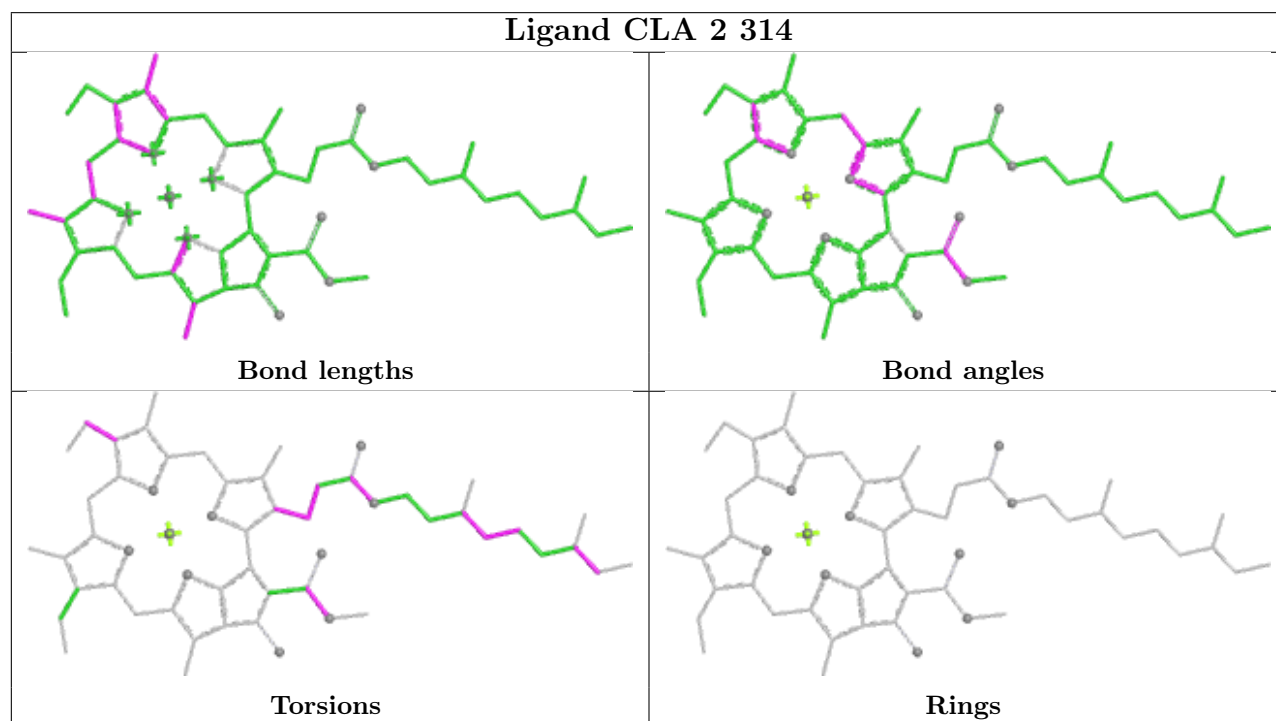
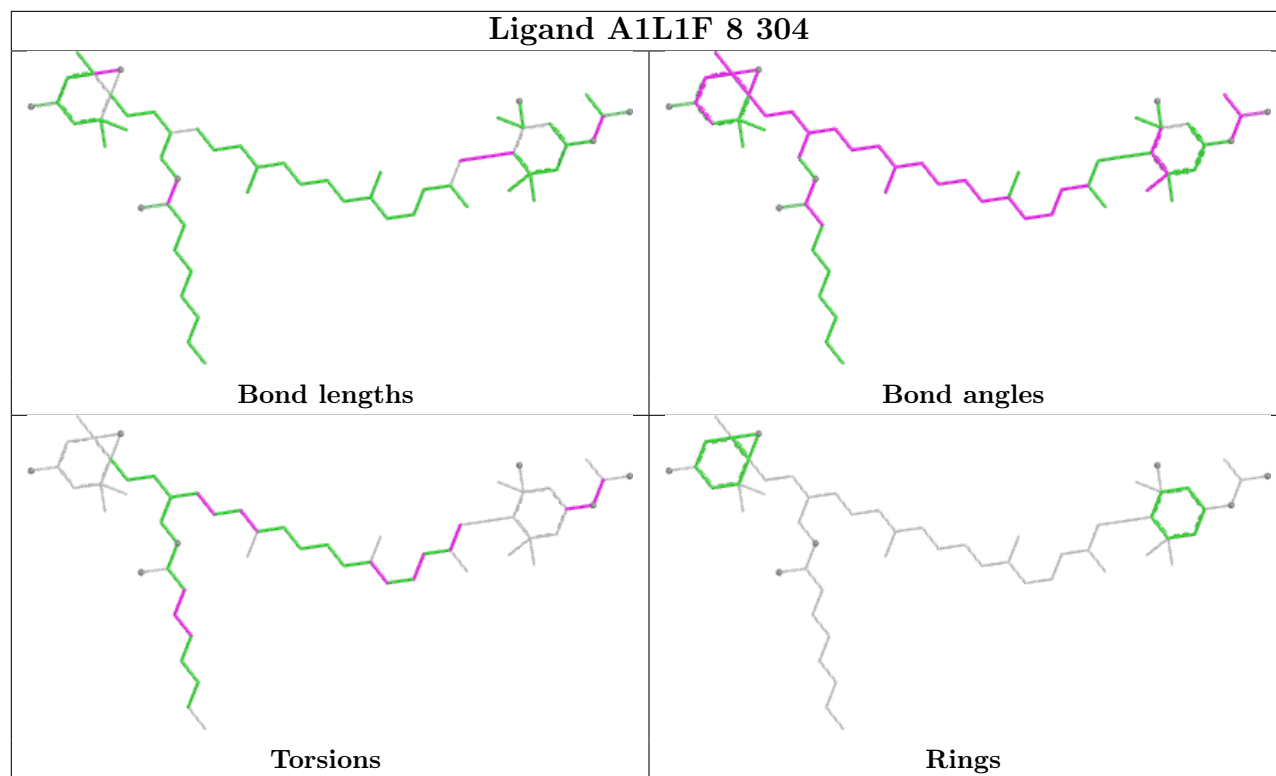
Bond angles



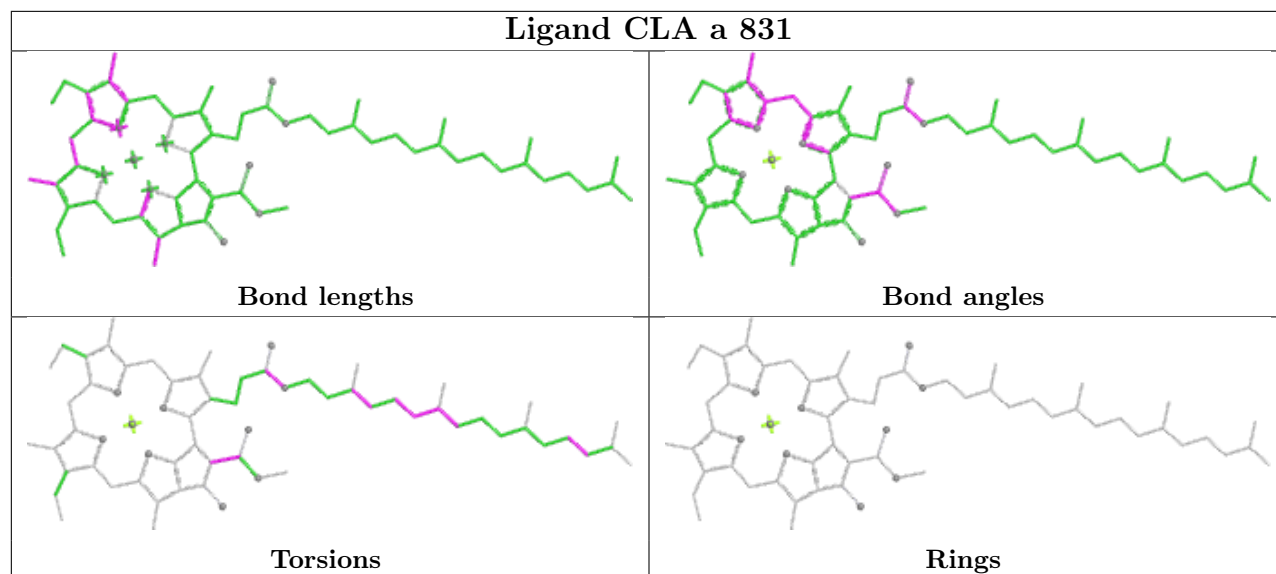
Torsions



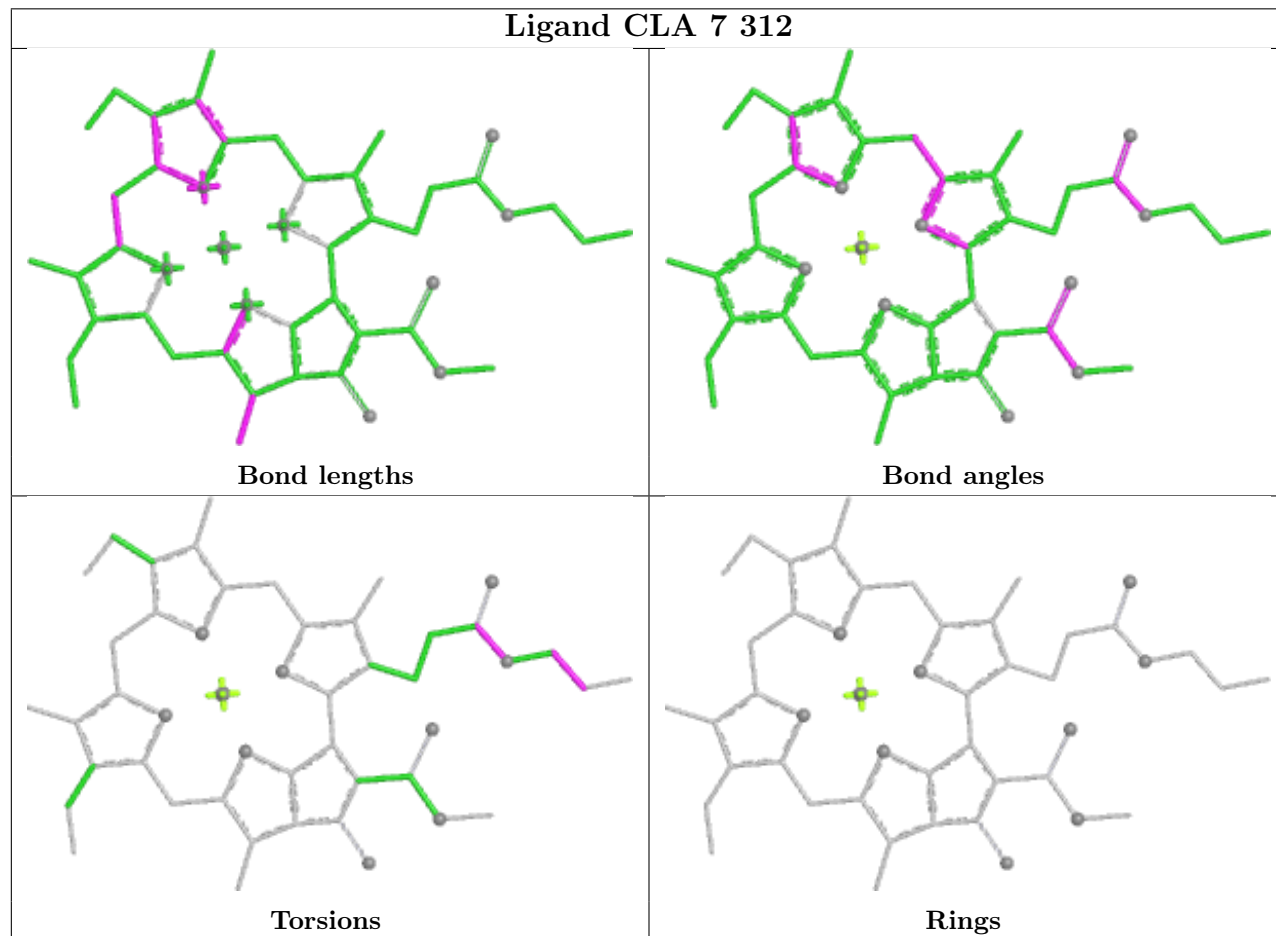
Rings

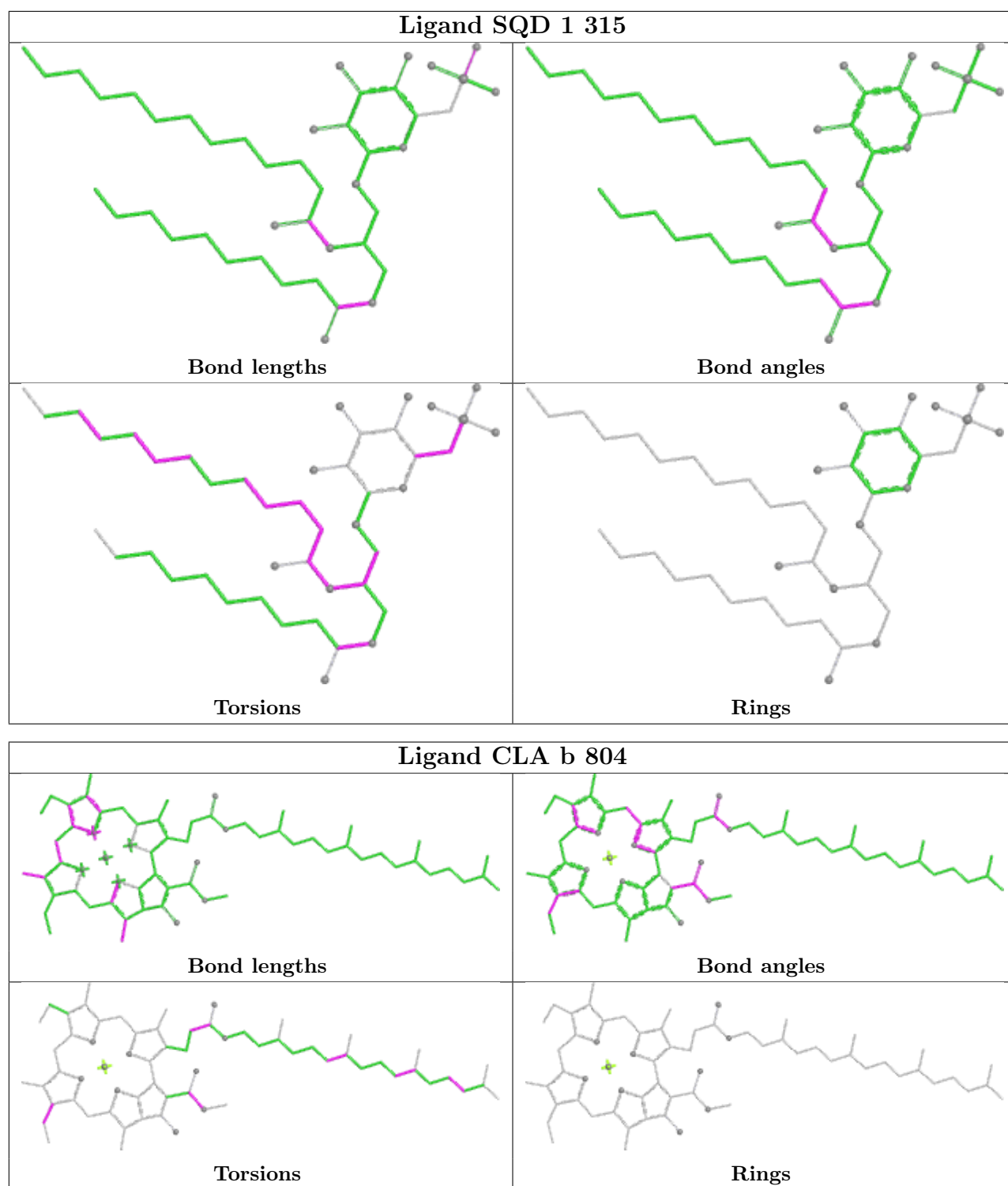


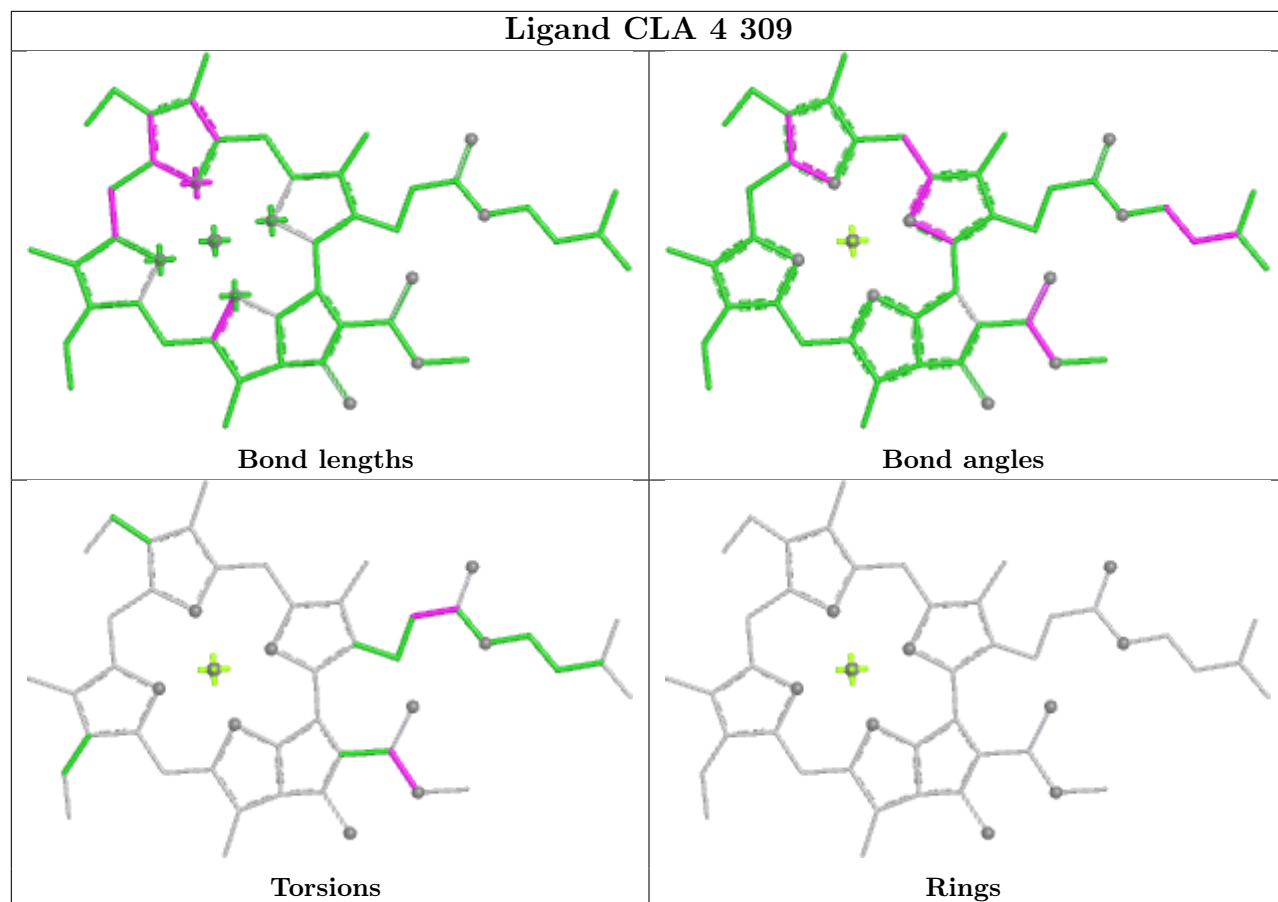
Ligand CLA a 831



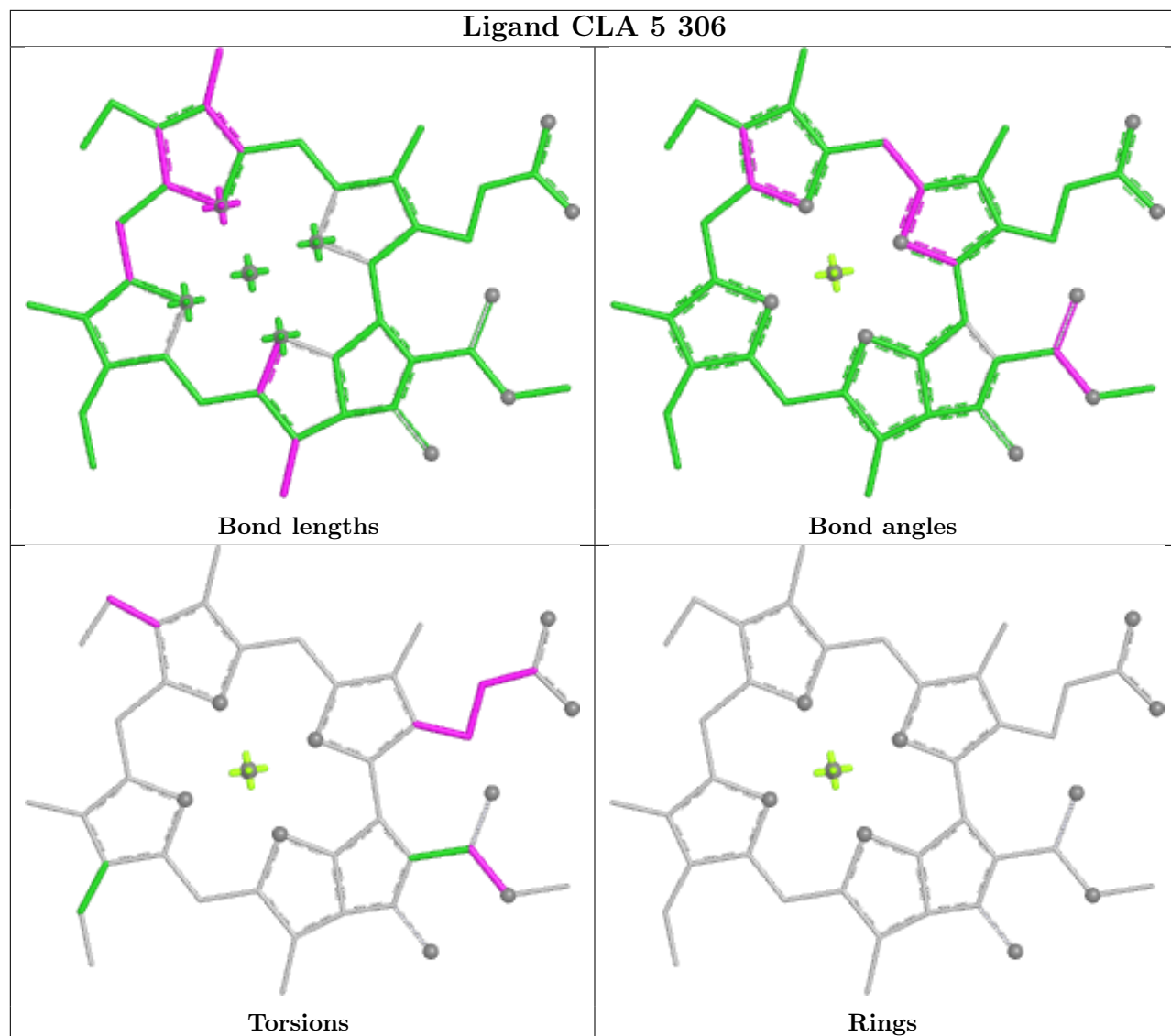
Ligand CLA 7 312



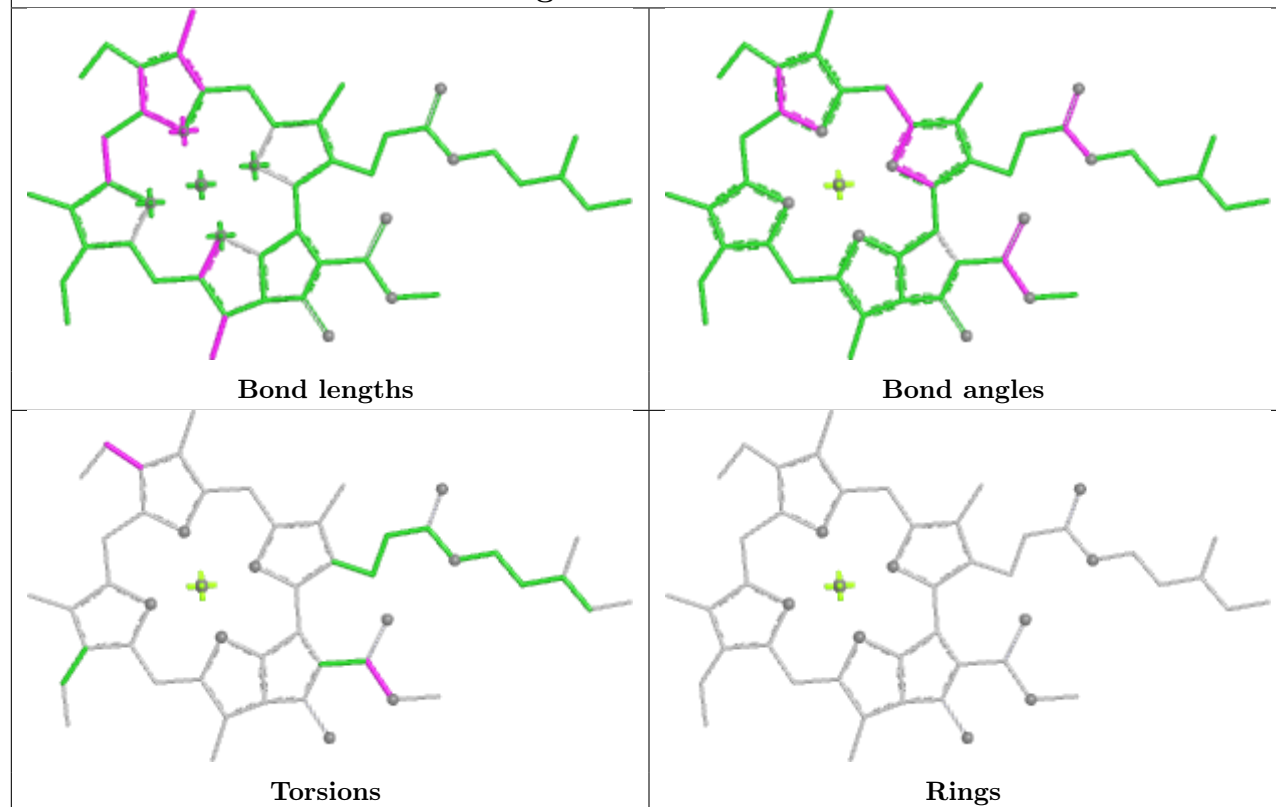




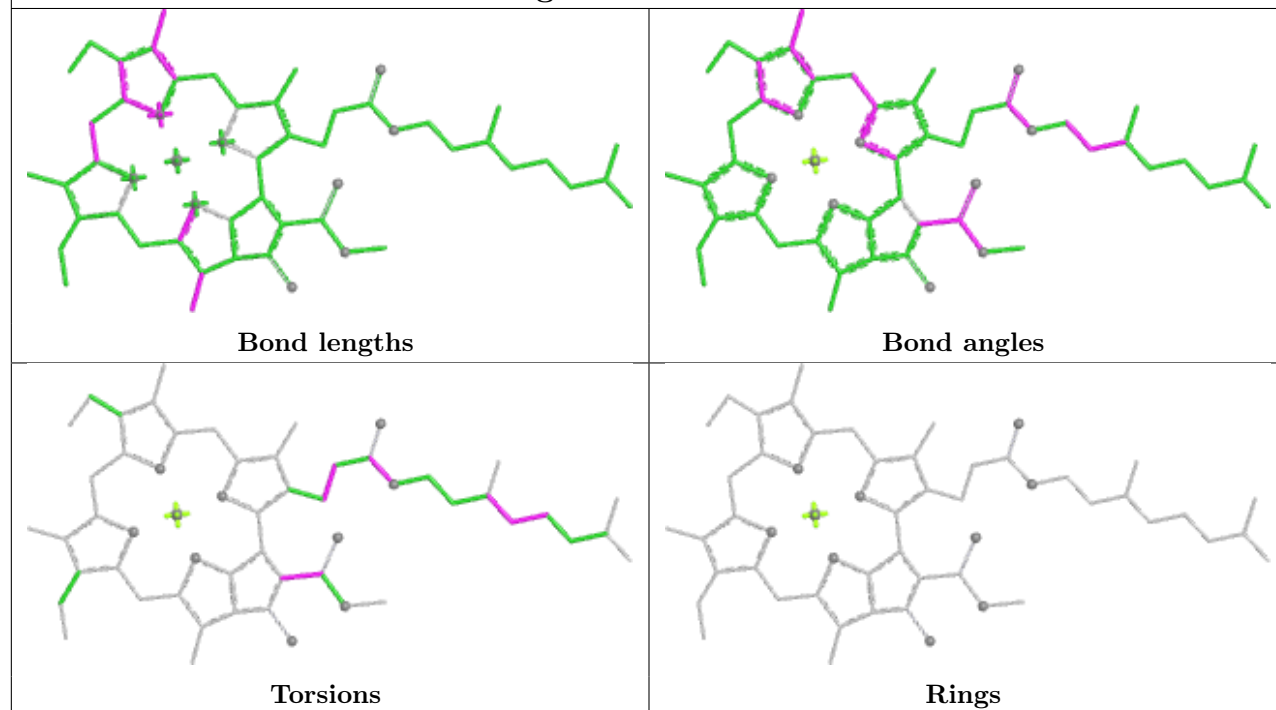
Ligand CLA 5 306

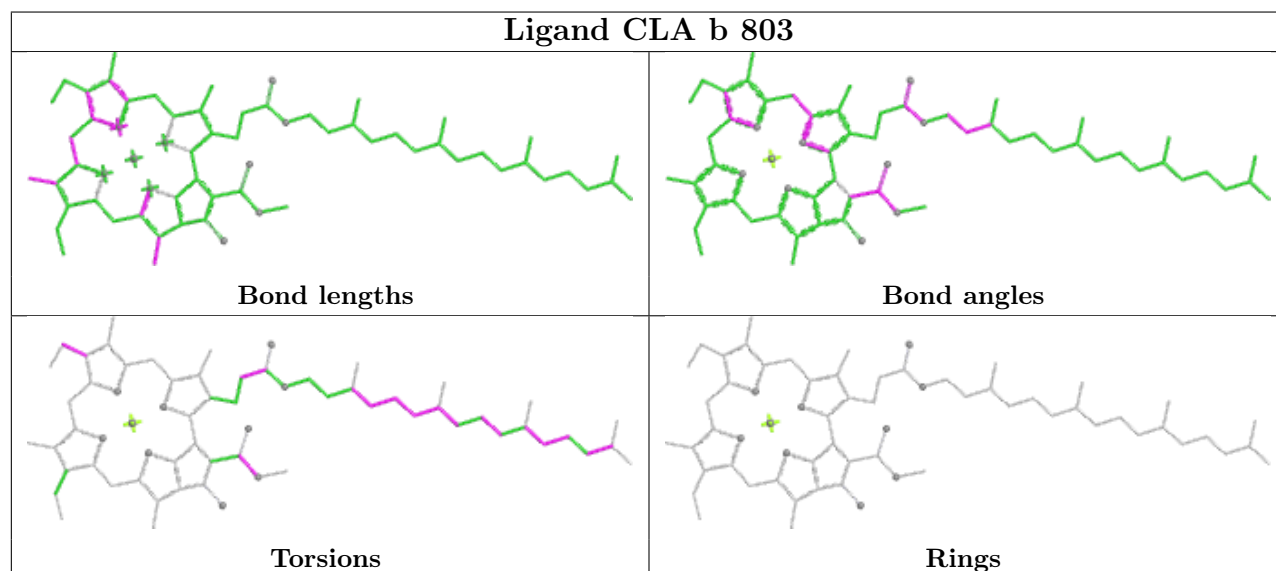
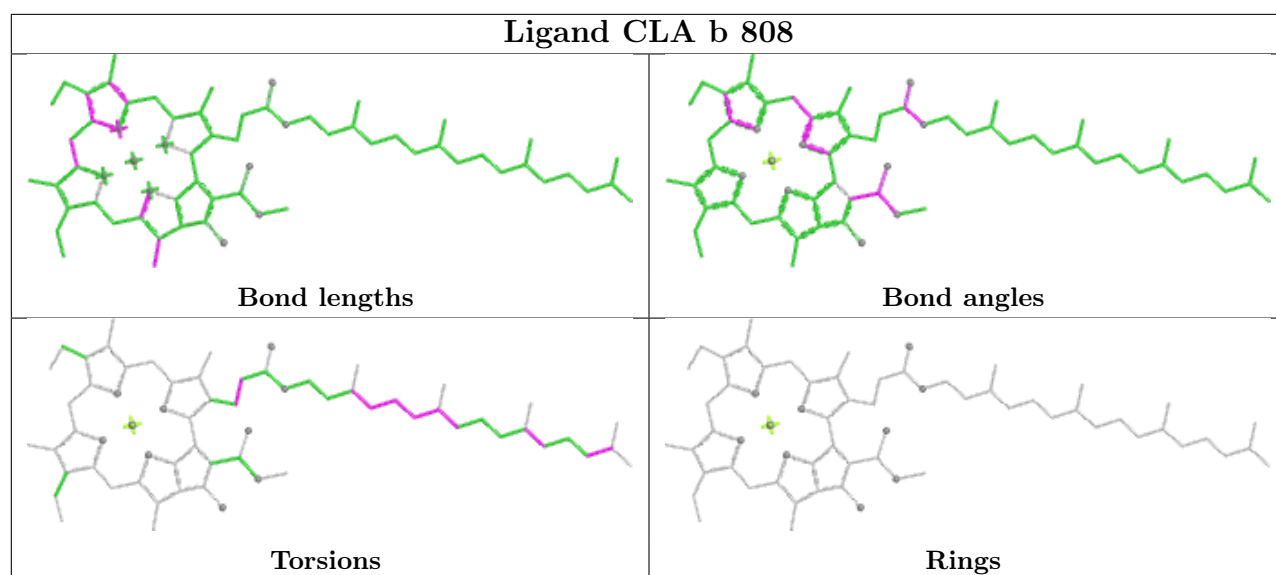


Ligand CLA a 808

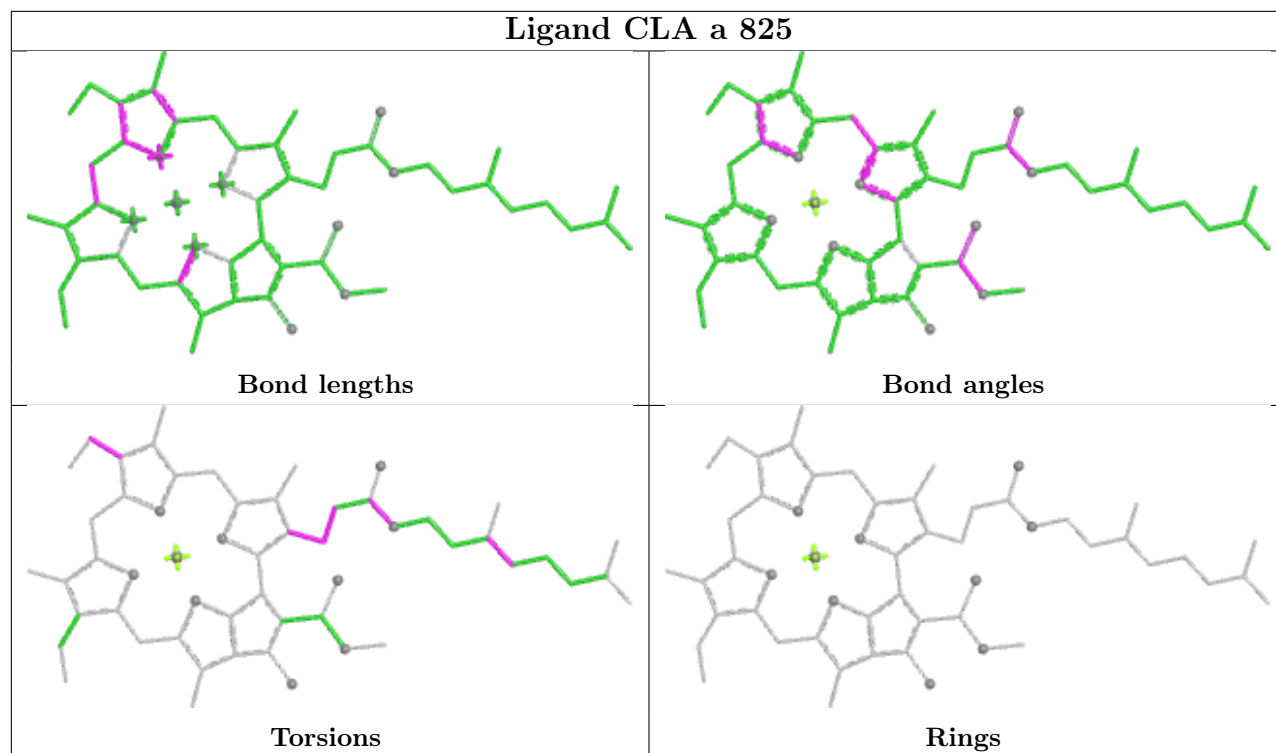


Ligand CLA 8 308

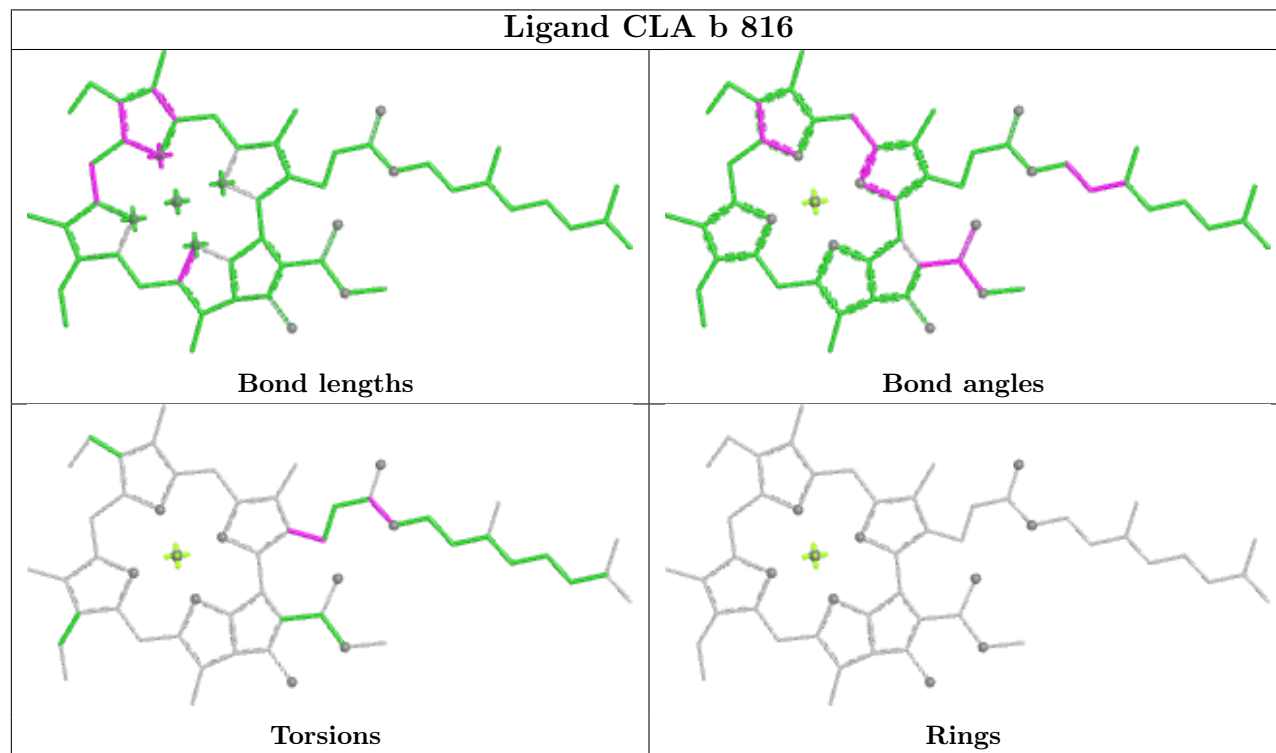


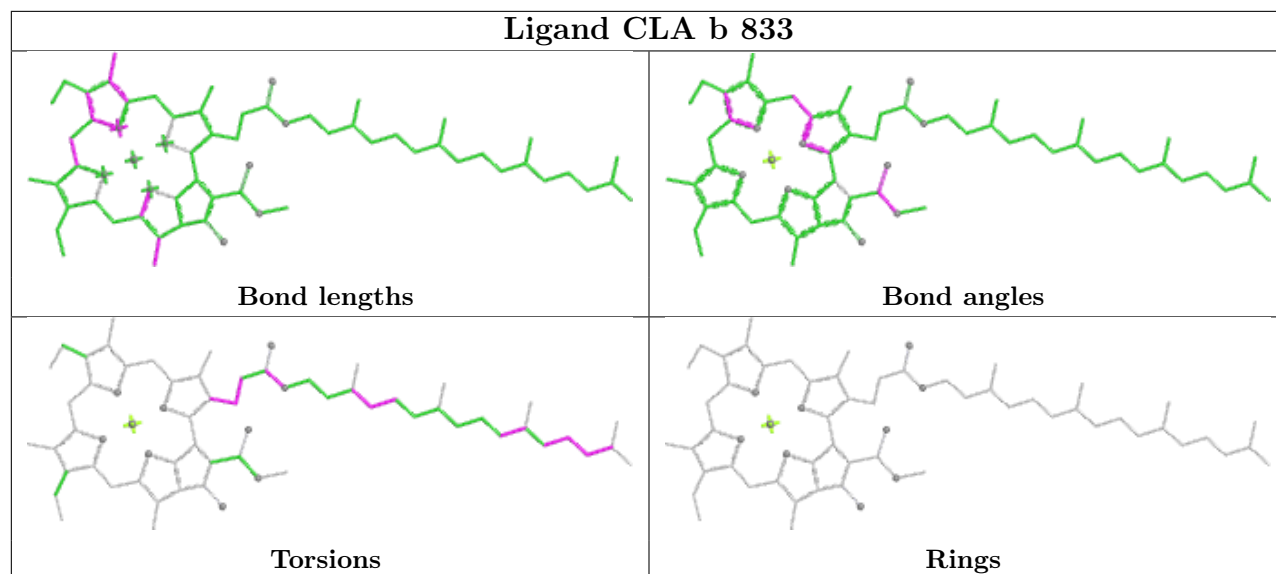
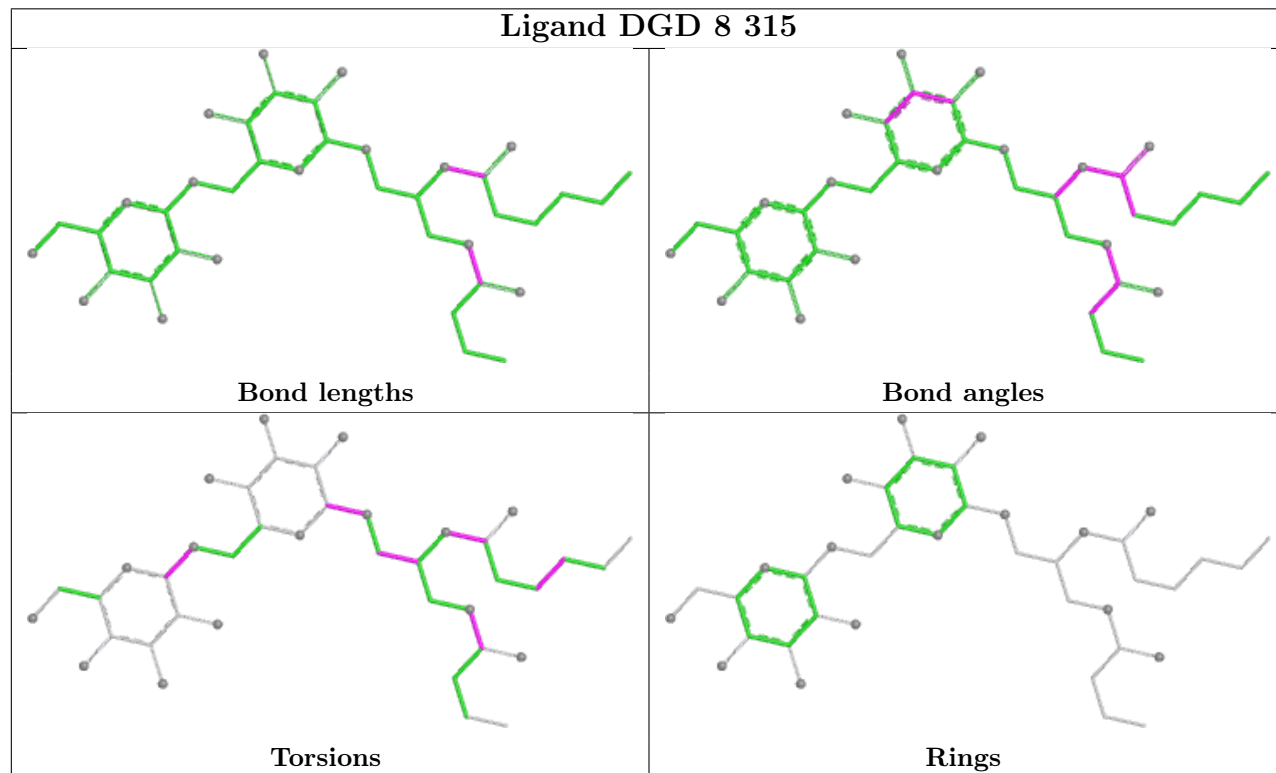


