



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 05:04 AM UTC

PDB ID : 8ZOD / pdb_00008zod
EMDB ID : EMD-60289
Title : Structure of the canthaxanthin mutant PSI-5VCPI supercomplex in Nan-
nochloropsis oceanica
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 2.88 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:

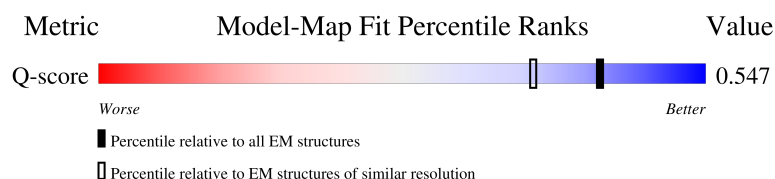
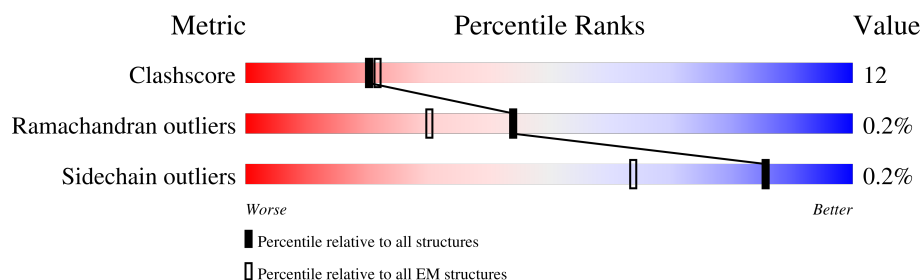
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

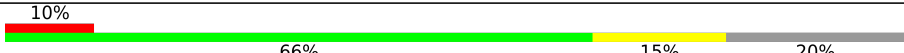
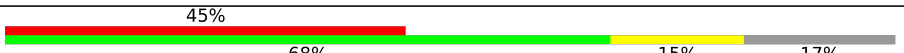
The reported resolution of this entry is 2.88 Å.

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	12111 (2.38 - 3.38)

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	4	202	
3	3	220	
4	2	223	

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Mol	Chain	Length	Quality of chain
5	1	208	
6	a	745	
7	b	737	
8	d	136	
9	e	67	
10	f	185	
11	i	45	
12	j	41	
13	l	172	
14	m	30	
15	g	55	
16	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
19	CLA	1	305	X	-	-	-
19	CLA	1	306	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	1	311	X	-	-	-
19	CLA	1	312	X	-	-	-
19	CLA	1	313	X	-	-	-
19	CLA	1	314	X	-	-	-
19	CLA	2	306	X	-	-	-
19	CLA	2	307	X	-	-	-
19	CLA	2	308	X	-	-	-
19	CLA	2	309	X	-	-	-
19	CLA	2	310	X	-	-	-
19	CLA	2	311	X	-	-	-
19	CLA	2	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	313	X	-	-	-
19	CLA	2	314	X	-	-	-
19	CLA	2	315	X	-	-	-
19	CLA	2	316	X	-	-	-
19	CLA	3	307	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	309	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	311	X	-	-	-
19	CLA	3	312	X	-	-	-
19	CLA	3	313	X	-	-	-
19	CLA	3	314	X	-	-	-
19	CLA	3	315	X	-	-	-
19	CLA	4	306	X	-	-	-
19	CLA	4	307	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	4	314	X	-	-	-
19	CLA	4	315	X	-	-	-
19	CLA	4	316	X	-	-	-
19	CLA	4	317	X	-	-	-
19	CLA	5	305	X	-	-	-
19	CLA	5	306	X	-	-	-
19	CLA	5	307	X	-	-	-
19	CLA	5	308	X	-	-	-
19	CLA	5	309	X	-	-	-
19	CLA	5	310	X	-	-	-
19	CLA	5	311	X	-	-	-
19	CLA	5	312	X	-	-	-
19	CLA	5	313	X	-	-	-
19	CLA	5	314	X	-	-	-
19	CLA	5	315	X	-	-	-
19	CLA	a	801	X	-	-	-
19	CLA	a	802	X	-	-	-
19	CLA	a	803	X	-	-	-
19	CLA	a	804	X	-	-	-
19	CLA	a	805	X	-	-	-
19	CLA	a	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	807	X	-	-	-
19	CLA	a	808	X	-	-	-
19	CLA	a	809	X	-	-	-
19	CLA	a	810	X	-	-	-
19	CLA	a	811	X	-	-	-
19	CLA	a	812	X	-	-	-
19	CLA	a	813	X	-	-	-
19	CLA	a	814	X	-	-	-
19	CLA	a	815	X	-	-	-
19	CLA	a	816	X	-	-	-
19	CLA	a	817	X	-	-	-
19	CLA	a	818	X	-	-	-
19	CLA	a	819	X	-	-	-
19	CLA	a	820	X	-	-	-
19	CLA	a	821	X	-	-	-
19	CLA	a	822	X	-	-	-
19	CLA	a	823	X	-	-	-
19	CLA	a	824	X	-	-	-
19	CLA	a	825	X	-	-	-
19	CLA	a	826	X	-	-	-
19	CLA	a	827	X	-	-	-
19	CLA	a	828	X	-	-	-
19	CLA	a	829	X	-	-	-
19	CLA	a	830	X	-	-	-
19	CLA	a	831	X	-	-	-
19	CLA	a	832	X	-	-	-
19	CLA	a	833	X	-	-	-
19	CLA	a	834	X	-	-	-
19	CLA	a	835	X	-	-	-
19	CLA	a	836	X	-	-	-
19	CLA	a	837	X	-	-	-
19	CLA	a	838	X	-	-	-
19	CLA	a	839	X	-	-	-
19	CLA	a	840	X	-	-	-
19	CLA	a	841	X	-	-	-
19	CLA	a	842	X	-	-	-
19	CLA	a	844	X	-	-	-
19	CLA	a	854	X	-	-	-
19	CLA	b	801	X	-	-	-
19	CLA	b	802	X	-	-	-
19	CLA	b	803	X	-	-	-
19	CLA	b	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	805	X	-	-	-
19	CLA	b	806	X	-	-	-
19	CLA	b	807	X	-	-	-
19	CLA	b	808	X	-	-	-
19	CLA	b	809	X	-	-	-
19	CLA	b	810	X	-	-	-
19	CLA	b	811	X	-	-	-
19	CLA	b	812	X	-	-	-
19	CLA	b	813	X	-	-	-
19	CLA	b	814	X	-	-	-
19	CLA	b	815	X	-	-	-
19	CLA	b	816	X	-	-	-
19	CLA	b	817	X	-	-	-
19	CLA	b	818	X	-	-	-
19	CLA	b	819	X	-	-	-
19	CLA	b	820	X	-	-	-
19	CLA	b	821	X	-	-	-
19	CLA	b	822	X	-	-	-
19	CLA	b	823	X	-	-	-
19	CLA	b	824	X	-	-	-
19	CLA	b	825	X	-	-	-
19	CLA	b	826	X	-	-	-
19	CLA	b	827	X	-	-	-
19	CLA	b	828	X	-	-	-
19	CLA	b	829	X	-	-	-
19	CLA	b	830	X	-	-	-
19	CLA	b	831	X	-	-	-
19	CLA	b	832	X	-	-	-
19	CLA	b	833	X	-	-	-
19	CLA	b	834	X	-	-	-
19	CLA	b	835	X	-	-	-
19	CLA	b	836	X	-	-	-
19	CLA	b	837	X	-	-	-
19	CLA	b	838	X	-	-	-
19	CLA	b	839	X	-	-	-
19	CLA	b	840	X	-	-	-
19	CLA	b	841	X	-	-	-
19	CLA	f	802	X	-	-	-
19	CLA	f	803	X	-	-	-
19	CLA	i	102	X	-	-	-
19	CLA	j	102	X	-	-	-
19	CLA	j	103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	l	202	X	-	-	-
19	CLA	l	203	X	-	-	-
19	CLA	l	204	X	-	-	-
27	SF4	c	102	-	-	X	-

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 34630 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-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	168	Total	C	N	O	S	0	0
			1268	822	211	229	6		

- Molecule 3 is a protein called VCPI-3.

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

- Molecule 4 is a protein called VCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	185	Total	C	N	O	S	0	0
			1372	892	224	249	7		

- Molecule 5 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called PSI subunit V.

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

- Molecule 14 is a protein called PsaM.

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

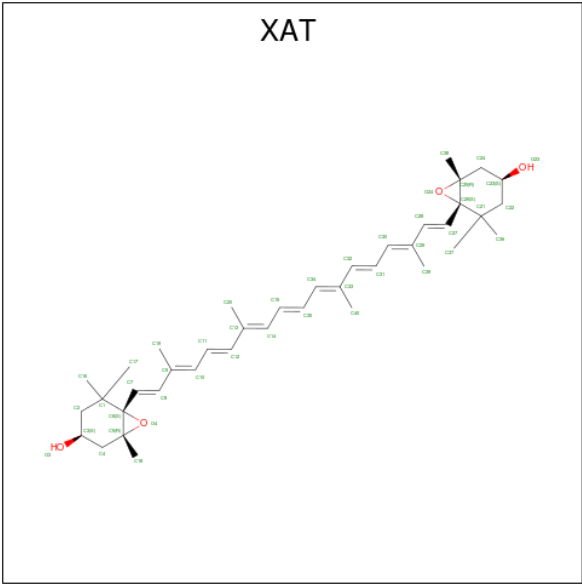
- Molecule 15 is a protein called PsaS.

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

- Molecule 16 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 17 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
17	5	1	Total	C	O	0
			44	40	4	
17	5	1	Total	C	O	0
			44	40	4	
17	5	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	4	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	3	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	2	1	Total	C	O	0
			44	40	4	
17	1	1	Total	C	O	0
			44	40	4	
17	1	1	Total	C	O	0
			44	40	4	
17	a	1	Total	C	O	0
			44	40	4	
17	j	1	Total	C	O	0
			44	40	4	

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



Mol	Chain	Residues	Atoms			AltCon
18	5	1	Total 45	C 40	O 5	0
18	3	1	Total 45	C 40	O 5	0
18	3	1	Total 45	C 40	O 5	0
18	1	1	Total 45	C 40	O 5	0

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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

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

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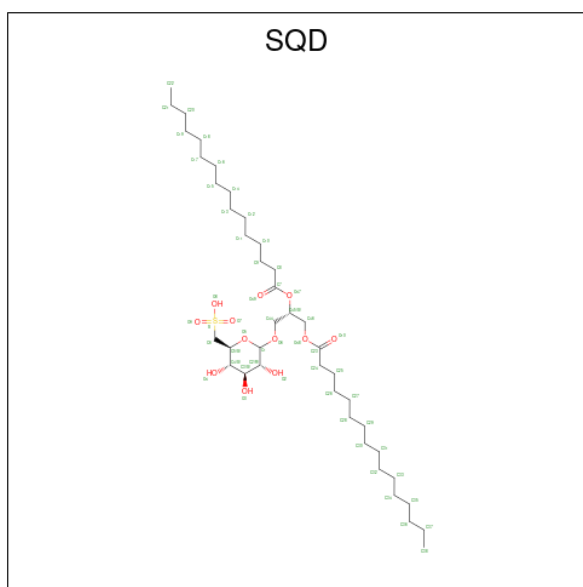
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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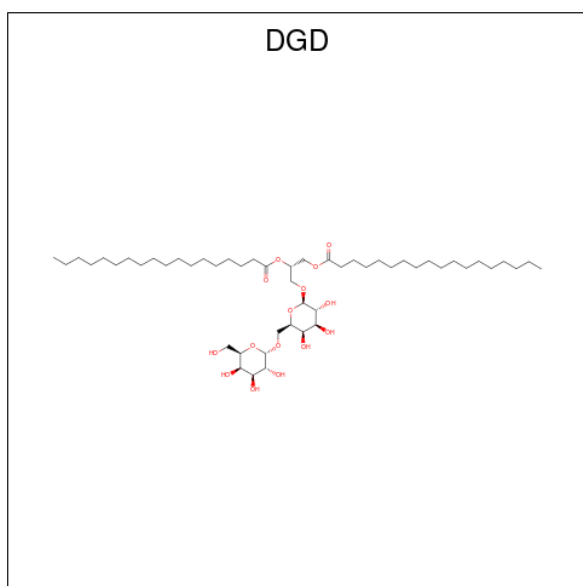
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	i	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 20 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
20	5	1	Total	C	O	S	0
			35	22	12	1	
20	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



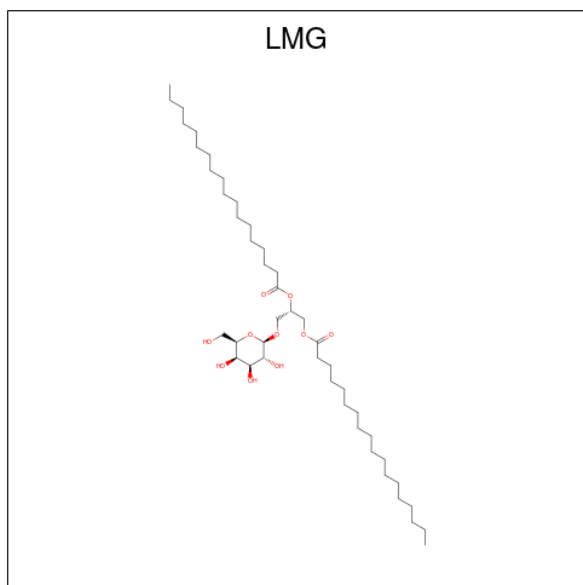
Mol	Chain	Residues	Atoms			AltConf
21	4	1	Total	C	O	0
			40	25	15	

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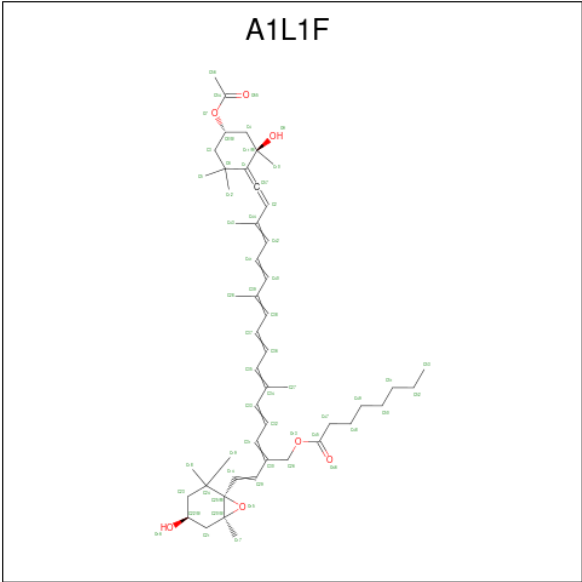
Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			57	42	15	

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



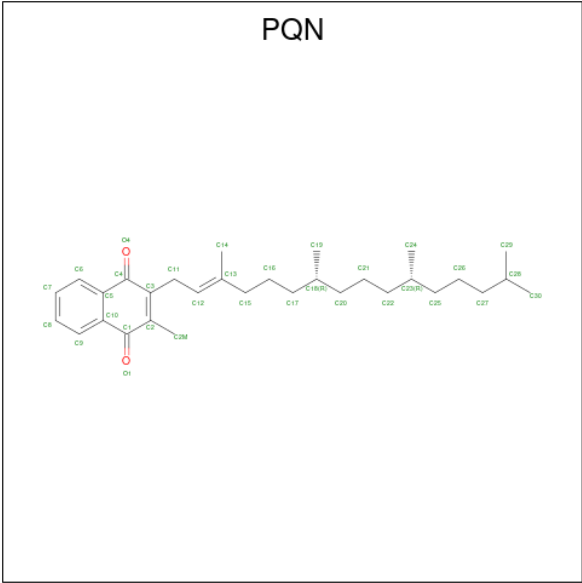
Mol	Chain	Residues	Atoms			AltConf
22	2	1	Total	C	O	0
			35	25	10	
22	a	1	Total	C	O	0
			34	24	10	
22	j	1	Total	C	O	0
			32	22	10	

- Molecule 23 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: $C_{50}H_{72}O_7$) (labeled as "Ligand of Interest" by depositor).



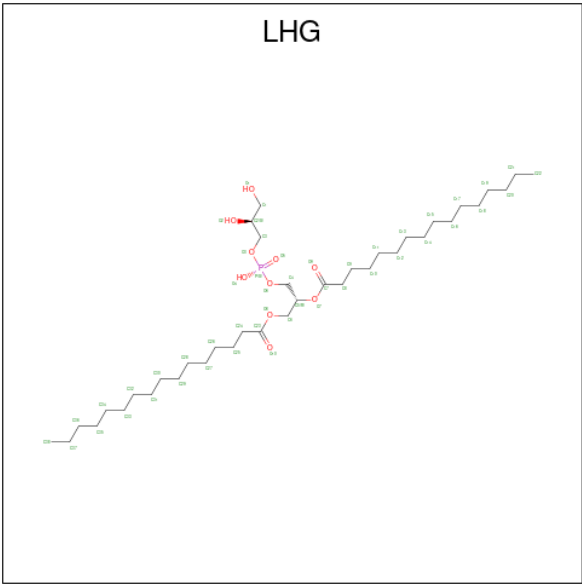
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			57	50	7	

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



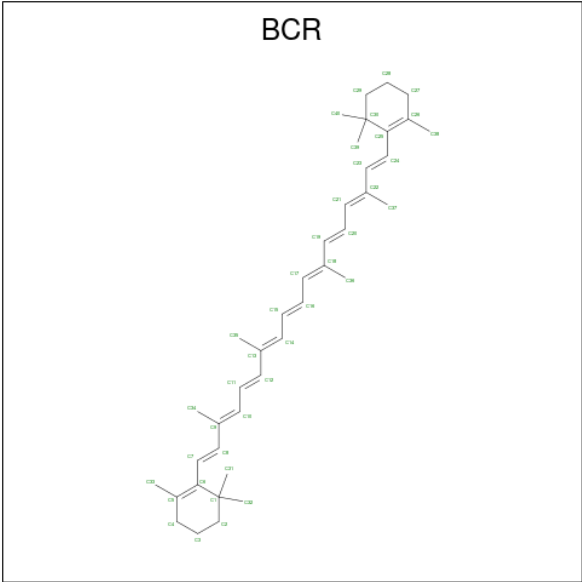
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			33	31	2	
24	b	1	Total	C	O	0
			33	31	2	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



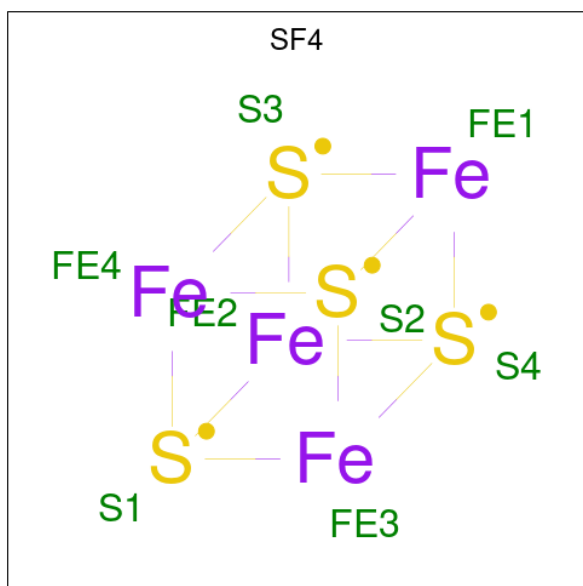
Mol	Chain	Residues	Atoms	AltConf
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C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

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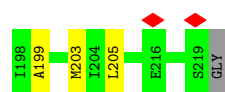
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Mol	Chain	Residues	Atoms	AltConf
26	i	1	Total C 40 40	0
26	j	1	Total C 40 40	0
26	l	1	Total C 40 40	0
26	l	1	Total C 40 40	0
26	m	1	Total C 40 40	0

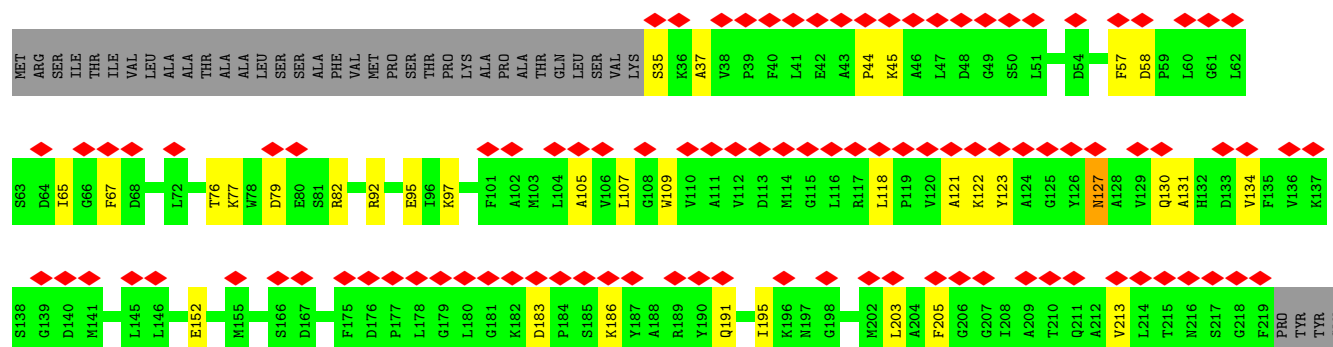
- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



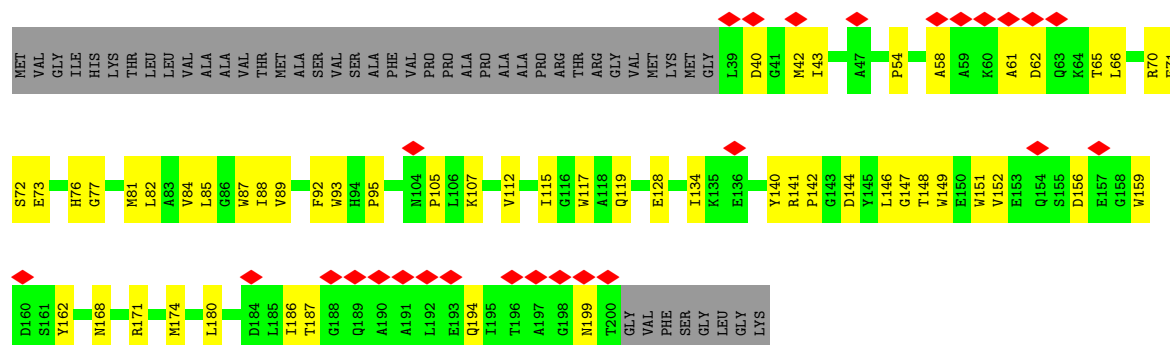
Mol	Chain	Residues	Atoms	AltConf
27	a	1	Total Fe S 8 4 4	0
27	c	1	Total Fe S 8 4 4	0
27	c	1	Total Fe S 8 4 4	0



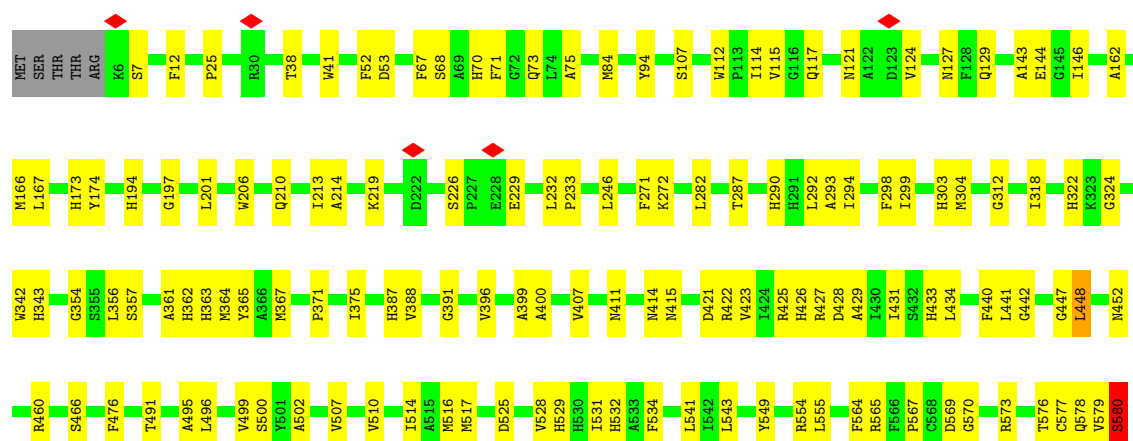
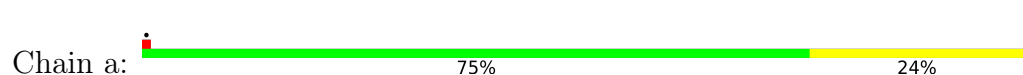
• Molecule 4: VCPI-2

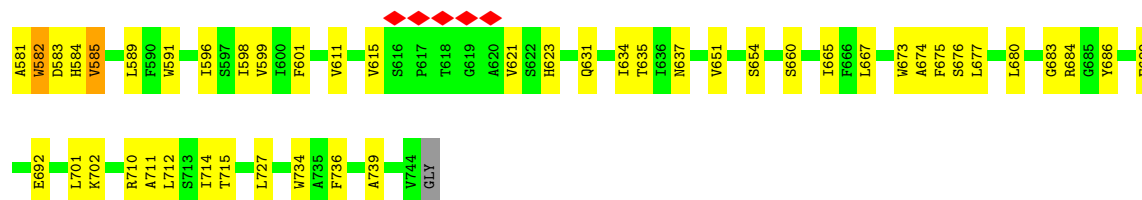


• Molecule 5: VCPI-1

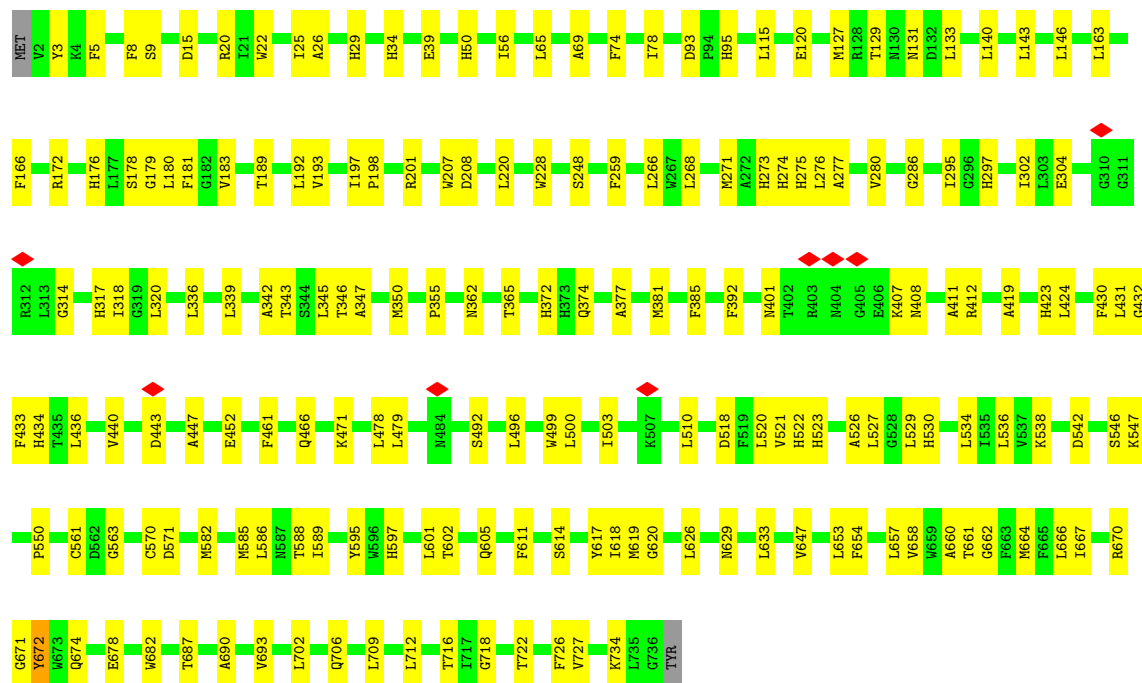
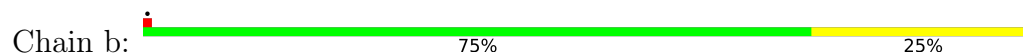


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

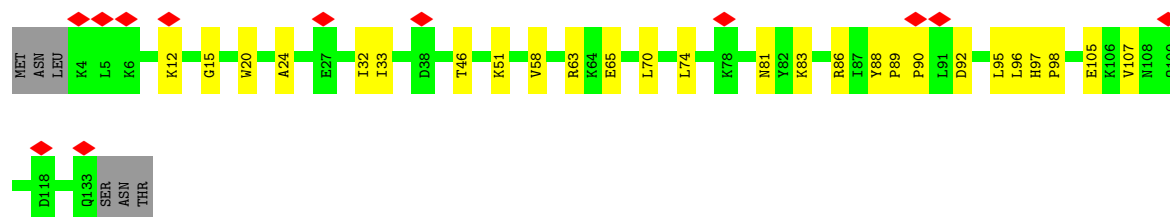
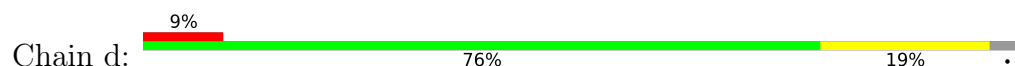




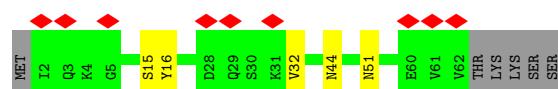
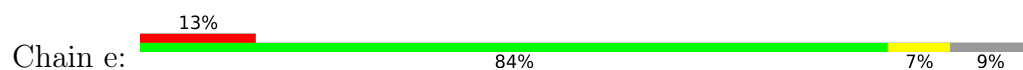
• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2



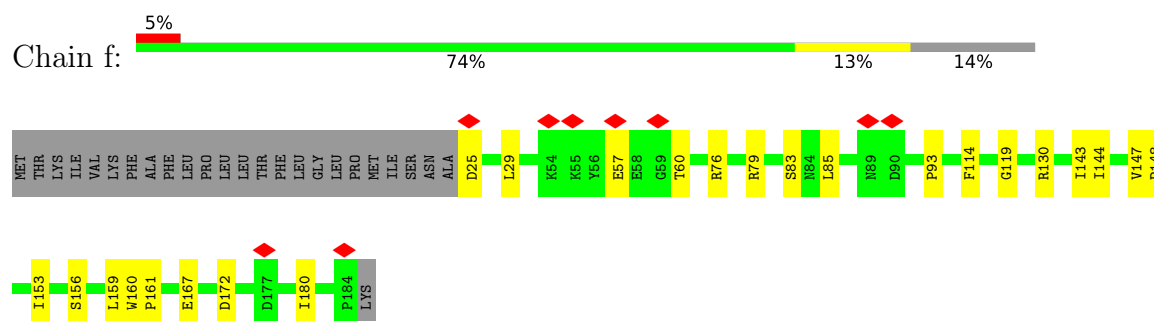
• Molecule 8: Photosystem I reaction center subunit II



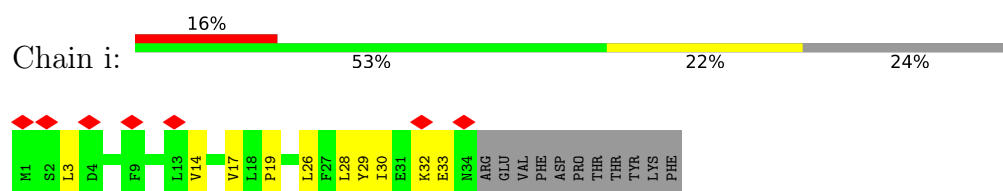
• Molecule 9: Photosystem I reaction center subunit IV



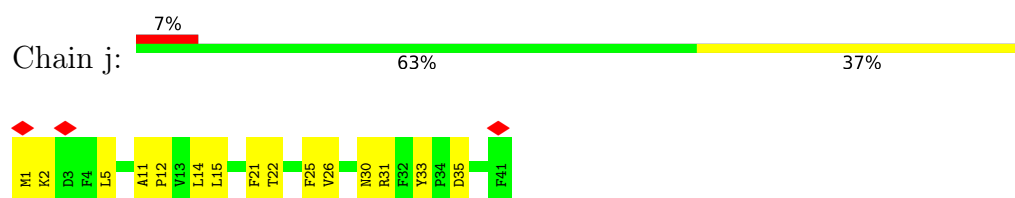
- Molecule 10: Photosystem I reaction center subunit III



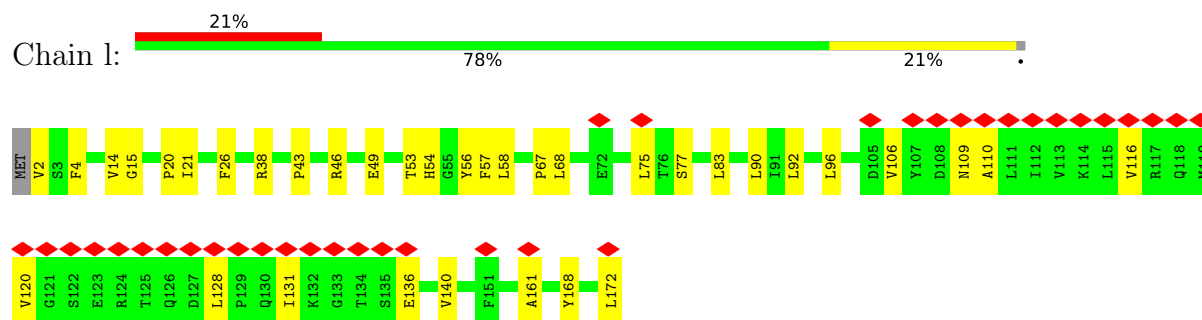
- Molecule 11: Photosystem I reaction center subunit VIII



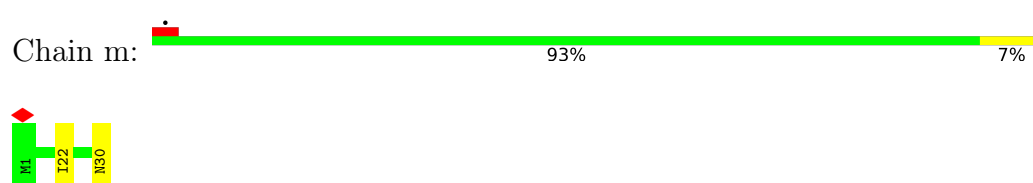
- Molecule 12: Photosystem I reaction center subunit IX



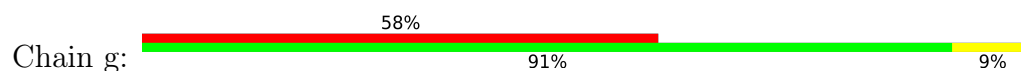
- Molecule 13: PSI subunit V

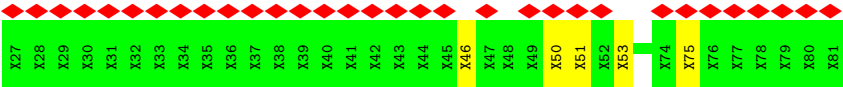


- Molecule 14: PsaM



- Molecule 15: PsaS





• Molecule 16: Photosystem I iron-sulfur center



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61296	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	1.724	Depositor
Minimum map value	-0.410	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.333	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: A1L1F, A1L1G, SF4, XAT, LHG, BCR, DGD, CLA, LMG, PQN, SQD

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	4	0.17	0/1298	0.32	0/1761
3	3	0.12	0/1350	0.27	0/1821
4	2	0.14	0/1405	0.36	0/1904
5	1	0.13	0/1293	0.33	0/1759
6	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
7	b	0.20	0/6080	0.32	1/8302 (0.0%)
8	d	0.12	0/1040	0.32	0/1402
9	e	0.09	0/502	0.20	0/681
10	f	0.14	0/1297	0.31	0/1762
11	i	0.14	0/278	0.33	0/378
12	j	0.15	0/351	0.36	0/478
13	l	0.14	0/1315	0.31	0/1796
14	m	0.09	0/210	0.28	0/288
16	c	0.13	0/606	0.34	0/822
All	All	0.20	3/24402 (0.0%)	0.32	5/33196 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	580	SER	CA-C	-7.01	1.43	1.52
6	a	581	ALA	CA-C	-5.42	1.45	1.52
6	a	582	TRP	CA-C	-5.04	1.45	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	581	ALA	N-CA-C	-8.62	102.52	113.72
6	a	448	LEU	N-CA-C	-6.13	104.15	111.69
6	a	584	HIS	N-CA-C	-5.84	106.50	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	672	TYR	N-CA-C	-5.61	106.28	113.23
6	a	585	VAL	N-CA-C	-5.07	105.46	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	4	1268	0	1288	22	0
3	3	1324	0	1340	22	0
4	2	1372	0	1347	22	0
5	1	1262	0	1237	39	0
6	a	5827	0	5697	140	0
7	b	5865	0	5710	152	0
8	d	1014	0	1015	20	0
9	e	494	0	495	5	0
10	f	1266	0	1262	21	0
11	i	271	0	292	12	0
12	j	339	0	342	21	0
13	l	1283	0	1278	26	0
14	m	210	0	226	2	0
15	g	275	0	62	3	0
16	c	596	0	583	19	0
17	1	88	0	112	6	0
17	2	220	0	280	24	0
17	3	176	0	224	15	0
17	4	220	0	280	28	0
17	5	132	0	168	18	0
17	a	44	0	56	4	0
17	j	44	0	56	5	0
18	1	45	0	0	1	0
18	3	90	0	0	0	0
18	5	45	0	0	1	0
19	1	547	0	508	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	544	0	452	10	0
19	3	458	0	378	10	0
19	4	613	0	522	30	0
19	5	563	0	472	22	0
19	a	2579	0	2562	139	0
19	b	2475	0	2536	129	0
19	f	117	0	115	1	0
19	i	62	0	63	5	0
19	j	100	0	86	8	0
19	l	148	0	123	3	0
20	1	45	0	54	2	0
20	5	35	0	34	1	0
21	4	40	0	38	11	0
21	b	57	0	72	5	0
22	2	35	0	40	2	0
22	a	34	0	38	11	0
22	j	32	0	34	6	0
23	1	57	0	0	2	0
24	a	33	0	46	3	0
24	b	33	0	46	2	0
25	a	75	0	93	6	0
25	b	31	0	32	0	0
25	m	46	0	65	3	0
26	a	160	0	224	14	0
26	b	320	0	448	30	0
26	f	80	0	112	13	0
26	i	40	0	56	2	0
26	j	40	0	56	8	0
26	l	80	0	112	13	0
26	m	40	0	56	1	0
27	a	8	0	0	0	0
27	c	16	0	0	2	0
All	All	34630	0	34141	839	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 12.