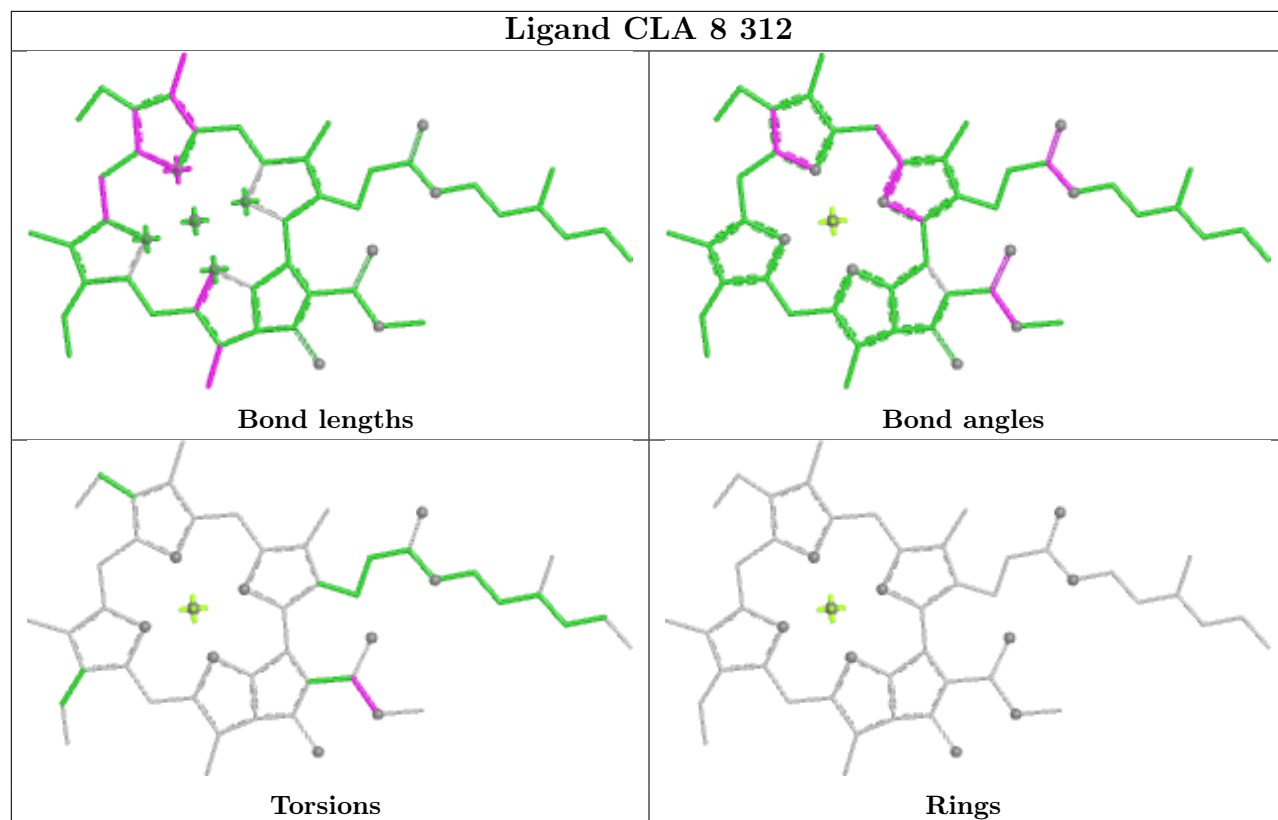
Ligand CLA a 825



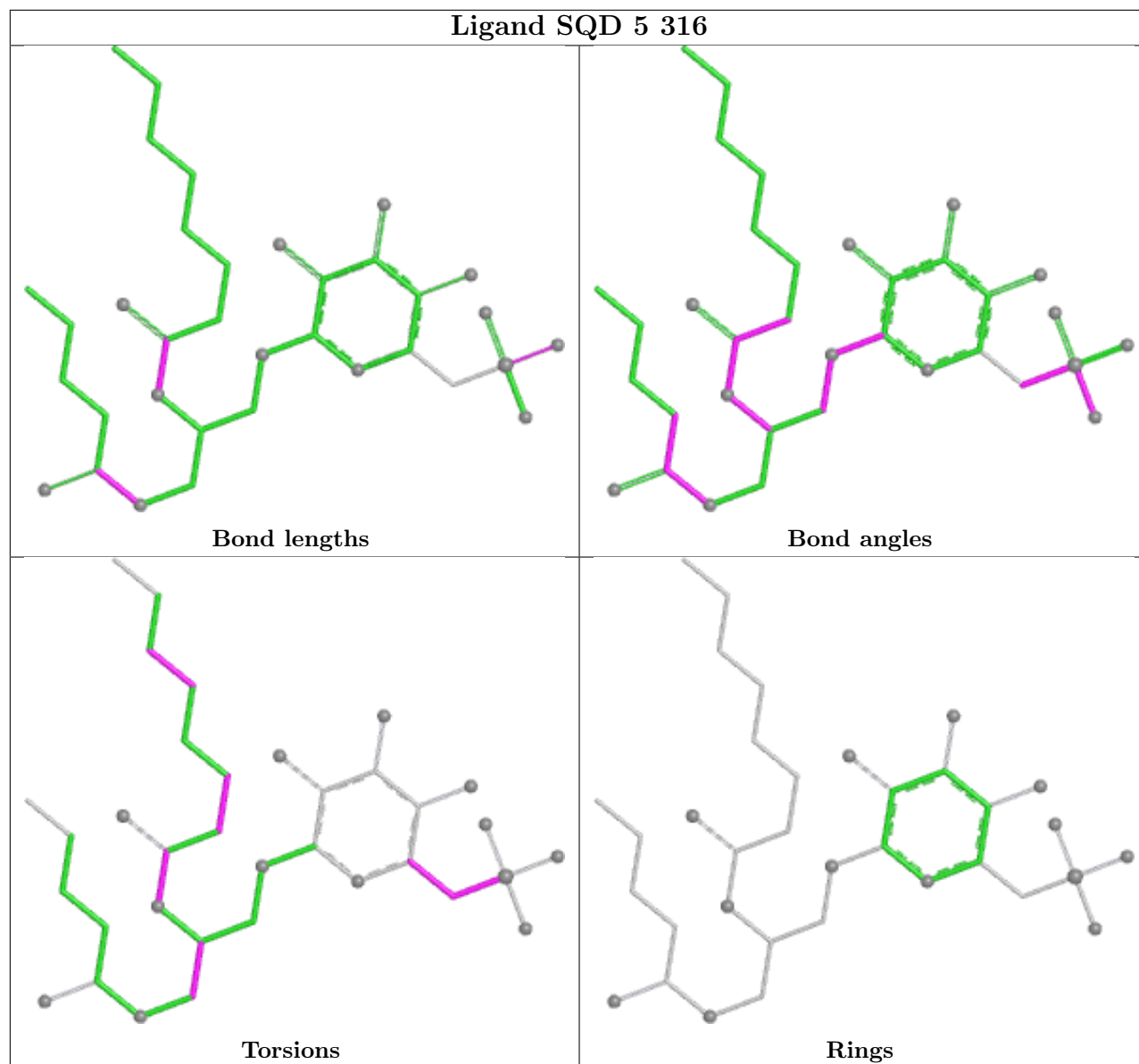
Ligand CLA b 816

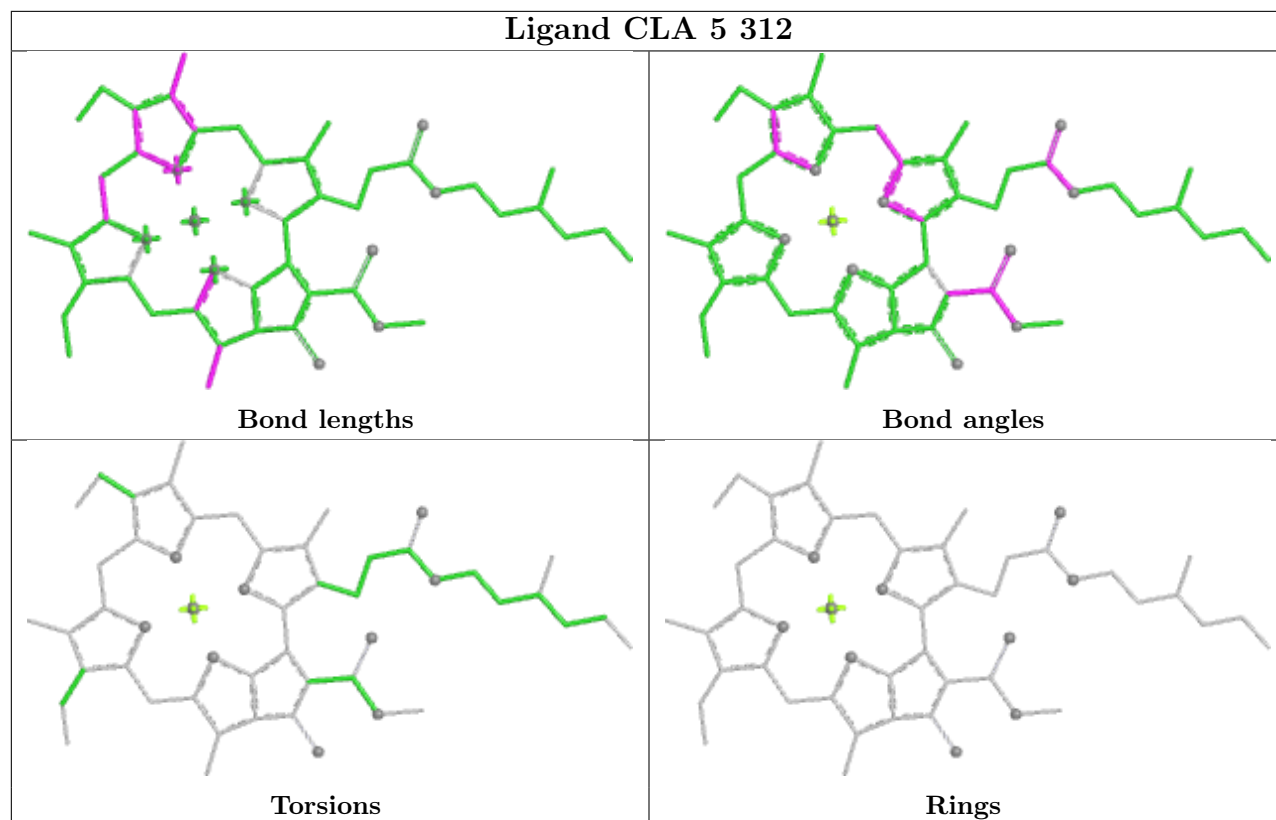


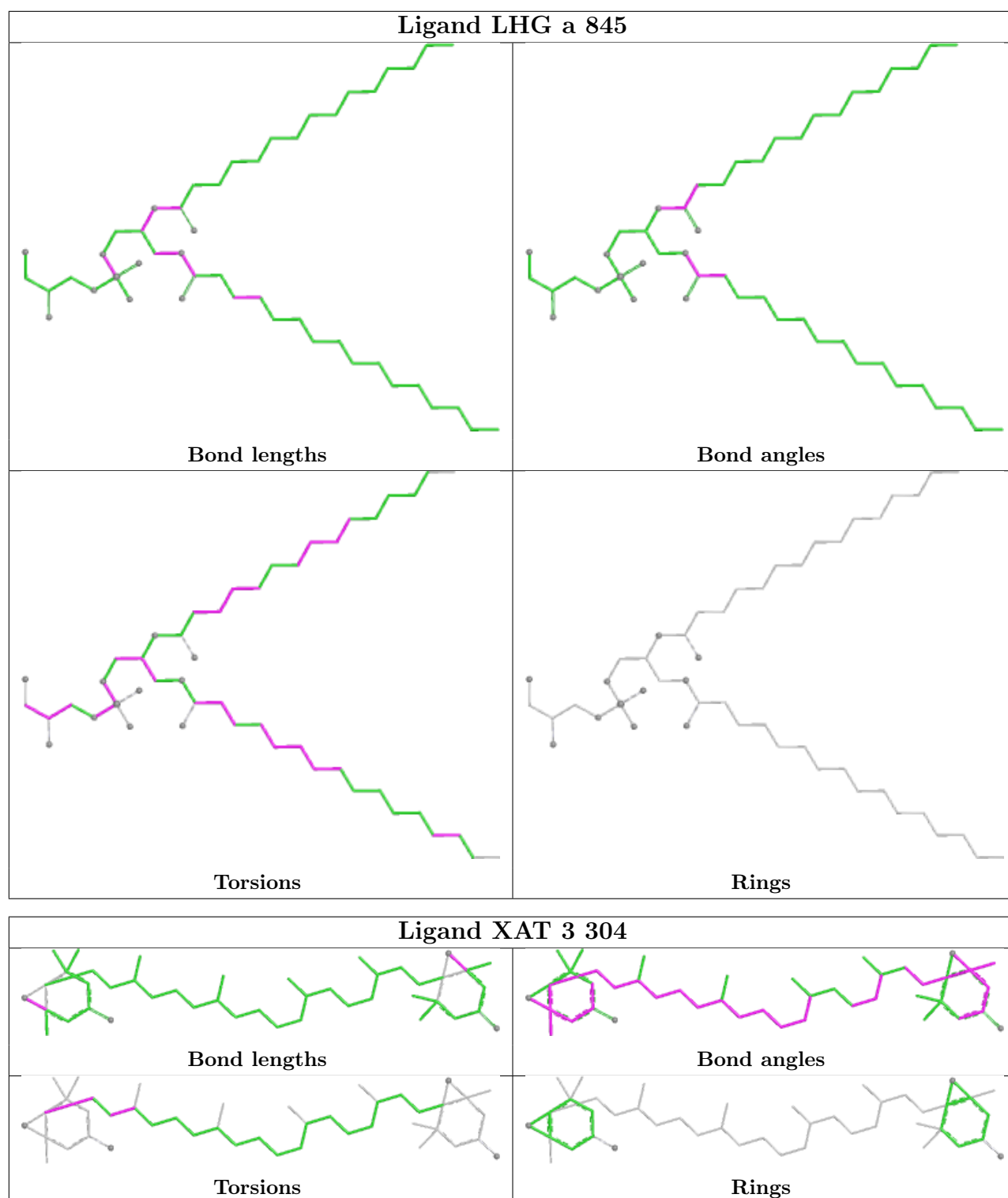
Ligand CLA b 833**Ligand DGD 8 315**

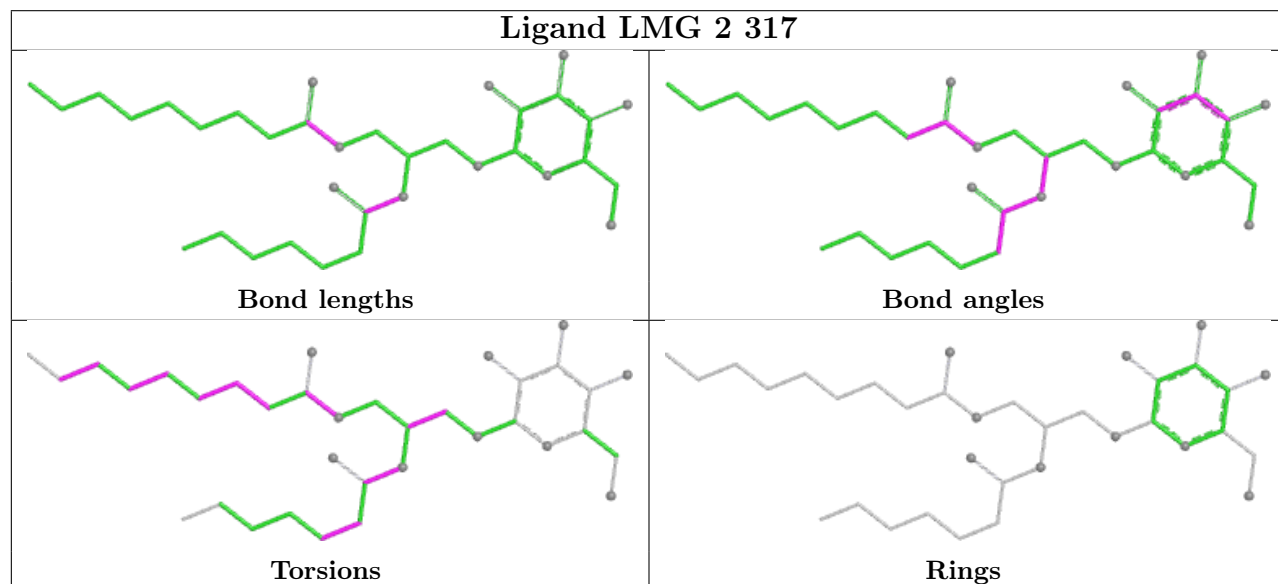
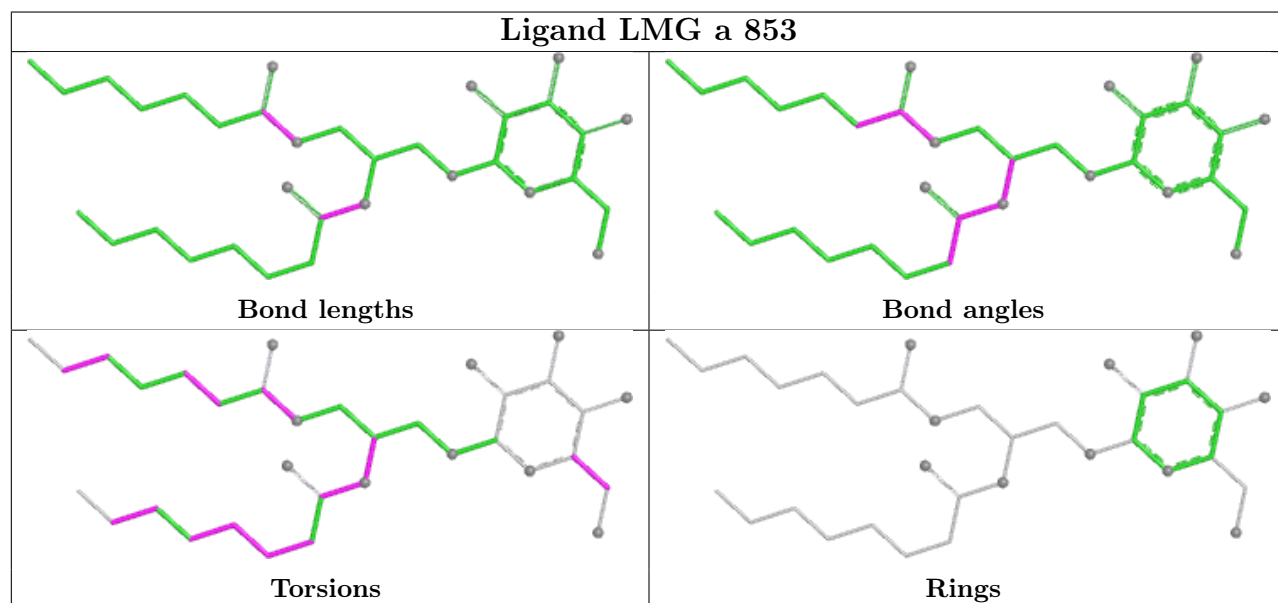
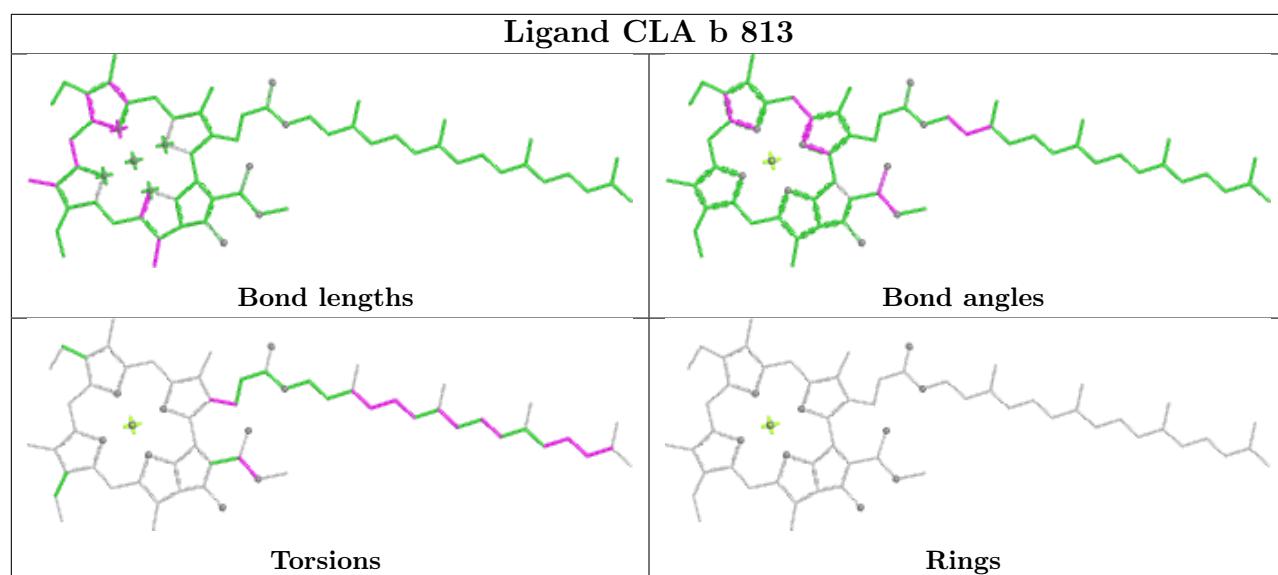


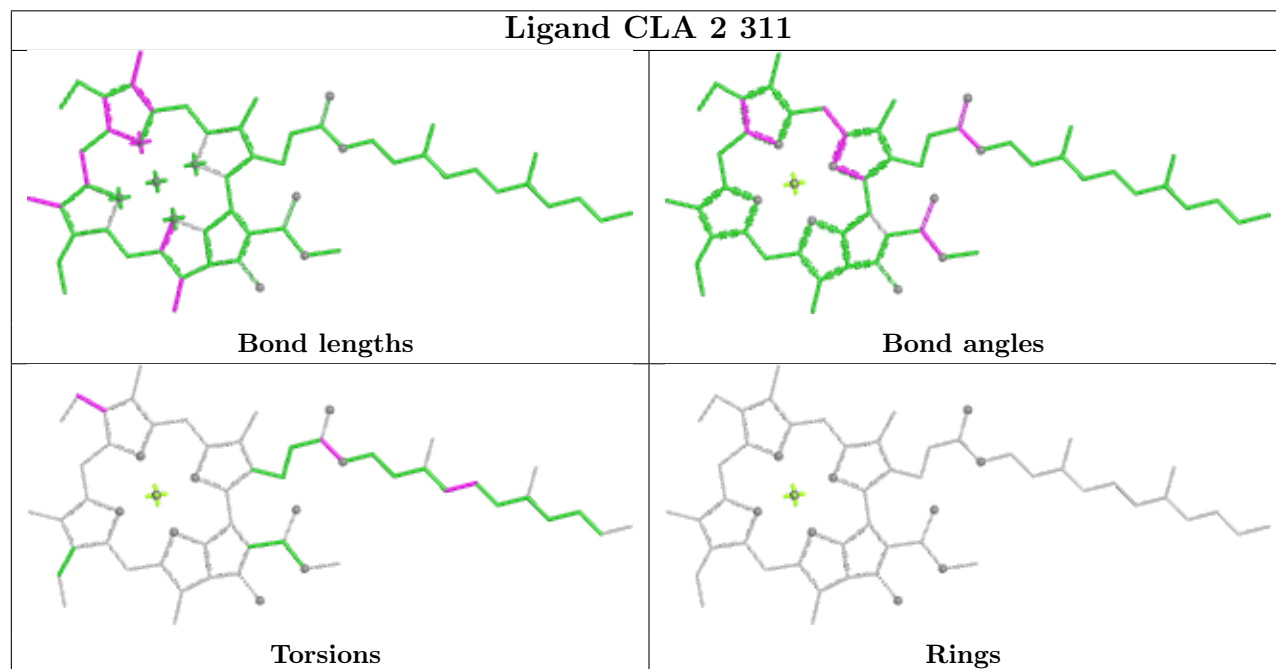
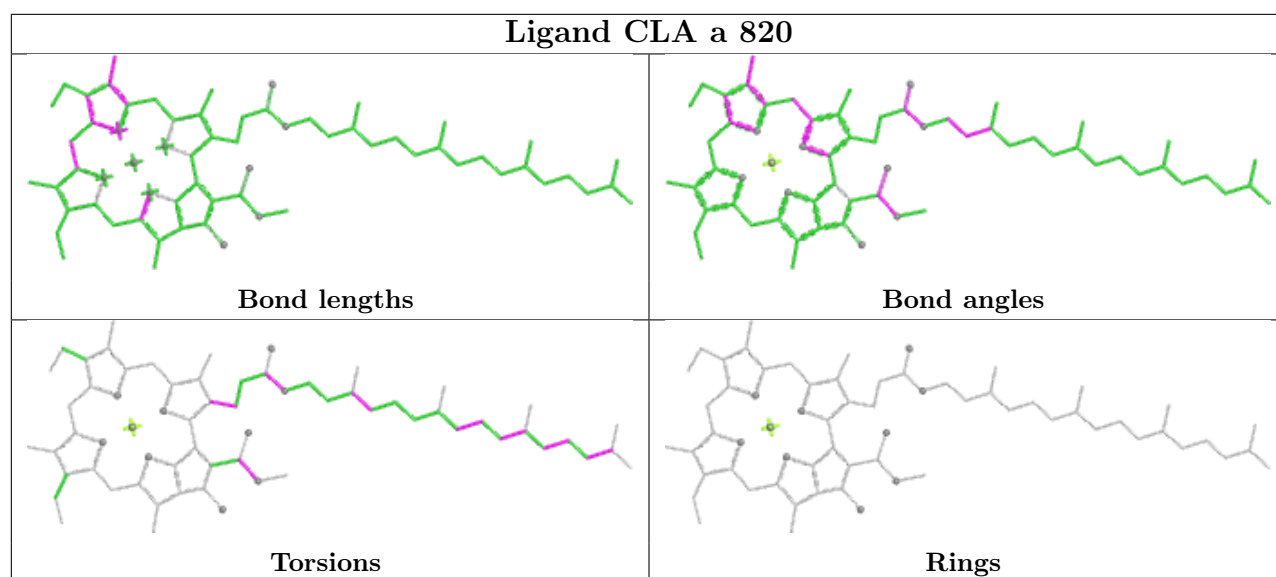
Ligand SQD 5 316



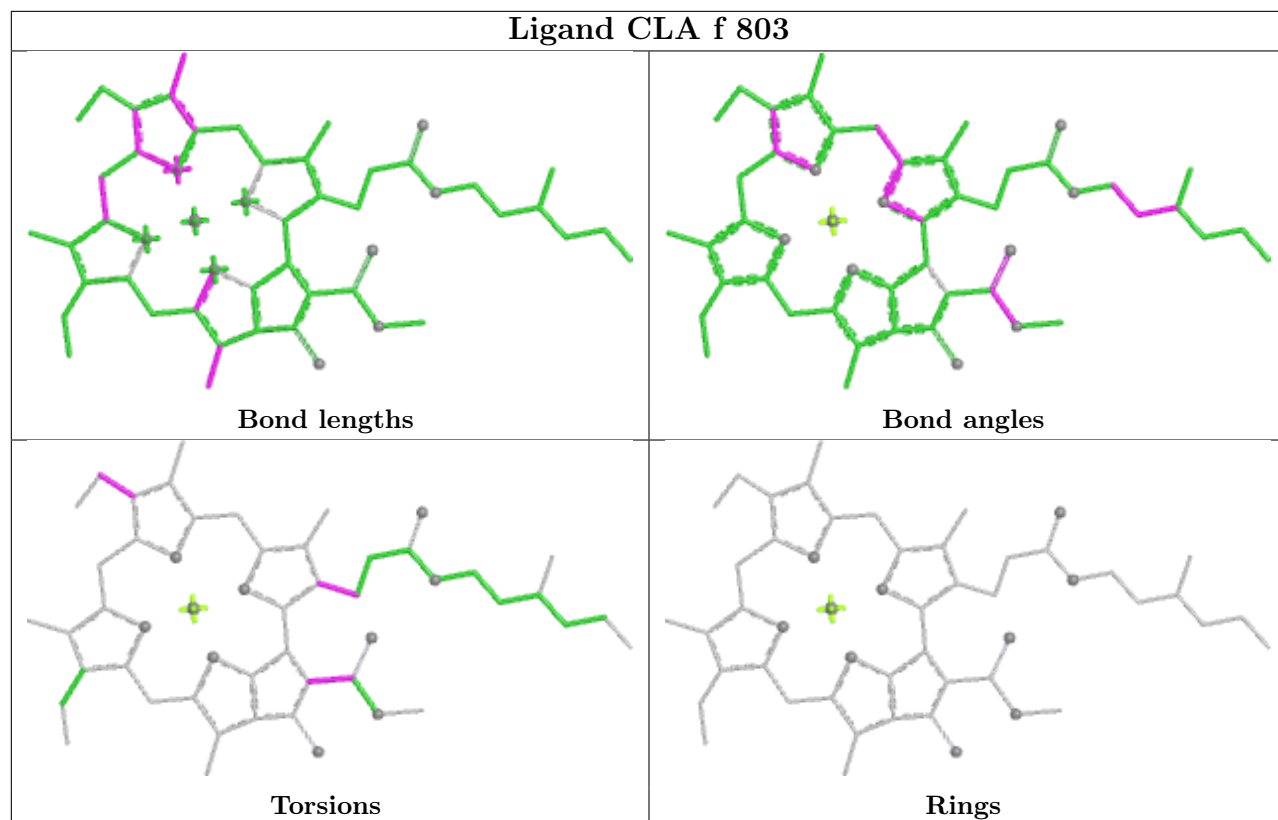




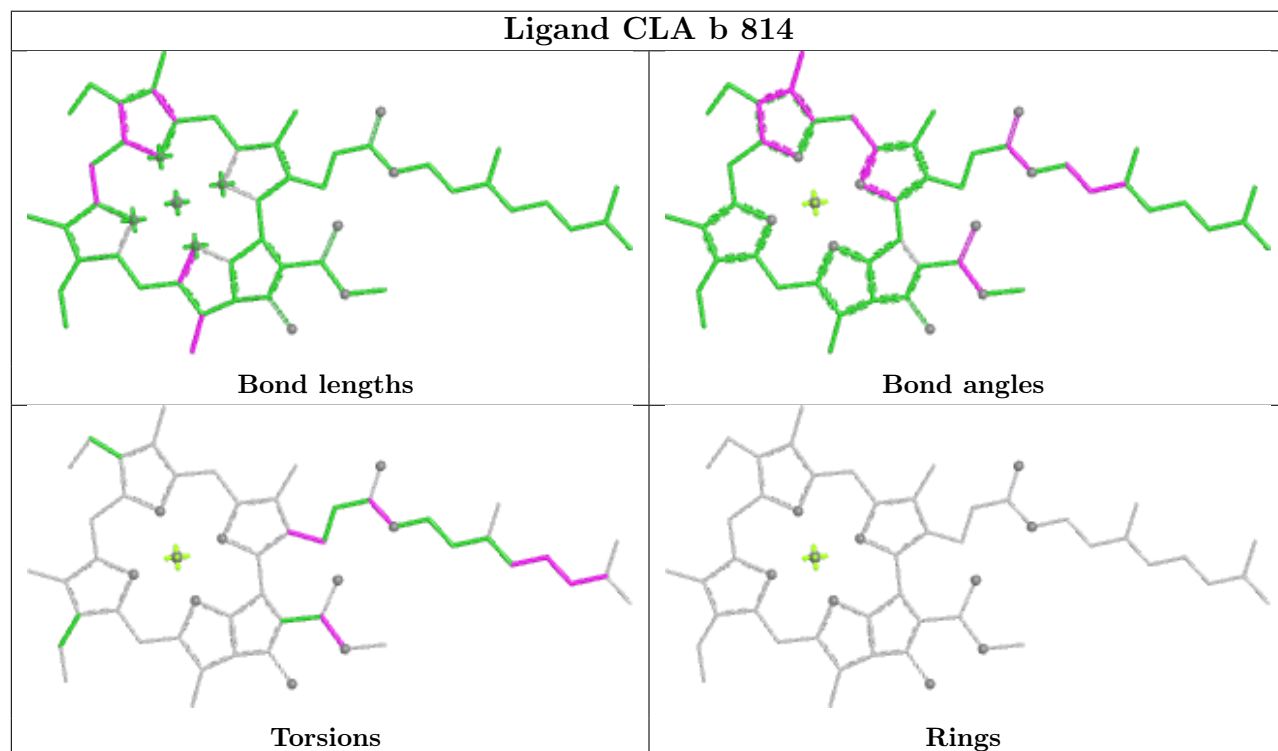




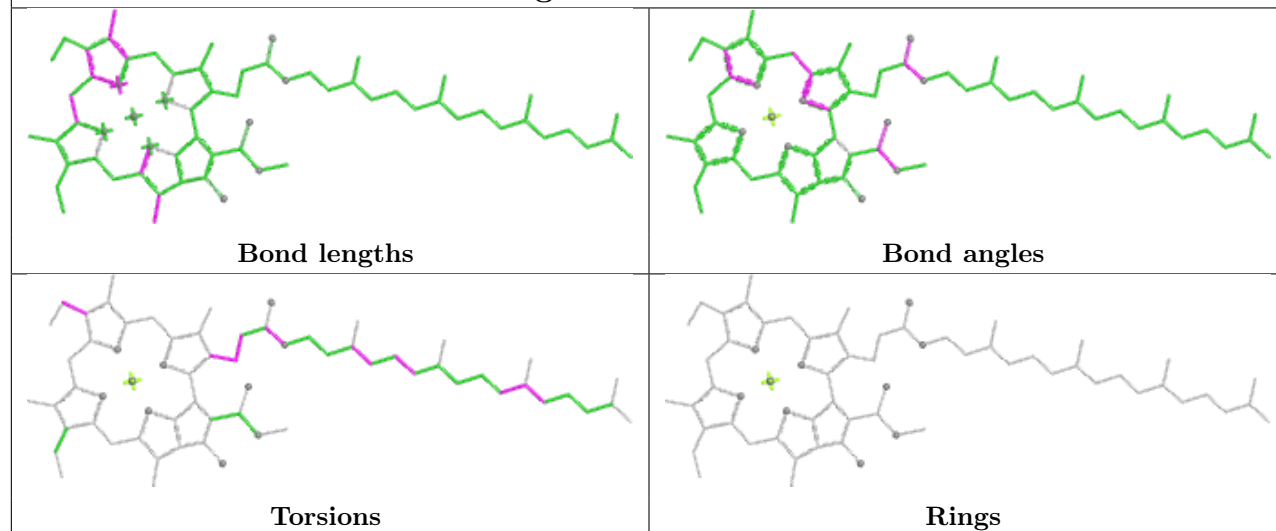
Ligand CLA f 803



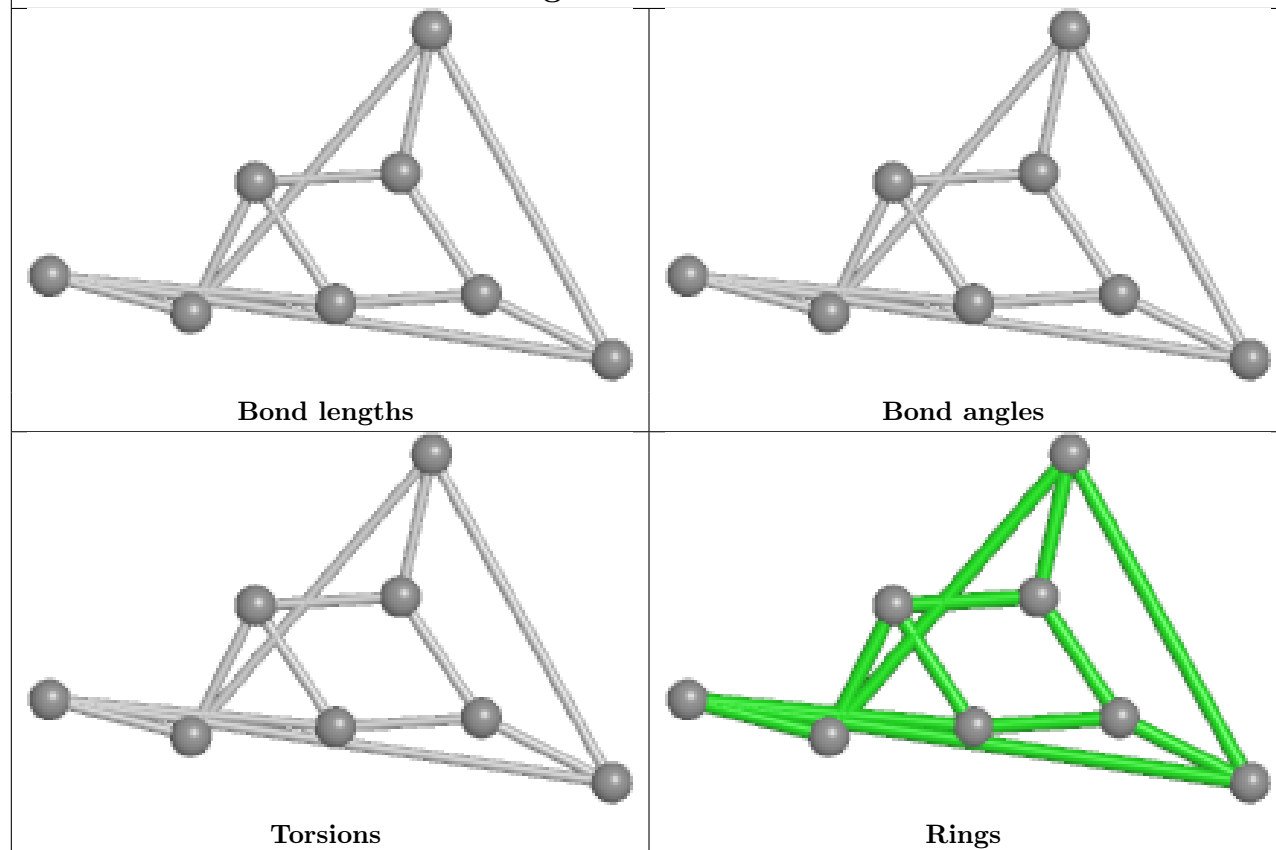
Ligand CLA b 814



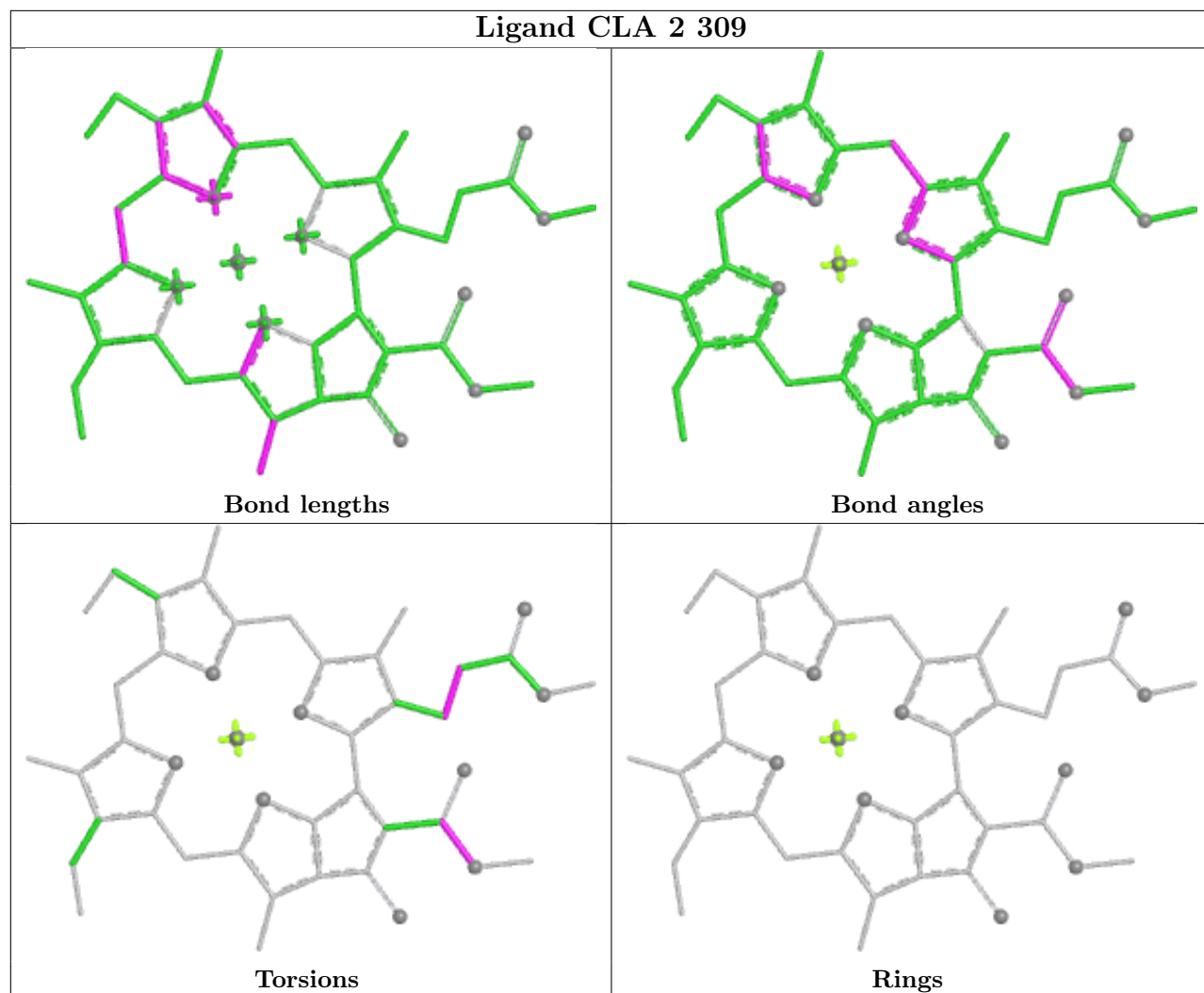
Ligand CLA b 828



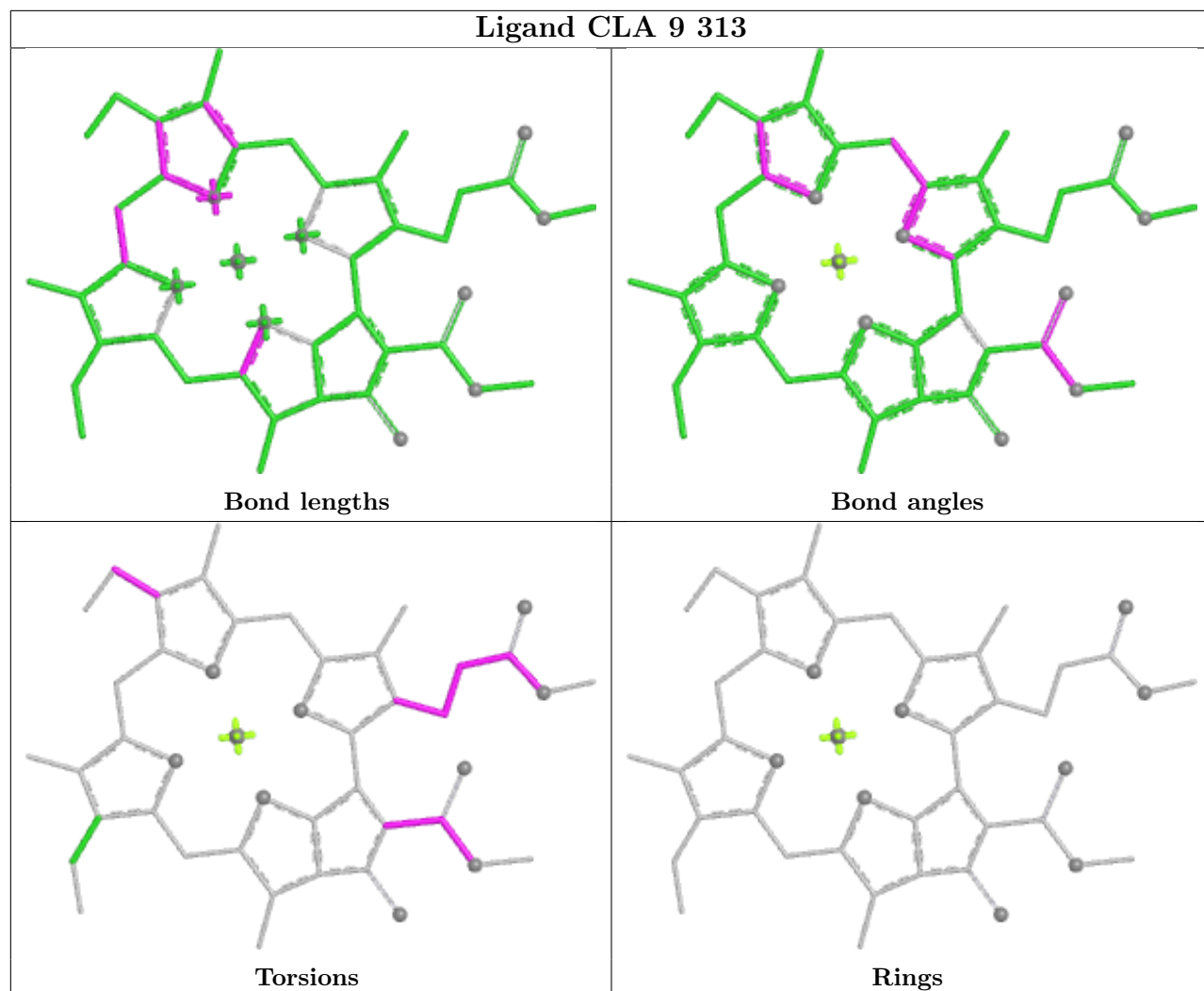
Ligand SF4 a 851



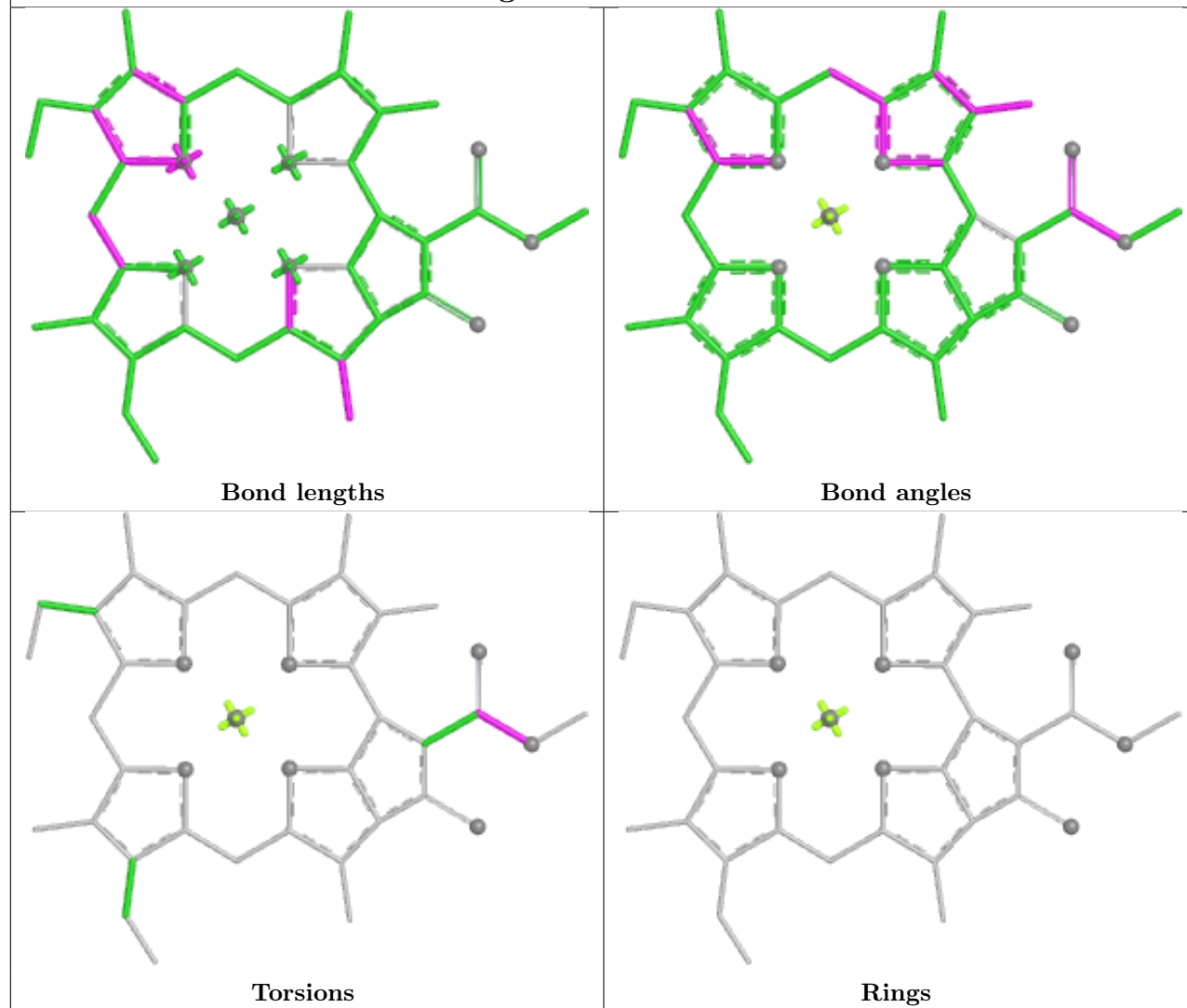
Ligand CLA 2 309



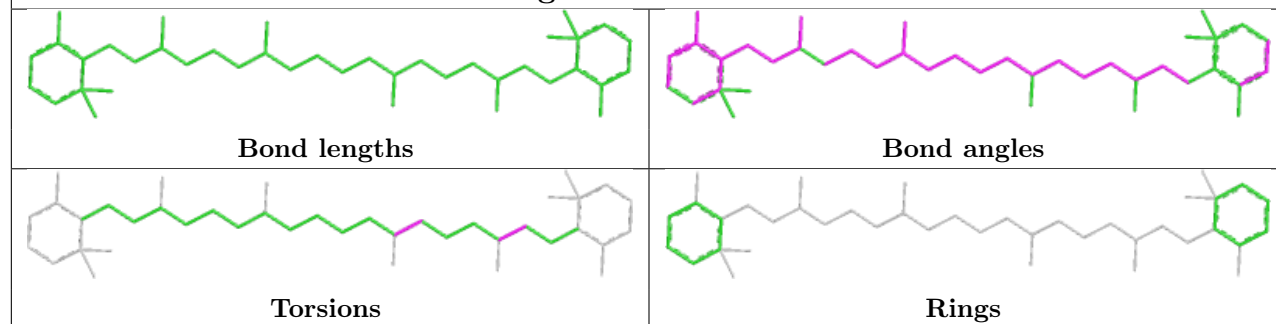
Ligand CLA 9 313

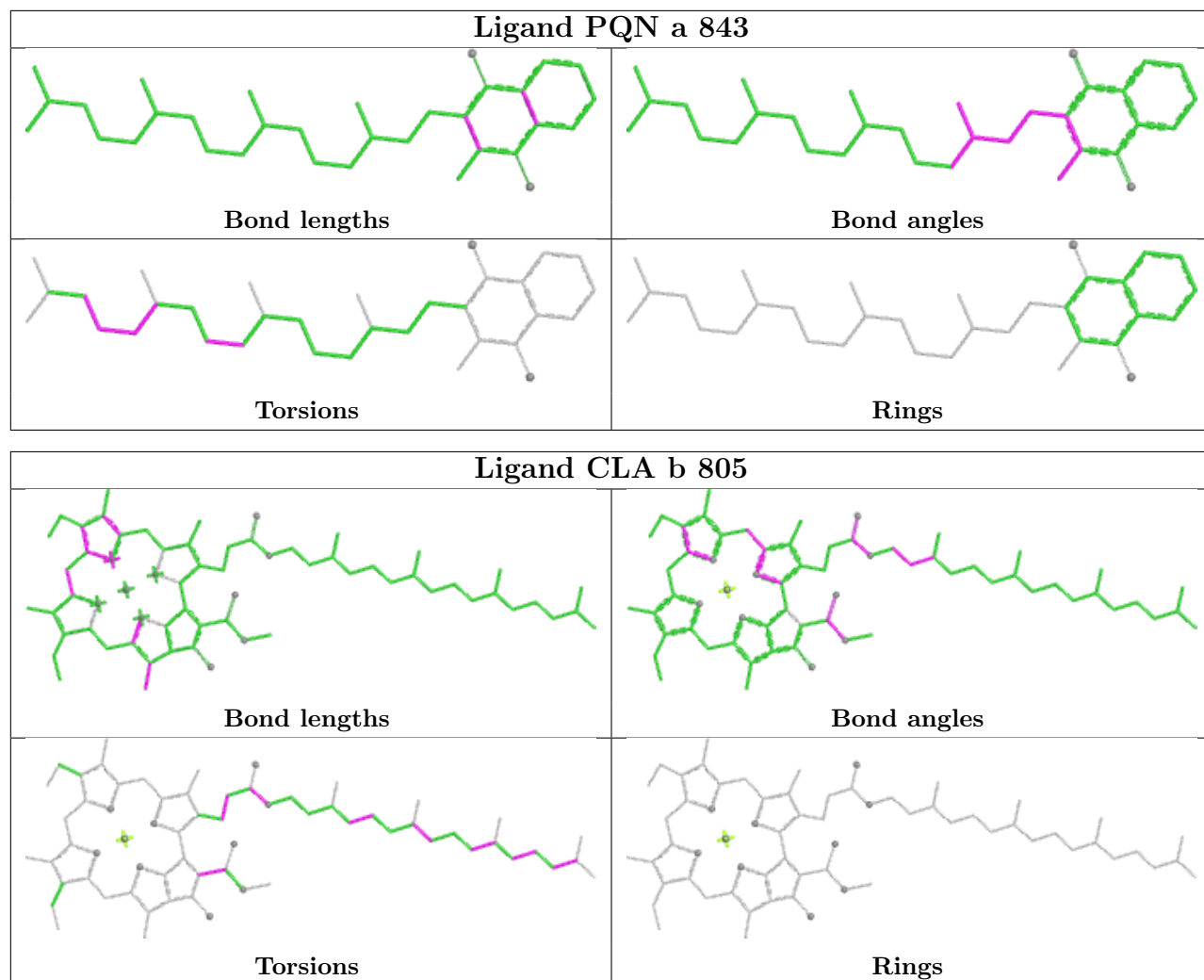


Ligand CLA 2 313

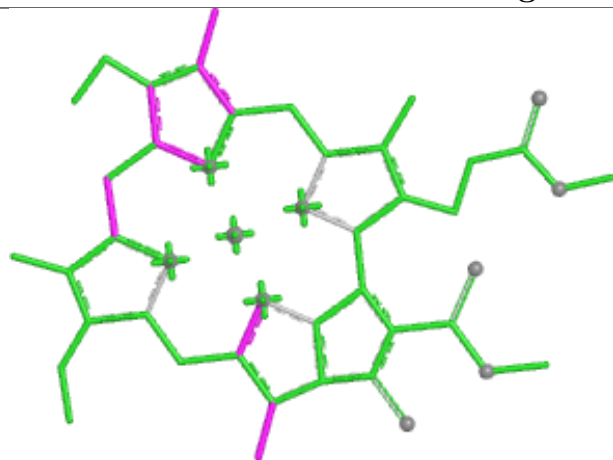


Ligand BCR f 801

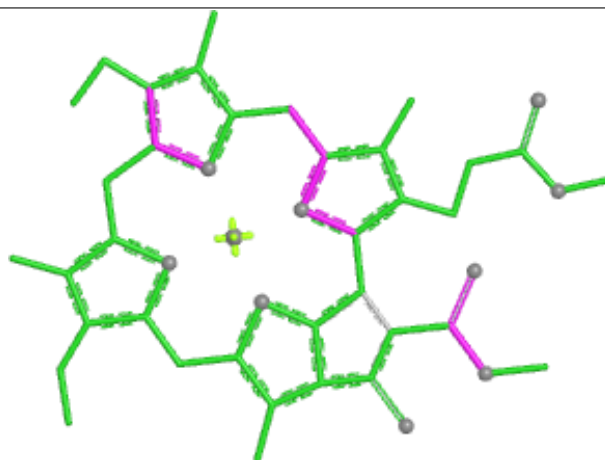




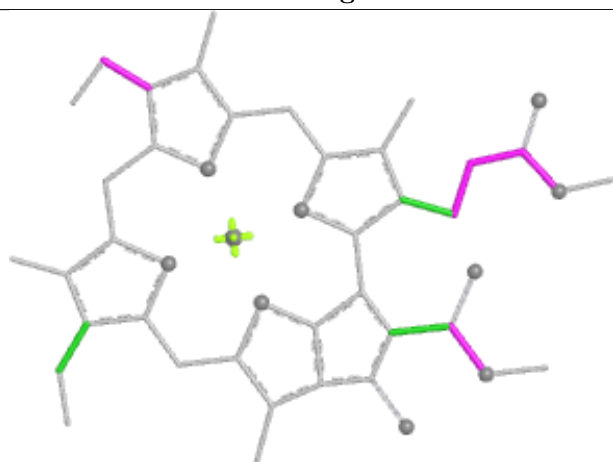
Ligand CLA 5 310



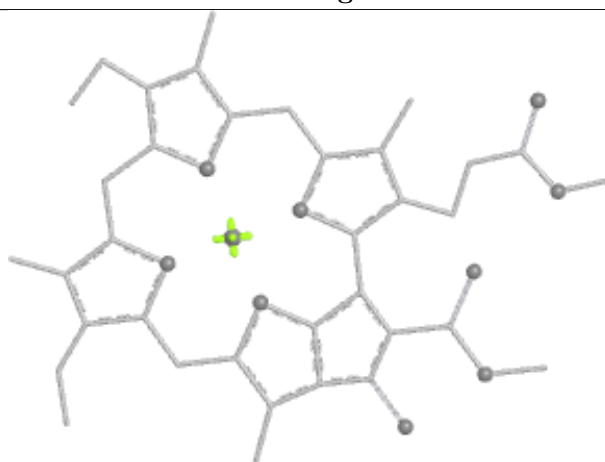
Bond lengths



Bond angles

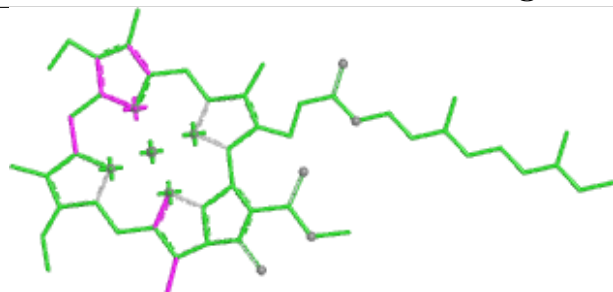


Torsions

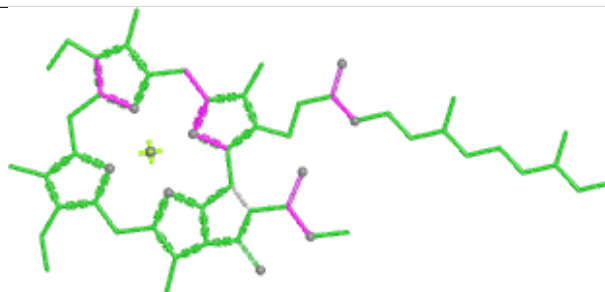


Rings

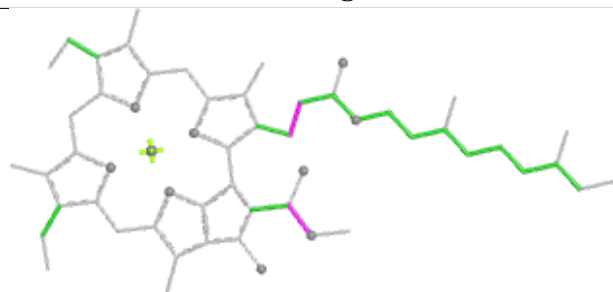
Ligand CLA 3 309



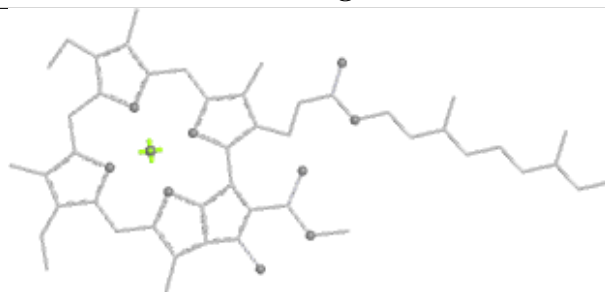
Bond lengths



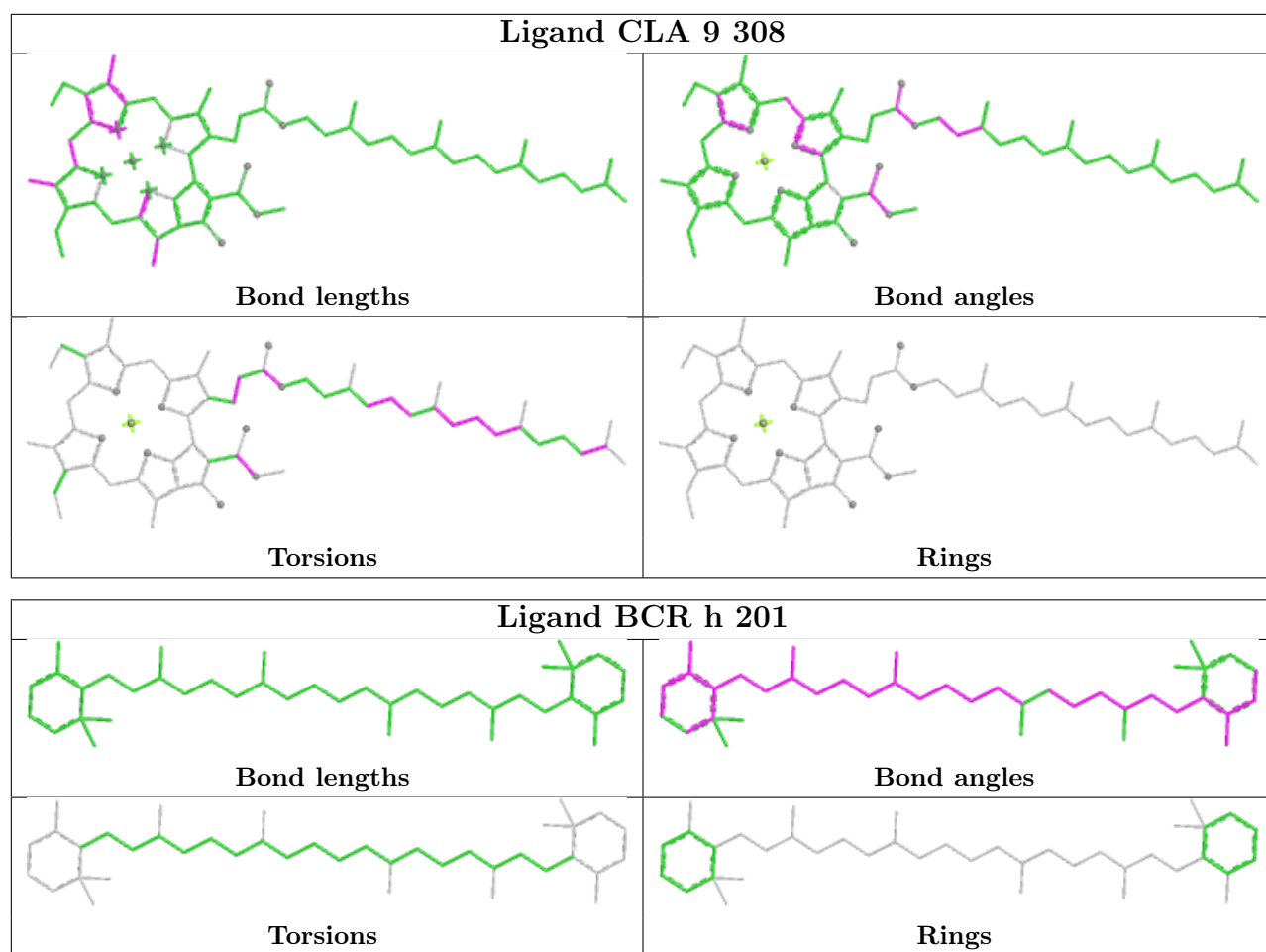
Bond angles



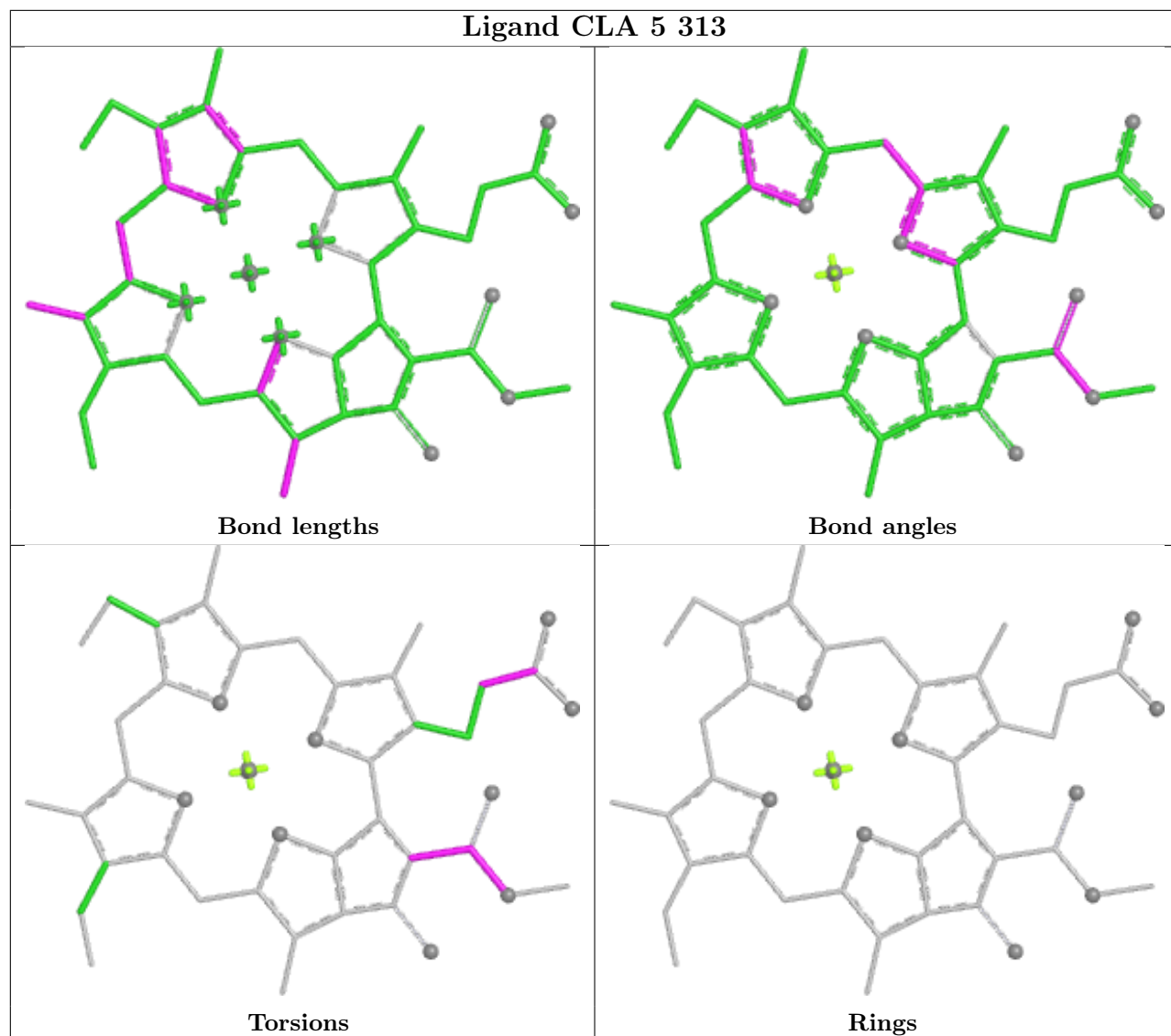
Torsions

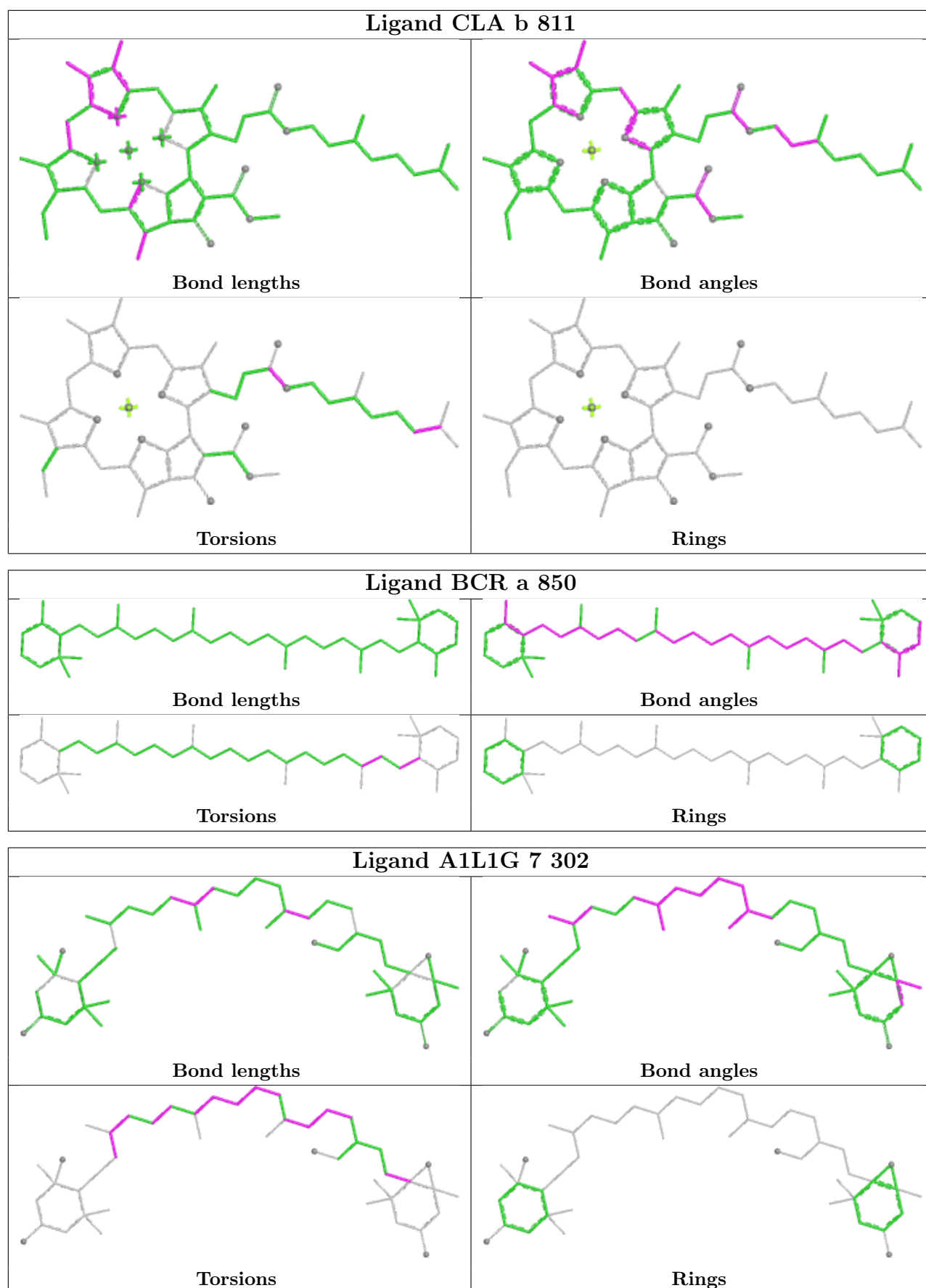


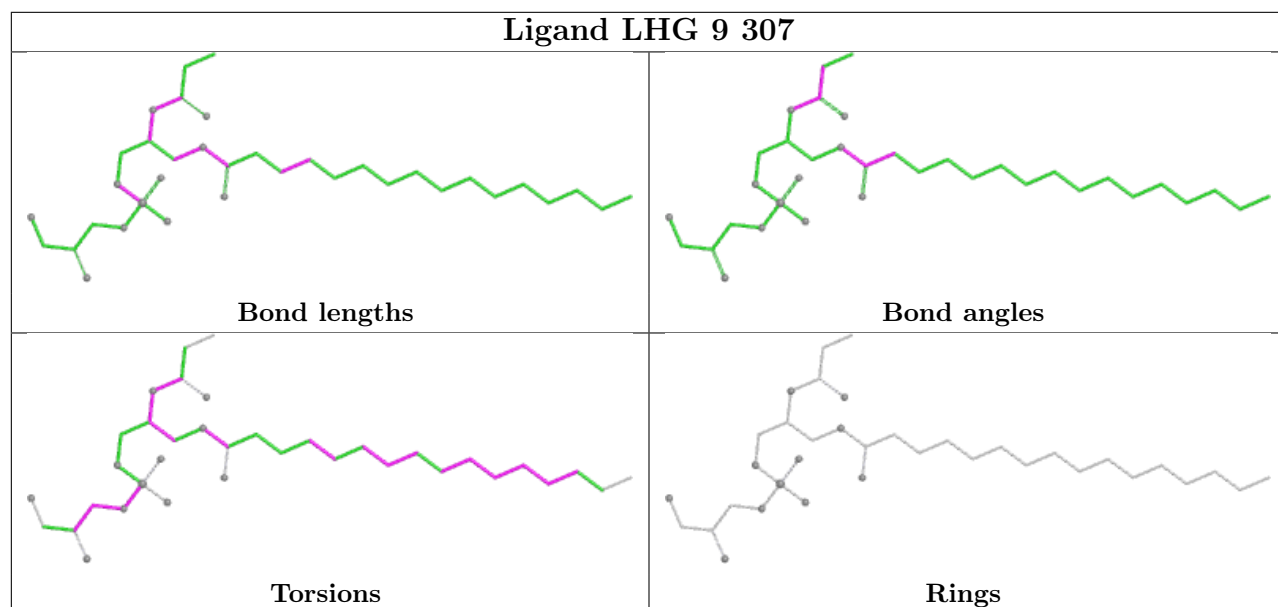
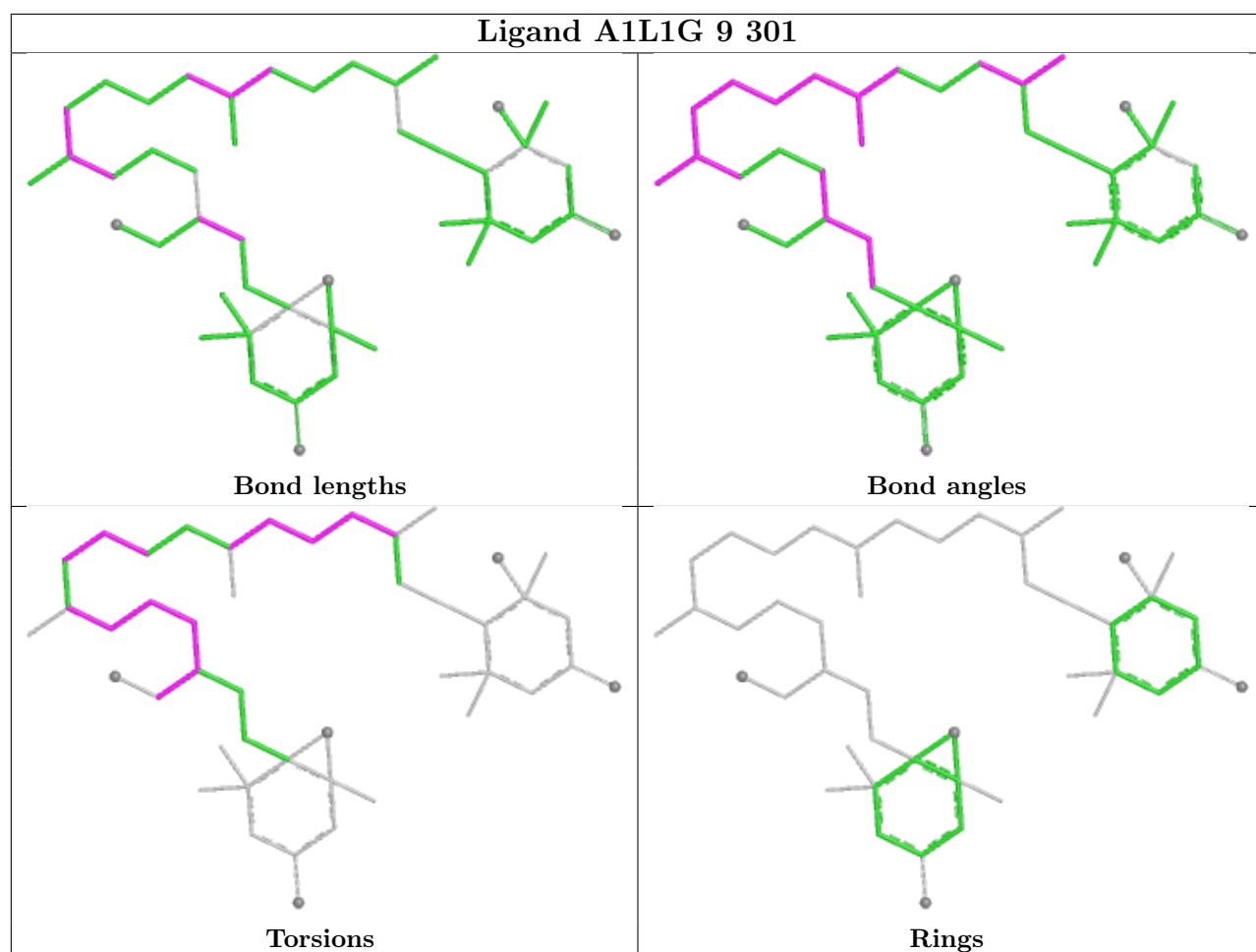
Rings



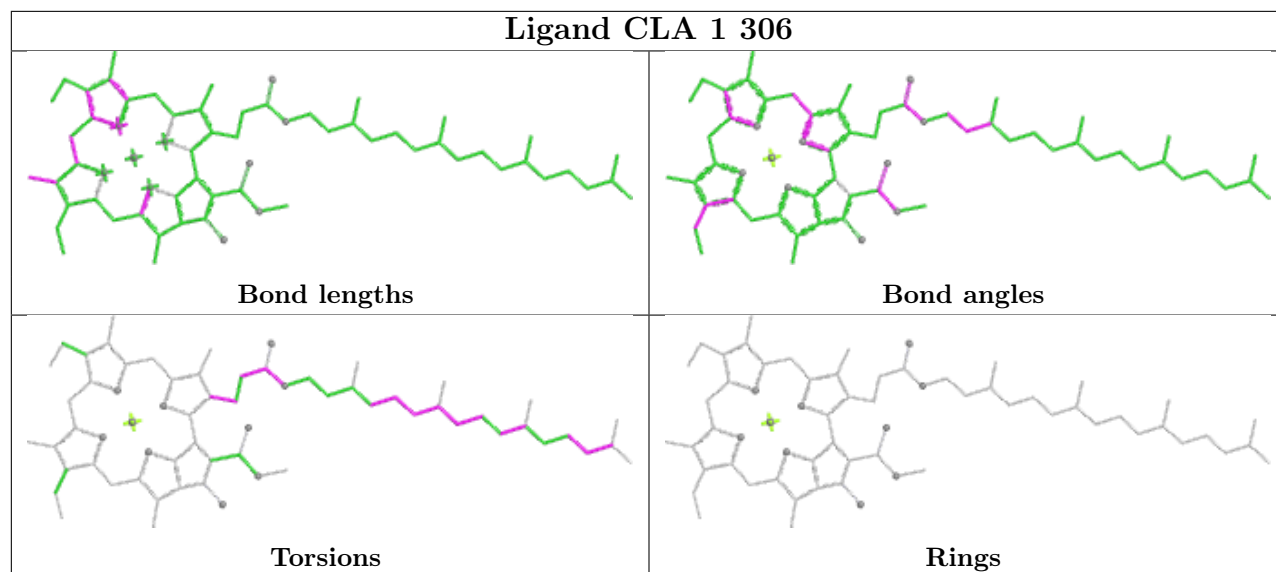
Ligand CLA 5 313



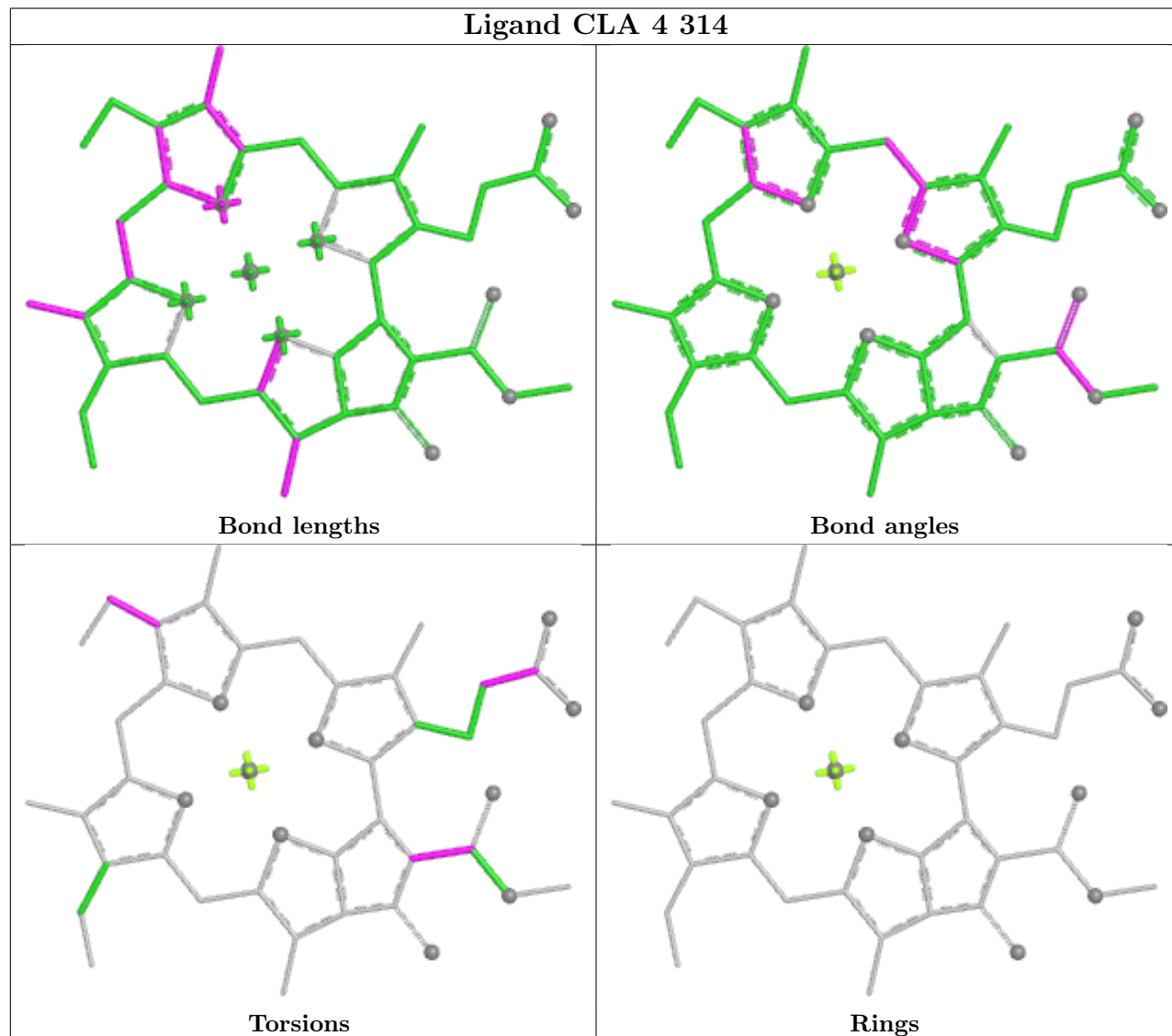




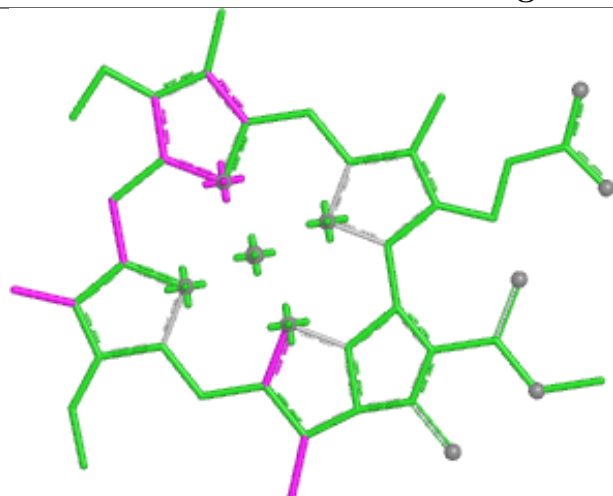
Ligand CLA 1 306



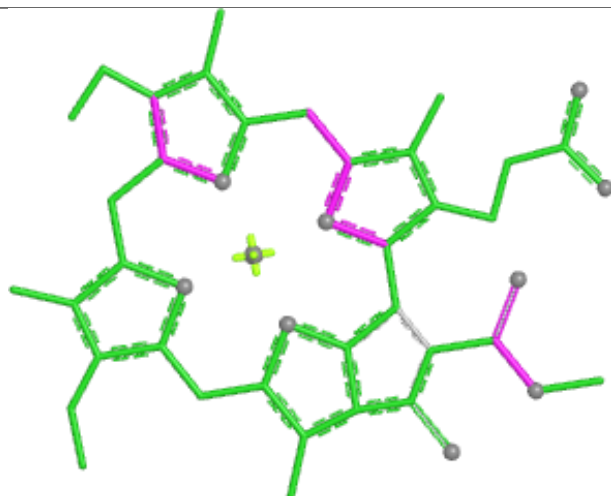
Ligand CLA 4 314



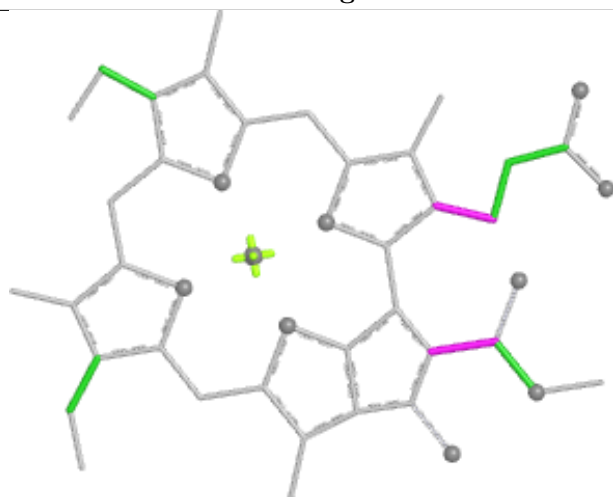
Ligand CLA b 815



Bond lengths



Bond angles

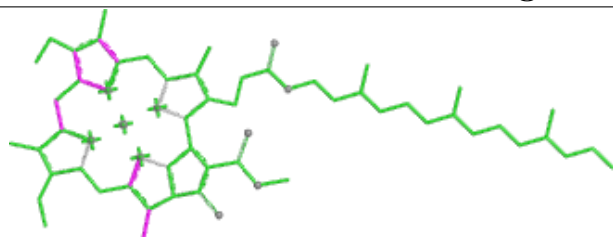


Torsions

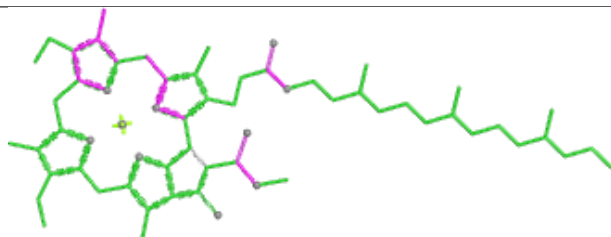


Rings

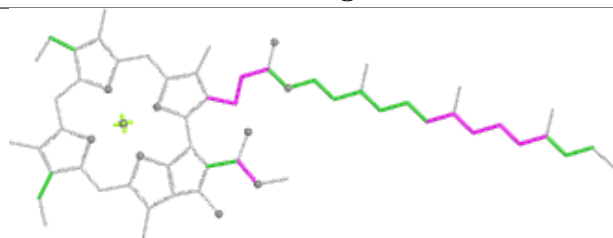
Ligand CLA a 829



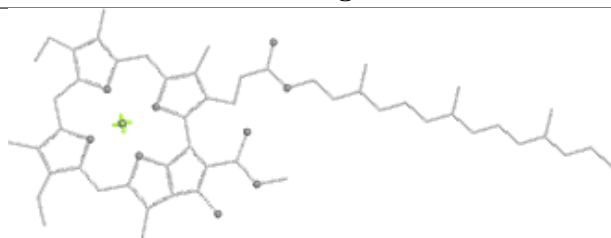
Bond lengths



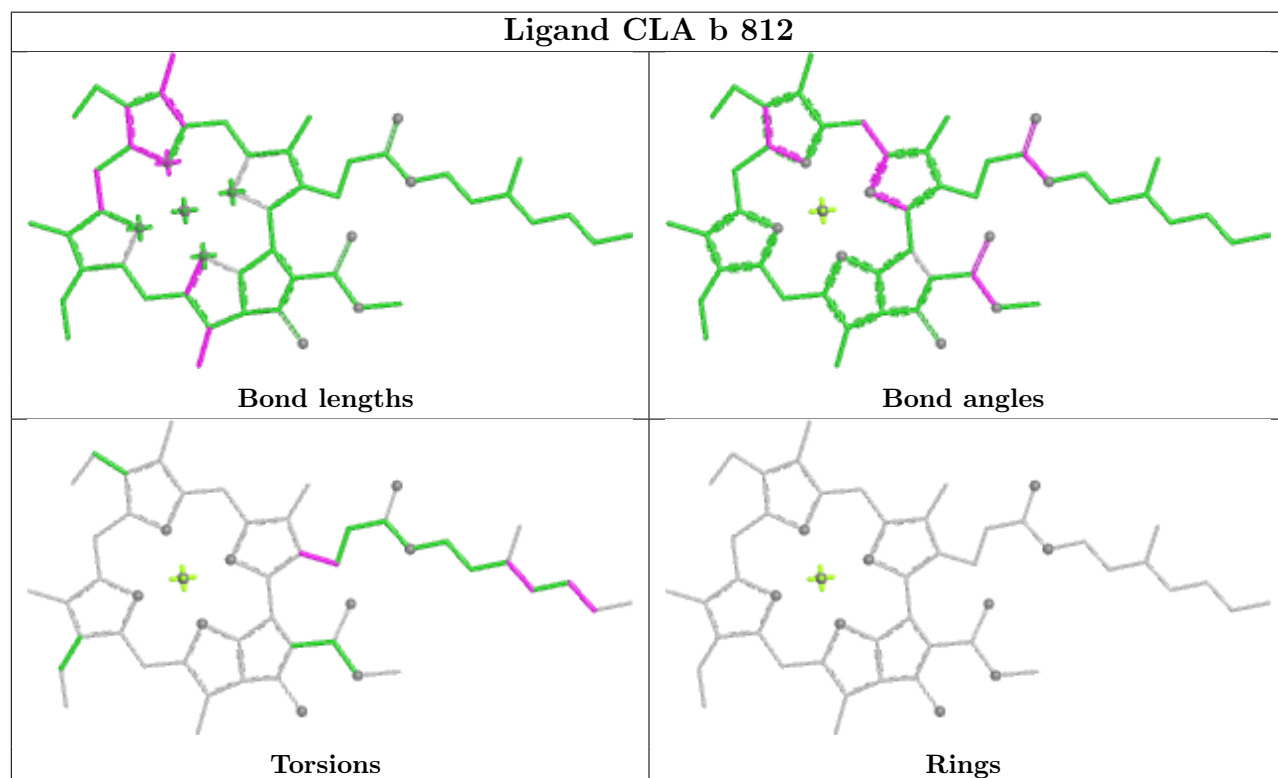
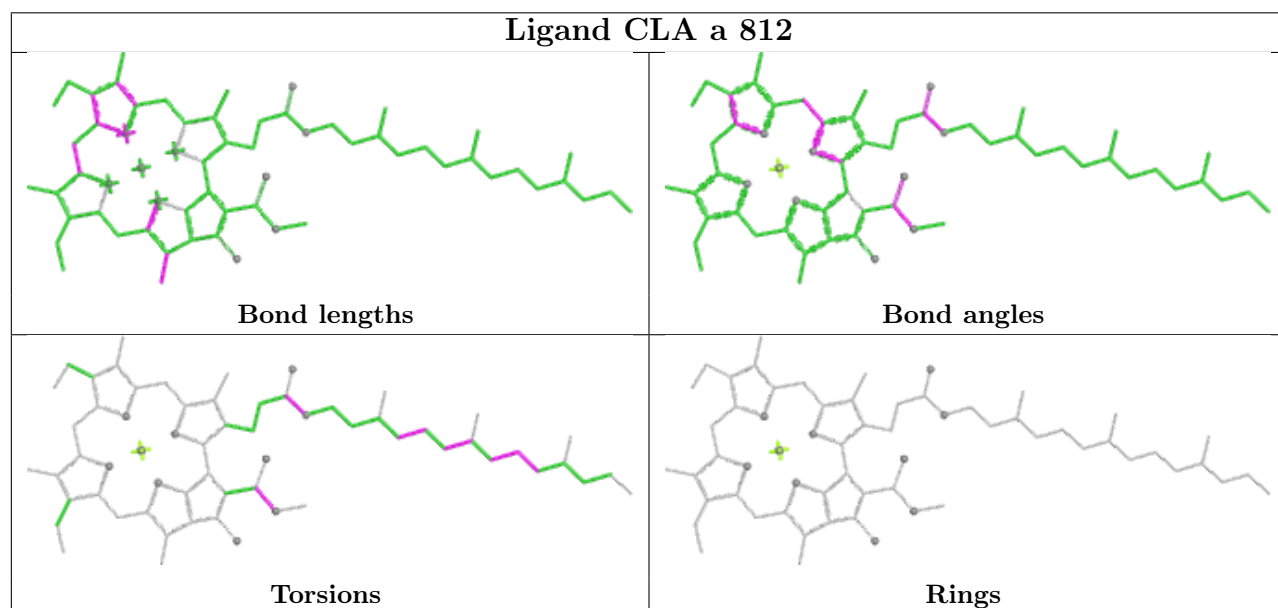
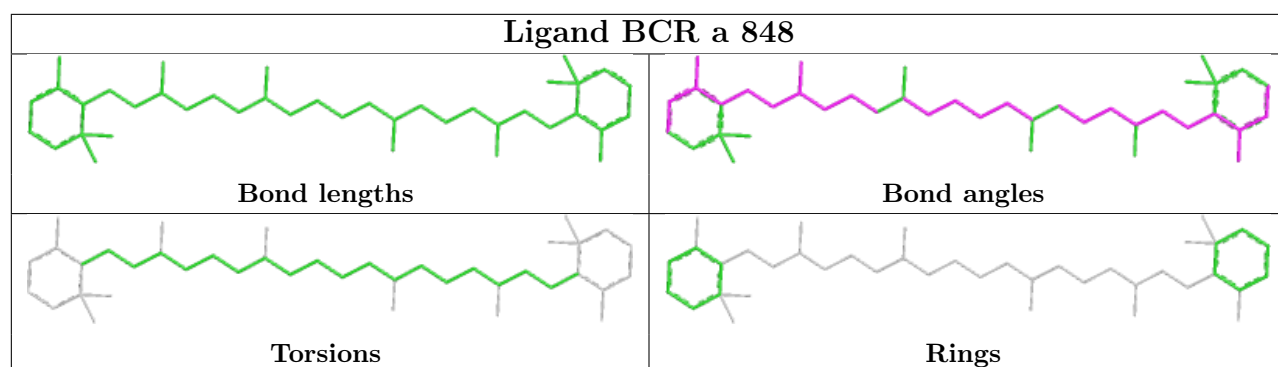
Bond angles



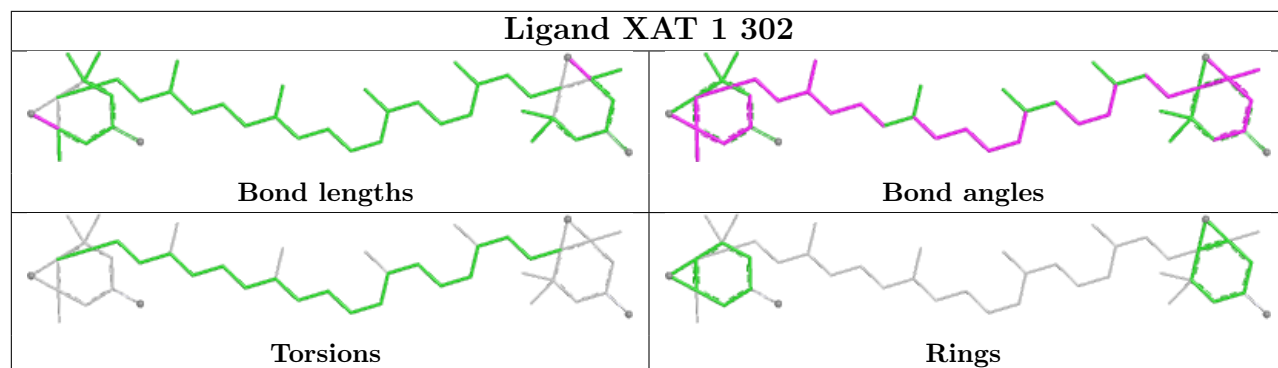
Torsions



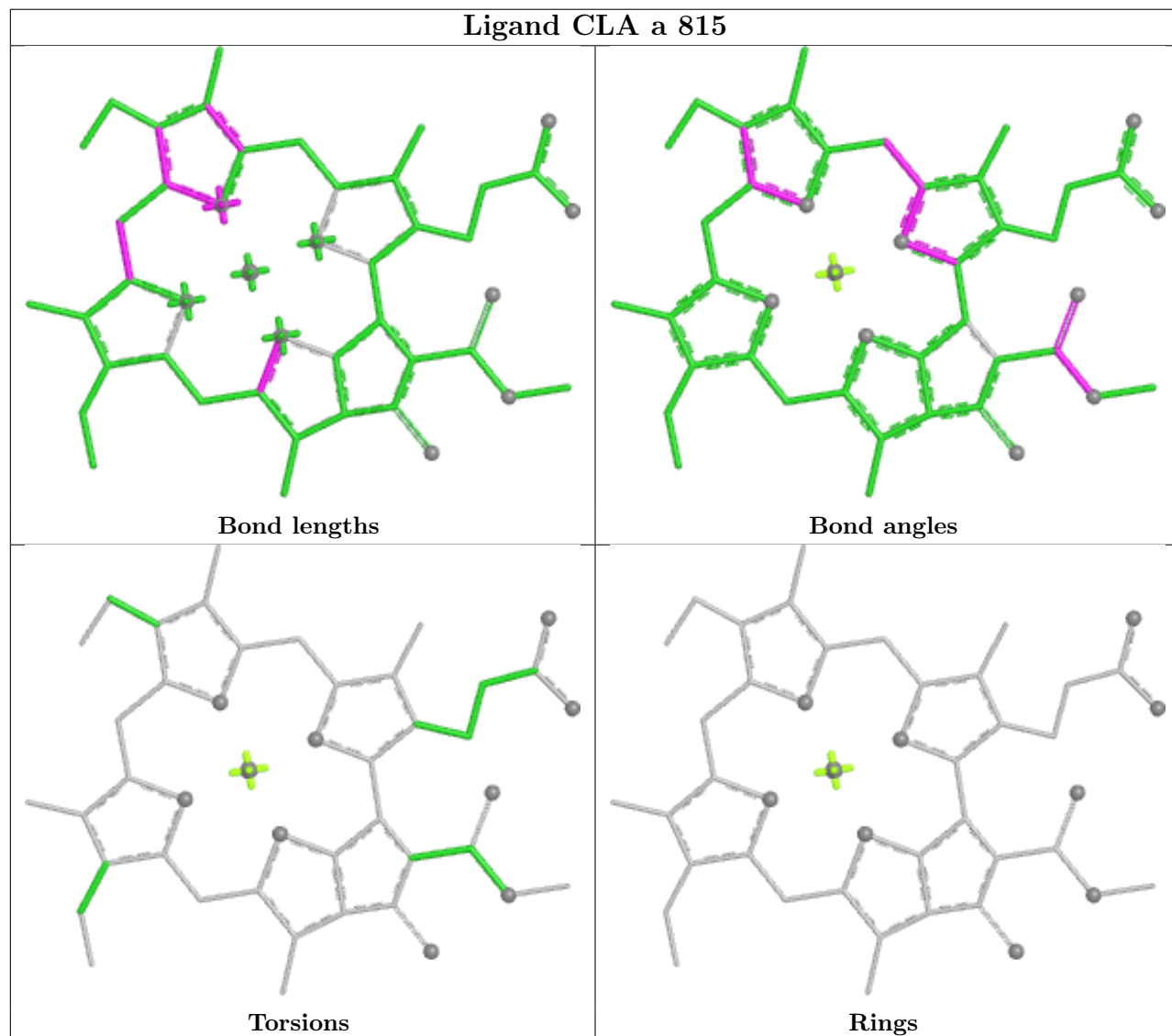
Rings



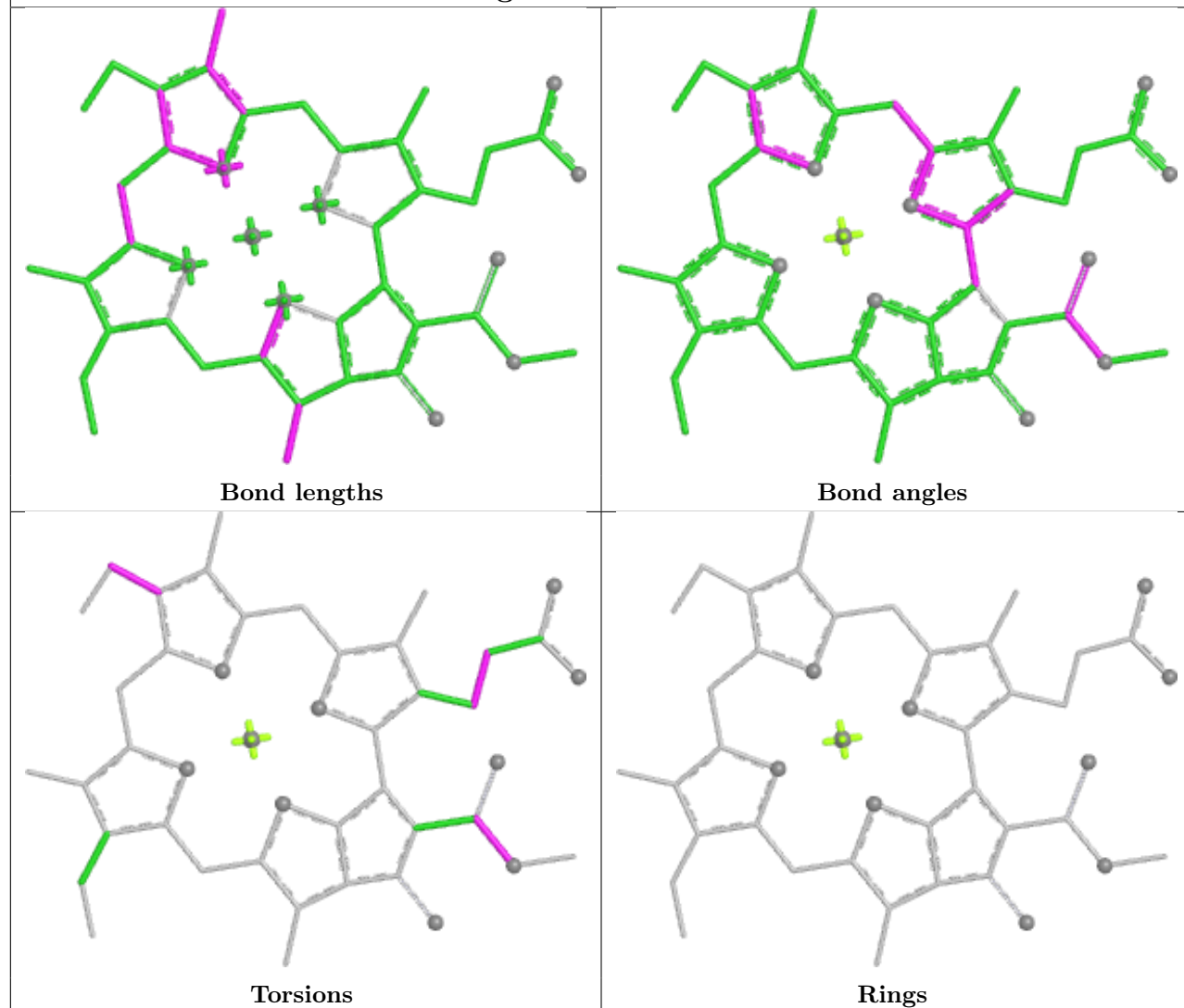
Ligand XAT 1 302



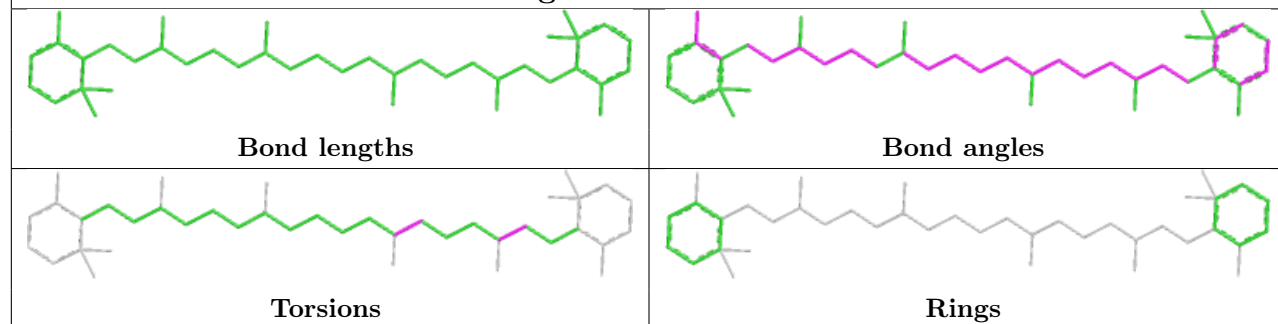
Ligand CLA a 815



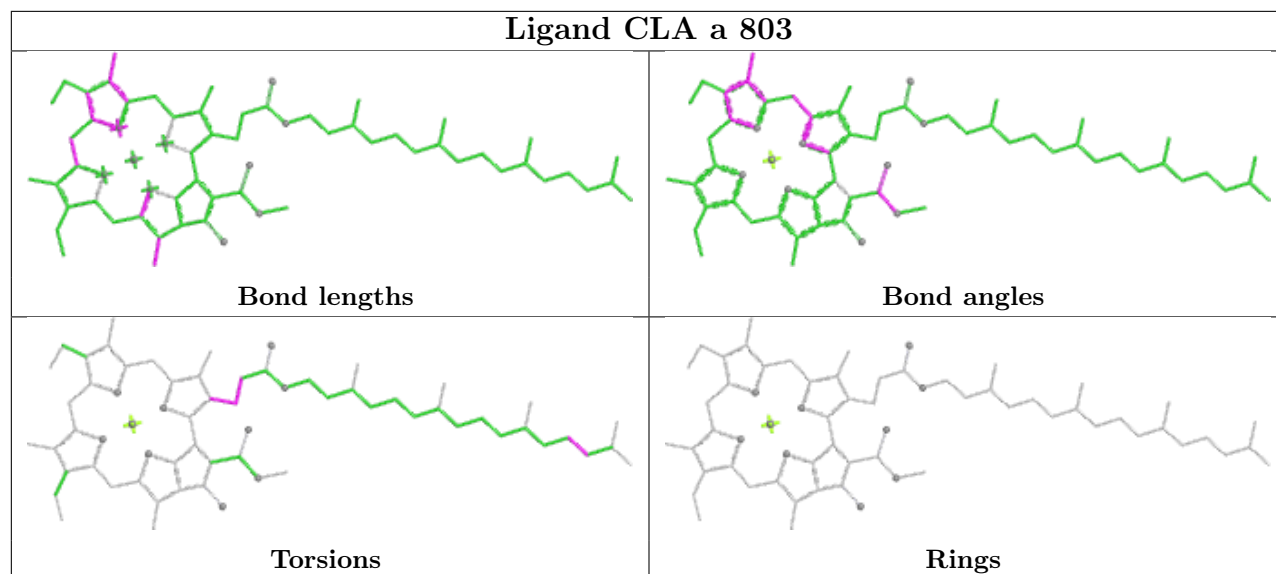
Ligand CLA 7 314



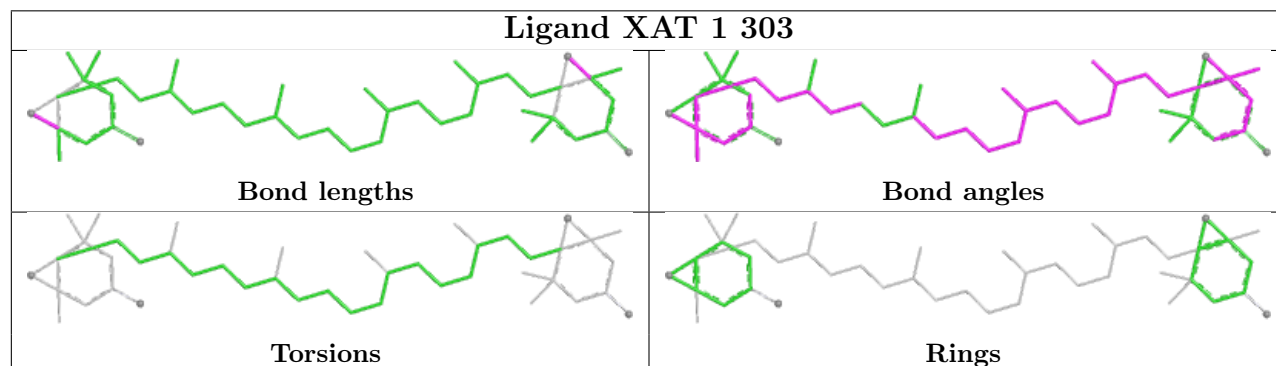
Ligand BCR i 101



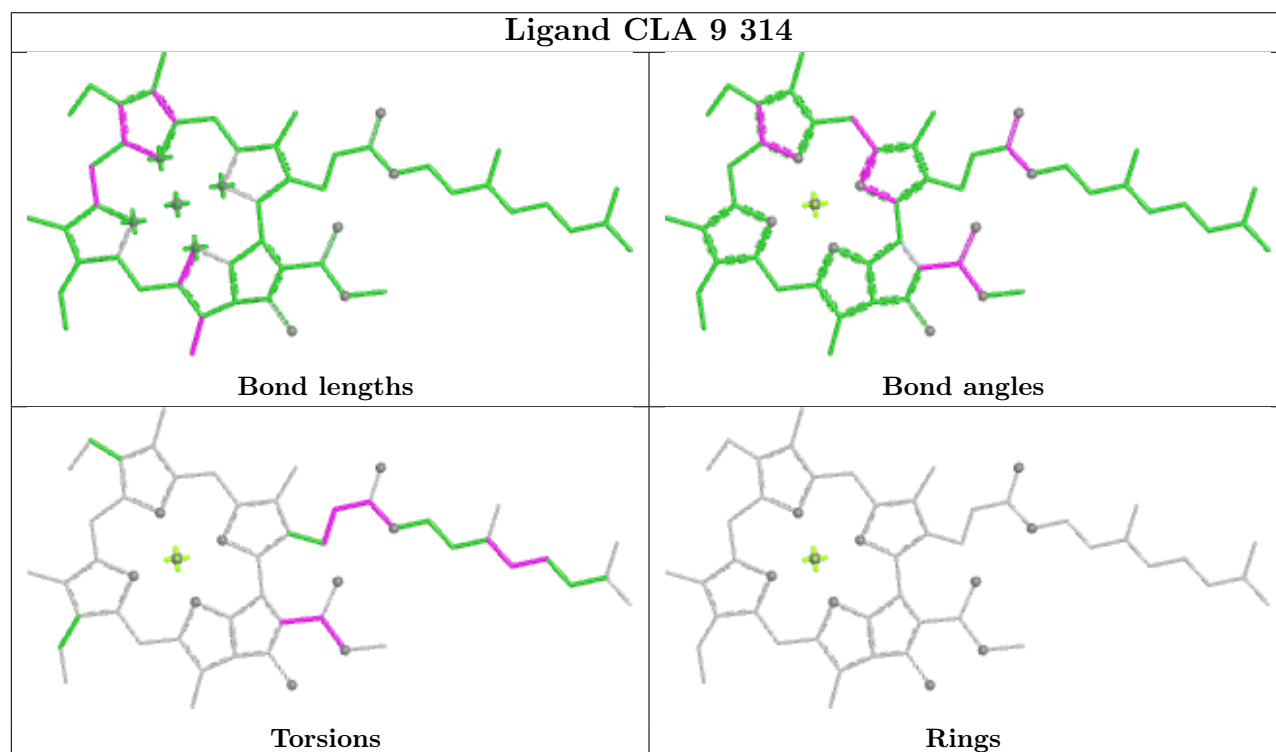
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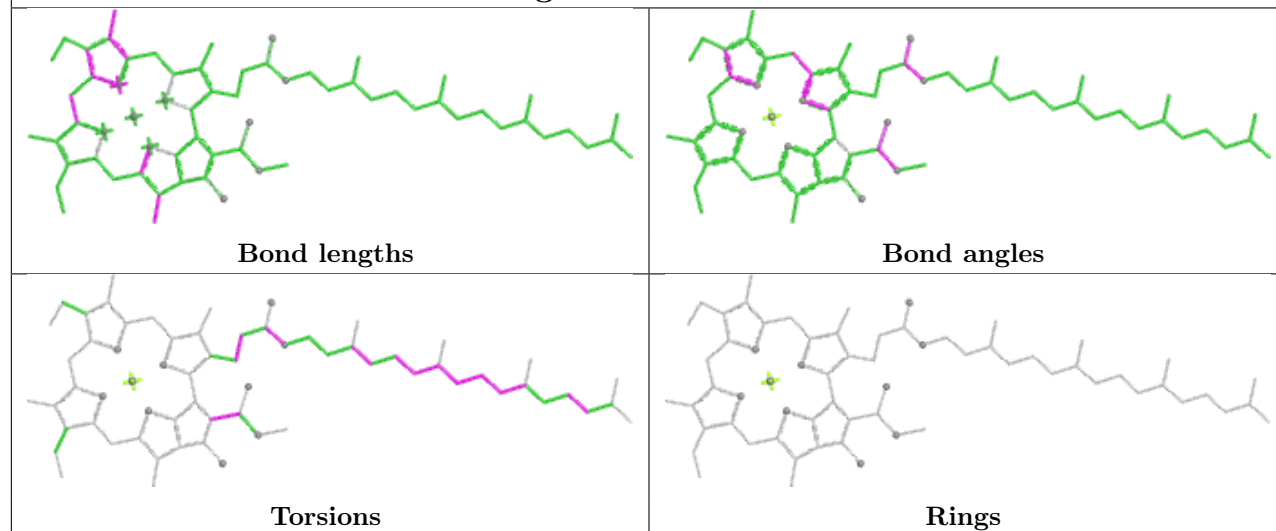
Ligand XAT 1 303



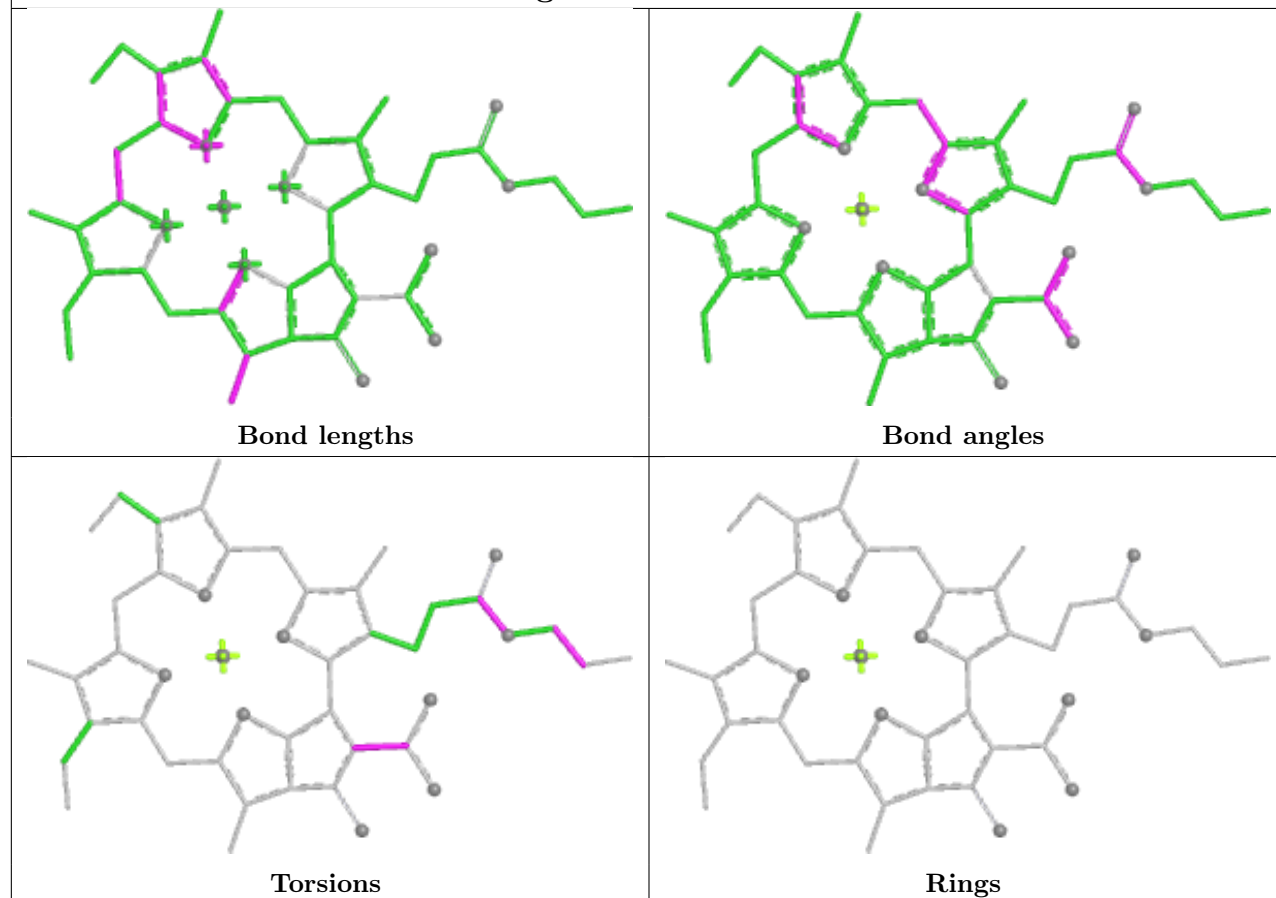
Ligand CLA 9 314

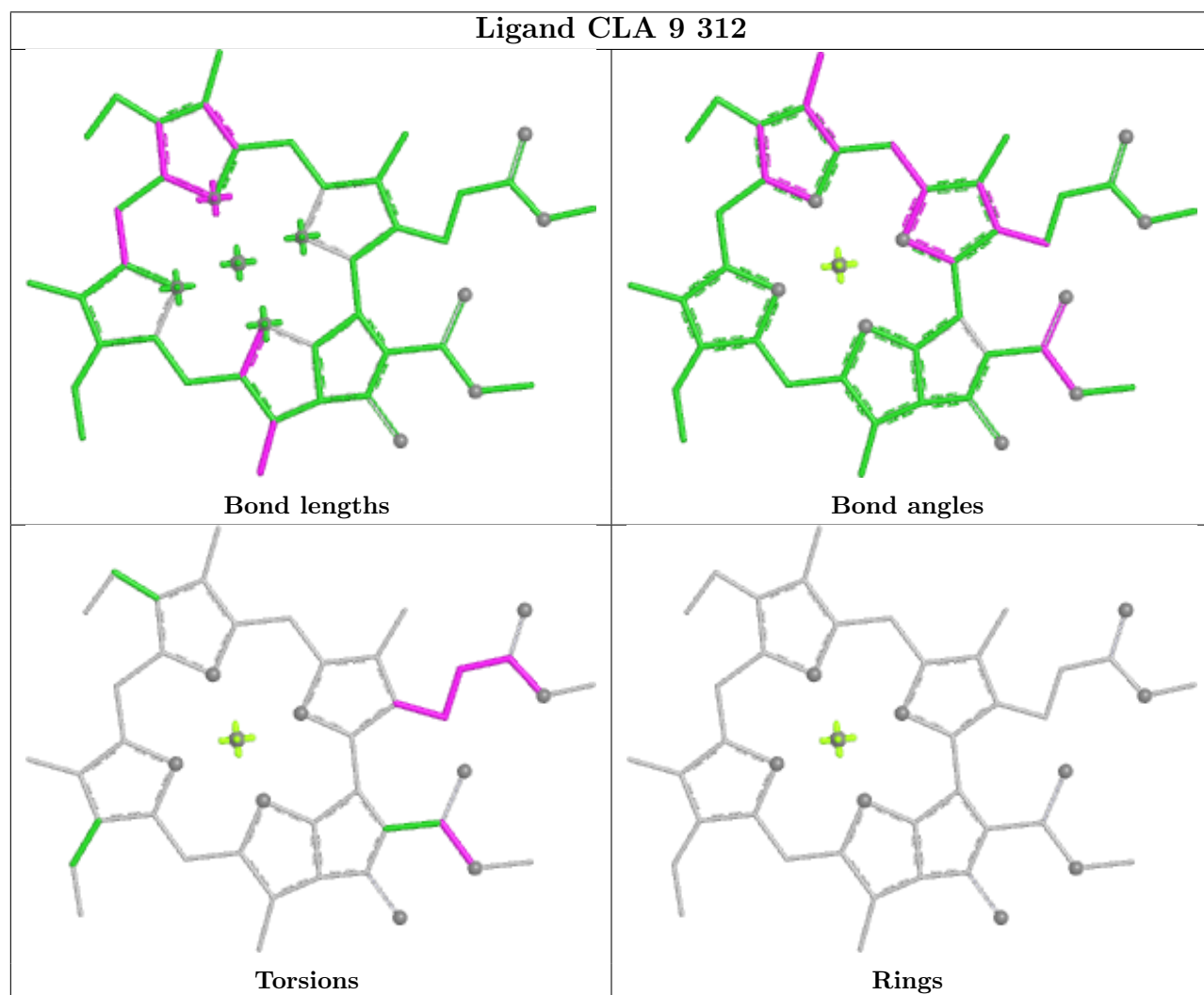
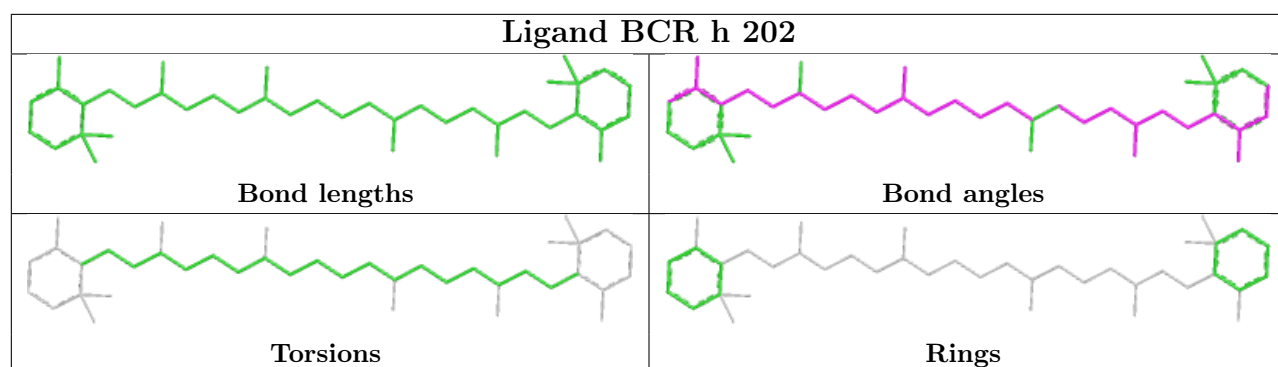