All (839) 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)
2:4:193:ALA:HB1	21:4:318:DGD:HE62	1.13	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:193:ALA:HB1	21:4:318:DGD:C6E	1.84	1.07
21:4:318:DGD:O4E	21:4:318:DGD:O5E	1.61	1.06
17:5:302:XAT:H12	19:5:307:CLA:HAB	1.53	0.90
17:2:303:XAT:H32	19:2:308:CLA:HAB	1.52	0.89
19:a:806:CLA:O1A	19:a:814:CLA:HBA1	1.81	0.79
6:a:531:ILE:HD12	19:a:801:CLA:H172	1.63	0.78
19:b:826:CLA:HMA1	26:b:847:BCR:H17C	1.66	0.78
2:4:193:ALA:CB	21:4:318:DGD:HE62	2.07	0.77
17:4:303:XAT:H12	19:4:308:CLA:HAB	1.67	0.75
17:2:303:XAT:H181	19:2:314:CLA:HBB1	1.70	0.73
19:1:312:CLA:HHC	19:1:312:CLA:HBB1	1.69	0.73
19:4:317:CLA:H2A	21:4:318:DGD:HE62	1.73	0.71
5:1:43:ILE:O	5:1:70:ARG:NH2	2.25	0.70
26:a:847:BCR:H362	26:a:848:BCR:H21C	1.73	0.70
19:b:807:CLA:H151	19:b:829:CLA:HBB2	1.74	0.70
19:b:834:CLA:H72	26:b:847:BCR:H391	1.72	0.69
12:j:22:THR:HA	12:j:25:PHE:CE1	2.28	0.69
7:b:273:HIS:HD1	19:b:818:CLA:HAB	1.58	0.69
10:f:167:GLU:HG3	10:f:172:ASP:HB3	1.73	0.69
6:a:569:ASP:OD2	6:a:573:ARG:NH2	2.27	0.68
19:a:804:CLA:HED1	12:j:15:LEU:HD22	1.76	0.68
1:5:179:LEU:HD12	10:f:159:LEU:HD11	1.75	0.67
5:1:194:GLN:HG3	5:1:199:ASN:HB3	1.77	0.67
6:a:363:HIS:ND1	19:a:819:CLA:OBD	2.26	0.67
7:b:295:ILE:HG13	19:b:821:CLA:HED1	1.77	0.67
17:4:302:XAT:H14	19:4:310:CLA:H12	1.76	0.67
12:j:31:ARG:HD3	17:j:101:XAT:H222	1.78	0.66
5:1:70:ARG:NH1	5:1:73:GLU:OE1	2.28	0.66
1:5:113:ARG:NH1	1:5:116:GLU:OE1	2.29	0.66
17:4:303:XAT:H193	19:4:308:CLA:H142	1.78	0.66
5:1:146:LEU:HD13	19:a:844:CLA:H91	1.77	0.65
7:b:9:SER:HB2	21:b:851:DGD:HE62	1.78	0.65
11:i:29:TYR:HA	11:i:32:LYS:HE2	1.79	0.65
19:4:317:CLA:HAA2	21:4:318:DGD:HE5	1.77	0.65
19:b:824:CLA:HBB1	19:b:838:CLA:H151	1.79	0.65
10:f:25:ASP:N	10:f:29:LEU:O	2.30	0.65
6:a:112:TRP:HB3	17:j:101:XAT:H373	1.77	0.64
19:a:834:CLA:H142	26:b:848:BCR:H15C	1.79	0.64
7:b:304:GLU:HG2	7:b:318:ILE:HG13	1.78	0.64
17:3:305:XAT:H32	19:3:313:CLA:HAB	1.80	0.64
19:a:808:CLA:HMB2	26:j:104:BCR:HC8	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:197:GLY:O	6:a:201:LEU:HB2	1.97	0.64
12:j:21:PHE:HA	19:j:103:CLA:HBB2	1.80	0.64
10:f:79:ARG:NH1	12:j:35:ASP:O	2.30	0.63
7:b:336:LEU:HD21	19:b:830:CLA:HAB	1.78	0.63
19:b:814:CLA:H121	19:b:819:CLA:H72	1.79	0.63
6:a:114:ILE:HB	17:j:101:XAT:H372	1.81	0.63
7:b:129:THR:HG22	7:b:131:ASN:H	1.63	0.63
1:5:120:GLY:O	1:5:124:MET:HG3	1.98	0.63
6:a:684:ARG:H	7:b:570:CYS:HB2	1.64	0.63
7:b:424:LEU:HD13	7:b:534:LEU:HA	1.81	0.63
1:5:130:PHE:CE1	17:5:302:XAT:O24	2.52	0.63
7:b:115:LEU:HA	7:b:365:THR:HG22	1.80	0.63
17:4:305:XAT:H363	17:3:301:XAT:H10	1.80	0.63
6:a:356:LEU:HD11	19:a:820:CLA:H71	1.79	0.63
6:a:589:LEU:HD21	19:a:831:CLA:HBC1	1.81	0.62
12:j:26:VAL:HG11	26:j:104:BCR:H24C	1.81	0.62
17:4:304:XAT:H32	19:4:313:CLA:HAB	1.80	0.62
6:a:362:HIS:HA	6:a:365:TYR:CE1	2.33	0.62
8:d:12:LYS:HB2	8:d:51:LYS:HB3	1.82	0.62
19:b:831:CLA:HAB	19:b:838:CLA:HBB2	1.82	0.62
8:d:86:ARG:HB2	8:d:96:LEU:HD11	1.82	0.62
6:a:298:PHE:CE1	19:a:822:CLA:HAB	2.35	0.61
1:5:225:ILE:HG22	19:5:314:CLA:HAB	1.82	0.61
17:5:302:XAT:H162	19:5:307:CLA:H2	1.82	0.61
20:5:316:SQD:H2	17:4:301:XAT:H373	1.82	0.61
7:b:15:ASP:HB3	7:b:20:ARG:HB2	1.82	0.61
19:4:317:CLA:H2A	21:4:318:DGD:C6E	2.30	0.61
7:b:660:ALA:HB3	19:b:804:CLA:HBB2	1.83	0.61
6:a:298:PHE:HE1	19:a:822:CLA:HAB	1.64	0.61
8:d:88:TYR:HB2	8:d:92:ASP:HB2	1.81	0.61
1:5:190:ARG:NH1	1:5:191:GLU:O	2.34	0.61
19:b:832:CLA:HBC3	26:f:804:BCR:H362	1.83	0.61
23:1:304:A1L1F:C2	19:a:844:CLA:H11	2.31	0.61
4:2:76:THR:O	4:2:82:ARG:NH1	2.33	0.60
6:a:162:ALA:O	6:a:166:MET:HG2	2.00	0.60
3:3:92:HIS:HB3	3:3:197:MET:SD	2.42	0.60
19:a:818:CLA:C3D	22:a:853:LMG:HC91	2.30	0.60
7:b:561:CYS:SG	7:b:563:GLY:N	2.71	0.60
6:a:167:LEU:HD11	19:a:810:CLA:H193	1.83	0.60
3:3:199:ALA:O	3:3:203:MET:HG3	2.01	0.60
5:1:186:ILE:HG13	5:1:187:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:833:CLA:HBC2	19:a:840:CLA:HMC2	1.83	0.60
7:b:412:ARG:NH2	19:b:831:CLA:O1D	2.35	0.60
4:2:44:PRO:HG3	4:2:58:ASP:HB3	1.83	0.60
6:a:53:ASP:OD2	6:a:343:HIS:NE2	2.35	0.60
1:5:111:TRP:NE1	19:5:308:CLA:O1A	2.33	0.59
5:1:72:SER:O	5:1:76:HIS:ND1	2.28	0.59
13:l:38:ARG:O	13:l:46:ARG:NH2	2.35	0.59
18:1:301:A1L1G:C18	19:1:306:CLA:HAC2	2.32	0.59
6:a:429:ALA:O	6:a:433:HIS:ND1	2.31	0.59
2:4:185:PHE:CZ	17:4:303:XAT:H30	2.37	0.59
3:3:83:TYR:OH	3:3:163:ARG:NH1	2.35	0.59
6:a:121:ASN:HB3	6:a:129:GLN:HB3	1.83	0.59
2:4:170:MET:HE1	19:4:313:CLA:H43	1.84	0.59
19:a:804:CLA:ND	12:j:12:PRO:HG3	2.17	0.59
17:2:303:XAT:H363	19:2:308:CLA:H2	1.84	0.58
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.58
19:3:312:CLA:H42	26:a:848:BCR:H272	1.85	0.58
6:a:507:VAL:HG22	6:a:517:MET:HG3	1.85	0.58
7:b:74:PHE:O	7:b:78:ILE:HG12	2.04	0.58
7:b:29:HIS:ND1	19:b:807:CLA:O1A	2.28	0.58
19:a:826:CLA:HBA1	19:a:830:CLA:H193	1.86	0.58
7:b:69:ALA:HB2	7:b:133:LEU:HB2	1.86	0.58
17:5:301:XAT:H14	19:5:309:CLA:H12	1.86	0.58
19:a:820:CLA:H92	19:a:830:CLA:H91	1.84	0.58
1:5:112:LEU:HD22	19:5:307:CLA:H12	1.86	0.58
3:3:87:GLU:OE2	3:3:163:ARG:NH2	2.31	0.57
6:a:517:MET:HE1	6:a:623:HIS:NE2	2.19	0.57
19:b:804:CLA:CGA	19:b:804:CLA:H3A	2.34	0.57
19:b:805:CLA:H18	11:i:14:VAL:HG22	1.86	0.57
1:5:155:VAL:HG21	19:5:309:CLA:HAA2	1.86	0.57
7:b:39:GLU:HB3	7:b:163:LEU:HD11	1.87	0.57
26:b:843:BCR:H23C	26:b:850:BCR:H323	1.86	0.57
26:f:801:BCR:HC32	19:j:102:CLA:H43	1.86	0.57
19:a:818:CLA:C1D	22:a:853:LMG:H291	2.34	0.57
7:b:93:ASP:OD1	7:b:95:HIS:ND1	2.33	0.57
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.57
6:a:107:SER:HB2	6:a:124:VAL:HG11	1.85	0.57
6:a:7:SER:H	6:a:12:PHE:HE2	1.53	0.57
19:a:802:CLA:CGA	19:a:802:CLA:H3A	2.35	0.57
22:a:853:LMG:O8	22:a:853:LMG:H112	2.05	0.57
22:a:853:LMG:H112	22:a:853:LMG:C9	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:693:VAL:HG11	19:b:801:CLA:HAB	1.87	0.57
3:3:86:ARG:NH1	3:3:89:GLU:OE1	2.38	0.56
3:3:182:PHE:HZ	19:3:313:CLA:HED3	1.70	0.56
6:a:70:HIS:ND1	19:a:814:CLA:OBD	2.31	0.56
6:a:292:LEU:HD21	19:a:818:CLA:CAB	2.34	0.56
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.56
6:a:651:VAL:HG22	6:a:739:ALA:HB3	1.87	0.56
7:b:178:SER:HB3	7:b:286:GLY:HA3	1.86	0.56
6:a:114:ILE:HG13	6:a:115:VAL:HG13	1.86	0.56
6:a:324:GLY:HA3	25:a:846:LHG:HC32	1.87	0.56
7:b:582:MET:HG3	7:b:712:LEU:HD21	1.87	0.56
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.56
19:a:818:CLA:CHD	22:a:853:LMG:H291	2.36	0.56
19:a:841:CLA:H72	26:f:801:BCR:H17C	1.88	0.56
19:b:822:CLA:HHB	19:b:823:CLA:H2	1.88	0.56
11:i:26:LEU:HD13	26:l:205:BCR:HC8	1.86	0.56
8:d:97:HIS:HB3	8:d:98:PRO:HD3	1.86	0.56
3:3:48:LEU:HD13	3:3:51:LEU:HD12	1.87	0.56
4:2:35:SER:OG	4:2:37:ALA:O	2.22	0.56
17:2:303:XAT:C36	19:2:308:CLA:H2	2.35	0.56
6:a:598:ILE:HG13	19:a:801:CLA:H192	1.86	0.56
6:a:734:TRP:NE1	19:a:829:CLA:O1A	2.36	0.56
13:l:54:HIS:HA	13:l:57:PHE:CE2	2.41	0.56
6:a:213:ILE:HG23	6:a:233:PRO:HB3	1.87	0.55
6:a:290:HIS:HB2	19:a:819:CLA:C1B	2.37	0.55
6:a:660:SER:HB2	7:b:447:ALA:HB1	1.88	0.55
2:4:185:PHE:CE2	17:4:303:XAT:H30	2.42	0.55
6:a:651:VAL:HG21	6:a:736:PHE:HA	1.88	0.55
19:a:841:CLA:H92	26:f:801:BCR:H15C	1.88	0.55
7:b:521:VAL:HG21	7:b:595:TYR:HB2	1.89	0.55
19:a:822:CLA:HBC3	19:a:828:CLA:H172	1.88	0.55
5:1:115:ILE:O	5:1:119:GLN:NE2	2.40	0.55
9:e:32:VAL:HG11	16:c:35:LYS:HD3	1.89	0.55
13:l:92:LEU:HB3	26:l:205:BCR:H401	1.88	0.55
19:a:854:CLA:H112	12:j:14:LEU:HD22	1.88	0.55
6:a:441:LEU:HB3	6:a:534:PHE:HB2	1.88	0.55
5:1:88:ILE:HG22	5:1:92:PHE:HE1	1.71	0.55
19:a:825:CLA:H12	26:a:849:BCR:H14C	1.88	0.55
7:b:5:PHE:HB2	11:i:30:ILE:HA	1.89	0.55
16:c:15:THR:HG22	16:c:28:MET:HG3	1.89	0.55
18:5:303:A1L1G:C41	19:5:312:CLA:HMC1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:136:VAL:HG22	19:4:312:CLA:HMA1	1.87	0.54
6:a:388:VAL:HG12	6:a:596:ILE:HG23	1.89	0.54
7:b:317:HIS:HB3	7:b:320:LEU:HD12	1.89	0.54
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.54
6:a:197:GLY:HA3	19:a:814:CLA:HBB1	1.89	0.54
6:a:573:ARG:HG3	16:c:78:GLY:HA3	1.90	0.54
6:a:219:LYS:HD3	6:a:246:LEU:HB3	1.90	0.54
6:a:591:TRP:HE1	19:b:804:CLA:C1D	2.21	0.54
8:d:105:GLU:HG2	16:c:19:ARG:HB3	1.88	0.54
6:a:210:GLN:HA	6:a:214:ALA:HB3	1.89	0.54
6:a:667:LEU:HD11	7:b:619:MET:HB2	1.89	0.54
19:a:820:CLA:HAB	19:a:820:CLA:H8	1.90	0.54
7:b:22:TRP:CG	7:b:706:GLN:HE22	2.26	0.54
19:b:806:CLA:HBA1	19:b:814:CLA:HBA1	1.87	0.54
2:4:140:SER:OG	12:j:1:MET:SD	2.57	0.53
7:b:140:LEU:HG	26:b:845:BCR:H382	1.90	0.53
2:4:121:LEU:HD23	2:4:124:ILE:HD12	1.90	0.53
6:a:702:LYS:HB3	10:f:130:ARG:HD3	1.89	0.53
7:b:443:ASP:OD1	7:b:617:TYR:HB2	2.08	0.53
19:b:824:CLA:HBB2	19:b:841:CLA:H52	1.90	0.53
12:j:14:LEU:HD21	22:j:105:LMG:H141	1.89	0.53
2:4:83:ILE:HD11	17:4:302:XAT:H362	1.90	0.53
19:a:829:CLA:H101	26:j:104:BCR:H341	1.89	0.53
7:b:633:LEU:HD22	7:b:726:PHE:HA	1.90	0.53
5:1:61:ALA:HB1	5:1:65:THR:HB	1.90	0.53
19:a:835:CLA:O2D	19:a:835:CLA:H2A	2.09	0.53
7:b:355:PRO:HG3	19:b:819:CLA:HBA1	1.90	0.53
19:a:825:CLA:HMA3	19:a:844:CLA:HAB	1.91	0.53
19:4:317:CLA:O2D	21:4:318:DGD:HE61	2.09	0.53
19:a:831:CLA:H42	25:a:845:LHG:H251	1.90	0.53
19:a:810:CLA:HAB	19:j:102:CLA:HMD2	1.91	0.53
7:b:419:ALA:O	7:b:423:HIS:ND1	2.40	0.53
19:b:830:CLA:H42	21:b:851:DGD:HB42	1.91	0.53
15:g:51:UNK:O	15:g:53:UNK:N	2.42	0.53
6:a:411:ASN:ND2	6:a:414:ASN:OD1	2.37	0.52
7:b:709:LEU:HD11	21:b:851:DGD:HB41	1.90	0.52
19:b:801:CLA:H101	19:b:801:CLA:HBB1	1.91	0.52
8:d:63:ARG:NH2	8:d:65:GLU:OE1	2.41	0.52
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.91	0.52
2:4:81:CYS:HB3	2:4:178:GLY:HA3	1.91	0.52
19:a:809:CLA:CHC	19:a:810:CLA:HMD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:l:38:ARG:NH1	13:l:49:GLU:OE1	2.40	0.52
7:b:661:THR:O	7:b:664:MET:HB3	2.08	0.52
8:d:95:LEU:HD22	15:g:75:UNK:HA	1.91	0.52
1:5:143:TYR:OH	19:5:310:CLA:OBD	2.23	0.52
19:a:834:CLA:H151	24:b:842:PQN:H202	1.91	0.52
7:b:718:GLY:O	7:b:722:THR:HG22	2.09	0.52
10:f:85:LEU:HD13	10:f:93:PRO:HB3	1.92	0.52
4:2:121:ALA:O	4:2:122:LYS:HG2	2.10	0.52
16:c:11:CYS:SG	16:c:39:ILE:HG13	2.50	0.52
7:b:208:ASP:OD1	7:b:208:ASP:N	2.43	0.52
17:5:302:XAT:C16	19:5:307:CLA:H2	2.39	0.51
3:3:79:GLY:O	3:3:158:ARG:NH1	2.43	0.51
6:a:577:CYS:O	7:b:671:GLY:HA3	2.11	0.51
19:a:827:CLA:H93	19:a:840:CLA:H52	1.92	0.51
16:c:58:CYS:SG	16:c:63:LEU:HA	2.51	0.51
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.51
8:d:33:ILE:HG22	8:d:58:VAL:HG22	1.92	0.51
19:a:818:CLA:HHC	19:a:818:CLA:HBB1	1.93	0.51
7:b:342:ALA:O	7:b:346:THR:HG23	2.11	0.51
7:b:662:GLY:O	7:b:666:LEU:HG	2.11	0.51
2:4:193:ALA:O	21:4:318:DGD:O6E	2.28	0.51
19:b:837:CLA:HBC3	26:f:804:BCR:H401	1.91	0.51
5:1:77:GLY:O	5:1:81:MET:HG3	2.09	0.51
5:1:85:LEU:HB3	19:1:308:CLA:HMC2	1.92	0.51
6:a:396:VAL:HG11	6:a:589:LEU:HG	1.91	0.51
7:b:189:THR:HG21	7:b:276:LEU:HB2	1.91	0.51
7:b:274:HIS:HB2	19:b:818:CLA:C1B	2.41	0.51
19:b:837:CLA:HBC3	26:f:804:BCR:H292	1.91	0.51
23:1:304:A1L1F:C56	25:a:846:LHG:H241	2.41	0.51
7:b:26:ALA:HA	19:b:830:CLA:H43	1.93	0.51
19:5:312:CLA:CGA	19:5:312:CLA:H3A	2.41	0.51
7:b:273:HIS:ND1	19:b:818:CLA:HAB	2.25	0.51
10:f:160:TRP:CD1	10:f:161:PRO:HD3	2.46	0.51
22:a:853:LMG:H131	22:a:853:LMG:H292	1.93	0.51
10:f:143:ILE:HG13	10:f:144:ILE:HG13	1.92	0.51
7:b:602:THR:HG21	7:b:611:PHE:HB2	1.93	0.51
17:4:303:XAT:C16	19:4:308:CLA:H2	2.41	0.50
3:3:93:CYS:HB3	3:3:193:GLY:HA3	1.93	0.50
7:b:179:GLY:O	7:b:183:VAL:HB	2.10	0.50
6:a:431:ILE:HG13	6:a:549:TYR:HE1	1.74	0.50
6:a:460:ARG:NH2	19:a:835:CLA:O1D	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:434:HIS:CD2	26:b:852:BCR:H333	2.46	0.50
17:5:301:XAT:H193	19:5:310:CLA:HBA2	1.94	0.50
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.50
19:b:824:CLA:HAB	19:b:831:CLA:HMD1	1.93	0.50
19:b:807:CLA:H52	21:b:851:DGD:HB72	1.92	0.50
13:l:106:VAL:H	13:l:140:VAL:HG23	1.77	0.50
6:a:440:PHE:HE2	19:a:839:CLA:HAB	1.76	0.50
19:b:833:CLA:HBB2	26:f:801:BCR:HC41	1.94	0.50
4:2:77:LYS:O	4:2:79:ASP:N	2.43	0.49
6:a:422:ARG:O	6:a:426:HIS:ND1	2.41	0.49
19:b:812:CLA:H72	19:b:813:CLA:HBC3	1.92	0.49
4:2:107:LEU:HB3	19:2:310:CLA:HMC2	1.94	0.49
5:1:112:VAL:HB	5:1:117:TRP:NE1	2.27	0.49
19:a:818:CLA:CHD	19:a:819:CLA:HBB2	2.43	0.49
7:b:25:ILE:HG12	26:l:205:BCR:H312	1.94	0.49
6:a:565:ARG:HG2	6:a:715:THR:HG21	1.93	0.49
22:a:853:LMG:C11	22:a:853:LMG:HC92	2.41	0.49
16:c:13:GLY:O	16:c:38:GLN:NE2	2.44	0.49
16:c:17:CYS:HB3	27:c:102:SF4:S4	2.52	0.49
6:a:615:VAL:HG22	6:a:621:VAL:HG22	1.95	0.49
7:b:3:TYR:HB2	11:i:33:GLU:HA	1.95	0.49
7:b:266:LEU:HD22	19:b:818:CLA:HBA1	1.94	0.49
19:4:309:CLA:HAC1	19:4:316:CLA:HAB	1.95	0.49
4:2:183:ASP:O	4:2:186:LYS:N	2.44	0.49
7:b:518:ASP:OD2	7:b:595:TYR:OH	2.23	0.49
19:a:818:CLA:O1A	22:a:853:LMG:O10	2.30	0.49
7:b:478:LEU:HG	7:b:479:LEU:HG	1.93	0.49
16:c:17:CYS:SG	16:c:18:VAL:N	2.85	0.49
6:a:423:VAL:HA	6:a:426:HIS:CE1	2.47	0.49
19:a:803:CLA:H2	7:b:657:LEU:HD22	1.95	0.49
1:5:171:GLU:HG3	19:5:311:CLA:NB	2.28	0.49
3:3:78:VAL:HG12	3:3:78:VAL:O	2.13	0.49
6:a:554:ARG:HB2	7:b:678:GLU:OE1	2.13	0.49
19:a:802:CLA:H41	7:b:436:LEU:HD22	1.95	0.49
7:b:722:THR:HG23	19:b:803:CLA:O1D	2.11	0.49
26:b:852:BCR:H23C	12:j:33:TYR:CD2	2.47	0.49
15:g:46:UNK:O	15:g:50:UNK:N	2.45	0.49
3:3:203:MET:HE2	17:3:305:XAT:O4	2.13	0.49
6:a:712:LEU:N	24:a:843:PQN:O4	2.45	0.49
7:b:443:ASP:OD1	7:b:618:ILE:N	2.46	0.48
13:l:43:PRO:HD3	13:l:136:GLU:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:292:LEU:HD12	19:a:816:CLA:HMC3	1.95	0.48
6:a:425:ARG:NH2	8:d:15:GLY:O	2.44	0.48
7:b:407:LYS:HB3	7:b:411:ALA:HB3	1.95	0.48
7:b:492:SER:HA	7:b:496:LEU:HD12	1.94	0.48
17:5:304:XAT:C10	19:5:315:CLA:HBC3	2.43	0.48
3:3:145:ILE:O	3:3:149:ILE:HG12	2.13	0.48
19:a:832:CLA:HAB	19:a:840:CLA:HBB2	1.96	0.48
7:b:595:TYR:CZ	19:b:836:CLA:HBC3	2.49	0.48
7:b:65:LEU:HD11	26:b:845:BCR:H281	1.95	0.48
7:b:526:ALA:O	7:b:530:HIS:ND1	2.37	0.48
7:b:597:HIS:CE1	7:b:601:LEU:HD11	2.48	0.48
9:e:51:ASN:CG	16:c:61:ASP:HB2	2.39	0.48
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.48
19:3:308:CLA:HED2	19:3:308:CLA:H2A	1.94	0.48
6:a:674:ALA:HB3	19:a:802:CLA:HBB2	1.94	0.48
2:4:184:ALA:HA	19:4:315:CLA:HBB1	1.95	0.48
19:3:308:CLA:H2A	19:3:308:CLA:CED	2.44	0.48
6:a:637:ASN:HB2	7:b:653:LEU:HD11	1.94	0.48
19:b:811:CLA:H202	13:l:90:LEU:HD22	1.96	0.48
2:4:159:ASN:C	2:4:161:ALA:H	2.20	0.48
3:3:81:ASP:N	3:3:81:ASP:OD1	2.46	0.48
5:1:144:ASP:OD2	5:1:148:THR:OG1	2.23	0.48
19:a:820:CLA:H203	19:a:828:CLA:H3A	1.96	0.48
7:b:670:ARG:C	7:b:672:TYR:H	2.22	0.48
26:b:852:BCR:H23C	12:j:33:TYR:HD2	1.78	0.48
11:i:26:LEU:HD22	26:l:205:BCR:H323	1.94	0.48
7:b:8:PHE:HB2	7:b:34:HIS:CG	2.49	0.48
19:b:824:CLA:H2A	19:b:824:CLA:HED3	1.95	0.48
8:d:95:LEU:HD11	8:d:98:PRO:HD2	1.95	0.48
19:i:102:CLA:H142	19:i:102:CLA:H111	1.61	0.48
13:l:109:ASN:OD1	13:l:110:ALA:N	2.35	0.48
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.48
4:2:92:ARG:NH1	4:2:95:GLU:OE1	2.47	0.48
5:1:88:ILE:HG22	5:1:92:PHE:CE1	2.49	0.48
7:b:271:MET:O	7:b:275:HIS:ND1	2.47	0.48
7:b:432:GLY:HA2	7:b:527:LEU:HD22	1.96	0.48
19:a:825:CLA:H71	19:a:840:CLA:H62	1.96	0.48
7:b:176:HIS:O	7:b:180:LEU:HB3	2.14	0.48
19:b:839:CLA:HAB	24:b:842:PQN:H172	1.96	0.48
19:b:841:CLA:H141	19:b:841:CLA:H161	1.74	0.48
6:a:127:ASN:HD21	10:f:60:THR:HG21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:290:HIS:HB2	19:a:819:CLA:CHB	2.44	0.47
11:i:26:LEU:HB3	26:l:205:BCR:H323	1.96	0.47
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.47
6:a:514:ILE:HD11	6:a:621:VAL:HG13	1.96	0.47
19:b:840:CLA:H13	26:i:101:BCR:H19C	1.95	0.47
17:2:305:XAT:H35	17:2:305:XAT:H401	1.74	0.47
6:a:38:THR:HB	6:a:710:ARG:HG3	1.97	0.47
6:a:114:ILE:HG23	6:a:115:VAL:HG22	1.96	0.47
7:b:166:PHE:O	7:b:172:ARG:NH2	2.46	0.47
7:b:297:HIS:HB3	7:b:302:ILE:HD11	1.97	0.47
7:b:538:LYS:O	7:b:542:ASP:HB2	2.14	0.47
26:b:845:BCR:H311	26:b:845:BCR:HC8	1.97	0.47
25:m:101:LHG:H321	25:m:101:LHG:H291	1.66	0.47
5:1:42:MET:HE1	5:1:66:LEU:HD22	1.95	0.47
7:b:586:LEU:HD21	7:b:716:THR:HG23	1.96	0.47
19:b:825:CLA:H193	19:b:825:CLA:H141	1.95	0.47
6:a:400:ALA:HB2	6:a:585:VAL:HG11	1.96	0.47
22:a:853:LMG:C9	22:a:853:LMG:C11	2.91	0.47
19:b:822:CLA:CHB	19:b:823:CLA:H2	2.44	0.47
19:2:316:CLA:C2C	22:2:317:LMG:H111	2.44	0.47
6:a:354:GLY:HA2	6:a:391:GLY:HA2	1.97	0.47
7:b:127:MET:HE1	26:b:845:BCR:H282	1.97	0.47
7:b:452:GLU:OE2	10:f:76:ARG:NE	2.42	0.47
19:b:802:CLA:H93	19:b:802:CLA:H112	1.70	0.47
19:b:811:CLA:HBA2	13:l:67:PRO:HG3	1.97	0.47
19:b:838:CLA:H101	19:b:838:CLA:H13	1.78	0.47
12:j:2:LYS:O	22:j:105:LMG:HC61	2.13	0.47
1:5:130:PHE:HE1	17:5:302:XAT:O24	1.94	0.47
19:4:317:CLA:CGD	21:4:318:DGD:HE61	2.45	0.47
6:a:502:ALA:HB2	6:a:516:MET:HE2	1.97	0.47
6:a:712:LEU:HD21	24:a:843:PQN:H151	1.96	0.47
19:a:841:CLA:H61	19:b:833:CLA:H42	1.95	0.47
7:b:143:LEU:HD23	7:b:146:LEU:HD12	1.97	0.47
7:b:181:PHE:HE2	19:b:820:CLA:HAB	1.78	0.47
19:b:831:CLA:HAB	19:b:838:CLA:CBB	2.44	0.47
19:b:839:CLA:H192	19:b:839:CLA:H162	1.73	0.47
8:d:20:TRP:CZ2	13:l:14:VAL:HG12	2.50	0.47
12:j:5:LEU:HB3	22:j:105:LMG:HC72	1.96	0.47
4:2:118:LEU:N	19:2:310:CLA:OBD	2.47	0.47
6:a:287:THR:HG23	19:a:820:CLA:HMA3	1.96	0.47
19:a:829:CLA:HBB1	19:a:829:CLA:HMB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:372:HIS:HB2	19:b:828:CLA:C1B	2.45	0.47
7:b:412:ARG:HH21	19:b:831:CLA:CGD	2.27	0.47
7:b:433:PHE:HZ	26:f:801:BCR:H372	1.80	0.47
7:b:687:THR:HG23	7:b:690:ALA:HB3	1.97	0.47
19:b:811:CLA:H71	13:l:83:LEU:HG	1.97	0.47
8:d:83:LYS:HG2	8:d:98:PRO:HG2	1.97	0.47
6:a:686:TYR:OH	19:a:802:CLA:OBD	2.22	0.47
19:a:827:CLA:H13	19:a:827:CLA:H172	1.77	0.47
7:b:277:ALA:HA	19:b:817:CLA:HMC2	1.96	0.47
7:b:385:PHE:HB3	7:b:536:LEU:HB3	1.97	0.47
1:5:96:VAL:HG12	19:5:307:CLA:OBD	2.15	0.47
2:4:185:PHE:CZ	17:4:303:XAT:H28	2.50	0.47
4:2:105:ALA:HB1	17:2:303:XAT:H161	1.97	0.47
19:b:807:CLA:H192	19:b:807:CLA:H161	1.72	0.46
19:b:819:CLA:HBA2	19:b:819:CLA:H3A	1.37	0.46
11:i:28:LEU:O	11:i:32:LYS:HG3	2.15	0.46
19:1:306:CLA:H93	19:1:306:CLA:H61	1.70	0.46
6:a:68:SER:OG	6:a:174:TYR:HB2	2.14	0.46
19:b:839:CLA:H41	19:b:839:CLA:H62	1.71	0.46
17:3:303:XAT:H35	17:3:303:XAT:H401	1.79	0.46
17:2:303:XAT:H11	17:2:303:XAT:H191	1.66	0.46
19:a:854:CLA:H142	19:a:854:CLA:H111	1.80	0.46
17:3:305:XAT:H35	17:3:305:XAT:H401	1.77	0.46
4:2:191:GLN:O	4:2:195:ILE:HD12	2.15	0.46
5:1:84:VAL:O	5:1:88:ILE:HG12	2.14	0.46
6:a:570:GLY:O	6:a:576:THR:OG1	2.32	0.46
19:a:801:CLA:H61	19:a:803:CLA:O1D	2.16	0.46
19:a:834:CLA:CAD	26:l:201:BCR:H10C	2.45	0.46
19:b:818:CLA:H41	19:b:834:CLA:HAA2	1.97	0.46
19:b:823:CLA:HHC	19:b:841:CLA:HED1	1.98	0.46
4:2:65:ILE:HG22	4:2:67:PHE:H	1.80	0.46
5:1:62:ASP:OD1	5:1:62:ASP:N	2.49	0.46
6:a:114:ILE:O	6:a:117:GLN:HG2	2.16	0.46
19:a:819:CLA:H3A	19:a:819:CLA:HBA2	1.53	0.46
7:b:50:HIS:HE1	19:b:806:CLA:H171	1.81	0.46
6:a:476:PHE:HB3	19:a:838:CLA:H11	1.96	0.46
19:a:818:CLA:NC	22:a:853:LMG:H302	2.31	0.46
19:b:839:CLA:H12	26:l:205:BCR:H15C	1.98	0.46
5:1:89:VAL:O	5:1:93:TRP:N	2.49	0.46
17:a:852:XAT:H15	17:a:852:XAT:H201	1.67	0.46
19:j:102:CLA:NB	26:j:104:BCR:H281	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:303:XAT:H35	17:4:303:XAT:H401	1.84	0.46
19:a:804:CLA:H41	19:a:841:CLA:HMC1	1.98	0.46
19:a:854:CLA:H143	22:j:105:LMG:H142	1.97	0.46
19:b:814:CLA:H141	19:b:814:CLA:H161	1.77	0.46
19:b:826:CLA:HAA2	19:b:827:CLA:OBD	2.16	0.46
19:b:840:CLA:HBA1	19:b:840:CLA:H3A	1.59	0.46
1:5:116:GLU:HB2	19:5:307:CLA:C1B	2.46	0.46
6:a:375:ILE:HG21	6:a:510:VAL:HB	1.96	0.46
7:b:268:LEU:HD23	7:b:271:MET:HE3	1.98	0.46
22:j:105:LMG:H292	22:j:105:LMG:H111	1.98	0.46
5:1:140:TYR:OH	5:1:142:PRO:O	2.25	0.46
6:a:25:PRO:HB2	6:a:41:TRP:HH2	1.81	0.46
6:a:665:ILE:HG23	19:a:809:CLA:H171	1.99	0.46
19:a:806:CLA:H72	26:a:848:BCR:HC8	1.98	0.46
7:b:392:PHE:CE2	26:b:847:BCR:HC42	2.51	0.46
13:l:168:TYR:O	13:l:172:LEU:HB2	2.16	0.46
1:5:124:MET:HE3	19:5:312:CLA:HMC2	1.98	0.45
17:4:305:XAT:H15	17:4:305:XAT:H201	1.71	0.45
3:3:179:PRO:C	3:3:181:LYS:H	2.24	0.45
5:1:105:PRO:C	5:1:107:LYS:H	2.24	0.45
6:a:282:LEU:HD21	6:a:367:MET:HB3	1.98	0.45
6:a:677:LEU:HB2	19:a:802:CLA:HMC2	1.97	0.45
19:a:822:CLA:H12	19:a:825:CLA:HBA2	1.98	0.45
4:2:131:ALA:HA	4:2:134:VAL:HG12	1.98	0.45
26:b:844:BCR:H11C	26:b:844:BCR:H341	1.76	0.45
17:5:302:XAT:H11	17:5:302:XAT:H191	1.65	0.45
17:4:302:XAT:H30	19:4:310:CLA:H151	1.98	0.45
19:3:310:CLA:H61	19:3:310:CLA:H41	1.86	0.45
5:1:141:ARG:HD3	5:1:149:TRP:HB3	1.99	0.45
19:b:812:CLA:H51	19:b:813:CLA:H43	1.97	0.45
10:f:119:GLY:HA3	10:f:160:TRP:CE2	2.51	0.45
12:j:26:VAL:CG1	26:j:104:BCR:H403	2.47	0.45
3:3:121:GLN:HA	3:3:124:VAL:HG12	1.99	0.45
5:1:73:GLU:HB2	19:1:306:CLA:C1B	2.45	0.45
7:b:339:LEU:O	7:b:343:THR:HG22	2.16	0.45
19:b:824:CLA:HBA1	26:b:846:BCR:H16C	1.98	0.45
10:f:143:ILE:O	12:j:11:ALA:N	2.48	0.45
17:4:305:XAT:H11	17:4:305:XAT:H191	1.81	0.45
6:a:144:GLU:HG2	6:a:206:TRP:HH2	1.80	0.45
7:b:466:GLN:NE2	19:b:836:CLA:OBD	2.34	0.45
19:b:811:CLA:H141	19:b:811:CLA:H162	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:232:HIS:HE1	17:5:304:XAT:H14	1.81	0.45
17:2:303:XAT:H15	17:2:303:XAT:H201	1.79	0.45
6:a:312:GLY:HA2	19:a:823:CLA:HMD2	1.99	0.45
19:b:833:CLA:H18	26:f:804:BCR:H17C	1.97	0.45
17:2:302:XAT:H15	17:2:302:XAT:H201	1.82	0.45
6:a:71:PHE:HD1	6:a:166:MET:HE3	1.82	0.45
6:a:304:MET:HG3	19:a:823:CLA:C3C	2.47	0.45
6:a:466:SER:HG	6:a:631:GLN:HE22	1.64	0.45
7:b:228:TRP:HZ3	26:b:850:BCR:H363	1.81	0.45
19:b:813:CLA:H62	19:b:813:CLA:H41	1.62	0.45
19:b:824:CLA:HHB	19:b:841:CLA:O1D	2.16	0.45
6:a:407:VAL:HG11	6:a:564:PHE:N	2.32	0.45
7:b:605:GLN:HE21	7:b:734:LYS:HB3	1.82	0.45
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.45
17:4:304:XAT:H35	17:4:304:XAT:H401	1.80	0.45
17:3:304:XAT:H15	17:3:304:XAT:H201	1.78	0.45
17:2:303:XAT:H31	17:2:303:XAT:H391	1.70	0.45
17:1:303:XAT:H183	19:1:308:CLA:C2B	2.47	0.45
1:5:164:PHE:HE1	19:f:802:CLA:H121	1.81	0.45
17:4:305:XAT:H391	17:4:305:XAT:H31	1.62	0.45
19:4:311:CLA:H2A	19:4:311:CLA:O2D	2.17	0.45
19:1:312:CLA:HMA2	20:1:315:SQD:H141	1.99	0.45
19:a:835:CLA:H61	26:l:201:BCR:H363	1.99	0.45
19:b:825:CLA:H41	19:b:825:CLA:H62	1.79	0.45
8:d:20:TRP:HB2	8:d:24:ALA:HB3	1.99	0.45
1:5:106:PHE:HB2	10:f:148:PRO:HG3	1.99	0.44
2:4:37:SER:HB3	2:4:45:ARG:HA	1.98	0.44
17:3:304:XAT:H35	17:3:304:XAT:H401	1.68	0.44
19:2:316:CLA:C1C	22:2:317:LMG:H111	2.46	0.44
20:1:315:SQD:H311	20:1:315:SQD:H282	1.84	0.44
6:a:683:GLY:HA3	7:b:571:ASP:HB2	1.99	0.44
7:b:50:HIS:ND1	19:b:814:CLA:OBD	2.38	0.44
7:b:259:PHE:CZ	7:b:510:LEU:HD12	2.53	0.44
7:b:280:VAL:HG21	19:b:817:CLA:HAB	1.98	0.44
26:b:845:BCR:H24C	26:b:845:BCR:H371	1.70	0.44
11:i:14:VAL:O	11:i:19:PRO:HD2	2.17	0.44
13:l:68:LEU:O	13:l:77:SER:OG	2.24	0.44
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.44
3:3:133:PRO:HB2	17:3:301:XAT:H23	2.00	0.44
17:2:302:XAT:H401	17:2:302:XAT:H35	1.71	0.44
5:1:156:ASP:OD2	13:l:2:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:801:CLA:CED	19:a:801:CLA:HAA2	2.46	0.44
10:f:79:ARG:O	10:f:83:SER:HB2	2.17	0.44
2:4:170:MET:CE	19:4:313:CLA:H12	2.47	0.44
17:2:303:XAT:H35	17:2:303:XAT:H401	1.71	0.44
5:1:40:ASP:HB2	5:1:42:MET:HG3	1.98	0.44
19:a:801:CLA:HED2	19:a:801:CLA:HBD	1.48	0.44
4:2:97:LYS:NZ	4:2:152:GLU:OE1	2.38	0.44
6:a:73:GLN:HG2	19:a:806:CLA:H3A	2.00	0.44
6:a:342:TRP:CD1	19:a:826:CLA:H192	2.51	0.44
6:a:447:GLY:HA3	19:a:835:CLA:HAB	1.98	0.44
19:a:826:CLA:HMB3	19:a:826:CLA:HBB1	1.99	0.44
7:b:172:ARG:HB2	19:b:814:CLA:HBC2	2.00	0.44
7:b:343:THR:HG23	7:b:377:ALA:HB2	2.00	0.44
19:b:811:CLA:H112	19:i:102:CLA:HAB	1.99	0.44
19:b:821:CLA:HBA2	19:b:821:CLA:H3A	1.33	0.44
19:b:836:CLA:H12	19:b:837:CLA:O1A	2.18	0.44
2:4:59:PHE:HE1	19:4:306:CLA:HBC3	1.83	0.44
6:a:367:MET:HG2	6:a:500:SER:HB2	1.99	0.44
6:a:580:SER:HB2	6:a:582:TRP:H	1.82	0.44
6:a:686:TYR:CE1	7:b:538:LYS:HD2	2.52	0.44
19:a:803:CLA:H151	19:b:811:CLA:HBC3	1.97	0.44
19:a:812:CLA:H142	19:a:812:CLA:H112	1.85	0.44
19:b:808:CLA:H93	19:b:808:CLA:H61	1.71	0.44
19:b:814:CLA:H143	19:b:825:CLA:H51	1.99	0.44
8:d:81:ASN:H	8:d:81:ASN:ND2	2.16	0.44
16:c:3:HIS:HB2	16:c:48:CYS:SG	2.56	0.44
5:1:95:PRO:HD2	19:1:308:CLA:HMD3	1.99	0.44
19:a:813:CLA:H62	19:a:813:CLA:H41	1.85	0.44
7:b:654:PHE:O	7:b:658:VAL:HG23	2.17	0.44
19:b:839:CLA:H161	13:l:92:LEU:HD21	1.99	0.44
26:b:843:BCR:H15C	26:b:843:BCR:H351	1.73	0.44
17:5:302:XAT:H383	19:5:309:CLA:C2B	2.48	0.44
17:2:305:XAT:H15	17:2:305:XAT:H201	1.78	0.44
6:a:532:HIS:CE1	6:a:599:VAL:HA	2.53	0.44
6:a:578:GLN:HA	6:a:583:ASP:OD2	2.18	0.44
19:a:829:CLA:H91	19:a:831:CLA:H192	2.00	0.44
19:a:834:CLA:H201	26:l:205:BCR:H343	1.98	0.44
7:b:682:TRP:NE1	13:l:15:GLY:O	2.43	0.44
26:b:852:BCR:H20C	26:b:852:BCR:H361	1.76	0.44
10:f:160:TRP:CG	10:f:161:PRO:HD3	2.52	0.44
17:j:101:XAT:H35	17:j:101:XAT:H401	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:c:59:PRO:HD2	27:c:102:SF4:S2	2.58	0.44
3:3:189:GLU:HB2	19:3:313:CLA:C1B	2.47	0.44
4:2:118:LEU:HB2	4:2:123:TYR:HD2	1.83	0.44
5:1:152:VAL:HG11	5:1:159:TRP:CD1	2.53	0.44
5:1:171:ARG:HA	5:1:174:MET:HE3	2.00	0.44
22:a:853:LMG:H112	22:a:853:LMG:HC92	1.98	0.44
7:b:678:GLU:HG2	16:c:81:TYR:HE1	1.81	0.44
19:b:818:CLA:HBA2	19:b:818:CLA:H3A	1.26	0.44
10:f:153:ILE:O	10:f:156:SER:OG	2.31	0.44
26:j:104:BCR:H341	26:j:104:BCR:H11C	1.72	0.44
13:l:116:VAL:HG11	13:l:128:LEU:C	2.42	0.44
25:m:101:LHG:H272	25:m:101:LHG:H302	1.86	0.44
17:4:302:XAT:H11	17:4:302:XAT:H191	1.89	0.44
4:2:127:ASN:OD1	4:2:130:GLN:N	2.46	0.44
17:1:302:XAT:H31	17:1:302:XAT:H391	1.88	0.44
6:a:52:PHE:CD2	19:a:806:CLA:HMC2	2.53	0.44
6:a:415:ASN:O	6:a:421:ASP:HB2	2.18	0.44
6:a:442:GLY:HA3	19:b:804:CLA:O1A	2.18	0.44
6:a:701:LEU:HD12	19:a:841:CLA:HMA2	2.00	0.44
7:b:302:ILE:HD13	19:b:823:CLA:HMD2	2.00	0.44
7:b:526:ALA:HB2	19:b:837:CLA:HMA1	2.00	0.44
19:b:826:CLA:H3A	19:b:826:CLA:HBA2	1.72	0.44
1:5:115:ALA:O	1:5:119:ASN:ND2	2.42	0.43
2:4:85:MET:HE3	2:4:177:ASN:HB3	2.00	0.43
19:a:807:CLA:H43	25:a:845:LHG:H252	2.00	0.43
7:b:26:ALA:HB1	21:b:851:DGD:O1B	2.17	0.43
7:b:520:LEU:HD23	7:b:520:LEU:HA	1.88	0.43
10:f:57:GLU:O	10:f:60:THR:OG1	2.32	0.43
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.43
19:a:806:CLA:H162	19:a:806:CLA:H141	1.59	0.43
7:b:518:ASP:O	7:b:522:HIS:ND1	2.38	0.43
19:b:805:CLA:H162	19:b:805:CLA:H141	1.67	0.43
16:c:54:CYS:SG	16:c:55:GLU:N	2.91	0.43
19:4:310:CLA:C1A	19:4:310:CLA:CGA	2.96	0.43
6:a:194:HIS:HE1	19:a:826:CLA:H72	1.83	0.43
6:a:565:ARG:HD2	25:a:845:LHG:HC61	2.00	0.43
19:a:822:CLA:OBD	19:a:824:CLA:HMD3	2.19	0.43
19:a:826:CLA:H202	19:a:826:CLA:H162	1.79	0.43
19:a:831:CLA:H92	19:a:831:CLA:H61	1.70	0.43
6:a:84:MET:SD	19:a:829:CLA:HED1	2.58	0.43
6:a:517:MET:HE2	6:a:611:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:807:CLA:H2	19:b:807:CLA:H62	1.79	0.43
9:e:16:TYR:CD2	9:e:44:ASN:HA	2.54	0.43
11:i:17:VAL:HG21	19:i:102:CLA:HMC2	2.01	0.43
13:l:96:LEU:HG	26:l:205:BCR:H24C	2.01	0.43
2:4:183:LEU:HD11	19:4:308:CLA:HAC1	2.00	0.43
7:b:201:ARG:HG2	7:b:248:SER:HB2	1.99	0.43
26:b:847:BCR:H15C	26:b:847:BCR:H351	1.85	0.43
12:j:30:ASN:ND2	19:j:102:CLA:O1A	2.47	0.43
19:a:844:CLA:C1C	25:a:846:LHG:HC31	2.48	0.43
17:a:852:XAT:H35	17:a:852:XAT:H401	1.85	0.43
7:b:172:ARG:HD2	19:b:825:CLA:OBD	2.18	0.43
19:b:841:CLA:H161	19:b:841:CLA:H192	1.82	0.43
19:j:103:CLA:O1D	19:j:103:CLA:H2A	2.18	0.43
17:4:301:XAT:H11	17:4:301:XAT:H191	1.86	0.43
5:1:171:ARG:HA	5:1:174:MET:CE	2.49	0.43
7:b:220:LEU:HD23	7:b:220:LEU:HA	1.87	0.43
7:b:350:MET:HE2	7:b:350:MET:HB3	1.89	0.43
19:b:807:CLA:H161	19:b:807:CLA:H102	2.01	0.43
19:b:814:CLA:H161	19:b:814:CLA:H192	1.76	0.43
19:5:307:CLA:HBC1	17:4:301:XAT:H383	2.01	0.43
17:2:304:XAT:H11	17:2:304:XAT:H191	1.89	0.43
5:1:128:GLU:HG3	17:1:302:XAT:H372	2.01	0.43
5:1:151:TRP:CH2	13:l:20:PRO:HA	2.54	0.43
5:1:168:ASN:HA	5:1:171:ARG:HD2	2.01	0.43
6:a:94:TYR:OH	6:a:146:ILE:O	2.24	0.43
19:a:833:CLA:H72	19:l:203:CLA:H12	2.00	0.43
7:b:207:TRP:HE1	19:b:815:CLA:H11	1.84	0.43
26:f:804:BCR:H11C	26:f:804:BCR:H341	1.73	0.43
3:3:103:ILE:HD11	17:3:304:XAT:H363	2.01	0.43
4:2:205:PHE:CD2	17:2:303:XAT:H12	2.54	0.43
19:2:310:CLA:H192	19:2:310:CLA:H162	1.71	0.43
5:1:58:ALA:HB1	5:1:66:LEU:HD21	2.00	0.43
5:1:82:LEU:HD11	19:1:311:CLA:HBC1	2.01	0.43
7:b:274:HIS:HB2	19:b:818:CLA:CHB	2.48	0.43
7:b:440:VAL:HG12	19:j:102:CLA:HAC1	2.01	0.43
7:b:547:LYS:NZ	9:e:15:SER:O	2.45	0.43
19:b:801:CLA:H91	19:b:801:CLA:H111	1.70	0.43
16:c:25:VAL:HG21	16:c:48:CYS:HA	2.00	0.43
17:4:304:XAT:H15	17:4:304:XAT:H201	1.87	0.43
3:3:56:ASN:HB3	3:3:82:LEU:HD22	2.01	0.43
17:2:301:XAT:H401	17:2:301:XAT:H35	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:555:LEU:HD11	7:b:674:GLN:HB3	2.01	0.43
7:b:140:LEU:HD23	7:b:143:LEU:HD12	2.01	0.43
7:b:345:LEU:CD1	19:b:827:CLA:HAA1	2.49	0.43
7:b:424:LEU:HG	19:b:838:CLA:CBB	2.48	0.43
7:b:626:LEU:HD22	19:b:803:CLA:HMD3	2.01	0.43
19:i:102:CLA:H91	19:i:102:CLA:H112	1.69	0.43
17:5:304:XAT:H15	17:5:304:XAT:H201	1.76	0.42
19:4:317:CLA:H92	19:4:317:CLA:H62	1.83	0.42
19:a:807:CLA:H92	19:a:807:CLA:H61	1.69	0.42
19:a:841:CLA:HED3	19:a:841:CLA:H2A	2.01	0.42
19:a:807:CLA:H102	19:a:807:CLA:H161	2.00	0.42
19:a:820:CLA:CAD	19:a:830:CLA:H41	2.48	0.42
26:a:848:BCR:H15C	26:a:848:BCR:H351	1.78	0.42
7:b:529:LEU:HD23	7:b:588:THR:HG21	2.00	0.42
2:4:193:ALA:HB1	21:4:318:DGD:O5E	2.16	0.42
19:4:309:CLA:HED2	19:4:309:CLA:HBD	1.83	0.42
6:a:727:LEU:HD22	19:a:842:CLA:HMA3	2.01	0.42
7:b:500:LEU:HA	7:b:503:ILE:HG22	2.02	0.42
8:d:88:TYR:HB3	8:d:89:PRO:HD2	2.01	0.42
12:j:12:PRO:HB2	17:j:101:XAT:H21	2.01	0.42
1:5:98:PHE:HE1	19:5:305:CLA:HBC3	1.84	0.42
17:5:301:XAT:H15	17:5:301:XAT:H201	1.85	0.42
17:5:301:XAT:H35	17:5:301:XAT:H401	1.77	0.42
19:4:306:CLA:CHA	19:4:306:CLA:HBA1	2.48	0.42
19:4:309:CLA:H3A	19:4:309:CLA:HBA1	1.77	0.42
6:a:75:ALA:HB2	6:a:166:MET:HB2	2.01	0.42
6:a:271:PHE:HE2	6:a:495:ALA:HB2	1.84	0.42
6:a:689:GLU:OE2	7:b:546:SER:OG	2.30	0.42
19:a:810:CLA:HBB1	26:j:104:BCR:H23C	2.00	0.42
8:d:32:ILE:HG21	8:d:70:LEU:HD23	2.00	0.42
3:3:172:PRO:HD2	17:3:305:XAT:H242	2.00	0.42
6:a:452:ASN:HD22	6:a:634:ILE:HB	1.85	0.42
7:b:381:MET:HE1	26:b:847:BCR:H352	2.02	0.42
19:b:817:CLA:CHD	19:b:818:CLA:HBB2	2.49	0.42
19:j:102:CLA:H111	19:j:102:CLA:H91	1.83	0.42
6:a:361:ALA:HB2	6:a:387:HIS:HB2	2.01	0.42
19:a:803:CLA:O1A	19:a:803:CLA:H3A	2.19	0.42
19:a:831:CLA:H93	19:a:842:CLA:HED3	2.01	0.42
7:b:347:ALA:HB3	7:b:374:GLN:HE21	1.85	0.42
19:b:827:CLA:HED1	26:b:847:BCR:H21C	2.02	0.42
26:b:845:BCR:HC7	26:b:845:BCR:H331	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5:304:XAT:H35	17:5:304:XAT:H401	1.80	0.42
17:2:305:XAT:H31	17:2:305:XAT:H391	1.71	0.42
6:a:143:ALA:HB2	6:a:371:PRO:HD2	2.00	0.42
19:a:804:CLA:C4D	12:j:12:PRO:HG3	2.50	0.42
26:a:850:BCR:H20C	26:a:850:BCR:H361	1.80	0.42
7:b:56:ILE:HD11	26:m:102:BCR:HC7	2.02	0.42
7:b:647:VAL:HG21	19:b:809:CLA:HAC1	2.00	0.42
19:b:815:CLA:H61	19:b:815:CLA:H2	1.77	0.42
19:b:836:CLA:H51	19:b:836:CLA:H11	1.73	0.42
19:b:840:CLA:H61	19:b:840:CLA:H92	1.73	0.42
12:j:14:LEU:CD2	22:j:105:LMG:H141	2.49	0.42
13:l:53:THR:HG22	19:l:202:CLA:C1B	2.49	0.42
17:3:304:XAT:H12	19:3:309:CLA:HAB	2.01	0.42
17:1:303:XAT:H35	17:1:303:XAT:H401	1.85	0.42
6:a:567:PRO:HB3	6:a:714:ILE:HB	2.00	0.42
19:a:807:CLA:H161	19:a:807:CLA:H192	1.82	0.42
19:a:823:CLA:CHD	17:a:852:XAT:H183	2.49	0.42
26:a:849:BCR:H15C	26:a:849:BCR:H351	1.79	0.42
26:a:849:BCR:H24C	26:a:849:BCR:H371	1.86	0.42
7:b:120:GLU:OE2	7:b:362:ASN:ND2	2.39	0.42
7:b:220:LEU:HD21	26:b:843:BCR:H391	2.01	0.42
19:b:805:CLA:H2	19:b:805:CLA:H61	1.62	0.42
19:b:817:CLA:CBB	26:b:850:BCR:H14C	2.50	0.42
26:l:201:BCR:H352	19:l:203:CLA:HAB	2.02	0.42
16:c:32:ASP:OD1	16:c:32:ASP:N	2.53	0.42
6:a:272:LYS:HG2	6:a:496:LEU:HD12	2.02	0.42
6:a:364:MET:HE1	19:a:830:CLA:CAD	2.49	0.42
6:a:440:PHE:CE2	19:a:839:CLA:HAB	2.55	0.42
6:a:680:LEU:HB3	7:b:667:ILE:HG12	2.02	0.42
26:a:849:BCR:H20C	26:a:849:BCR:H361	1.89	0.42
26:b:843:BCR:H11C	26:b:843:BCR:H341	1.74	0.42
2:4:75:GLU:OE1	2:4:148:ARG:NH2	2.47	0.42
17:4:303:XAT:H163	19:4:308:CLA:H2	2.02	0.42
4:2:205:PHE:HE1	17:2:303:XAT:H162	1.84	0.42
17:2:305:XAT:H11	17:2:305:XAT:H191	1.90	0.42
6:a:290:HIS:O	6:a:294:ILE:HG12	2.20	0.42
6:a:601:PHE:CZ	19:a:801:CLA:HED3	2.55	0.42
6:a:684:ARG:NH1	6:a:711:ALA:O	2.52	0.42
6:a:692:GLU:CD	7:b:547:LYS:HB2	2.44	0.42
19:a:806:CLA:H202	19:a:806:CLA:H161	1.70	0.42
19:a:840:CLA:H72	26:a:850:BCR:H373	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:192:LEU:HA	7:b:192:LEU:HD23	1.83	0.42
7:b:597:HIS:CE1	7:b:727:VAL:HG23	2.54	0.42
19:b:802:CLA:HMA1	19:b:803:CLA:H161	2.02	0.42
19:1:306:CLA:H3A	19:1:306:CLA:O2A	2.20	0.41
6:a:491:THR:OG1	19:a:836:CLA:OBD	2.32	0.41
6:a:525:ASP:HA	6:a:528:VAL:HG12	2.01	0.41
19:a:816:CLA:C4B	17:a:852:XAT:H242	2.50	0.41
19:a:840:CLA:H112	19:a:840:CLA:H152	1.80	0.41
7:b:197:ILE:HB	7:b:198:PRO:HD3	2.02	0.41
7:b:585:MET:O	7:b:589:ILE:HG12	2.20	0.41
19:b:828:CLA:H13	19:b:830:CLA:H141	2.02	0.41
8:d:70:LEU:O	8:d:74:LEU:HG	2.19	0.41
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.41
17:5:301:XAT:H31	17:5:301:XAT:H391	1.88	0.41
6:a:67:PHE:HE2	6:a:173:HIS:CG	2.38	0.41
6:a:399:ALA:HB1	6:a:543:LEU:HB3	2.02	0.41
6:a:427:ARG:NH2	8:d:46:THR:O	2.53	0.41
19:a:805:CLA:H61	19:a:805:CLA:H41	1.91	0.41
19:a:834:CLA:H142	26:b:848:BCR:H17C	2.01	0.41
7:b:430:PHE:O	7:b:434:HIS:ND1	2.40	0.41
19:b:801:CLA:H141	19:b:801:CLA:H161	1.63	0.41
13:l:75:LEU:HD23	13:l:75:LEU:HA	1.89	0.41
4:2:109:TRP:CE3	17:2:303:XAT:H22	2.54	0.41
4:2:203:LEU:HD13	17:2:301:XAT:C10	2.50	0.41
5:1:162:TYR:CE2	19:a:844:CLA:HBD	2.56	0.41
6:a:293:ALA:HB1	19:a:818:CLA:HBC2	2.02	0.41
19:a:826:CLA:HMD2	19:a:826:CLA:H143	2.03	0.41
19:a:839:CLA:H141	19:a:839:CLA:H161	1.68	0.41
7:b:471:LYS:HB2	7:b:471:LYS:HE2	1.89	0.41
19:b:836:CLA:HBB1	19:b:836:CLA:HMB1	2.02	0.41
10:f:114:PHE:HB2	26:f:801:BCR:C32	2.49	0.41
17:5:302:XAT:H15	17:5:302:XAT:H201	1.74	0.41
5:1:54:PRO:HD2	17:1:303:XAT:H242	2.02	0.41
19:1:311:CLA:H72	13:l:21:ILE:HG12	2.02	0.41
7:b:193:VAL:O	7:b:198:PRO:HD3	2.20	0.41
7:b:314:GLY:HA3	7:b:412:ARG:HD2	2.02	0.41
7:b:702:LEU:HD22	7:b:706:GLN:NE2	2.35	0.41
19:4:307:CLA:HBD	19:4:314:CLA:OBD	2.20	0.41
17:3:303:XAT:H15	17:3:303:XAT:H201	1.79	0.41
17:2:301:XAT:H31	17:2:301:XAT:H391	1.72	0.41
5:1:147:GLY:HA2	5:1:149:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:310:CLA:H41	19:1:310:CLA:H62	1.80	0.41
6:a:194:HIS:ND1	19:a:826:CLA:OBD	2.48	0.41
6:a:357:SER:HB2	19:a:830:CLA:HMC2	2.01	0.41
26:a:847:BCR:H24C	26:a:847:BCR:H371	1.92	0.41
19:b:801:CLA:H51	19:b:839:CLA:H102	2.01	0.41
17:3:301:XAT:H201	17:3:301:XAT:H15	1.79	0.41
19:a:834:CLA:H143	19:a:834:CLA:H161	1.93	0.41
7:b:342:ALA:HB2	19:b:825:CLA:H43	2.02	0.41
19:b:809:CLA:C4A	19:b:809:CLA:HBA2	2.50	0.41
19:b:825:CLA:H52	19:b:825:CLA:H12	1.85	0.41
26:l:205:BCR:H15C	26:l:205:BCR:H351	1.74	0.41
1:5:149:VAL:HG22	17:5:304:XAT:H182	2.02	0.41
4:2:57:PHE:CZ	17:2:305:XAT:H172	2.55	0.41
6:a:232:LEU:HD23	6:a:232:LEU:HA	1.92	0.41
6:a:356:LEU:HB2	19:a:828:CLA:H41	2.02	0.41
6:a:434:LEU:HG	6:a:541:LEU:HB2	2.03	0.41
6:a:651:VAL:O	6:a:654:SER:OG	2.29	0.41
19:a:841:CLA:HAA2	19:b:832:CLA:HMB1	2.02	0.41
24:a:843:PQN:H211	24:a:843:PQN:H252	1.82	0.41
7:b:181:PHE:CE2	19:b:820:CLA:HAB	2.56	0.41
10:f:114:PHE:HB2	26:f:801:BCR:H321	2.02	0.41
17:4:303:XAT:H11	17:4:303:XAT:H191	1.74	0.41
19:a:806:CLA:H52	26:a:848:BCR:HC8	2.03	0.41
19:a:818:CLA:OBD	19:a:837:CLA:HED2	2.21	0.41
19:a:820:CLA:H3A	19:a:820:CLA:HBA2	1.48	0.41
19:a:828:CLA:H2	19:a:828:CLA:H61	1.78	0.41
7:b:433:PHE:CZ	26:f:801:BCR:H372	2.56	0.41
11:i:3:LEU:HD23	11:i:3:LEU:HA	1.92	0.41
17:4:305:XAT:H363	17:3:301:XAT:C10	2.49	0.41
17:2:304:XAT:H31	17:2:304:XAT:H391	1.85	0.41
5:1:71:GLU:HG2	5:1:142:PRO:O	2.20	0.41
5:1:87:TRP:CG	5:1:180:LEU:HD13	2.56	0.41
19:1:310:CLA:H111	19:1:310:CLA:H71	1.89	0.41
6:a:226:SER:OG	6:a:229:GLU:HG2	2.21	0.41
6:a:499:VAL:HG12	19:a:819:CLA:H11	2.03	0.41
6:a:675:PHE:HZ	19:a:842:CLA:HBC2	1.86	0.41
7:b:346:THR:HG21	19:b:829:CLA:HHD	2.03	0.41
7:b:547:LYS:HE2	10:f:180:ILE:HD11	2.03	0.41
7:b:585:MET:HE3	7:b:585:MET:HB3	1.83	0.41
19:b:802:CLA:H122	19:b:802:CLA:H162	1.60	0.41
19:b:804:CLA:HBC2	19:b:804:CLA:HHD	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:813:CLA:H3A	19:b:813:CLA:HBA2	1.61	0.41
19:b:827:CLA:HMB2	19:b:834:CLA:HBA1	2.03	0.41
26:b:845:BCR:H15C	26:b:845:BCR:H351	1.78	0.41
9:e:51:ASN:ND2	16:c:61:ASP:HB2	2.35	0.41
11:i:29:TYR:HE1	14:m:30:ASN:HD21	1.67	0.41
17:1:302:XAT:H11	17:1:302:XAT:H191	1.86	0.41
6:a:318:ILE:O	6:a:322:HIS:ND1	2.54	0.41
6:a:342:TRP:HB3	19:a:806:CLA:HAC1	2.02	0.41
7:b:499:TRP:CD1	19:b:834:CLA:HED2	2.57	0.41
7:b:629:ASN:HA	7:b:734:LYS:HE2	2.02	0.41
19:b:822:CLA:H12	19:b:823:CLA:H52	2.03	0.41
8:d:107:VAL:HG21	16:c:38:GLN:HB3	2.01	0.41
4:2:92:ARG:NH2	19:2:308:CLA:HED3	2.36	0.40
6:a:452:ASN:HB3	6:a:635:THR:HG22	2.04	0.40
6:a:529:HIS:CG	19:a:839:CLA:HED2	2.56	0.40
7:b:523:HIS:CE1	26:b:852:BCR:H322	2.56	0.40
7:b:614:SER:O	7:b:620:GLY:HA3	2.21	0.40
26:j:104:BCR:H20C	26:j:104:BCR:H361	1.91	0.40
13:l:56:TYR:CD2	13:l:161:ALA:HB2	2.56	0.40
14:m:22:ILE:HD12	25:m:101:LHG:H312	2.02	0.40
17:4:303:XAT:H383	19:4:310:CLA:C2B	2.51	0.40
19:3:312:CLA:H11	19:3:312:CLA:H51	1.89	0.40
6:a:673:TRP:O	6:a:676:SER:OG	2.32	0.40
26:a:847:BCR:H20C	26:a:847:BCR:H361	1.80	0.40
7:b:401:ASN:HB3	7:b:408:ASN:OD1	2.22	0.40
7:b:431:LEU:HD11	19:b:837:CLA:HMB1	2.03	0.40
19:b:815:CLA:CHA	19:b:815:CLA:HBA1	2.49	0.40
19:b:840:CLA:H111	19:b:840:CLA:H152	1.87	0.40
26:b:852:BCR:H11C	26:b:852:BCR:H341	1.73	0.40
26:i:101:BCR:H11C	26:i:101:BCR:H341	1.86	0.40
26:l:205:BCR:H20C	26:l:205:BCR:H361	1.91	0.40
17:4:301:XAT:H35	17:4:301:XAT:H401	1.66	0.40
17:4:302:XAT:H35	17:4:302:XAT:H401	1.76	0.40
19:4:307:CLA:H41	19:4:307:CLA:H61	1.86	0.40
3:3:106:VAL:HG11	19:3:311:CLA:HED1	2.03	0.40
3:3:205:LEU:HD12	3:3:205:LEU:HA	1.86	0.40
6:a:299:ILE:O	6:a:303:HIS:ND1	2.53	0.40
19:a:820:CLA:H122	19:a:820:CLA:H161	1.83	0.40
19:a:828:CLA:H152	19:a:840:CLA:H191	2.03	0.40
19:a:829:CLA:O1D	19:a:830:CLA:HMA1	2.21	0.40
26:a:847:BCR:H15C	26:a:847:BCR:H351	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:850:BCR:H361	26:b:850:BCR:H20C	1.88	0.40
8:d:89:PRO:HB2	8:d:90:PRO:HD3	2.03	0.40
19:i:102:CLA:H41	19:i:102:CLA:H62	1.88	0.40
19:5:308:CLA:CBB	19:5:315:CLA:HAB	2.51	0.40
17:4:304:XAT:H30	19:4:313:CLA:H71	2.02	0.40
19:4:317:CLA:HMB3	17:3:301:XAT:H392	2.03	0.40
6:a:226:SER:HG	6:a:229:GLU:HG2	1.86	0.40
19:a:825:CLA:H62	19:a:825:CLA:H41	1.84	0.40
7:b:339:LEU:HD11	19:b:806:CLA:H51	2.04	0.40
10:f:147:VAL:HG22	12:j:14:LEU:HD11	2.04	0.40
13:l:54:HIS:O	13:l:58:LEU:HB2	2.22	0.40
1:5:98:PHE:CD2	19:5:305:CLA:HMD2	2.56	0.40
5:1:134:ILE:HD11	13:l:26:PHE:HA	2.03	0.40
19:a:828:CLA:H122	19:a:828:CLA:H162	1.66	0.40
7:b:461:PHE:HB2	19:b:837:CLA:CAD	2.52	0.40
7:b:550:PRO:HD2	16:c:62:PHE:CE1	2.57	0.40
19:b:834:CLA:H61	19:b:834:CLA:H102	1.98	0.40
13:l:4:PHE:HB3	13:l:20:PRO:HG3	2.03	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	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	21	48
3	3	175/220 (80%)	166 (95%)	9 (5%)	0	100	100
4	2	183/223 (82%)	155 (85%)	25 (14%)	3 (2%)	7	24
5	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
6	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
8	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
9	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
10	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
11	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
12	j	39/41 (95%)	39 (100%)	0	0	100	100
13	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	10	31
14	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	3012/3336 (90%)	2834 (94%)	171 (6%)	7 (0%)	44	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	45	LYS
13	1	120	VAL
4	2	127	ASN
4	2	213	VAL
6	a	580	SER
13	1	131	ILE
2	4	146	SER