Ligand CLA b 824

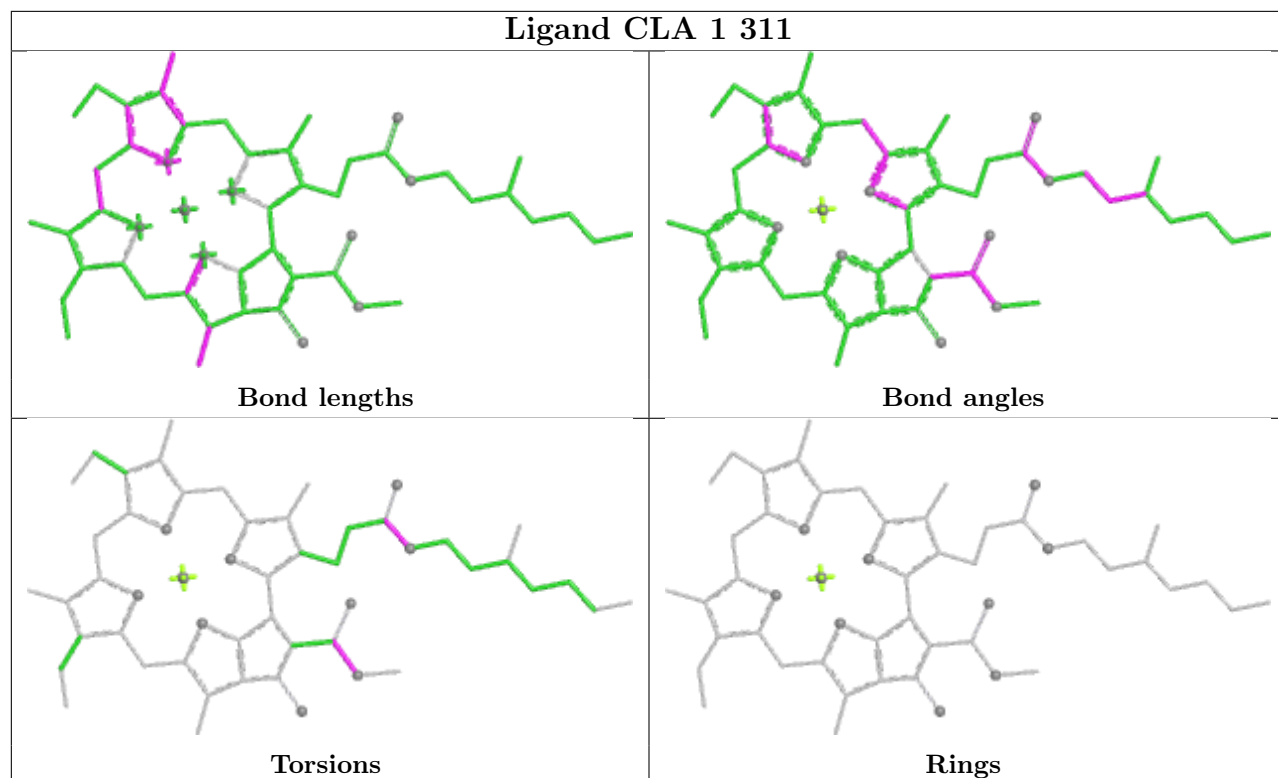


Ligand CLA 7 309

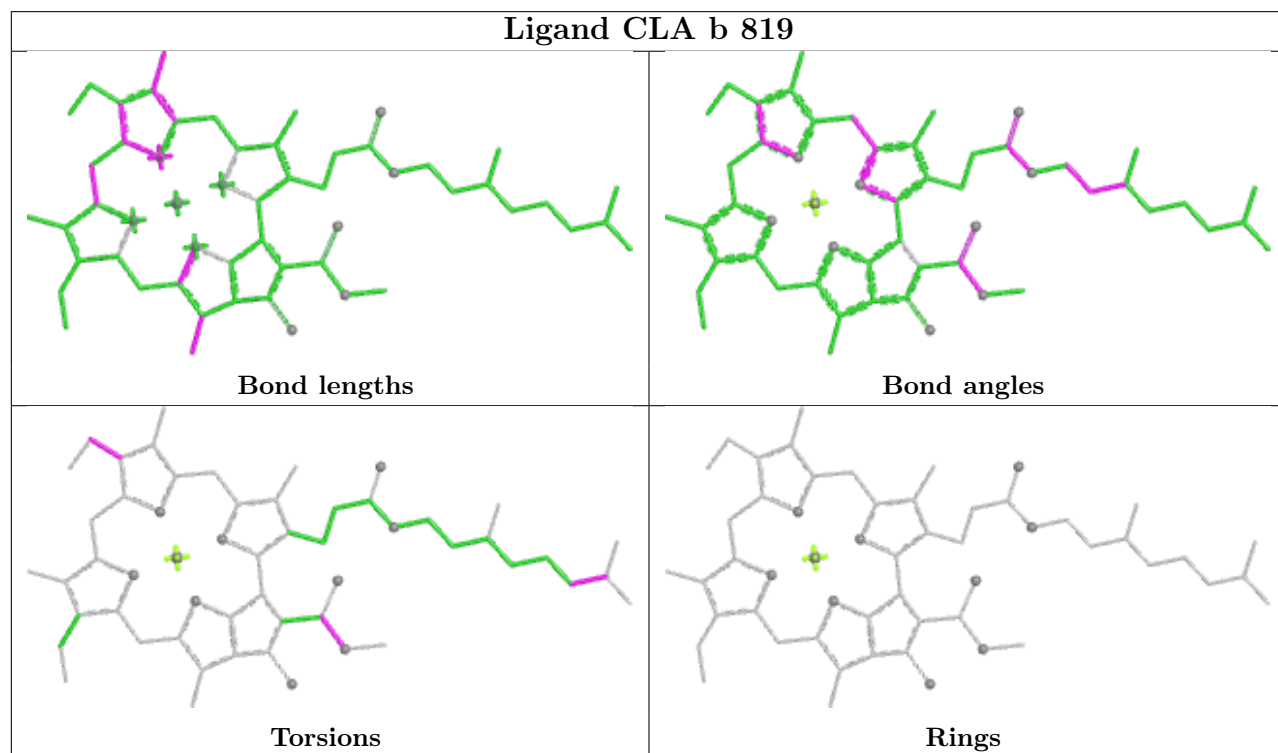


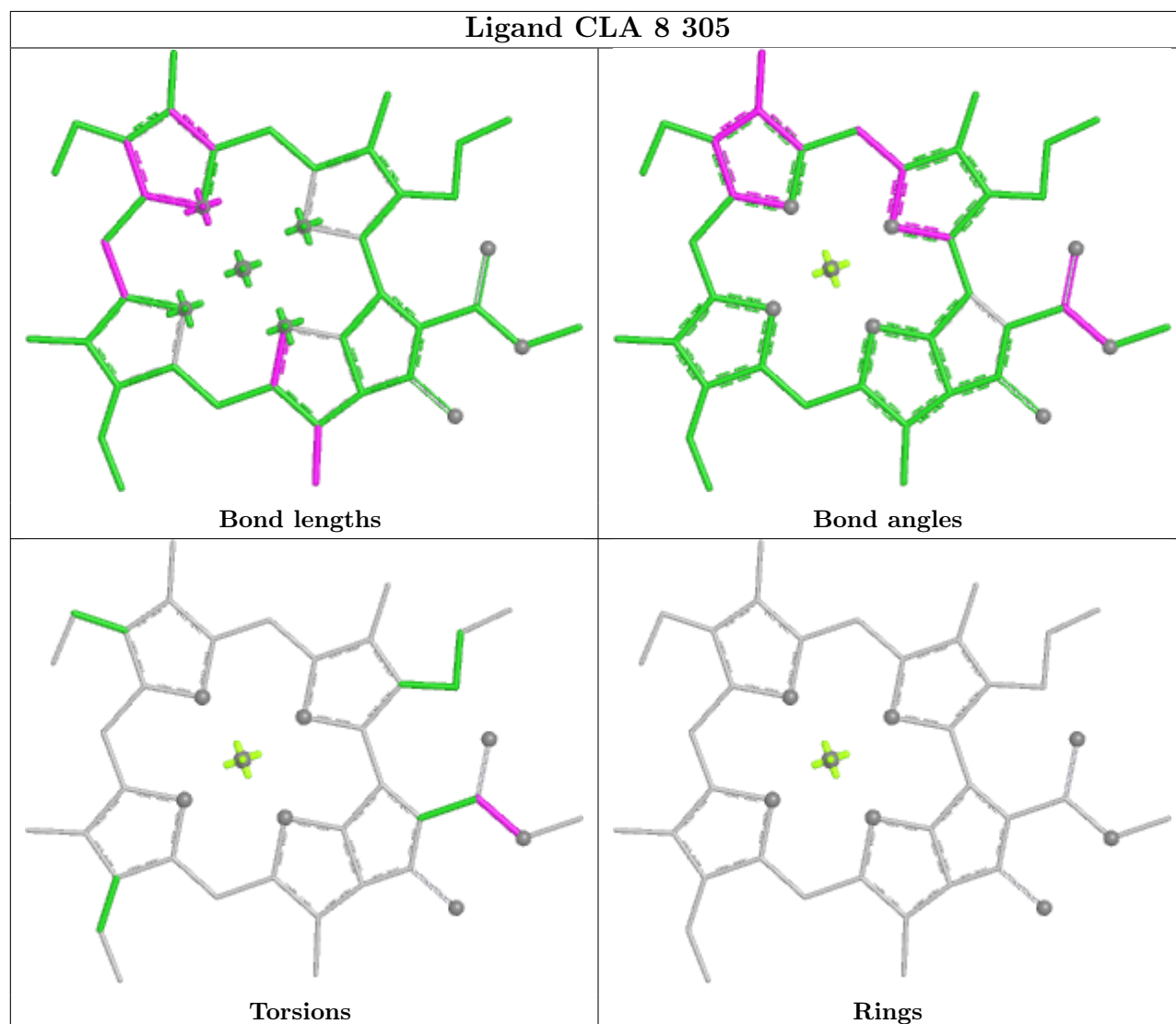
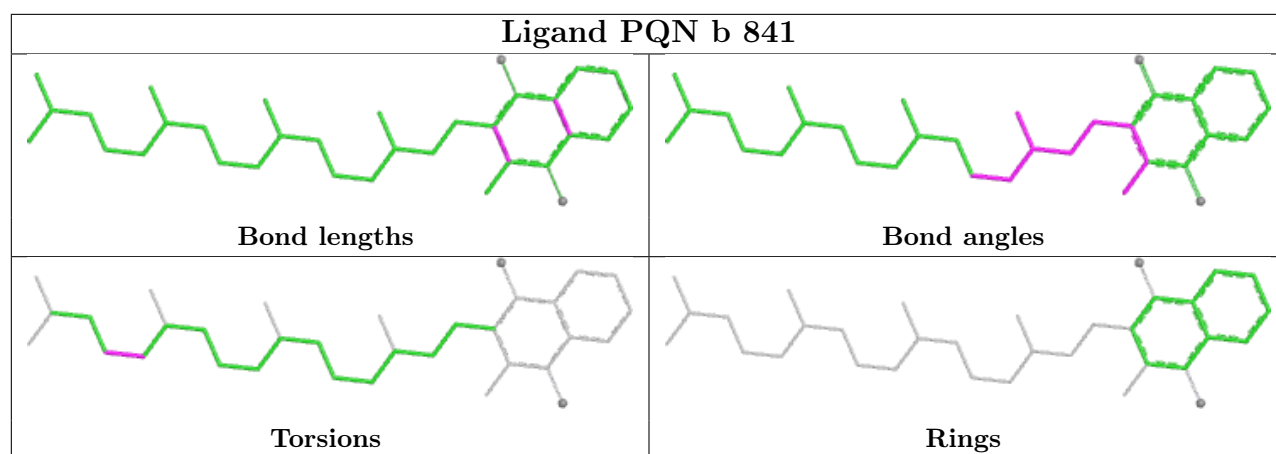


Ligand CLA 1 311

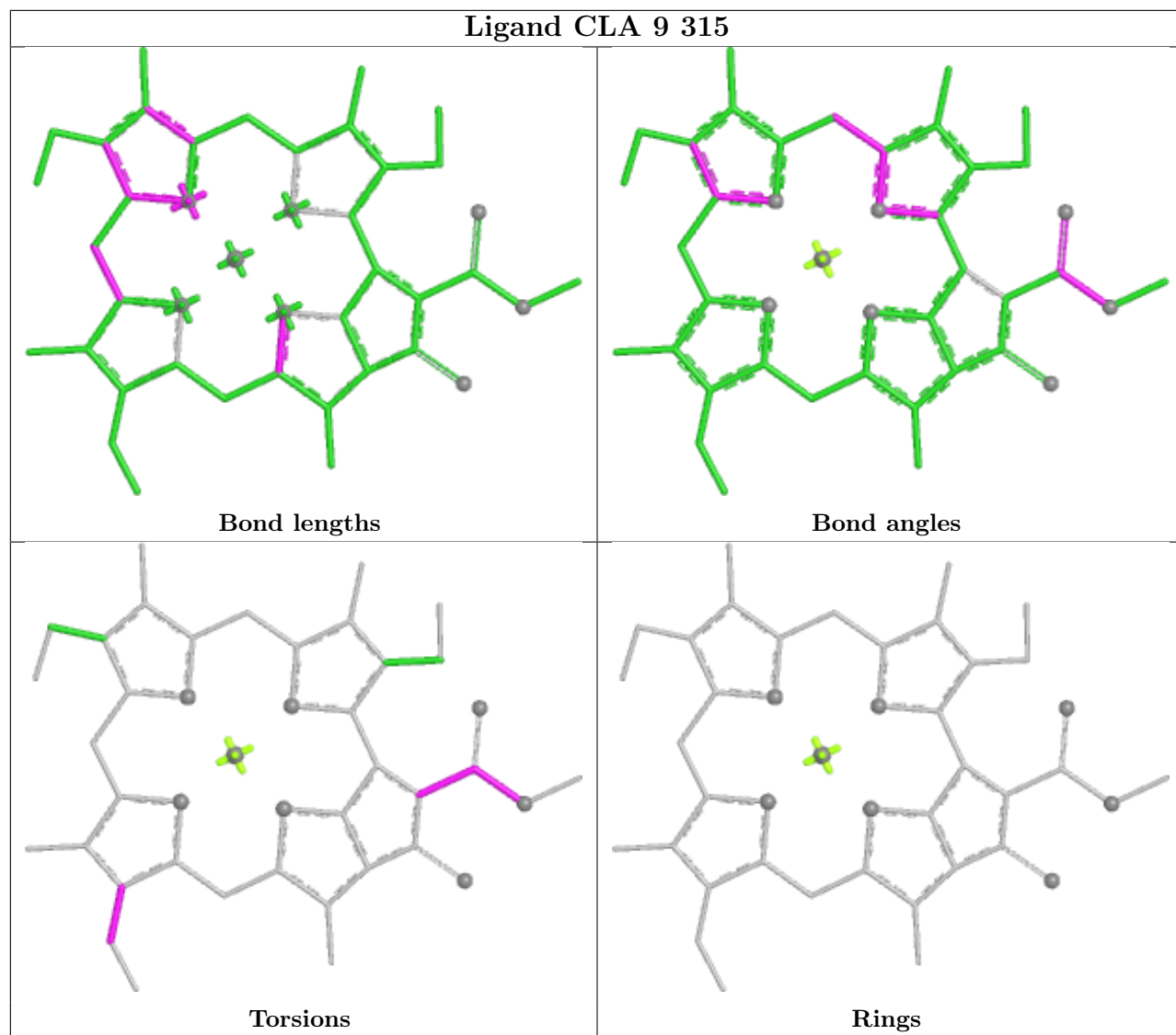


Ligand CLA b 819

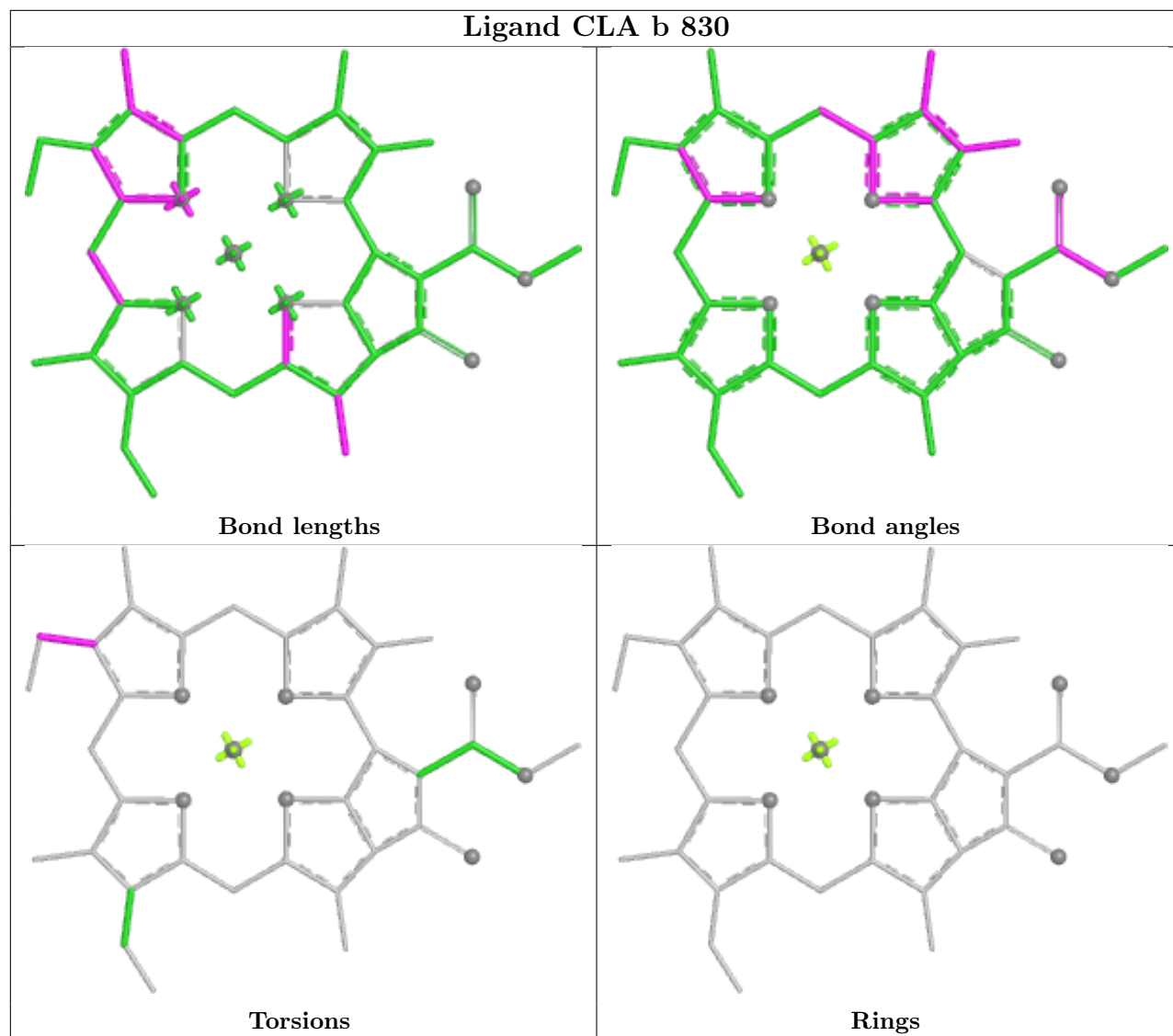




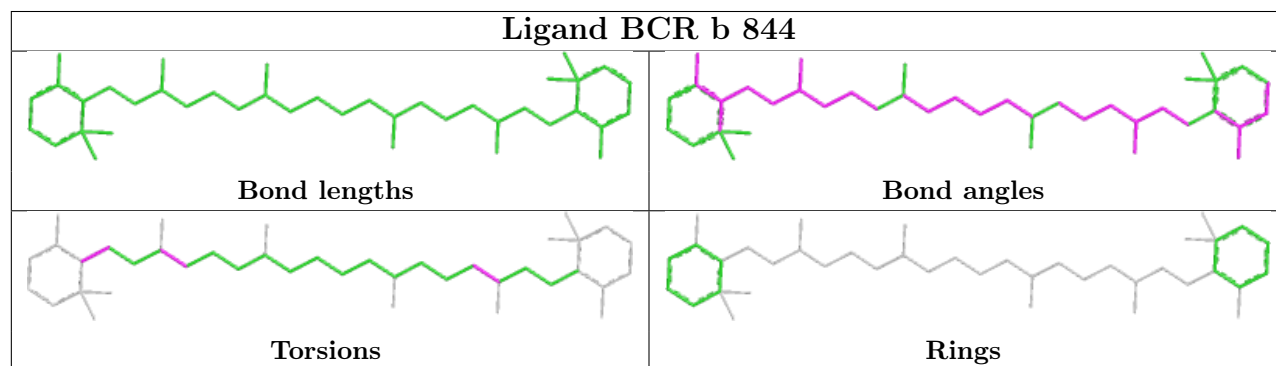
Ligand CLA 9 315



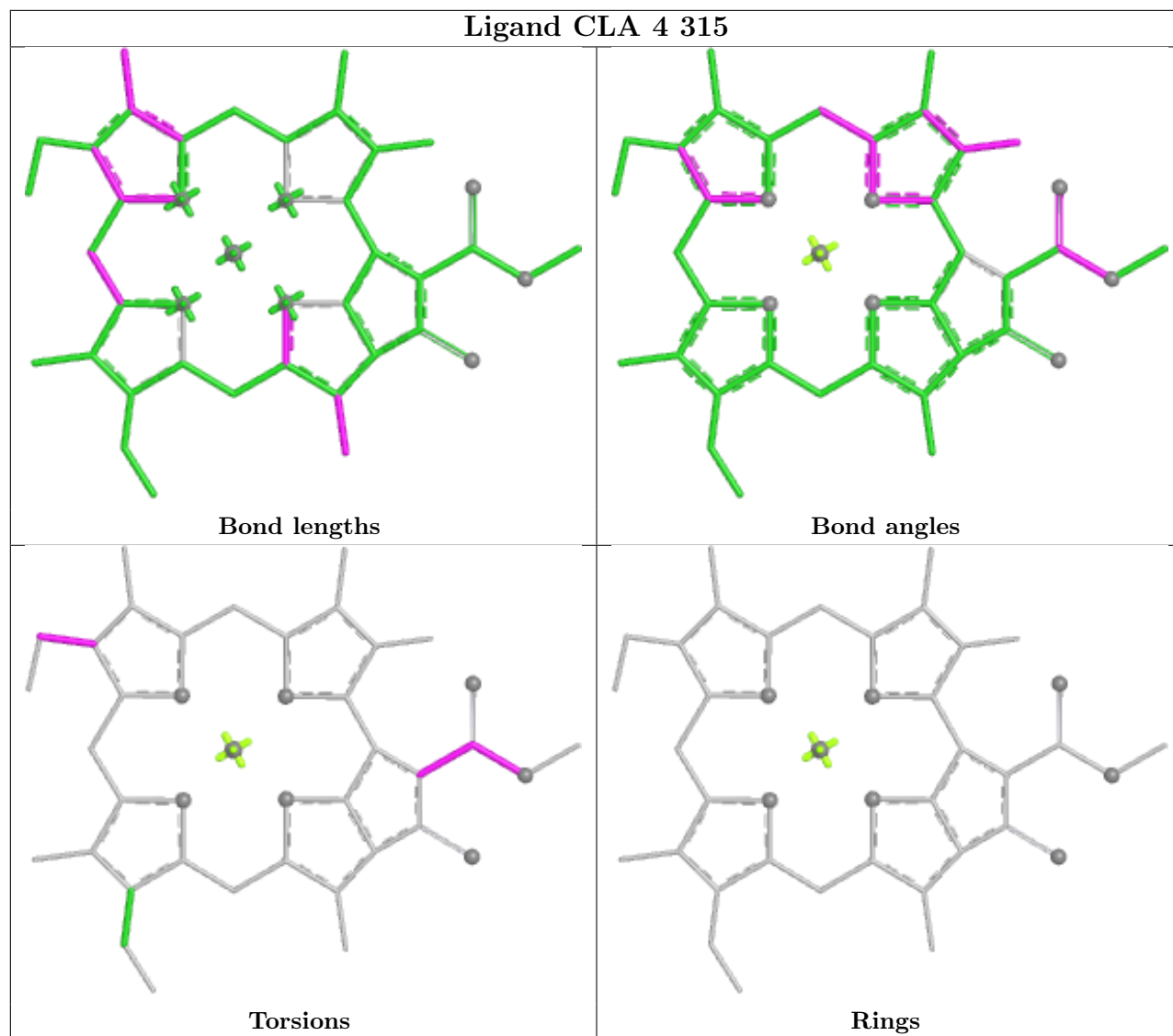
Ligand CLA b 830



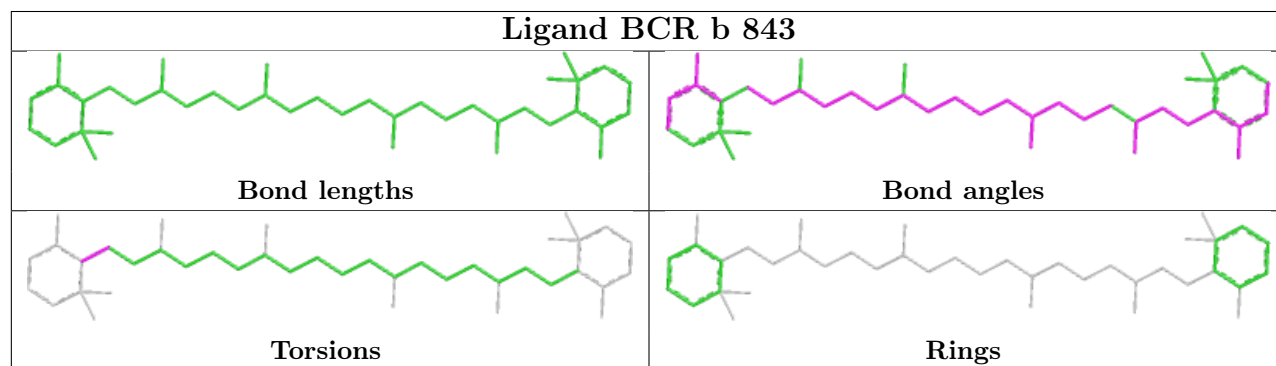
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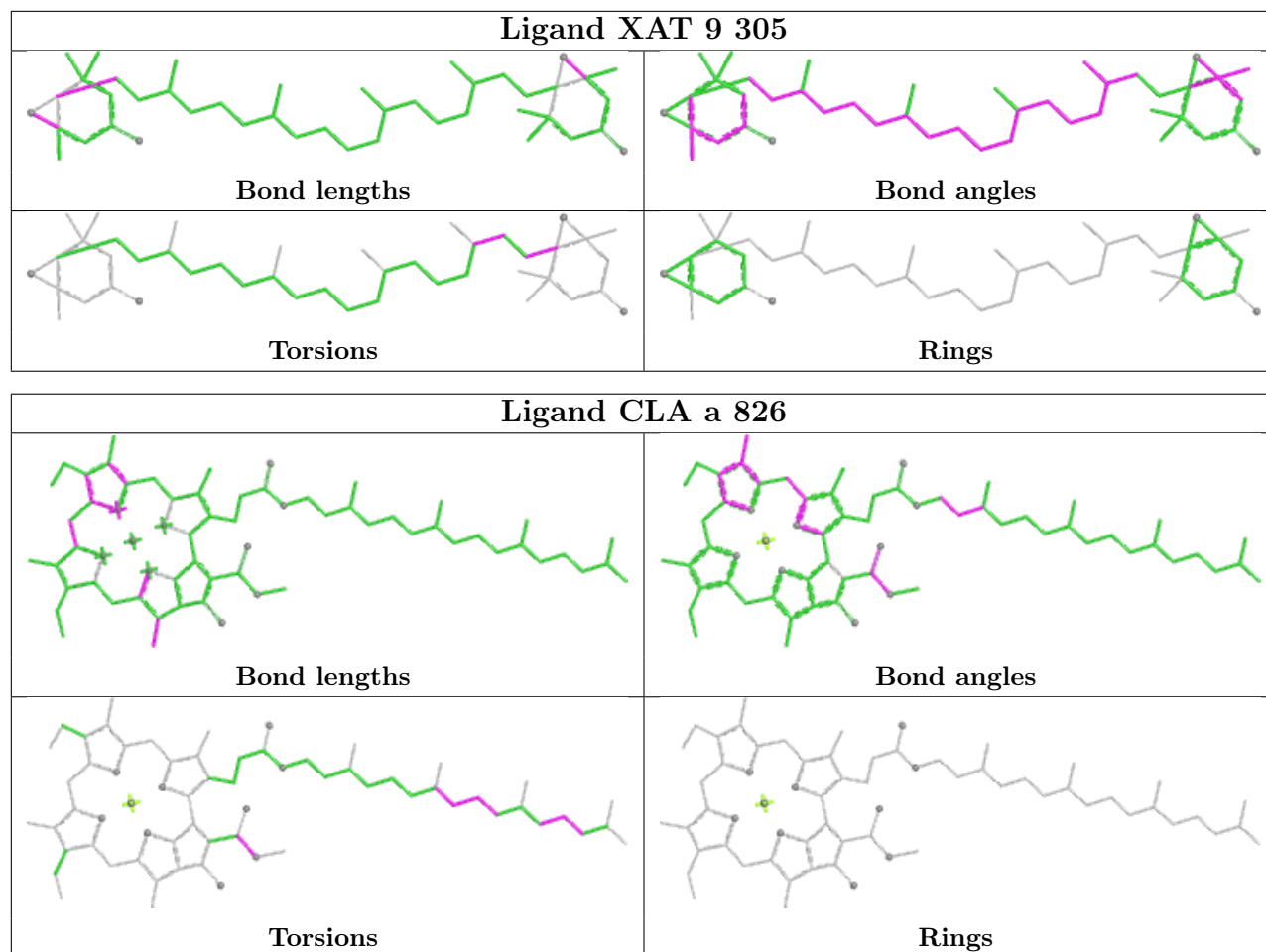


Ligand CLA 4 315

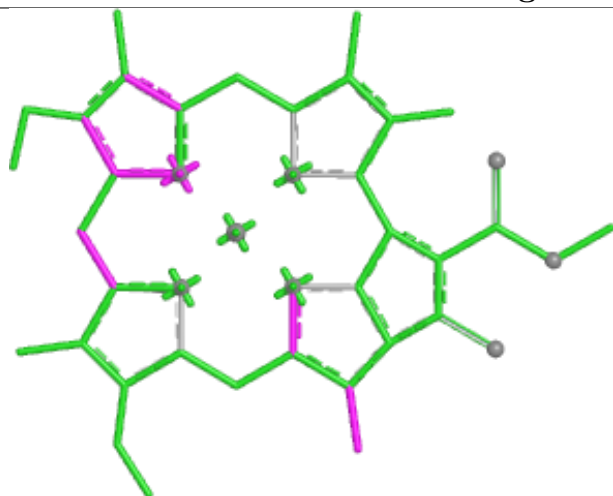


Ligand BCR b 843

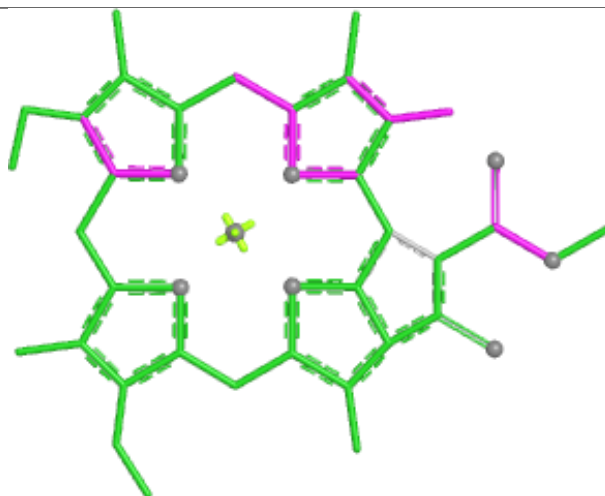




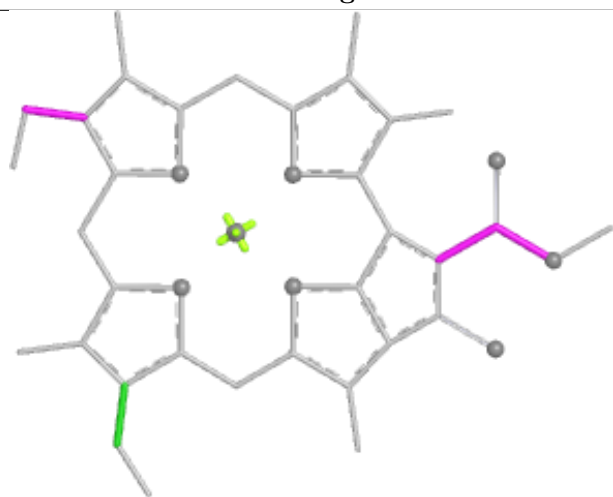
Ligand CLA 1 313



Bond lengths



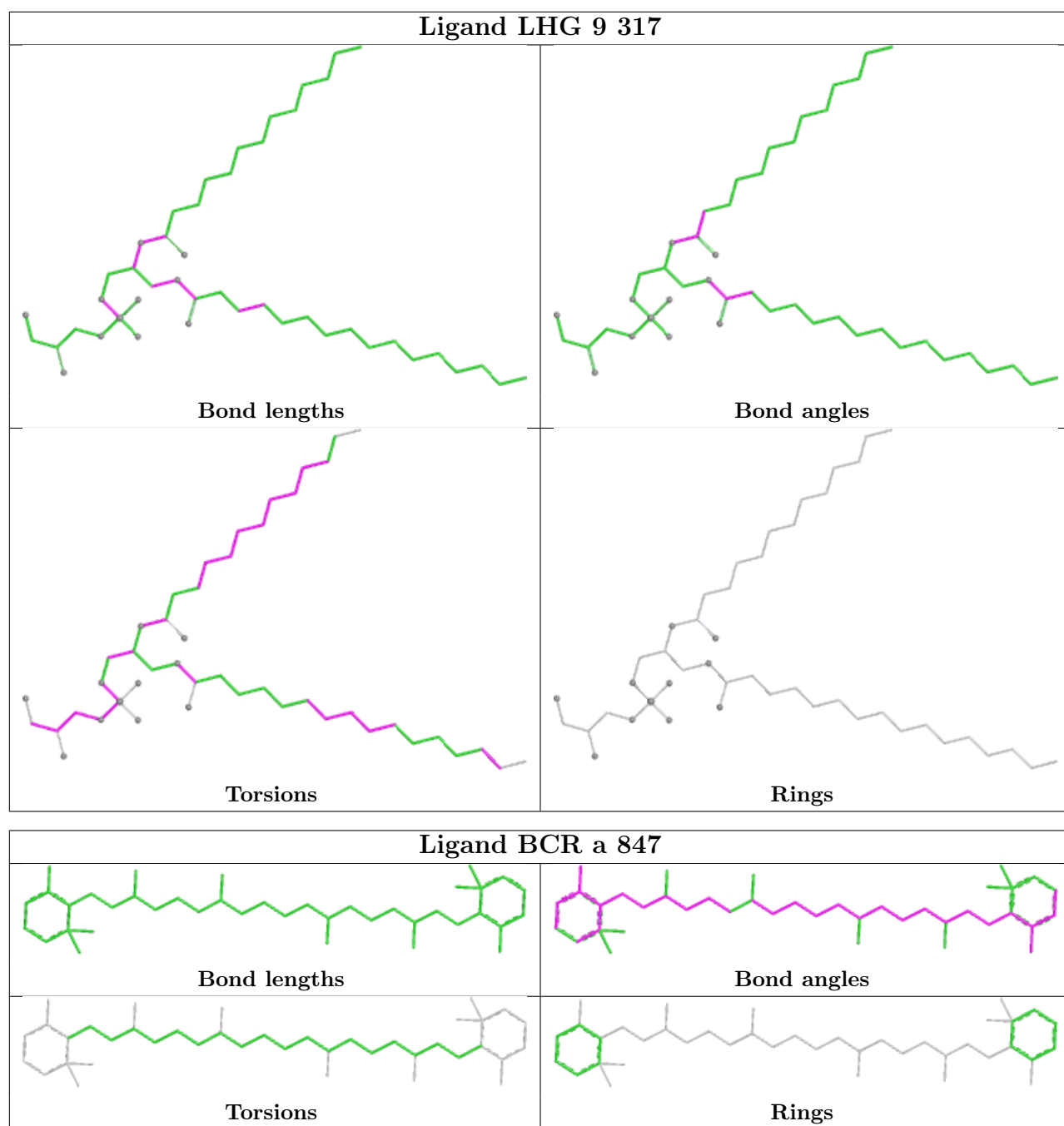
Bond angles



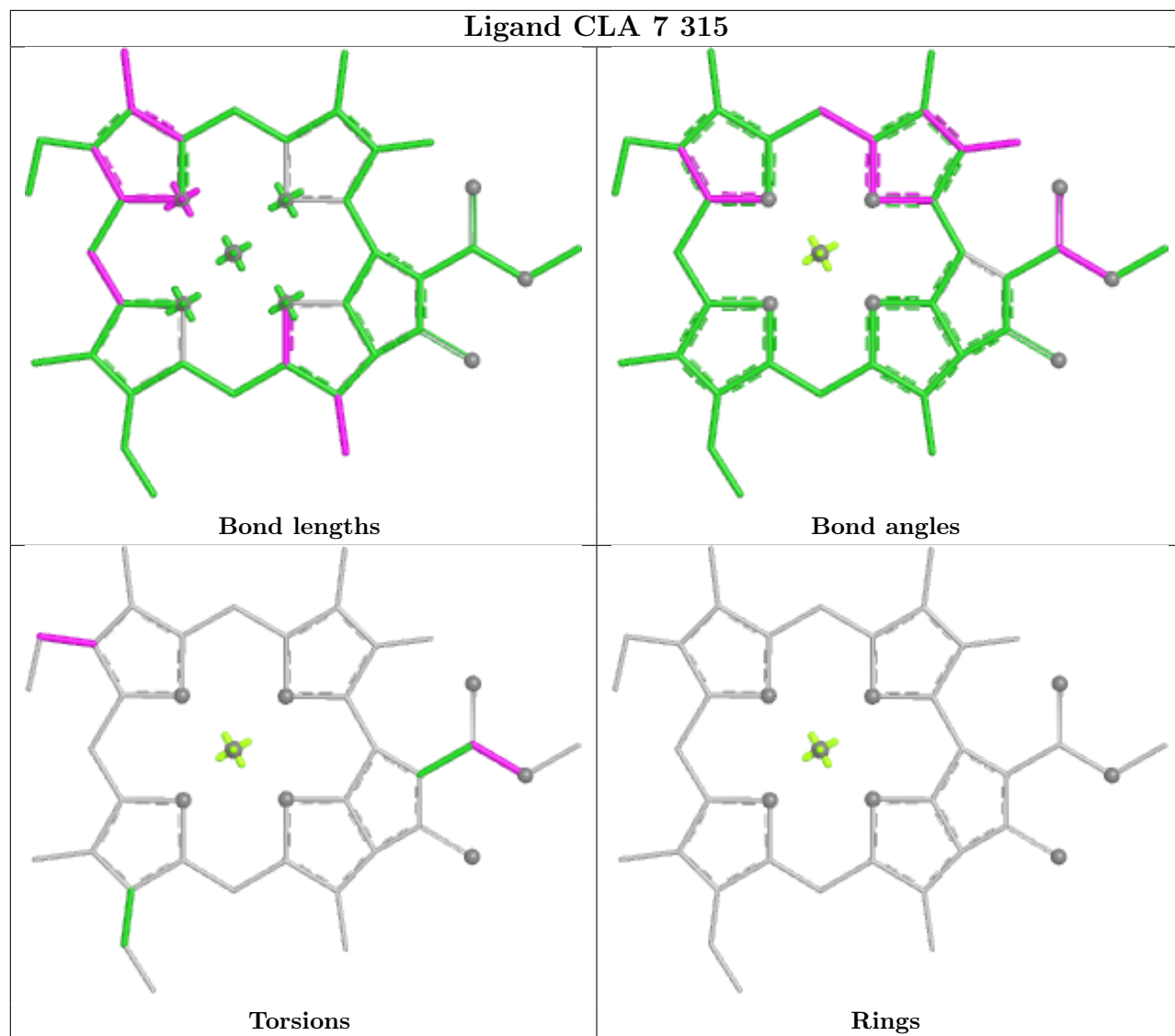
Torsions



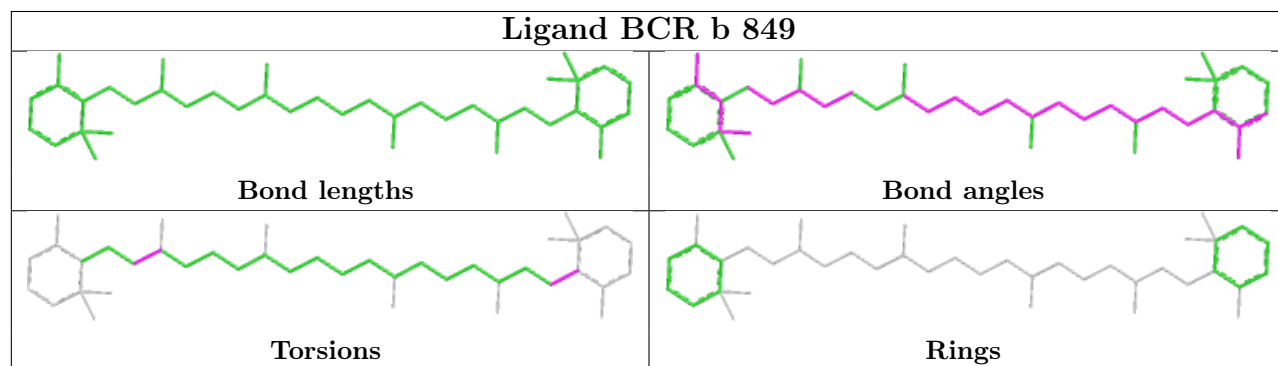
Rings

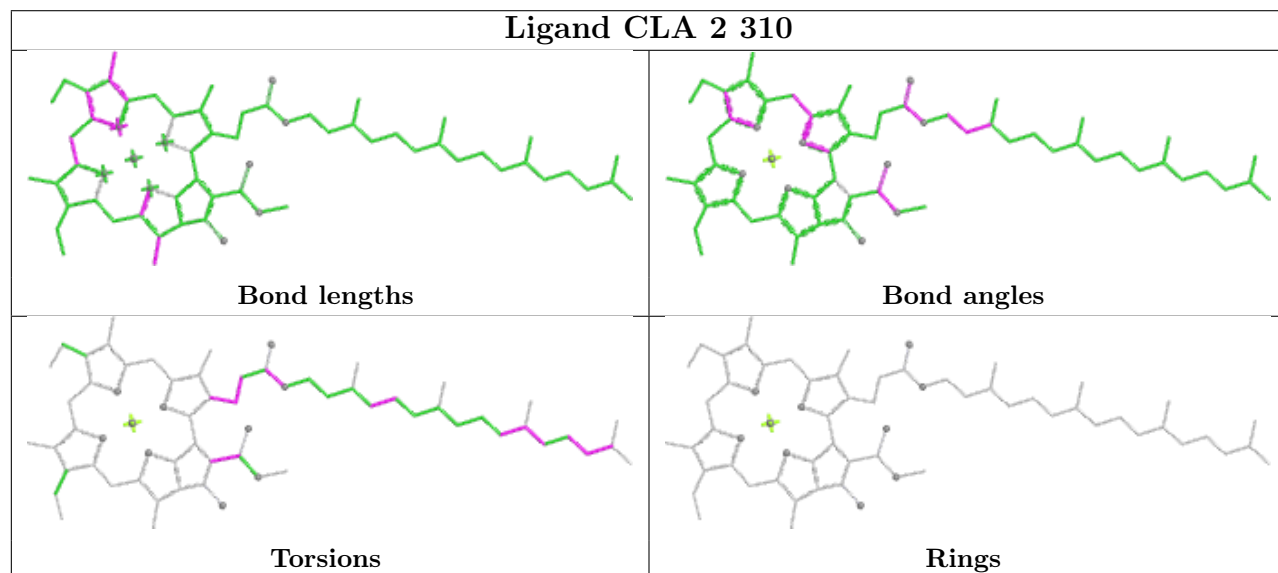
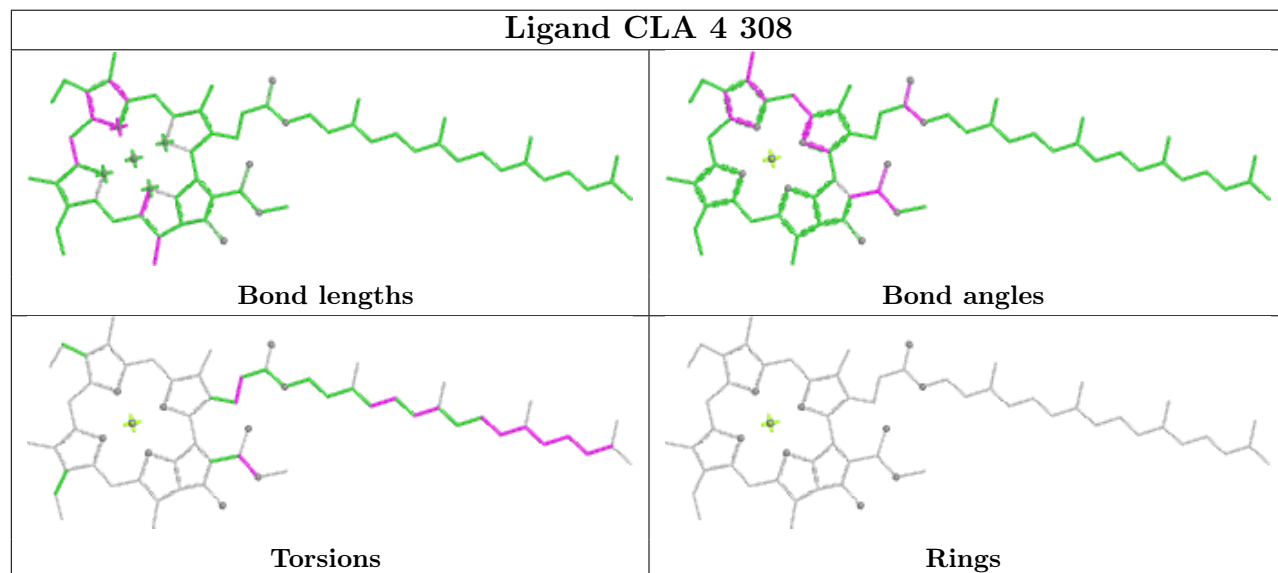
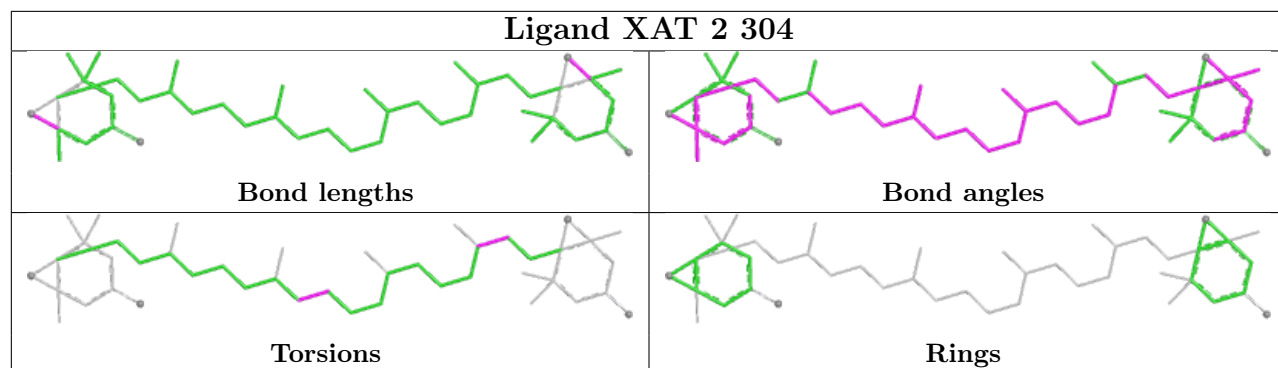