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	4	133/159 (84%)	133 (100%)	0	100	100
3	3	136/164 (83%)	136 (100%)	0	100	100
4	2	134/172 (78%)	134 (100%)	0	100	100
5	1	128/165 (78%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	a	607/613 (99%)	603 (99%)	4 (1%)	76	90
7	b	599/602 (100%)	599 (100%)	0	100	100
8	d	107/113 (95%)	107 (100%)	0	100	100
9	e	56/62 (90%)	56 (100%)	0	100	100
10	f	138/162 (85%)	138 (100%)	0	100	100
11	i	32/43 (74%)	32 (100%)	0	100	100
12	j	36/36 (100%)	36 (100%)	0	100	100
13	l	130/141 (92%)	130 (100%)	0	100	100
14	m	21/24 (88%)	21 (100%)	0	100	100
16	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2457/2706 (91%)	2453 (100%)	4 (0%)	85	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	a	428	ASP
6	a	448	LEU
6	a	579	VAL
6	a	580	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	133	GLN
3	3	156	GLN
3	3	169	ASN
3	3	211	HIS
5	1	63	GLN
5	1	119	GLN
5	1	132	ASN
5	1	194	GLN
6	a	127	ASN
6	a	186	ASN
6	a	435	ASN
7	b	80	ASN
7	b	112	ASN
7	b	169	ASN

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Mol	Chain	Res	Type
7	b	234	ASN
7	b	326	ASN
7	b	605	GLN
7	b	629	ASN
8	d	7	GLN
10	f	166	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

207 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	$\# Z > 2$
19	CLA	1	311	-	57,61,73	1.28	7 (12%)	67,98,113	1.35	6 (8%)
19	CLA	j	102	-	62,66,73	1.23	8 (12%)	73,104,113	1.30	5 (6%)
19	CLA	b	837	-	69,73,73	1.16	6 (8%)	82,113,113	1.29	6 (7%)
19	CLA	b	832	-	53,57,73	1.32	6 (11%)	61,93,113	1.38	5 (8%)
26	BCR	b	852	-	41,41,41	0.71	0	56,56,56	2.06	13 (23%)
21	DGD	4	318	-	41,41,67	1.07	2 (4%)	55,55,81	1.79	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	b	813	-	57,61,73	1.30	8 (14%)	67,98,113	1.36	5 (7%)
19	CLA	1	310	5	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
26	BCR	f	801	-	41,41,41	0.65	0	56,56,56	2.16	15 (26%)
18	A1L1G	3	302	-	40,47,47	1.17	5 (12%)	49,71,71	1.32	7 (14%)
19	CLA	a	805	19	59,63,73	1.26	6 (10%)	70,101,113	1.35	6 (8%)
26	BCR	i	101	-	41,41,41	0.72	0	56,56,56	2.15	13 (23%)
19	CLA	2	312	-	51,55,73	1.35	8 (15%)	60,91,113	1.40	5 (8%)
19	CLA	a	804	-	59,63,73	1.28	8 (13%)	70,101,113	1.40	8 (11%)
19	CLA	a	811	-	60,64,73	1.25	7 (11%)	71,102,113	1.34	6 (8%)
19	CLA	2	311	-	62,66,73	1.24	6 (9%)	73,104,113	1.29	5 (6%)
19	CLA	b	809	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
17	XAT	j	101	-	41,47,47	0.86	2 (4%)	54,74,74	2.74	18 (33%)
19	CLA	1	306	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	7 (8%)
27	SF4	a	851	-	0,12,12	-	-	-	-	-
19	CLA	a	809	6	69,73,73	1.16	7 (10%)	82,113,113	1.29	8 (9%)
26	BCR	b	844	-	41,41,41	0.68	0	56,56,56	1.93	16 (28%)
19	CLA	4	308	-	69,73,73	1.16	7 (10%)	82,113,113	1.22	7 (8%)
20	SQD	5	316	19	33,35,54	1.39	3 (9%)	43,46,65	1.31	5 (11%)
19	CLA	4	313	-	57,61,73	1.29	7 (12%)	67,98,113	1.31	7 (10%)
19	CLA	a	802	-	62,66,73	1.22	8 (12%)	73,104,113	1.35	7 (9%)
26	BCR	b	847	-	41,41,41	0.65	0	56,56,56	2.22	22 (39%)
19	CLA	a	815	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
19	CLA	a	814	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
19	CLA	2	307	-	51,55,73	1.35	8 (15%)	60,91,113	1.45	8 (13%)
19	CLA	b	817	-	59,63,73	1.26	7 (11%)	70,101,113	1.32	6 (8%)
19	CLA	1	308	5	69,73,73	1.17	5 (7%)	82,113,113	1.30	6 (7%)
19	CLA	a	824	-	50,54,73	1.38	8 (16%)	59,90,113	1.35	4 (6%)
19	CLA	b	816	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
19	CLA	b	818	-	63,67,73	1.23	8 (12%)	74,105,113	1.36	9 (12%)
19	CLA	b	840	-	69,73,73	1.18	7 (10%)	82,113,113	1.31	6 (7%)
19	CLA	b	819	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	5 (6%)
19	CLA	b	826	-	68,72,73	1.18	8 (11%)	80,111,113	1.30	8 (10%)
23	A1L1F	1	304	-	52,59,59	1.41	6 (11%)	63,85,85	2.26	18 (28%)
17	XAT	2	304	-	41,47,47	0.88	2 (4%)	54,74,74	2.55	20 (37%)
19	CLA	a	827	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	XAT	2	305	-	41,47,47	0.95	2 (4%)	54,74,74	2.43	18 (33%)
19	CLA	a	831	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
17	XAT	2	301	-	41,47,47	0.91	2 (4%)	54,74,74	2.73	18 (33%)
19	CLA	b	802	-	69,73,73	1.17	6 (8%)	82,113,113	1.17	5 (6%)
19	CLA	b	836	-	62,66,73	1.24	7 (11%)	73,104,113	1.37	8 (10%)
19	CLA	2	306	-	45,50,73	1.42	7 (15%)	52,85,113	1.39	4 (7%)
19	CLA	a	833	-	59,63,73	1.25	7 (11%)	70,101,113	1.39	8 (11%)
19	CLA	a	839	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	6 (7%)
19	CLA	a	841	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
27	SF4	c	102	-	0,12,12	-	-	-	-	-
26	BCR	b	845	-	41,41,41	0.66	0	56,56,56	2.10	17 (30%)
19	CLA	5	307	1	64,68,73	1.21	8 (12%)	76,107,113	1.27	6 (7%)
26	BCR	m	102	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	6 (10%)
19	CLA	a	825	-	59,63,73	1.27	6 (10%)	70,101,113	1.33	5 (7%)
19	CLA	1	204	-	50,54,73	1.37	9 (18%)	59,90,113	1.41	4 (6%)
19	CLA	2	309	-	50,54,73	1.37	8 (16%)	59,90,113	1.40	4 (6%)
19	CLA	1	309	5	50,54,73	1.37	8 (16%)	59,90,113	1.35	4 (6%)
19	CLA	b	835	-	57,61,73	1.31	8 (14%)	67,98,113	1.36	6 (8%)
19	CLA	5	314	-	56,60,73	1.30	6 (10%)	65,97,113	1.40	5 (7%)
17	XAT	5	301	-	41,47,47	0.93	2 (4%)	54,74,74	2.60	19 (35%)
18	A1L1G	5	303	-	40,47,47	1.16	4 (10%)	49,71,71	1.37	7 (14%)
19	CLA	a	818	-	60,64,73	1.26	7 (11%)	71,102,113	1.31	7 (9%)
19	CLA	5	309	1	69,73,73	1.18	6 (8%)	82,113,113	1.25	4 (4%)
19	CLA	a	826	-	69,73,73	1.18	7 (10%)	82,113,113	1.31	7 (8%)
19	CLA	3	315	3	50,54,73	1.38	8 (16%)	59,90,113	1.37	4 (6%)
19	CLA	4	314	2	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
17	XAT	3	301	-	41,47,47	0.91	2 (4%)	54,74,74	2.56	19 (35%)
19	CLA	a	808	-	55,59,73	1.32	8 (14%)	64,96,113	1.38	5 (7%)
19	CLA	b	829	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	5 (6%)
25	LHG	b	849	19	30,30,48	1.39	6 (20%)	33,36,54	1.16	2 (6%)
19	CLA	b	825	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
19	CLA	a	806	-	69,73,73	1.21	9 (13%)	82,113,113	1.56	12 (14%)
19	CLA	b	828	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
19	CLA	i	102	-	66,70,73	1.21	8 (12%)	78,109,113	1.27	6 (7%)
17	XAT	3	304	-	41,47,47	0.93	2 (4%)	54,74,74	2.63	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	5	312	-	56,60,73	1.30	7 (12%)	65,97,113	1.39	6 (9%)
17	XAT	4	301	-	41,47,47	0.95	2 (4%)	54,74,74	2.63	19 (35%)
19	CLA	3	311	-	54,58,73	1.33	8 (14%)	64,95,113	1.38	6 (9%)
19	CLA	a	830	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
19	CLA	b	801	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
26	BCR	l	205	-	41,41,41	0.65	0	56,56,56	2.05	15 (26%)
17	XAT	a	852	-	41,47,47	0.91	2 (4%)	54,74,74	2.71	18 (33%)
22	LMG	2	317	-	35,35,55	1.10	2 (5%)	43,43,63	1.31	4 (9%)
19	CLA	2	310	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
24	PQN	a	843	-	34,34,34	1.62	2 (5%)	43,45,45	1.15	4 (9%)
27	SF4	c	101	-	0,12,12	-	-	-	-	-
19	CLA	a	812	19	66,70,73	1.20	7 (10%)	78,109,113	1.31	5 (6%)
19	CLA	b	808	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
19	CLA	f	803	10	56,60,73	1.30	7 (12%)	65,97,113	1.37	5 (7%)
26	BCR	b	850	-	41,41,41	0.67	0	56,56,56	1.90	17 (30%)
19	CLA	b	833	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
17	XAT	3	305	-	41,47,47	0.89	2 (4%)	54,74,74	2.58	17 (31%)
19	CLA	b	827	-	69,73,73	1.17	7 (10%)	82,113,113	1.23	5 (6%)
19	CLA	f	802	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
17	XAT	5	302	-	41,47,47	0.95	2 (4%)	54,74,74	2.59	19 (35%)
19	CLA	a	810	6	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
25	LHG	m	101	-	45,45,48	1.19	6 (13%)	48,51,54	0.96	2 (4%)
19	CLA	j	103	12	46,50,73	1.40	7 (15%)	53,85,113	1.48	4 (7%)
26	BCR	b	843	-	41,41,41	0.64	0	56,56,56	2.31	21 (37%)
19	CLA	a	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.28	5 (6%)
19	CLA	a	817	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
19	CLA	a	820	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
19	CLA	a	838	-	55,59,73	1.30	8 (14%)	64,96,113	1.41	6 (9%)
19	CLA	4	315	2	45,49,73	1.43	8 (17%)	54,84,113	1.49	5 (9%)
19	CLA	a	840	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	5 (6%)
18	A1L1G	3	306	-	40,47,47	1.18	4 (10%)	49,71,71	1.40	8 (16%)
22	LMG	j	105	-	32,32,55	1.14	2 (6%)	40,40,63	1.16	4 (10%)
18	A1L1G	1	301	-	40,47,47	1.14	5 (12%)	49,71,71	1.46	10 (20%)
19	CLA	4	309	-	54,58,73	1.31	6 (11%)	64,95,113	1.40	5 (7%)
19	CLA	1	305	-	65,69,73	1.22	8 (12%)	77,108,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	b	812	-	58,62,73	1.35	9 (15%)	71,100,113	1.34	9 (12%)
17	XAT	2	303	-	41,47,47	1.01	2 (4%)	54,74,74	2.63	17 (31%)
19	CLA	b	821	-	54,58,73	1.31	7 (12%)	64,95,113	1.43	7 (10%)
19	CLA	b	841	25	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
19	CLA	2	314	-	60,64,73	1.27	8 (13%)	71,102,113	1.31	4 (5%)
19	CLA	b	815	-	59,63,73	1.26	6 (10%)	70,101,113	1.40	8 (11%)
25	LHG	a	846	19	26,26,48	1.30	5 (19%)	29,32,54	1.18	2 (6%)
19	CLA	a	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
19	CLA	b	823	-	64,68,73	1.21	7 (10%)	76,107,113	1.25	5 (6%)
19	CLA	b	839	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
19	CLA	b	804	-	69,73,73	1.14	7 (10%)	82,113,113	1.43	8 (9%)
19	CLA	b	811	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	7 (8%)
17	XAT	4	303	-	41,47,47	0.92	2 (4%)	54,74,74	2.58	17 (31%)
19	CLA	b	830	-	69,73,73	1.20	8 (11%)	82,113,113	1.30	9 (10%)
19	CLA	4	316	-	50,54,73	1.36	5 (10%)	59,90,113	1.43	4 (6%)
19	CLA	b	831	-	45,49,73	1.41	8 (17%)	54,84,113	1.47	6 (11%)
19	CLA	a	803	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
26	BCR	b	846	-	41,41,41	0.67	0	56,56,56	1.99	21 (37%)
19	CLA	3	312	3	63,67,73	1.23	7 (11%)	74,105,113	1.29	4 (5%)
17	XAT	1	303	-	41,47,47	0.90	2 (4%)	54,74,74	2.53	19 (35%)
19	CLA	2	316	4	50,54,73	1.37	9 (18%)	59,90,113	1.41	4 (6%)
19	CLA	1	312	5	56,60,73	1.33	7 (12%)	65,97,113	1.35	5 (7%)
19	CLA	a	842	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
19	CLA	b	810	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)
19	CLA	5	306	20	49,53,73	1.39	6 (12%)	58,89,113	1.42	4 (6%)
19	CLA	2	315	-	46,50,73	1.41	7 (15%)	53,85,113	1.38	4 (7%)
17	XAT	3	303	-	41,47,47	0.89	2 (4%)	54,74,74	2.60	20 (37%)
19	CLA	4	312	-	50,54,73	1.37	8 (16%)	59,90,113	1.37	4 (6%)
17	XAT	4	305	-	41,47,47	0.92	2 (4%)	54,74,74	2.75	18 (33%)
19	CLA	5	310	-	50,54,73	1.36	7 (14%)	59,90,113	1.40	4 (6%)
19	CLA	a	819	-	58,62,73	1.27	8 (13%)	68,99,113	1.34	5 (7%)
19	CLA	1	313	-	45,49,73	1.41	8 (17%)	54,84,113	1.47	5 (9%)
25	LHG	a	845	-	47,47,48	1.16	6 (12%)	50,53,54	0.99	2 (4%)
19	CLA	5	311	-	55,59,73	1.31	8 (14%)	64,96,113	1.37	7 (10%)
19	CLA	5	313	1	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	XAT	4	304	-	41,47,47	0.91	2 (4%)	54,74,74	2.57	19 (35%)
19	CLA	4	307	-	60,64,73	1.27	6 (10%)	71,102,113	1.32	6 (8%)
19	CLA	3	313	-	56,60,73	1.31	8 (14%)	65,97,113	1.38	6 (9%)
20	SQD	1	315	-	43,45,54	1.22	3 (6%)	53,56,65	1.13	2 (3%)
26	BCR	l	201	-	41,41,41	0.67	0	56,56,56	1.98	17 (30%)
19	CLA	a	816	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	7 (10%)
19	CLA	l	203	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	5 (6%)
19	CLA	a	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
19	CLA	b	822	-	55,59,73	1.31	7 (12%)	64,96,113	1.42	7 (10%)
19	CLA	1	307	-	58,62,73	1.28	8 (13%)	68,99,113	1.36	6 (8%)
26	BCR	a	847	-	41,41,41	0.68	0	56,56,56	1.95	16 (28%)
19	CLA	a	821	-	49,53,73	1.38	7 (14%)	58,89,113	1.45	4 (6%)
19	CLA	a	832	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	6 (9%)
26	BCR	f	804	-	41,41,41	0.69	0	56,56,56	2.06	14 (25%)
19	CLA	4	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.42	5 (8%)
19	CLA	3	310	-	60,64,73	1.26	7 (11%)	71,102,113	1.29	6 (8%)
26	BCR	a	848	-	41,41,41	0.68	0	56,56,56	1.95	18 (32%)
19	CLA	2	308	4	58,62,73	1.28	7 (12%)	68,99,113	1.28	6 (8%)
19	CLA	a	835	-	69,73,73	1.16	6 (8%)	82,113,113	1.31	6 (7%)
19	CLA	b	806	-	69,73,73	1.16	6 (8%)	82,113,113	1.30	6 (7%)
17	XAT	1	302	-	41,47,47	0.91	2 (4%)	54,74,74	2.61	18 (33%)
19	CLA	3	307	3	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
19	CLA	b	824	-	57,61,73	1.28	8 (14%)	67,98,113	1.35	6 (8%)
21	DGD	b	851	-	58,58,67	1.13	4 (6%)	72,72,81	1.50	10 (13%)
19	CLA	b	807	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	7 (8%)
19	CLA	2	313	4	45,49,73	1.43	6 (13%)	54,84,113	1.50	5 (9%)
22	LMG	a	853	-	34,34,55	1.15	2 (5%)	42,42,63	1.17	3 (7%)
24	PQN	b	842	-	34,34,34	1.59	2 (5%)	43,45,45	1.24	5 (11%)
19	CLA	4	310	-	69,73,73	1.18	7 (10%)	82,113,113	1.30	5 (6%)
26	BCR	j	104	-	41,41,41	0.68	0	56,56,56	2.09	17 (30%)
19	CLA	b	814	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
19	CLA	a	844	25	69,73,73	1.17	7 (10%)	82,113,113	1.27	8 (9%)
19	CLA	b	834	-	69,73,73	1.18	6 (8%)	82,113,113	1.24	4 (4%)
19	CLA	a	834	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
26	BCR	b	848	-	41,41,41	0.69	0	56,56,56	1.81	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	a	836	-	54,58,73	1.32	6 (11%)	64,95,113	1.38	6 (9%)
19	CLA	b	803	-	69,73,73	1.16	7 (10%)	82,113,113	1.25	7 (8%)
19	CLA	1	314	-	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
19	CLA	4	317	-	59,63,73	1.28	8 (13%)	70,101,113	1.34	5 (7%)
19	CLA	a	801	-	69,73,73	1.18	9 (13%)	82,113,113	1.28	5 (6%)
26	BCR	a	849	-	41,41,41	0.67	0	56,56,56	2.19	22 (39%)
19	CLA	a	837	6	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
19	CLA	b	805	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
19	CLA	5	305	1	50,54,73	1.38	7 (14%)	59,90,113	1.39	4 (6%)
19	CLA	b	820	-	59,63,73	1.26	8 (13%)	70,101,113	1.32	6 (8%)
19	CLA	a	813	-	58,62,73	1.28	6 (10%)	68,99,113	1.31	5 (7%)
19	CLA	4	306	2	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
19	CLA	a	823	-	53,57,73	1.31	7 (13%)	61,93,113	1.43	6 (9%)
17	XAT	4	302	-	41,47,47	0.89	2 (4%)	54,74,74	2.59	19 (35%)
19	CLA	1	202	-	46,50,73	1.41	8 (17%)	53,85,113	1.44	4 (7%)
19	CLA	a	829	-	66,70,73	1.19	7 (10%)	78,109,113	1.24	7 (8%)
26	BCR	a	850	-	41,41,41	0.69	0	56,56,56	2.17	14 (25%)
19	CLA	3	308	-	51,55,73	1.36	7 (13%)	60,91,113	1.41	6 (10%)
19	CLA	3	314	3	51,55,73	1.36	9 (17%)	60,91,113	1.41	4 (6%)
19	CLA	b	838	-	69,73,73	1.18	7 (10%)	82,113,113	1.22	6 (7%)
17	XAT	5	304	-	41,47,47	0.86	2 (4%)	54,74,74	2.85	20 (37%)
19	CLA	3	309	3	60,64,73	1.25	7 (11%)	71,102,113	1.30	5 (7%)
19	CLA	5	315	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
19	CLA	a	854	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
17	XAT	2	302	-	41,47,47	0.94	2 (4%)	54,74,74	2.52	18 (33%)
19	CLA	5	308	-	59,63,73	1.27	7 (11%)	70,101,113	1.34	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	311	-	1/1/12/20	4/25/101/115	-
19	CLA	j	102	-	1/1/13/20	18/31/107/115	-
19	CLA	b	837	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	832	-	1/1/11/20	5/20/96/115	-
26	BCR	b	852	-	-	4/29/63/63	0/2/2/2
21	DGD	4	318	-	-	10/29/69/95	0/2/2/2
19	CLA	b	813	-	1/1/12/20	5/25/101/115	-
19	CLA	1	310	5	1/1/15/20	17/39/115/115	-
26	BCR	f	801	-	-	3/29/63/63	0/2/2/2
18	A1L1G	3	302	-	-	17/29/85/85	0/3/3/3
19	CLA	a	805	19	1/1/13/20	6/27/103/115	-
26	BCR	i	101	-	-	3/29/63/63	0/2/2/2
19	CLA	2	312	-	1/1/11/20	4/18/94/115	-
19	CLA	a	804	-	1/1/13/20	9/27/103/115	-
19	CLA	a	811	-	1/1/13/20	6/29/105/115	-
19	CLA	2	311	-	1/1/13/20	5/31/107/115	-
19	CLA	b	809	-	1/1/15/20	13/39/115/115	-
17	XAT	j	101	-	-	5/31/93/93	0/4/4/4
19	CLA	1	306	-	1/1/15/20	15/39/115/115	-
27	SF4	a	851	-	-	-	0/6/5/5
19	CLA	a	809	6	1/1/15/20	15/39/115/115	-
26	BCR	b	844	-	-	2/29/63/63	0/2/2/2
19	CLA	4	308	-	1/1/15/20	13/39/115/115	-
20	SQD	5	316	19	-	11/30/50/69	0/1/1/1
19	CLA	4	313	-	1/1/12/20	4/25/101/115	-
19	CLA	a	802	-	1/1/13/20	5/31/107/115	-
26	BCR	b	847	-	-	0/29/63/63	0/2/2/2
19	CLA	a	815	-	1/1/11/20	0/15/91/115	-
19	CLA	a	814	-	1/1/15/20	19/39/115/115	-
19	CLA	2	307	-	1/1/11/20	7/18/94/115	-
19	CLA	b	817	-	1/1/13/20	3/27/103/115	-
19	CLA	1	308	5	1/1/15/20	13/39/115/115	-
19	CLA	a	824	-	1/1/11/20	5/17/93/115	-
19	CLA	b	816	-	1/1/11/20	3/15/91/115	-
19	CLA	b	818	-	1/1/13/20	11/32/108/115	-
19	CLA	b	840	-	1/1/15/20	15/39/115/115	-
19	CLA	b	819	-	1/1/14/20	15/33/109/115	-
19	CLA	b	826	-	1/1/14/20	4/38/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
17	XAT	2	304	-	-	3/31/93/93	0/4/4/4
19	CLA	a	827	-	1/1/15/20	6/39/115/115	-
19	CLA	a	831	-	1/1/15/20	11/39/115/115	-
17	XAT	2	305	-	-	2/31/93/93	0/4/4/4
17	XAT	2	301	-	-	3/31/93/93	0/4/4/4
19	CLA	b	802	-	1/1/15/20	15/39/115/115	-
19	CLA	b	836	-	1/1/13/20	10/31/107/115	-
19	CLA	2	306	-	1/1/10/20	4/11/87/115	-
19	CLA	a	833	-	1/1/13/20	2/27/103/115	-
19	CLA	a	839	-	1/1/15/20	14/39/115/115	-
19	CLA	a	841	-	1/1/15/20	15/39/115/115	-
27	SF4	c	102	-	-	-	0/6/5/5
26	BCR	b	845	-	-	6/29/63/63	0/2/2/2
19	CLA	5	307	1	1/1/14/20	5/33/109/115	-
26	BCR	m	102	-	-	8/29/63/63	0/2/2/2
19	CLA	a	825	-	1/1/13/20	8/27/103/115	-
19	CLA	1	204	-	1/1/11/20	3/17/93/115	-
19	CLA	2	309	-	1/1/11/20	3/17/93/115	-
19	CLA	1	309	5	1/1/11/20	7/17/93/115	-
19	CLA	b	835	-	1/1/12/20	9/25/101/115	-
19	CLA	5	314	-	1/1/12/20	4/24/100/115	-
17	XAT	5	301	-	-	3/31/93/93	0/4/4/4
18	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
19	CLA	a	818	-	1/1/13/20	11/29/105/115	-
19	CLA	5	309	1	1/1/15/20	10/39/115/115	-
19	CLA	a	826	-	1/1/15/20	8/39/115/115	-
19	CLA	3	315	3	1/1/11/20	9/17/93/115	-
19	CLA	4	314	2	1/1/11/20	6/15/91/115	-
17	XAT	3	301	-	-	3/31/93/93	0/4/4/4
19	CLA	a	808	-	1/1/12/20	4/23/99/115	-
19	CLA	b	829	-	1/1/15/20	13/39/115/115	-
25	LHG	b	849	19	-	20/35/35/53	-
19	CLA	b	825	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	806	-	1/1/15/20	11/39/115/115	-
19	CLA	b	828	-	1/1/15/20	14/39/115/115	-
19	CLA	i	102	-	1/1/14/20	11/36/112/115	-
17	XAT	3	304	-	-	3/31/93/93	0/4/4/4
19	CLA	5	312	-	1/1/12/20	0/24/100/115	-
19	CLA	3	311	-	1/1/12/20	4/21/97/115	-
17	XAT	4	301	-	-	4/31/93/93	0/4/4/4
19	CLA	a	830	-	1/1/15/20	13/39/115/115	-
19	CLA	b	801	-	1/1/15/20	20/39/115/115	-
26	BCR	l	205	-	-	8/29/63/63	0/2/2/2
17	XAT	a	852	-	-	7/31/93/93	0/4/4/4
22	LMG	2	317	-	-	11/30/50/70	0/1/1/1
19	CLA	2	310	-	1/1/15/20	14/39/115/115	-
24	PQN	a	843	-	-	5/23/43/43	0/2/2/2
27	SF4	c	101	-	-	-	0/6/5/5
19	CLA	a	812	19	1/1/14/20	9/36/112/115	-
19	CLA	b	808	-	1/1/15/20	11/39/115/115	-
19	CLA	f	803	10	1/1/12/20	5/24/100/115	-
26	BCR	b	850	-	-	0/29/63/63	0/2/2/2
19	CLA	b	833	-	1/1/15/20	13/39/115/115	-
17	XAT	3	305	-	-	0/31/93/93	0/4/4/4
19	CLA	b	827	-	1/1/15/20	3/39/115/115	-
19	CLA	f	802	-	1/1/15/20	13/39/115/115	-
19	CLA	a	810	6	1/1/15/20	15/39/115/115	-
17	XAT	5	302	-	-	3/31/93/93	0/4/4/4
25	LHG	m	101	-	-	28/50/50/53	-
19	CLA	j	103	12	1/1/10/20	7/12/88/115	-
26	BCR	b	843	-	-	2/29/63/63	0/2/2/2
19	CLA	a	807	-	1/1/15/20	18/39/115/115	-
19	CLA	a	817	-	1/1/11/20	8/15/91/115	-
19	CLA	a	820	-	1/1/15/20	12/39/115/115	-
19	CLA	a	838	-	1/1/12/20	6/23/99/115	-
19	CLA	4	315	2	1/1/10/20	6/10/86/115	-
19	CLA	a	840	-	1/1/15/20	7/39/115/115	-
18	A1L1G	3	306	-	-	19/29/85/85	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMG	j	105	-	-	11/27/47/70	0/1/1/1
19	CLA	b	821	-	1/1/12/20	5/21/97/115	-
19	CLA	4	309	-	1/1/12/20	4/21/97/115	-
19	CLA	1	305	-	1/1/14/20	9/35/111/115	-
19	CLA	b	812	-	1/1/13/20	4/25/101/115	-
19	CLA	b	841	25	1/1/15/20	11/39/115/115	-
17	XAT	2	303	-	-	6/31/93/93	0/4/4/4
18	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
19	CLA	2	314	-	1/1/13/20	14/29/105/115	-
19	CLA	b	815	-	1/1/13/20	10/27/103/115	-
25	LHG	a	846	19	-	15/31/31/53	-
19	CLA	a	822	-	1/1/15/20	5/39/115/115	-
19	CLA	b	823	-	1/1/14/20	7/33/109/115	-
19	CLA	b	839	-	1/1/15/20	15/39/115/115	-
19	CLA	b	804	-	1/1/15/20	7/39/115/115	-
19	CLA	b	811	-	1/1/15/20	16/39/115/115	-
19	CLA	b	830	-	1/1/15/20	11/39/115/115	-
17	XAT	4	303	-	-	3/31/93/93	0/4/4/4
19	CLA	4	316	-	1/1/11/20	7/17/93/115	-
19	CLA	b	831	-	1/1/10/20	2/10/86/115	-
19	CLA	a	803	-	1/1/15/20	3/39/115/115	-
26	BCR	b	846	-	-	0/29/63/63	0/2/2/2
19	CLA	3	312	3	1/1/13/20	10/32/108/115	-
19	CLA	2	316	4	1/1/11/20	6/17/93/115	-
17	XAT	1	303	-	-	0/31/93/93	0/4/4/4
19	CLA	1	312	5	1/1/12/20	3/24/100/115	-
19	CLA	a	842	-	1/1/15/20	8/39/115/115	-
19	CLA	b	810	-	1/1/15/20	14/39/115/115	-
19	CLA	5	306	20	1/1/11/20	8/15/91/115	-
19	CLA	2	315	-	1/1/10/20	3/12/88/115	-
17	XAT	3	303	-	-	3/31/93/93	0/4/4/4
19	CLA	4	312	-	1/1/11/20	6/17/93/115	-
17	XAT	4	305	-	-	4/31/93/93	0/4/4/4
19	CLA	5	310	-	1/1/11/20	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	819	-	1/1/12/20	6/26/102/115	-
19	CLA	1	313	-	1/1/10/20	6/10/86/115	-
25	LHG	a	845	-	-	26/52/52/53	-
19	CLA	5	311	-	1/1/12/20	7/23/99/115	-
19	CLA	5	313	1	1/1/11/20	6/15/91/115	-
17	XAT	4	304	-	-	0/31/93/93	0/4/4/4
19	CLA	4	307	-	1/1/13/20	9/29/105/115	-
19	CLA	3	313	-	1/1/12/20	1/24/100/115	-
20	SQD	1	315	-	-	19/40/60/69	0/1/1/1
26	BCR	l	201	-	-	4/29/63/63	0/2/2/2
19	CLA	a	816	-	1/1/12/20	4/21/97/115	-
19	CLA	l	203	-	1/1/14/20	4/33/109/115	-
19	CLA	a	828	-	1/1/15/20	8/39/115/115	-
19	CLA	b	822	-	1/1/12/20	4/23/99/115	-
19	CLA	1	307	-	1/1/12/20	5/26/102/115	-
26	BCR	a	847	-	-	0/29/63/63	0/2/2/2
19	CLA	a	821	-	1/1/11/20	1/15/91/115	-
19	CLA	a	832	-	1/1/12/20	7/21/97/115	-
26	BCR	f	804	-	-	4/29/63/63	0/2/2/2
19	CLA	4	311	-	1/1/11/20	9/17/93/115	-
19	CLA	3	310	-	1/1/13/20	3/29/105/115	-
26	BCR	a	848	-	-	0/29/63/63	0/2/2/2
19	CLA	2	308	4	1/1/12/20	3/26/102/115	-
19	CLA	a	835	-	1/1/15/20	11/39/115/115	-
19	CLA	b	806	-	1/1/15/20	13/39/115/115	-
19	CLA	b	824	-	1/1/12/20	7/25/101/115	-
19	CLA	3	307	3	1/1/11/20	2/15/91/115	-
17	XAT	1	302	-	-	0/31/93/93	0/4/4/4
21	DGD	b	851	-	-	20/46/86/95	0/2/2/2
19	CLA	b	807	-	1/1/15/20	18/39/115/115	-
19	CLA	2	313	4	1/1/10/20	2/10/86/115	-
22	LMG	a	853	-	-	13/29/49/70	0/1/1/1
24	PQN	b	842	-	-	1/23/43/43	0/2/2/2
19	CLA	4	310	-	1/1/15/20	14/39/115/115	-
26	BCR	j	104	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	814	-	1/1/15/20	13/39/115/115	-
19	CLA	a	844	25	1/1/15/20	15/39/115/115	-
19	CLA	b	834	-	1/1/15/20	13/39/115/115	-
19	CLA	a	834	-	1/1/15/20	9/39/115/115	-
26	BCR	b	848	-	-	2/29/63/63	0/2/2/2
19	CLA	a	836	-	1/1/12/20	8/21/97/115	-
19	CLA	b	803	-	1/1/15/20	17/39/115/115	-
19	CLA	1	314	-	1/1/11/20	7/15/91/115	-
19	CLA	4	317	-	1/1/13/20	9/27/103/115	-
19	CLA	a	801	-	1/1/15/20	22/39/115/115	-
26	BCR	a	849	-	-	0/29/63/63	0/2/2/2
19	CLA	a	837	6	1/1/11/20	4/15/91/115	-
19	CLA	b	805	-	1/1/15/20	11/39/115/115	-
19	CLA	5	305	1	1/1/11/20	6/17/93/115	-
19	CLA	b	820	-	1/1/13/20	5/27/103/115	-
19	CLA	a	813	-	1/1/12/20	10/26/102/115	-
19	CLA	4	306	2	1/1/11/20	9/15/91/115	-
19	CLA	a	823	-	1/1/11/20	7/20/96/115	-
19	CLA	1	202	-	1/1/10/20	0/12/88/115	-
17	XAT	4	302	-	-	0/31/93/93	0/4/4/4
19	CLA	a	829	-	1/1/14/20	13/36/112/115	-
26	BCR	a	850	-	-	4/29/63/63	0/2/2/2
19	CLA	3	308	-	1/1/11/20	7/18/94/115	-
19	CLA	3	314	3	1/1/11/20	8/18/94/115	-
19	CLA	b	838	-	1/1/15/20	9/39/115/115	-
17	XAT	5	304	-	-	1/31/93/93	0/4/4/4
19	CLA	3	309	3	1/1/13/20	3/29/105/115	-
19	CLA	5	315	-	1/1/11/20	5/17/93/115	-
19	CLA	a	854	-	1/1/15/20	14/39/115/115	-
17	XAT	2	302	-	-	0/31/93/93	0/4/4/4
19	CLA	5	308	-	1/1/13/20	6/27/103/115	-