Ligand CLA 7 315

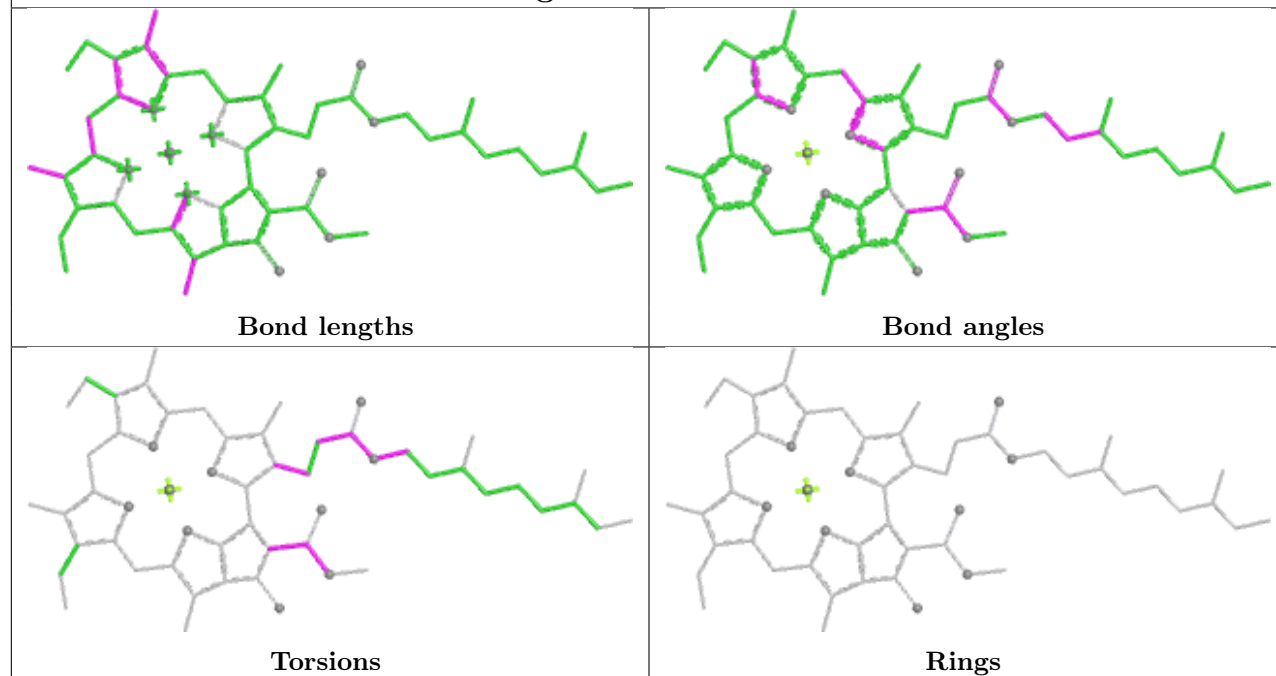


Ligand BCR b 849

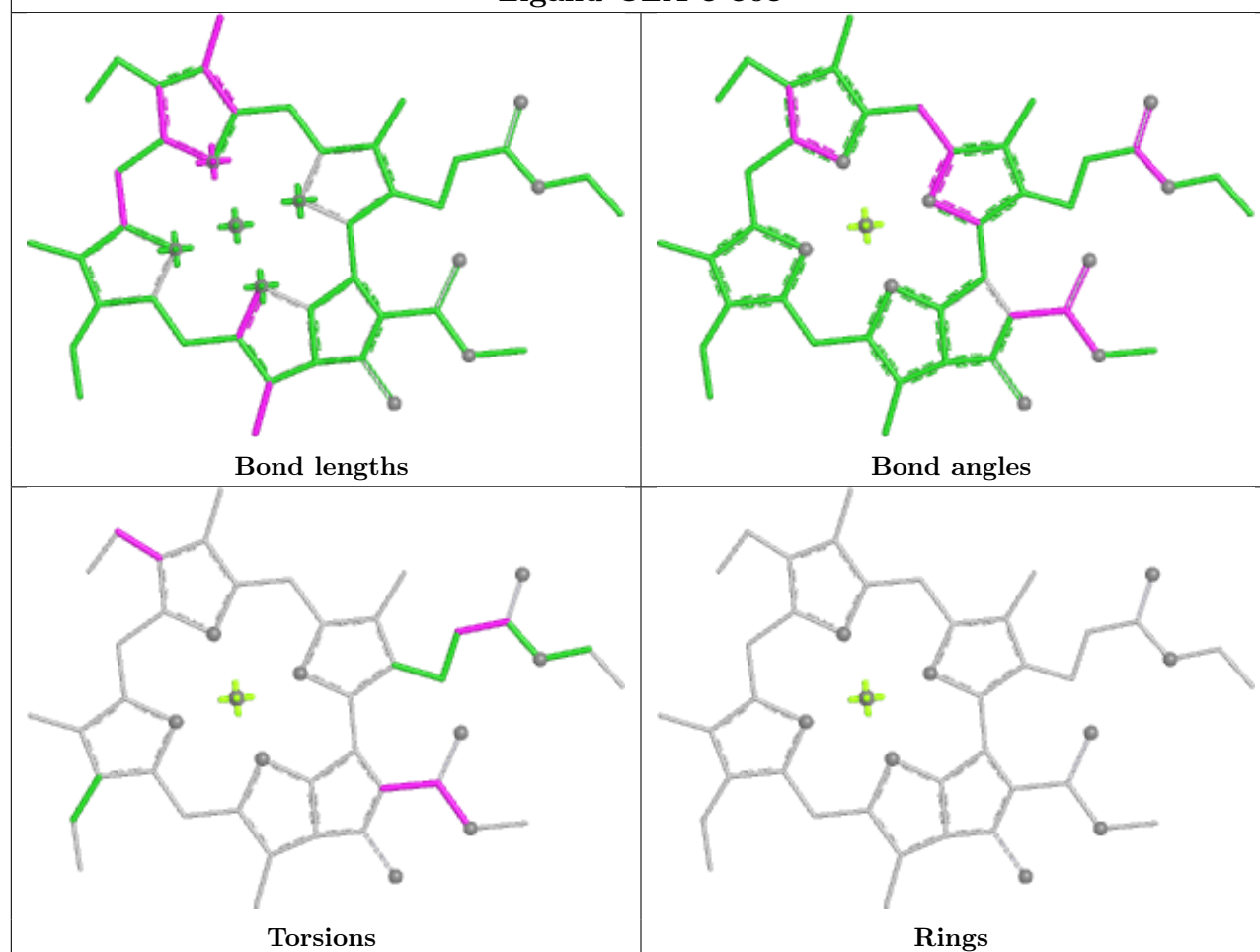


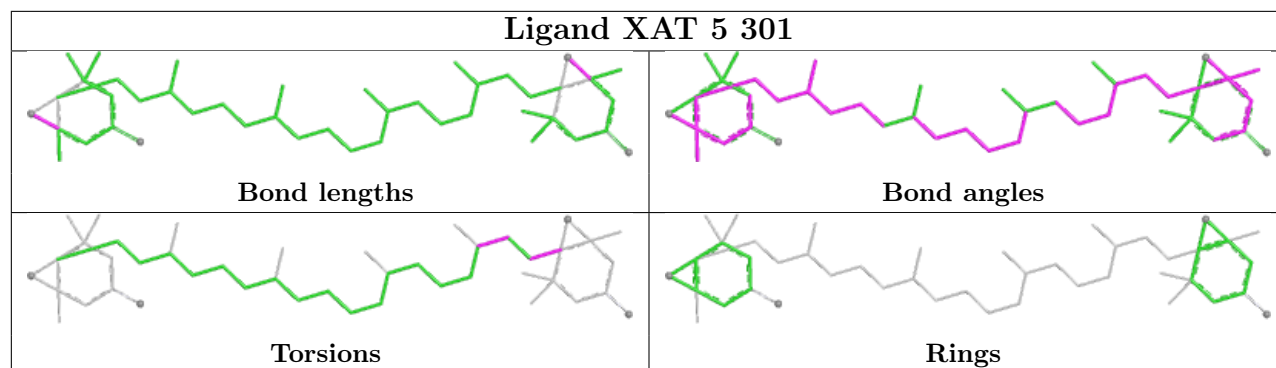
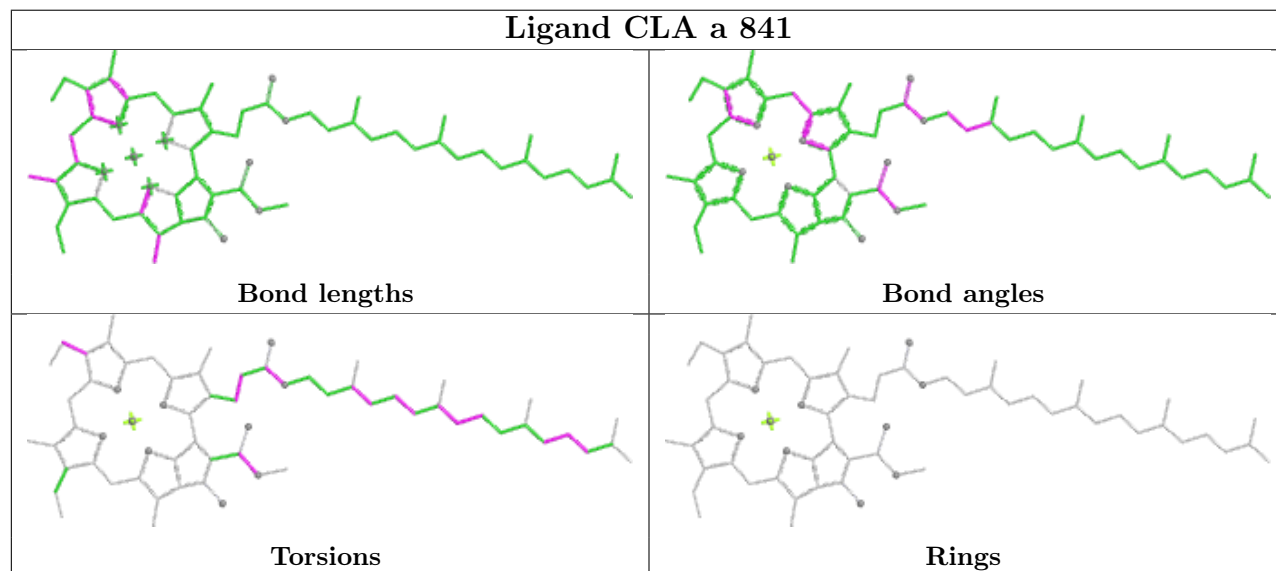
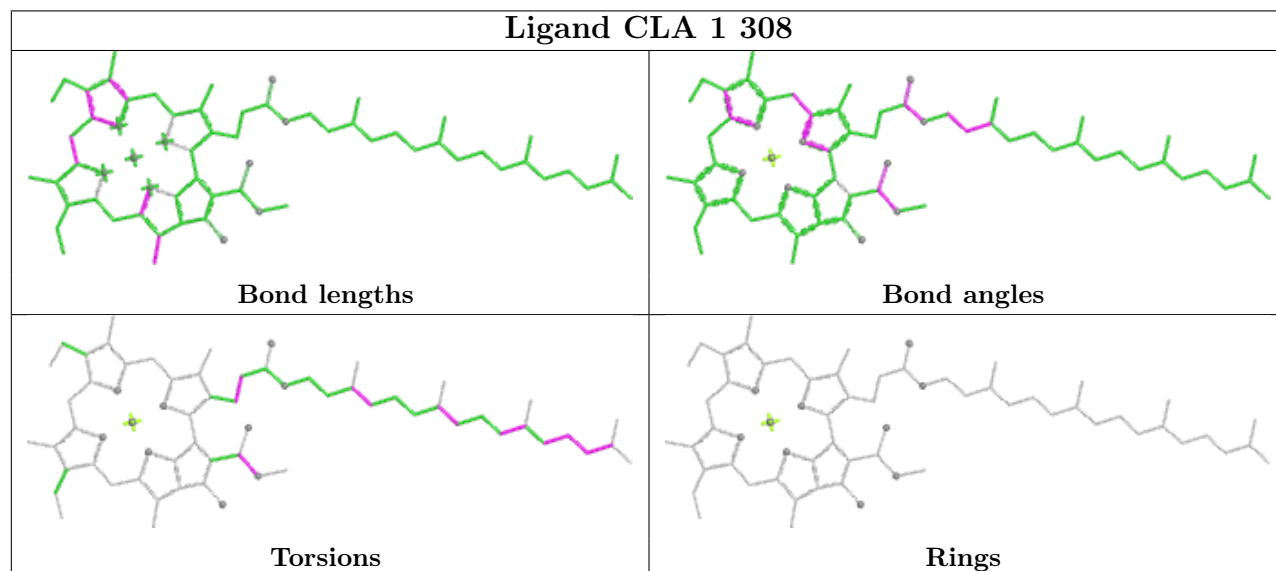


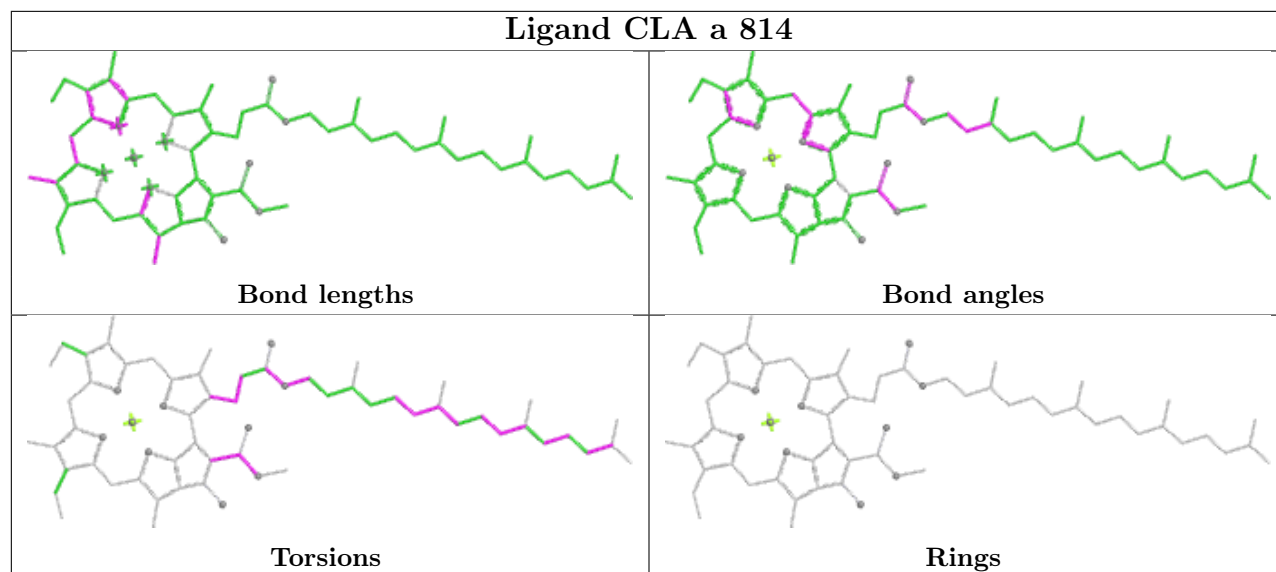
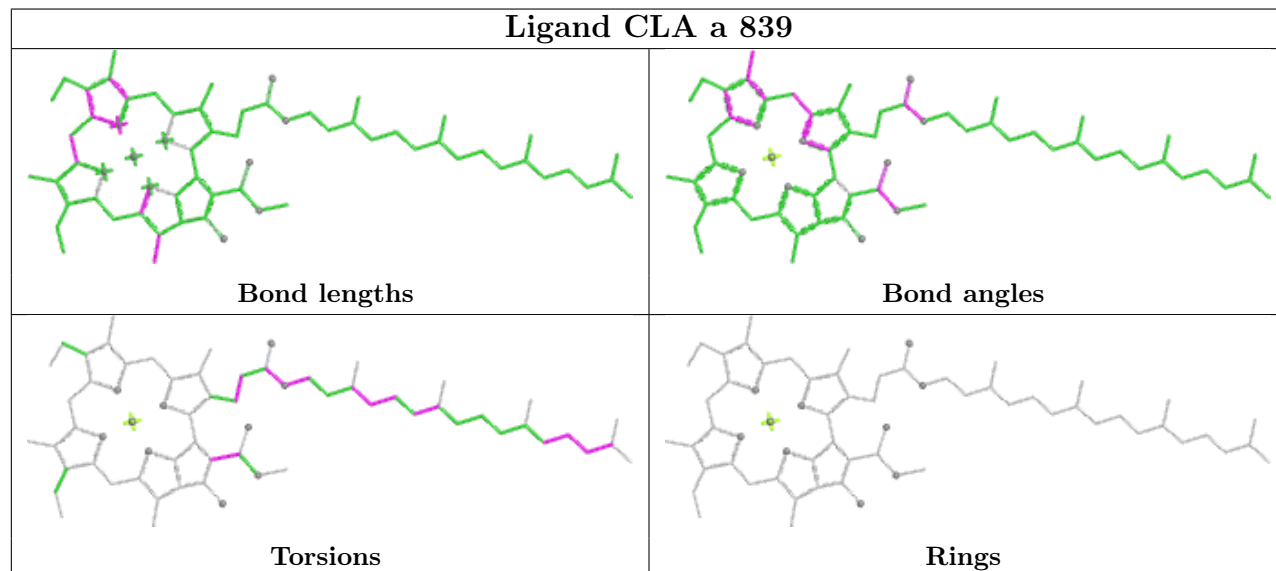
Ligand CLA a 818



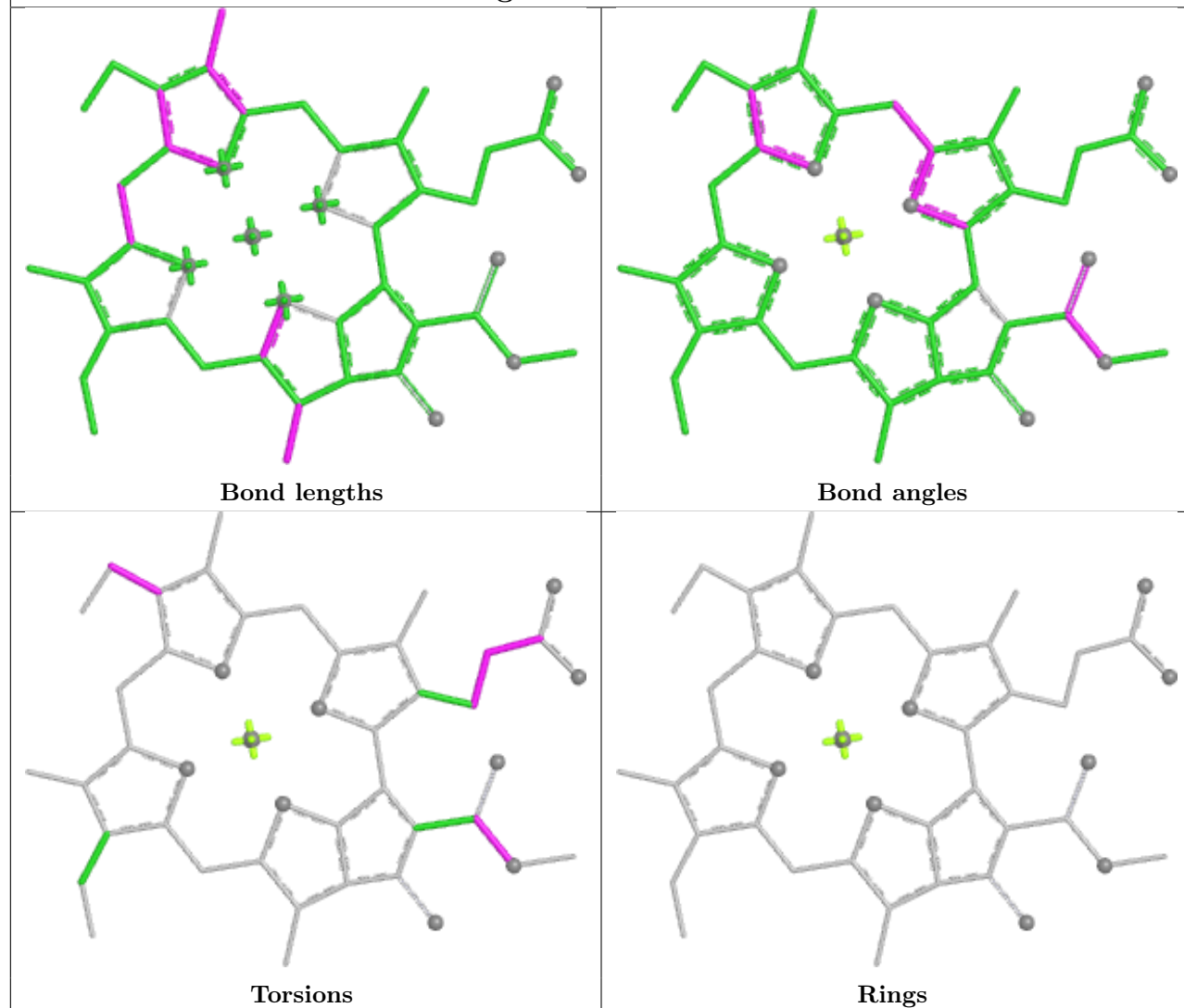
Ligand CLA 3 308



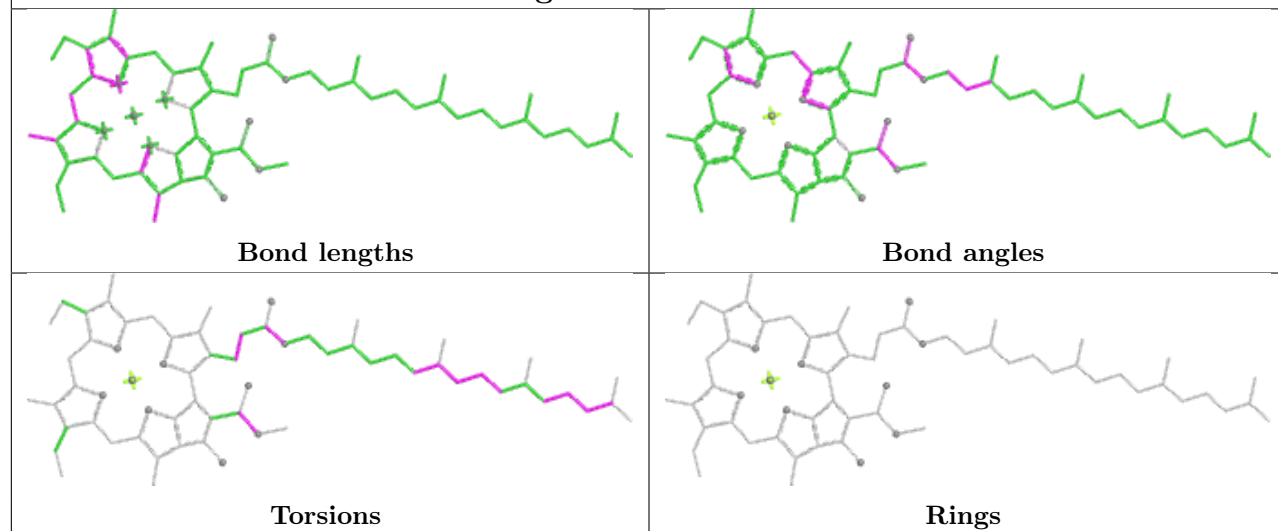
Ligand XAT 5 301**Ligand CLA a 841****Ligand CLA 1 308**

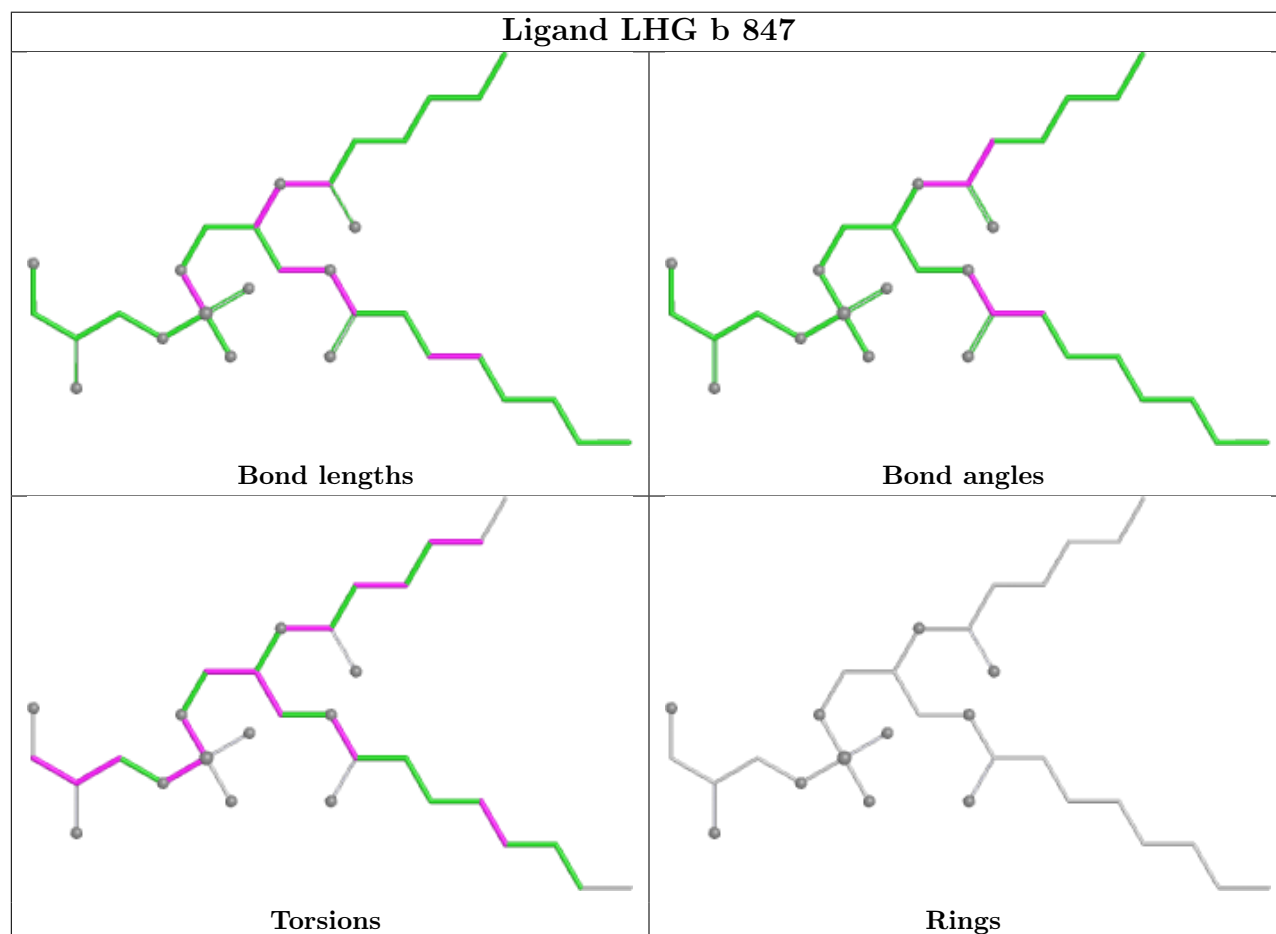
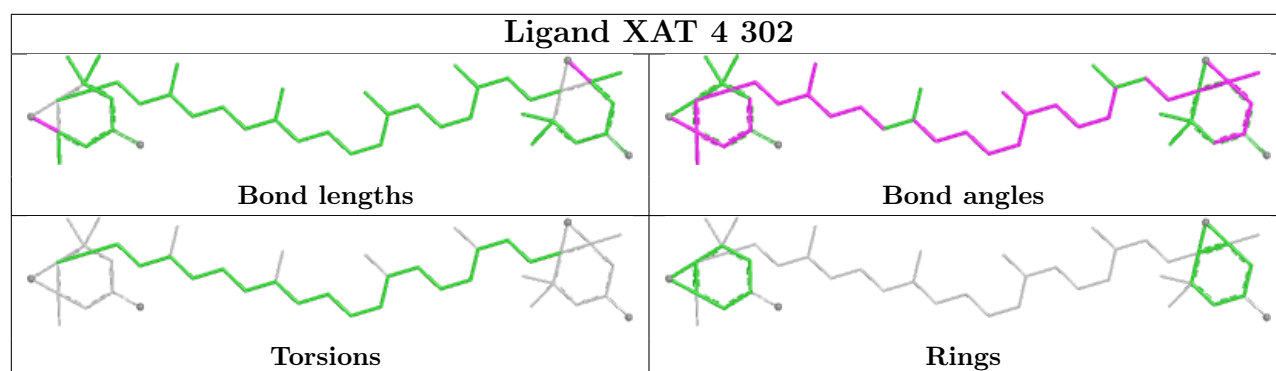
Ligand CLA a 814**Ligand CLA a 839**

Ligand CLA 7 317

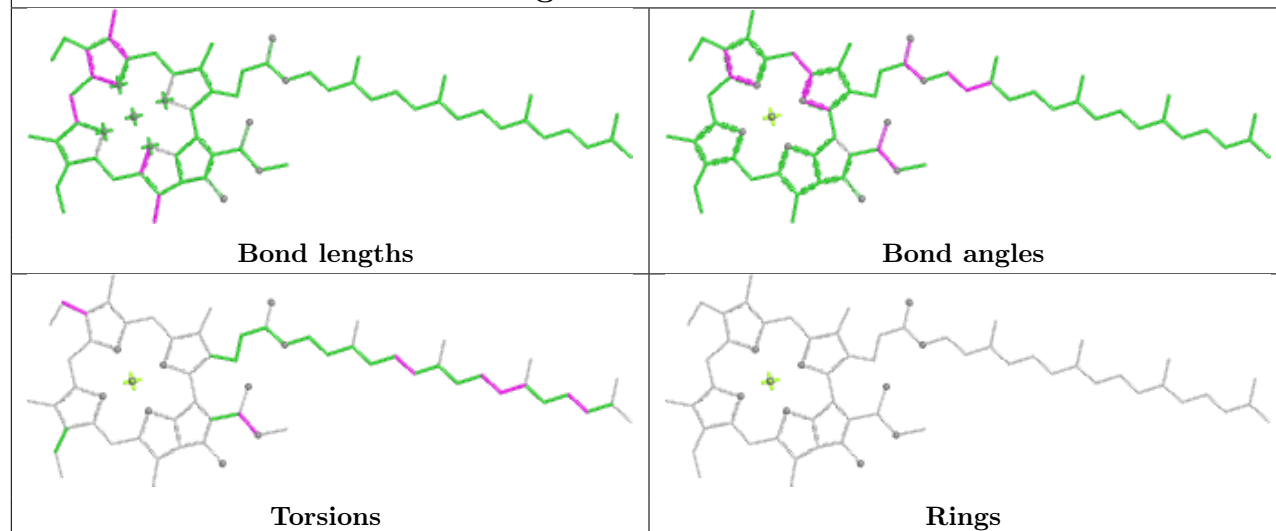


Ligand CLA b 827

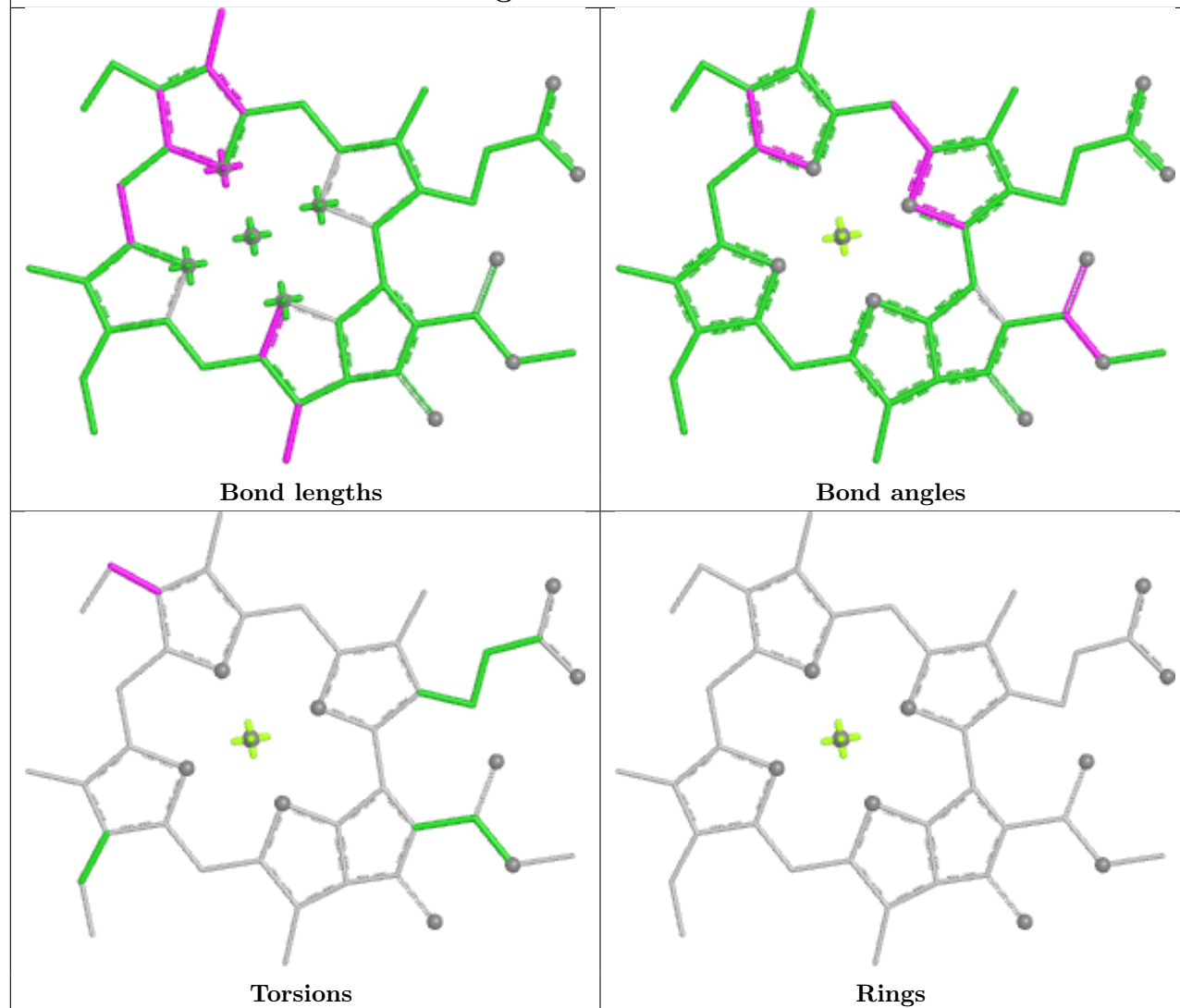




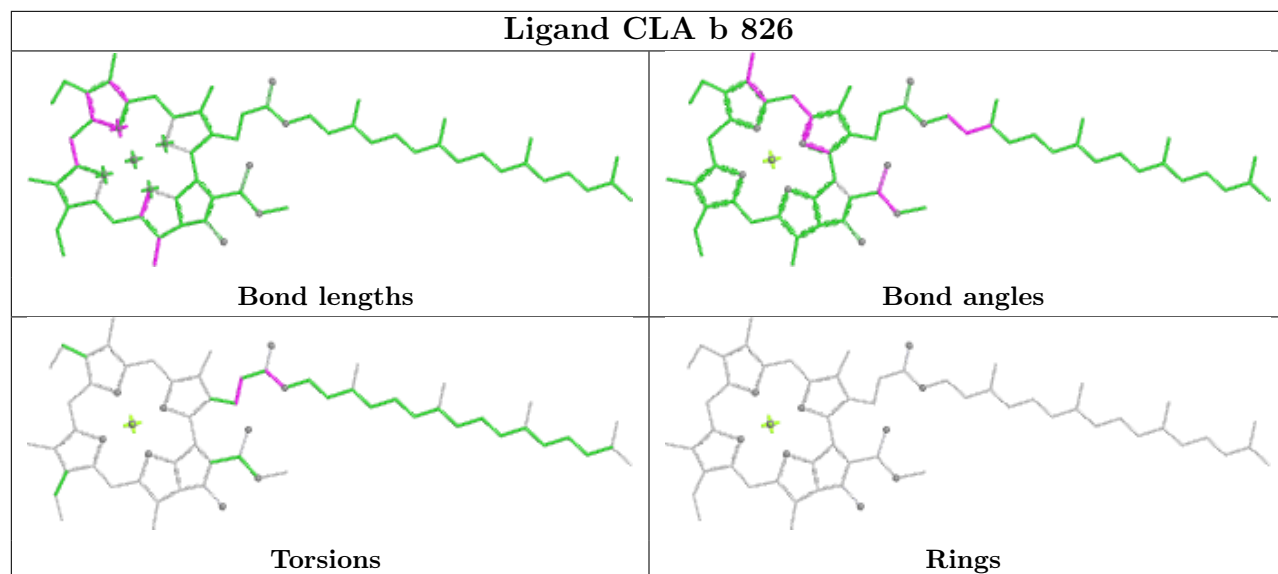
Ligand CLA a 834



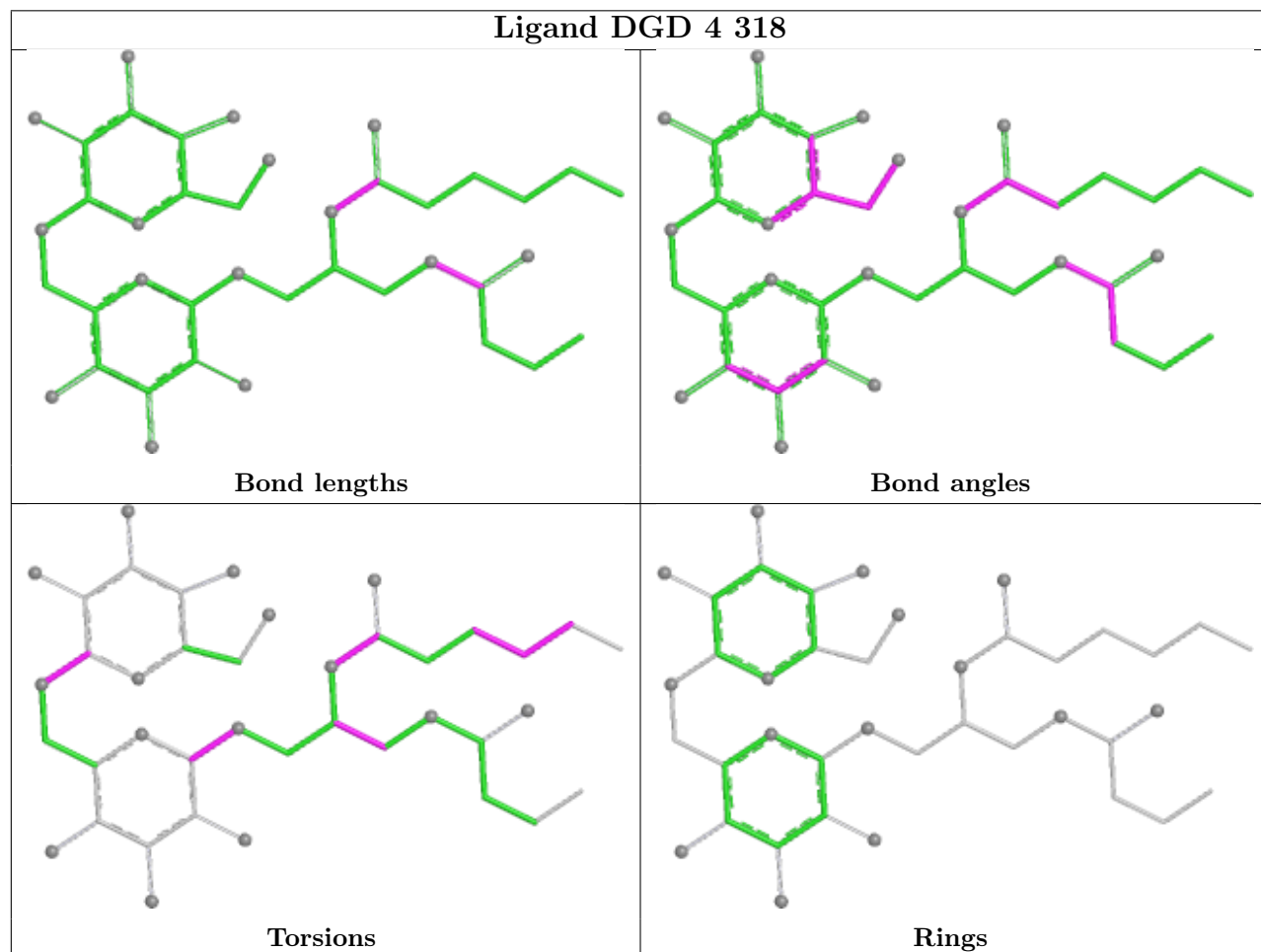
Ligand CLA 3 307



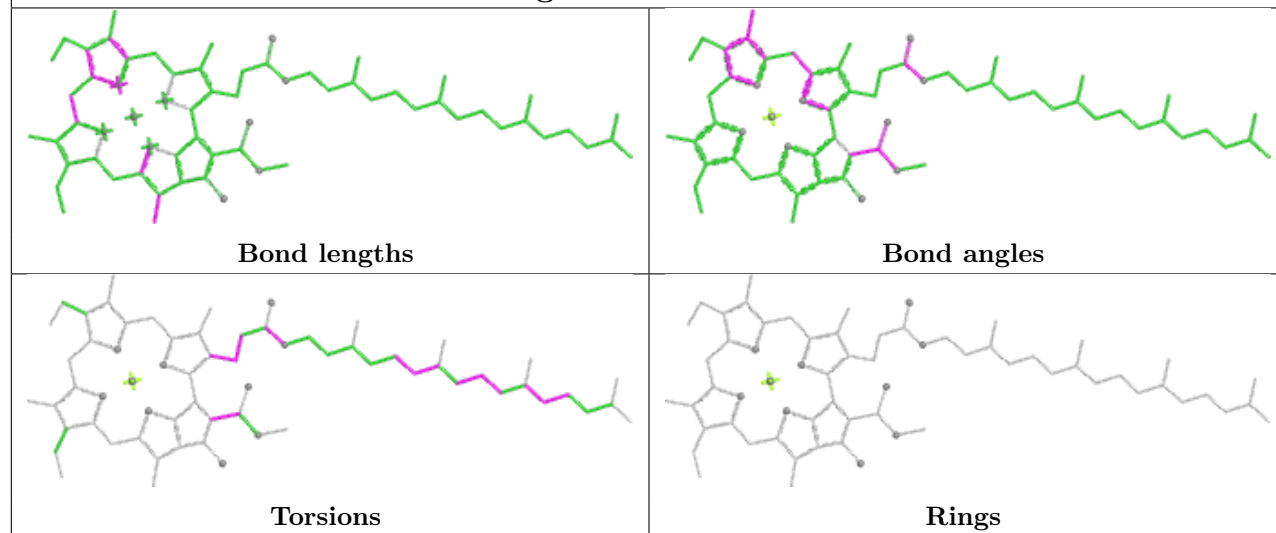
Ligand CLA b 826



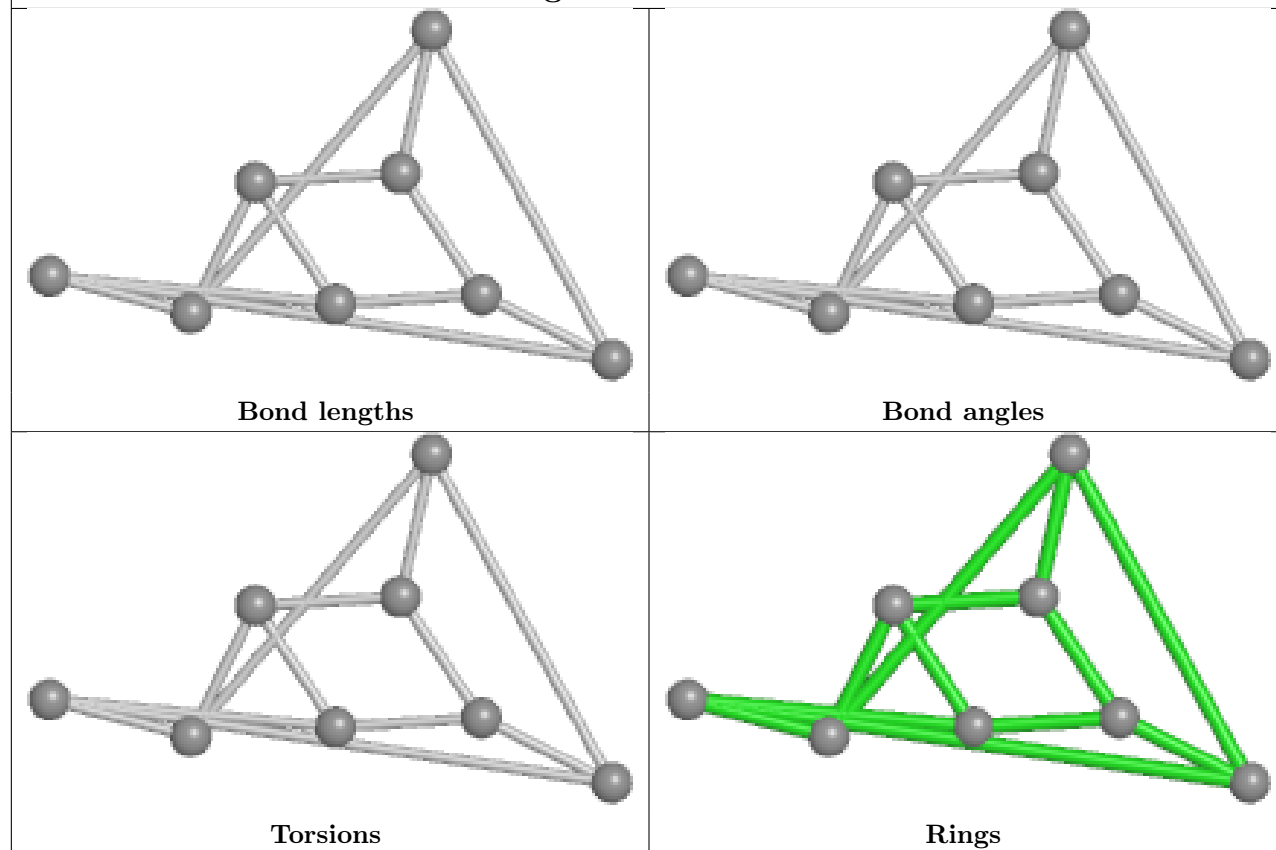
Ligand DGD 4 318



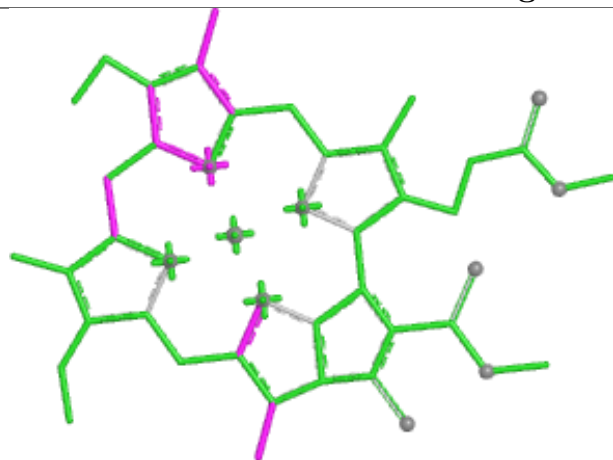
Ligand CLA a 809



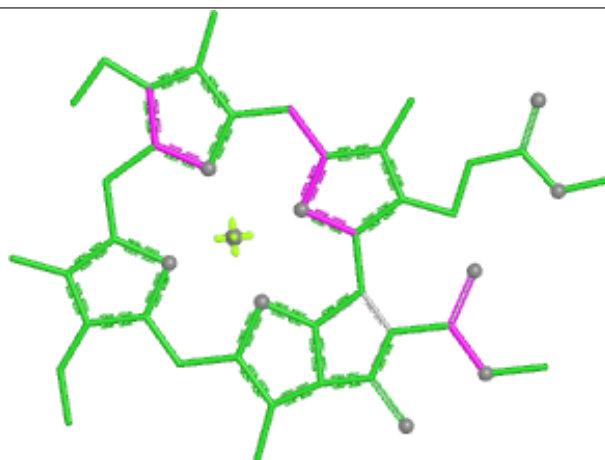
Ligand SF4 c 101



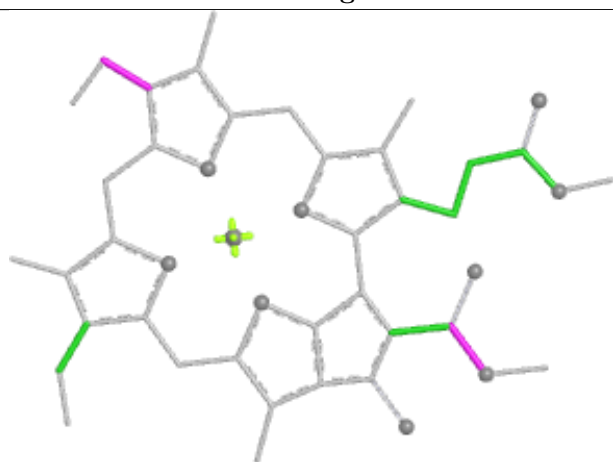
Ligand CLA 8 306



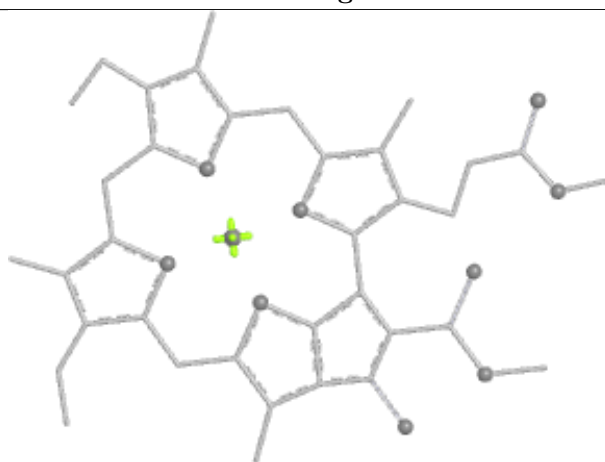
Bond lengths



Bond angles

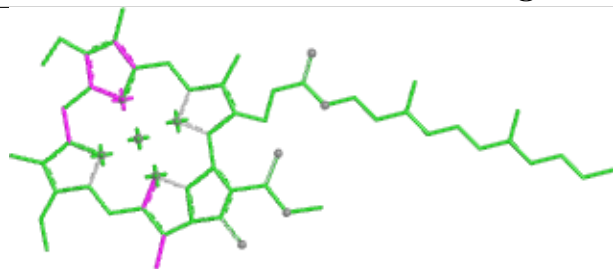


Torsions

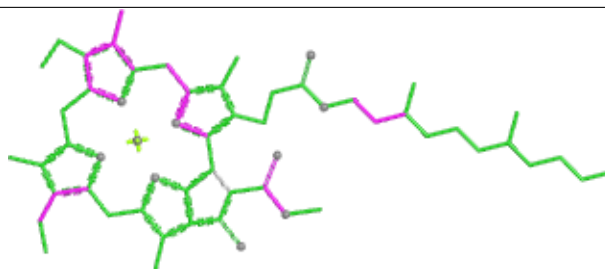


Rings

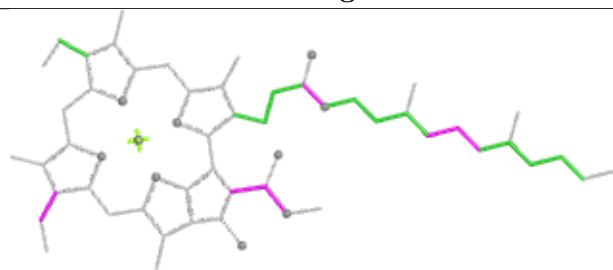
Ligand CLA b 835



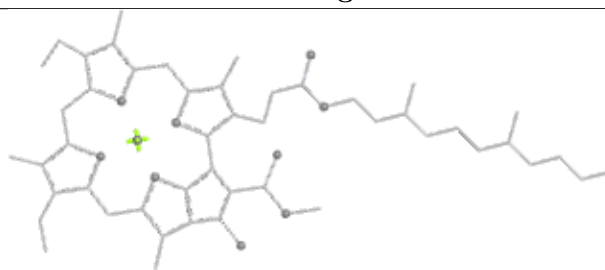
Bond lengths



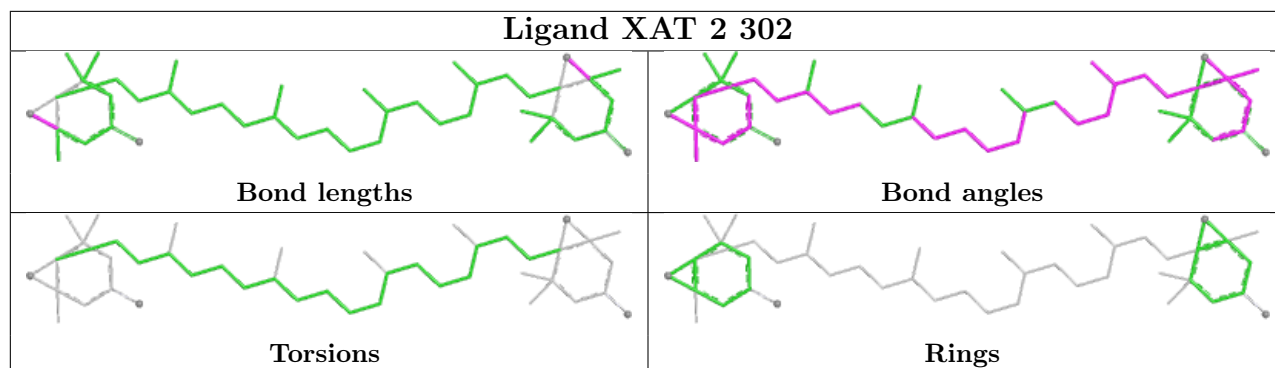
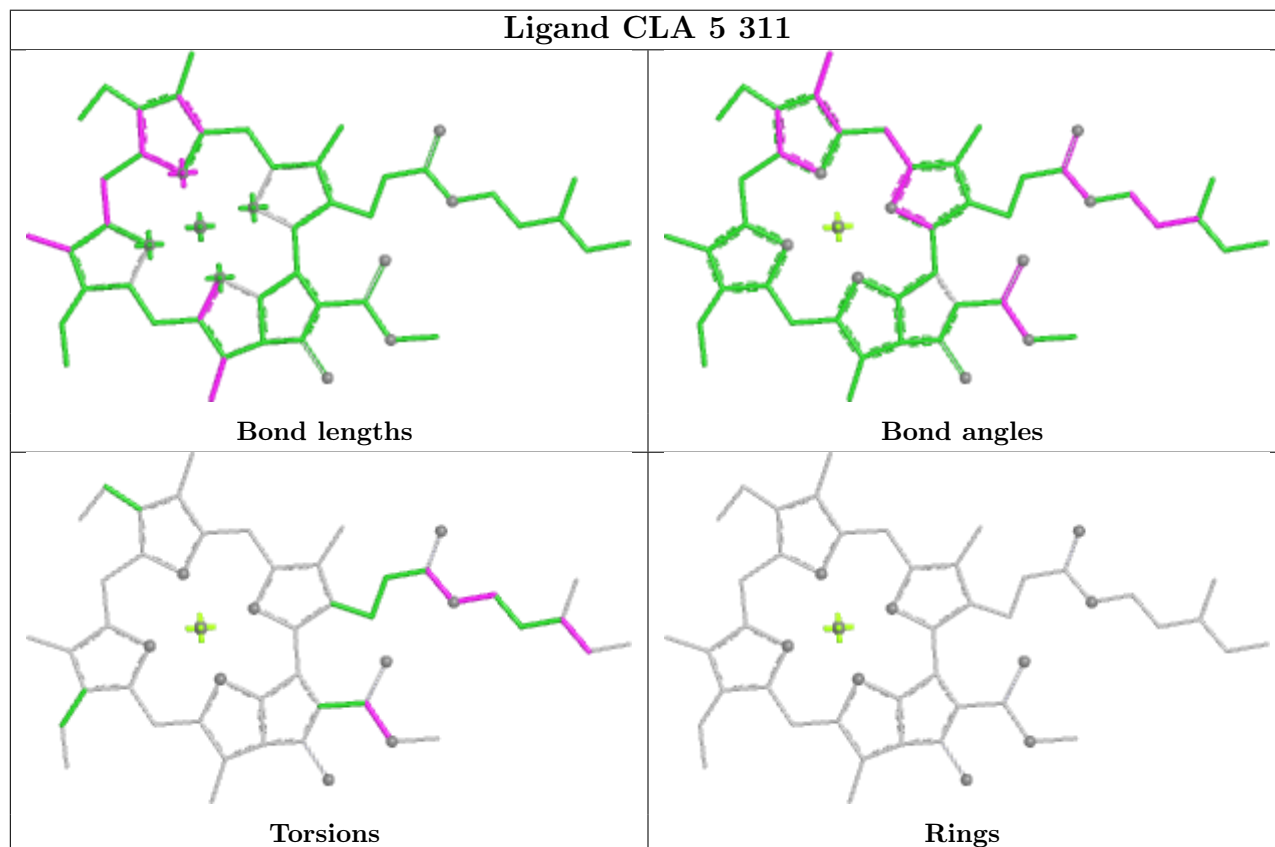
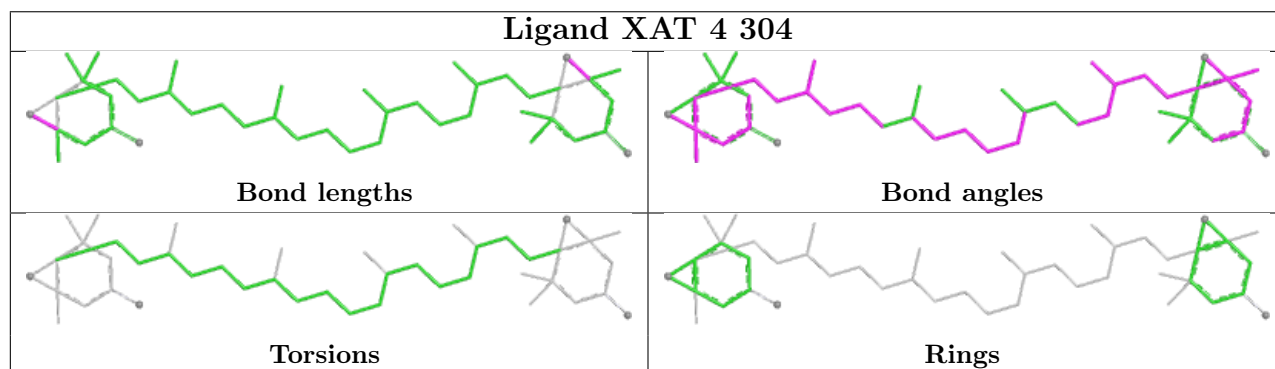
Bond angles



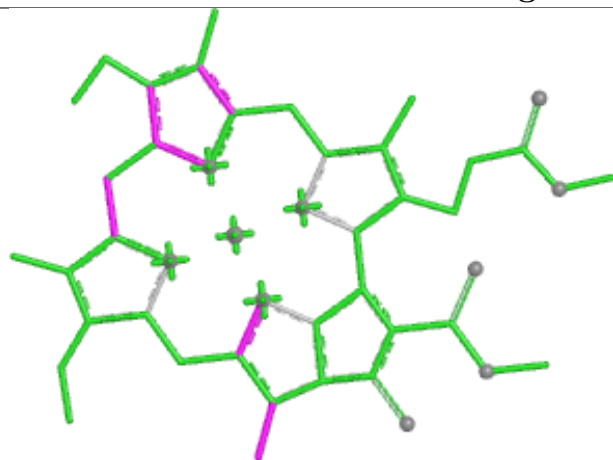
Torsions



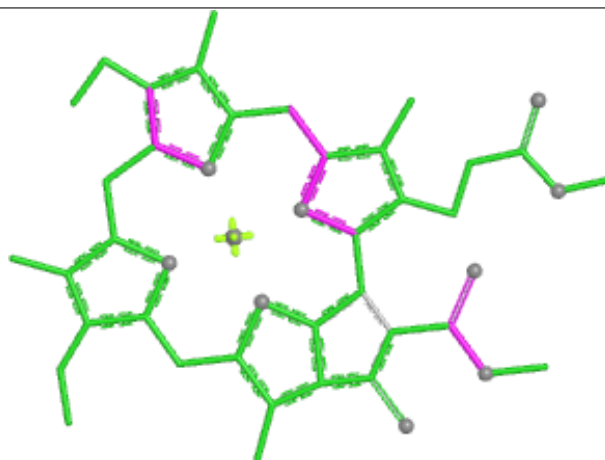
Rings

Ligand XAT 2 302**Ligand CLA 5 311****Ligand XAT 4 304**

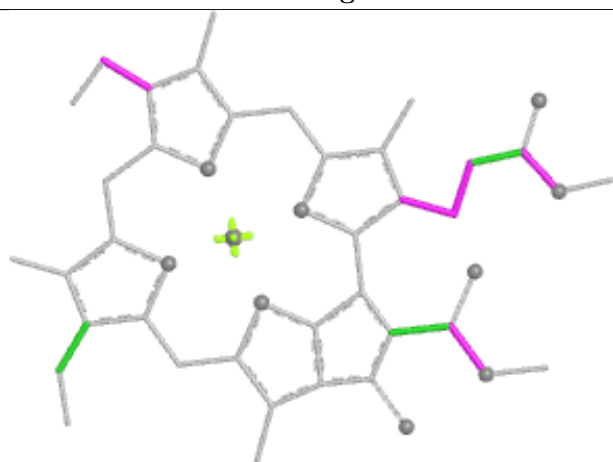
Ligand CLA 4 316



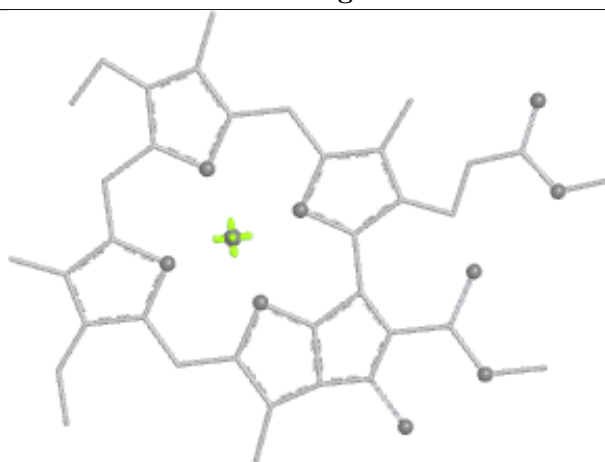
Bond lengths



Bond angles

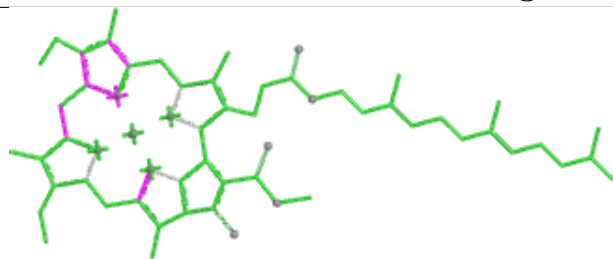


Torsions

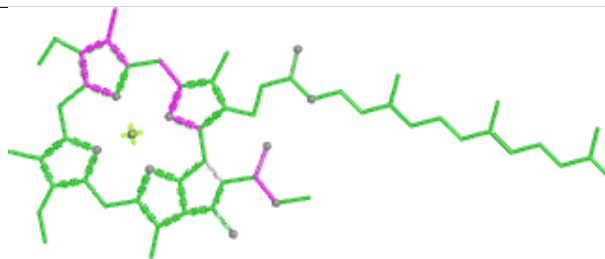


Rings

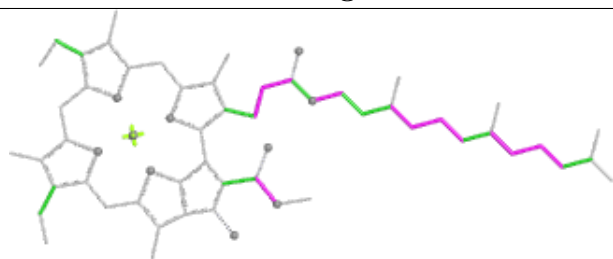
Ligand CLA 7 308



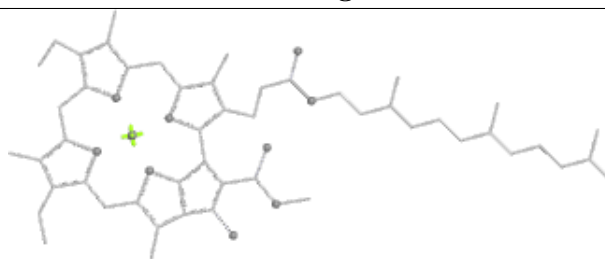
Bond lengths



Bond angles

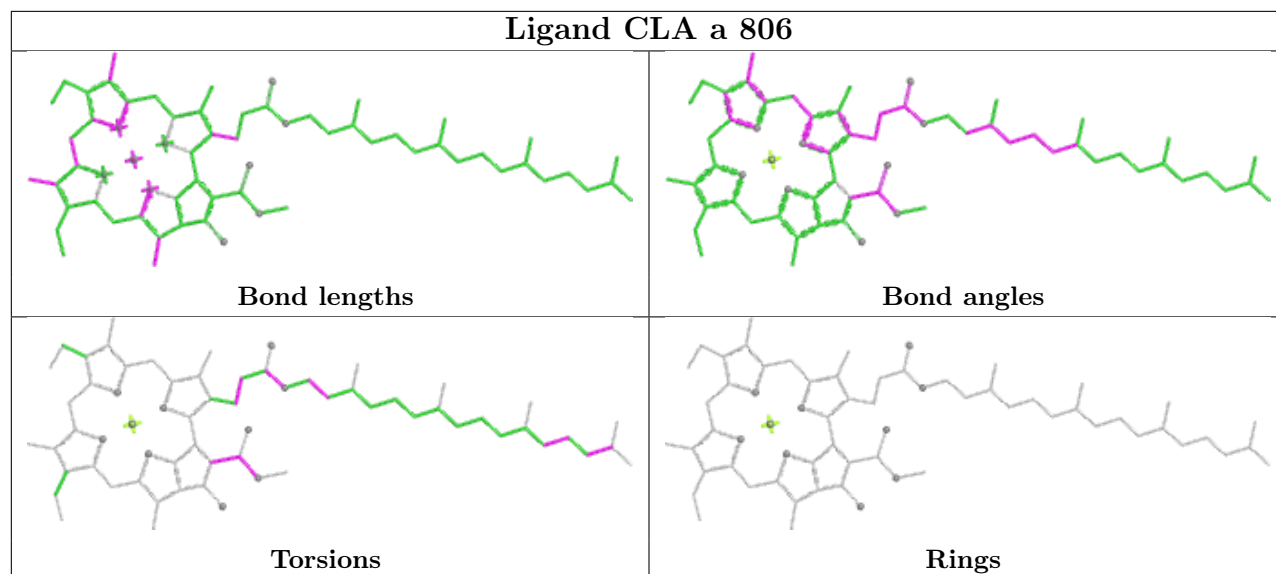


Torsions

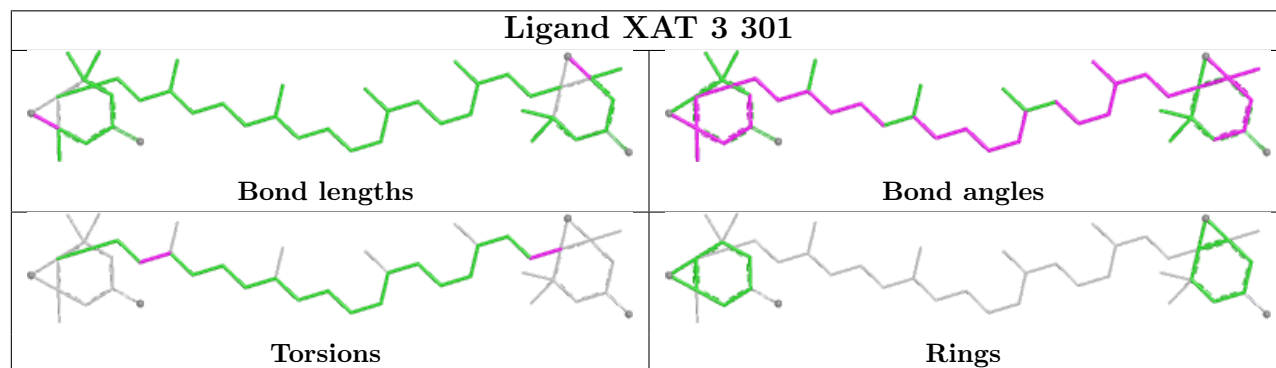


Rings

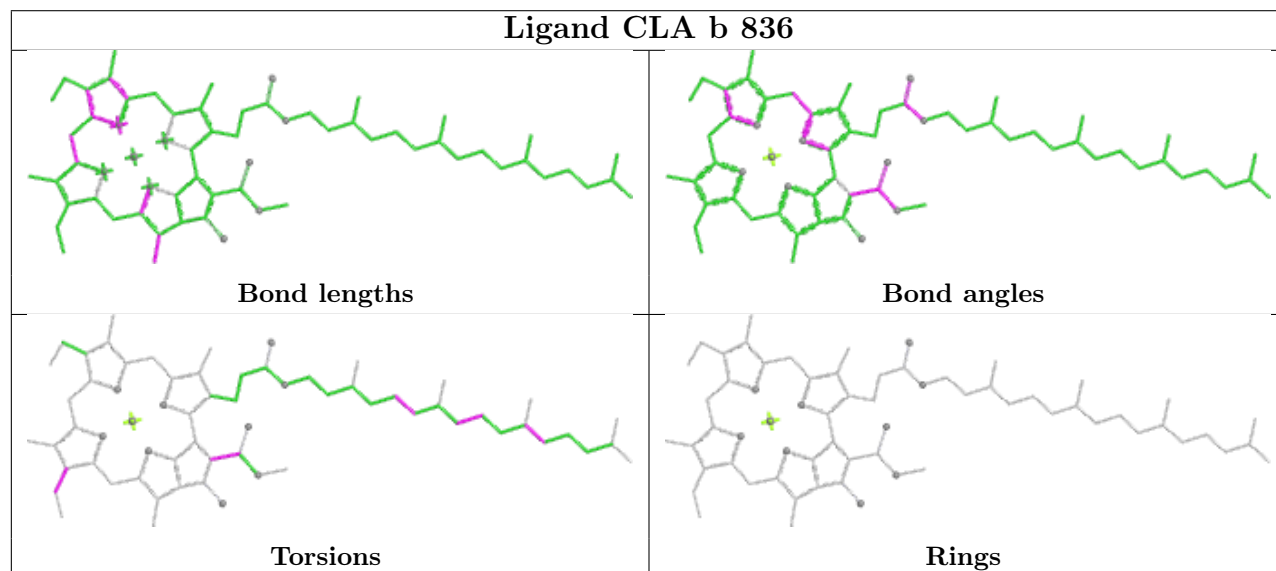
Ligand CLA a 806

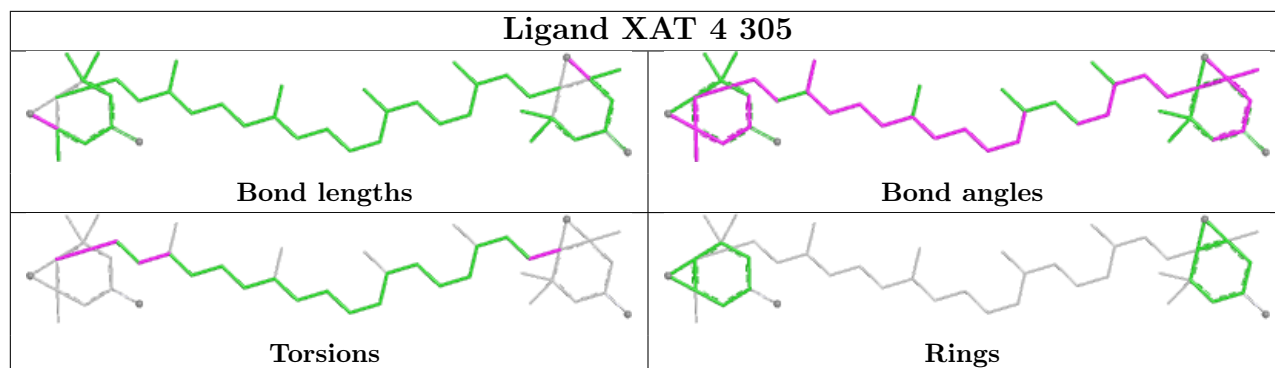
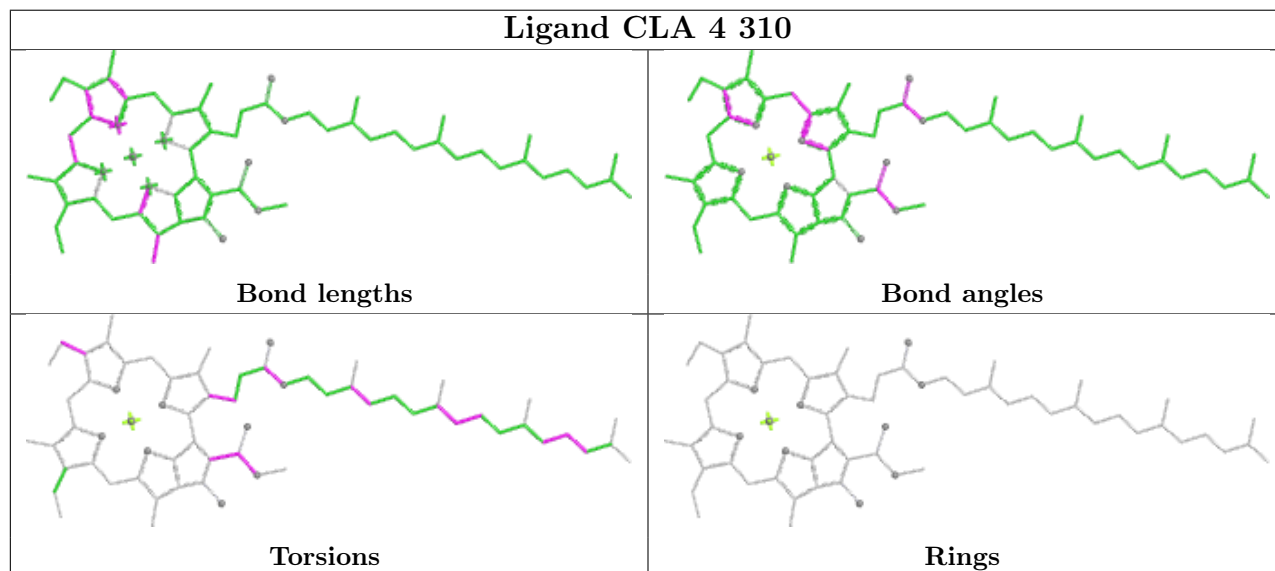
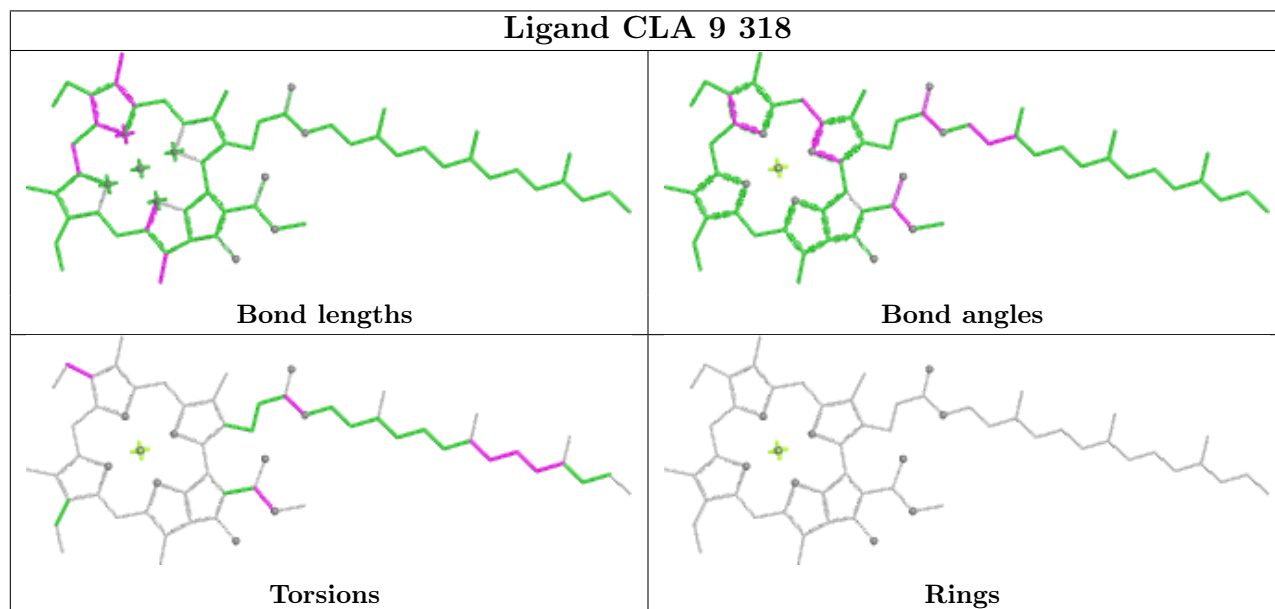