All (1193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	843	PQN	C3-C2	7.72	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	842	PQN	C3-C2	7.54	1.48	1.35
24	b	842	PQN	C10-C5	4.92	1.48	1.40
24	a	843	PQN	C10-C5	4.91	1.48	1.40
23	1	304	A1L1F	O7-C54	4.58	1.45	1.35
20	5	316	SQD	O8-S	4.45	1.64	1.47
20	1	315	SQD	O8-S	4.42	1.63	1.47
20	1	315	SQD	O48-C23	4.32	1.45	1.33
22	a	853	LMG	O8-C28	4.27	1.45	1.33
23	1	304	A1L1F	C57-C1	-4.26	1.25	1.30
20	5	316	SQD	O48-C23	4.23	1.45	1.33
23	1	304	A1L1F	O13-C45	4.22	1.45	1.33
20	1	315	SQD	O47-C7	4.17	1.46	1.34
22	a	853	LMG	O7-C10	4.14	1.46	1.34
22	j	105	LMG	O8-C28	4.10	1.45	1.33
20	5	316	SQD	O47-C7	4.09	1.45	1.34
22	2	317	LMG	O8-C28	4.06	1.45	1.33
21	4	318	DGD	O1G-C1A	4.03	1.45	1.33
21	b	851	DGD	O2G-C1B	3.99	1.45	1.34
21	b	851	DGD	O1G-C1A	3.96	1.44	1.33
22	2	317	LMG	O7-C10	3.94	1.45	1.34
22	j	105	LMG	O7-C10	3.90	1.45	1.34
26	m	102	BCR	C1-C6	-3.89	1.48	1.53
21	4	318	DGD	O2G-C1B	3.83	1.45	1.34
19	2	313	CLA	C1D-ND	3.68	1.42	1.37
19	b	827	CLA	C1D-ND	3.65	1.42	1.37
19	a	804	CLA	C1D-ND	3.64	1.42	1.37
19	1	310	CLA	C1D-ND	3.63	1.42	1.37
19	a	837	CLA	C1D-ND	3.62	1.42	1.37
19	3	308	CLA	C1D-ND	3.62	1.42	1.37
23	1	304	A1L1F	C57-C2	-3.62	1.26	1.31
19	5	308	CLA	C1D-ND	3.61	1.42	1.37
19	3	314	CLA	C1D-ND	3.61	1.42	1.37
19	3	313	CLA	C1D-ND	3.59	1.42	1.37
19	a	828	CLA	C1D-ND	3.59	1.42	1.37
19	1	312	CLA	C1D-ND	3.58	1.42	1.37
19	5	310	CLA	C1D-ND	3.58	1.42	1.37
19	4	307	CLA	C1D-ND	3.58	1.42	1.37
19	a	840	CLA	C1D-ND	3.58	1.42	1.37
19	4	316	CLA	C1D-ND	3.58	1.42	1.37
19	2	307	CLA	C1D-ND	3.58	1.42	1.37
19	5	314	CLA	C1D-ND	3.58	1.42	1.37
19	a	814	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	j	103	CLA	C1D-ND	3.57	1.42	1.37
19	a	839	CLA	C1D-ND	3.56	1.42	1.37
19	4	314	CLA	C1D-ND	3.56	1.42	1.37
19	5	311	CLA	C1D-ND	3.56	1.42	1.37
19	5	305	CLA	C1D-ND	3.56	1.42	1.37
19	2	314	CLA	C1D-ND	3.56	1.42	1.37
19	b	834	CLA	C1D-ND	3.55	1.42	1.37
19	b	825	CLA	C1D-ND	3.55	1.42	1.37
19	a	825	CLA	C1D-ND	3.55	1.42	1.37
19	4	315	CLA	C1D-ND	3.54	1.42	1.37
19	l	204	CLA	C1D-ND	3.54	1.42	1.37
19	b	819	CLA	C1D-ND	3.53	1.42	1.37
19	b	840	CLA	C1D-ND	3.53	1.42	1.37
19	b	821	CLA	C1D-ND	3.53	1.42	1.37
19	a	816	CLA	C1D-ND	3.53	1.42	1.37
19	3	311	CLA	C1D-ND	3.53	1.42	1.37
19	3	315	CLA	C1D-ND	3.53	1.42	1.37
19	2	315	CLA	C1D-ND	3.53	1.42	1.37
19	b	841	CLA	C1D-ND	3.53	1.42	1.37
19	2	312	CLA	C1D-ND	3.53	1.42	1.37
19	l	202	CLA	C1D-ND	3.53	1.42	1.37
19	b	839	CLA	C1D-ND	3.52	1.42	1.37
19	3	312	CLA	C1D-ND	3.52	1.42	1.37
19	a	811	CLA	C1D-ND	3.52	1.42	1.37
19	2	311	CLA	C1D-ND	3.52	1.42	1.37
19	1	309	CLA	C1D-ND	3.52	1.42	1.37
19	b	816	CLA	C1D-ND	3.52	1.42	1.37
19	a	829	CLA	C1D-ND	3.51	1.42	1.37
19	a	815	CLA	C1D-ND	3.51	1.42	1.37
19	2	306	CLA	C1D-ND	3.51	1.42	1.37
19	b	836	CLA	C1D-ND	3.51	1.42	1.37
19	1	307	CLA	C1D-ND	3.51	1.42	1.37
19	a	835	CLA	C1D-ND	3.50	1.42	1.37
19	b	818	CLA	C1D-ND	3.50	1.42	1.37
19	4	310	CLA	C1D-ND	3.50	1.42	1.37
19	3	310	CLA	C1D-ND	3.50	1.42	1.37
19	b	835	CLA	C1D-ND	3.50	1.42	1.37
19	a	832	CLA	C1D-ND	3.50	1.42	1.37
19	5	309	CLA	C1D-ND	3.50	1.42	1.37
19	4	317	CLA	C1D-ND	3.50	1.42	1.37
19	b	813	CLA	C1D-ND	3.50	1.42	1.37
19	4	312	CLA	C1D-ND	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	809	CLA	C1D-ND	3.50	1.42	1.37
19	a	842	CLA	C1D-ND	3.49	1.42	1.37
19	a	826	CLA	C1D-ND	3.49	1.42	1.37
19	f	802	CLA	C1D-ND	3.49	1.42	1.37
19	a	836	CLA	C1D-ND	3.49	1.42	1.37
19	a	813	CLA	C1D-ND	3.49	1.42	1.37
19	b	805	CLA	C1D-ND	3.49	1.42	1.37
19	a	838	CLA	C1D-ND	3.49	1.42	1.37
19	5	315	CLA	C1D-ND	3.48	1.42	1.37
19	1	314	CLA	C1D-ND	3.48	1.42	1.37
19	b	820	CLA	C1D-ND	3.48	1.42	1.37
19	a	844	CLA	C1D-ND	3.48	1.42	1.37
19	b	832	CLA	C1D-ND	3.48	1.42	1.37
19	i	102	CLA	C1D-ND	3.48	1.42	1.37
19	2	308	CLA	C1D-ND	3.48	1.42	1.37
19	4	309	CLA	C1D-ND	3.48	1.42	1.37
19	a	817	CLA	C1D-ND	3.47	1.42	1.37
19	4	306	CLA	C1D-ND	3.47	1.42	1.37
19	b	807	CLA	C1D-ND	3.47	1.42	1.37
19	f	803	CLA	C1D-ND	3.47	1.42	1.37
19	a	824	CLA	C1D-ND	3.47	1.42	1.37
19	a	854	CLA	C1D-ND	3.46	1.42	1.37
19	5	306	CLA	C1D-ND	3.46	1.42	1.37
19	a	834	CLA	C1D-ND	3.46	1.42	1.37
19	2	309	CLA	C1D-ND	3.46	1.42	1.37
19	b	814	CLA	C1D-ND	3.46	1.42	1.37
19	4	313	CLA	C1D-ND	3.46	1.42	1.37
19	a	822	CLA	C1D-ND	3.46	1.42	1.37
19	a	808	CLA	C1D-ND	3.46	1.42	1.37
19	a	819	CLA	C1D-ND	3.45	1.42	1.37
19	5	313	CLA	C1D-ND	3.45	1.42	1.37
19	a	841	CLA	C1D-ND	3.45	1.42	1.37
19	5	312	CLA	C1D-ND	3.45	1.42	1.37
19	b	817	CLA	C1D-ND	3.45	1.42	1.37
19	3	309	CLA	C1D-ND	3.45	1.42	1.37
19	b	822	CLA	C1D-ND	3.45	1.42	1.37
19	1	306	CLA	C1D-ND	3.45	1.42	1.37
19	a	807	CLA	C1D-ND	3.45	1.42	1.37
19	1	311	CLA	C1D-ND	3.45	1.42	1.37
19	1	308	CLA	C1D-ND	3.44	1.42	1.37
19	b	815	CLA	C1D-ND	3.44	1.42	1.37
19	b	829	CLA	C1D-ND	3.44	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	808	CLA	C1D-ND	3.44	1.42	1.37
19	b	830	CLA	C1D-ND	3.44	1.42	1.37
19	b	838	CLA	C1D-ND	3.44	1.42	1.37
19	b	828	CLA	C1D-ND	3.44	1.42	1.37
19	a	805	CLA	C1D-ND	3.43	1.42	1.37
19	a	823	CLA	C1D-ND	3.43	1.42	1.37
19	4	308	CLA	C1D-ND	3.43	1.42	1.37
19	1	305	CLA	C1D-ND	3.43	1.42	1.37
19	b	811	CLA	C1D-ND	3.43	1.42	1.37
19	b	823	CLA	C1D-ND	3.43	1.42	1.37
19	3	307	CLA	C1D-ND	3.43	1.42	1.37
19	a	821	CLA	C1D-ND	3.43	1.42	1.37
19	b	801	CLA	C1D-ND	3.43	1.42	1.37
19	a	818	CLA	C1D-ND	3.42	1.42	1.37
19	a	820	CLA	C1D-ND	3.42	1.42	1.37
19	b	826	CLA	C1D-ND	3.42	1.42	1.37
19	a	831	CLA	C1D-ND	3.42	1.42	1.37
19	a	827	CLA	C1D-ND	3.41	1.42	1.37
19	1	313	CLA	C1D-ND	3.41	1.42	1.37
19	1	312	CLA	C4B-NB	3.41	1.42	1.37
19	a	810	CLA	C1D-ND	3.41	1.42	1.37
19	j	102	CLA	C1D-ND	3.40	1.42	1.37
19	a	812	CLA	C1D-ND	3.39	1.42	1.37
19	b	809	CLA	C1D-ND	3.39	1.42	1.37
19	5	307	CLA	C1D-ND	3.39	1.42	1.37
19	l	203	CLA	C1D-ND	3.37	1.42	1.37
19	b	810	CLA	C1D-ND	3.37	1.42	1.37
19	2	310	CLA	C1D-ND	3.37	1.42	1.37
19	a	830	CLA	C1D-ND	3.37	1.42	1.37
19	a	803	CLA	C1D-ND	3.36	1.42	1.37
26	m	102	BCR	C30-C25	-3.36	1.49	1.53
19	b	837	CLA	C1D-ND	3.35	1.42	1.37
19	b	802	CLA	C1D-ND	3.35	1.42	1.37
19	2	316	CLA	C1D-ND	3.35	1.42	1.37
19	a	802	CLA	C1D-ND	3.32	1.42	1.37
19	b	806	CLA	C1D-ND	3.32	1.42	1.37
19	4	311	CLA	C1D-ND	3.32	1.42	1.37
19	b	824	CLA	C1D-ND	3.31	1.42	1.37
19	b	812	CLA	C1D-ND	3.31	1.42	1.37
19	b	833	CLA	C1D-ND	3.29	1.42	1.37
19	b	803	CLA	C1D-ND	3.29	1.42	1.37
25	a	845	LHG	C26-C25	-3.27	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	801	CLA	C1D-ND	3.25	1.42	1.37
19	a	818	CLA	C4B-NB	3.25	1.42	1.37
25	m	101	LHG	C26-C25	-3.25	1.35	1.51
19	b	831	CLA	C1D-ND	3.24	1.42	1.37
19	a	840	CLA	C4B-NB	3.23	1.42	1.37
19	2	315	CLA	C4B-NB	3.23	1.42	1.37
19	4	315	CLA	C4B-NB	3.22	1.42	1.37
25	b	849	LHG	C26-C25	-3.22	1.35	1.51
19	b	838	CLA	C4B-NB	3.21	1.42	1.37
19	5	313	CLA	C4B-NB	3.20	1.42	1.37
19	4	306	CLA	C4B-NB	3.20	1.42	1.37
19	1	309	CLA	C4B-NB	3.19	1.42	1.37
19	a	833	CLA	C1D-ND	3.19	1.42	1.37
19	1	314	CLA	C4B-NB	3.18	1.42	1.37
19	a	842	CLA	C4B-NB	3.18	1.42	1.37
19	1	305	CLA	C4B-NB	3.17	1.42	1.37
19	b	821	CLA	C4B-NB	3.17	1.42	1.37
19	3	315	CLA	C4B-NB	3.17	1.42	1.37
19	i	102	CLA	C4B-NB	3.16	1.42	1.37
19	4	307	CLA	C4B-NB	3.16	1.42	1.37
19	a	808	CLA	C4B-NB	3.16	1.42	1.37
19	b	835	CLA	C4B-NB	3.15	1.42	1.37
19	a	825	CLA	C4B-NB	3.15	1.42	1.37
19	b	830	CLA	C4B-NB	3.14	1.42	1.37
19	f	803	CLA	C4B-NB	3.14	1.42	1.37
19	a	831	CLA	C4B-NB	3.13	1.42	1.37
19	4	317	CLA	C4B-NB	3.13	1.42	1.37
19	b	802	CLA	C4B-NB	3.12	1.42	1.37
19	j	102	CLA	C4B-NB	3.12	1.42	1.37
19	4	311	CLA	C4B-NB	3.12	1.42	1.37
19	b	840	CLA	C4B-NB	3.11	1.41	1.37
19	b	801	CLA	C4B-NB	3.11	1.41	1.37
19	b	812	CLA	CAB-C3B	-3.11	1.44	1.50
19	4	314	CLA	C4B-NB	3.11	1.41	1.37
19	3	311	CLA	C4B-NB	3.11	1.41	1.37
19	a	804	CLA	C4B-NB	3.11	1.41	1.37
19	2	312	CLA	C4B-NB	3.10	1.41	1.37
19	a	824	CLA	C4B-NB	3.10	1.41	1.37
19	b	841	CLA	C4B-NB	3.10	1.41	1.37
19	2	308	CLA	C4B-NB	3.10	1.41	1.37
19	4	310	CLA	C4B-NB	3.10	1.41	1.37
19	4	312	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	313	CLA	C4B-NB	3.10	1.41	1.37
19	4	316	CLA	C4B-NB	3.10	1.41	1.37
19	1	202	CLA	C4B-NB	3.10	1.41	1.37
19	2	311	CLA	C4B-NB	3.10	1.41	1.37
19	5	310	CLA	C4B-NB	3.09	1.41	1.37
19	a	817	CLA	C4B-NB	3.09	1.41	1.37
19	b	827	CLA	C4B-NB	3.09	1.41	1.37
19	a	813	CLA	C4B-NB	3.09	1.41	1.37
19	2	314	CLA	C4B-NB	3.08	1.41	1.37
19	a	805	CLA	C4B-NB	3.08	1.41	1.37
19	5	305	CLA	C4B-NB	3.08	1.41	1.37
19	2	310	CLA	C4B-NB	3.08	1.41	1.37
19	b	837	CLA	C4B-NB	3.08	1.41	1.37
19	3	313	CLA	C4B-NB	3.07	1.41	1.37
19	5	306	CLA	C4B-NB	3.07	1.41	1.37
19	5	315	CLA	C4B-NB	3.07	1.41	1.37
19	1	313	CLA	C4B-NB	3.07	1.41	1.37
19	1	310	CLA	C4B-NB	3.07	1.41	1.37
19	b	829	CLA	C4B-NB	3.07	1.41	1.37
19	a	820	CLA	C4B-NB	3.06	1.41	1.37
19	b	805	CLA	C4B-NB	3.06	1.41	1.37
19	3	310	CLA	C4B-NB	3.06	1.41	1.37
19	a	841	CLA	C4B-NB	3.06	1.41	1.37
19	a	829	CLA	C4B-NB	3.06	1.41	1.37
19	b	828	CLA	C4B-NB	3.05	1.41	1.37
19	3	307	CLA	C4B-NB	3.05	1.41	1.37
19	2	309	CLA	C4B-NB	3.05	1.41	1.37
19	2	316	CLA	C4B-NB	3.05	1.41	1.37
19	a	822	CLA	C4B-NB	3.05	1.41	1.37
19	b	825	CLA	C4B-NB	3.04	1.41	1.37
19	b	817	CLA	C4B-NB	3.04	1.41	1.37
19	3	312	CLA	C4B-NB	3.04	1.41	1.37
19	b	823	CLA	C4B-NB	3.04	1.41	1.37
19	5	309	CLA	C4B-NB	3.04	1.41	1.37
19	f	802	CLA	C4B-NB	3.04	1.41	1.37
19	b	804	CLA	C4B-NB	3.04	1.41	1.37
19	b	819	CLA	C4B-NB	3.04	1.41	1.37
19	b	808	CLA	C4B-NB	3.03	1.41	1.37
19	a	854	CLA	C4B-NB	3.03	1.41	1.37
19	4	309	CLA	C4B-NB	3.03	1.41	1.37
19	1	307	CLA	C4B-NB	3.03	1.41	1.37
19	b	815	CLA	C4B-NB	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	834	CLA	C4B-NB	3.03	1.41	1.37
19	3	308	CLA	C4B-NB	3.03	1.41	1.37
19	b	832	CLA	C4B-NB	3.03	1.41	1.37
19	a	810	CLA	C4B-NB	3.02	1.41	1.37
19	b	812	CLA	C4B-NB	3.02	1.41	1.37
19	a	837	CLA	C4B-NB	3.02	1.41	1.37
19	b	834	CLA	C4B-NB	3.02	1.41	1.37
19	a	812	CLA	C4B-NB	3.01	1.41	1.37
19	2	306	CLA	C4B-NB	3.01	1.41	1.37
19	j	103	CLA	C4B-NB	3.01	1.41	1.37
19	a	826	CLA	C4B-NB	3.00	1.41	1.37
19	2	313	CLA	C4B-NB	3.00	1.41	1.37
19	a	827	CLA	C4B-NB	3.00	1.41	1.37
19	a	830	CLA	C4B-NB	2.99	1.41	1.37
19	5	307	CLA	C4B-NB	2.99	1.41	1.37
19	l	203	CLA	C4B-NB	2.99	1.41	1.37
19	a	816	CLA	C4B-NB	2.99	1.41	1.37
19	l	204	CLA	C4B-NB	2.98	1.41	1.37
19	b	804	CLA	C1D-ND	2.98	1.41	1.37
19	b	809	CLA	C4B-NB	2.98	1.41	1.37
19	5	311	CLA	C4B-NB	2.98	1.41	1.37
19	a	821	CLA	C4B-NB	2.98	1.41	1.37
19	1	306	CLA	C4B-NB	2.97	1.41	1.37
19	1	308	CLA	C4B-NB	2.97	1.41	1.37
19	a	836	CLA	C4B-NB	2.97	1.41	1.37
19	b	833	CLA	C4B-NB	2.96	1.41	1.37
19	a	811	CLA	C4B-NB	2.96	1.41	1.37
19	a	835	CLA	C4B-NB	2.96	1.41	1.37
19	b	803	CLA	C4B-NB	2.96	1.41	1.37
19	b	810	CLA	C4B-NB	2.96	1.41	1.37
19	a	815	CLA	C4B-NB	2.96	1.41	1.37
19	a	832	CLA	C4B-NB	2.96	1.41	1.37
19	a	839	CLA	C4B-NB	2.96	1.41	1.37
19	3	309	CLA	C4B-NB	2.96	1.41	1.37
19	b	839	CLA	C4B-NB	2.96	1.41	1.37
19	a	823	CLA	C4B-NB	2.95	1.41	1.37
19	a	844	CLA	C4B-NB	2.95	1.41	1.37
19	a	803	CLA	C4B-NB	2.95	1.41	1.37
19	b	803	CLA	C1B-C2B	2.95	1.50	1.43
19	5	312	CLA	C4B-NB	2.95	1.41	1.37
19	5	308	CLA	C4B-NB	2.94	1.41	1.37
19	b	816	CLA	C4B-NB	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	314	CLA	C4B-NB	2.92	1.41	1.37
19	b	814	CLA	C4B-NB	2.92	1.41	1.37
19	b	820	CLA	C4B-NB	2.92	1.41	1.37
19	a	819	CLA	C4B-NB	2.92	1.41	1.37
19	a	833	CLA	C4B-NB	2.91	1.41	1.37
19	b	831	CLA	C4B-NB	2.91	1.41	1.37
19	3	314	CLA	C4B-NB	2.90	1.41	1.37
19	a	802	CLA	C4B-NB	2.90	1.41	1.37
19	a	814	CLA	C4B-NB	2.90	1.41	1.37
19	b	826	CLA	C4B-NB	2.90	1.41	1.37
19	b	824	CLA	C4B-NB	2.90	1.41	1.37
19	b	813	CLA	C4B-NB	2.89	1.41	1.37
19	1	311	CLA	C4B-NB	2.89	1.41	1.37
19	a	807	CLA	C4B-NB	2.89	1.41	1.37
19	b	836	CLA	C4B-NB	2.88	1.41	1.37
19	b	806	CLA	C4B-NB	2.87	1.41	1.37
19	a	801	CLA	C4B-NB	2.87	1.41	1.37
19	a	838	CLA	C4B-NB	2.87	1.41	1.37
19	2	307	CLA	C4B-NB	2.87	1.41	1.37
19	b	818	CLA	C4B-NB	2.86	1.41	1.37
19	a	823	CLA	C1B-C2B	2.85	1.49	1.43
19	b	807	CLA	C4B-NB	2.85	1.41	1.37
19	a	828	CLA	C4B-NB	2.84	1.41	1.37
19	b	822	CLA	C4B-NB	2.84	1.41	1.37
19	4	308	CLA	C4B-NB	2.84	1.41	1.37
19	b	840	CLA	C1B-C2B	2.84	1.49	1.43
19	1	305	CLA	C1B-C2B	2.83	1.49	1.43
19	a	809	CLA	C4B-NB	2.82	1.41	1.37
19	b	811	CLA	C4B-NB	2.82	1.41	1.37
19	3	308	CLA	C1B-C2B	2.82	1.49	1.43
19	b	822	CLA	C1B-C2B	2.81	1.49	1.43
19	b	828	CLA	C1B-C2B	2.81	1.49	1.43
19	b	808	CLA	C1B-C2B	2.81	1.49	1.43
19	3	314	CLA	C1B-C2B	2.81	1.49	1.43
19	2	313	CLA	C1B-C2B	2.80	1.49	1.43
19	1	306	CLA	C1B-C2B	2.80	1.49	1.43
19	3	311	CLA	C1B-C2B	2.79	1.49	1.43
19	a	844	CLA	C1B-C2B	2.79	1.49	1.43
19	3	309	CLA	C1B-C2B	2.79	1.49	1.43
19	1	311	CLA	C1B-C2B	2.79	1.49	1.43
19	b	811	CLA	C1B-C2B	2.78	1.49	1.43
19	a	830	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	824	CLA	C1B-C2B	2.78	1.49	1.43
19	b	813	CLA	C1B-C2B	2.77	1.49	1.43
19	3	310	CLA	C1B-C2B	2.77	1.49	1.43
19	a	821	CLA	C1B-C2B	2.77	1.49	1.43
19	a	810	CLA	C1B-C2B	2.77	1.49	1.43
19	b	807	CLA	C1B-C2B	2.77	1.49	1.43
19	2	309	CLA	C1B-C2B	2.77	1.49	1.43
19	2	316	CLA	C1B-C2B	2.77	1.49	1.43
19	b	821	CLA	C1B-C2B	2.77	1.49	1.43
19	f	802	CLA	C1B-C2B	2.77	1.49	1.43
19	4	310	CLA	C1B-C2B	2.76	1.49	1.43
19	j	103	CLA	C1B-C2B	2.76	1.49	1.43
19	4	316	CLA	C1B-C2B	2.76	1.49	1.43
19	2	315	CLA	C1B-C2B	2.76	1.49	1.43
19	a	812	CLA	C1B-C2B	2.75	1.49	1.43
19	b	833	CLA	C1B-C2B	2.75	1.49	1.43
19	5	315	CLA	C1B-C2B	2.75	1.49	1.43
19	a	834	CLA	C1B-C2B	2.75	1.49	1.43
19	a	817	CLA	C1B-C2B	2.75	1.49	1.43
19	b	805	CLA	C1B-C2B	2.75	1.49	1.43
19	3	313	CLA	C1B-C2B	2.74	1.49	1.43
19	1	308	CLA	C1B-C2B	2.74	1.49	1.43
19	l	204	CLA	C1B-C2B	2.74	1.49	1.43
19	b	834	CLA	C1B-C2B	2.74	1.49	1.43
19	2	311	CLA	C1B-C2B	2.74	1.49	1.43
19	a	809	CLA	C1B-C2B	2.74	1.49	1.43
19	4	308	CLA	C1B-C2B	2.73	1.49	1.43
19	1	309	CLA	C1B-C2B	2.73	1.49	1.43
19	a	828	CLA	C1B-C2B	2.73	1.49	1.43
19	a	835	CLA	C1B-C2B	2.73	1.49	1.43
19	1	314	CLA	C1B-C2B	2.73	1.49	1.43
19	4	314	CLA	C1B-C2B	2.73	1.49	1.43
19	5	311	CLA	C1B-C2B	2.73	1.49	1.43
19	a	838	CLA	C1B-C2B	2.73	1.49	1.43
19	b	837	CLA	C1B-C2B	2.73	1.49	1.43
19	a	807	CLA	C1B-C2B	2.73	1.49	1.43
19	1	313	CLA	C1B-C2B	2.73	1.49	1.43
19	a	805	CLA	C1B-C2B	2.72	1.49	1.43
19	a	839	CLA	C1B-C2B	2.72	1.49	1.43
19	4	312	CLA	C1B-C2B	2.72	1.49	1.43
19	a	811	CLA	C1B-C2B	2.72	1.49	1.43
19	5	309	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	305	CLA	C1B-C2B	2.72	1.49	1.43
19	b	832	CLA	C1B-C2B	2.72	1.49	1.43
19	b	812	CLA	C4B-C3B	2.72	1.49	1.43
19	a	806	CLA	MG-NB	-2.72	2.00	2.05
19	5	312	CLA	C1B-C2B	2.72	1.49	1.43
19	4	317	CLA	C1B-C2B	2.72	1.49	1.43
19	j	102	CLA	C1B-C2B	2.72	1.49	1.43
19	2	312	CLA	C1B-C2B	2.72	1.49	1.43
19	a	824	CLA	C1B-C2B	2.72	1.49	1.43
19	l	202	CLA	C1B-C2B	2.72	1.49	1.43
19	2	306	CLA	C1B-C2B	2.71	1.49	1.43
19	a	842	CLA	C1B-C2B	2.71	1.49	1.43
19	b	812	CLA	C1B-C2B	2.71	1.49	1.43
19	5	306	CLA	C1B-C2B	2.71	1.49	1.43
19	a	829	CLA	C1B-C2B	2.71	1.49	1.43
19	5	310	CLA	C1B-C2B	2.70	1.49	1.43
19	2	308	CLA	C1B-C2B	2.70	1.49	1.43
19	b	838	CLA	C1B-C2B	2.70	1.49	1.43
19	4	307	CLA	C1B-C2B	2.70	1.49	1.43
19	b	802	CLA	C1B-C2B	2.69	1.49	1.43
19	b	801	CLA	C1B-C2B	2.69	1.49	1.43
19	a	818	CLA	C3B-C4B	2.69	1.50	1.42
19	a	816	CLA	C1B-C2B	2.69	1.49	1.43
19	a	840	CLA	C1B-C2B	2.69	1.49	1.43
19	a	825	CLA	C1B-C2B	2.69	1.49	1.43
19	b	806	CLA	C1B-C2B	2.69	1.49	1.43
19	b	841	CLA	C1B-C2B	2.69	1.49	1.43
19	f	803	CLA	C1B-C2B	2.69	1.49	1.43
19	a	826	CLA	C1B-C2B	2.69	1.49	1.43
19	5	314	CLA	C1B-C2B	2.69	1.49	1.43
19	b	827	CLA	C1B-C2B	2.69	1.49	1.43
19	3	312	CLA	C1B-C2B	2.69	1.49	1.43
19	2	314	CLA	C1B-C2B	2.68	1.49	1.43
19	i	102	CLA	C1B-C2B	2.68	1.49	1.43
19	4	306	CLA	C1B-C2B	2.68	1.49	1.43
19	5	307	CLA	C1B-C2B	2.68	1.49	1.43
19	5	313	CLA	C1B-C2B	2.68	1.49	1.43
19	b	814	CLA	C1B-C2B	2.68	1.49	1.43
19	4	311	CLA	C1B-C2B	2.67	1.49	1.43
19	1	307	CLA	C1B-C2B	2.67	1.49	1.43
19	1	312	CLA	C3B-C4B	2.67	1.50	1.42
19	a	836	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	309	CLA	C1B-C2B	2.67	1.49	1.43
19	2	310	CLA	C1B-C2B	2.67	1.49	1.43
19	a	854	CLA	C1B-C2B	2.67	1.49	1.43
19	b	816	CLA	C1B-C2B	2.67	1.49	1.43
19	a	804	CLA	C1B-C2B	2.67	1.49	1.43
19	b	810	CLA	C1B-C2B	2.67	1.49	1.43
19	b	823	CLA	C1B-C2B	2.67	1.49	1.43
19	b	830	CLA	CMB-C2B	-2.67	1.45	1.50
19	b	815	CLA	C1B-C2B	2.66	1.49	1.43
19	a	813	CLA	C1B-C2B	2.66	1.49	1.43
19	a	819	CLA	C1B-C2B	2.66	1.49	1.43
19	b	826	CLA	C1B-C2B	2.66	1.49	1.43
19	3	307	CLA	C1B-C2B	2.66	1.49	1.43
19	4	315	CLA	C1B-C2B	2.66	1.49	1.43
19	a	814	CLA	C1B-C2B	2.66	1.49	1.43
19	3	315	CLA	C1B-C2B	2.65	1.49	1.43
19	a	827	CLA	C1B-C2B	2.65	1.49	1.43
19	a	815	CLA	C1B-C2B	2.65	1.49	1.43
19	a	808	CLA	C1B-C2B	2.65	1.49	1.43
19	b	836	CLA	C1B-C2B	2.65	1.49	1.43
19	b	819	CLA	C1B-C2B	2.65	1.49	1.43
19	b	825	CLA	C1B-C2B	2.64	1.49	1.43
18	5	303	A1L1G	C33-C34	-2.64	1.40	1.46
19	b	809	CLA	C1B-C2B	2.64	1.49	1.43
19	a	837	CLA	C1B-C2B	2.64	1.49	1.43
19	a	831	CLA	CMB-C2B	-2.64	1.45	1.50
19	a	801	CLA	C1B-C2B	2.63	1.49	1.43
19	5	308	CLA	C1B-C2B	2.63	1.49	1.43
19	b	817	CLA	C1B-C2B	2.63	1.49	1.43
18	3	306	A1L1G	C40-C39	-2.63	1.40	1.46
19	a	833	CLA	C1B-C2B	2.62	1.49	1.43
19	1	312	CLA	C1B-C2B	2.62	1.49	1.43
18	3	306	A1L1G	C33-C34	-2.62	1.40	1.46
19	b	829	CLA	C1B-C2B	2.61	1.49	1.43
19	l	203	CLA	C1B-C2B	2.61	1.49	1.43
19	b	839	CLA	C1B-C2B	2.61	1.49	1.43
19	a	841	CLA	C1B-C2B	2.61	1.49	1.43
19	1	310	CLA	C1B-C2B	2.61	1.49	1.43
19	a	832	CLA	C1B-C2B	2.60	1.49	1.43
19	a	822	CLA	C1B-C2B	2.59	1.49	1.43
19	b	835	CLA	C1B-C2B	2.57	1.49	1.43
19	a	806	CLA	CMD-C2D	-2.56	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	831	CLA	C1B-C2B	2.56	1.49	1.43
19	4	313	CLA	CHC-C1C	2.53	1.43	1.38
18	3	302	A1L1G	C33-C34	-2.53	1.40	1.46
19	b	820	CLA	C1B-C2B	2.53	1.49	1.43
19	a	818	CLA	C1B-C2B	2.50	1.49	1.43
19	4	313	CLA	C3B-C4B	2.50	1.50	1.42
19	3	315	CLA	C3B-C4B	2.50	1.50	1.42
18	1	301	A1L1G	C33-C34	-2.50	1.40	1.46
19	b	830	CLA	CMD-C2D	-2.49	1.45	1.50
18	5	303	A1L1G	C40-C39	-2.49	1.40	1.46
19	5	313	CLA	C3B-C4B	2.48	1.50	1.42
19	4	313	CLA	C1B-C2B	2.48	1.48	1.43
19	4	315	CLA	C3B-C4B	2.48	1.50	1.42
19	a	803	CLA	C1B-C2B	2.48	1.48	1.43
19	a	820	CLA	C1B-C2B	2.48	1.48	1.43
23	1	304	A1L1F	O15-C20	-2.48	1.43	1.46
19	a	831	CLA	C1B-C2B	2.47	1.48	1.43
19	a	802	CLA	C1B-C2B	2.47	1.48	1.43
19	a	840	CLA	C3B-C4B	2.47	1.49	1.42
19	b	830	CLA	C1B-C2B	2.47	1.48	1.43
19	b	817	CLA	C3B-C4B	2.47	1.49	1.42
18	3	302	A1L1G	C40-C39	-2.46	1.40	1.46
19	2	307	CLA	C1B-C2B	2.45	1.48	1.43
19	a	813	CLA	C3B-C4B	2.45	1.49	1.42
19	b	804	CLA	C3B-C4B	2.45	1.49	1.42
19	a	801	CLA	CMD-C2D	-2.45	1.45	1.50
19	2	314	CLA	C3B-C4B	2.44	1.49	1.42
19	a	806	CLA	CMC-C2C	-2.44	1.45	1.50
19	a	842	CLA	C3B-C4B	2.44	1.49	1.42
19	a	814	CLA	C3B-C4B	2.44	1.49	1.42
19	b	835	CLA	C3B-C4B	2.44	1.49	1.42
19	b	815	CLA	C3B-C4B	2.44	1.49	1.42
25	b	849	LHG	O8-C6	-2.44	1.39	1.45
19	4	307	CLA	C3B-C4B	2.43	1.49	1.42
19	a	830	CLA	CMC-C2C	-2.43	1.45	1.50
19	b	806	CLA	C3B-C4B	2.43	1.49	1.42
19	a	827	CLA	C3B-C4B	2.43	1.49	1.42
19	b	809	CLA	C3B-C4B	2.43	1.49	1.42
19	a	822	CLA	C3B-C4B	2.42	1.49	1.42
19	a	819	CLA	C3B-C4B	2.42	1.49	1.42
25	a	846	LHG	O7-C5	-2.42	1.40	1.46
25	a	846	LHG	O8-C6	-2.42	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	817	CLA	CHC-C1C	2.42	1.43	1.38
19	b	814	CLA	C3B-C4B	2.42	1.49	1.42
19	a	841	CLA	C3B-C4B	2.42	1.49	1.42
19	5	306	CLA	C3B-C4B	2.42	1.49	1.42
19	a	802	CLA	CHC-C1C	2.42	1.43	1.38
19	i	102	CLA	C3B-C4B	2.42	1.49	1.42
19	a	802	CLA	C3B-C4B	2.42	1.49	1.42
19	2	311	CLA	C3B-C4B	2.41	1.49	1.42
19	b	829	CLA	C3B-C4B	2.41	1.49	1.42
19	a	805	CLA	C3B-C4B	2.40	1.49	1.42
19	a	808	CLA	C3B-C4B	2.40	1.49	1.42
17	4	304	XAT	O24-C25	-2.40	1.43	1.46
17	1	302	XAT	O4-C5	-2.40	1.43	1.46
19	b	839	CLA	CHC-C1C	2.40	1.43	1.38
19	4	311	CLA	CMD-C2D	-2.40	1.45	1.50
19	i	102	CLA	CHC-C1C	2.40	1.43	1.38
19	5	305	CLA	C3B-C4B	2.40	1.49	1.42
19	a	822	CLA	CHC-C1C	2.40	1.43	1.38
19	5	315	CLA	C3B-C4B	2.40	1.49	1.42
19	2	308	CLA	CHC-C1C	2.40	1.43	1.38
19	4	308	CLA	C3B-C4B	2.40	1.49	1.42
19	a	804	CLA	C3B-C4B	2.39	1.49	1.42
19	f	803	CLA	C3B-C4B	2.39	1.49	1.42
19	a	818	CLA	CHC-C1C	2.39	1.43	1.38
19	2	315	CLA	C3B-C4B	2.39	1.49	1.42
19	a	829	CLA	C3B-C4B	2.39	1.49	1.42
19	a	816	CLA	C3B-C4B	2.39	1.49	1.42
19	b	836	CLA	C3B-C4B	2.39	1.49	1.42
19	j	103	CLA	C3B-C4B	2.39	1.49	1.42
17	4	301	XAT	O24-C25	-2.39	1.43	1.46
19	b	818	CLA	C1B-C2B	2.39	1.48	1.43
19	4	316	CLA	C3B-C4B	2.39	1.49	1.42
19	2	306	CLA	C3B-C4B	2.39	1.49	1.42
19	b	802	CLA	C3B-C4B	2.39	1.49	1.42
25	a	845	LHG	O8-C6	-2.39	1.39	1.45
19	5	314	CLA	C3B-C4B	2.39	1.49	1.42
19	4	312	CLA	C3B-C4B	2.39	1.49	1.42
19	a	837	CLA	C3B-C4B	2.38	1.49	1.42
19	2	308	CLA	C3B-C4B	2.38	1.49	1.42
19	5	309	CLA	C3B-C4B	2.38	1.49	1.42
19	5	312	CLA	C3B-C4B	2.38	1.49	1.42
19	a	828	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	809	CLA	C3B-C4B	2.38	1.49	1.42
19	2	313	CLA	C3B-C4B	2.38	1.49	1.42
19	2	316	CLA	C3B-C4B	2.38	1.49	1.42
19	a	839	CLA	C3B-C4B	2.38	1.49	1.42
19	b	837	CLA	C3B-C4B	2.38	1.49	1.42
25	m	101	LHG	O8-C6	-2.37	1.39	1.45
19	a	844	CLA	C3B-C4B	2.37	1.49	1.42
19	b	805	CLA	C3B-C4B	2.37	1.49	1.42
19	b	804	CLA	C1B-C2B	2.37	1.48	1.43
19	b	838	CLA	C3B-C4B	2.37	1.49	1.42
19	4	312	CLA	CHC-C1C	2.37	1.43	1.38
19	b	812	CLA	CHC-C1C	2.37	1.43	1.38
19	b	816	CLA	C3B-C4B	2.37	1.49	1.42
25	a	845	LHG	O7-C5	-2.37	1.41	1.46
19	b	832	CLA	C3B-C4B	2.37	1.49	1.42
19	l	203	CLA	C3B-C4B	2.37	1.49	1.42
25	b	849	LHG	O7-C5	-2.37	1.41	1.46
19	a	806	CLA	CMB-C2B	-2.37	1.45	1.50
19	1	313	CLA	C3B-C4B	2.37	1.49	1.42
19	a	833	CLA	C3B-C4B	2.37	1.49	1.42
19	4	314	CLA	C3B-C4B	2.37	1.49	1.42
19	1	309	CLA	C3B-C4B	2.37	1.49	1.42
19	a	817	CLA	C3B-C4B	2.37	1.49	1.42
19	a	820	CLA	C3B-C4B	2.37	1.49	1.42
19	b	815	CLA	CHC-C1C	2.36	1.43	1.38
19	3	312	CLA	C3B-C4B	2.36	1.49	1.42
19	b	825	CLA	C3B-C4B	2.36	1.49	1.42
19	3	307	CLA	C3B-C4B	2.36	1.49	1.42
19	5	310	CLA	C3B-C4B	2.36	1.49	1.42
19	a	819	CLA	CHC-C1C	2.36	1.43	1.38
25	b	849	LHG	O8-C23	2.36	1.40	1.33
19	1	308	CLA	CHC-C1C	2.36	1.43	1.38
19	a	804	CLA	CHC-C1C	2.36	1.43	1.38
19	4	306	CLA	C3B-C4B	2.36	1.49	1.42
19	a	835	CLA	C3B-C4B	2.36	1.49	1.42
19	3	309	CLA	C3B-C4B	2.36	1.49	1.42
19	a	820	CLA	CHC-C1C	2.36	1.43	1.38
19	a	826	CLA	C3B-C4B	2.36	1.49	1.42
19	l	204	CLA	C3B-C4B	2.36	1.49	1.42
19	3	313	CLA	C3B-C4B	2.35	1.49	1.42
19	b	826	CLA	C3B-C4B	2.35	1.49	1.42
17	3	301	XAT	O24-C25	-2.35	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	812	CLA	C3B-C4B	2.35	1.49	1.42
19	a	811	CLA	C3B-C4B	2.35	1.49	1.42
19	b	807	CLA	C3B-C4B	2.35	1.49	1.42
19	b	805	CLA	CHC-C1C	2.35	1.43	1.38
19	4	317	CLA	C3B-C4B	2.35	1.49	1.42
19	b	837	CLA	CHC-C1C	2.35	1.43	1.38
19	2	309	CLA	C3B-C4B	2.35	1.49	1.42
19	b	839	CLA	C3B-C4B	2.35	1.49	1.42
19	1	314	CLA	C3B-C4B	2.35	1.49	1.42
19	b	822	CLA	C3B-C4B	2.35	1.49	1.42
19	b	833	CLA	C3B-C4B	2.35	1.49	1.42
17	3	305	XAT	O4-C5	-2.35	1.43	1.46
19	b	834	CLA	C3B-C4B	2.35	1.49	1.42
19	a	813	CLA	CHC-C1C	2.35	1.43	1.38
19	a	824	CLA	C3B-C4B	2.34	1.49	1.42
19	5	311	CLA	C3B-C4B	2.34	1.49	1.42
19	a	836	CLA	C3B-C4B	2.34	1.49	1.42
19	a	826	CLA	CHC-C1C	2.34	1.43	1.38
19	1	308	CLA	C3B-C4B	2.34	1.49	1.42
19	5	315	CLA	CHC-C1C	2.34	1.43	1.38
19	b	826	CLA	CHC-C1C	2.34	1.43	1.38
19	b	836	CLA	CHC-C1C	2.34	1.43	1.38
19	a	815	CLA	C3B-C4B	2.34	1.49	1.42
19	j	102	CLA	C3B-C4B	2.34	1.49	1.42
25	m	101	LHG	O8-C23	2.34	1.40	1.33
19	2	315	CLA	CHC-C1C	2.34	1.43	1.38
19	2	309	CLA	CHC-C1C	2.34	1.43	1.38
17	2	302	XAT	O4-C5	-2.34	1.43	1.46
19	3	311	CLA	C3B-C4B	2.34	1.49	1.42
19	1	310	CLA	CHC-C1C	2.34	1.43	1.38
19	f	802	CLA	C3B-C4B	2.34	1.49	1.42
19	b	814	CLA	CHC-C1C	2.33	1.43	1.38
19	5	311	CLA	CHC-C1C	2.33	1.43	1.38
19	5	307	CLA	C3B-C4B	2.33	1.49	1.42
19	b	823	CLA	C3B-C4B	2.33	1.49	1.42
19	4	310	CLA	C3B-C4B	2.33	1.49	1.42
19	a	841	CLA	CHC-C1C	2.33	1.43	1.38
19	b	829	CLA	CHC-C1C	2.33	1.43	1.38
19	a	825	CLA	C3B-C4B	2.33	1.49	1.42
19	b	818	CLA	C3B-C4B	2.33	1.49	1.42
19	5	312	CLA	CHC-C1C	2.33	1.43	1.38
19	3	315	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	808	CLA	CHC-C1C	2.33	1.43	1.38
19	b	813	CLA	C3B-C4B	2.33	1.49	1.42
25	m	101	LHG	O7-C7	2.33	1.40	1.34
19	1	310	CLA	C3B-C4B	2.33	1.49	1.42
19	b	813	CLA	CHC-C1C	2.33	1.43	1.38
19	4	309	CLA	C3B-C4B	2.32	1.49	1.42
19	b	835	CLA	CHC-C1C	2.32	1.43	1.38
19	5	313	CLA	CHC-C1C	2.32	1.43	1.38
19	2	312	CLA	C3B-C4B	2.32	1.49	1.42
19	a	823	CLA	C3B-C4B	2.32	1.49	1.42
19	a	829	CLA	CHC-C1C	2.32	1.43	1.38
19	b	806	CLA	CHC-C1C	2.32	1.43	1.38
19	3	308	CLA	C3B-C4B	2.32	1.49	1.42
19	l	202	CLA	C3B-C4B	2.32	1.49	1.42
19	a	827	CLA	CHC-C1C	2.32	1.43	1.38
19	a	854	CLA	C3B-C4B	2.32	1.49	1.42
19	5	308	CLA	C3B-C4B	2.32	1.49	1.42
19	5	314	CLA	CHC-C1C	2.32	1.43	1.38
19	b	816	CLA	CHC-C1C	2.31	1.43	1.38
18	3	302	A1L1G	C29-C30	-2.31	1.40	1.45
19	a	801	CLA	CMB-C2B	-2.31	1.46	1.50
19	b	820	CLA	CMB-C2B	-2.31	1.46	1.50
19	4	308	CLA	CHC-C1C	2.31	1.43	1.38
19	a	837	CLA	CHC-C1C	2.31	1.43	1.38
19	1	309	CLA	CHC-C1C	2.31	1.43	1.38
19	a	854	CLA	CHC-C1C	2.31	1.43	1.38
19	b	801	CLA	C3B-C4B	2.31	1.49	1.42
19	a	834	CLA	C3B-C4B	2.31	1.49	1.42
19	b	809	CLA	CHC-C1C	2.31	1.43	1.38
19	b	818	CLA	CHC-C1C	2.31	1.43	1.38
19	1	311	CLA	C3B-C4B	2.31	1.49	1.42
19	a	809	CLA	CHC-C1C	2.31	1.43	1.38
19	1	307	CLA	C3B-C4B	2.31	1.49	1.42
19	3	313	CLA	CHC-C1C	2.31	1.43	1.38
19	4	311	CLA	C3B-C4B	2.31	1.49	1.42
19	1	312	CLA	CHC-C1C	2.31	1.43	1.38
17	5	301	XAT	O4-C5	-2.31	1.43	1.46
25	m	101	LHG	O7-C5	-2.31	1.41	1.46
19	5	309	CLA	CHC-C1C	2.31	1.43	1.38
19	3	307	CLA	CHC-C1C	2.31	1.43	1.38
23	1	304	A1L1F	C6-C1	-2.31	1.50	1.54
19	3	314	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	840	CLA	C3B-C4B	2.31	1.49	1.42
19	3	311	CLA	CHC-C1C	2.30	1.43	1.38
19	a	821	CLA	C3B-C4B	2.30	1.49	1.42
19	a	830	CLA	C3B-C4B	2.30	1.49	1.42
19	5	306	CLA	CHC-C1C	2.30	1.43	1.38
19	b	838	CLA	CHC-C1C	2.30	1.43	1.38
18	1	301	A1L1G	C40-C39	-2.30	1.41	1.46
19	b	802	CLA	CHC-C1C	2.30	1.43	1.38
19	1	307	CLA	CHC-C1C	2.30	1.43	1.38
25	a	845	LHG	O8-C23	2.30	1.40	1.33
19	a	844	CLA	CHC-C1C	2.30	1.43	1.38
19	2	310	CLA	C3B-C4B	2.30	1.49	1.42
19	a	833	CLA	CHC-C1C	2.30	1.43	1.38
19	2	311	CLA	CHC-C1C	2.30	1.43	1.38
17	5	302	XAT	O4-C5	-2.29	1.43	1.46
19	b	832	CLA	CHC-C1C	2.29	1.43	1.38
19	b	831	CLA	CMD-C2D	-2.29	1.46	1.50
19	2	316	CLA	CHC-C1C	2.29	1.43	1.38
19	2	307	CLA	C3B-C4B	2.29	1.49	1.42
17	5	302	XAT	O24-C25	-2.29	1.43	1.46
19	b	811	CLA	C3B-C4B	2.29	1.49	1.42
19	3	309	CLA	CHC-C1C	2.29	1.43	1.38
19	b	834	CLA	CHC-C1C	2.29	1.43	1.38
25	a	845	LHG	O7-C7	2.29	1.40	1.34
19	a	815	CLA	CHC-C1C	2.29	1.43	1.38
17	1	303	XAT	O4-C5	-2.29	1.43	1.46
19	b	821	CLA	C3B-C4B	2.29	1.49	1.42
19	b	831	CLA	C3B-C4B	2.29	1.49	1.42
19	b	807	CLA	CHC-C1C	2.29	1.43	1.38
17	a	852	XAT	O4-C5	-2.29	1.43	1.46
19	b	833	CLA	CHC-C1C	2.29	1.43	1.38
19	4	314	CLA	CHC-C1C	2.29	1.43	1.38
19	b	823	CLA	CMD-C2D	-2.29	1.46	1.50
19	1	311	CLA	CHC-C1C	2.29	1.43	1.38
19	a	828	CLA	CHC-C1C	2.28	1.43	1.38
19	1	314	CLA	CHC-C1C	2.28	1.43	1.38
19	4	315	CLA	CHC-C1C	2.28	1.43	1.38
19	2	313	CLA	CHC-C1C	2.28	1.43	1.38
19	a	832	CLA	C3B-C4B	2.28	1.49	1.42
19	b	820	CLA	C3B-C4B	2.28	1.49	1.42
17	4	305	XAT	O4-C5	-2.28	1.43	1.46
19	4	309	CLA	CHC-C1C	2.28	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	808	CLA	C3B-C4B	2.28	1.49	1.42
19	a	814	CLA	CHC-C1C	2.28	1.43	1.38
19	l	202	CLA	CHC-C1C	2.28	1.43	1.38
19	b	828	CLA	C3B-C4B	2.28	1.49	1.42
25	a	846	LHG	O8-C23	2.28	1.40	1.33
19	3	310	CLA	C3B-C4B	2.28	1.49	1.42
19	a	811	CLA	CHC-C1C	2.28	1.43	1.38
19	j	102	CLA	CHC-C1C	2.28	1.43	1.38
19	b	809	CLA	CMD-C2D	-2.28	1.46	1.50
19	l	204	CLA	CHC-C1C	2.28	1.43	1.38
19	5	310	CLA	CHC-C1C	2.28	1.43	1.38
19	b	824	CLA	CHC-C1C	2.28	1.43	1.38
19	4	310	CLA	CHC-C1C	2.28	1.43	1.38
19	a	805	CLA	CHC-C1C	2.28	1.43	1.38
19	a	816	CLA	CHC-C1C	2.28	1.43	1.38
19	a	842	CLA	CHC-C1C	2.28	1.43	1.38
19	a	839	CLA	CHC-C1C	2.28	1.43	1.38
19	a	832	CLA	CHC-C1C	2.27	1.43	1.38
19	b	831	CLA	CHC-C1C	2.27	1.43	1.38
19	f	803	CLA	CHC-C1C	2.27	1.43	1.38
19	1	306	CLA	C3B-C4B	2.27	1.49	1.42
19	a	803	CLA	CHC-C1C	2.27	1.43	1.38
19	l	203	CLA	CHC-C1C	2.27	1.43	1.38
19	b	803	CLA	C3B-C4B	2.27	1.49	1.42
19	b	818	CLA	MG-NB	-2.27	2.01	2.05
25	a	846	LHG	O7-C7	2.27	1.40	1.34
19	2	312	CLA	CHC-C1C	2.27	1.43	1.38
19	a	838	CLA	C3B-C4B	2.27	1.49	1.42
19	4	317	CLA	CHC-C1C	2.27	1.43	1.38
19	a	806	CLA	C1D-ND	2.27	1.40	1.37
17	3	303	XAT	O4-C5	-2.27	1.43	1.46
19	4	307	CLA	CHC-C1C	2.27	1.43	1.38
19	a	824	CLA	CHC-C1C	2.26	1.43	1.38
19	b	827	CLA	C3B-C4B	2.26	1.49	1.42
17	2	303	XAT	O4-C5	-2.26	1.43	1.46
19	b	828	CLA	CHC-C1C	2.26	1.43	1.38
19	1	305	CLA	C3B-C4B	2.26	1.49	1.42
19	5	305	CLA	CHC-C1C	2.26	1.43	1.38
19	a	840	CLA	CHC-C1C	2.26	1.43	1.38
19	b	804	CLA	CHC-C1C	2.26	1.43	1.38
19	b	824	CLA	C3B-C4B	2.26	1.49	1.42
19	a	817	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	841	CLA	CHC-C1C	2.26	1.43	1.38
19	a	834	CLA	CHC-C1C	2.26	1.43	1.38
19	b	801	CLA	CMB-C2B	-2.26	1.46	1.50
19	a	812	CLA	CHC-C1C	2.26	1.43	1.38
17	a	852	XAT	O24-C25	-2.26	1.43	1.46
19	5	307	CLA	CHC-C1C	2.25	1.43	1.38
17	2	301	XAT	O4-C5	-2.25	1.43	1.46
19	3	312	CLA	CHC-C1C	2.25	1.43	1.38
19	a	810	CLA	C3B-C4B	2.25	1.49	1.42
19	2	310	CLA	CHC-C1C	2.25	1.43	1.38
19	a	824	CLA	CMD-C2D	-2.25	1.46	1.50
19	b	840	CLA	CMB-C2B	-2.25	1.46	1.50
19	1	313	CLA	CHC-C1C	2.25	1.43	1.38
19	3	314	CLA	CHC-C1C	2.25	1.43	1.38
19	a	803	CLA	C3B-C4B	2.25	1.49	1.42
25	b	849	LHG	O7-C7	2.25	1.40	1.34
19	b	810	CLA	CMB-C2B	-2.25	1.46	1.50
19	b	819	CLA	C3B-C4B	2.25	1.49	1.42
19	4	306	CLA	CHC-C1C	2.25	1.43	1.38
17	2	305	XAT	O4-C5	-2.24	1.43	1.46
17	3	304	XAT	O24-C25	-2.24	1.43	1.46
19	a	825	CLA	CHC-C1C	2.24	1.43	1.38
19	b	831	CLA	MG-NB	-2.24	2.01	2.05
19	3	310	CLA	CHC-C1C	2.24	1.43	1.38
19	f	802	CLA	CHC-C1C	2.24	1.43	1.38
18	1	301	A1L1G	C38-C39	2.24	1.41	1.35
19	3	307	CLA	CMD-C2D	-2.24	1.46	1.50
19	a	830	CLA	CHC-C1C	2.24	1.43	1.38
19	b	822	CLA	CHC-C1C	2.24	1.43	1.38
19	a	836	CLA	CHC-C1C	2.24	1.43	1.38
19	1	305	CLA	CHC-C1C	2.24	1.43	1.38
19	b	824	CLA	CMD-C2D	-2.23	1.46	1.50
19	2	314	CLA	CHC-C1C	2.23	1.43	1.38
19	b	823	CLA	CHC-C1C	2.23	1.43	1.38
19	a	807	CLA	C3B-C4B	2.23	1.49	1.42
19	2	307	CLA	CMB-C2B	-2.23	1.46	1.50
19	b	803	CLA	CHC-C1C	2.23	1.43	1.38
19	a	823	CLA	CHC-C1C	2.23	1.43	1.38
19	a	806	CLA	CAA-C2A	-2.23	1.50	1.54
19	a	838	CLA	CHC-C1C	2.23	1.42	1.38
19	a	801	CLA	CMC-C2C	-2.23	1.46	1.50
17	4	304	XAT	O4-C5	-2.23	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	305	CLA	CMD-C2D	-2.22	1.46	1.50
19	b	821	CLA	CHC-C1C	2.22	1.42	1.38
19	a	810	CLA	CMD-C2D	-2.22	1.46	1.50
17	3	301	XAT	O4-C5	-2.22	1.43	1.46
19	b	841	CLA	C3B-C4B	2.22	1.49	1.42
19	a	831	CLA	C3B-C4B	2.22	1.49	1.42
19	2	306	CLA	CHC-C1C	2.22	1.42	1.38
19	a	821	CLA	CHC-C1C	2.22	1.42	1.38
19	b	830	CLA	MG-NB	-2.22	2.01	2.05
19	b	831	CLA	CMB-C2B	-2.22	1.46	1.50
19	5	308	CLA	CHC-C1C	2.21	1.42	1.38
19	a	830	CLA	CMD-C2D	-2.21	1.46	1.50
17	3	304	XAT	O4-C5	-2.21	1.43	1.46
19	4	316	CLA	CHC-C1C	2.21	1.42	1.38
19	b	801	CLA	CHC-C1C	2.21	1.42	1.38
19	3	308	CLA	CHC-C1C	2.21	1.42	1.38
17	2	305	XAT	O24-C25	-2.21	1.43	1.46
19	b	820	CLA	CHC-C1C	2.21	1.42	1.38
17	4	303	XAT	O4-C5	-2.21	1.43	1.46
17	5	304	XAT	O4-C5	-2.20	1.43	1.46
19	a	804	CLA	CMC-C2C	-2.20	1.46	1.50
19	b	825	CLA	CHC-C1C	2.20	1.42	1.38
19	2	310	CLA	CMB-C2B	-2.20	1.46	1.50
19	a	835	CLA	CHC-C1C	2.20	1.42	1.38
19	a	828	CLA	CMC-C2C	-2.20	1.46	1.50
19	b	810	CLA	C3B-C4B	2.20	1.49	1.42
19	1	306	CLA	CHC-C1C	2.20	1.42	1.38
19	a	810	CLA	CHC-C1C	2.20	1.42	1.38
18	3	306	A1L1G	C29-C30	-2.20	1.40	1.45
19	4	311	CLA	CHC-C1C	2.20	1.42	1.38
19	4	311	CLA	CMB-C2B	-2.19	1.46	1.50
19	b	808	CLA	CHC-C1C	2.19	1.42	1.38
19	2	310	CLA	MG-NB	-2.19	2.01	2.05
17	1	302	XAT	O24-C25	-2.19	1.43	1.46
19	a	832	CLA	CMB-C2B	-2.19	1.46	1.50
17	5	301	XAT	O24-C25	-2.19	1.43	1.46
19	b	830	CLA	C3B-C4B	2.19	1.49	1.42
19	a	832	CLA	MG-NB	-2.19	2.01	2.05
17	2	304	XAT	O24-C25	-2.19	1.43	1.46
19	a	803	CLA	MG-NB	-2.19	2.01	2.05
19	b	803	CLA	CMD-C2D	-2.19	1.46	1.50
17	4	303	XAT	O24-C25	-2.19	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	811	CLA	CHC-C1C	2.19	1.42	1.38
19	b	829	CLA	CMD-C2D	-2.18	1.46	1.50
19	b	838	CLA	CMD-C2D	-2.18	1.46	1.50
19	a	833	CLA	MG-NB	-2.18	2.01	2.05
19	a	836	CLA	CMB-C2B	-2.18	1.46	1.50
18	5	303	A1L1G	C29-C30	-2.18	1.40	1.45
19	a	801	CLA	C3B-C4B	2.18	1.49	1.42
19	2	310	CLA	CMD-C2D	-2.17	1.46	1.50
17	j	101	XAT	O4-C5	-2.17	1.43	1.46
17	2	302	XAT	O24-C25	-2.17	1.43	1.46
19	a	828	CLA	MG-NB	-2.17	2.01	2.05
19	a	801	CLA	CHC-C1C	2.17	1.42	1.38
19	3	307	CLA	MG-NB	-2.17	2.01	2.05
19	a	831	CLA	MG-NB	-2.17	2.01	2.05
19	b	818	CLA	CMB-C2B	-2.17	1.46	1.50
19	b	801	CLA	CMD-C2D	-2.17	1.46	1.50
17	4	301	XAT	O4-C5	-2.16	1.43	1.46
19	b	839	CLA	CMD-C2D	-2.16	1.46	1.50
19	b	804	CLA	MG-NB	-2.16	2.01	2.05
19	b	815	CLA	CMD-C2D	-2.16	1.46	1.50
19	a	820	CLA	MG-NB	-2.16	2.01	2.05
19	a	807	CLA	MG-NB	-2.16	2.01	2.05
19	a	807	CLA	CHC-C1C	2.16	1.42	1.38
19	b	835	CLA	CMB-C2B	-2.15	1.46	1.50
18	1	301	A1L1G	C35-C34	2.15	1.40	1.35
19	2	307	CLA	CHC-C1C	2.15	1.42	1.38
19	a	806	CLA	C1B-NB	-2.15	1.35	1.37
18	1	301	A1L1G	C29-C30	-2.15	1.40	1.45
19	j	103	CLA	CHC-C1C	2.15	1.42	1.38
19	a	812	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	832	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	820	CLA	CMB-C2B	-2.15	1.46	1.50
19	b	819	CLA	CMB-C2B	-2.15	1.46	1.50
19	b	826	CLA	MG-NB	-2.15	2.01	2.05
19	b	808	CLA	MG-NB	-2.15	2.01	2.05
19	b	820	CLA	MG-NB	-2.15	2.01	2.05
19	5	312	CLA	MG-NB	-2.15	2.01	2.05
19	a	842	CLA	CMD-C2D	-2.15	1.46	1.50
17	2	303	XAT	O24-C25	-2.15	1.43	1.46
17	3	303	XAT	O24-C25	-2.14	1.43	1.46
17	2	301	XAT	O24-C25	-2.14	1.43	1.46
19	a	803	CLA	CMB-C2B	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	j	101	XAT	O24-C25	-2.14	1.43	1.46
19	b	829	CLA	CMB-C2B	-2.14	1.46	1.50
17	5	304	XAT	O24-C25	-2.14	1.43	1.46
19	1	307	CLA	MG-NB	-2.14	2.01	2.05
17	4	302	XAT	O4-C5	-2.13	1.43	1.46
19	b	825	CLA	MG-NB	-2.13	2.01	2.05
19	a	826	CLA	MG-NB	-2.13	2.01	2.05
19	b	827	CLA	CHC-C1C	2.13	1.42	1.38
19	4	308	CLA	MG-NB	-2.13	2.01	2.05
19	4	317	CLA	CMB-C2B	-2.13	1.46	1.50
19	b	812	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	810	CLA	CHC-C1C	2.13	1.42	1.38
18	3	302	A1L1G	C35-C34	2.13	1.40	1.35
19	2	307	CLA	MG-NB	-2.13	2.01	2.05
19	2	316	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	823	CLA	MG-NB	-2.13	2.01	2.05
19	a	821	CLA	CMD-C2D	-2.12	1.46	1.50
19	3	307	CLA	CMB-C2B	-2.12	1.46	1.50
19	b	816	CLA	CMC-C2C	-2.12	1.46	1.50
19	b	817	CLA	MG-NB	-2.12	2.01	2.05
19	1	313	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	824	CLA	MG-NB	-2.12	2.01	2.05
19	a	838	CLA	MG-NB	-2.12	2.01	2.05
25	m	101	LHG	P-O6	2.12	1.67	1.59
19	b	826	CLA	CMD-C2D	-2.12	1.46	1.50
17	2	304	XAT	O4-C5	-2.12	1.43	1.46
19	b	819	CLA	CHC-C1C	2.12	1.42	1.38
19	i	102	CLA	CMD-C2D	-2.12	1.46	1.50
25	b	849	LHG	P-O6	2.12	1.67	1.59
19	a	810	CLA	MG-NB	-2.11	2.01	2.05
19	b	836	CLA	MG-NB	-2.11	2.01	2.05
19	a	816	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	827	CLA	MG-NB	-2.11	2.01	2.05
19	b	833	CLA	MG-NB	-2.11	2.01	2.05
25	a	845	LHG	P-O6	2.11	1.67	1.59
19	b	814	CLA	MG-NB	-2.11	2.01	2.05
19	a	826	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	801	CLA	MG-NB	-2.11	2.01	2.05
19	a	802	CLA	MG-NB	-2.11	2.01	2.05
19	3	309	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	827	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	802	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	313	CLA	MG-NB	-2.10	2.01	2.05
17	1	303	XAT	O24-C25	-2.10	1.43	1.46
19	a	834	CLA	CMD-C2D	-2.10	1.46	1.50
17	4	302	XAT	O24-C25	-2.10	1.43	1.46
19	b	807	CLA	MG-NB	-2.10	2.01	2.05
19	l	203	CLA	CMB-C2B	-2.10	1.46	1.50
19	2	309	CLA	MG-NB	-2.10	2.01	2.05
17	4	305	XAT	O24-C25	-2.10	1.43	1.46
19	a	839	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	808	CLA	CMB-C2B	-2.10	1.46	1.50
19	4	314	CLA	MG-NB	-2.10	2.01	2.05
19	a	806	CLA	MG-ND	-2.10	2.01	2.05
19	a	824	CLA	CMB-C2B	-2.10	1.46	1.50
19	3	311	CLA	MG-NB	-2.10	2.01	2.05
19	b	841	CLA	MG-NB	-2.10	2.01	2.05
19	a	822	CLA	CMB-C2B	-2.10	1.46	1.50
19	a	816	CLA	MG-NB	-2.10	2.01	2.05
19	b	825	CLA	CMB-C2B	-2.10	1.46	1.50
19	1	309	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	837	CLA	CMB-C2B	-2.10	1.46	1.50
19	1	310	CLA	MG-NB	-2.10	2.01	2.05
19	3	310	CLA	MG-NB	-2.10	2.01	2.05
19	4	313	CLA	CMB-C2B	-2.09	1.46	1.50
19	b	820	CLA	CMD-C2D	-2.09	1.46	1.50
19	4	308	CLA	CMD-C2D	-2.09	1.46	1.50
19	5	308	CLA	MG-NB	-2.09	2.01	2.05
19	a	822	CLA	MG-NB	-2.09	2.01	2.05
19	b	803	CLA	CMC-C2C	-2.09	1.46	1.50
19	b	835	CLA	MG-NB	-2.09	2.01	2.05
19	a	808	CLA	MG-NB	-2.09	2.01	2.05
19	b	809	CLA	CMC-C2C	-2.09	1.46	1.50
19	b	810	CLA	MG-NB	-2.09	2.01	2.05
19	5	307	CLA	MG-NB	-2.09	2.01	2.05
19	a	825	CLA	MG-NB	-2.09	2.01	2.05
19	a	807	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	824	CLA	MG-NB	-2.09	2.01	2.05
19	2	306	CLA	CMD-C2D	-2.09	1.46	1.50
19	b	832	CLA	MG-NB	-2.09	2.01	2.05
19	3	314	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	834	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	835	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	806	CLA	C4B-NB	2.08	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	828	CLA	MG-NB	-2.08	2.01	2.05
19	2	312	CLA	MG-NB	-2.08	2.01	2.05
19	5	312	CLA	CMB-C2B	-2.08	1.46	1.50
19	2	314	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	836	CLA	CMD-C2D	-2.08	1.46	1.50
18	3	302	A1L1G	C38-C39	2.08	1.40	1.35
19	l	204	CLA	CMC-C2C	-2.08	1.46	1.50
19	3	315	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	807	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	814	CLA	MG-NB	-2.08	2.01	2.05
19	1	306	CLA	MG-NB	-2.08	2.01	2.05
19	4	312	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	829	CLA	MG-NB	-2.08	2.01	2.05
19	a	854	CLA	MG-NB	-2.08	2.01	2.05
19	b	809	CLA	CMB-C2B	-2.07	1.46	1.50
19	b	808	CLA	CMD-C2D	-2.07	1.46	1.50
19	2	312	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	813	CLA	MG-NB	-2.07	2.01	2.05
19	b	839	CLA	MG-NB	-2.07	2.01	2.05
19	j	102	CLA	CMD-C2D	-2.07	1.46	1.50
19	3	309	CLA	MG-NB	-2.07	2.01	2.05
19	4	309	CLA	MG-NB	-2.07	2.01	2.05
19	f	802	CLA	MG-NB	-2.07	2.01	2.05
19	4	307	CLA	CMD-C2D	-2.07	1.46	1.50
19	a	844	CLA	MG-NB	-2.07	2.01	2.05
19	1	307	CLA	CMB-C2B	-2.07	1.46	1.50
19	4	314	CLA	CMD-C2D	-2.07	1.46	1.50
19	2	316	CLA	MG-NB	-2.07	2.01	2.05
19	b	816	CLA	MG-NB	-2.07	2.01	2.05
19	a	838	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	810	CLA	CMD-C2D	-2.07	1.46	1.50
19	4	311	CLA	MG-NB	-2.07	2.01	2.05
19	a	830	CLA	MG-NB	-2.07	2.01	2.05
18	3	306	A1L1G	C38-C39	2.07	1.40	1.35
19	b	821	CLA	CMD-C2D	-2.07	1.46	1.50
19	3	314	CLA	MG-NB	-2.07	2.01	2.05
19	b	812	CLA	MG-NB	-2.07	2.01	2.05
19	2	314	CLA	CMC-C2C	-2.06	1.46	1.50
19	b	813	CLA	CMD-C2D	-2.06	1.46	1.50
19	5	315	CLA	MG-NB	-2.06	2.01	2.05
19	b	814	CLA	CMD-C2D	-2.06	1.46	1.50
19	l	203	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	802	CLA	CMD-C2D	-2.06	1.46	1.50
19	l	202	CLA	CMB-C2B	-2.06	1.46	1.50
17	3	305	XAT	O24-C25	-2.06	1.43	1.46
19	b	801	CLA	MG-NB	-2.06	2.01	2.05
19	a	817	CLA	CMB-C2B	-2.06	1.46	1.50
19	5	311	CLA	CMD-C2D	-2.06	1.46	1.50
19	l	204	CLA	CMB-C2B	-2.06	1.46	1.50
19	3	312	CLA	CMD-C2D	-2.06	1.46	1.50
19	b	841	CLA	CMB-C2B	-2.06	1.46	1.50
19	l	203	CLA	CMC-C2C	-2.06	1.46	1.50
19	b	840	CLA	MG-NB	-2.06	2.01	2.05
19	b	826	CLA	CMB-C2B	-2.06	1.46	1.50
19	b	827	CLA	MG-NB	-2.06	2.01	2.05
19	l	202	CLA	MG-NB	-2.06	2.01	2.05
19	a	810	CLA	CMB-C2B	-2.06	1.46	1.50
25	a	846	LHG	P-O6	2.06	1.67	1.59
19	b	838	CLA	MG-NB	-2.06	2.01	2.05
21	b	851	DGD	C1E-C2E	2.06	1.58	1.52
19	3	313	CLA	MG-NB	-2.06	2.01	2.05
19	a	842	CLA	CMB-C2B	-2.05	1.46	1.50
19	b	833	CLA	CMD-C2D	-2.05	1.46	1.50
19	b	821	CLA	MG-NB	-2.05	2.01	2.05
19	2	308	CLA	CMD-C2D	-2.05	1.46	1.50
19	1	305	CLA	CMB-C2B	-2.05	1.46	1.50
19	4	310	CLA	CMD-C2D	-2.05	1.46	1.50
19	5	311	CLA	MG-NB	-2.05	2.01	2.05
19	a	815	CLA	CMD-C2D	-2.05	1.46	1.50
19	b	818	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	811	CLA	MG-NB	-2.05	2.01	2.05
19	4	315	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	819	CLA	CMC-C2C	-2.05	1.46	1.50
19	b	822	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	840	CLA	CMD-C2D	-2.05	1.46	1.50
19	5	308	CLA	CMD-C2D	-2.05	1.46	1.50
19	1	305	CLA	MG-NB	-2.05	2.01	2.05
19	a	815	CLA	MG-NB	-2.05	2.01	2.05
19	a	817	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	803	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	818	CLA	CMC-C2C	-2.05	1.46	1.50
19	a	804	CLA	CMD-C2D	-2.05	1.46	1.50
19	1	312	CLA	CMB-C2B	-2.05	1.46	1.50
19	a	822	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	808	CLA	CMD-C2D	-2.04	1.46	1.50
19	3	314	CLA	CMC-C2C	-2.04	1.46	1.50
19	f	803	CLA	CMD-C2D	-2.04	1.46	1.50
19	1	311	CLA	MG-NB	-2.04	2.01	2.05
19	a	812	CLA	MG-NB	-2.04	2.01	2.05
19	1	309	CLA	CMB-C2B	-2.04	1.46	1.50
19	f	802	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	819	CLA	MG-NB	-2.04	2.01	2.05
19	b	837	CLA	MG-NB	-2.04	2.01	2.05
19	a	805	CLA	CMD-C2D	-2.04	1.46	1.50
19	3	308	CLA	CMD-C2D	-2.04	1.46	1.50
19	3	313	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	831	CLA	CMC-C2C	-2.04	1.46	1.50
19	l	202	CLA	CMD-C2D	-2.04	1.46	1.50
19	4	314	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	814	CLA	CMD-C2D	-2.04	1.46	1.50
19	1	306	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	819	CLA	CMD-C2D	-2.04	1.46	1.50
19	b	828	CLA	CMD-C2D	-2.04	1.46	1.50
19	j	103	CLA	CMD-C2D	-2.04	1.46	1.50
19	3	310	CLA	CMD-C2D	-2.04	1.46	1.50
19	b	805	CLA	MG-NB	-2.04	2.01	2.05
19	a	840	CLA	CMB-C2B	-2.04	1.46	1.50
19	2	308	CLA	MG-NB	-2.04	2.01	2.05
19	a	813	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	816	CLA	CMC-C2C	-2.04	1.46	1.50
19	4	310	CLA	MG-NB	-2.04	2.01	2.05
19	5	310	CLA	CMD-C2D	-2.04	1.46	1.50
19	2	309	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	802	CLA	CMD-C2D	-2.04	1.46	1.50
19	b	819	CLA	MG-NB	-2.04	2.01	2.05
19	2	314	CLA	CMB-C2B	-2.04	1.46	1.50
19	2	315	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	835	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	804	CLA	MG-NB	-2.04	2.01	2.05
19	a	818	CLA	CMB-C2B	-2.04	1.46	1.50
19	b	816	CLA	CMD-C2D	-2.04	1.46	1.50
19	2	316	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	837	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	809	CLA	CMD-C2D	-2.03	1.46	1.50
19	1	309	CLA	MG-NB	-2.03	2.01	2.05
19	b	819	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	830	CLA	CHC-C1C	2.03	1.42	1.38
19	4	312	CLA	MG-NB	-2.03	2.01	2.05
19	a	854	CLA	CMB-C2B	-2.03	1.46	1.50
19	4	317	CLA	CMD-C2D	-2.03	1.46	1.50
19	a	831	CLA	CMD-C2D	-2.03	1.46	1.50
19	a	809	CLA	MG-NB	-2.03	2.01	2.05
19	a	841	CLA	MG-NB	-2.03	2.01	2.05
19	2	311	CLA	CMD-C2D	-2.03	1.46	1.50
19	1	310	CLA	CMB-C2B	-2.03	1.46	1.50
19	b	825	CLA	CMD-C2D	-2.03	1.46	1.50
19	1	204	CLA	MG-NB	-2.03	2.01	2.05
19	5	309	CLA	MG-NB	-2.03	2.01	2.05
19	b	804	CLA	CMD-C2D	-2.03	1.46	1.50
19	5	307	CLA	CMD-C2D	-2.03	1.46	1.50
19	4	312	CLA	CMB-C2B	-2.03	1.46	1.50
19	b	812	CLA	CMB-C2B	-2.03	1.46	1.50
19	a	829	CLA	MG-NB	-2.03	2.01	2.05
19	5	315	CLA	CMB-C2B	-2.03	1.46	1.50
19	a	837	CLA	MG-NB	-2.03	2.01	2.05
19	b	809	CLA	MG-NB	-2.03	2.01	2.05
19	2	309	CLA	CMB-C2B	-2.03	1.46	1.50
19	a	831	CLA	CHC-C1C	2.03	1.42	1.38
19	5	310	CLA	MG-NB	-2.03	2.01	2.05
19	a	823	CLA	MG-NB	-2.03	2.01	2.05
19	3	308	CLA	CMB-C2B	-2.02	1.46	1.50
19	2	306	CLA	CMB-C2B	-2.02	1.46	1.50
19	1	314	CLA	CMB-C2B	-2.02	1.46	1.50
19	2	307	CLA	CMD-C2D	-2.02	1.46	1.50
19	j	103	CLA	CMB-C2B	-2.02	1.46	1.50
19	a	839	CLA	MG-NB	-2.02	2.01	2.05
19	1	312	CLA	CMD-C2D	-2.02	1.46	1.50
19	a	811	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	814	CLA	CMC-C2C	-2.02	1.46	1.50
19	1	307	CLA	CMD-C2D	-2.02	1.46	1.50
19	1	310	CLA	CMD-C2D	-2.02	1.46	1.50
19	a	841	CLA	CMC-C2C	-2.02	1.46	1.50
18	5	303	A1L1G	C38-C39	2.02	1.40	1.35
19	a	842	CLA	MG-NB	-2.02	2.01	2.05
19	b	813	CLA	CMB-C2B	-2.02	1.46	1.50
19	b	822	CLA	MG-NB	-2.02	2.01	2.05
19	b	817	CLA	CMD-C2D	-2.02	1.46	1.50
19	1	313	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	815	CLA	CMB-C2B	-2.02	1.46	1.50
19	5	305	CLA	MG-NB	-2.02	2.01	2.05
19	4	306	CLA	MG-NB	-2.02	2.01	2.05
19	2	313	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	840	CLA	CMD-C2D	-2.02	1.46	1.50
26	m	102	BCR	C33-C5	-2.02	1.47	1.50
19	5	313	CLA	CMD-C2D	-2.02	1.46	1.50
19	a	854	CLA	CMD-C2D	-2.02	1.46	1.50
19	l	203	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	811	CLA	MG-NB	-2.02	2.01	2.05
19	1	306	CLA	CMD-C2D	-2.02	1.46	1.50
19	a	814	CLA	CMC-C2C	-2.02	1.46	1.50
19	i	102	CLA	CMC-C2C	-2.02	1.46	1.50
19	a	821	CLA	MG-NB	-2.02	2.01	2.05
19	3	314	CLA	CMB-C2B	-2.02	1.46	1.50
19	a	820	CLA	CMD-C2D	-2.02	1.46	1.50
19	2	315	CLA	MG-NB	-2.02	2.01	2.05
19	l	204	CLA	CMD-C2D	-2.01	1.46	1.50
19	1	314	CLA	CMD-C2D	-2.01	1.46	1.50
19	1	305	CLA	CMD-C2D	-2.01	1.46	1.50
19	j	102	CLA	CMB-C2B	-2.01	1.46	1.50
19	f	803	CLA	MG-NB	-2.01	2.01	2.05
19	5	311	CLA	CMC-C2C	-2.01	1.46	1.50
19	5	314	CLA	CMD-C2D	-2.01	1.46	1.50
19	4	315	CLA	CMB-C2B	-2.01	1.46	1.50
19	b	824	CLA	CMC-C2C	-2.01	1.46	1.50
19	3	311	CLA	CMB-C2B	-2.01	1.46	1.50
19	4	315	CLA	MG-NB	-2.01	2.01	2.05
19	b	806	CLA	MG-NB	-2.01	2.01	2.05
19	2	312	CLA	CMC-C2C	-2.01	1.46	1.50
19	b	839	CLA	CMB-C2B	-2.01	1.46	1.50
19	3	315	CLA	CMB-C2B	-2.01	1.46	1.50
19	4	313	CLA	CMD-C2D	-2.01	1.46	1.50
19	a	817	CLA	MG-NB	-2.01	2.01	2.05
19	5	307	CLA	CMB-C2B	-2.01	1.46	1.50
19	j	102	CLA	MG-NB	-2.01	2.01	2.05
19	5	306	CLA	CMD-C2D	-2.01	1.46	1.50
19	a	841	CLA	CMD-C2D	-2.01	1.46	1.50
19	4	306	CLA	CMD-C2D	-2.01	1.46	1.50
21	b	851	DGD	O3D-C3D	-2.01	1.38	1.43
19	2	316	CLA	CMB-C2B	-2.01	1.46	1.50
19	a	833	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	811	CLA	CMD-C2D	-2.01	1.46	1.50
19	i	102	CLA	CMB-C2B	-2.01	1.46	1.50
19	3	313	CLA	CMB-C2B	-2.00	1.46	1.50
19	a	829	CLA	CMD-C2D	-2.00	1.46	1.50
19	a	844	CLA	CMD-C2D	-2.00	1.46	1.50
19	a	838	CLA	CMB-C2B	-2.00	1.46	1.50
19	4	317	CLA	MG-NB	-2.00	2.01	2.05
19	3	312	CLA	MG-NB	-2.00	2.01	2.05
19	a	834	CLA	CMB-C2B	-2.00	1.46	1.50
19	3	315	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	827	CLA	CMD-C2D	-2.00	1.46	1.50
19	a	823	CLA	CMD-C2D	-2.00	1.46	1.50
19	a	828	CLA	CMD-C2D	-2.00	1.46	1.50
19	b	805	CLA	CMD-C2D	-2.00	1.46	1.50
19	3	311	CLA	CMD-C2D	-2.00	1.46	1.50
19	1	311	CLA	CMD-C2D	-2.00	1.46	1.50