Ligand XAT 3 301

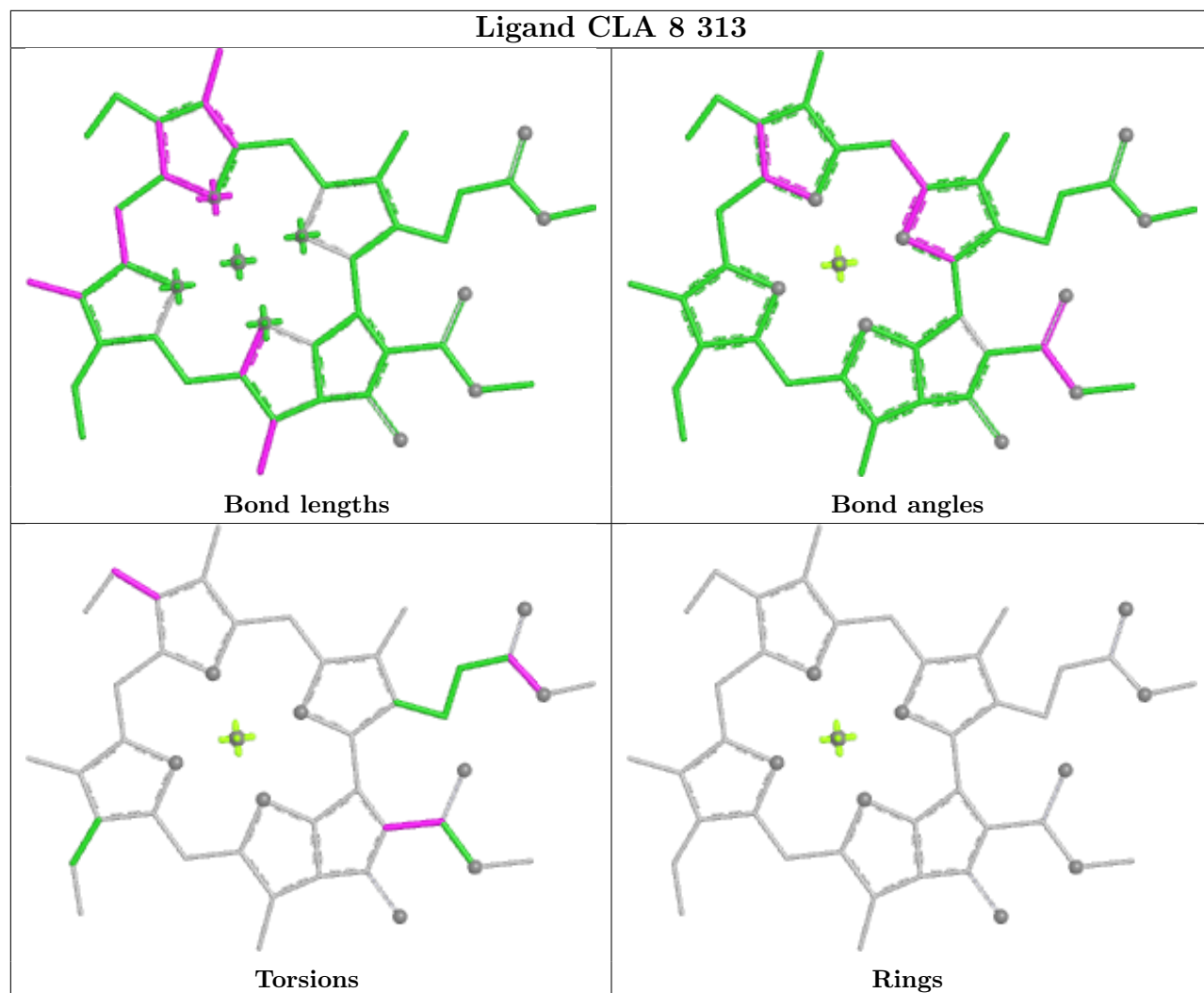


Ligand CLA b 836

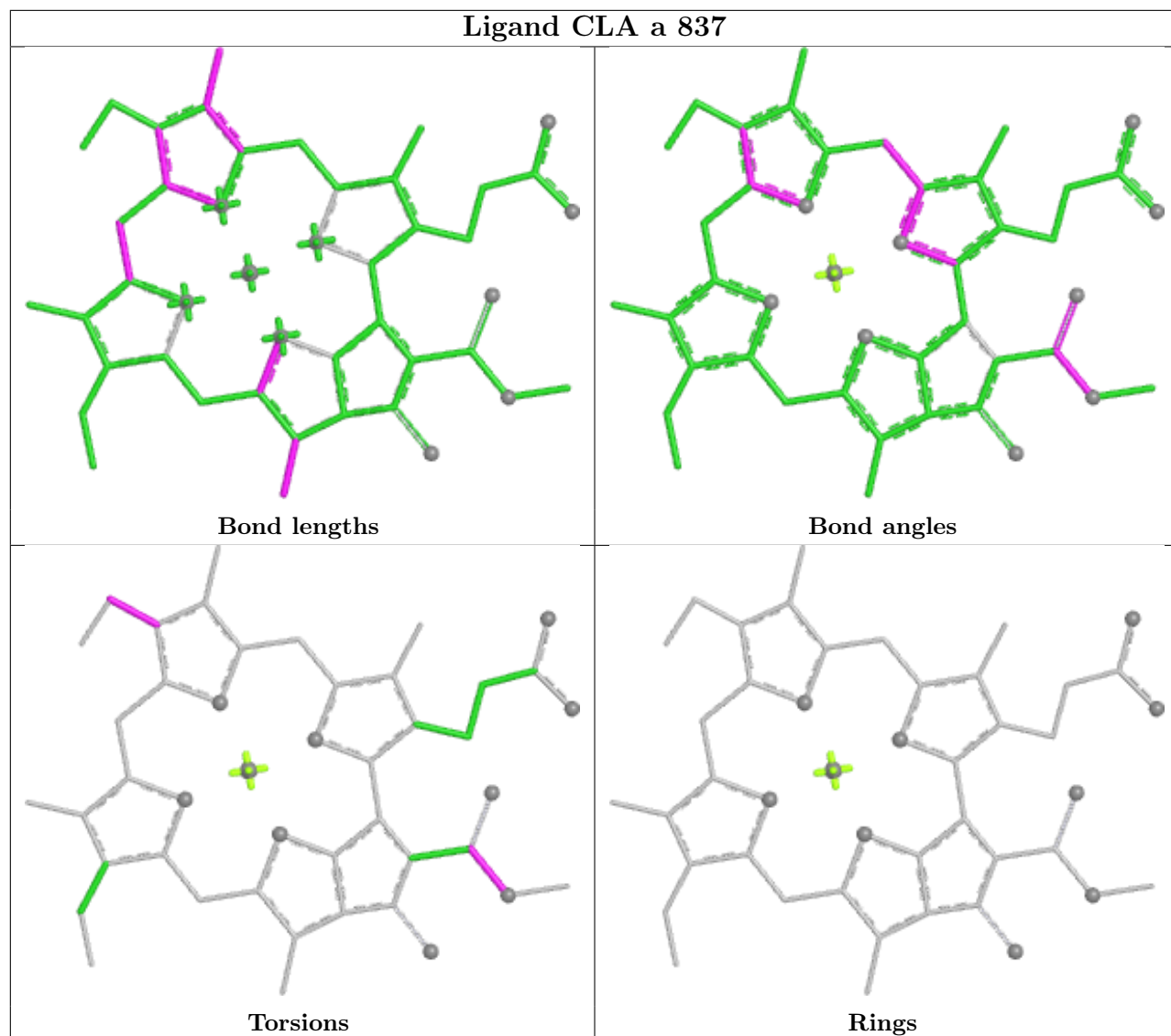


Ligand XAT 4 305**Ligand CLA 4 310****Ligand CLA 9 318**

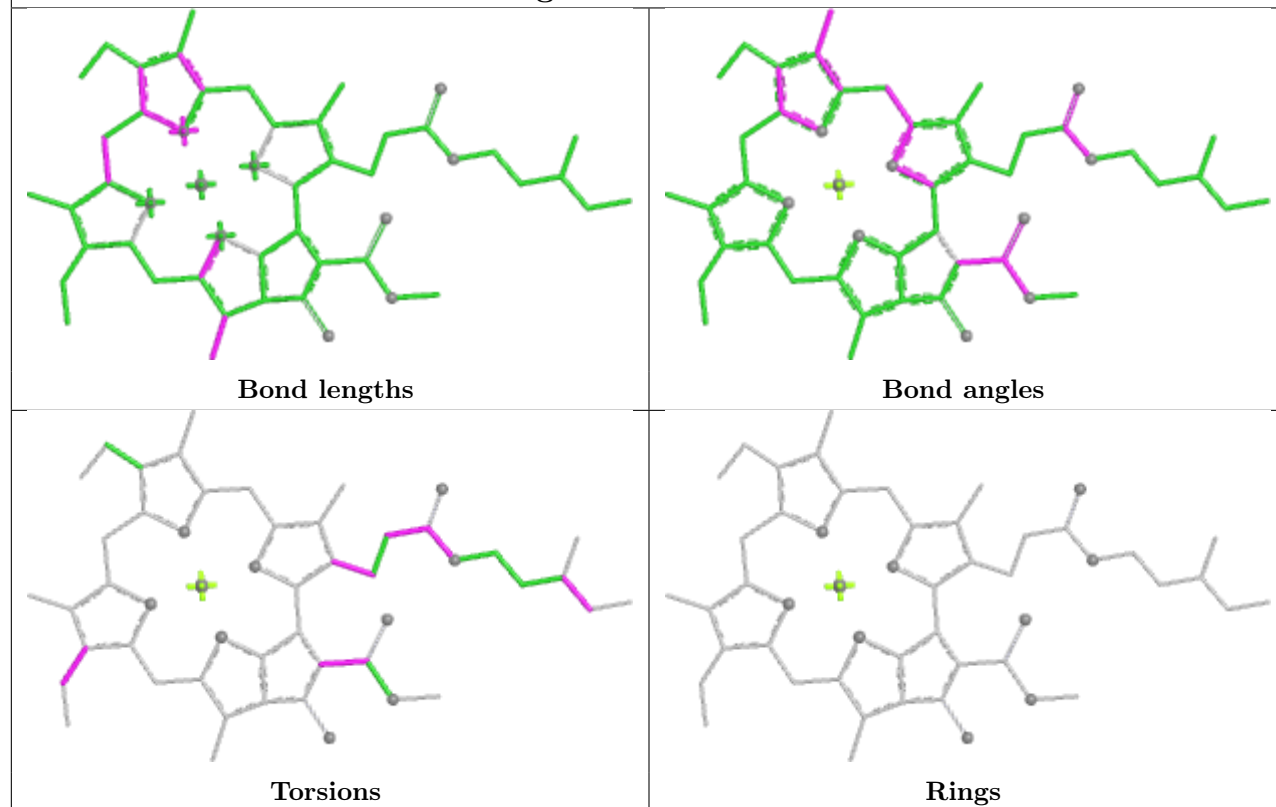
Ligand CLA 8 313



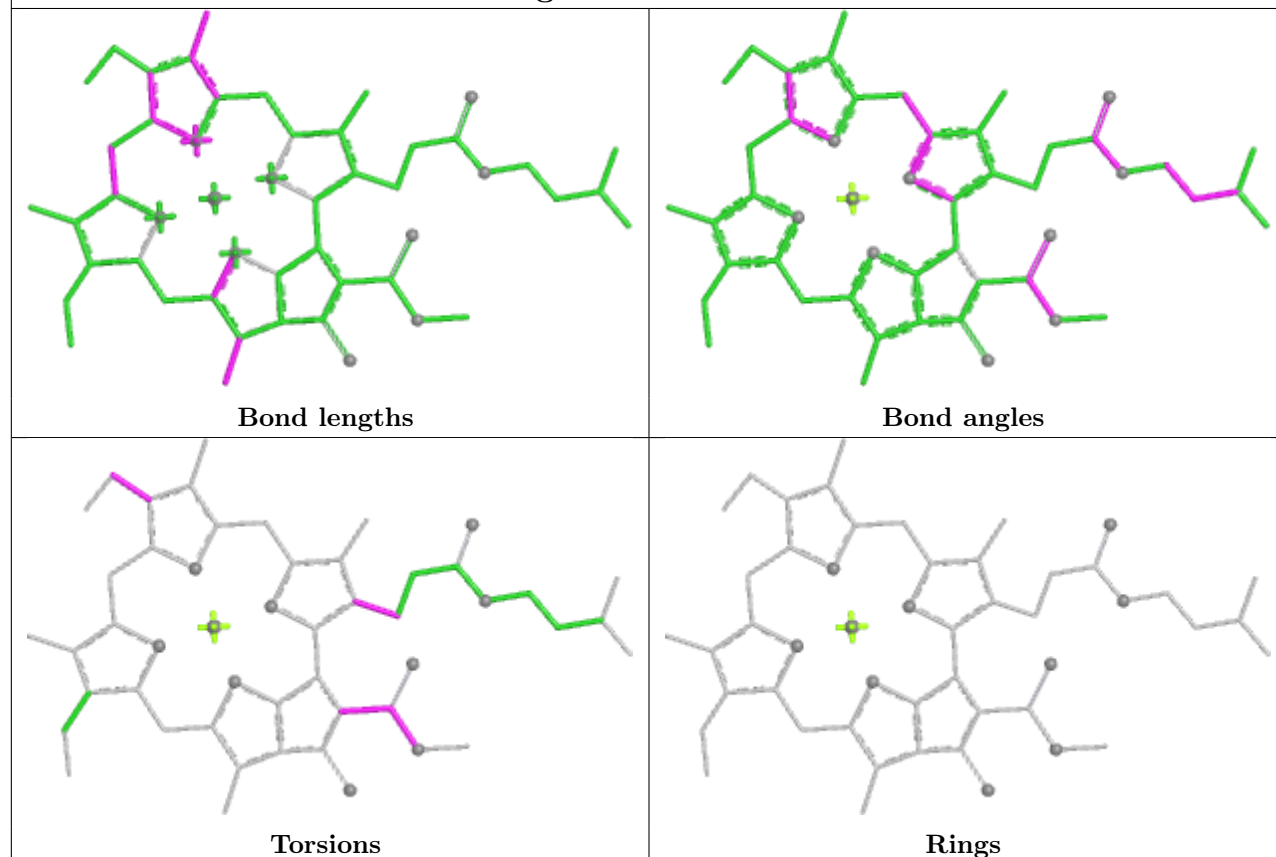
Ligand CLA a 837

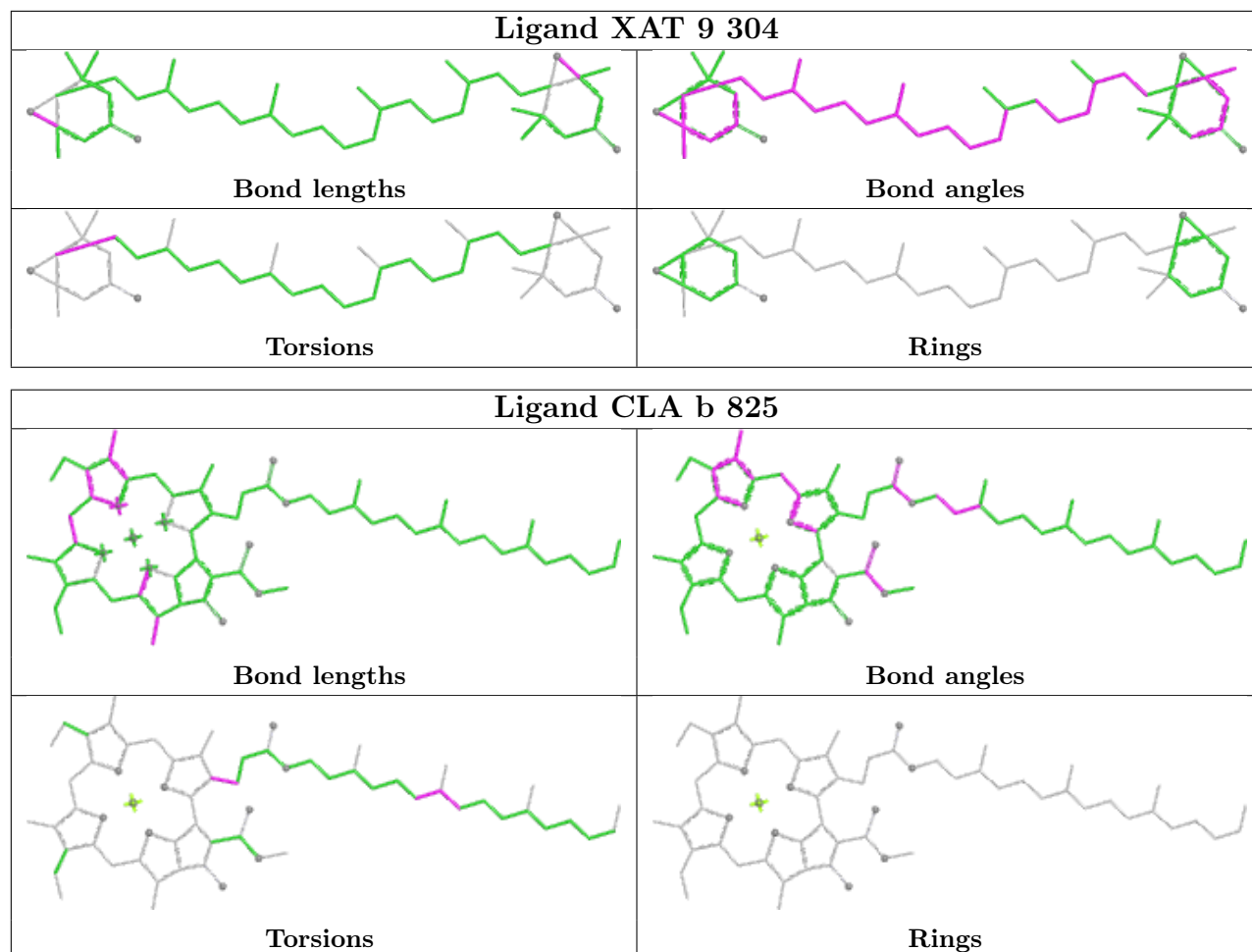


Ligand CLA 7 316

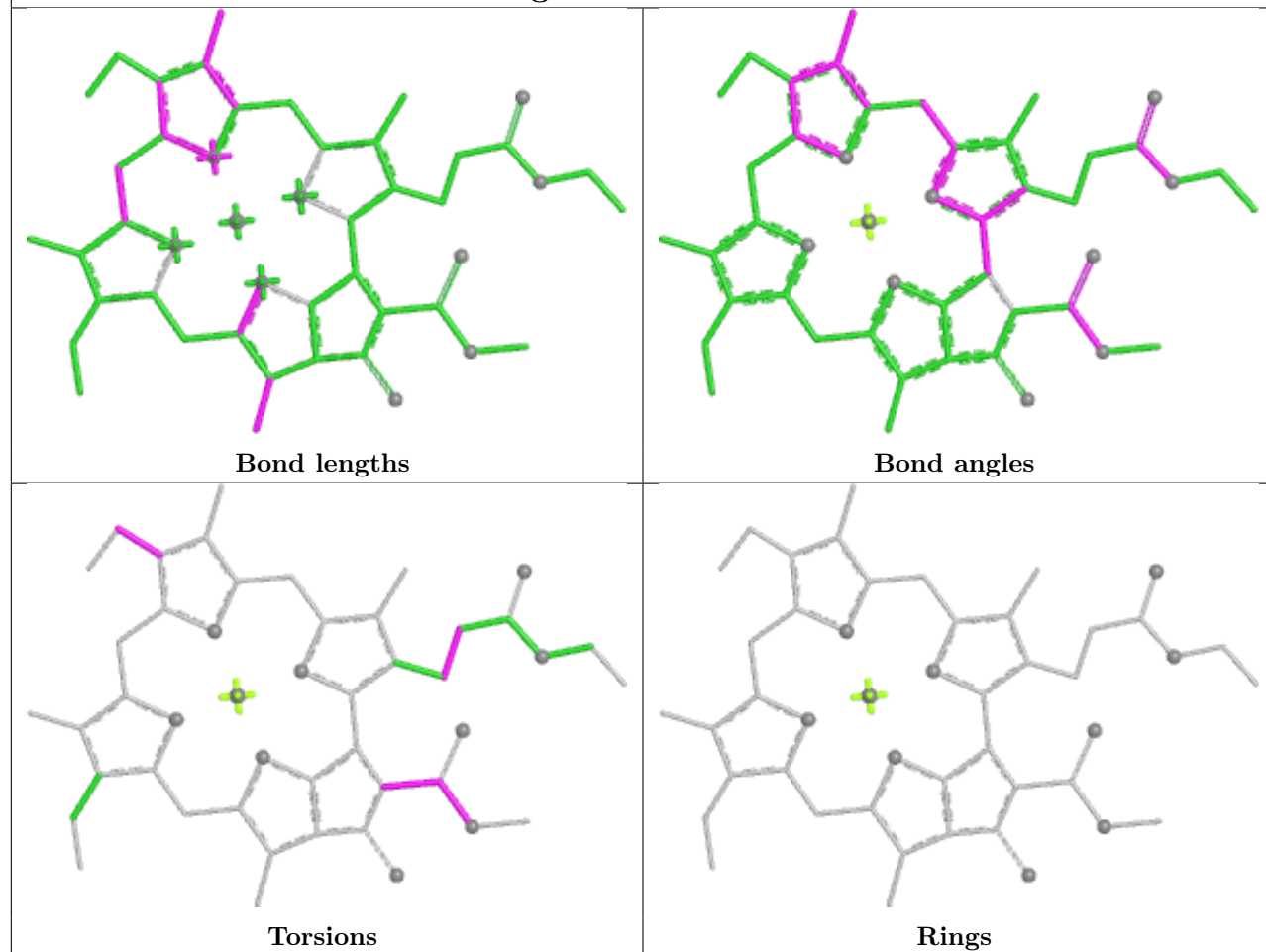


Ligand CLA a 832

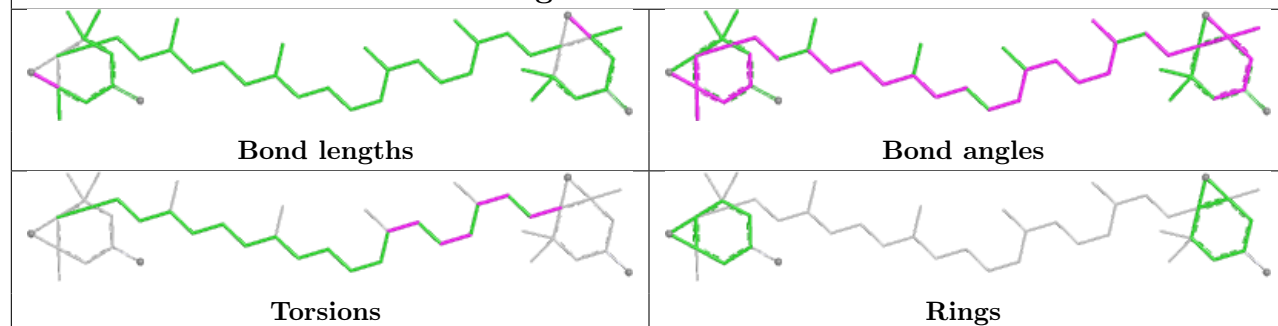




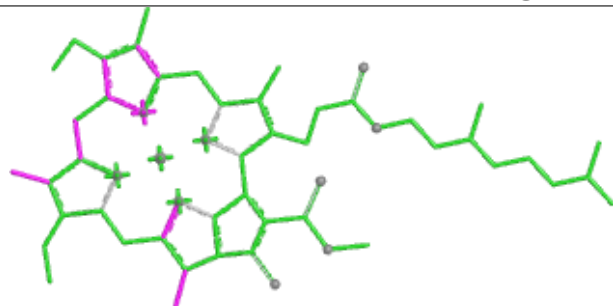
Ligand CLA 2 307



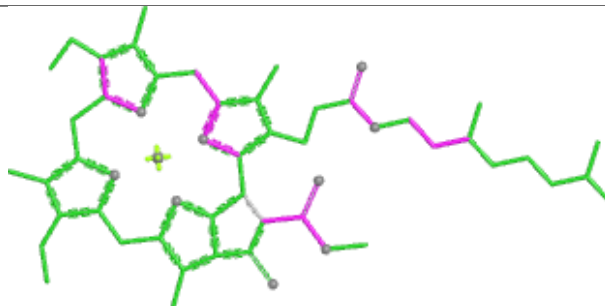
Ligand XAT 7 304



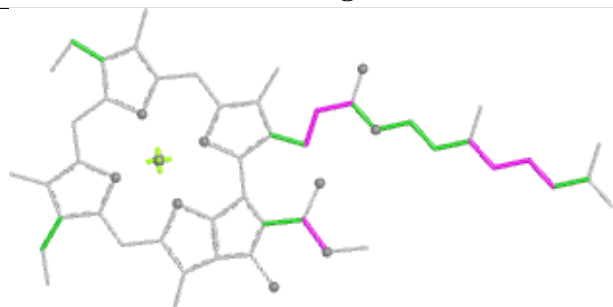
Ligand CLA h 205



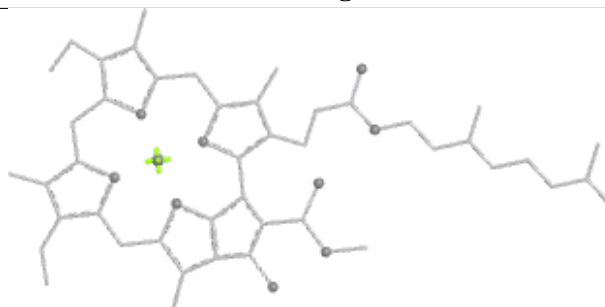
Bond lengths



Bond angles

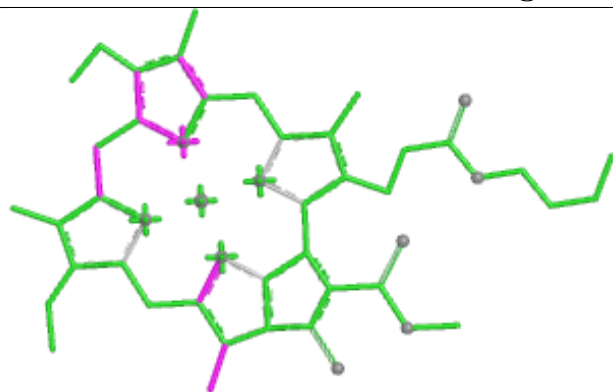


Torsions

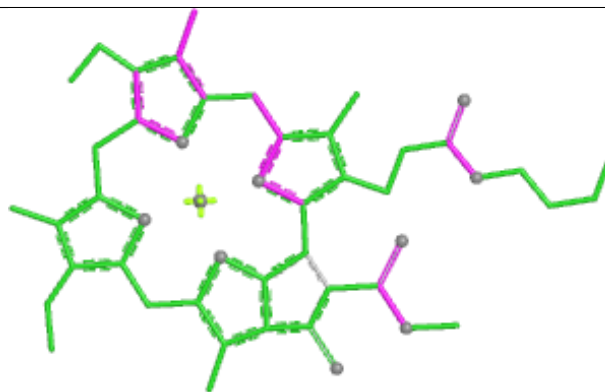


Rings

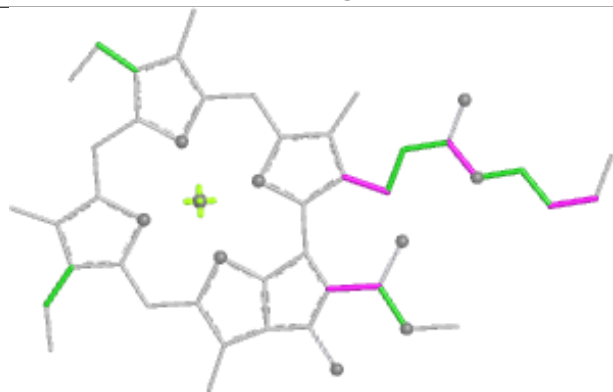
Ligand CLA a 823



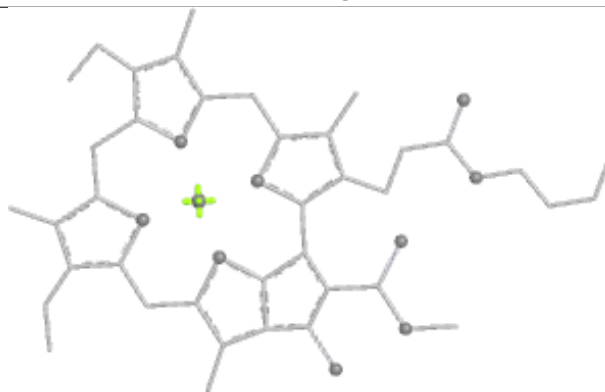
Bond lengths



Bond angles

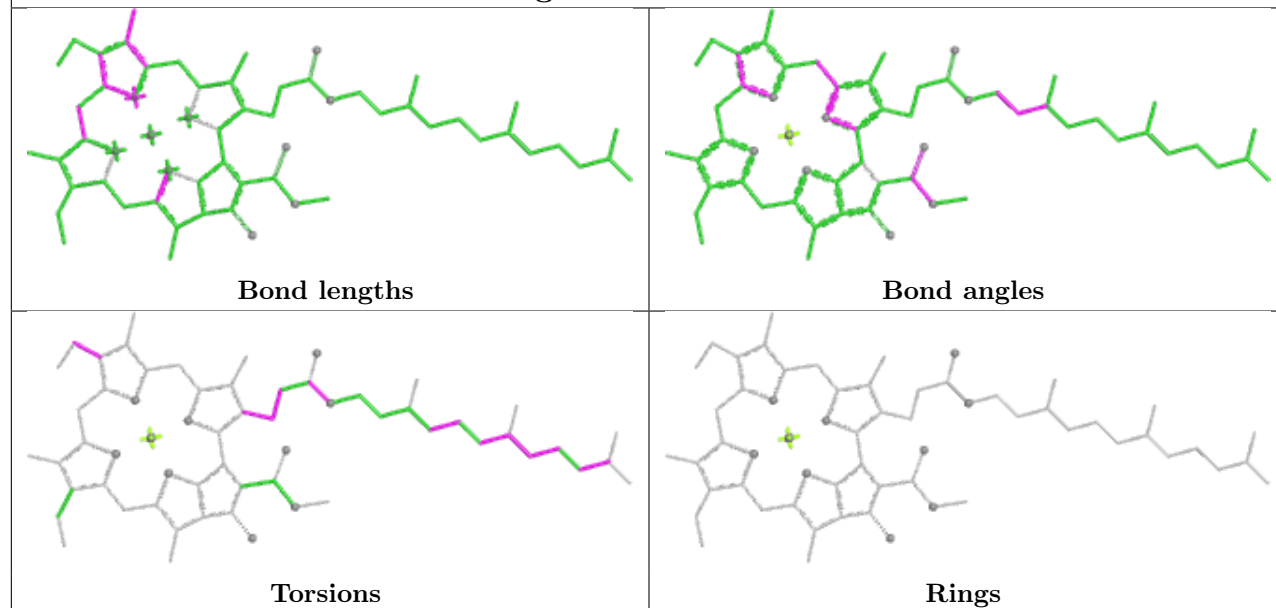


Torsions

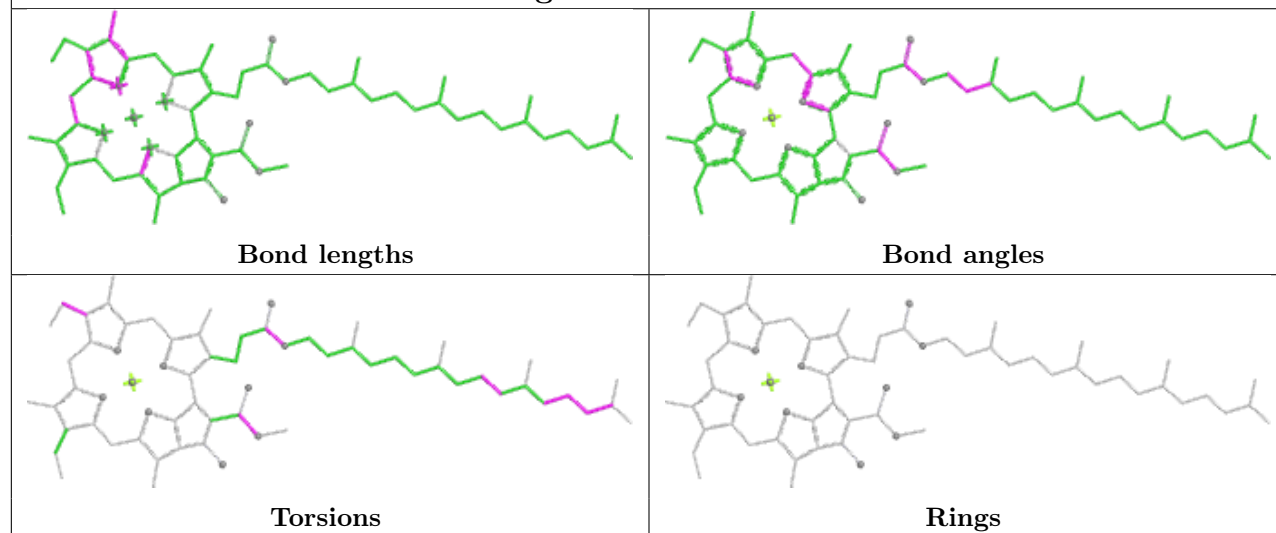


Rings

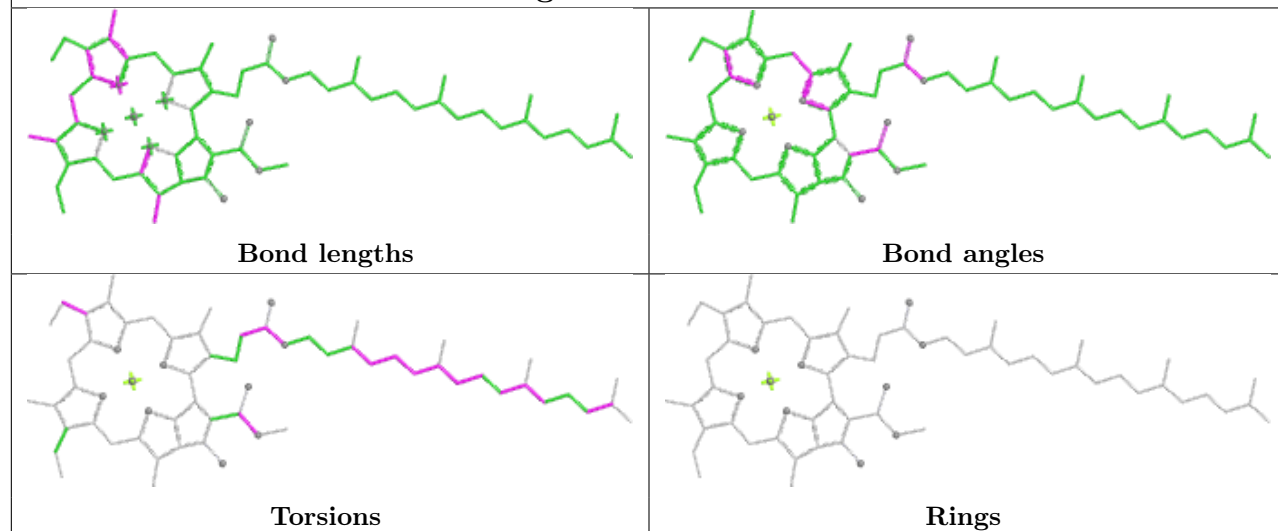
Ligand CLA b 818



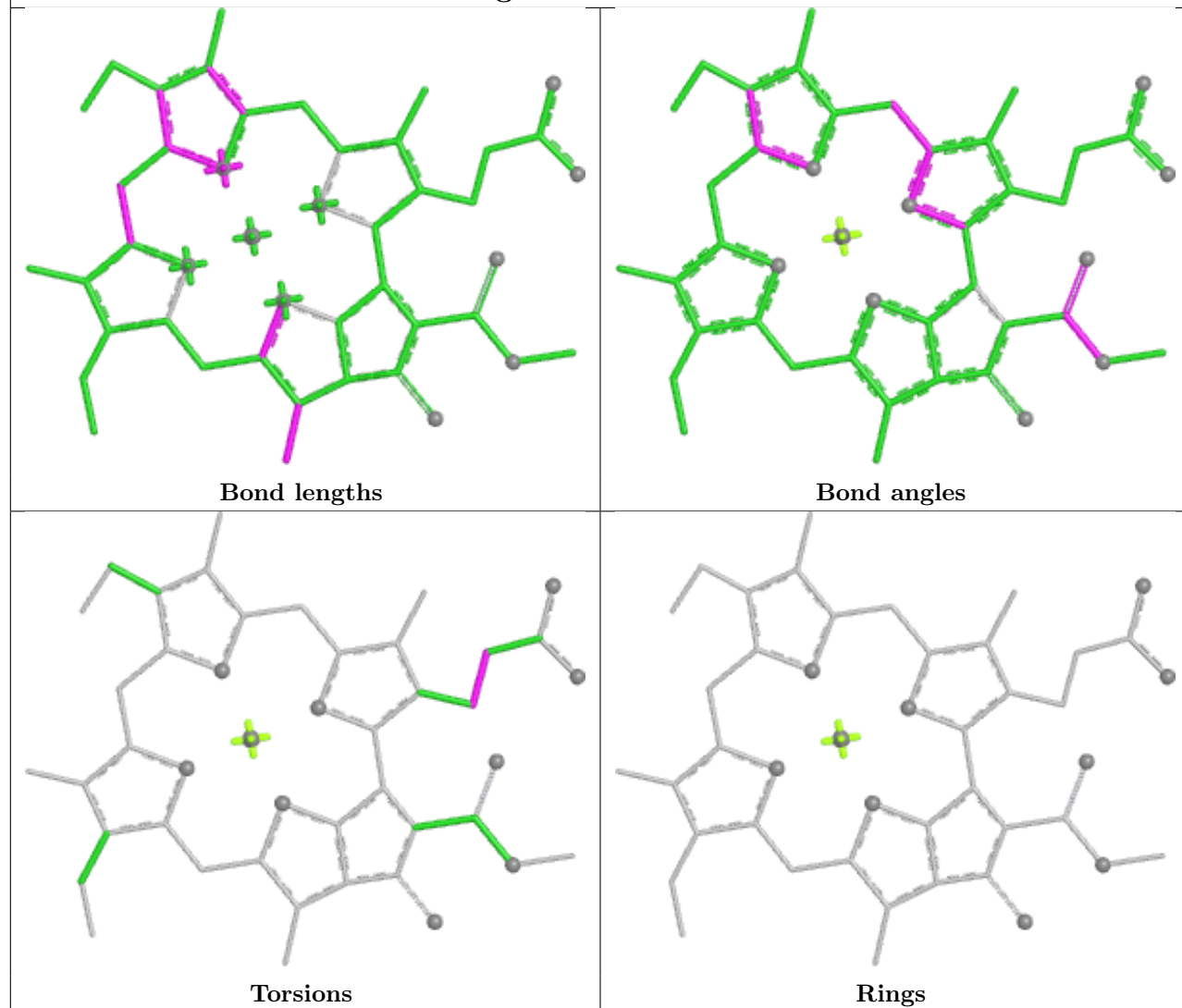
Ligand CLA b 840



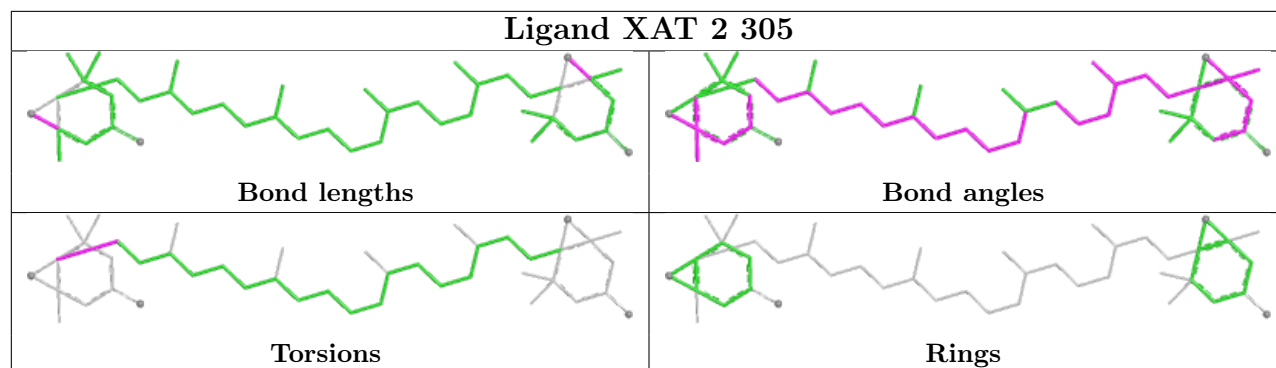
Ligand CLA a 801



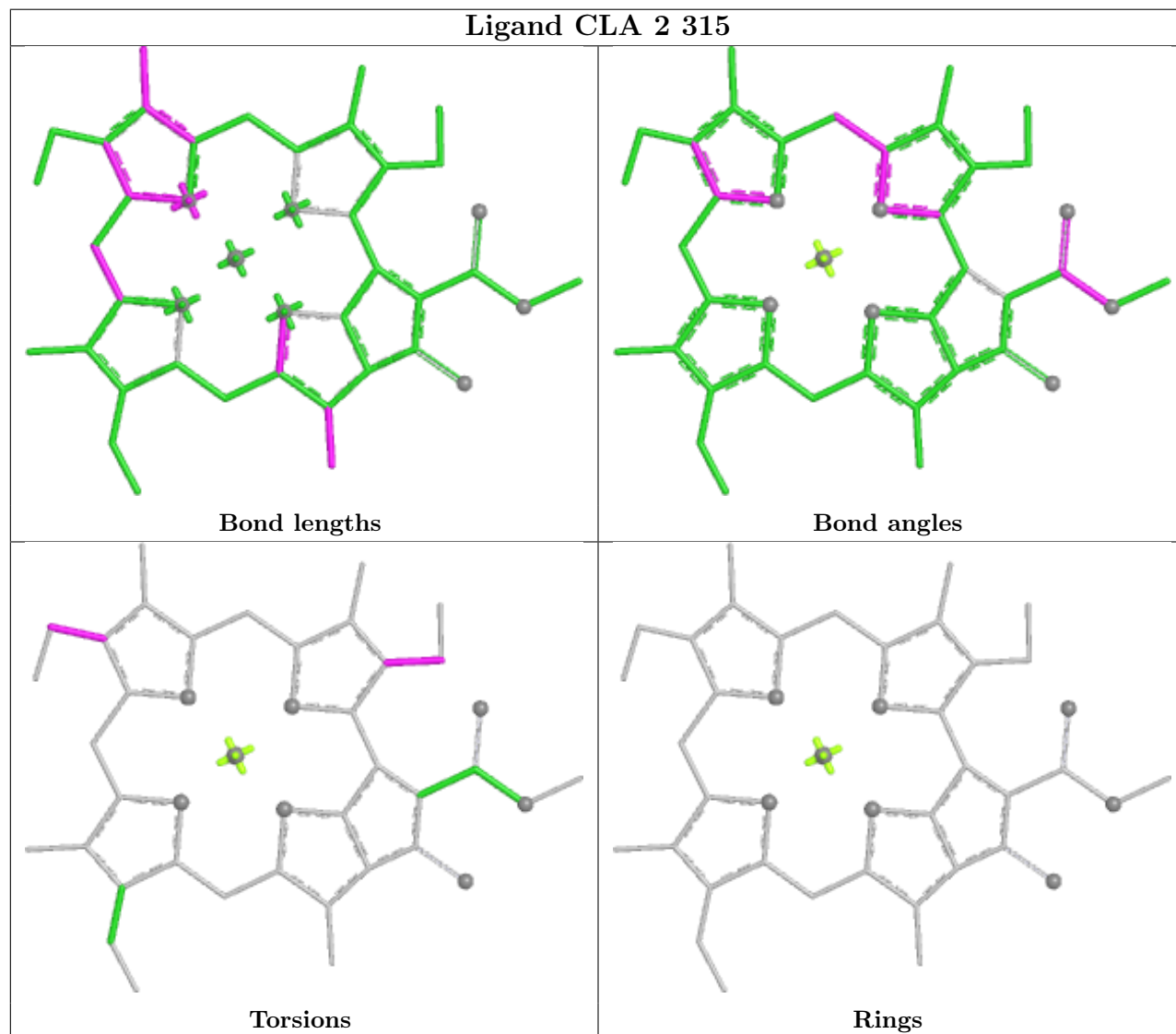
Ligand CLA a 821



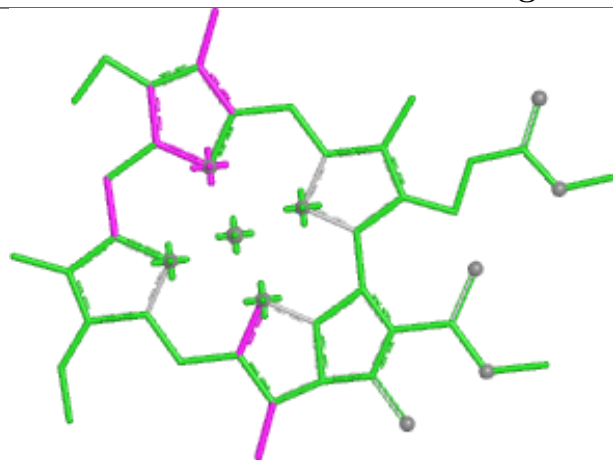
Ligand XAT 2 305



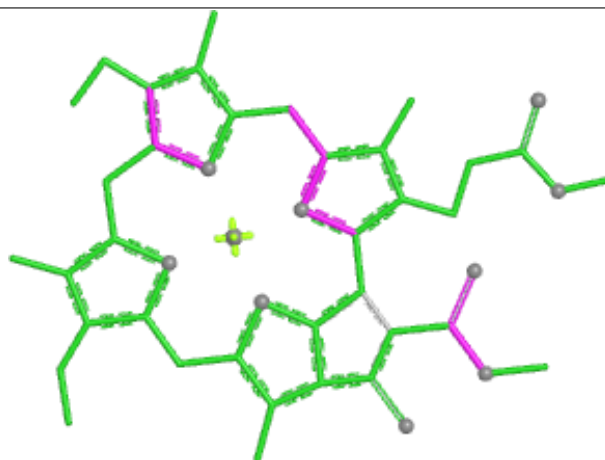
Ligand CLA 2 315



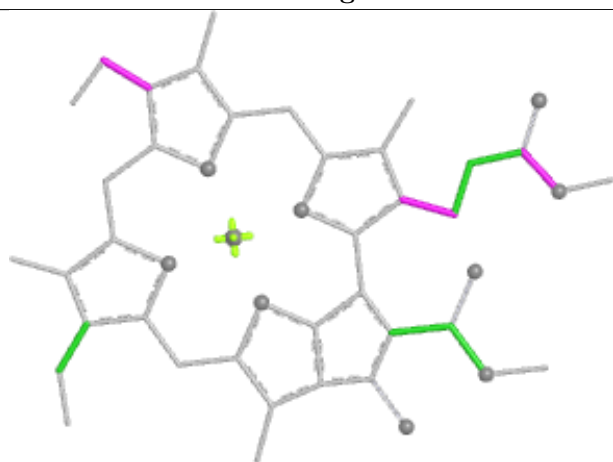
Ligand CLA a 824



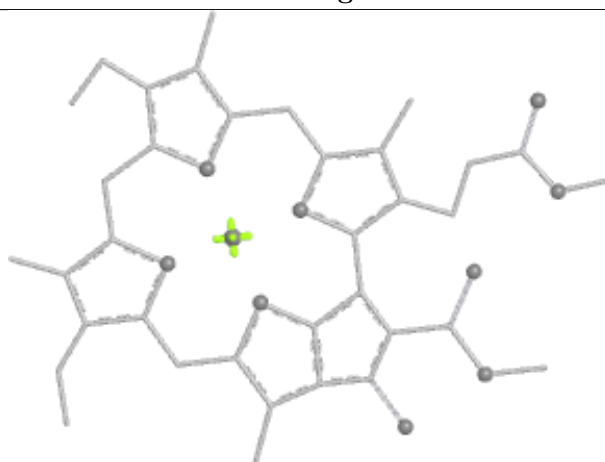
Bond lengths



Bond angles

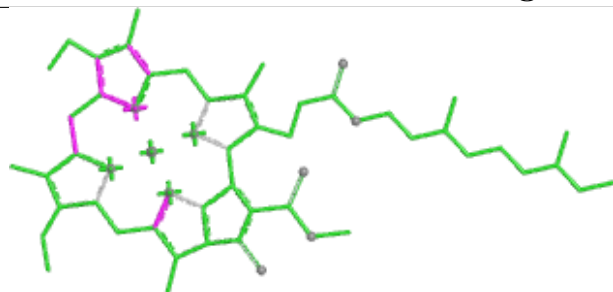


Torsions

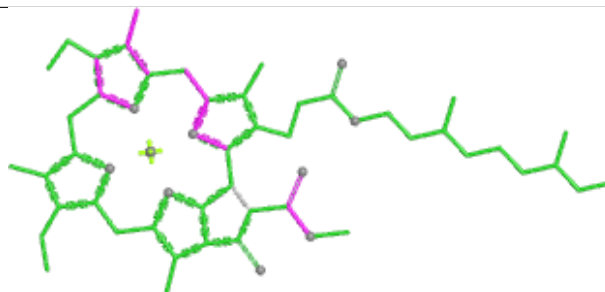


Rings

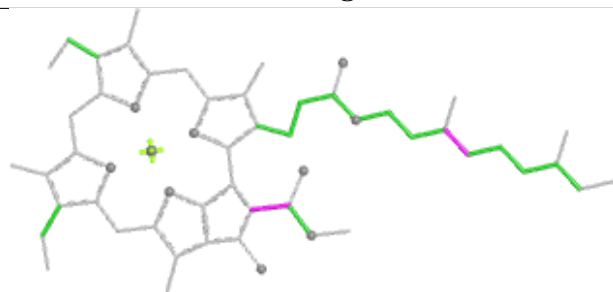
Ligand CLA 3 310



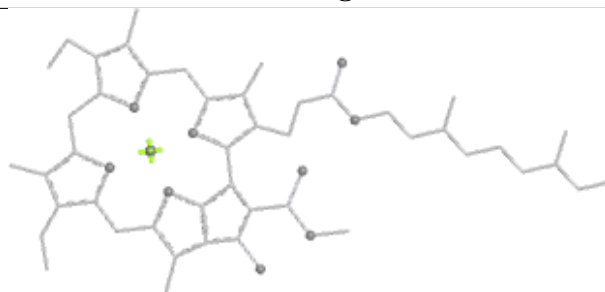
Bond lengths



Bond angles

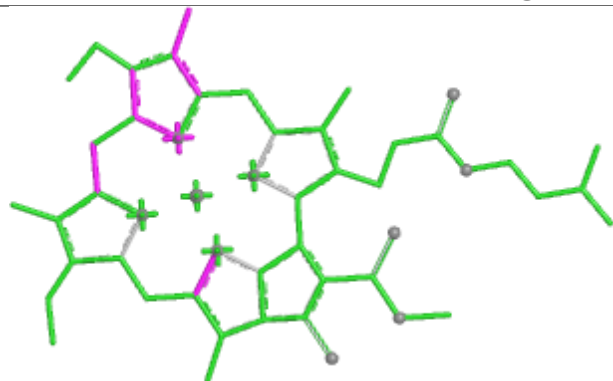


Torsions

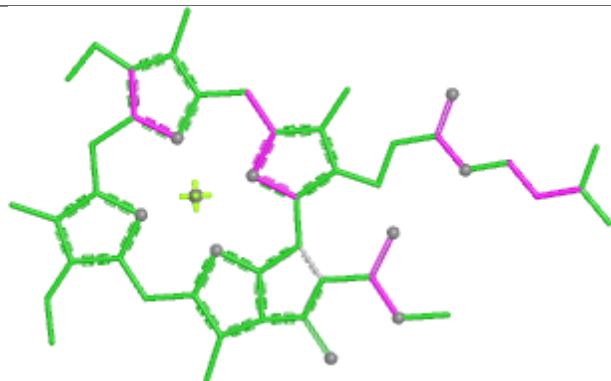


Rings

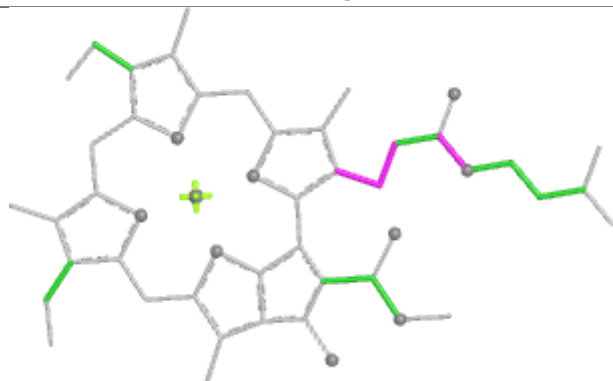
Ligand CLA 3 311



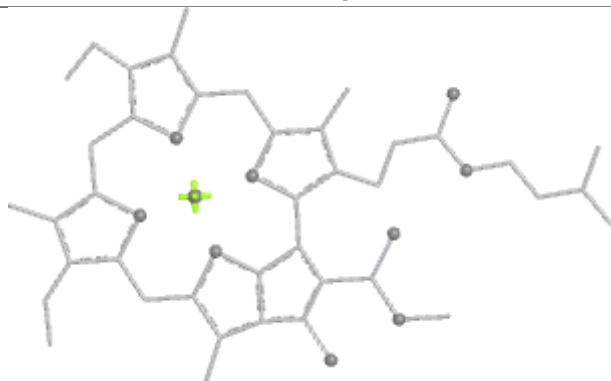
Bond lengths



Bond angles

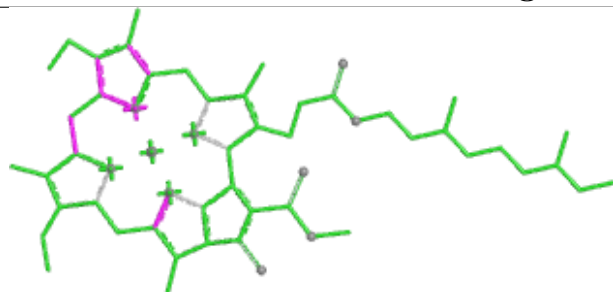


Torsions

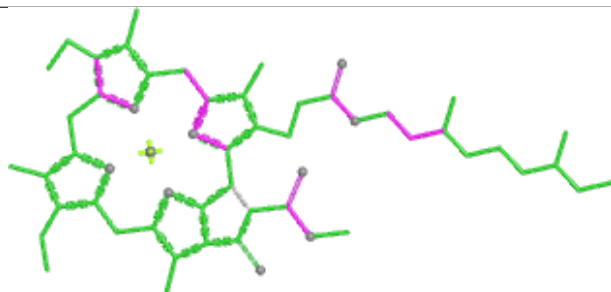


Rings

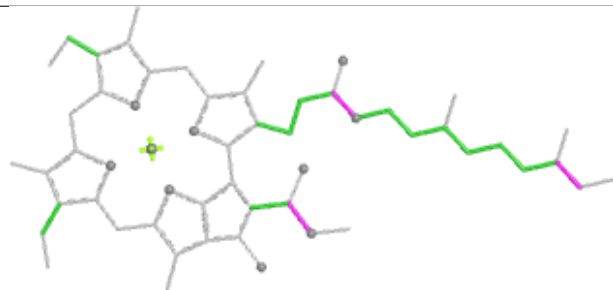
Ligand CLA a 811



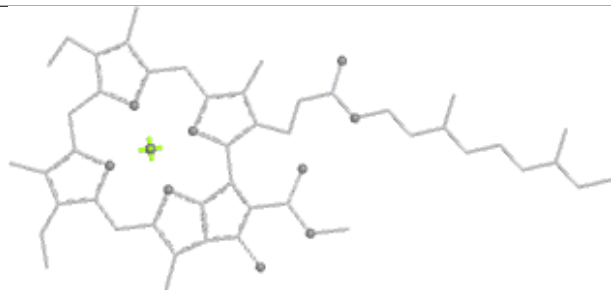
Bond lengths



Bond angles

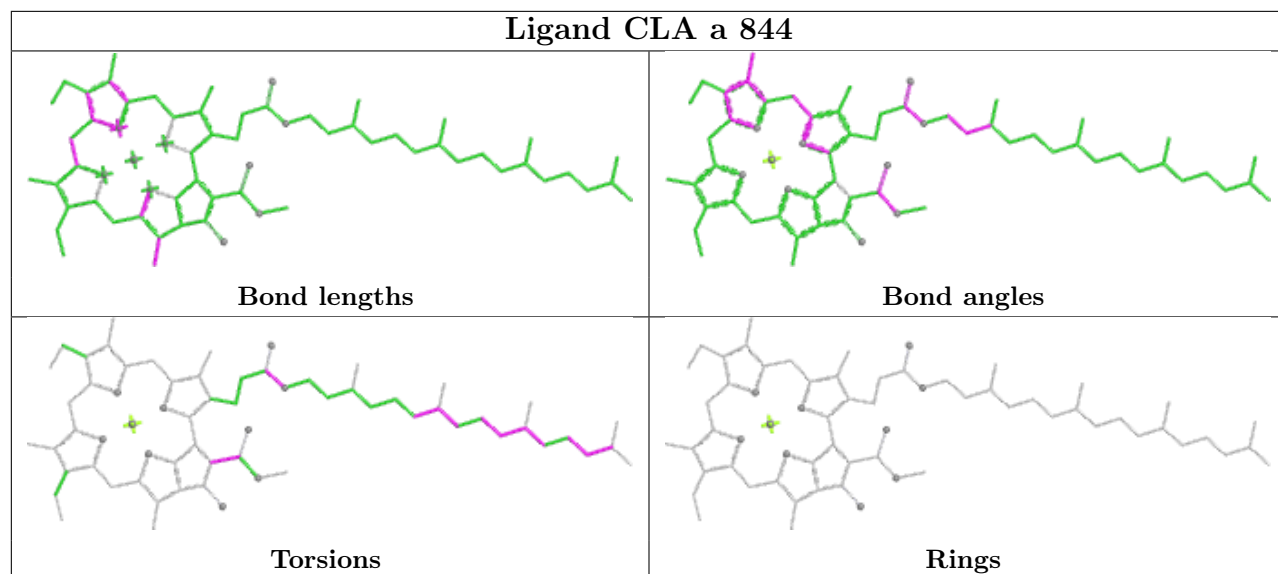


Torsions

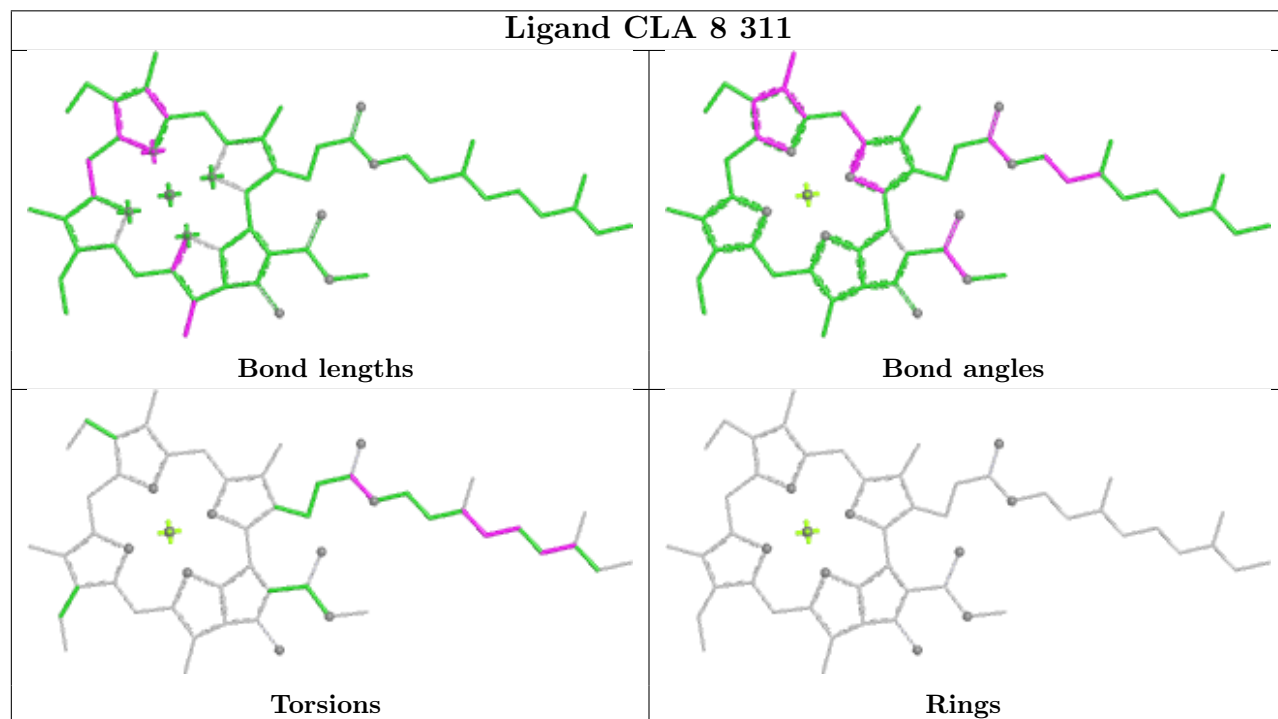


Rings

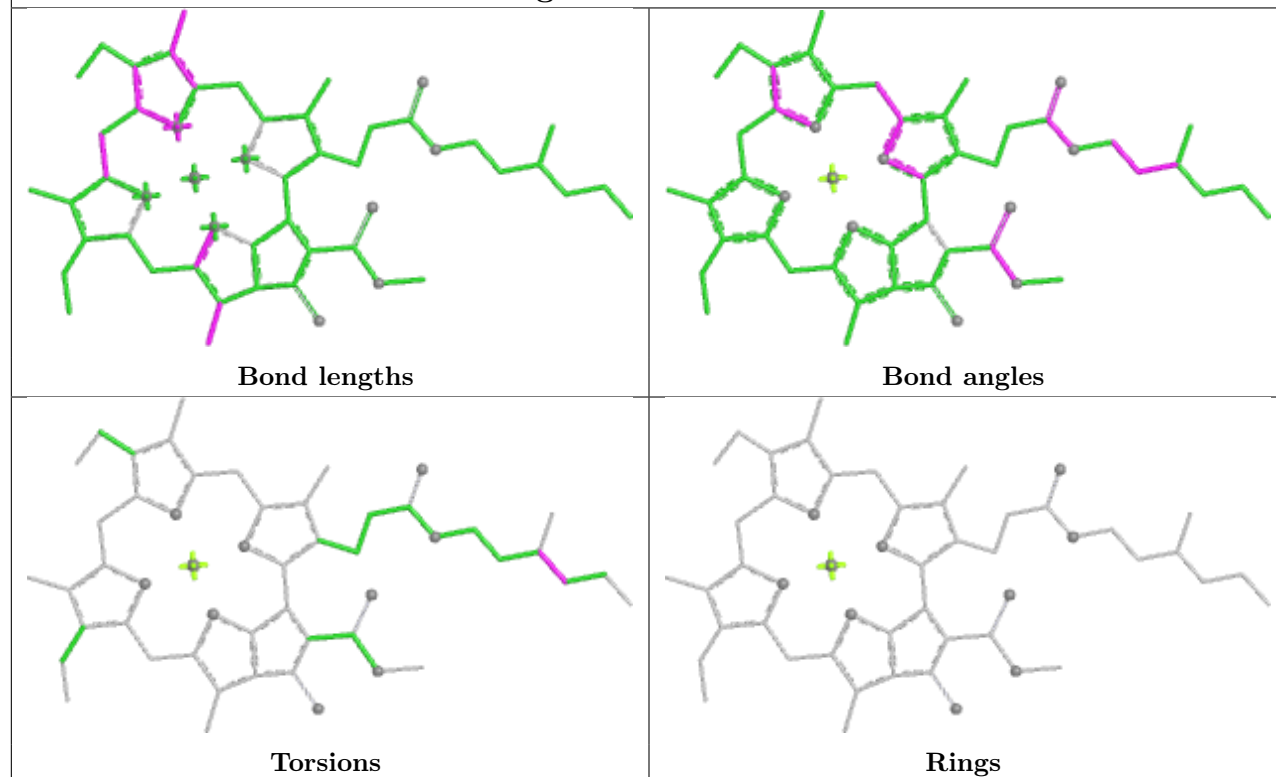
Ligand CLA a 844



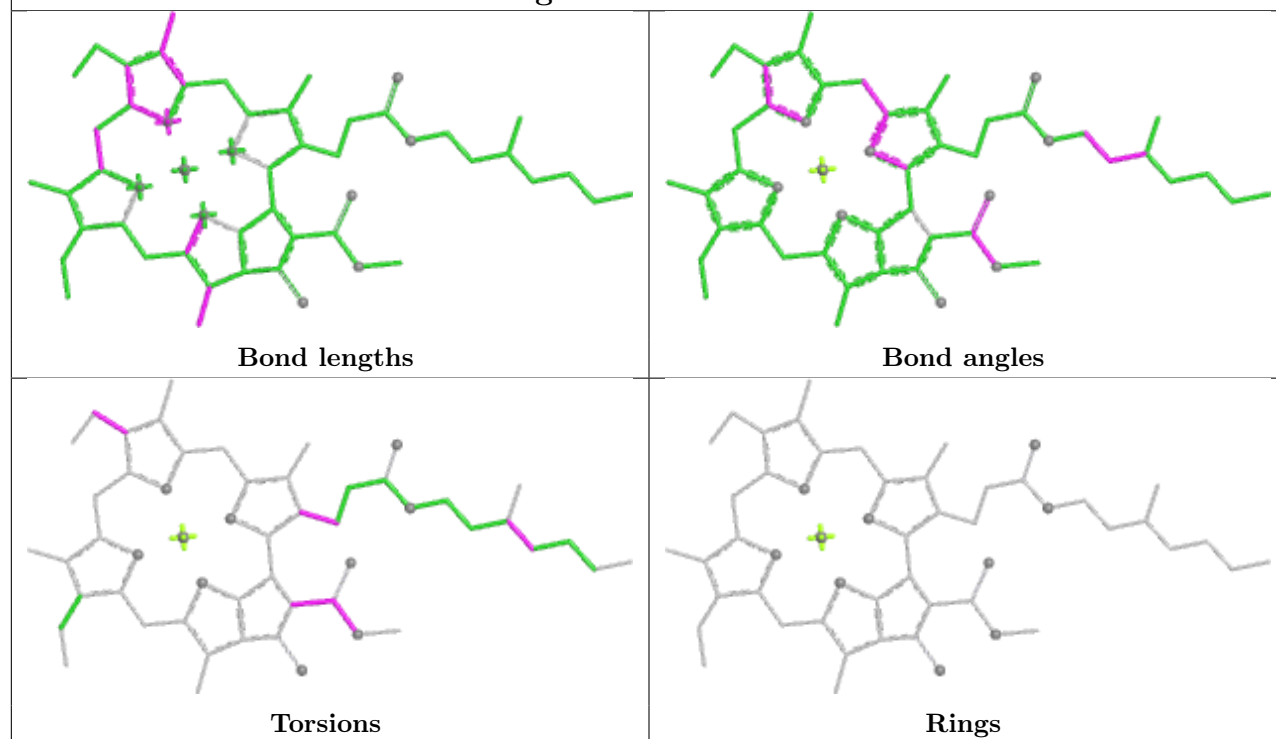
Ligand CLA 8 311



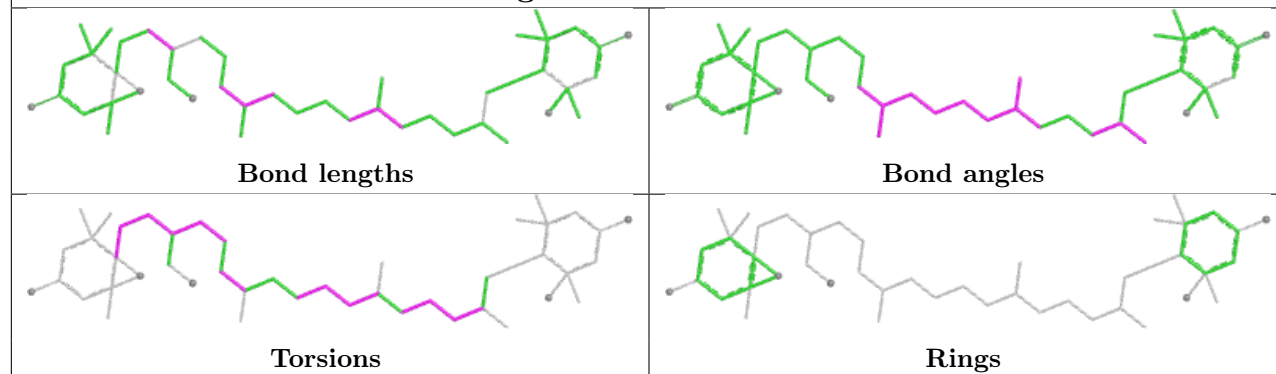
Ligand CLA 3 313



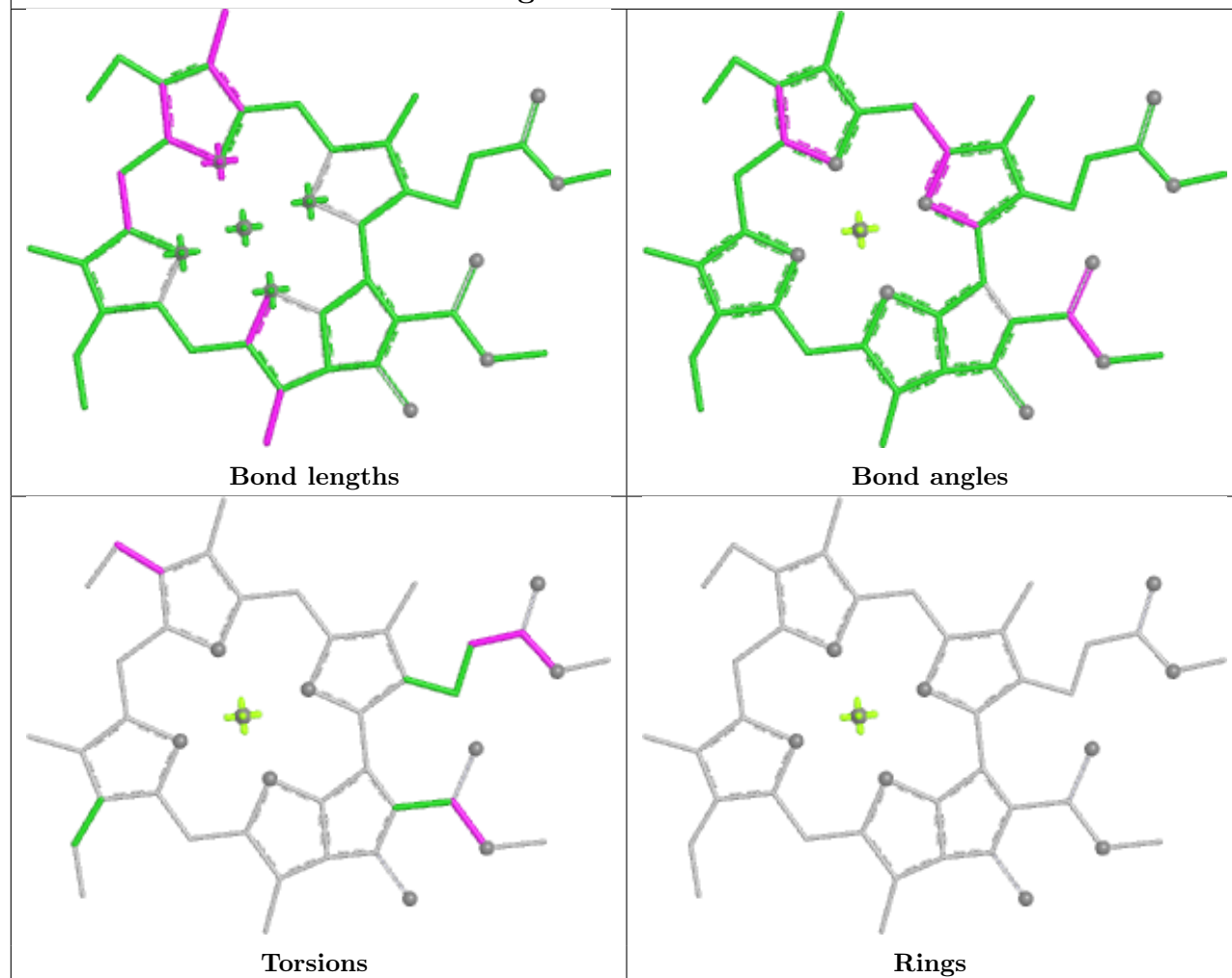
Ligand CLA b 834



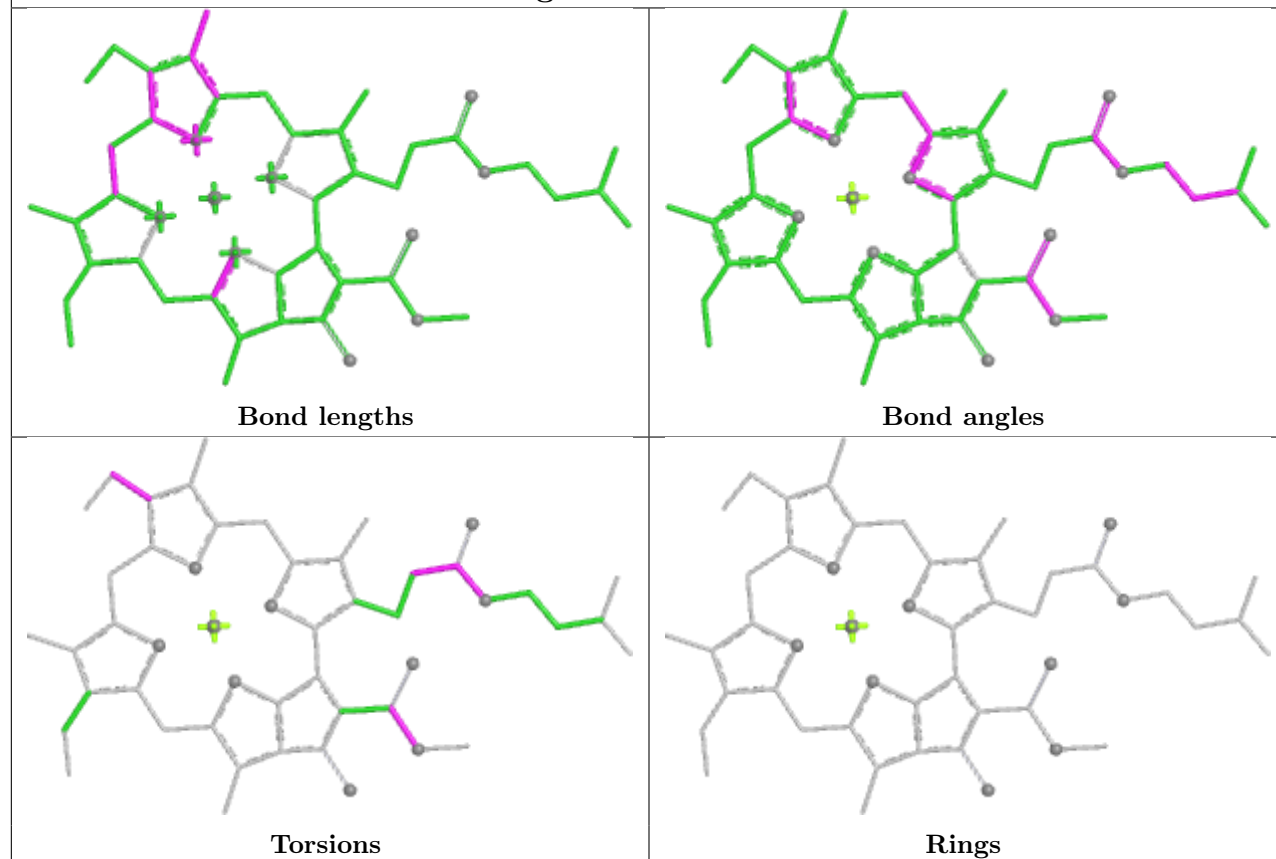
Ligand A1L1G 3 302



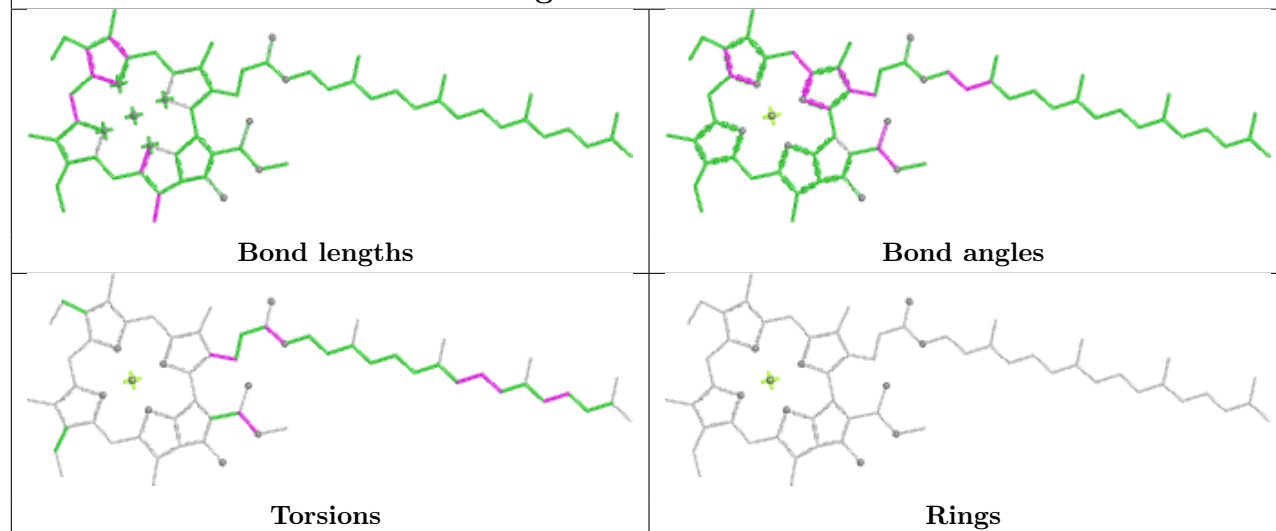
Ligand CLA 1 309



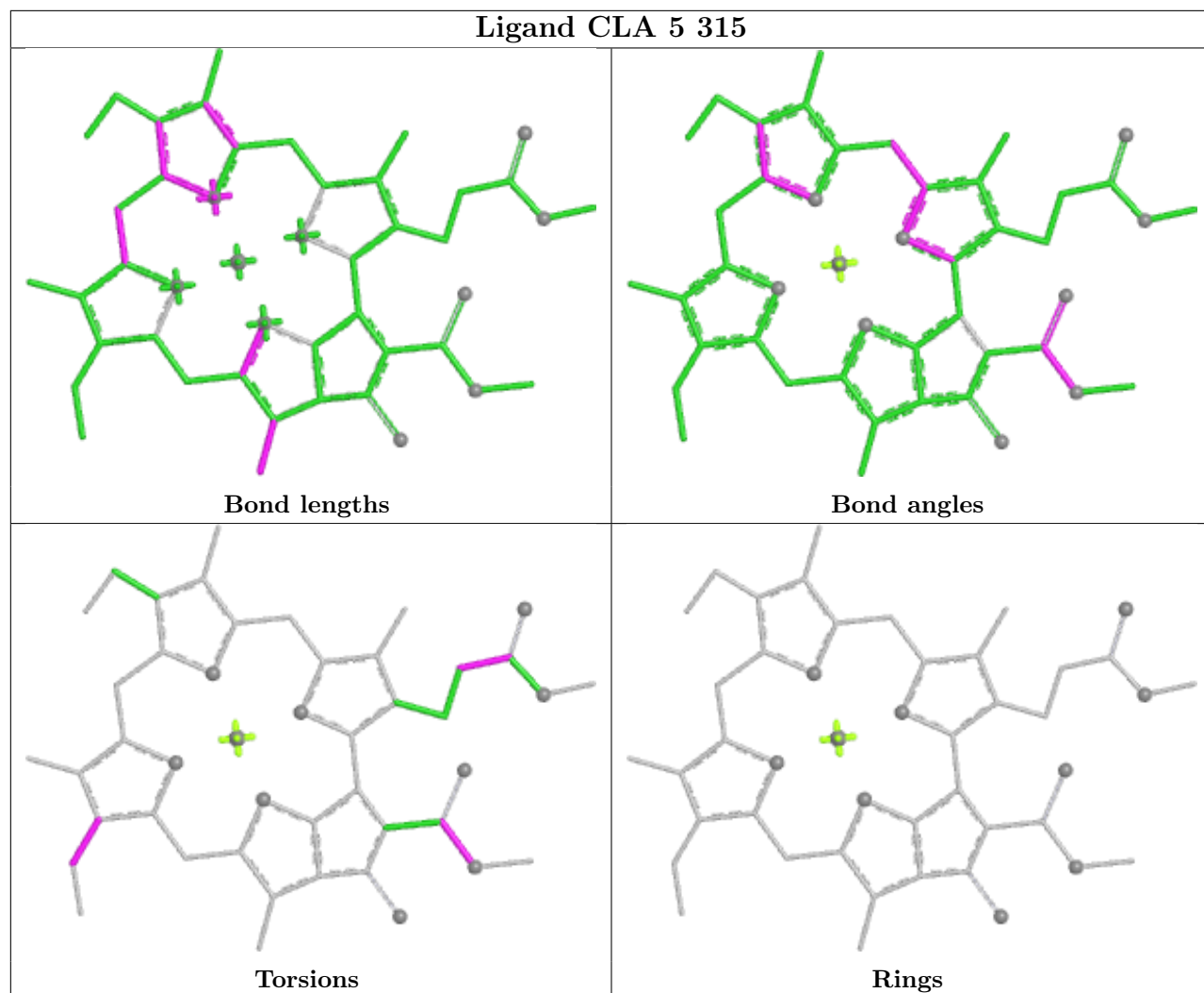
Ligand CLA a 836



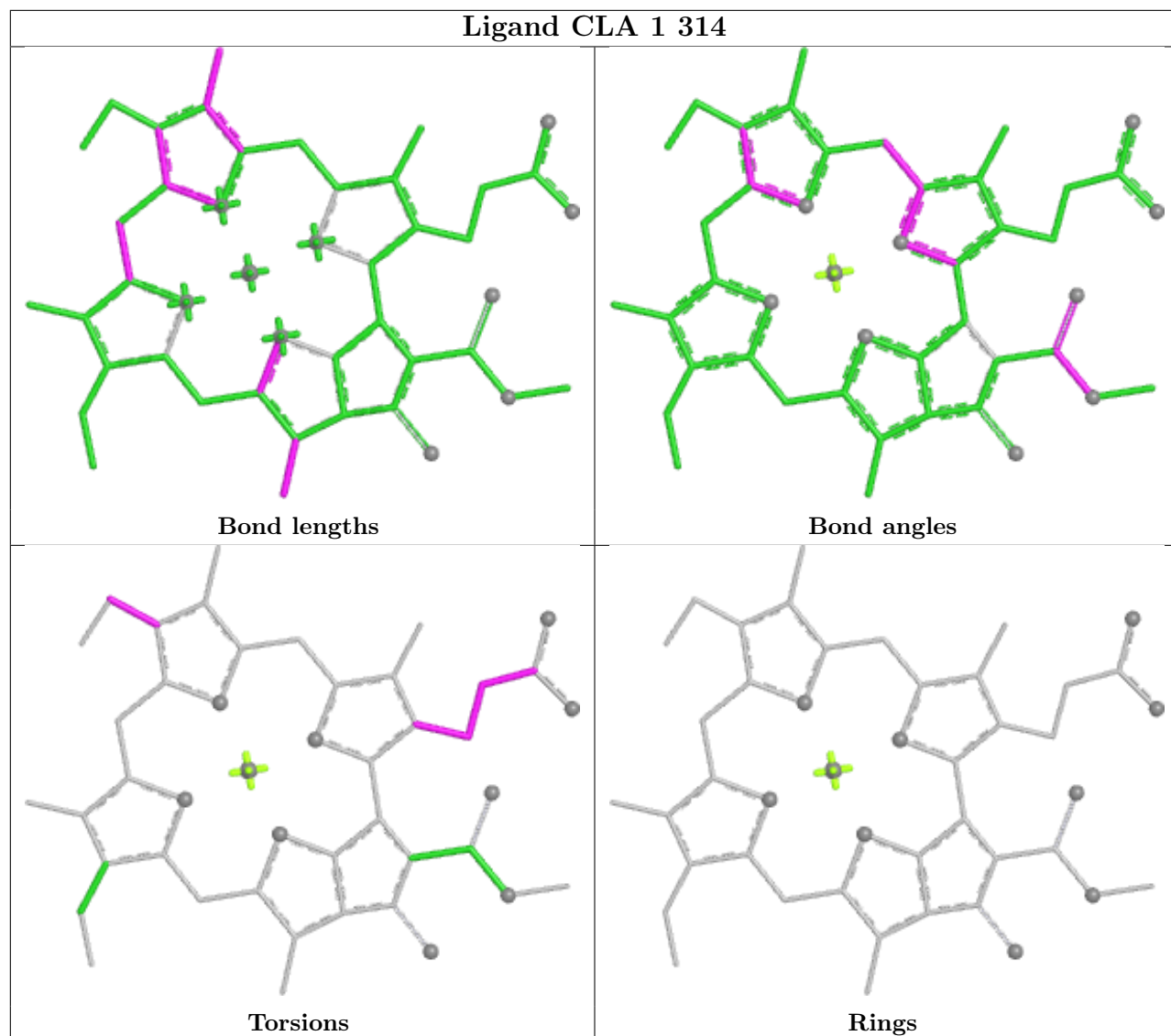
Ligand CLA h 203



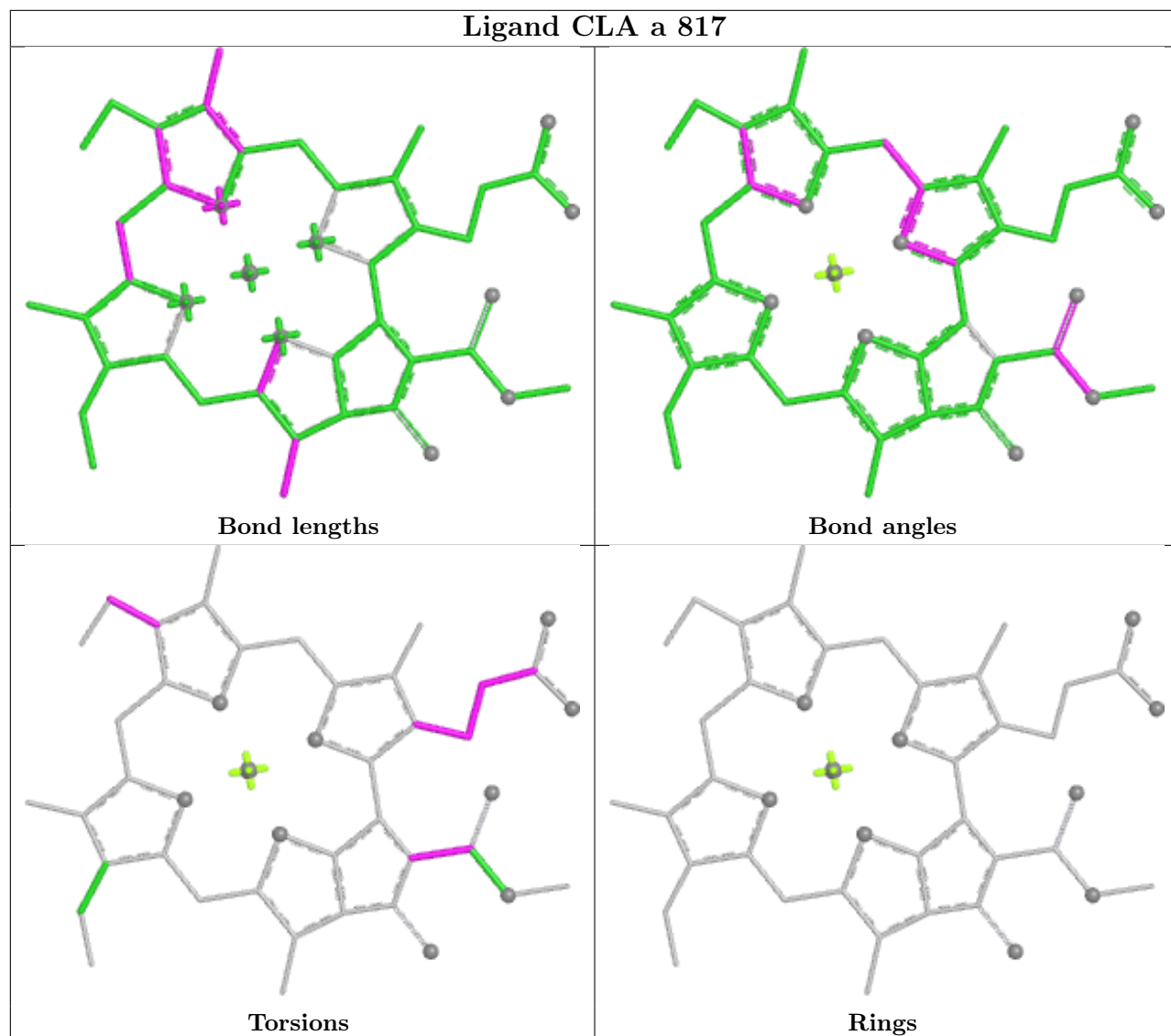
Ligand CLA 5 315



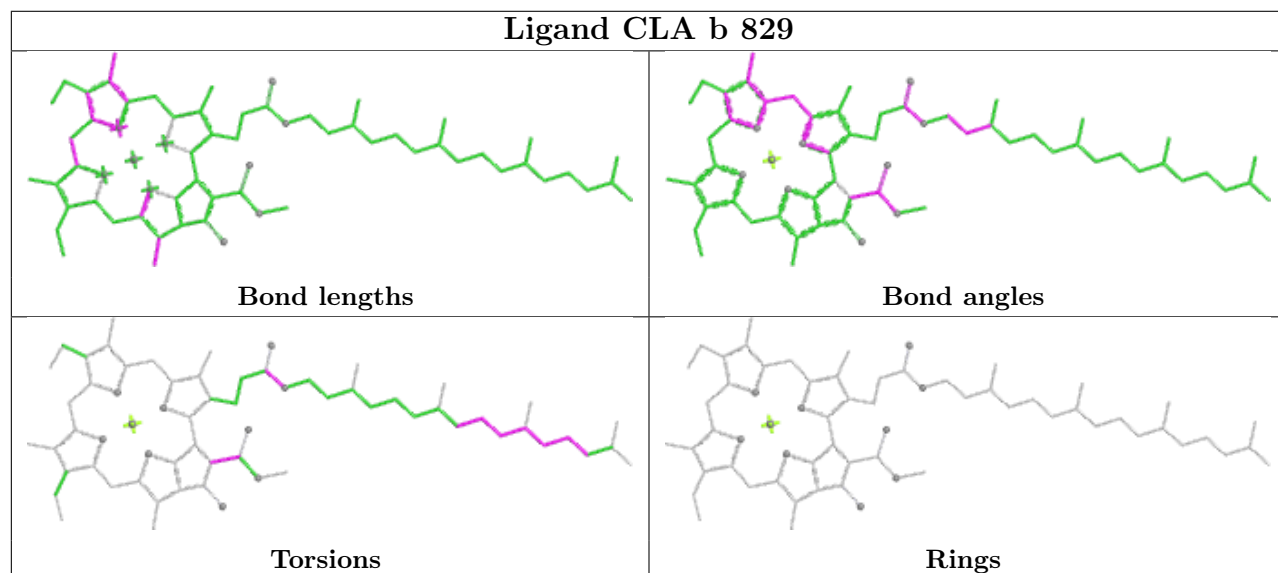
Ligand CLA 1 314



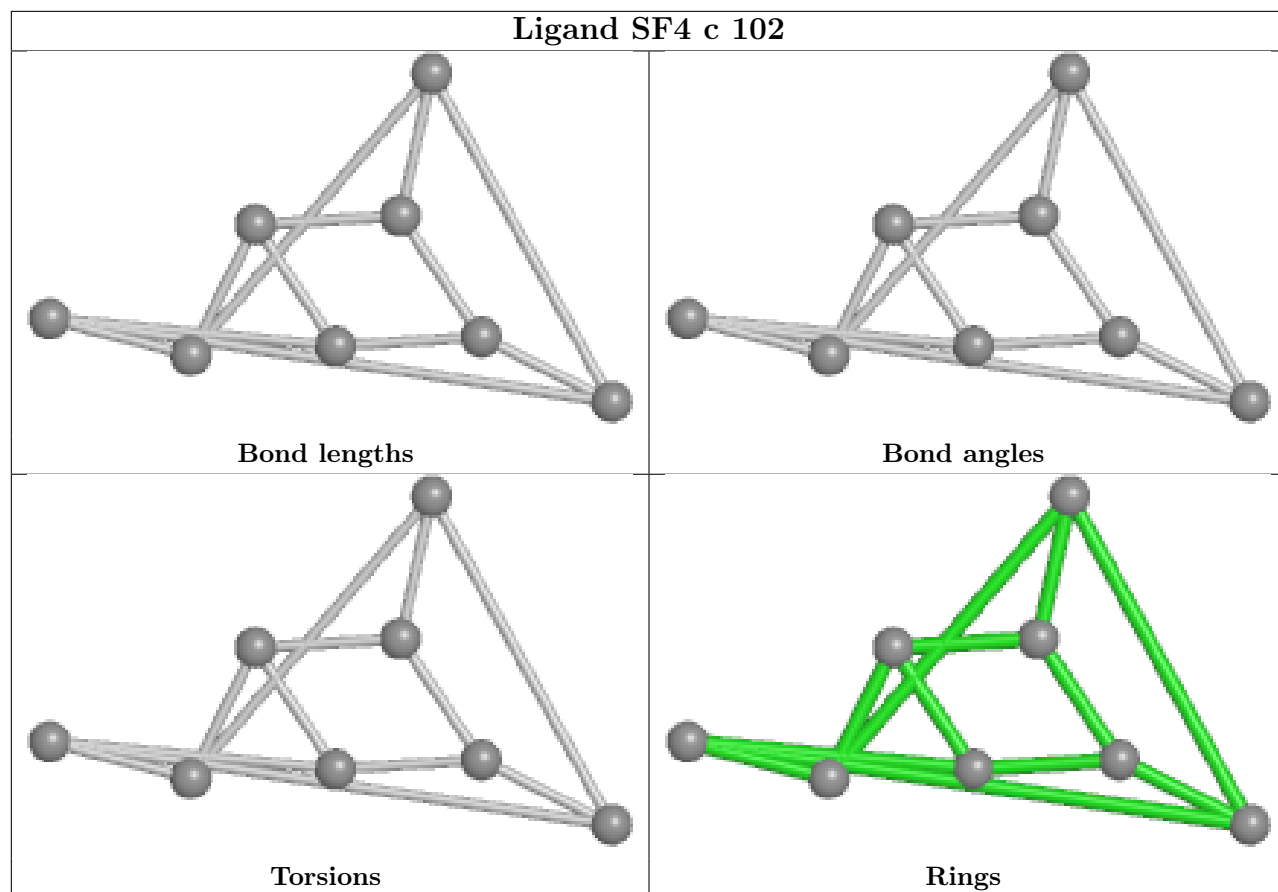
Ligand CLA a 817



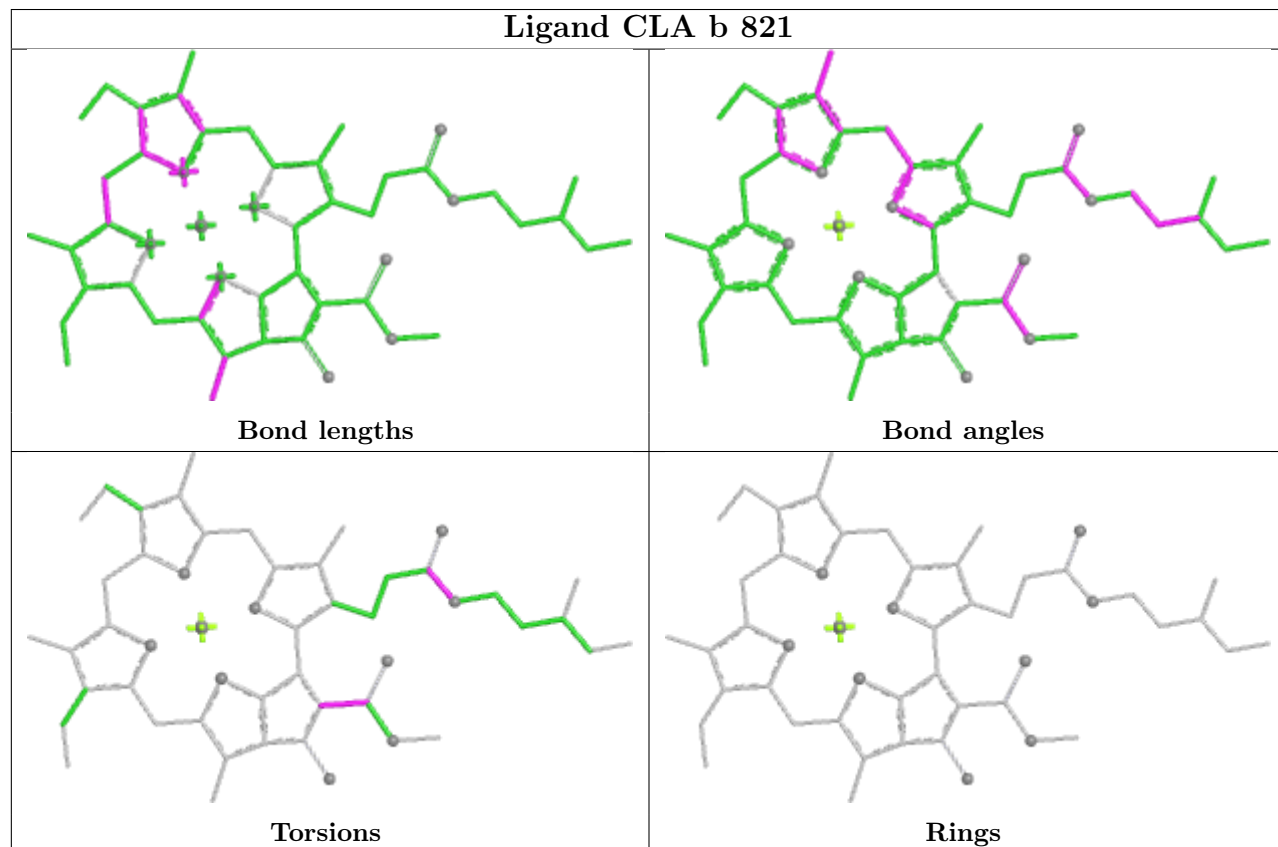
Ligand CLA b 829



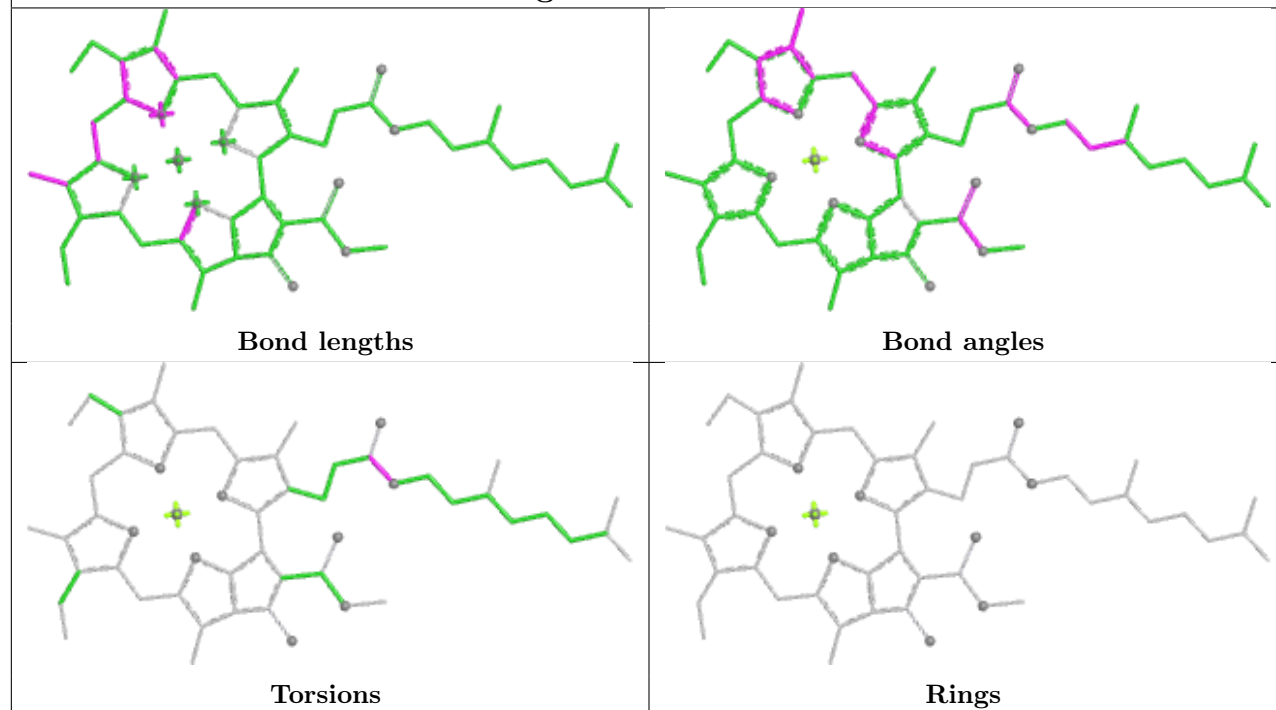
Ligand SF4 c 102



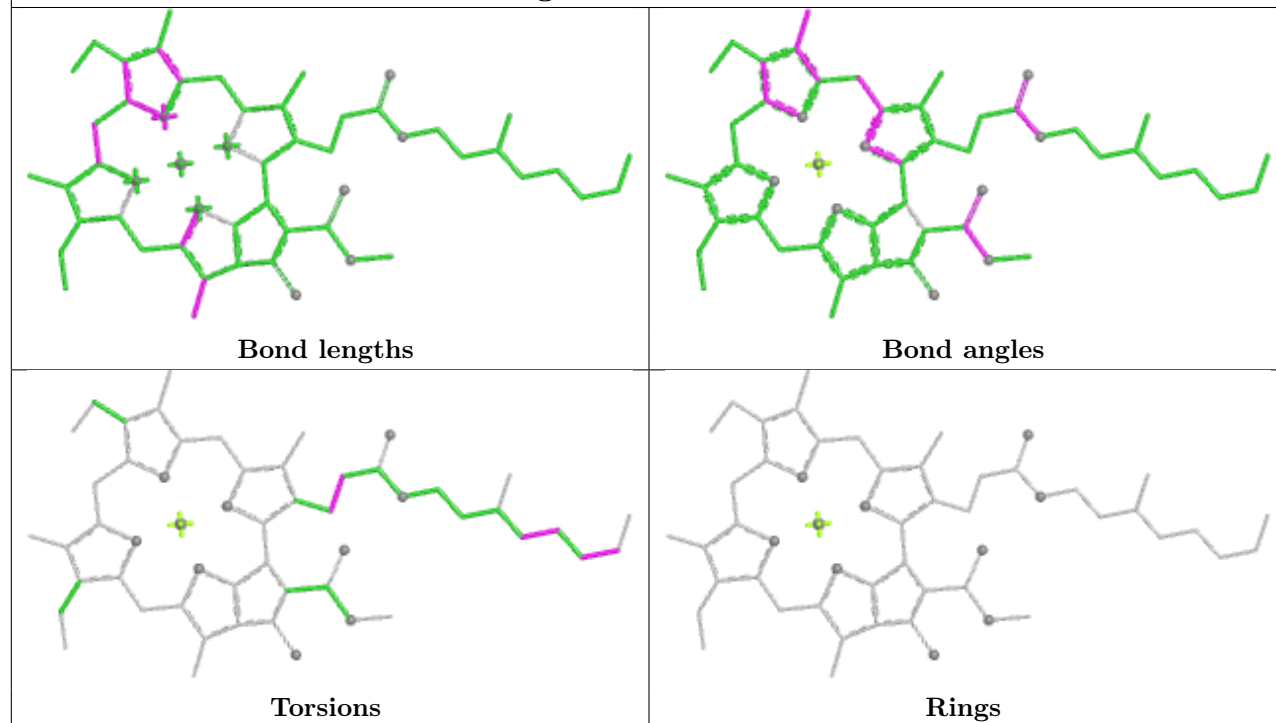
Ligand CLA b 821

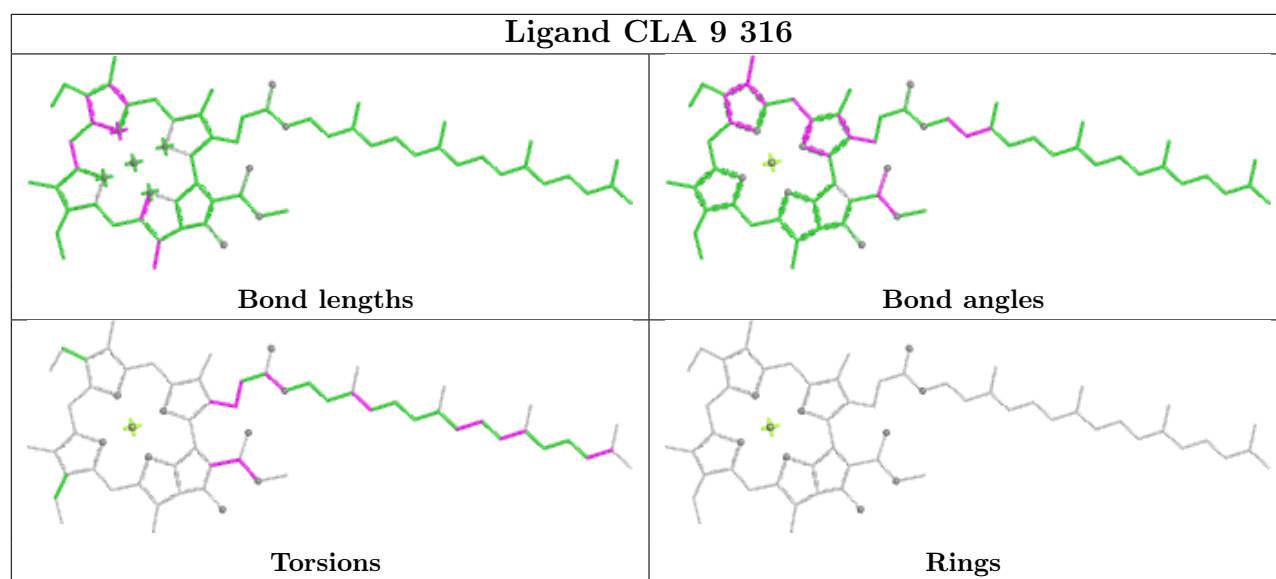


Ligand CLA a 833



Ligand CLA 2 308





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.

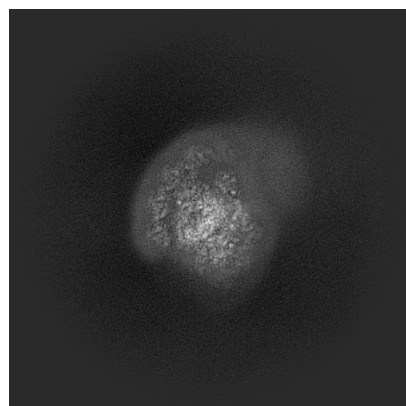
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60286. These allow visual inspection of the internal detail of the map and identification of artifacts.

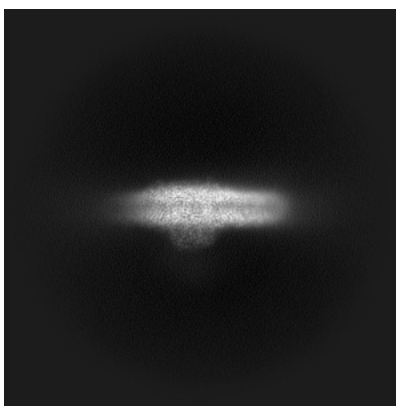
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

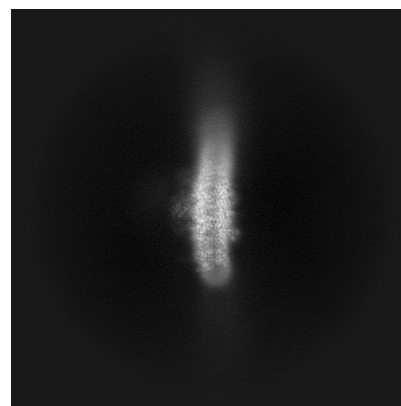
6.1.1 Primary map



X

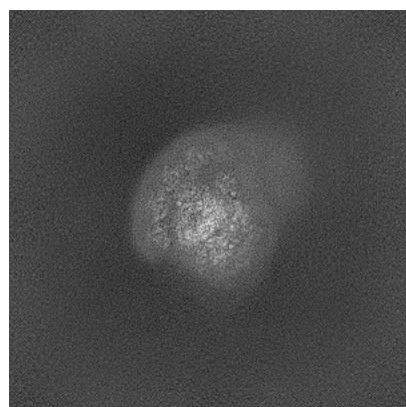


Y

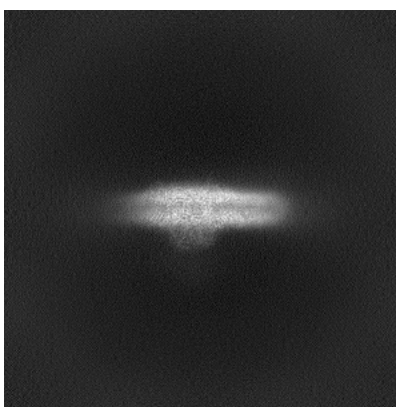


Z

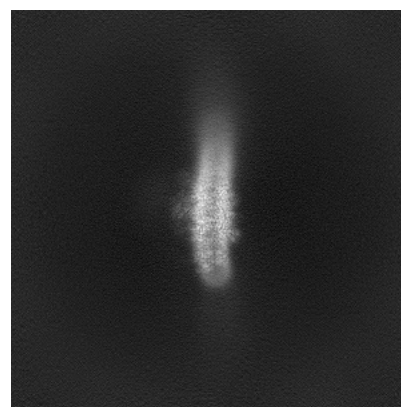
6.1.2 Raw map



X



Y

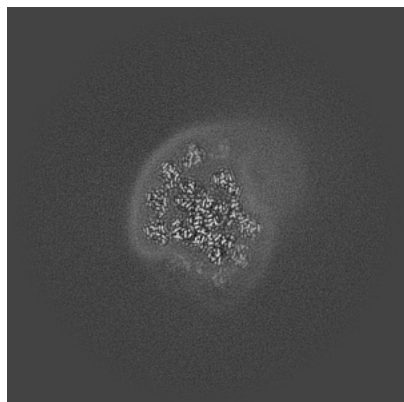


Z

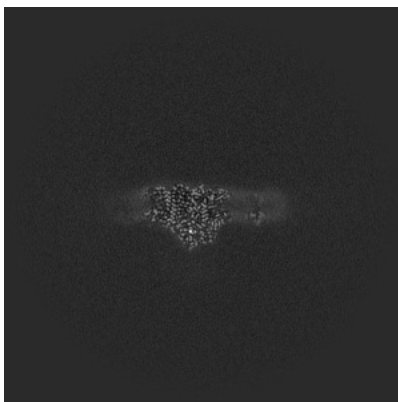
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

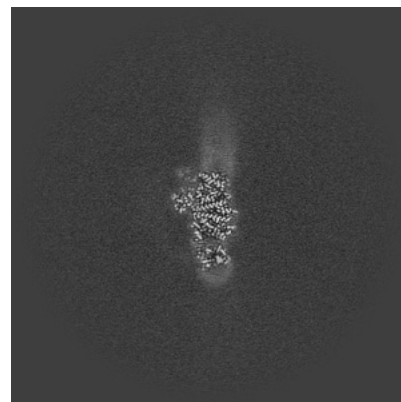
6.2.1 Primary map



X Index: 256

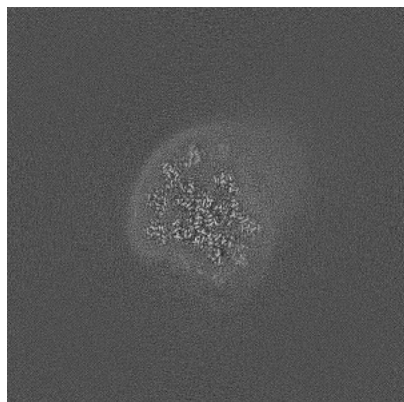


Y Index: 256

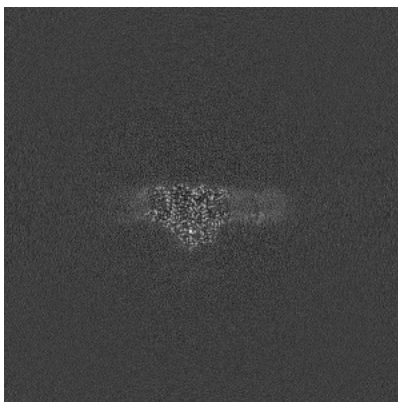


Z Index: 256

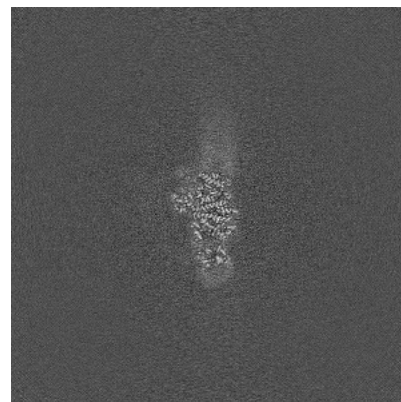
6.2.2 Raw map



X Index: 256



Y Index: 256

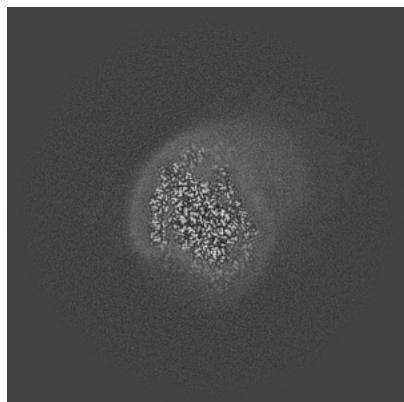


Z Index: 256

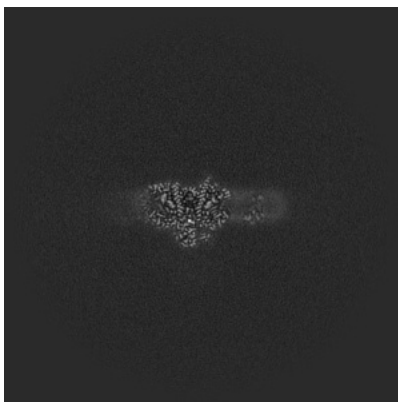
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

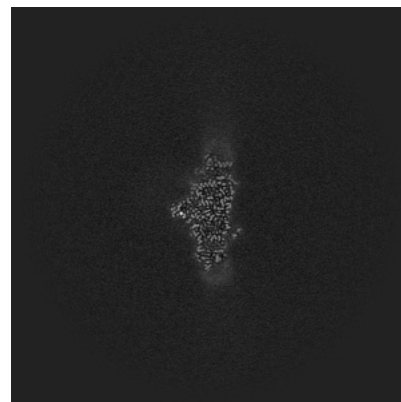
6.3.1 Primary map



X Index: 268

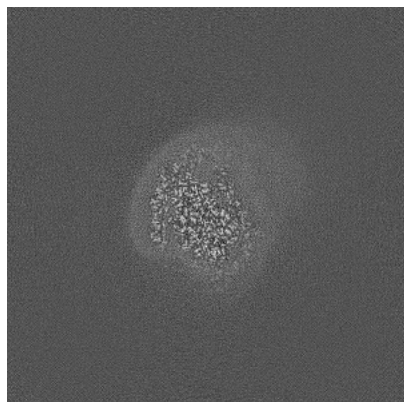


Y Index: 251

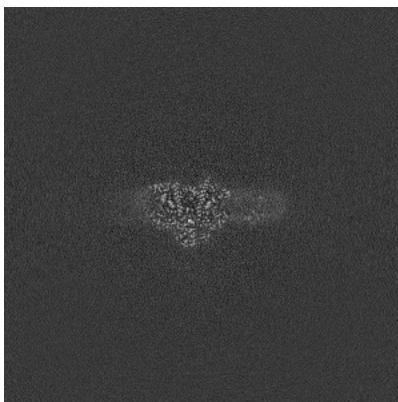


Z Index: 234

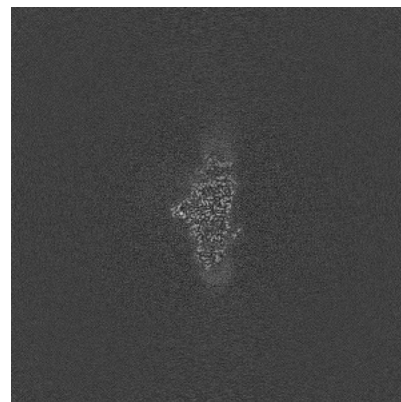
6.3.2 Raw map



X Index: 268



Y Index: 251

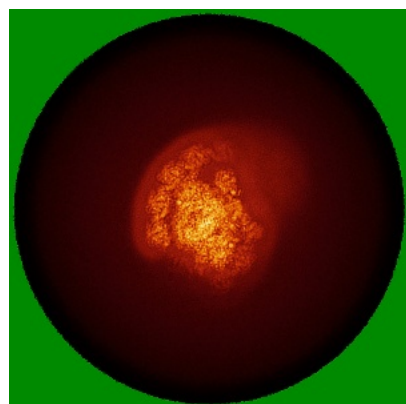


Z Index: 234

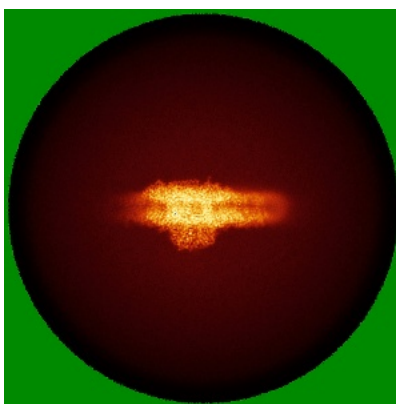
The images above show the largest variance slices of the map in three orthogonal directions.

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

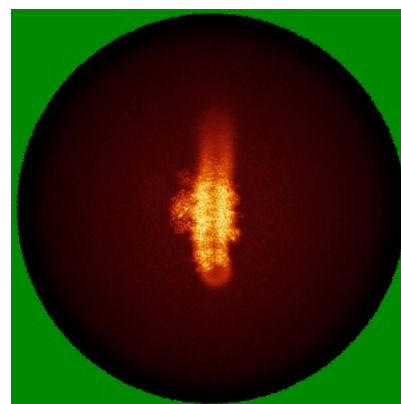
6.4.1 Primary map



X

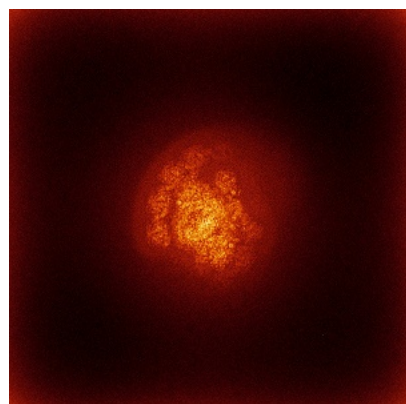


Y

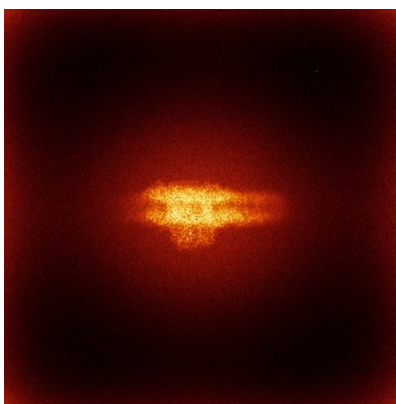


Z

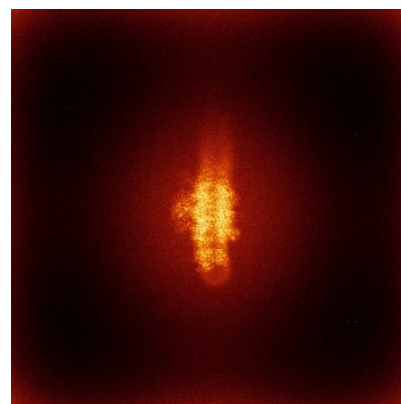
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.295. 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



X



Y



Z

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.

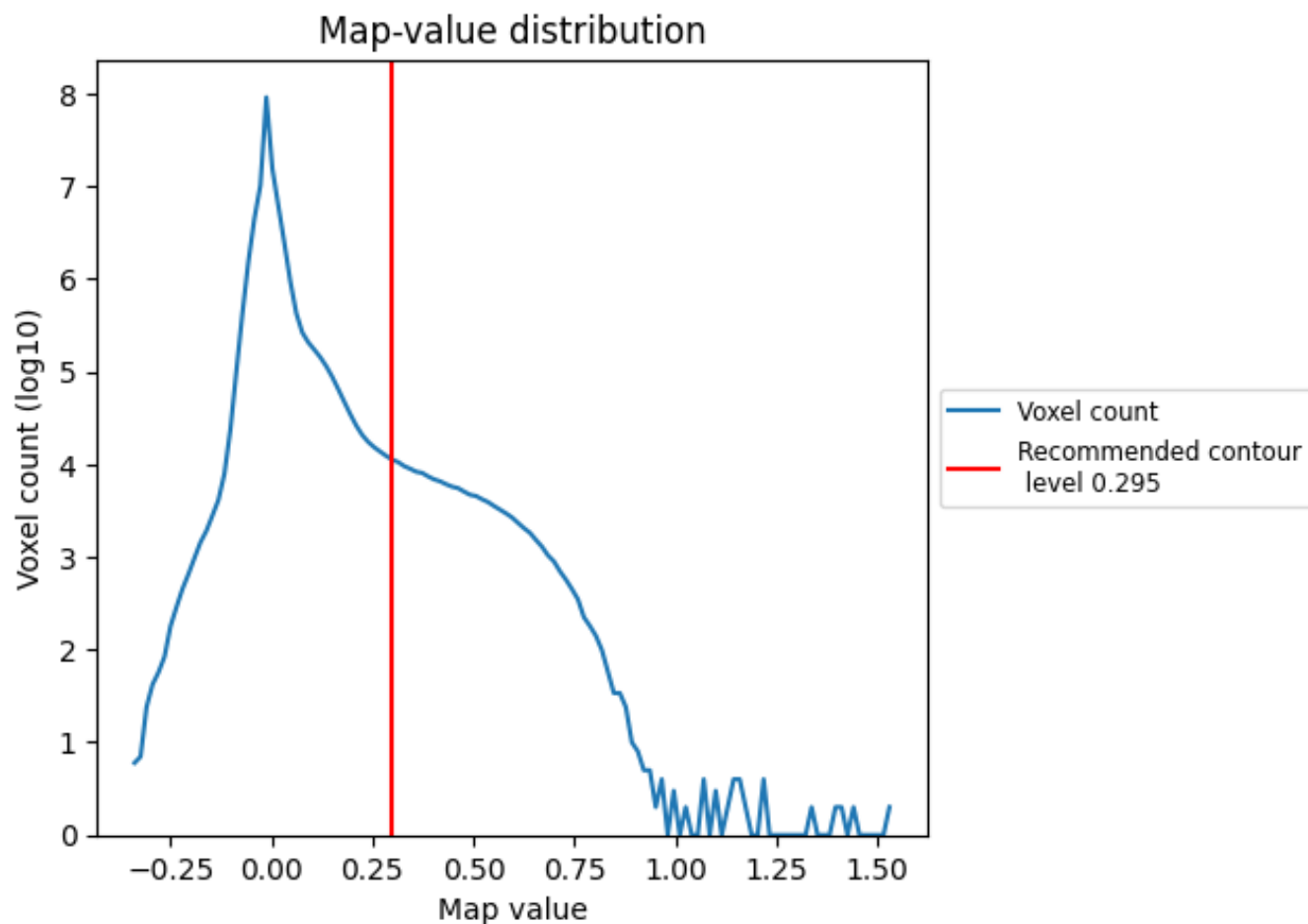
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

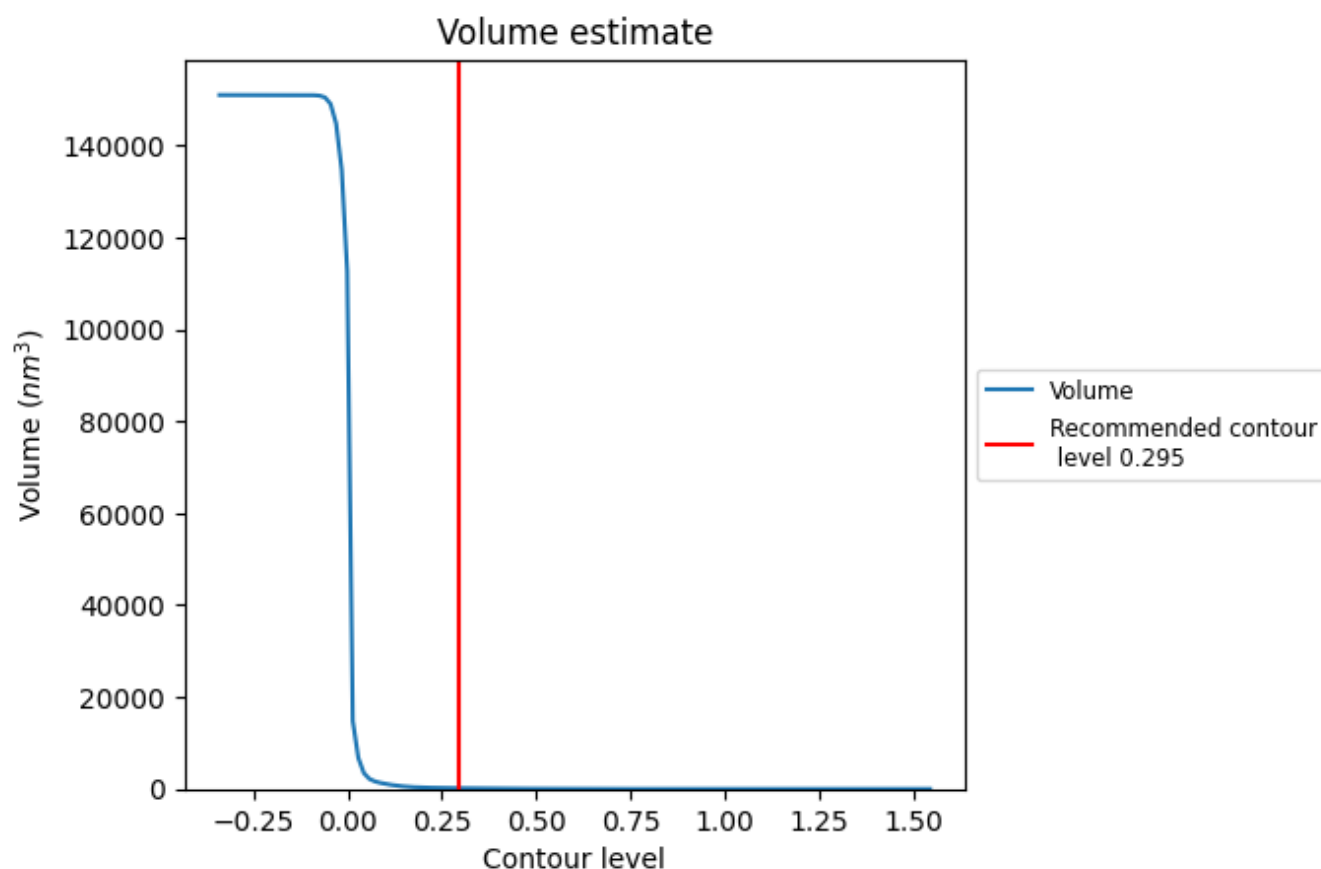
This section contains the results of statistical analysis of the map.

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.

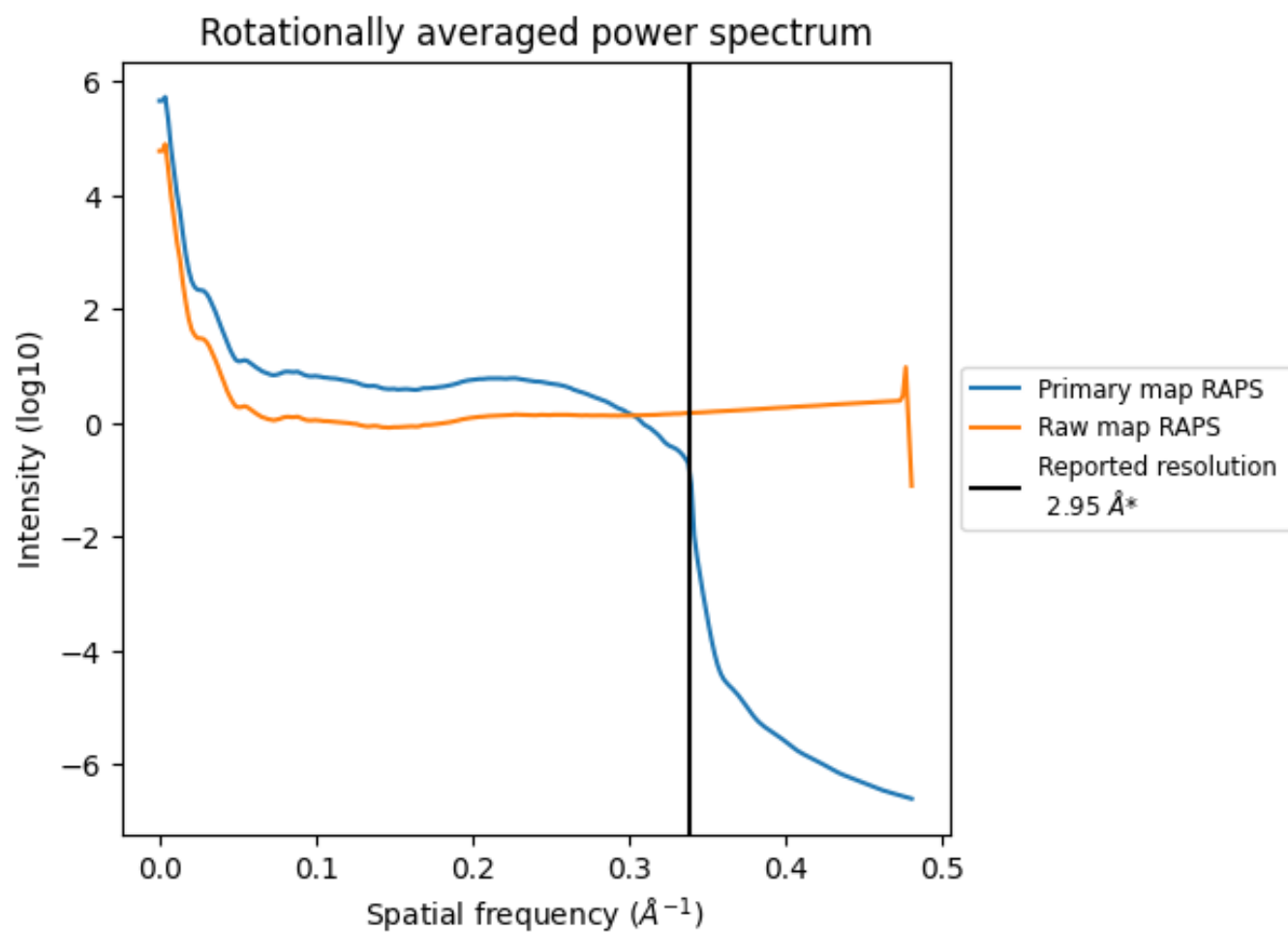
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm³; this corresponds to an approximate mass of 149 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 ⓘ

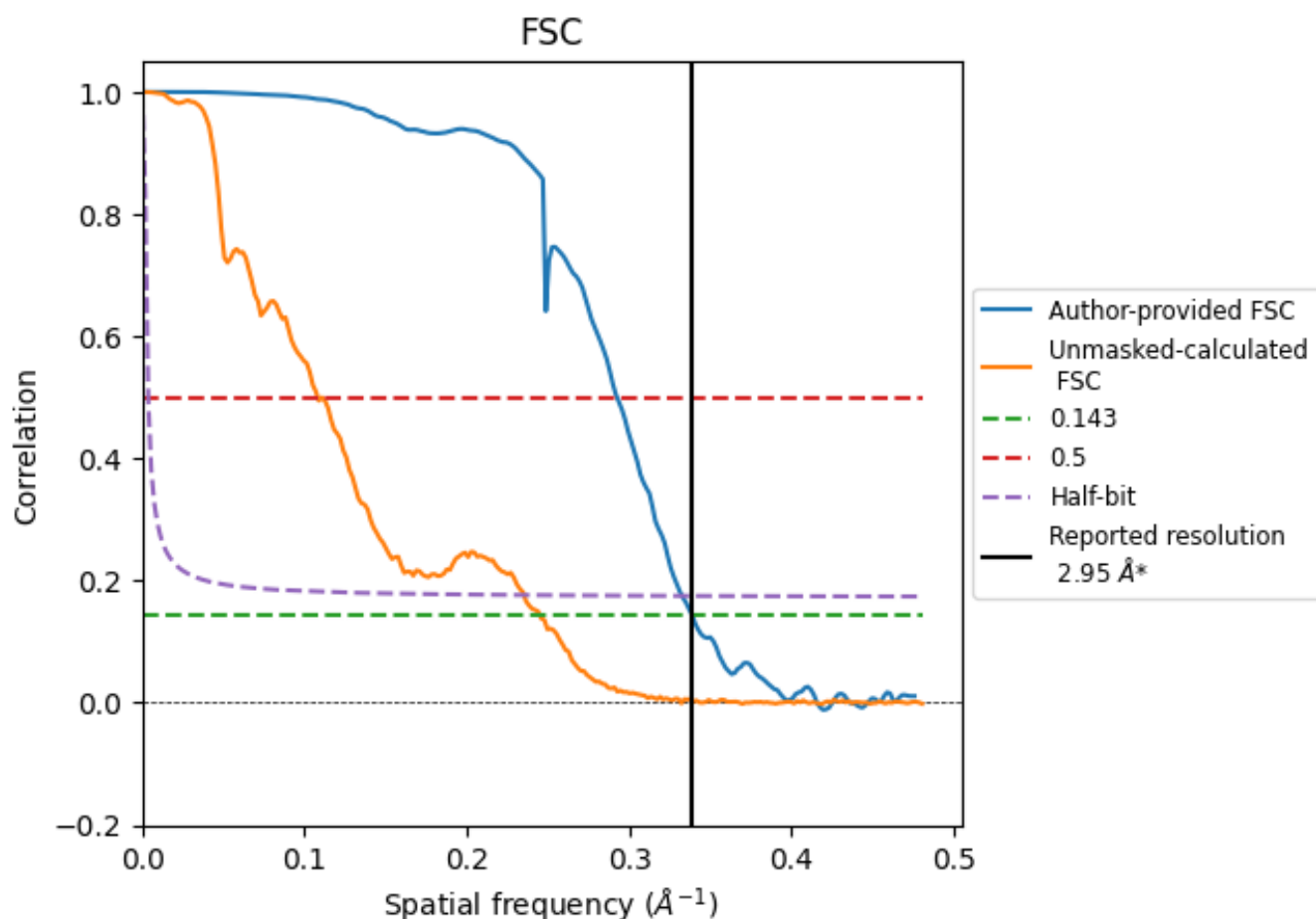


*Reported resolution corresponds to spatial frequency of 0.339 $\text{\AA}^{-1}$

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 $0.339 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

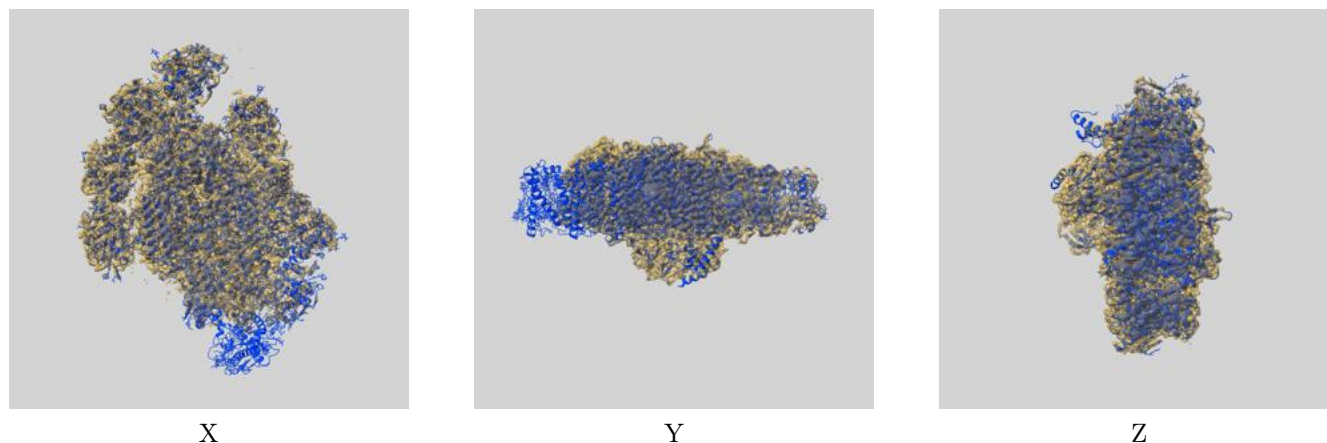
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.42	3.00
Unmasked-calculated*	4.08	9.24	4.25

*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 4.08 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

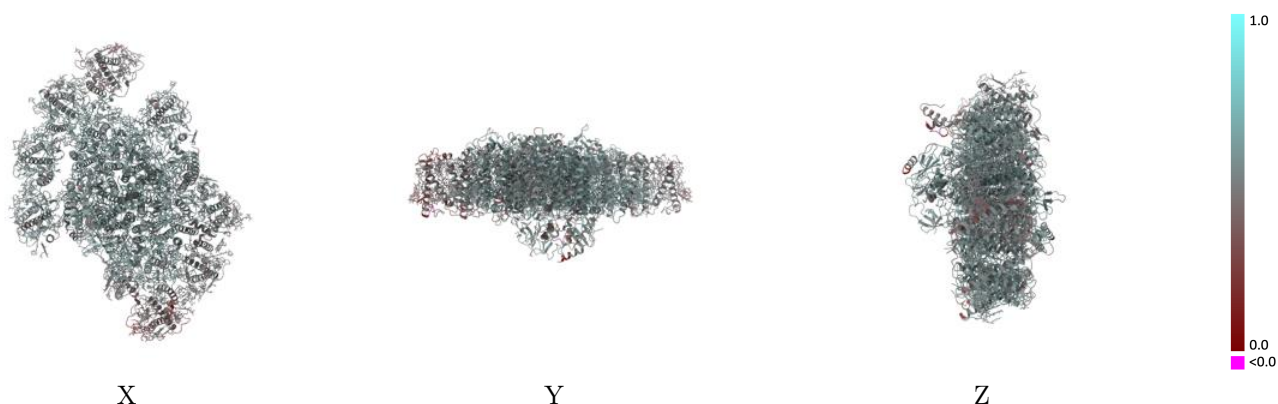
This section contains information regarding the fit between EMDB map EMD-60286 and PDB model 8ZOA. Per-residue inclusion information can be found in section 3 on page 30.

9.1 Map-model overlay [i](#)



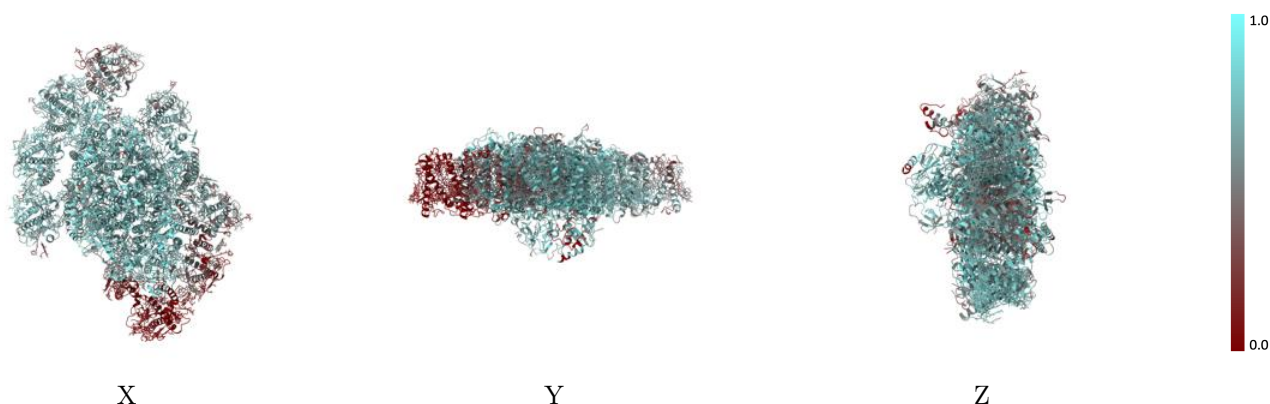
The images above show the 3D surface view of the map at the recommended contour level 0.295 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



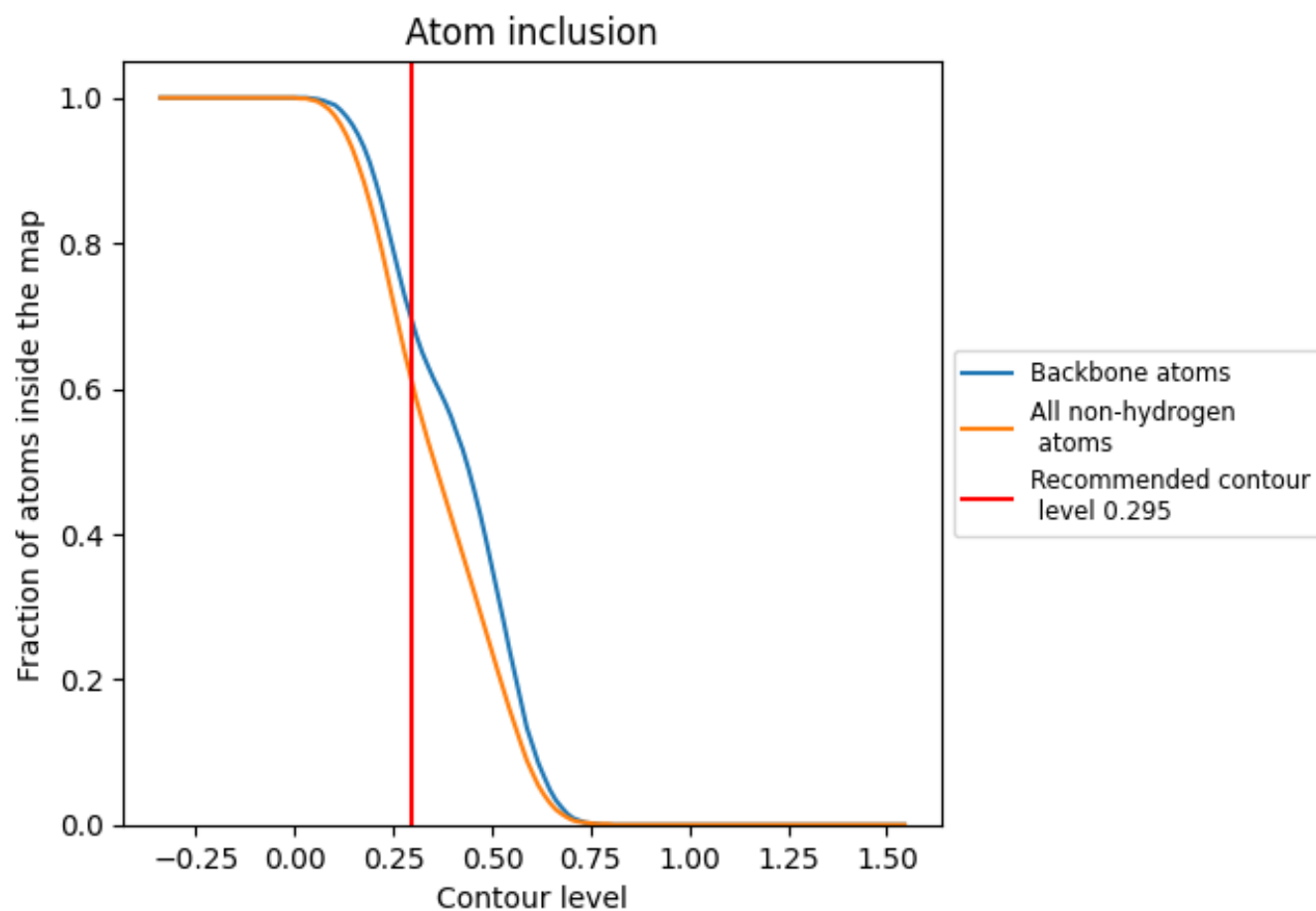
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.295).

9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 61% 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 (0.295) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6140	0.5290
1	0.6330	0.5250
2	0.4790	0.4640
3	0.6590	0.5320
4	0.6850	0.5340
5	0.6530	0.5180
7	0.0110	0.3890
8	0.2650	0.4850
9	0.4640	0.4980
a	0.7450	0.5690
b	0.7440	0.5620
c	0.7780	0.5450
d	0.6890	0.5510
e	0.6530	0.5370
f	0.6770	0.5320
g	0.4180	0.4380
h	0.0880	0.4680
i	0.6840	0.5390
j	0.7160	0.5590
l	0.6510	0.5180
m	0.6600	0.5110