All (1624) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	318	DGD	C6E-C5E-C4E	-8.96	91.01	113.02
23	1	304	A1L1F	C17-C20-C25	-8.25	108.73	122.30
17	5	304	XAT	C38-C25-C24	7.25	122.38	114.24
17	3	305	XAT	C38-C25-C24	7.25	122.38	114.24
17	1	303	XAT	C38-C25-C24	7.22	122.36	114.24
19	b	840	CLA	C4A-NA-C1A	7.22	109.97	106.68
17	4	305	XAT	C38-C25-C24	7.22	122.35	114.24
19	a	806	CLA	C4A-NA-C1A	7.20	109.97	106.68
19	l	203	CLA	C4A-NA-C1A	7.19	109.96	106.68
17	a	852	XAT	C15-C14-C13	-7.18	117.21	127.28
17	j	101	XAT	C38-C25-C24	7.16	122.28	114.24
26	f	801	BCR	C24-C23-C22	-7.12	115.70	126.23
19	b	803	CLA	C4A-NA-C1A	7.11	109.92	106.68
17	5	304	XAT	C18-C5-C4	7.05	122.16	114.24
19	a	823	CLA	C4A-NA-C1A	7.04	109.89	106.68
19	b	809	CLA	C4A-NA-C1A	7.04	109.89	106.68
17	5	301	XAT	C38-C25-C26	-7.03	110.73	122.30
19	4	310	CLA	C4A-NA-C1A	7.02	109.88	106.68
17	4	304	XAT	C38-C25-C24	7.02	122.12	114.24
17	2	301	XAT	C18-C5-C6	-7.01	110.76	122.30
19	a	835	CLA	C4A-NA-C1A	7.01	109.88	106.68
17	3	304	XAT	C38-C25-C24	7.01	122.11	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	810	CLA	C4A-NA-C1A	6.98	109.86	106.68
17	4	305	XAT	C38-C25-C26	-6.96	110.84	122.30
19	a	826	CLA	C4A-NA-C1A	6.95	109.85	106.68
19	a	833	CLA	C4A-NA-C1A	6.95	109.85	106.68
19	a	821	CLA	C4A-NA-C1A	6.94	109.85	106.68
17	3	304	XAT	C38-C25-C26	-6.93	110.90	122.30
19	j	103	CLA	C4A-NA-C1A	6.92	109.84	106.68
17	1	302	XAT	C38-C25-C24	6.90	121.99	114.24
19	a	828	CLA	C4A-NA-C1A	6.89	109.82	106.68
19	b	821	CLA	C4A-NA-C1A	6.87	109.81	106.68
19	4	316	CLA	C4A-NA-C1A	6.87	109.81	106.68
19	b	801	CLA	C4A-NA-C1A	6.85	109.80	106.68
17	5	304	XAT	C6-C7-C8	-6.84	111.53	125.99
17	a	852	XAT	C38-C25-C24	6.84	121.93	114.24
17	4	303	XAT	C38-C25-C24	6.84	121.92	114.24
17	5	304	XAT	C18-C5-C6	-6.84	111.05	122.30
17	2	304	XAT	C38-C25-C24	6.83	121.91	114.24
19	b	806	CLA	C4A-NA-C1A	6.83	109.79	106.68
19	b	822	CLA	C4A-NA-C1A	6.82	109.79	106.68
19	b	805	CLA	C4A-NA-C1A	6.82	109.79	106.68
17	3	304	XAT	C18-C5-C6	-6.81	111.10	122.30
17	j	101	XAT	C38-C25-C26	-6.80	111.11	122.30
19	2	316	CLA	C4A-NA-C1A	6.80	109.78	106.68
19	1	308	CLA	C4A-NA-C1A	6.79	109.78	106.68
19	b	815	CLA	C4A-NA-C1A	6.79	109.78	106.68
19	4	317	CLA	C4A-NA-C1A	6.79	109.78	106.68
19	b	811	CLA	C4A-NA-C1A	6.78	109.77	106.68
19	f	802	CLA	C4A-NA-C1A	6.78	109.77	106.68
26	i	101	BCR	C24-C23-C22	-6.78	116.20	126.23
19	b	828	CLA	C4A-NA-C1A	6.77	109.77	106.68
19	b	813	CLA	C4A-NA-C1A	6.76	109.76	106.68
19	1	306	CLA	C4A-NA-C1A	6.75	109.76	106.68
19	a	807	CLA	C4A-NA-C1A	6.75	109.76	106.68
19	b	825	CLA	C4A-NA-C1A	6.75	109.76	106.68
19	a	801	CLA	C4A-NA-C1A	6.75	109.76	106.68
17	2	304	XAT	C18-C5-C4	6.75	121.82	114.24
17	4	302	XAT	C38-C25-C24	6.74	121.82	114.24
19	a	825	CLA	C4A-NA-C1A	6.74	109.75	106.68
19	4	311	CLA	C4A-NA-C1A	6.74	109.75	106.68
19	a	840	CLA	C4A-NA-C1A	6.74	109.75	106.68
17	5	302	XAT	C18-C5-C6	-6.74	111.21	122.30
17	3	303	XAT	C38-C25-C24	6.73	121.80	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	808	CLA	C4A-NA-C1A	6.73	109.75	106.68
19	l	204	CLA	C4A-NA-C1A	6.72	109.75	106.68
19	5	310	CLA	C4A-NA-C1A	6.72	109.75	106.68
19	a	812	CLA	C4A-NA-C1A	6.72	109.75	106.68
19	b	810	CLA	C4A-NA-C1A	6.72	109.74	106.68
19	a	841	CLA	C4A-NA-C1A	6.71	109.74	106.68
17	2	301	XAT	C18-C5-C4	6.71	121.78	114.24
19	4	315	CLA	C4A-NA-C1A	6.71	109.74	106.68
19	3	314	CLA	C4A-NA-C1A	6.71	109.74	106.68
19	2	311	CLA	C4A-NA-C1A	6.70	109.74	106.68
17	4	301	XAT	C31-C30-C29	-6.69	117.89	127.28
19	a	838	CLA	C4A-NA-C1A	6.69	109.73	106.68
17	3	301	XAT	C18-C5-C4	6.68	121.75	114.24
19	a	817	CLA	C4A-NA-C1A	6.68	109.73	106.68
19	b	807	CLA	C4A-NA-C1A	6.68	109.73	106.68
19	b	837	CLA	C4A-NA-C1A	6.68	109.73	106.68
17	2	303	XAT	C18-C5-C6	-6.68	111.31	122.30
17	4	301	XAT	C18-C5-C6	-6.67	111.32	122.30
17	4	303	XAT	C18-C5-C6	-6.67	111.32	122.30
19	3	313	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	a	831	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	a	805	CLA	C4A-NA-C1A	6.66	109.72	106.68
19	a	839	CLA	C4A-NA-C1A	6.66	109.72	106.68
17	5	304	XAT	C38-C25-C26	-6.65	111.35	122.30
19	2	312	CLA	C4A-NA-C1A	6.65	109.71	106.68
19	3	308	CLA	C4A-NA-C1A	6.65	109.71	106.68
19	5	306	CLA	C4A-NA-C1A	6.64	109.71	106.68
19	5	311	CLA	C4A-NA-C1A	6.64	109.71	106.68
19	a	809	CLA	C4A-NA-C1A	6.63	109.71	106.68
17	5	301	XAT	C38-C25-C24	6.63	121.69	114.24
19	3	312	CLA	C4A-NA-C1A	6.63	109.70	106.68
19	a	834	CLA	C4A-NA-C1A	6.63	109.70	106.68
17	3	305	XAT	C38-C25-C26	-6.63	111.39	122.30
19	5	313	CLA	C4A-NA-C1A	6.62	109.70	106.68
17	4	301	XAT	C18-C5-C4	6.62	121.68	114.24
17	2	305	XAT	C18-C5-C6	-6.62	111.40	122.30
17	4	303	XAT	C38-C25-C26	-6.62	111.41	122.30
19	1	305	CLA	C4A-NA-C1A	6.61	109.69	106.68
19	b	833	CLA	C4A-NA-C1A	6.61	109.69	106.68
26	a	850	BCR	C24-C23-C22	-6.61	116.46	126.23
17	2	303	XAT	C38-C25-C26	-6.60	111.44	122.30
19	5	314	CLA	C4A-NA-C1A	6.60	109.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	304	XAT	C18-C5-C6	-6.59	111.45	122.30
17	2	304	XAT	C38-C25-C26	-6.59	111.45	122.30
19	j	102	CLA	C4A-NA-C1A	6.59	109.68	106.68
19	a	811	CLA	C4A-NA-C1A	6.58	109.68	106.68
19	5	312	CLA	C4A-NA-C1A	6.57	109.68	106.68
19	l	202	CLA	C4A-NA-C1A	6.56	109.67	106.68
17	3	303	XAT	C18-C5-C6	-6.56	111.50	122.30
19	a	837	CLA	C4A-NA-C1A	6.56	109.67	106.68
17	j	101	XAT	C18-C5-C6	-6.56	111.50	122.30
17	3	301	XAT	C18-C5-C6	-6.56	111.51	122.30
19	4	307	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	f	803	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	a	844	CLA	C4A-NA-C1A	6.55	109.67	106.68
19	4	306	CLA	C4A-NA-C1A	6.54	109.66	106.68
19	a	842	CLA	C4A-NA-C1A	6.54	109.66	106.68
17	4	302	XAT	C18-C5-C4	6.54	121.59	114.24
19	a	804	CLA	C4A-NA-C1A	6.53	109.66	106.68
17	1	302	XAT	C38-C25-C26	-6.52	111.57	122.30
19	2	313	CLA	C4A-NA-C1A	6.52	109.65	106.68
19	4	314	CLA	C4A-NA-C1A	6.51	109.65	106.68
19	b	816	CLA	C4A-NA-C1A	6.51	109.65	106.68
19	a	829	CLA	C4A-NA-C1A	6.51	109.65	106.68
19	b	823	CLA	C4A-NA-C1A	6.51	109.65	106.68
17	3	303	XAT	C38-C25-C26	-6.51	111.59	122.30
19	2	307	CLA	C4A-NA-C1A	6.50	109.64	106.68
19	a	832	CLA	C4A-NA-C1A	6.49	109.64	106.68
19	1	307	CLA	C4A-NA-C1A	6.49	109.64	106.68
17	4	304	XAT	C18-C5-C6	-6.49	111.62	122.30
19	a	808	CLA	C4A-NA-C1A	6.49	109.64	106.68
19	a	854	CLA	C4A-NA-C1A	6.49	109.64	106.68
17	4	302	XAT	C18-C5-C6	-6.49	111.63	122.30
19	5	308	CLA	C4A-NA-C1A	6.48	109.64	106.68
19	a	827	CLA	C4A-NA-C1A	6.48	109.64	106.68
19	b	824	CLA	C4A-NA-C1A	6.47	109.63	106.68
19	4	309	CLA	C4A-NA-C1A	6.46	109.62	106.68
17	4	305	XAT	C18-C5-C6	-6.45	111.68	122.30
19	5	315	CLA	C4A-NA-C1A	6.45	109.62	106.68
19	b	814	CLA	C4A-NA-C1A	6.45	109.62	106.68
19	3	309	CLA	C4A-NA-C1A	6.45	109.62	106.68
19	a	836	CLA	C4A-NA-C1A	6.44	109.62	106.68
19	2	309	CLA	C4A-NA-C1A	6.44	109.61	106.68
17	1	302	XAT	C18-C5-C6	-6.43	111.72	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	j	101	XAT	C18-C5-C4	6.43	121.46	114.24
17	2	302	XAT	C18-C5-C6	-6.43	111.72	122.30
19	a	819	CLA	C4A-NA-C1A	6.42	109.61	106.68
17	2	302	XAT	C38-C25-C24	6.42	121.45	114.24
19	3	311	CLA	C4A-NA-C1A	6.42	109.61	106.68
19	a	830	CLA	C4A-NA-C1A	6.42	109.61	106.68
19	i	102	CLA	C4A-NA-C1A	6.41	109.60	106.68
17	4	302	XAT	C38-C25-C26	-6.41	111.75	122.30
19	a	822	CLA	C4A-NA-C1A	6.41	109.60	106.68
17	4	305	XAT	C31-C30-C29	-6.41	118.29	127.28
17	3	305	XAT	C18-C5-C6	-6.41	111.76	122.30
19	b	834	CLA	C4A-NA-C1A	6.40	109.60	106.68
19	1	313	CLA	C4A-NA-C1A	6.40	109.60	106.68
17	a	852	XAT	C38-C25-C26	-6.40	111.77	122.30
19	b	836	CLA	C4A-NA-C1A	6.40	109.60	106.68
17	5	302	XAT	C26-C27-C28	-6.40	112.46	125.99
17	3	305	XAT	C18-C5-C4	6.40	121.43	114.24
17	3	301	XAT	C38-C25-C26	-6.40	111.77	122.30
17	1	303	XAT	C18-C5-C6	-6.39	111.78	122.30
17	2	303	XAT	C38-C25-C24	6.39	121.42	114.24
17	4	304	XAT	C38-C25-C26	-6.39	111.79	122.30
19	3	310	CLA	C4A-NA-C1A	6.38	109.59	106.68
19	b	832	CLA	C4A-NA-C1A	6.38	109.59	106.68
19	3	315	CLA	C4A-NA-C1A	6.38	109.59	106.68
19	b	827	CLA	C4A-NA-C1A	6.37	109.59	106.68
19	2	314	CLA	C4A-NA-C1A	6.37	109.58	106.68
17	1	303	XAT	C38-C25-C26	-6.36	111.83	122.30
17	1	302	XAT	C18-C5-C4	6.36	121.39	114.24
26	i	101	BCR	C20-C21-C22	-6.36	118.36	127.28
19	1	312	CLA	C4A-NA-C1A	6.35	109.58	106.68
17	5	301	XAT	C18-C5-C6	-6.35	111.85	122.30
19	b	819	CLA	C4A-NA-C1A	6.35	109.58	106.68
19	a	814	CLA	C4A-NA-C1A	6.35	109.58	106.68
19	a	816	CLA	C4A-NA-C1A	6.35	109.58	106.68
19	2	306	CLA	C4A-NA-C1A	6.35	109.57	106.68
19	1	310	CLA	C4A-NA-C1A	6.35	109.57	106.68
19	b	826	CLA	C4A-NA-C1A	6.34	109.57	106.68
19	b	839	CLA	C4A-NA-C1A	6.34	109.57	106.68
19	3	307	CLA	C4A-NA-C1A	6.33	109.57	106.68
17	2	302	XAT	C38-C25-C26	-6.33	111.89	122.30
19	a	818	CLA	C4A-NA-C1A	6.33	109.56	106.68
17	4	303	XAT	C18-C5-C4	6.32	121.34	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	303	XAT	C18-C5-C4	6.32	121.34	114.24
17	3	304	XAT	C18-C5-C4	6.32	121.34	114.24
19	b	820	CLA	C4A-NA-C1A	6.31	109.56	106.68
19	5	305	CLA	C4A-NA-C1A	6.31	109.56	106.68
19	1	314	CLA	C4A-NA-C1A	6.30	109.55	106.68
19	4	308	CLA	C4A-NA-C1A	6.30	109.55	106.68
19	5	309	CLA	C4A-NA-C1A	6.30	109.55	106.68
19	1	309	CLA	C4A-NA-C1A	6.30	109.55	106.68
19	2	315	CLA	C4A-NA-C1A	6.29	109.55	106.68
19	a	815	CLA	C4A-NA-C1A	6.29	109.55	106.68
19	b	835	CLA	C4A-NA-C1A	6.29	109.55	106.68
19	4	312	CLA	C4A-NA-C1A	6.28	109.55	106.68
17	2	301	XAT	C38-C25-C24	6.28	121.30	114.24
19	2	310	CLA	C4A-NA-C1A	6.27	109.54	106.68
19	5	307	CLA	C4A-NA-C1A	6.26	109.53	106.68
19	a	813	CLA	C4A-NA-C1A	6.25	109.53	106.68
19	1	311	CLA	C4A-NA-C1A	6.24	109.53	106.68
19	a	824	CLA	C4A-NA-C1A	6.24	109.52	106.68
19	b	841	CLA	C4A-NA-C1A	6.23	109.52	106.68
17	4	304	XAT	C18-C5-C4	6.22	121.23	114.24
19	a	802	CLA	C4A-NA-C1A	6.22	109.52	106.68
17	3	301	XAT	C38-C25-C24	6.19	121.20	114.24
19	b	830	CLA	C4A-NA-C1A	6.18	109.50	106.68
17	2	301	XAT	C38-C25-C26	-6.18	112.13	122.30
17	5	302	XAT	C38-C25-C24	6.18	121.18	114.24
19	b	829	CLA	C4A-NA-C1A	6.15	109.48	106.68
17	2	301	XAT	C31-C30-C29	-6.15	118.66	127.28
17	1	303	XAT	C18-C5-C4	6.14	121.14	114.24
19	b	812	CLA	C4A-NA-C1A	6.14	109.48	106.68
17	a	852	XAT	C26-C27-C28	-6.12	113.06	125.99
17	2	305	XAT	C18-C5-C4	6.09	121.08	114.24
26	b	843	BCR	C7-C8-C9	-6.08	117.24	126.23
19	a	820	CLA	C4A-NA-C1A	6.08	109.45	106.68
17	4	305	XAT	C18-C5-C4	6.08	121.06	114.24
19	b	838	CLA	C4A-NA-C1A	6.07	109.45	106.68
23	1	304	AI1F	O15-C20-C17	6.05	121.81	115.05
19	b	804	CLA	C4A-NA-C1A	6.03	109.43	106.68
17	2	302	XAT	C18-C5-C4	6.01	121.00	114.24
19	b	818	CLA	C4A-NA-C1A	5.98	109.41	106.68
19	4	313	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	5	302	XAT	C18-C5-C4	5.96	120.93	114.24
26	b	852	BCR	C16-C17-C18	-5.94	118.95	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	5	304	XAT	C26-C27-C28	-5.92	113.47	125.99
17	5	302	XAT	C38-C25-C26	-5.92	112.56	122.30
19	b	817	CLA	C4A-NA-C1A	5.92	109.38	106.68
19	2	308	CLA	C4A-NA-C1A	5.91	109.38	106.68
17	5	301	XAT	C18-C5-C4	5.90	120.87	114.24
17	j	101	XAT	C6-C7-C8	-5.86	113.61	125.99
17	2	303	XAT	C18-C5-C4	5.84	120.80	114.24
19	b	831	CLA	C4A-NA-C1A	5.83	109.34	106.68
19	b	802	CLA	C4A-NA-C1A	5.81	109.33	106.68
17	4	301	XAT	C35-C34-C33	-5.81	119.13	127.28
26	a	850	BCR	C20-C21-C22	-5.78	119.17	127.28
26	b	845	BCR	C24-C23-C22	-5.75	117.73	126.23
26	f	801	BCR	C16-C17-C18	-5.73	119.25	127.28
17	5	302	XAT	C11-C10-C9	-5.72	119.26	127.28
23	1	304	AIL1F	O15-C20-C21	5.71	118.84	113.49
17	4	301	XAT	C38-C25-C24	5.69	120.63	114.24
26	b	843	BCR	C11-C10-C9	-5.68	119.31	127.28
26	b	845	BCR	C7-C8-C9	-5.63	117.91	126.23
26	b	847	BCR	C16-C17-C18	-5.56	119.48	127.28
26	f	801	BCR	C20-C21-C22	-5.49	119.58	127.28
17	3	304	XAT	C35-C34-C33	-5.47	119.60	127.28
26	b	845	BCR	C33-C5-C6	-5.45	118.53	124.48
17	a	852	XAT	C18-C5-C6	-5.45	113.33	122.30
26	f	804	BCR	C15-C14-C13	-5.45	119.64	127.28
17	3	301	XAT	C6-C7-C8	-5.44	114.50	125.99
17	4	301	XAT	C38-C25-C26	-5.44	113.35	122.30
17	2	303	XAT	C35-C34-C33	-5.44	119.65	127.28
26	j	104	BCR	C28-C27-C26	-5.43	104.37	114.06
17	2	303	XAT	C31-C30-C29	-5.39	119.72	127.28
17	4	305	XAT	C15-C14-C13	-5.35	119.77	127.28
26	b	843	BCR	C15-C14-C13	-5.35	119.77	127.28
26	b	843	BCR	C3-C4-C5	-5.33	104.55	114.06
26	l	201	BCR	C7-C8-C9	-5.32	118.36	126.23
17	2	305	XAT	C31-C30-C29	-5.32	119.82	127.28
17	2	303	XAT	C11-C10-C9	-5.30	119.84	127.28
19	a	803	CLA	C4A-NA-C1A	5.29	109.09	106.68
17	4	303	XAT	C26-C27-C28	-5.29	114.81	125.99
17	2	301	XAT	C35-C34-C33	-5.29	119.87	127.28
17	a	852	XAT	C18-C5-C4	5.28	120.17	114.24
17	2	302	XAT	C35-C34-C33	-5.28	119.87	127.28
21	b	851	DGD	O2G-C1B-C2B	5.27	122.88	111.48
26	a	849	BCR	C3-C4-C5	-5.27	104.67	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	304	XAT	C26-C27-C28	-5.26	114.87	125.99
26	l	205	BCR	C24-C23-C22	-5.25	118.47	126.23
17	a	852	XAT	C6-C7-C8	-5.23	114.93	125.99
17	2	304	XAT	C6-C7-C8	-5.20	115.01	125.99
17	j	101	XAT	C26-C27-C28	-5.16	115.08	125.99
17	2	305	XAT	C35-C34-C33	-5.13	120.09	127.28
26	a	847	BCR	C16-C17-C18	-5.12	120.10	127.28
26	b	846	BCR	C3-C4-C5	-5.11	104.94	114.06
17	1	302	XAT	C35-C34-C33	-5.10	120.12	127.28
17	3	305	XAT	C26-C27-C28	-5.04	115.33	125.99
26	a	850	BCR	C16-C17-C18	-5.03	120.22	127.28
26	b	852	BCR	C11-C10-C9	-5.03	120.22	127.28
26	b	852	BCR	C20-C21-C22	-5.02	120.24	127.28
26	f	804	BCR	C11-C10-C9	-5.01	120.25	127.28
17	5	301	XAT	C26-C27-C28	-5.01	115.41	125.99
17	2	301	XAT	C15-C14-C13	-5.00	120.27	127.28
17	1	302	XAT	C26-C27-C28	-4.99	115.44	125.99
17	4	304	XAT	C6-C7-C8	-4.99	115.44	125.99
26	a	849	BCR	C16-C17-C18	-4.97	120.31	127.28
17	3	305	XAT	C6-C7-C8	-4.96	115.50	125.99
26	j	104	BCR	C11-C10-C9	-4.93	120.36	127.28
17	1	303	XAT	C6-C7-C8	-4.91	115.60	125.99
17	4	303	XAT	C11-C10-C9	-4.91	120.40	127.28
17	j	101	XAT	C11-C10-C9	-4.90	120.41	127.28
26	b	852	BCR	C38-C26-C25	-4.90	119.14	124.48
17	5	302	XAT	C15-C14-C13	-4.87	120.44	127.28
17	2	305	XAT	C6-C7-C8	-4.86	115.71	125.99
17	2	301	XAT	C6-C7-C8	-4.86	115.72	125.99
26	l	205	BCR	C15-C14-C13	-4.86	120.47	127.28
26	b	850	BCR	C16-C17-C18	-4.83	120.51	127.28
17	5	304	XAT	C15-C14-C13	-4.81	120.53	127.28
26	i	101	BCR	C16-C17-C18	-4.81	120.53	127.28
17	1	302	XAT	C6-C7-C8	-4.81	115.83	125.99
26	b	852	BCR	C7-C8-C9	-4.80	119.13	126.23
17	4	302	XAT	C26-C27-C28	-4.73	115.99	125.99
17	4	302	XAT	C35-C34-C33	-4.69	120.70	127.28
17	3	303	XAT	C26-C27-C28	-4.68	116.09	125.99
17	4	302	XAT	C6-C7-C8	-4.67	116.11	125.99
26	b	848	BCR	C16-C17-C18	-4.66	120.74	127.28
26	b	844	BCR	C7-C8-C9	-4.64	119.37	126.23
17	5	301	XAT	C35-C34-C33	-4.63	120.79	127.28
17	3	304	XAT	C6-C7-C8	-4.62	116.22	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	305	XAT	C15-C14-C13	-4.60	120.82	127.28
26	b	844	BCR	C11-C10-C9	-4.59	120.84	127.28
17	4	305	XAT	C26-C27-C28	-4.54	116.40	125.99
17	3	305	XAT	C35-C34-C33	-4.52	120.93	127.28
17	3	303	XAT	C6-C7-C8	-4.49	116.49	125.99
17	2	302	XAT	C6-C7-C8	-4.49	116.49	125.99
26	a	850	BCR	C15-C14-C13	-4.47	121.01	127.28
17	2	304	XAT	C26-C27-C28	-4.46	116.55	125.99
26	a	848	BCR	C15-C14-C13	-4.46	121.02	127.28
26	a	848	BCR	C16-C17-C18	-4.46	121.03	127.28
26	b	848	BCR	C33-C5-C6	-4.44	119.64	124.48
26	b	845	BCR	C16-C17-C18	-4.44	121.06	127.28
26	j	104	BCR	C15-C14-C13	-4.43	121.07	127.28
26	a	849	BCR	C15-C14-C13	-4.42	121.07	127.28
26	b	843	BCR	C16-C17-C18	-4.42	121.08	127.28
17	3	303	XAT	C35-C34-C33	-4.39	121.12	127.28
22	2	317	LMG	O7-C10-C11	4.37	120.94	111.48
17	j	101	XAT	C35-C34-C33	-4.37	121.15	127.28
17	3	303	XAT	C15-C14-C13	-4.37	121.16	127.28
21	4	318	DGD	O6E-C5E-C6E	4.35	117.23	106.44
17	5	304	XAT	C35-C34-C33	-4.35	121.18	127.28
26	j	104	BCR	C16-C17-C18	-4.34	121.19	127.28
17	3	304	XAT	C31-C30-C29	-4.31	121.23	127.28
26	f	804	BCR	C24-C23-C22	-4.31	119.85	126.23
23	1	304	A1L1F	O7-C54-C56	4.30	118.76	111.09
26	b	844	BCR	C15-C14-C13	-4.30	121.25	127.28
17	4	301	XAT	C6-C7-C8	-4.29	116.92	125.99
17	4	304	XAT	C35-C34-C33	-4.29	121.27	127.28
26	b	845	BCR	C15-C14-C13	-4.28	121.27	127.28
23	1	304	A1L1F	C37-C38-C39	-4.27	121.29	127.28
17	3	301	XAT	C15-C14-C13	-4.27	121.29	127.28
26	b	847	BCR	C24-C23-C22	-4.27	119.92	126.23
26	j	104	BCR	C7-C8-C9	-4.26	119.94	126.23
26	b	850	BCR	C33-C5-C6	-4.25	119.85	124.48
17	2	305	XAT	C38-C25-C24	4.24	119.01	114.24
26	l	201	BCR	C33-C5-C6	-4.24	119.86	124.48
17	4	305	XAT	C35-C34-C33	-4.23	121.35	127.28
26	l	205	BCR	C20-C21-C22	-4.22	121.36	127.28
25	a	845	LHG	O7-C7-C8	4.22	120.60	111.48
26	l	201	BCR	C15-C14-C13	-4.21	121.37	127.28
21	4	318	DGD	O2G-C1B-C2B	4.21	120.59	111.48
26	b	846	BCR	C16-C17-C18	-4.20	121.38	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	804	BCR	C7-C8-C9	-4.20	120.02	126.23
17	3	304	XAT	C15-C14-C13	-4.18	121.42	127.28
23	1	304	A1L1F	C17-C20-C21	4.17	118.93	114.24
26	a	850	BCR	C38-C26-C25	-4.17	119.94	124.48
26	b	847	BCR	C20-C21-C22	-4.16	121.44	127.28
17	5	301	XAT	C11-C10-C9	-4.16	121.45	127.28
26	b	847	BCR	C7-C8-C9	-4.15	120.10	126.23
26	l	205	BCR	C38-C26-C25	-4.12	119.98	124.48
22	a	853	LMG	O7-C10-C11	4.11	120.38	111.48
24	b	842	PQN	C11-C12-C13	-4.10	119.77	126.83
26	a	847	BCR	C38-C26-C25	-4.09	120.03	124.48
17	4	301	XAT	C15-C14-C13	-4.08	121.55	127.28
26	b	847	BCR	C16-C15-C14	-4.08	115.17	123.52
26	f	801	BCR	C3-C4-C5	-4.08	106.78	114.06
25	b	849	LHG	O7-C7-C8	4.08	120.30	111.48
26	a	848	BCR	C11-C10-C9	-4.08	121.56	127.28
26	i	101	BCR	C7-C8-C9	-4.05	120.24	126.23
17	3	301	XAT	C35-C34-C33	-4.05	121.60	127.28
26	f	804	BCR	C33-C5-C6	-4.05	120.07	124.48
26	b	843	BCR	C28-C27-C26	-4.02	106.89	114.06
26	b	847	BCR	C15-C14-C13	-4.00	121.67	127.28
17	4	305	XAT	C11-C10-C9	-4.00	121.67	127.28
17	a	852	XAT	C31-C30-C29	-4.00	121.67	127.28
17	4	305	XAT	C6-C7-C8	-3.98	117.57	125.99
26	l	201	BCR	C11-C10-C9	-3.97	121.70	127.28
26	b	847	BCR	C28-C27-C26	-3.97	106.98	114.06
25	a	846	LHG	O7-C7-C8	3.97	120.06	111.48
25	m	101	LHG	O7-C7-C8	3.96	120.05	111.48
17	4	303	XAT	C15-C14-C13	-3.96	121.73	127.28
17	2	302	XAT	C31-C30-C29	-3.96	121.73	127.28
22	j	105	LMG	O7-C10-C11	3.95	120.03	111.48
26	a	847	BCR	C20-C21-C22	-3.95	121.74	127.28
26	l	205	BCR	C33-C5-C6	-3.95	120.18	124.48
17	j	101	XAT	C15-C14-C13	-3.95	121.74	127.28
17	2	303	XAT	C15-C14-C13	-3.94	121.75	127.28
17	2	302	XAT	C15-C14-C13	-3.94	121.75	127.28
26	f	804	BCR	C38-C26-C25	-3.93	120.19	124.48
17	1	303	XAT	C26-C27-C28	-3.93	117.68	125.99
19	b	804	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
26	f	804	BCR	C20-C21-C22	-3.91	121.79	127.28
17	2	305	XAT	C27-C28-C29	-3.91	119.46	125.53
26	l	205	BCR	C16-C17-C18	-3.89	121.82	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	201	BCR	C16-C17-C18	-3.89	121.82	127.28
26	f	804	BCR	C16-C17-C18	-3.86	121.86	127.28
18	1	301	A1L1G	C37-C36-C35	3.84	131.38	123.52
26	b	848	BCR	C15-C14-C13	-3.84	121.89	127.28
18	3	306	A1L1G	C36-C37-C38	3.83	131.36	123.52
17	5	301	XAT	C15-C14-C13	-3.83	121.91	127.28
17	2	302	XAT	C26-C27-C28	-3.83	117.90	125.99
21	b	851	DGD	O5D-C6D-C5D	-3.81	100.83	109.42
17	1	303	XAT	C35-C34-C33	-3.80	121.94	127.28
26	a	849	BCR	C28-C27-C26	-3.80	107.28	114.06
26	a	850	BCR	C33-C5-C6	-3.79	120.34	124.48
26	b	846	BCR	C15-C14-C13	-3.79	121.96	127.28
26	j	104	BCR	C20-C21-C22	-3.79	121.96	127.28
26	f	801	BCR	C16-C15-C14	-3.76	115.82	123.52
19	a	806	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
17	a	852	XAT	C35-C34-C33	-3.75	122.02	127.28
20	1	315	SQD	O47-C7-C8	3.75	119.58	111.48
17	3	301	XAT	C31-C30-C29	-3.73	122.05	127.28
18	5	303	A1L1G	C36-C37-C38	3.73	131.15	123.52
26	a	849	BCR	C4-C5-C6	-3.71	117.69	122.70
26	b	850	BCR	C7-C8-C9	-3.70	120.76	126.23
17	2	303	XAT	C26-C27-C28	-3.70	118.17	125.99
26	b	844	BCR	C3-C4-C5	-3.70	107.46	114.06
17	3	301	XAT	C26-C27-C28	-3.70	118.18	125.99
26	a	849	BCR	C20-C21-C22	-3.69	122.11	127.28
17	2	301	XAT	C27-C28-C29	-3.67	119.84	125.53
17	2	303	XAT	C6-C7-C8	-3.66	118.25	125.99
26	a	847	BCR	C33-C5-C6	-3.66	120.49	124.48
17	1	302	XAT	C11-C10-C9	-3.64	122.18	127.28
26	a	849	BCR	C11-C10-C9	-3.63	122.18	127.28
17	4	302	XAT	C35-C15-C14	-3.63	116.10	123.52
26	b	844	BCR	C33-C5-C6	-3.61	120.54	124.48
26	b	847	BCR	C3-C4-C5	-3.61	107.62	114.06
17	j	101	XAT	C10-C11-C12	-3.60	112.75	123.20
26	b	847	BCR	C10-C11-C12	-3.59	112.79	123.20
19	a	806	CLA	CAA-CBA-CGA	-3.59	103.03	113.21
26	i	101	BCR	C33-C5-C6	-3.59	120.57	124.48
17	4	303	XAT	C35-C34-C33	-3.58	122.26	127.28
26	l	205	BCR	C11-C10-C9	-3.58	122.26	127.28
26	a	847	BCR	C7-C8-C9	-3.57	120.95	126.23
26	b	846	BCR	C24-C23-C22	-3.57	120.96	126.23
26	b	850	BCR	C38-C26-C25	-3.57	120.59	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	305	XAT	C24-C23-C22	-3.56	104.14	110.79
26	a	847	BCR	C15-C14-C13	-3.55	122.29	127.28
17	1	303	XAT	C15-C14-C13	-3.54	122.31	127.28
26	a	848	BCR	C24-C23-C22	-3.54	121.00	126.23
23	1	304	A1L1F	C8-O7-C54	-3.53	111.61	117.85
17	4	302	XAT	C11-C10-C9	-3.52	122.34	127.28
26	l	205	BCR	C3-C4-C5	-3.52	107.78	114.06
26	a	849	BCR	C7-C8-C9	-3.50	121.06	126.23
20	5	316	SQD	O47-C7-C8	3.50	119.05	111.48
26	i	101	BCR	C28-C27-C26	-3.50	107.82	114.06
26	a	847	BCR	C24-C23-C22	-3.50	121.06	126.23
19	a	806	CLA	C3B-C4B-NB	-3.49	107.41	110.53
17	3	303	XAT	C11-C10-C9	-3.48	122.40	127.28
17	2	304	XAT	C11-C10-C9	-3.47	122.41	127.28
17	2	304	XAT	C31-C30-C29	-3.47	122.42	127.28
26	a	849	BCR	C24-C23-C22	-3.46	121.11	126.23
17	3	305	XAT	C15-C14-C13	-3.46	122.43	127.28
18	3	302	A1L1G	C36-C37-C38	3.45	130.58	123.52
26	a	848	BCR	C20-C21-C22	-3.45	122.44	127.28
26	a	847	BCR	C11-C10-C9	-3.44	122.45	127.28
17	a	852	XAT	C10-C11-C12	-3.44	113.22	123.20
19	b	804	CLA	CHB-C4A-NA	3.44	129.36	124.40
17	1	303	XAT	C24-C23-C22	-3.43	104.38	110.79
18	3	302	A1L1G	C37-C36-C35	3.42	130.52	123.52
21	b	851	DGD	C2G-O2G-C1B	-3.41	109.63	117.80
17	5	302	XAT	C6-C7-C8	-3.40	118.81	125.99
17	5	304	XAT	C24-C23-C22	-3.39	104.44	110.79
17	5	301	XAT	C7-C8-C9	-3.39	120.27	125.53
17	5	304	XAT	C4-C3-C2	-3.38	104.48	110.79
26	b	850	BCR	C11-C10-C9	-3.37	122.56	127.28
17	1	303	XAT	C31-C30-C29	-3.37	122.56	127.28
18	5	303	A1L1G	C37-C36-C35	3.35	130.38	123.52
17	5	301	XAT	C6-C7-C8	-3.35	118.90	125.99
26	b	848	BCR	C10-C11-C12	-3.35	113.49	123.20
19	b	804	CLA	C3B-C4B-NB	-3.35	107.54	110.53
26	i	101	BCR	C15-C14-C13	-3.35	122.58	127.28
17	4	301	XAT	C11-C10-C9	-3.34	122.59	127.28
17	5	301	XAT	C24-C23-C22	-3.34	104.54	110.79
26	a	850	BCR	C7-C8-C9	-3.34	121.29	126.23
26	a	847	BCR	C3-C4-C5	-3.34	108.09	114.06
26	j	104	BCR	C24-C23-C22	-3.34	121.30	126.23
23	1	304	A1L1F	C14-C29-C30	-3.33	119.80	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	312	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
18	1	301	A1L1G	C36-C37-C38	3.30	130.28	123.52
26	l	201	BCR	C38-C26-C25	-3.30	120.88	124.48
26	i	101	BCR	C11-C10-C9	-3.30	122.65	127.28
17	4	303	XAT	C6-C7-C8	-3.28	119.06	125.99
26	b	852	BCR	C24-C23-C22	-3.28	121.38	126.23
17	4	303	XAT	C24-C23-C22	-3.28	104.66	110.79
26	a	848	BCR	C33-C5-C6	-3.28	120.91	124.48
19	b	809	CLA	O2A-CGA-O1A	-3.27	115.45	123.63
24	a	843	PQN	C14-C13-C15	3.26	120.88	115.23
19	j	103	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
17	4	304	XAT	C24-C23-C22	-3.25	104.71	110.79
17	3	303	XAT	C24-C23-C22	-3.25	104.72	110.79
17	4	304	XAT	C15-C14-C13	-3.24	122.74	127.28
19	b	831	CLA	C3B-C4B-NB	-3.23	107.64	110.53
26	l	201	BCR	C24-C23-C22	-3.23	121.46	126.23
17	3	304	XAT	C26-C27-C28	-3.23	119.17	125.99
21	4	318	DGD	O1G-C1A-C2A	3.23	121.67	111.83
19	b	821	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
17	1	302	XAT	C15-C14-C13	-3.22	122.77	127.28
19	a	835	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
17	a	852	XAT	C11-C10-C9	-3.21	122.77	127.28
26	a	850	BCR	C11-C10-C9	-3.21	122.77	127.28
26	b	846	BCR	C20-C21-C22	-3.21	122.77	127.28
26	a	848	BCR	C38-C26-C25	-3.20	121.00	124.48
17	2	301	XAT	C11-C10-C9	-3.20	122.80	127.28
26	b	844	BCR	C16-C17-C18	-3.19	122.81	127.28
17	3	304	XAT	C11-C10-C9	-3.19	122.81	127.28
19	b	818	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	a	804	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
26	b	852	BCR	C33-C5-C6	-3.16	121.03	124.48
18	3	306	A1L1G	C37-C36-C35	3.16	129.99	123.52
17	3	304	XAT	C4-C3-C2	-3.16	104.89	110.79
19	b	833	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
26	a	848	BCR	C3-C4-C5	-3.14	108.45	114.06
26	b	846	BCR	C38-C26-C25	-3.14	121.06	124.48
19	a	818	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
19	a	819	CLA	C3B-C4B-NB	-3.14	107.73	110.53
26	l	205	BCR	C8-C7-C6	-3.14	118.62	127.00
17	4	303	XAT	C30-C31-C32	-3.14	114.12	123.20
19	1	313	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
26	a	849	BCR	C38-C26-C25	-3.13	121.07	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	301	XAT	C26-C27-C28	-3.12	119.39	125.99
26	a	848	BCR	C8-C7-C6	-3.11	118.68	127.00
17	4	305	XAT	C24-C23-C22	-3.11	104.97	110.79
17	a	852	XAT	C35-C15-C14	-3.11	117.16	123.52
17	3	305	XAT	C4-C3-C2	-3.10	104.99	110.79
26	b	843	BCR	C20-C21-C22	-3.10	122.93	127.28
19	4	311	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
26	f	801	BCR	C8-C7-C6	-3.10	118.72	127.00
19	a	809	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
17	4	304	XAT	C35-C15-C14	-3.09	117.20	123.52
19	4	316	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
19	b	809	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
19	3	308	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
17	5	301	XAT	C31-C30-C29	-3.08	122.96	127.28
17	a	852	XAT	C31-C32-C33	-3.08	117.93	126.36
19	i	102	CLA	C3B-C4B-NB	-3.07	107.79	110.53
19	4	307	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
17	1	302	XAT	C31-C30-C29	-3.07	122.98	127.28
18	1	301	A1L1G	C33-C34-C35	3.06	123.83	119.01
19	a	807	CLA	C3B-C4B-NB	-3.06	107.80	110.53
26	b	850	BCR	C15-C14-C13	-3.06	122.99	127.28
18	5	303	A1L1G	C40-C39-C38	3.05	123.81	119.01
19	a	802	CLA	C3B-C4B-NB	-3.05	107.81	110.53
26	b	848	BCR	C8-C7-C6	-3.05	118.85	127.00
26	b	847	BCR	C11-C10-C9	-3.05	123.00	127.28
25	a	846	LHG	O8-C23-C24	3.05	120.40	111.15
19	4	312	CLA	C3B-C4B-NB	-3.05	107.81	110.53
17	3	301	XAT	C4-C3-C2	-3.04	105.11	110.79
17	4	304	XAT	C4-C3-C2	-3.04	105.11	110.79
17	3	305	XAT	C24-C23-C22	-3.03	105.12	110.79
19	b	817	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
19	a	831	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
26	b	850	BCR	C16-C15-C14	-3.02	117.34	123.52
26	b	846	BCR	C4-C5-C6	-3.02	118.62	122.70
19	4	315	CLA	C3B-C4B-NB	-3.02	107.83	110.53
17	4	301	XAT	C31-C32-C33	-3.02	118.08	126.36
17	2	304	XAT	C24-C23-C22	-3.02	105.15	110.79
26	b	846	BCR	C8-C7-C6	-3.01	118.95	127.00
26	b	848	BCR	C21-C20-C19	-3.01	114.47	123.20
19	1	314	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
19	3	315	CLA	C3B-C4B-NB	-3.01	107.84	110.53
19	a	832	CLA	C3B-C4B-NB	-3.01	107.84	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	808	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
17	1	302	XAT	C4-C3-C2	-3.00	105.17	110.79
19	a	813	CLA	C3B-C4B-NB	-3.00	107.85	110.53
17	4	302	XAT	C24-C23-C22	-3.00	105.17	110.79
17	2	303	XAT	C4-C3-C2	-3.00	105.18	110.79
19	a	822	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	a	820	CLA	C1-C2-C3	-3.00	121.28	126.20
19	3	307	CLA	C3B-C4B-NB	-3.00	107.86	110.53
19	a	854	CLA	C3B-C4B-NB	-2.99	107.86	110.53
24	b	842	PQN	C16-C15-C13	-2.99	106.18	113.47
17	5	302	XAT	C24-C23-C22	-2.99	105.20	110.79
19	b	835	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
19	b	812	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
19	b	837	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
19	a	830	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
26	b	844	BCR	C21-C20-C19	-2.98	114.57	123.20
19	4	308	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
17	1	302	XAT	C24-C23-C22	-2.97	105.23	110.79
17	3	305	XAT	C31-C30-C29	-2.97	123.11	127.28
18	3	306	A1L1G	C40-C39-C38	2.97	123.68	119.01
19	b	820	CLA	C3B-C4B-NB	-2.97	107.88	110.53
26	b	844	BCR	C38-C26-C25	-2.96	121.25	124.48
17	a	852	XAT	C24-C23-C22	-2.96	105.25	110.79
19	f	803	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	4	309	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
19	a	828	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	a	839	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
18	1	301	A1L1G	C40-C39-C38	2.96	123.66	119.01
19	b	825	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
19	a	841	CLA	C3B-C4B-NB	-2.96	107.89	110.53
26	a	848	BCR	C7-C8-C9	-2.96	121.86	126.23
19	2	309	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
26	b	852	BCR	C16-C15-C14	-2.96	117.47	123.52
19	a	808	CLA	C3B-C4B-NB	-2.95	107.89	110.53
18	3	302	A1L1G	C33-C34-C35	2.95	123.65	119.01
26	b	845	BCR	C38-C26-C25	-2.95	121.27	124.48
17	1	302	XAT	C35-C15-C14	-2.95	117.49	123.52
17	4	302	XAT	C4-C3-C2	-2.95	105.28	110.79
17	2	304	XAT	C4-C3-C2	-2.95	105.28	110.79
19	1	311	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
19	4	317	CLA	C3B-C4B-NB	-2.94	107.90	110.53
19	3	309	CLA	O2D-CGD-O1D	-2.94	118.12	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	304	A1L1F	C26-O13-C45	2.94	121.81	115.64
17	4	301	XAT	C4-C3-C2	-2.94	105.29	110.79
26	a	850	BCR	C28-C27-C26	-2.94	108.81	114.06
19	b	815	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
19	2	313	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
26	b	850	BCR	C23-C24-C25	-2.94	119.15	127.00
19	a	818	CLA	C3B-C4B-NB	-2.94	107.91	110.53
26	b	843	BCR	C4-C5-C6	-2.94	118.73	122.70
19	b	840	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
19	b	815	CLA	CHB-C4A-NA	2.94	128.64	124.40
19	a	817	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
19	1	310	CLA	C3B-C4B-NB	-2.94	107.91	110.53
17	3	301	XAT	C10-C11-C12	-2.94	114.69	123.20
17	1	303	XAT	C4-C3-C2	-2.94	105.30	110.79
19	b	830	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
17	3	303	XAT	C4-C3-C2	-2.93	105.30	110.79
26	f	801	BCR	C20-C19-C18	-2.93	118.32	126.36
26	a	849	BCR	C2-C1-C6	2.93	114.70	110.44
19	2	309	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	b	809	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	b	819	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
21	b	851	DGD	O3E-C3E-C2E	-2.93	103.47	110.38
19	a	812	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
19	a	840	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
26	b	847	BCR	C33-C5-C6	-2.92	121.29	124.48
19	b	817	CLA	C3B-C4B-NB	-2.92	107.92	110.53
19	5	312	CLA	O2D-CGD-CBD	2.92	116.33	111.23
19	a	836	CLA	C3B-C4B-NB	-2.92	107.93	110.53
19	3	307	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
19	4	312	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
19	2	316	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
19	l	202	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	j	101	XAT	C4-C3-C2	-2.92	105.34	110.79
19	b	818	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
19	5	315	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
19	5	306	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	1	314	CLA	C3B-C4B-NB	-2.91	107.93	110.53
19	b	827	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
19	a	813	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
18	5	303	A1L1G	C28-C39-C38	-2.91	118.10	122.82
17	2	305	XAT	C11-C10-C9	-2.91	123.20	127.28
19	b	824	CLA	C3B-C4B-NB	-2.91	107.94	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	801	BCR	C33-C5-C6	-2.90	121.31	124.48
19	b	805	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
19	b	806	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
19	5	307	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
21	b	851	DGD	O1G-C1A-C2A	2.90	120.68	111.83
19	j	102	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
18	1	301	A1L1G	C27-C34-C35	-2.90	118.12	122.82
19	a	820	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
19	2	310	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
19	a	804	CLA	C1-C2-C3	-2.90	121.45	126.20
17	1	303	XAT	C10-C11-C12	-2.89	114.81	123.20
17	3	304	XAT	C24-C23-C22	-2.89	105.38	110.79
19	1	312	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	5	304	XAT	C19-C9-C8	2.89	122.50	118.09
19	a	837	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
18	3	302	A1L1G	C28-C39-C38	-2.89	118.13	122.82
17	2	301	XAT	C4-C3-C2	-2.89	105.39	110.79
18	3	302	A1L1G	C40-C39-C38	2.89	123.55	119.01
19	b	839	CLA	C3B-C4B-NB	-2.89	107.95	110.53
19	2	314	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
22	2	317	LMG	O8-C28-C29	2.88	120.62	111.83
18	3	306	A1L1G	C27-C34-C35	-2.88	118.15	122.82
19	5	309	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
19	a	842	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	5	305	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	b	835	CLA	C3B-C4B-NB	-2.88	107.96	110.53
26	b	848	BCR	C15-C16-C17	-2.87	117.64	123.52
19	2	316	CLA	C3B-C4B-NB	-2.87	107.97	110.53
26	b	846	BCR	C10-C11-C12	-2.87	114.88	123.20
19	a	833	CLA	C3B-C4B-NB	-2.87	107.97	110.53
19	a	825	CLA	C3B-C4B-NB	-2.87	107.97	110.53
21	4	318	DGD	O5E-C6E-C5E	-2.87	101.57	111.33
19	5	309	CLA	C3B-C4B-NB	-2.87	107.97	110.53
19	4	307	CLA	C3B-C4B-NB	-2.87	107.97	110.53
19	1	305	CLA	C3B-C4B-NB	-2.87	107.97	110.53
26	i	101	BCR	C29-C30-C25	2.87	114.60	110.44
19	1	312	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
17	5	304	XAT	C10-C11-C12	-2.86	114.90	123.20
17	4	305	XAT	C4-C3-C2	-2.86	105.43	110.79
19	a	823	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
18	1	301	A1L1G	C28-C39-C38	-2.86	118.18	122.82
19	4	314	CLA	C3B-C4B-NB	-2.86	107.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	816	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
17	5	302	XAT	C35-C34-C33	-2.86	123.27	127.28
19	2	307	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	5	315	CLA	C3B-C4B-NB	-2.86	107.98	110.53
18	5	303	A1L1G	C33-C34-C35	2.86	123.50	119.01
19	b	839	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
19	4	306	CLA	C3B-C4B-NB	-2.86	107.98	110.53
19	b	838	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
19	3	312	CLA	C3B-C4B-NB	-2.85	107.98	110.53
19	1	307	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
18	3	306	A1L1G	C33-C34-C35	2.85	123.49	119.01
19	a	825	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
19	a	826	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
19	b	828	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
19	a	833	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
19	a	802	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
19	a	811	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
19	a	827	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	2	301	XAT	C24-C23-C22	-2.84	105.48	110.79
19	5	310	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
19	1	305	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
18	3	302	A1L1G	C27-C34-C35	-2.84	118.22	122.82
18	3	306	A1L1G	C28-C39-C38	-2.84	118.22	122.82
19	a	832	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
17	4	304	XAT	C11-C10-C9	-2.83	123.31	127.28
19	5	313	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	3	311	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
19	a	837	CLA	C3B-C4B-NB	-2.83	108.00	110.53
17	2	305	XAT	C38-C25-C26	-2.82	117.65	122.30
19	5	314	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	j	102	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	1	310	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	4	316	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	b	813	CLA	C3B-C4B-NB	-2.82	108.01	110.53
26	f	801	BCR	C10-C11-C12	-2.82	115.03	123.20
17	2	305	XAT	C4-C3-C2	-2.82	105.52	110.79
24	a	843	PQN	C11-C3-C2	-2.82	120.06	124.89
19	3	313	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	2	314	CLA	C3B-C4B-NB	-2.82	108.02	110.53
19	b	816	CLA	C3B-C4B-NB	-2.82	108.02	110.53
19	b	837	CLA	C3B-C4B-NB	-2.82	108.02	110.53
18	5	303	A1L1G	C27-C34-C35	-2.82	118.25	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	308	CLA	C1-C2-C3	-2.82	121.58	126.20
19	4	313	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
19	a	805	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
19	2	310	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	a	834	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	1	306	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
19	b	822	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
22	a	853	LMG	O8-C28-C29	2.81	120.41	111.83
19	2	307	CLA	CHB-C4A-NA	2.81	128.46	124.40
19	b	832	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
26	b	850	BCR	C21-C20-C19	-2.81	115.06	123.20
17	2	302	XAT	C24-C23-C22	-2.81	105.53	110.79
19	3	314	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
19	a	817	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	b	814	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	b	829	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	b	841	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
19	a	836	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
26	a	849	BCR	C33-C5-C4	2.81	119.58	113.60
17	j	101	XAT	C24-C23-C22	-2.81	105.54	110.79
19	a	821	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
19	a	824	CLA	C3B-C4B-NB	-2.80	108.03	110.53
26	m	102	BCR	C27-C26-C25	2.80	126.49	122.70
26	b	843	BCR	C2-C1-C6	2.80	114.51	110.44
19	a	831	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
19	2	308	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
19	a	815	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
19	l	203	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
20	1	315	SQD	O48-C23-C24	2.80	120.38	111.83
19	5	308	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
19	3	313	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	4	310	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	b	801	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	a	803	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
19	a	844	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
19	a	839	CLA	C3B-C4B-NB	-2.80	108.03	110.53
26	b	846	BCR	C33-C5-C4	2.80	119.56	113.60
19	b	801	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	b	833	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	5	313	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	4	306	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	b	816	CLA	O2D-CGD-O1D	-2.79	118.42	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	811	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	b	829	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	b	841	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	3	315	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
26	b	843	BCR	C38-C26-C25	-2.79	121.44	124.48
19	2	315	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
19	1	308	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	1	304	A1L1F	C36-C35-C34	-2.78	123.37	127.28
19	b	830	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
26	b	845	BCR	C20-C21-C22	-2.78	123.38	127.28
19	2	313	CLA	CAA-C2A-C3A	-2.78	109.86	116.23
19	b	831	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	b	846	BCR	C2-C1-C6	2.78	114.47	110.44
19	j	103	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	5	310	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	l	203	CLA	C3B-C4B-NB	-2.78	108.05	110.53
26	j	104	BCR	C23-C24-C25	-2.78	119.58	127.00
19	b	823	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
26	b	850	BCR	C24-C23-C22	-2.78	122.13	126.23
19	5	314	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
19	1	313	CLA	C3B-C4B-NB	-2.77	108.05	110.53
19	2	307	CLA	C3B-C4B-NB	-2.77	108.05	110.53
17	5	302	XAT	C4-C3-C2	-2.77	105.60	110.79
17	3	303	XAT	C31-C30-C29	-2.77	123.39	127.28
26	i	101	BCR	C20-C19-C18	-2.77	118.76	126.36
19	2	306	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	b	805	CLA	C3B-C4B-NB	-2.77	108.06	110.53
25	m	101	LHG	O8-C23-C24	2.77	120.28	111.83
20	5	316	SQD	O48-C23-C24	2.77	120.28	111.83
19	a	819	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
17	4	302	XAT	C31-C30-C29	-2.77	123.39	127.28
19	a	811	CLA	C3B-C4B-NB	-2.77	108.06	110.53
26	b	843	BCR	C24-C23-C22	-2.77	122.14	126.23
19	4	311	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	b	820	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
19	b	826	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	a	828	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	a	841	CLA	CHB-C4A-NA	2.76	128.39	124.40
26	b	847	BCR	C35-C13-C12	2.76	122.31	118.09
19	b	813	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
19	b	824	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	4	301	XAT	C26-C27-C28	-2.76	120.16	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	843	BCR	C23-C24-C25	-2.76	119.64	127.00
17	2	301	XAT	C31-C32-C33	-2.76	118.81	126.36
19	a	841	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	3	301	XAT	C19-C9-C8	2.75	122.30	118.09
19	f	803	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
19	a	838	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
17	3	305	XAT	C35-C15-C14	-2.75	117.89	123.52
19	l	204	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
19	a	820	CLA	C3B-C4B-NB	-2.75	108.08	110.53
17	2	302	XAT	C35-C15-C14	-2.75	117.90	123.52
19	a	807	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
19	f	802	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
19	3	314	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	a	816	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	3	312	CLA	CHB-C4A-NA	2.74	128.36	124.40
26	m	102	BCR	C33-C5-C6	-2.74	121.49	124.48
26	b	852	BCR	C20-C19-C18	-2.74	118.85	126.36
19	b	806	CLA	C3B-C4B-NB	-2.74	108.08	110.53
19	4	314	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
18	1	301	A1L1G	C43-C44-C42	-2.74	118.38	122.82
26	b	846	BCR	C7-C8-C9	-2.74	122.19	126.23
26	b	845	BCR	C11-C10-C9	-2.74	123.44	127.28
19	b	831	CLA	CAA-C2A-C3A	-2.74	109.96	116.23
19	2	312	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
19	b	836	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
19	a	824	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
19	5	305	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
19	1	309	CLA	C3B-C4B-NB	-2.73	108.09	110.53
19	a	802	CLA	C1-C2-C3	-2.73	121.73	126.20
17	4	303	XAT	C4-C3-C2	-2.73	105.69	110.79
23	1	304	A1L1F	C26-C30-C31	-2.73	121.51	124.97
19	a	815	CLA	C3B-C4B-NB	-2.73	108.10	110.53
17	3	301	XAT	C24-C23-C22	-2.73	105.69	110.79
19	a	827	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	2	313	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	b	810	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
19	3	311	CLA	C3B-C4B-NB	-2.72	108.10	110.53
19	a	808	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
19	l	202	CLA	C3B-C4B-NB	-2.72	108.11	110.53
17	j	101	XAT	C31-C32-C33	-2.71	118.92	126.36
17	5	304	XAT	C31-C30-C29	-2.71	123.47	127.28
26	b	850	BCR	C20-C21-C22	-2.71	123.47	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	814	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	j	101	XAT	C31-C30-C29	-2.71	123.48	127.28
19	a	814	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
17	4	305	XAT	C31-C32-C33	-2.71	118.94	126.36
19	a	841	CLA	C1-C2-C3	-2.71	121.76	126.20
17	j	101	XAT	C15-C35-C34	-2.70	117.99	123.52
17	4	303	XAT	C39-C29-C28	2.70	122.22	118.09
19	a	812	CLA	C3B-C4B-NB	-2.70	108.12	110.53
19	b	825	CLA	C3B-C4B-NB	-2.70	108.12	110.53
17	4	302	XAT	C15-C14-C13	-2.70	123.49	127.28
19	4	313	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	b	849	LHG	O8-C23-C24	2.70	120.06	111.83
22	j	105	LMG	O8-C28-C29	2.70	120.06	111.83
19	b	818	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
19	4	315	CLA	CHB-C4A-NA	2.70	128.29	124.40
19	4	315	CLA	CAA-C2A-C3A	-2.69	110.05	116.23
19	b	803	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	3	312	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
19	4	315	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
19	5	307	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	4	309	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	b	815	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	a	805	CLA	CHB-C4A-NA	2.69	128.28	124.40
19	a	822	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
23	1	304	A1L1F	O15-C25-C14	-2.69	109.19	116.88
19	4	310	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
19	l	203	CLA	CHB-C4A-NA	2.68	128.27	124.40
19	b	832	CLA	C3B-C4B-NB	-2.68	108.14	110.53
23	1	304	A1L1F	O13-C45-C47	2.68	120.01	111.83
17	5	304	XAT	C30-C31-C32	-2.68	115.44	123.20
24	b	842	PQN	C2M-C2-C3	-2.68	120.05	124.45
19	2	315	CLA	C3B-C4B-NB	-2.68	108.14	110.53
19	5	308	CLA	C3B-C4B-NB	-2.68	108.14	110.53
20	5	316	SQD	C44-O6-C1	-2.67	108.06	113.80
17	3	301	XAT	C27-C28-C29	-2.67	121.38	125.53
17	5	301	XAT	C35-C15-C14	-2.67	118.06	123.52
19	b	807	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
17	2	305	XAT	C31-C32-C33	-2.66	119.06	126.36
25	a	845	LHG	O8-C23-C24	2.66	119.95	111.83
19	5	306	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
19	a	810	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
19	b	834	CLA	C3B-C4B-NB	-2.66	108.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	847	BCR	C16-C15-C14	-2.66	118.08	123.52
19	5	312	CLA	C3B-C4B-NB	-2.66	108.16	110.53
19	a	829	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
19	2	311	CLA	C3B-C4B-NB	-2.66	108.16	110.53
19	a	801	CLA	C3B-C4B-NB	-2.66	108.16	110.53
19	a	835	CLA	C3B-C4B-NB	-2.66	108.16	110.53
26	f	801	BCR	C2-C1-C6	2.65	114.29	110.44
19	a	834	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
19	b	801	CLA	CHB-C4A-NA	2.65	128.23	124.40
19	5	311	CLA	C3B-C4B-NB	-2.65	108.16	110.53
17	2	304	XAT	C15-C14-C13	-2.65	123.56	127.28
19	a	840	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	b	838	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	a	826	CLA	CHB-C4A-NA	2.65	128.22	124.40
19	a	835	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	j	104	BCR	C27-C26-C25	-2.64	119.13	122.70
19	a	842	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
19	5	314	CLA	CHB-C4A-NA	2.63	128.20	124.40
19	b	806	CLA	CHB-C4A-NA	2.63	128.20	124.40
19	a	805	CLA	C3B-C4B-NB	-2.63	108.18	110.53
17	4	301	XAT	C27-C28-C29	-2.63	121.45	125.53
19	b	826	CLA	C3B-C4B-NB	-2.62	108.19	110.53
26	b	848	BCR	C34-C9-C8	2.62	122.10	118.09
19	a	810	CLA	C3B-C4B-NB	-2.62	108.19	110.53
19	i	102	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
26	l	201	BCR	C20-C21-C22	-2.62	123.60	127.28
26	b	846	BCR	C21-C20-C19	-2.62	115.60	123.20
26	a	849	BCR	C16-C15-C14	-2.62	118.16	123.52
19	1	308	CLA	C3B-C4B-NB	-2.62	108.19	110.53
19	l	204	CLA	C3B-C4B-NB	-2.62	108.19	110.53
17	4	304	XAT	C31-C30-C29	-2.62	123.60	127.28
26	a	849	BCR	C23-C24-C25	-2.62	120.00	127.00
19	1	309	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
26	b	848	BCR	C24-C23-C22	-2.62	122.36	126.23
26	b	850	BCR	C28-C27-C26	-2.62	109.39	114.06
17	2	302	XAT	C4-C3-C2	-2.62	105.90	110.79
17	4	305	XAT	C7-C8-C9	-2.62	121.47	125.53
19	b	825	CLA	CHB-C4A-NA	2.62	128.17	124.40
19	a	810	CLA	C1-C2-C3	-2.61	121.91	126.20
19	a	821	CLA	C3B-C4B-NB	-2.61	108.20	110.53
26	b	847	BCR	C38-C26-C25	-2.61	121.64	124.48
19	4	317	CLA	O2D-CGD-O1D	-2.61	118.77	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	819	CLA	CHB-C4A-NA	2.61	128.17	124.40
19	b	802	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
26	l	201	BCR	C21-C20-C19	-2.61	115.64	123.20
19	4	317	CLA	CHB-C4A-NA	2.61	128.16	124.40
19	b	809	CLA	CHB-C4A-NA	2.61	128.16	124.40
19	b	823	CLA	C3B-C4B-NB	-2.61	108.20	110.53
26	b	847	BCR	C8-C7-C6	-2.61	120.03	127.00
19	a	821	CLA	CHB-C4A-NA	2.61	128.16	124.40
19	a	814	CLA	CHB-C4A-NA	2.61	128.16	124.40
17	2	304	XAT	C35-C15-C14	-2.61	118.19	123.52
19	5	311	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
19	b	834	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
19	2	311	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
19	3	310	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
19	3	309	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	4	311	CLA	CHB-C4A-NA	2.60	128.16	124.40
26	m	102	BCR	C15-C16-C17	-2.60	118.20	123.52
21	b	851	DGD	C1E-O6E-C5E	2.60	118.80	113.72
19	a	807	CLA	CHB-C4A-NA	2.60	128.15	124.40
19	3	308	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	a	804	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	1	307	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	4	310	CLA	CHB-C4A-NA	2.60	128.15	124.40
17	4	302	XAT	C10-C11-C12	-2.59	115.68	123.20
19	b	814	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
19	b	811	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	a	853	LMG	C8-O7-C10	-2.59	111.60	117.80
19	a	838	CLA	C3B-C4B-NB	-2.59	108.22	110.53
26	b	844	BCR	C24-C23-C22	-2.58	122.41	126.23
19	a	844	CLA	C3B-C4B-NB	-2.58	108.23	110.53
19	a	854	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
19	b	807	CLA	C1-C2-C3	-2.58	121.97	126.20
19	2	312	CLA	C3B-C4B-NB	-2.58	108.23	110.53
19	b	808	CLA	C3B-C4B-NB	-2.58	108.23	110.53
19	a	833	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	a	809	CLA	CHB-C4A-NA	2.57	128.12	124.40
17	3	305	XAT	C10-C11-C12	-2.57	115.74	123.20
19	j	103	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	j	104	BCR	C33-C5-C6	-2.57	121.68	124.48
26	l	205	BCR	C28-C27-C26	-2.57	109.47	114.06
26	b	843	BCR	C29-C30-C25	2.57	114.17	110.44
26	b	843	BCR	C21-C20-C19	-2.57	115.75	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	303	XAT	C19-C9-C10	-2.57	118.65	122.82
17	2	302	XAT	C11-C10-C9	-2.57	123.67	127.28
19	b	821	CLA	C1-C2-C3	-2.57	122.61	126.76
19	5	313	CLA	CHB-C4A-NA	2.57	128.10	124.40
19	a	828	CLA	C1-C2-C3	-2.56	122.00	126.20
19	a	832	CLA	CHB-C4A-NA	2.56	128.10	124.40
17	5	301	XAT	C4-C3-C2	-2.56	106.00	110.79
19	2	306	CLA	O2D-CGD-O1D	-2.56	118.28	124.08
19	b	818	CLA	CHB-C4A-NA	2.56	128.09	124.40
19	1	314	CLA	CHB-C4A-NA	2.56	128.09	124.40
26	a	850	BCR	C10-C11-C12	-2.56	115.80	123.20
26	b	848	BCR	C20-C21-C22	-2.55	123.69	127.28
17	1	303	XAT	C35-C15-C14	-2.55	118.29	123.52
19	1	311	CLA	C3B-C4B-NB	-2.55	108.25	110.53
19	1	306	CLA	CHB-C4A-NA	2.55	128.08	124.40
19	a	830	CLA	C1-C2-C3	-2.55	122.02	126.20
19	a	801	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
18	3	306	A1L1G	C43-C44-C42	-2.55	118.69	122.82
19	b	821	CLA	O2D-CGD-CBD	2.55	115.68	111.23
19	3	315	CLA	CHB-C4A-NA	2.54	128.07	124.40
26	j	104	BCR	C38-C26-C27	2.54	119.02	113.60
19	3	314	CLA	CHB-C4A-NA	2.54	128.07	124.40
26	b	852	BCR	C15-C14-C13	-2.54	123.72	127.28
26	f	804	BCR	C15-C16-C17	-2.54	118.33	123.52
19	a	804	CLA	CHB-C4A-NA	2.54	128.06	124.40
19	a	832	CLA	C1-C2-C3	-2.54	122.66	126.76
19	b	822	CLA	C3B-C4B-NB	-2.53	108.27	110.53
19	l	204	CLA	CHB-C4A-NA	2.53	128.06	124.40
19	a	840	CLA	CHB-C4A-NA	2.53	128.06	124.40
19	b	803	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
19	b	814	CLA	CHB-C4A-NA	2.53	128.05	124.40
17	3	303	XAT	C30-C31-C32	-2.53	115.87	123.20
17	5	304	XAT	C39-C29-C28	2.53	121.95	118.09
26	b	850	BCR	C10-C11-C12	-2.53	115.87	123.20
26	l	205	BCR	C15-C16-C17	-2.53	118.34	123.52
21	b	851	DGD	O2G-C1B-O1B	-2.53	117.80	123.70
19	a	806	CLA	C6-C5-C3	-2.53	107.31	113.47
19	4	306	CLA	CHB-C4A-NA	2.53	128.04	124.40
19	a	838	CLA	CHB-C4A-NA	2.53	128.04	124.40
17	5	304	XAT	C15-C35-C34	-2.53	118.35	123.52
19	a	817	CLA	CHB-C4A-NA	2.52	128.04	124.40
19	a	806	CLA	CHB-C4A-NA	2.52	128.04	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	825	CLA	CHB-C4A-NA	2.52	128.03	124.40
19	4	307	CLA	CHB-C4A-NA	2.52	128.03	124.40
17	4	302	XAT	C30-C31-C32	-2.52	115.91	123.20
18	3	306	A1L1G	C17-C20-C21	2.52	117.07	114.24
17	5	304	XAT	C8-C9-C10	-2.52	115.05	119.01
19	b	813	CLA	CHB-C4A-NA	2.52	128.03	124.40
26	b	843	BCR	C33-C5-C4	2.52	118.96	113.60
19	a	806	CLA	O1D-CGD-CBD	2.52	129.48	124.52
19	1	308	CLA	CHB-C4A-NA	2.51	128.03	124.40
19	2	313	CLA	CHB-C4A-NA	2.51	128.03	124.40
19	3	313	CLA	CHB-C4A-NA	2.51	128.02	124.40
19	a	827	CLA	CHB-C4A-NA	2.51	128.02	124.40
19	4	314	CLA	CHB-C4A-NA	2.51	128.02	124.40
19	f	802	CLA	CHB-C4A-NA	2.51	128.02	124.40
19	5	310	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	l	201	BCR	C28-C27-C26	-2.50	109.59	114.06
19	5	312	CLA	CHB-C4A-NA	2.50	128.01	124.40
19	b	836	CLA	CHB-C4A-NA	2.50	128.01	124.40
19	a	810	CLA	CHB-C4A-NA	2.50	128.01	124.40
19	2	316	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	b	847	BCR	C39-C30-C25	-2.50	106.32	110.24
19	b	836	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	b	807	CLA	CHB-C4A-NA	2.50	128.01	124.40
19	a	802	CLA	CHB-C4A-NA	2.50	128.00	124.40
19	b	821	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	1	307	CLA	CHB-C4A-NA	2.50	128.00	124.40
23	1	304	A1L1F	C31-C32-C33	-2.50	115.97	123.20
26	b	844	BCR	C15-C16-C17	-2.49	118.41	123.52
19	b	807	CLA	C3B-C4B-NB	-2.49	108.30	110.53
19	a	836	CLA	CHB-C4A-NA	2.49	128.00	124.40
19	f	803	CLA	CHB-C4A-NA	2.49	128.00	124.40
19	1	306	CLA	C3B-C4B-NB	-2.49	108.31	110.53
21	b	851	DGD	C6D-O5D-C1E	2.49	119.14	113.80
19	a	812	CLA	CHB-C4A-NA	2.49	128.00	124.40
19	5	306	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	a	822	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	1	304	A1L1F	C27-C34-C33	2.49	121.89	118.09
19	1	312	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	3	308	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	b	832	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	b	837	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	a	802	CLA	CMB-C2B-C1B	-2.49	121.63	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	821	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	a	816	CLA	CHB-C4A-NA	2.48	127.99	124.40
26	b	843	BCR	C15-C16-C17	-2.48	118.44	123.52
17	4	301	XAT	C35-C15-C14	-2.48	118.44	123.52
19	1	313	CLA	CAA-C2A-C3A	-2.48	110.54	116.23
19	b	805	CLA	CHB-C4A-NA	2.48	127.98	124.40
19	5	308	CLA	CHB-C4A-NA	2.48	127.98	124.40
17	2	301	XAT	C10-C11-C12	-2.48	116.02	123.20
19	a	808	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	a	848	BCR	C10-C11-C12	-2.48	116.02	123.20
17	2	303	XAT	C24-C23-C22	-2.48	106.16	110.79
19	1	310	CLA	CHB-C4A-NA	2.48	127.97	124.40
19	b	834	CLA	CHB-C4A-NA	2.47	127.97	124.40
19	a	804	CLA	O2D-CGD-CBD	2.47	115.55	111.23
19	a	830	CLA	C3B-C4B-NB	-2.47	108.32	110.53
19	3	307	CLA	CHB-C4A-NA	2.47	127.97	124.40
19	b	822	CLA	CHB-C4A-NA	2.47	127.97	124.40
26	a	850	BCR	C38-C26-C27	2.47	118.86	113.60
19	5	305	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	a	823	CLA	CHB-C4A-NA	2.47	127.96	124.40
19	l	202	CLA	CHB-C4A-NA	2.47	127.96	124.40
26	j	104	BCR	C15-C16-C17	-2.47	118.47	123.52
19	a	809	CLA	C3B-C4B-NB	-2.47	108.33	110.53
19	a	826	CLA	C3B-C4B-NB	-2.47	108.33	110.53
19	b	812	CLA	CMB-C2B-C3B	2.47	130.09	123.53
17	2	302	XAT	C10-C11-C12	-2.46	116.06	123.20
19	5	315	CLA	CHB-C4A-NA	2.46	127.96	124.40
19	4	316	CLA	CHB-C4A-NA	2.46	127.96	124.40
19	2	314	CLA	CHB-C4A-NA	2.46	127.95	124.40
19	a	828	CLA	CHB-C4A-NA	2.46	127.95	124.40
19	b	840	CLA	CHB-C4A-NA	2.46	127.95	124.40
19	b	810	CLA	C1-C2-C3	-2.46	122.17	126.20
18	5	303	A1L1G	C43-C44-C42	-2.46	118.83	122.82
19	2	312	CLA	CHB-C4A-NA	2.46	127.95	124.40
19	a	837	CLA	CHB-C4A-NA	2.46	127.95	124.40
26	j	104	BCR	C38-C26-C25	-2.46	121.80	124.48
26	a	850	BCR	C8-C7-C6	-2.46	120.44	127.00
22	j	105	LMG	C8-O7-C10	-2.46	111.92	117.80
19	b	822	CLA	C1-C2-C3	-2.46	122.17	126.20
26	b	846	BCR	C33-C5-C6	-2.45	121.81	124.48
19	2	308	CLA	C3B-C4B-NB	-2.45	108.34	110.53
19	2	309	CLA	CHB-C4A-NA	2.45	127.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	820	CLA	CHB-C4A-NA	2.45	127.94	124.40
19	b	808	CLA	CHB-C4A-NA	2.45	127.94	124.40
19	a	811	CLA	CHB-C4A-NA	2.45	127.93	124.40
17	5	302	XAT	C31-C30-C29	-2.45	123.85	127.28
19	a	839	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	a	835	CLA	O2D-CGD-CBD	2.44	115.50	111.23
19	a	820	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	b	816	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	2	311	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	a	803	CLA	C3B-C4B-NB	-2.44	108.35	110.53
26	a	850	BCR	C16-C15-C14	-2.44	118.53	123.52
26	b	847	BCR	C21-C20-C19	-2.44	116.14	123.20
19	4	313	CLA	CHB-C4A-NA	2.43	127.91	124.40
19	b	839	CLA	CHB-C4A-NA	2.43	127.91	124.40
19	f	802	CLA	C3B-C4B-NB	-2.43	108.36	110.53
19	b	828	CLA	C3B-C4B-NB	-2.43	108.36	110.53
26	b	850	BCR	C8-C7-C6	-2.43	120.51	127.00
19	a	815	CLA	CHB-C4A-NA	2.43	127.90	124.40
24	b	842	PQN	C11-C3-C2	-2.43	120.73	124.89
17	3	304	XAT	C31-C32-C33	-2.43	119.71	126.36
19	b	840	CLA	C3B-C4B-NB	-2.42	108.37	110.53
26	f	804	BCR	C28-C27-C26	-2.42	109.74	114.06
26	b	848	BCR	C38-C26-C25	-2.42	121.85	124.48
19	b	812	CLA	CAB-C3B-C2B	2.42	129.95	123.53
19	2	306	CLA	CHB-C4A-NA	2.42	127.89	124.40
19	b	835	CLA	CHB-C4A-NA	2.41	127.88	124.40
26	b	846	BCR	C16-C15-C14	-2.41	118.59	123.52
19	4	308	CLA	C3B-C4B-NB	-2.41	108.38	110.53
26	a	847	BCR	C23-C24-C25	-2.41	120.56	127.00
19	a	818	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	b	842	PQN	C14-C13-C15	2.40	119.40	115.23
19	b	814	CLA	C1-C2-C3	-2.40	122.26	126.20
19	b	826	CLA	CHB-C4A-NA	2.40	127.86	124.40
19	4	309	CLA	CHB-C4A-NA	2.40	127.86	124.40
26	b	845	BCR	C28-C27-C26	-2.40	109.78	114.06
19	3	309	CLA	CHB-C4A-NA	2.40	127.86	124.40
18	3	302	A1L1G	C43-C44-C42	-2.40	118.93	122.82
19	3	311	CLA	C1-C2-C3	-2.39	122.89	126.76
19	a	829	CLA	C3B-C4B-NB	-2.39	108.39	110.53
26	a	848	BCR	C21-C20-C19	-2.39	116.27	123.20
19	5	311	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	b	844	BCR	C23-C24-C25	-2.39	120.62	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	313	CLA	CHB-C4A-NA	2.39	127.85	124.40
19	b	828	CLA	CHB-C4A-NA	2.39	127.84	124.40
19	3	311	CLA	CHB-C4A-NA	2.38	127.83	124.40
17	5	301	XAT	O24-C25-C38	2.38	117.71	115.05
26	b	845	BCR	C34-C9-C10	-2.38	118.96	122.82
19	b	836	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
26	f	801	BCR	C33-C5-C4	2.38	118.66	113.60
19	4	312	CLA	CHB-C4A-NA	2.37	127.83	124.40
19	b	823	CLA	CHB-C4A-NA	2.37	127.83	124.40
19	4	308	CLA	CHB-C4A-NA	2.37	127.82	124.40
19	5	309	CLA	CHB-C4A-NA	2.37	127.82	124.40
19	b	810	CLA	CHB-C4A-NA	2.37	127.82	124.40
19	a	834	CLA	C1-C2-C3	-2.37	122.31	126.20
19	a	833	CLA	C1-C2-C3	-2.37	122.32	126.20
19	a	854	CLA	CHB-C4A-NA	2.37	127.82	124.40
19	j	102	CLA	CHB-C4A-NA	2.37	127.82	124.40
26	a	849	BCR	C21-C20-C19	-2.37	116.34	123.20
26	b	844	BCR	C28-C27-C26	-2.37	109.84	114.06
26	f	804	BCR	C11-C12-C13	-2.36	119.88	126.36
19	a	842	CLA	CHB-C4A-NA	2.36	127.81	124.40
26	b	843	BCR	C11-C12-C13	-2.36	119.89	126.36
19	i	102	CLA	CHB-C4A-NA	2.36	127.81	124.40
19	b	812	CLA	CHB-C4A-NA	2.36	127.81	124.40
19	a	823	CLA	C3B-C4B-NB	-2.36	108.42	110.53
19	a	834	CLA	CHB-C4A-NA	2.36	127.80	124.40
19	3	310	CLA	CHB-C4A-NA	2.36	127.80	124.40
19	a	813	CLA	CHB-C4A-NA	2.35	127.80	124.40
17	j	101	XAT	C39-C29-C28	2.35	121.69	118.09
19	b	833	CLA	CHB-C4A-NA	2.35	127.80	124.40
26	l	201	BCR	C15-C16-C17	-2.35	118.70	123.52
19	a	841	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
17	5	301	XAT	C30-C31-C32	-2.35	116.38	123.20
19	a	844	CLA	C1-C2-C3	-2.35	122.34	126.20
19	b	824	CLA	CHB-C4A-NA	2.35	127.79	124.40
19	b	836	CLA	C1-C2-C3	-2.35	122.35	126.20
19	b	810	CLA	C3B-C4B-NB	-2.35	108.44	110.53
26	a	848	BCR	C15-C16-C17	-2.35	118.72	123.52
26	i	101	BCR	C16-C15-C14	-2.35	118.72	123.52
26	m	102	BCR	C8-C7-C6	-2.35	120.73	127.00
19	1	311	CLA	CHB-C4A-NA	2.34	127.78	124.40
19	2	307	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
17	3	303	XAT	O24-C25-C38	2.34	117.67	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	817	CLA	CHB-C4A-NA	2.34	127.78	124.40
23	1	304	A1L1F	O7-C54-O55	-2.34	118.47	122.99
19	b	819	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	1	201	BCR	C29-C30-C25	2.34	113.83	110.44
19	1	305	CLA	CHB-C4A-NA	2.34	127.77	124.40
19	b	840	CLA	C1-C2-C3	-2.33	122.37	126.20
26	b	852	BCR	C23-C24-C25	-2.33	120.76	127.00
19	1	309	CLA	CHB-C4A-NA	2.33	127.77	124.40
23	1	304	A1L1F	C37-C36-C35	-2.33	118.75	123.52
19	b	812	CLA	C3B-C4B-NB	-2.33	107.91	110.33
19	b	838	CLA	C1-C2-C3	-2.33	122.38	126.20
19	5	314	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
17	4	305	XAT	O24-C25-C38	2.33	117.65	115.05
26	b	845	BCR	C7-C6-C5	-2.33	116.20	121.56
19	b	817	CLA	C1-C2-C3	-2.33	122.39	126.20
19	2	315	CLA	CHB-C4A-NA	2.32	127.75	124.40
19	a	810	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
17	4	303	XAT	O24-C25-C38	2.32	117.64	115.05
19	a	844	CLA	CHB-C4A-NA	2.32	127.75	124.40
26	b	845	BCR	C37-C22-C21	-2.32	119.06	122.82
17	3	301	XAT	C15-C35-C34	-2.32	118.77	123.52
17	a	852	XAT	C19-C9-C8	2.32	121.63	118.09
18	1	301	A1L1G	C14-C29-C30	-2.32	121.53	125.47
26	m	102	BCR	C24-C23-C22	-2.32	122.81	126.23
19	a	831	CLA	CHB-C4A-NA	2.32	127.74	124.40
19	a	816	CLA	C1-C2-C3	-2.31	123.02	126.76
19	a	824	CLA	CHB-C4A-NA	2.31	127.74	124.40
26	b	847	BCR	C29-C30-C25	2.31	113.80	110.44
17	5	302	XAT	C15-C35-C34	-2.31	118.79	123.52
19	a	826	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
19	b	835	CLA	C1-C2-C3	-2.31	122.41	126.20
18	1	301	A1L1G	C17-C20-C21	2.31	116.83	114.24
17	5	304	XAT	O24-C25-C38	2.31	117.63	115.05
19	b	830	CLA	C1-C2-C3	-2.31	122.42	126.20
17	2	304	XAT	C35-C34-C33	-2.31	124.04	127.28
19	b	811	CLA	C3B-C4B-NB	-2.31	108.47	110.53
19	a	836	CLA	C1-C2-C3	-2.31	123.03	126.76
19	a	805	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
19	a	844	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
17	2	303	XAT	C8-C9-C10	2.30	122.63	119.01
19	5	307	CLA	CHB-C4A-NA	2.30	127.72	124.40
19	4	313	CLA	CMB-C2B-C1B	-2.30	121.92	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	833	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
26	l	201	BCR	C23-C24-C25	-2.29	120.87	127.00
17	2	304	XAT	C20-C13-C12	2.29	121.59	118.09
26	b	850	BCR	C37-C22-C23	2.29	121.59	118.09
26	a	849	BCR	C10-C11-C12	-2.29	116.56	123.20
19	4	310	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
20	5	316	SQD	C45-O47-C7	-2.29	112.32	117.80
19	b	841	CLA	CHB-C4A-NA	2.29	127.70	124.40
17	1	303	XAT	C27-C28-C29	-2.29	121.98	125.53
26	b	847	BCR	C33-C5-C4	2.29	118.47	113.60
17	j	101	XAT	O24-C25-C38	2.28	117.60	115.05
17	2	304	XAT	O24-C25-C38	2.28	117.60	115.05
19	b	809	CLA	O2D-CGD-CBD	2.28	115.22	111.23
26	b	847	BCR	C34-C9-C8	2.28	121.58	118.09
19	1	306	CLA	C1-C2-C3	-2.28	122.46	126.20
19	b	831	CLA	CHB-C4A-NA	2.28	127.69	124.40
19	2	310	CLA	CHB-C4A-NA	2.28	127.69	124.40
26	i	101	BCR	C10-C11-C12	-2.28	116.59	123.20
19	b	826	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
19	b	824	CLA	C1-C2-C3	-2.28	122.46	126.20
19	b	822	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
19	3	310	CLA	C3B-C4B-NB	-2.28	108.50	110.53
26	b	848	BCR	C35-C13-C12	2.28	121.56	118.09
26	f	801	BCR	C34-C9-C8	2.28	121.56	118.09
26	f	804	BCR	C3-C4-C5	-2.28	110.00	114.06
26	a	848	BCR	C16-C15-C14	-2.28	118.86	123.52
17	3	304	XAT	O4-C5-C18	2.27	117.59	115.05
19	b	819	CLA	C3B-C4B-NB	-2.27	108.50	110.53
17	4	304	XAT	O4-C5-C18	2.27	117.59	115.05
17	1	303	XAT	C19-C9-C8	2.27	121.56	118.09
26	f	801	BCR	C35-C13-C12	2.27	121.56	118.09
17	2	303	XAT	O4-C5-C18	2.27	117.59	115.05
19	a	818	CLA	O2D-CGD-CBD	2.27	115.20	111.23
17	5	302	XAT	C11-C12-C13	-2.27	120.14	126.36
17	2	304	XAT	C10-C11-C12	-2.27	116.62	123.20
26	1	205	BCR	C38-C26-C27	2.27	118.43	113.60
17	3	301	XAT	O24-C25-C38	2.27	117.58	115.05
19	3	313	CLA	C1-C2-C3	-2.26	122.49	126.20
17	a	852	XAT	O24-C25-C38	2.26	117.58	115.05
17	2	301	XAT	O24-C25-C38	2.26	117.58	115.05
19	b	804	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
19	2	311	CLA	O2A-CGA-O1A	-2.26	117.97	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	818	CLA	CMB-C2B-C3B	2.26	131.87	126.55
26	l	205	BCR	C33-C5-C4	2.26	118.41	113.60
19	a	809	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
19	b	838	CLA	CHB-C4A-NA	2.26	127.66	124.40
17	3	303	XAT	C10-C11-C12	-2.26	116.66	123.20
17	2	305	XAT	C19-C9-C8	2.26	121.53	118.09
19	a	827	CLA	CAA-C2A-C1A	-2.26	104.58	111.97
26	b	847	BCR	C23-C24-C25	-2.25	120.98	127.00
17	2	305	XAT	O4-C5-C18	2.25	117.56	115.05
24	a	843	PQN	C11-C12-C13	-2.25	122.95	126.83
17	3	303	XAT	O4-C5-C18	2.25	117.56	115.05
17	1	302	XAT	O24-C25-C38	2.25	117.56	115.05
17	3	304	XAT	C27-C28-C29	-2.25	122.04	125.53
26	a	850	BCR	C20-C19-C18	-2.25	120.20	126.36
17	5	302	XAT	O4-C5-C18	2.25	117.56	115.05
19	5	311	CLA	C1-C2-C3	-2.24	122.52	126.20
19	f	803	CLA	C1-C2-C3	-2.24	122.52	126.20
19	b	818	CLA	C1-C2-C3	-2.24	122.52	126.20
26	f	801	BCR	C28-C27-C26	-2.24	110.06	114.06
26	b	846	BCR	C11-C10-C9	-2.24	124.13	127.28
19	b	803	CLA	CHB-C4A-NA	2.24	127.63	124.40
19	a	820	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
19	a	806	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
19	f	802	CLA	C1-C2-C3	-2.24	122.53	126.20
19	a	838	CLA	C1-C2-C3	-2.24	122.53	126.20
17	5	304	XAT	O4-C5-C18	2.24	117.55	115.05
19	3	310	CLA	CMB-C2B-C1B	-2.24	122.02	125.42
17	3	305	XAT	O24-C25-C38	2.23	117.55	115.05
17	4	305	XAT	C15-C35-C34	-2.23	118.95	123.52
19	a	840	CLA	C1-C2-C3	-2.23	122.54	126.20
19	a	811	CLA	C1-C2-C3	-2.23	122.54	126.20
19	b	837	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
19	b	804	CLA	O1D-CGD-CBD	2.23	128.92	124.52
17	3	305	XAT	C19-C9-C8	2.23	121.50	118.09
17	5	302	XAT	C30-C31-C32	-2.23	116.74	123.20
17	2	303	XAT	O24-C25-C38	2.23	117.54	115.05
17	3	301	XAT	O4-C5-C18	2.23	117.54	115.05
19	a	820	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
26	j	104	BCR	C29-C30-C25	2.23	113.67	110.44
17	4	301	XAT	C39-C29-C30	-2.23	119.21	122.82
19	a	819	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
26	f	801	BCR	C15-C14-C13	-2.22	124.16	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	829	CLA	CHB-C4A-NA	2.22	127.61	124.40
19	5	307	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
19	1	312	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
19	b	827	CLA	CHB-C4A-NA	2.22	127.61	124.40
19	a	831	CLA	O2D-CGD-CBD	2.22	115.11	111.23
17	3	303	XAT	C15-C35-C34	-2.22	118.97	123.52
26	b	844	BCR	C36-C18-C19	2.22	121.48	118.09
19	b	815	CLA	C1-C2-C3	-2.22	122.56	126.20
17	4	302	XAT	C39-C29-C28	2.22	121.48	118.09
26	b	846	BCR	C34-C9-C8	2.22	121.48	118.09
19	b	836	CLA	CAC-C3C-C4C	2.22	127.68	124.79
26	b	844	BCR	C37-C22-C23	2.22	121.48	118.09
17	1	303	XAT	O24-C25-C38	2.22	117.53	115.05
17	2	305	XAT	C15-C35-C34	-2.22	118.98	123.52
26	b	850	BCR	C35-C13-C12	2.22	121.47	118.09
17	2	302	XAT	O24-C25-C38	2.22	117.52	115.05
17	4	305	XAT	O4-C5-C18	2.21	117.52	115.05
19	b	811	CLA	C1-C2-C3	-2.21	122.57	126.20
19	5	311	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
19	a	806	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
17	1	302	XAT	O4-C5-C18	2.21	117.52	115.05
19	a	829	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
19	a	823	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
17	5	301	XAT	O4-C5-C18	2.20	117.51	115.05
26	a	848	BCR	C33-C5-C4	2.20	118.29	113.60
19	b	830	CLA	CHB-C4A-NA	2.20	127.58	124.40
17	a	852	XAT	C40-C33-C32	2.20	121.45	118.09
17	2	303	XAT	C31-C32-C33	-2.20	120.33	126.36
17	3	304	XAT	O24-C25-C38	2.20	117.50	115.05
19	b	815	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
17	4	305	XAT	C39-C29-C30	-2.20	119.25	122.82
19	b	805	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
26	a	848	BCR	C23-C24-C25	-2.20	121.13	127.00
19	3	311	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
17	4	302	XAT	O4-C5-C18	2.20	117.50	115.05
26	a	849	BCR	C8-C7-C6	-2.20	121.13	127.00
26	l	201	BCR	C39-C30-C25	-2.20	106.80	110.24
26	b	850	BCR	C33-C5-C4	2.19	118.27	113.60
17	2	305	XAT	C10-C11-C12	-2.19	116.85	123.20
19	b	828	CLA	C1-C2-C3	-2.19	122.61	126.20
26	b	844	BCR	C11-C12-C13	-2.19	120.36	126.36
26	f	804	BCR	C21-C20-C19	-2.19	116.86	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	304	XAT	O24-C25-C38	2.19	117.49	115.05
17	4	302	XAT	C20-C13-C12	2.19	121.43	118.09
22	2	317	LMG	C8-O7-C10	-2.19	112.56	117.80
17	3	305	XAT	O4-C5-C18	2.18	117.49	115.05
17	3	303	XAT	C35-C15-C14	-2.18	119.05	123.52
17	3	301	XAT	C8-C9-C10	-2.18	115.58	119.01
19	1	308	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
19	a	804	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
17	2	304	XAT	O4-C5-C18	2.18	117.48	115.05
26	a	848	BCR	C34-C9-C8	2.18	121.42	118.09
26	m	102	BCR	C15-C14-C13	-2.18	124.22	127.28
19	a	834	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
19	b	829	CLA	CHB-C4A-NA	2.18	127.54	124.40
19	4	307	CLA	O2D-CGD-CBD	2.17	115.03	111.23
19	i	102	CLA	C1-C2-C3	-2.17	122.64	126.20
19	5	312	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
19	b	819	CLA	C1-C2-C3	-2.17	122.64	126.20
17	4	302	XAT	O24-C25-C38	2.17	117.47	115.05
19	2	308	CLA	CHB-C4A-NA	2.17	127.53	124.40
26	l	201	BCR	C37-C22-C23	2.17	121.40	118.09
19	5	308	CLA	C1-C2-C3	-2.17	122.65	126.20
19	a	831	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
26	b	846	BCR	C23-C24-C25	-2.16	121.22	127.00
17	3	303	XAT	C39-C29-C28	2.16	121.39	118.09
17	2	304	XAT	C30-C31-C32	-2.16	116.94	123.20
19	a	839	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
26	b	848	BCR	C37-C22-C23	2.16	121.39	118.09
19	b	831	CLA	CMA-C3A-C2A	-2.16	111.28	116.23
24	a	843	PQN	C2M-C2-C3	-2.16	120.90	124.45
17	4	303	XAT	O4-C5-C18	2.16	117.46	115.05
19	4	311	CLA	O2D-CGD-CBD	2.15	114.99	111.23
19	3	313	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
19	a	801	CLA	CHB-C4A-NA	2.15	127.50	124.40
26	l	201	BCR	C3-C4-C5	-2.15	110.22	114.06
26	a	847	BCR	C8-C7-C6	-2.15	121.25	127.00
19	a	806	CLA	C5-C3-C2	-2.15	116.34	121.17
17	4	301	XAT	O4-C5-C18	2.15	117.45	115.05
19	b	807	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
26	a	849	BCR	C15-C16-C17	-2.15	119.12	123.52
26	j	104	BCR	C21-C20-C19	-2.15	116.98	123.20
17	5	302	XAT	O24-C25-C38	2.15	117.45	115.05
19	b	823	CLA	O2A-CGA-O1A	-2.15	118.26	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	803	CLA	CMB-C2B-C3B	2.15	131.60	126.55
19	b	801	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
19	b	824	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
19	4	308	CLA	O2D-CGD-CBD	2.14	114.98	111.23
19	f	802	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
19	b	841	CLA	C1-C2-C3	-2.14	122.69	126.20
17	4	303	XAT	C7-C8-C9	-2.14	122.20	125.53
17	1	302	XAT	C30-C31-C32	-2.14	116.99	123.20
26	b	847	BCR	C2-C1-C6	2.14	113.55	110.44
17	5	302	XAT	O24-C25-C26	-2.14	57.23	58.93
19	a	812	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
26	b	845	BCR	C1-C6-C7	2.14	121.45	115.65
19	i	102	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
19	a	809	CLA	O2D-CGD-CBD	2.14	114.97	111.23
26	b	846	BCR	C15-C16-C17	-2.14	119.14	123.52
19	a	838	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
19	b	821	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
19	a	826	CLA	CMB-C2B-C3B	2.14	131.57	126.55
19	a	816	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
19	a	830	CLA	CHB-C4A-NA	2.13	127.48	124.40
19	a	836	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
26	j	104	BCR	C16-C15-C14	-2.13	119.15	123.52
17	1	302	XAT	C10-C11-C12	-2.13	117.02	123.20
19	b	839	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
19	a	842	CLA	C1-C2-C3	-2.13	122.70	126.20
17	2	302	XAT	O4-C5-C18	2.13	117.43	115.05
19	b	830	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
19	1	307	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
26	b	843	BCR	C37-C22-C23	2.13	121.34	118.09
19	b	827	CLA	C1-C2-C3	-2.13	122.71	126.20
26	b	843	BCR	C38-C26-C27	2.13	118.14	113.60
19	4	308	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
19	b	802	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
17	1	303	XAT	O4-C5-C18	2.13	117.43	115.05
19	a	807	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
26	b	848	BCR	C23-C24-C25	-2.13	121.32	127.00
19	b	833	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
19	b	813	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
17	j	101	XAT	O4-C5-C18	2.12	117.42	115.05
17	a	852	XAT	C39-C29-C28	2.12	121.33	118.09
17	2	304	XAT	C40-C33-C32	2.12	121.33	118.09
19	2	308	CLA	O2A-CGA-O1A	-2.12	118.33	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	818	CLA	C1-C2-C3	-2.12	122.73	126.20
19	4	313	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	a	829	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	b	832	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	a	827	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
19	b	836	CLA	CMB-C2B-C3B	2.11	131.52	126.55
17	4	303	XAT	C35-C15-C14	-2.11	119.20	123.52
19	b	820	CLA	C1-C2-C3	-2.11	122.74	126.20
19	b	826	CLA	C1-C2-C3	-2.11	122.74	126.20
17	5	301	XAT	C39-C29-C28	2.11	121.31	118.09
19	b	820	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
17	5	302	XAT	C19-C9-C10	-2.11	119.40	122.82
20	5	316	SQD	O7-S-C6	2.11	109.90	106.76
26	l	201	BCR	C34-C9-C10	-2.11	119.41	122.82
26	a	849	BCR	C37-C22-C23	2.10	121.30	118.09
19	b	808	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
19	a	802	CLA	CMB-C2B-C3B	2.10	131.50	126.55
19	b	830	CLA	CHB-C1B-NB	2.10	127.20	124.05
21	b	851	DGD	O3D-C3D-C4D	-2.10	105.43	110.38
19	b	811	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
26	a	847	BCR	C33-C5-C4	2.10	118.07	113.60
19	b	830	CLA	O2D-CGD-CBD	2.10	114.90	111.23
19	3	309	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
17	4	304	XAT	C19-C9-C8	2.10	121.29	118.09
17	1	303	XAT	C20-C13-C12	2.10	121.29	118.09
19	a	825	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
17	3	304	XAT	C35-C15-C14	-2.10	119.23	123.52
19	a	803	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
26	b	852	BCR	C32-C1-C6	-2.10	106.96	110.24
19	b	805	CLA	C1-C2-C3	-2.10	122.76	126.20
26	b	844	BCR	C33-C5-C4	2.10	118.06	113.60
19	2	312	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
17	5	304	XAT	C35-C15-C14	-2.09	119.23	123.52
19	1	310	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
19	a	844	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
19	a	801	CLA	O1D-CGD-CBD	2.09	128.64	124.52
26	j	104	BCR	C3-C4-C5	-2.09	110.33	114.06
19	a	854	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
19	b	841	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
19	4	309	CLA	C1-C2-C3	-2.09	123.39	126.76
19	b	803	CLA	O2D-CGD-CBD	2.09	114.88	111.23
19	b	838	CLA	O2A-CGA-O1A	-2.09	118.41	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	847	BCR	C28-C27-C26	-2.08	110.34	114.06
19	a	826	CLA	C1-C2-C3	-2.08	122.78	126.20
19	a	806	CLA	C6-C7-C8	-2.08	109.04	115.97
26	b	845	BCR	C16-C15-C14	-2.08	119.25	123.52
19	b	802	CLA	C3B-C4B-NB	-2.08	108.67	110.53
19	a	808	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
19	b	808	CLA	O2D-CGD-CBD	2.08	114.87	111.23
19	b	817	CLA	O2D-CGD-CBD	2.08	114.87	111.23
19	a	818	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
17	2	301	XAT	C19-C9-C8	2.08	121.27	118.09
19	a	822	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	b	811	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
17	2	302	XAT	C19-C9-C8	2.08	121.26	118.09
17	4	304	XAT	C30-C31-C32	-2.08	117.18	123.20
19	b	804	CLA	O2D-CGD-CBD	2.08	114.86	111.23
19	5	308	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
19	a	804	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
19	1	306	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
19	b	828	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
19	b	840	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
19	a	827	CLA	C1-C2-C3	-2.07	122.80	126.20
19	a	806	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
19	2	307	CLA	CMB-C2B-C3B	2.07	131.43	126.55
19	3	308	CLA	O2D-CGD-CBD	2.07	114.85	111.23
19	2	308	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
19	2	310	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	2	317	LMG	C4-C3-C2	-2.07	107.19	110.83
17	2	304	XAT	C15-C35-C34	-2.07	119.28	123.52
19	j	102	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	1	311	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	b	822	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
19	1	307	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	a	832	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	a	814	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	a	805	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
19	1	306	CLA	CAC-C3C-C4C	2.07	127.48	124.79
17	4	301	XAT	C10-C11-C12	-2.07	117.21	123.20
26	f	804	BCR	C8-C7-C6	-2.07	121.48	127.00
19	1	311	CLA	O2D-CGD-CBD	2.07	114.84	111.23
19	4	317	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
19	5	307	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
17	4	301	XAT	C24-C23-C22	-2.06	106.93	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	303	XAT	C11-C10-C9	-2.06	124.39	127.28
21	b	851	DGD	O5E-C6E-C5E	-2.06	104.32	111.33
19	a	814	CLA	C1-C2-C3	-2.06	122.82	126.20
19	a	829	CLA	CMB-C2B-C3B	2.06	131.40	126.55
19	b	818	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
17	2	302	XAT	C27-C28-C29	-2.06	122.33	125.53
19	b	818	CLA	CHB-C1B-NB	2.06	127.14	124.05
19	2	307	CLA	C2A-C1A-CHA	2.06	127.44	123.87
19	a	830	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	b	806	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
26	a	847	BCR	C20-C19-C18	-2.05	120.73	126.36
19	b	839	CLA	C1-C2-C3	-2.05	122.83	126.20
19	a	823	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
17	3	303	XAT	C19-C9-C8	2.05	121.22	118.09
26	i	101	BCR	C23-C22-C21	2.05	122.23	119.01
19	a	844	CLA	CMB-C2B-C3B	2.05	131.37	126.55
19	b	837	CLA	O2D-CGD-CBD	2.05	114.81	111.23
19	a	809	CLA	CMB-C2B-C3B	2.05	131.37	126.55
19	3	308	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
19	5	311	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
19	l	203	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
19	a	816	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
19	4	307	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
17	4	304	XAT	C20-C13-C12	2.04	121.21	118.09
19	b	810	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	b	812	CLA	C1-C2-C3	-2.04	122.85	126.20
19	b	804	CLA	CAC-C3C-C4C	2.04	127.45	124.79
19	a	809	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	b	835	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	b	826	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
18	1	301	A1L1G	C29-C30-C31	2.04	122.16	119.00
17	4	304	XAT	C39-C29-C28	2.04	121.20	118.09
19	b	806	CLA	C1-C2-C3	-2.04	122.86	126.20
19	b	810	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
19	a	833	CLA	CMB-C2B-C3B	2.04	131.34	126.55
26	b	846	BCR	C35-C13-C12	2.03	121.19	118.09
26	b	852	BCR	C38-C26-C27	2.03	117.93	113.60
26	b	845	BCR	C21-C20-C19	-2.03	117.31	123.20
17	5	301	XAT	C10-C11-C12	-2.03	117.31	123.20
19	b	827	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
19	a	835	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
17	3	305	XAT	C20-C13-C12	2.03	121.19	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	302	XAT	C39-C29-C28	2.03	121.19	118.09
22	j	105	LMG	O7-C10-O9	-2.03	118.97	123.70
19	b	825	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
26	b	843	BCR	C16-C15-C14	-2.03	119.37	123.52
26	b	847	BCR	C38-C26-C27	2.03	117.92	113.60
26	l	205	BCR	C10-C11-C12	-2.03	117.33	123.20
26	a	848	BCR	C28-C27-C26	-2.03	110.44	114.06
19	b	812	CLA	O2D-CGD-CBD	2.03	114.77	111.23
19	a	839	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
19	2	307	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	4	308	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
19	b	815	CLA	CMB-C2B-C3B	2.02	131.31	126.55
19	b	803	CLA	C1-C2-C3	-2.02	122.88	126.20
26	a	849	BCR	C29-C30-C25	2.02	113.38	110.44
19	b	826	CLA	CMB-C2B-C3B	2.02	131.31	126.55
19	a	831	CLA	C3B-C4B-NB	-2.02	108.72	110.53
19	b	829	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	b	846	BCR	C28-C27-C26	-2.02	110.45	114.06
26	a	847	BCR	C10-C11-C12	-2.02	117.34	123.20
19	a	842	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	a	849	BCR	C38-C26-C27	2.02	117.91	113.60
26	b	845	BCR	C10-C11-C12	-2.02	117.34	123.20
26	a	849	BCR	C35-C13-C12	2.02	121.18	118.09
19	4	313	CLA	CMB-C2B-C3B	2.02	131.30	126.55
19	a	813	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
19	b	802	CLA	C1-C2-C3	-2.02	122.89	126.20
17	4	301	XAT	C28-C29-C30	2.02	122.18	119.01
19	a	833	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
26	b	843	BCR	C33-C5-C6	-2.02	122.28	124.48
17	2	301	XAT	O4-C5-C18	2.02	117.30	115.05
19	b	830	CLA	C3B-C4B-NB	-2.01	108.73	110.53
19	2	310	CLA	C1-C2-C3	-2.01	122.90	126.20
19	a	811	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
26	b	845	BCR	C8-C9-C10	2.01	122.17	119.01
19	b	812	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
19	b	815	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
19	3	310	CLA	CMB-C2B-C3B	2.01	131.27	126.55
19	a	822	CLA	C1-C2-C3	-2.01	122.91	126.20
19	1	305	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
23	1	304	A1L1F	C25-C14-C29	-2.01	121.75	125.99
21	4	318	DGD	C4D-C3D-C2D	-2.01	107.31	110.83
19	b	809	CLA	C1-C2-C3	-2.00	122.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	205	BCR	C7-C8-C9	-2.00	123.27	126.23
19	b	807	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
19	b	814	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
17	2	305	XAT	O24-C25-C38	2.00	117.28	115.05
19	b	803	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
17	3	301	XAT	C30-C31-C32	-2.00	117.40	123.20

All (146) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	5	305	CLA	ND
19	5	306	CLA	ND
19	5	307	CLA	ND
19	5	308	CLA	ND
19	5	309	CLA	ND
19	5	310	CLA	ND
19	5	311	CLA	ND
19	5	312	CLA	ND
19	5	313	CLA	ND
19	5	314	CLA	ND
19	5	315	CLA	ND
19	4	306	CLA	ND
19	4	307	CLA	ND
19	4	308	CLA	ND
19	4	309	CLA	ND
19	4	310	CLA	ND
19	4	311	CLA	ND
19	4	312	CLA	ND
19	4	313	CLA	ND
19	4	314	CLA	ND
19	4	315	CLA	ND
19	4	316	CLA	ND
19	4	317	CLA	ND
19	3	307	CLA	ND
19	3	308	CLA	ND
19	3	309	CLA	ND
19	3	310	CLA	ND
19	3	311	CLA	ND
19	3	312	CLA	ND
19	3	313	CLA	ND
19	3	314	CLA	ND
19	3	315	CLA	ND

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Mol	Chain	Res	Type	Atom
19	2	306	CLA	ND
19	2	307	CLA	ND
19	2	308	CLA	ND
19	2	309	CLA	ND
19	2	310	CLA	ND
19	2	311	CLA	ND
19	2	312	CLA	ND
19	2	313	CLA	ND
19	2	314	CLA	ND
19	2	315	CLA	ND
19	2	316	CLA	ND
19	1	305	CLA	ND
19	1	306	CLA	ND
19	1	307	CLA	ND
19	1	308	CLA	ND
19	1	309	CLA	ND
19	1	310	CLA	ND
19	1	311	CLA	ND
19	1	312	CLA	ND
19	1	313	CLA	ND
19	1	314	CLA	ND
19	a	801	CLA	ND
19	a	802	CLA	ND
19	a	803	CLA	ND
19	a	804	CLA	ND
19	a	805	CLA	ND
19	a	806	CLA	ND
19	a	807	CLA	ND
19	a	808	CLA	ND
19	a	809	CLA	ND
19	a	810	CLA	ND
19	a	811	CLA	ND
19	a	812	CLA	ND
19	a	813	CLA	ND
19	a	814	CLA	ND
19	a	815	CLA	ND
19	a	816	CLA	ND
19	a	817	CLA	ND
19	a	818	CLA	ND
19	a	819	CLA	ND
19	a	820	CLA	ND
19	a	821	CLA	ND

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Mol	Chain	Res	Type	Atom
19	a	822	CLA	ND
19	a	823	CLA	ND
19	a	824	CLA	ND
19	a	825	CLA	ND
19	a	826	CLA	ND
19	a	827	CLA	ND
19	a	828	CLA	ND
19	a	829	CLA	ND
19	a	830	CLA	ND
19	a	831	CLA	ND
19	a	832	CLA	ND
19	a	833	CLA	ND
19	a	834	CLA	ND
19	a	835	CLA	ND
19	a	836	CLA	ND
19	a	837	CLA	ND
19	a	838	CLA	ND
19	a	839	CLA	ND
19	a	840	CLA	ND
19	a	841	CLA	ND
19	a	842	CLA	ND
19	a	844	CLA	ND
19	a	854	CLA	ND
19	b	801	CLA	ND
19	b	802	CLA	ND
19	b	803	CLA	ND
19	b	804	CLA	ND
19	b	805	CLA	ND
19	b	806	CLA	ND
19	b	807	CLA	ND
19	b	808	CLA	ND
19	b	809	CLA	ND
19	b	810	CLA	ND
19	b	811	CLA	ND
19	b	812	CLA	ND
19	b	813	CLA	ND
19	b	814	CLA	ND
19	b	815	CLA	ND
19	b	816	CLA	ND
19	b	817	CLA	ND
19	b	818	CLA	ND
19	b	819	CLA	ND

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Mol	Chain	Res	Type	Atom
19	b	820	CLA	ND
19	b	821	CLA	ND
19	b	822	CLA	ND
19	b	823	CLA	ND
19	b	824	CLA	ND
19	b	825	CLA	ND
19	b	826	CLA	ND
19	b	827	CLA	ND
19	b	828	CLA	ND
19	b	829	CLA	ND
19	b	830	CLA	ND
19	b	831	CLA	ND
19	b	832	CLA	ND
19	b	833	CLA	ND
19	b	834	CLA	ND
19	b	835	CLA	ND
19	b	836	CLA	ND
19	b	837	CLA	ND
19	b	838	CLA	ND
19	b	839	CLA	ND
19	b	840	CLA	ND
19	b	841	CLA	ND
19	f	802	CLA	ND
19	f	803	CLA	ND
19	i	102	CLA	ND
19	j	102	CLA	ND
19	j	103	CLA	ND
19	l	202	CLA	ND
19	l	203	CLA	ND
19	l	204	CLA	ND

All (1598) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	5	302	XAT	O4-C6-C7-C8
17	5	302	XAT	C7-C8-C9-C10
17	5	302	XAT	C7-C8-C9-C19
17	4	301	XAT	C27-C28-C29-C30
17	4	301	XAT	C27-C28-C29-C39
17	4	303	XAT	O4-C6-C7-C8
17	4	303	XAT	C7-C8-C9-C10
17	4	303	XAT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
17	4	305	XAT	O24-C26-C27-C28
17	3	301	XAT	O4-C6-C7-C8
17	3	301	XAT	C27-C28-C29-C30
17	3	301	XAT	C27-C28-C29-C39
17	3	303	XAT	C27-C28-C29-C30
17	3	304	XAT	O24-C26-C27-C28
17	3	304	XAT	C27-C28-C29-C30
17	3	304	XAT	C27-C28-C29-C39
17	2	303	XAT	O4-C6-C7-C8
17	2	303	XAT	O24-C26-C27-C28
17	2	303	XAT	C27-C28-C29-C30
17	2	303	XAT	C27-C28-C29-C39
17	2	305	XAT	C25-C26-C27-C28
17	a	852	XAT	C7-C8-C9-C10
17	a	852	XAT	C7-C8-C9-C19
17	a	852	XAT	C11-C12-C13-C14
17	a	852	XAT	C27-C28-C29-C30
17	j	101	XAT	O4-C6-C7-C8
17	j	101	XAT	C7-C8-C9-C10
17	j	101	XAT	O24-C26-C27-C28
18	5	303	A1L1G	C26-C30-C31-C32
18	5	303	A1L1G	C31-C32-C33-C34
18	5	303	A1L1G	C32-C33-C34-C27
18	5	303	A1L1G	C32-C33-C34-C35
18	5	303	A1L1G	C41-C42-C44-C2
18	5	303	A1L1G	C41-C42-C44-C43
18	3	302	A1L1G	C25-C14-C29-C30
18	3	302	A1L1G	C14-C29-C30-C26
18	3	302	A1L1G	C26-C30-C31-C32
18	3	302	A1L1G	C29-C30-C31-C32
18	3	302	A1L1G	C41-C42-C44-C2
18	3	302	A1L1G	C41-C42-C44-C43
18	3	306	A1L1G	C45-C2-C44-C42
18	3	306	A1L1G	C45-C2-C44-C43
18	3	306	A1L1G	O13-C26-C30-C29
18	3	306	A1L1G	C37-C38-C39-C28
18	3	306	A1L1G	C37-C38-C39-C40
18	3	306	A1L1G	C39-C40-C41-C42
18	3	306	A1L1G	C41-C42-C44-C2
18	3	306	A1L1G	C41-C42-C44-C43
18	1	301	A1L1G	C45-C2-C44-C42
18	1	301	A1L1G	C45-C2-C44-C43

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Mol	Chain	Res	Type	Atoms
18	1	301	A1L1G	O13-C26-C30-C29
18	1	301	A1L1G	C27-C34-C35-C36
18	1	301	A1L1G	C33-C34-C35-C36
18	1	301	A1L1G	C35-C36-C37-C38
18	1	301	A1L1G	C38-C39-C40-C41
18	1	301	A1L1G	C39-C40-C41-C42
19	5	308	CLA	CBD-CGD-O2D-CED
19	5	309	CLA	CAD-CBD-CGD-O1D
19	5	309	CLA	CAD-CBD-CGD-O2D
19	5	310	CLA	CBD-CGD-O2D-CED
19	5	314	CLA	C1A-C2A-CAA-CBA
19	5	314	CLA	C3A-C2A-CAA-CBA
19	5	315	CLA	CBD-CGD-O2D-CED
19	5	315	CLA	O1D-CGD-O2D-CED
19	4	306	CLA	C1A-C2A-CAA-CBA
19	4	307	CLA	CHA-CBD-CGD-O1D
19	4	307	CLA	CHA-CBD-CGD-O2D
19	4	309	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	C1A-C2A-CAA-CBA
19	4	311	CLA	CBA-CGA-O2A-C1
19	4	311	CLA	CBD-CGD-O2D-CED
19	4	312	CLA	C1A-C2A-CAA-CBA
19	4	312	CLA	C3A-C2A-CAA-CBA
19	4	315	CLA	CAD-CBD-CGD-O2D
19	4	316	CLA	CBD-CGD-O2D-CED
19	4	317	CLA	CBD-CGD-O2D-CED
19	3	308	CLA	CHA-CBD-CGD-O1D
19	3	308	CLA	CHA-CBD-CGD-O2D
19	3	312	CLA	C1A-C2A-CAA-CBA
19	3	315	CLA	C1A-C2A-CAA-CBA
19	2	307	CLA	CHA-CBD-CGD-O2D
19	2	307	CLA	CBD-CGD-O2D-CED
19	2	309	CLA	CBD-CGD-O2D-CED
19	2	310	CLA	CHA-CBD-CGD-O1D
19	2	310	CLA	CHA-CBD-CGD-O2D
19	2	312	CLA	CBD-CGD-O2D-CED
19	2	313	CLA	CBD-CGD-O2D-CED
19	1	305	CLA	C11-C10-C8-C9
19	1	310	CLA	CBD-CGD-O2D-CED
19	1	313	CLA	CBD-CGD-O2D-CED
19	1	314	CLA	C1A-C2A-CAA-CBA
19	1	314	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	a	801	CLA	CBD-CGD-O2D-CED
19	a	804	CLA	CHA-CBD-CGD-O1D
19	a	804	CLA	CHA-CBD-CGD-O2D
19	a	805	CLA	C1A-C2A-CAA-CBA
19	a	805	CLA	C3A-C2A-CAA-CBA
19	a	806	CLA	CAD-CBD-CGD-O2D
19	a	809	CLA	C1A-C2A-CAA-CBA
19	a	809	CLA	C3A-C2A-CAA-CBA
19	a	809	CLA	CHA-CBD-CGD-O1D
19	a	809	CLA	CHA-CBD-CGD-O2D
19	a	811	CLA	CBD-CGD-O2D-CED
19	a	817	CLA	CHA-CBD-CGD-O1D
19	a	817	CLA	CHA-CBD-CGD-O2D
19	a	818	CLA	C1A-C2A-CAA-CBA
19	a	818	CLA	C3A-C2A-CAA-CBA
19	a	818	CLA	CHA-CBD-CGD-O1D
19	a	818	CLA	CHA-CBD-CGD-O2D
19	a	819	CLA	C3A-C2A-CAA-CBA
19	a	820	CLA	C1A-C2A-CAA-CBA
19	a	820	CLA	C3A-C2A-CAA-CBA
19	a	823	CLA	C1A-C2A-CAA-CBA
19	a	823	CLA	C3A-C2A-CAA-CBA
19	a	823	CLA	CHA-CBD-CGD-O1D
19	a	823	CLA	CHA-CBD-CGD-O2D
19	a	829	CLA	C1A-C2A-CAA-CBA
19	a	829	CLA	CBD-CGD-O2D-CED
19	a	831	CLA	CHA-CBD-CGD-O1D
19	a	831	CLA	CHA-CBD-CGD-O2D
19	a	832	CLA	C1A-C2A-CAA-CBA
19	a	832	CLA	C3A-C2A-CAA-CBA
19	a	834	CLA	C2B-C3B-CAB-CBB
19	a	834	CLA	C4B-C3B-CAB-CBB
19	a	838	CLA	C1A-C2A-CAA-CBA
19	a	838	CLA	C2-C3-C5-C6
19	a	838	CLA	C4-C3-C5-C6
19	a	854	CLA	C1A-C2A-CAA-CBA
19	a	854	CLA	C2B-C3B-CAB-CBB
19	a	854	CLA	C4B-C3B-CAB-CBB
19	b	803	CLA	CBD-CGD-O2D-CED
19	b	804	CLA	CBD-CGD-O2D-CED
19	b	805	CLA	CHA-CBD-CGD-O1D
19	b	805	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	b	806	CLA	C1A-C2A-CAA-CBA
19	b	806	CLA	C3A-C2A-CAA-CBA
19	b	806	CLA	CAD-CBD-CGD-O1D
19	b	806	CLA	CAD-CBD-CGD-O2D
19	b	809	CLA	CHA-CBD-CGD-O1D
19	b	809	CLA	CHA-CBD-CGD-O2D
19	b	810	CLA	C1A-C2A-CAA-CBA
19	b	811	CLA	C1A-C2A-CAA-CBA
19	b	811	CLA	CAD-CBD-CGD-O1D
19	b	811	CLA	CAD-CBD-CGD-O2D
19	b	813	CLA	C1A-C2A-CAA-CBA
19	b	813	CLA	C2-C3-C5-C6
19	b	813	CLA	C4-C3-C5-C6
19	b	815	CLA	C1A-C2A-CAA-CBA
19	b	815	CLA	CBD-CGD-O2D-CED
19	b	816	CLA	CHA-CBD-CGD-O1D
19	b	816	CLA	CHA-CBD-CGD-O2D
19	b	818	CLA	C3A-C2A-CAA-CBA
19	b	819	CLA	C1A-C2A-CAA-CBA
19	b	819	CLA	C3A-C2A-CAA-CBA
19	b	820	CLA	C4B-C3B-CAB-CBB
19	b	821	CLA	C1A-C2A-CAA-CBA
19	b	821	CLA	C3A-C2A-CAA-CBA
19	b	822	CLA	CHA-CBD-CGD-O2D
19	b	825	CLA	CHA-CBD-CGD-O1D
19	b	825	CLA	CHA-CBD-CGD-O2D
19	b	829	CLA	C1A-C2A-CAA-CBA
19	b	829	CLA	C3A-C2A-CAA-CBA
19	b	830	CLA	CHA-CBD-CGD-O1D
19	b	830	CLA	CHA-CBD-CGD-O2D
19	b	833	CLA	C1A-C2A-CAA-CBA
19	b	833	CLA	C3A-C2A-CAA-CBA
19	b	834	CLA	C1A-C2A-CAA-CBA
19	b	834	CLA	C3A-C2A-CAA-CBA
19	b	834	CLA	C11-C12-C13-C14
19	b	835	CLA	CHA-CBD-CGD-O1D
19	b	835	CLA	CHA-CBD-CGD-O2D
19	b	835	CLA	CBD-CGD-O2D-CED
19	b	839	CLA	C4B-C3B-CAB-CBB
19	b	840	CLA	C1A-C2A-CAA-CBA
19	b	840	CLA	C3A-C2A-CAA-CBA
19	b	840	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	b	840	CLA	CAD-CBD-CGD-O2D
19	b	840	CLA	CBD-CGD-O2D-CED
19	j	102	CLA	C1A-C2A-CAA-CBA
19	j	103	CLA	CAD-CBD-CGD-O1D
19	j	103	CLA	CAD-CBD-CGD-O2D
19	j	103	CLA	CBD-CGD-O2D-CED
19	l	203	CLA	C6-C7-C8-C9
20	5	316	SQD	O49-C7-O47-C45
20	5	316	SQD	C8-C7-O47-C45
20	5	316	SQD	C5-C6-S-O7
20	5	316	SQD	C5-C6-S-O8
20	5	316	SQD	C5-C6-S-O9
20	1	315	SQD	O5-C5-C6-S
20	1	315	SQD	C5-C6-S-O7
20	1	315	SQD	C5-C6-S-O8
20	1	315	SQD	C5-C6-S-O9
21	4	318	DGD	C2B-C1B-O2G-C2G
21	4	318	DGD	O1B-C1B-O2G-C2G
22	2	317	LMG	O1-C7-C8-O7
22	a	853	LMG	C11-C10-O7-C8
22	j	105	LMG	O9-C10-O7-C8
22	j	105	LMG	C11-C10-O7-C8
23	1	304	A1L1F	C32-C33-C34-C35
23	1	304	A1L1F	C38-C39-C40-C41
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	849	LHG	O1-C1-C2-C3
25	b	849	LHG	C1-C2-C3-O3
25	b	849	LHG	O2-C2-C3-O3
25	b	849	LHG	C3-O3-P-O5
25	b	849	LHG	C3-O3-P-O6
25	b	849	LHG	C4-O6-P-O3
25	b	849	LHG	C4-O6-P-O4
25	b	849	LHG	C4-O6-P-O5
25	m	101	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	m	101	LHG	C3-O3-P-O4
25	m	101	LHG	O9-C7-O7-C5
25	m	101	LHG	C8-C7-O7-C5
26	a	850	BCR	C23-C24-C25-C26
26	b	843	BCR	C7-C8-C9-C10
26	b	843	BCR	C7-C8-C9-C34
26	b	845	BCR	C1-C6-C7-C8
26	b	845	BCR	C5-C6-C7-C8
26	i	101	BCR	C21-C22-C23-C24
26	i	101	BCR	C37-C22-C23-C24
26	j	104	BCR	C7-C8-C9-C10
26	j	104	BCR	C7-C8-C9-C34
26	m	102	BCR	C21-C22-C23-C24
26	m	102	BCR	C37-C22-C23-C24
19	5	310	CLA	O1D-CGD-O2D-CED
19	4	309	CLA	O1D-CGD-O2D-CED
19	2	314	CLA	O1D-CGD-O2D-CED
19	2	307	CLA	O1D-CGD-O2D-CED
19	2	309	CLA	O1D-CGD-O2D-CED
19	2	313	CLA	O1D-CGD-O2D-CED
19	1	313	CLA	O1D-CGD-O2D-CED
19	a	812	CLA	O1D-CGD-O2D-CED
19	b	803	CLA	O1D-CGD-O2D-CED
19	b	835	CLA	O1D-CGD-O2D-CED
19	5	313	CLA	CBD-CGD-O2D-CED
19	4	306	CLA	CBD-CGD-O2D-CED
19	2	314	CLA	CBD-CGD-O2D-CED
19	1	309	CLA	CBD-CGD-O2D-CED
19	a	812	CLA	CBD-CGD-O2D-CED
19	i	102	CLA	CBD-CGD-O2D-CED
19	1	307	CLA	O1A-CGA-O2A-C1
19	a	806	CLA	O1A-CGA-O2A-C1
19	b	815	CLA	O1A-CGA-O2A-C1
22	2	317	LMG	O10-C28-O8-C9
25	m	101	LHG	O10-C23-O8-C6
19	4	316	CLA	O1D-CGD-O2D-CED
19	b	804	CLA	O1D-CGD-O2D-CED
19	a	801	CLA	O1D-CGD-O2D-CED
19	1	307	CLA	CBA-CGA-O2A-C1
19	a	806	CLA	CBA-CGA-O2A-C1
19	b	815	CLA	CBA-CGA-O2A-C1
25	m	101	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
19	4	310	CLA	O1A-CGA-O2A-C1
19	2	310	CLA	O1A-CGA-O2A-C1
19	2	311	CLA	O1A-CGA-O2A-C1
19	a	805	CLA	O1A-CGA-O2A-C1
19	a	818	CLA	O1A-CGA-O2A-C1
19	b	822	CLA	O1A-CGA-O2A-C1
19	f	802	CLA	O1A-CGA-O2A-C1
22	a	853	LMG	O10-C28-O8-C9
25	b	849	LHG	O10-C23-O8-C6
19	4	311	CLA	O1A-CGA-O2A-C1
19	2	312	CLA	O1D-CGD-O2D-CED
19	b	815	CLA	O1D-CGD-O2D-CED
19	5	308	CLA	O1D-CGD-O2D-CED
19	4	317	CLA	O1D-CGD-O2D-CED
19	1	310	CLA	O1D-CGD-O2D-CED
19	a	811	CLA	O1D-CGD-O2D-CED
19	a	829	CLA	O1D-CGD-O2D-CED
19	b	840	CLA	O1D-CGD-O2D-CED
19	j	103	CLA	O1D-CGD-O2D-CED
22	a	853	LMG	O9-C10-O7-C8
19	1	309	CLA	CBA-CGA-O2A-C1
19	1	309	CLA	O1A-CGA-O2A-C1
19	1	204	CLA	O1A-CGA-O2A-C1
19	3	312	CLA	C3-C5-C6-C7
19	2	310	CLA	C3-C5-C6-C7
19	2	311	CLA	C3-C5-C6-C7
19	2	314	CLA	C3-C5-C6-C7
19	a	810	CLA	C3-C5-C6-C7
19	b	802	CLA	C3-C5-C6-C7
19	b	805	CLA	C3-C5-C6-C7
19	b	807	CLA	C3-C5-C6-C7
19	b	809	CLA	C3-C5-C6-C7
19	2	310	CLA	CBA-CGA-O2A-C1
19	2	311	CLA	CBA-CGA-O2A-C1
19	a	805	CLA	CBA-CGA-O2A-C1
19	a	818	CLA	CBA-CGA-O2A-C1
19	a	836	CLA	CBA-CGA-O2A-C1
19	b	822	CLA	CBA-CGA-O2A-C1
19	b	824	CLA	CBA-CGA-O2A-C1
19	f	802	CLA	CBA-CGA-O2A-C1
22	2	317	LMG	C29-C28-O8-C9
22	a	853	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
23	1	304	A1L1F	C56-C54-O7-C8
23	1	304	A1L1F	O55-C54-O7-C8
19	5	305	CLA	CBD-CGD-O2D-CED
19	5	309	CLA	CBD-CGD-O2D-CED
19	3	308	CLA	CBD-CGD-O2D-CED
19	2	316	CLA	CBD-CGD-O2D-CED
19	a	804	CLA	CBD-CGD-O2D-CED
19	a	814	CLA	CBD-CGD-O2D-CED
19	b	806	CLA	CBD-CGD-O2D-CED
19	b	820	CLA	CBD-CGD-O2D-CED
19	b	836	CLA	CBD-CGD-O2D-CED
19	4	311	CLA	O1D-CGD-O2D-CED
19	3	310	CLA	C4-C3-C5-C6
19	a	825	CLA	C4-C3-C5-C6
19	a	831	CLA	C4-C3-C5-C6
19	a	839	CLA	C4-C3-C5-C6
19	j	102	CLA	C4-C3-C5-C6
19	3	310	CLA	C2-C3-C5-C6
19	a	831	CLA	C2-C3-C5-C6
19	a	839	CLA	C2-C3-C5-C6
19	j	102	CLA	C2-C3-C5-C6
19	l	204	CLA	CBA-CGA-O2A-C1
19	5	306	CLA	CBD-CGD-O2D-CED
19	1	309	CLA	O1D-CGD-O2D-CED
19	a	817	CLA	C2A-CAA-CBA-CGA
19	b	810	CLA	C2A-CAA-CBA-CGA
19	1	307	CLA	C3-C5-C6-C7
19	1	310	CLA	C3-C5-C6-C7
19	b	819	CLA	C3-C5-C6-C7
19	4	310	CLA	CBA-CGA-O2A-C1
19	1	305	CLA	CBA-CGA-O2A-C1
19	a	807	CLA	CBA-CGA-O2A-C1
19	a	811	CLA	CBA-CGA-O2A-C1
19	b	806	CLA	CBA-CGA-O2A-C1
19	b	811	CLA	CBA-CGA-O2A-C1
19	b	819	CLA	CBA-CGA-O2A-C1
22	j	105	LMG	C29-C28-O8-C9
25	b	849	LHG	C24-C23-O8-C6
22	j	105	LMG	C4-C5-C6-O5
18	3	302	A1L1G	C30-C31-C32-C33
19	5	311	CLA	O1A-CGA-O2A-C1
19	1	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	811	CLA	O1A-CGA-O2A-C1
19	a	812	CLA	O1A-CGA-O2A-C1
19	a	820	CLA	O1A-CGA-O2A-C1
19	b	806	CLA	O1A-CGA-O2A-C1
19	b	819	CLA	O1A-CGA-O2A-C1
22	j	105	LMG	O10-C28-O8-C9
19	4	307	CLA	CBD-CGD-O2D-CED
19	a	818	CLA	CBD-CGD-O2D-CED
19	a	837	CLA	CBD-CGD-O2D-CED
22	j	105	LMG	C12-C13-C14-C15
25	a	845	LHG	O2-C2-C3-O3
25	m	101	LHG	O2-C2-C3-O3
19	a	812	CLA	CBA-CGA-O2A-C1
19	b	840	CLA	CBA-CGA-O2A-C1
19	a	836	CLA	O1A-CGA-O2A-C1
19	b	824	CLA	O1A-CGA-O2A-C1
19	3	309	CLA	CBD-CGD-O2D-CED
19	3	315	CLA	CBD-CGD-O2D-CED
19	b	811	CLA	CBD-CGD-O2D-CED
19	b	840	CLA	O1A-CGA-O2A-C1
19	i	102	CLA	O1D-CGD-O2D-CED
19	5	309	CLA	C3-C5-C6-C7
19	a	807	CLA	C3-C5-C6-C7
19	a	835	CLA	C3-C5-C6-C7
19	a	841	CLA	CBD-CGD-O2D-CED
19	b	824	CLA	CBD-CGD-O2D-CED
19	b	828	CLA	CBD-CGD-O2D-CED
21	b	851	DGD	O6E-C5E-C6E-O5E
19	4	306	CLA	O1D-CGD-O2D-CED
19	5	311	CLA	CBA-CGA-O2A-C1
19	a	820	CLA	CBA-CGA-O2A-C1
19	a	813	CLA	C4-C3-C5-C6
19	b	829	CLA	C4-C3-C5-C6
19	a	825	CLA	C2-C3-C5-C6
19	a	807	CLA	O1A-CGA-O2A-C1
19	b	811	CLA	O1A-CGA-O2A-C1
19	1	312	CLA	C3-C5-C6-C7
21	4	318	DGD	O6E-C1E-O5D-C6D
19	4	308	CLA	CBD-CGD-O2D-CED
19	a	807	CLA	CBD-CGD-O2D-CED
19	a	810	CLA	CBD-CGD-O2D-CED
19	a	834	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	a	835	CLA	CBD-CGD-O2D-CED
19	b	841	CLA	CBD-CGD-O2D-CED
25	a	845	LHG	C23-C24-C25-C26
22	a	853	LMG	O6-C5-C6-O5
22	j	105	LMG	O6-C5-C6-O5
19	5	313	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	C12-C13-C14-C15
18	5	303	A1L1G	C40-C41-C42-C44
25	a	845	LHG	C1-C2-C3-O3
19	5	308	CLA	CBA-CGA-O2A-C1
19	3	311	CLA	CBA-CGA-O2A-C1
19	a	809	CLA	CBA-CGA-O2A-C1
19	a	839	CLA	CBA-CGA-O2A-C1
19	a	854	CLA	CBA-CGA-O2A-C1
19	b	821	CLA	CBA-CGA-O2A-C1
19	b	827	CLA	CBA-CGA-O2A-C1
19	b	834	CLA	CBA-CGA-O2A-C1
19	5	311	CLA	CBD-CGD-O2D-CED
19	b	823	CLA	CBD-CGD-O2D-CED
22	a	853	LMG	C4-C5-C6-O5
19	a	804	CLA	O1D-CGD-O2D-CED
19	b	806	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	C28-C29-C30-C31
19	a	813	CLA	C2-C3-C5-C6
19	2	310	CLA	C11-C12-C13-C14
19	1	306	CLA	C6-C7-C8-C9
19	1	306	CLA	C11-C12-C13-C14
19	1	310	CLA	C14-C13-C15-C16
19	a	829	CLA	C11-C10-C8-C9
19	b	801	CLA	C11-C10-C8-C9
19	b	801	CLA	C14-C13-C15-C16
19	b	805	CLA	C11-C10-C8-C9
19	b	819	CLA	C11-C10-C8-C9
19	b	825	CLA	C6-C7-C8-C9
19	b	830	CLA	C14-C13-C15-C16
19	b	839	CLA	C6-C7-C8-C9
19	f	802	CLA	C11-C12-C13-C14
19	i	102	CLA	C11-C10-C8-C9
19	i	102	CLA	C11-C12-C13-C14
22	2	317	LMG	C29-C30-C31-C32
21	4	318	DGD	C2E-C1E-O5D-C6D
25	a	846	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
19	b	836	CLA	O1D-CGD-O2D-CED
19	a	809	CLA	O1A-CGA-O2A-C1
19	a	854	CLA	O1A-CGA-O2A-C1
17	3	303	XAT	C27-C28-C29-C39
17	2	301	XAT	C27-C28-C29-C39
17	a	852	XAT	C11-C12-C13-C20
17	a	852	XAT	C27-C28-C29-C39
17	j	101	XAT	C7-C8-C9-C19
18	3	306	A1L1G	C28-C39-C40-C41
18	1	301	A1L1G	C28-C39-C40-C41
23	1	304	A1L1F	C32-C33-C34-C27
23	1	304	A1L1F	C28-C39-C40-C41
26	b	852	BCR	C7-C8-C9-C34
26	l	205	BCR	C7-C8-C9-C34
26	l	205	BCR	C37-C22-C23-C24
26	m	102	BCR	C7-C8-C9-C34
17	2	301	XAT	C27-C28-C29-C30
18	3	306	A1L1G	C38-C39-C40-C41
26	b	852	BCR	C7-C8-C9-C10
26	l	205	BCR	C7-C8-C9-C10
26	l	205	BCR	C21-C22-C23-C24
19	5	310	CLA	C2A-CAA-CBA-CGA
19	4	311	CLA	C2A-CAA-CBA-CGA
19	4	316	CLA	C2A-CAA-CBA-CGA
19	b	805	CLA	C2A-CAA-CBA-CGA
19	b	827	CLA	C2A-CAA-CBA-CGA
22	a	853	LMG	C28-C29-C30-C31
19	5	305	CLA	O1D-CGD-O2D-CED
19	3	311	CLA	O1A-CGA-O2A-C1
19	b	821	CLA	O1A-CGA-O2A-C1
19	4	316	CLA	CBA-CGA-O2A-C1
19	2	312	CLA	CBA-CGA-O2A-C1
19	b	839	CLA	CBA-CGA-O2A-C1
19	a	810	CLA	C13-C15-C16-C17
19	5	308	CLA	O1A-CGA-O2A-C1
19	b	827	CLA	O1A-CGA-O2A-C1
19	2	316	CLA	O1D-CGD-O2D-CED
18	3	302	A1L1G	C35-C36-C37-C38
19	a	807	CLA	C5-C6-C7-C8
19	b	809	CLA	C5-C6-C7-C8
19	i	102	CLA	C8-C10-C11-C12
19	a	814	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	b	824	CLA	C3-C5-C6-C7
19	b	807	CLA	C15-C16-C17-C18
19	4	315	CLA	CBD-CGD-O2D-CED
19	b	807	CLA	CBD-CGD-O2D-CED
19	1	310	CLA	C11-C10-C8-C7
19	a	801	CLA	C12-C13-C15-C16
19	a	809	CLA	C12-C13-C15-C16
19	a	828	CLA	C12-C13-C15-C16
19	a	844	CLA	C12-C13-C15-C16
19	b	808	CLA	C12-C13-C15-C16
19	b	834	CLA	C13-C15-C16-C17
21	b	851	DGD	C1A-C2A-C3A-C4A
19	5	309	CLA	O1D-CGD-O2D-CED
25	b	849	LHG	C7-C8-C9-C10
19	a	839	CLA	O1A-CGA-O2A-C1
19	b	834	CLA	O1A-CGA-O2A-C1
19	2	310	CLA	C15-C16-C17-C18
19	a	809	CLA	C5-C6-C7-C8
19	a	834	CLA	C15-C16-C17-C18
19	b	801	CLA	C15-C16-C17-C18
19	a	825	CLA	C2A-CAA-CBA-CGA
19	a	830	CLA	C2A-CAA-CBA-CGA
19	a	842	CLA	C2A-CAA-CBA-CGA
19	b	821	CLA	C2A-CAA-CBA-CGA
19	b	834	CLA	C2A-CAA-CBA-CGA
19	b	839	CLA	C2A-CAA-CBA-CGA
18	3	302	A1L1G	C39-C40-C41-C42
19	4	308	CLA	C10-C11-C12-C13
19	a	802	CLA	C5-C6-C7-C8
19	a	814	CLA	C13-C15-C16-C17
19	b	809	CLA	C8-C10-C11-C12
19	b	833	CLA	C13-C15-C16-C17
19	b	841	CLA	C13-C15-C16-C17
19	i	102	CLA	C10-C11-C12-C13
22	a	853	LMG	C10-C11-C12-C13
23	1	304	A1L1F	C45-C47-C48-C49
25	a	846	LHG	C7-C8-C9-C10
19	a	801	CLA	C3-C5-C6-C7
23	1	304	A1L1F	C49-C50-C51-C52
19	3	308	CLA	O1D-CGD-O2D-CED
19	b	820	CLA	O1D-CGD-O2D-CED
19	5	309	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	1	306	CLA	C5-C6-C7-C8
19	1	306	CLA	C8-C10-C11-C12
19	a	809	CLA	C8-C10-C11-C12
19	a	830	CLA	C13-C15-C16-C17
19	a	831	CLA	C5-C6-C7-C8
19	b	814	CLA	C15-C16-C17-C18
19	b	830	CLA	C8-C10-C11-C12
19	l	203	CLA	C10-C11-C12-C13
19	b	828	CLA	CBA-CGA-O2A-C1
19	a	807	CLA	C15-C16-C17-C18
19	a	841	CLA	C5-C6-C7-C8
19	b	815	CLA	C5-C6-C7-C8
19	b	837	CLA	C5-C6-C7-C8
19	5	305	CLA	CBA-CGA-O2A-C1
19	5	306	CLA	O1D-CGD-O2D-CED
19	a	837	CLA	O1D-CGD-O2D-CED
19	2	312	CLA	O1A-CGA-O2A-C1
19	1	306	CLA	C15-C16-C17-C18
19	a	841	CLA	C15-C16-C17-C18
19	b	841	CLA	C10-C11-C12-C13
19	4	317	CLA	CBA-CGA-O2A-C1
19	a	816	CLA	CBA-CGA-O2A-C1
19	b	802	CLA	CBA-CGA-O2A-C1
19	b	832	CLA	CBA-CGA-O2A-C1
19	b	802	CLA	CBD-CGD-O2D-CED
19	f	802	CLA	CBD-CGD-O2D-CED
19	a	818	CLA	O1D-CGD-O2D-CED
19	4	313	CLA	C3-C5-C6-C7
21	b	851	DGD	C4E-C5E-C6E-O5E
19	b	801	CLA	C2A-CAA-CBA-CGA
19	a	814	CLA	CBA-CGA-O2A-C1
19	a	838	CLA	CBA-CGA-O2A-C1
19	a	801	CLA	C8-C10-C11-C12
19	a	828	CLA	C13-C15-C16-C17
19	a	828	CLA	C15-C16-C17-C18
19	f	802	CLA	C13-C15-C16-C17
24	b	842	PQN	C23-C25-C26-C27
19	4	307	CLA	O1D-CGD-O2D-CED
19	a	826	CLA	CBD-CGD-O2D-CED
19	3	315	CLA	O1D-CGD-O2D-CED
19	a	831	CLA	C15-C16-C17-C18
19	b	837	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	f	802	CLA	C5-C6-C7-C8
19	a	839	CLA	C13-C15-C16-C17
19	b	802	CLA	C8-C10-C11-C12
19	b	828	CLA	C13-C15-C16-C17
19	a	833	CLA	CBA-CGA-O2A-C1
19	a	844	CLA	CBA-CGA-O2A-C1
21	4	318	DGD	C3B-C4B-C5B-C6B
19	b	829	CLA	C2-C3-C5-C6
19	b	801	CLA	C8-C10-C11-C12
19	b	801	CLA	C13-C15-C16-C17
19	l	203	CLA	C8-C10-C11-C12
20	1	315	SQD	C8-C7-O47-C45
19	b	811	CLA	O1D-CGD-O2D-CED
20	1	315	SQD	O49-C7-O47-C45
19	a	824	CLA	CBA-CGA-O2A-C1
20	1	315	SQD	C24-C23-O48-C46
19	a	801	CLA	C16-C17-C18-C20
19	b	811	CLA	C16-C17-C18-C20
19	b	839	CLA	O1A-CGA-O2A-C1
18	3	302	A1L1G	C14-C29-C30-C31
18	3	302	A1L1G	C37-C38-C39-C28
18	3	306	A1L1G	C27-C34-C35-C36
17	2	303	XAT	C7-C8-C9-C19
17	2	304	XAT	C7-C8-C9-C19
18	3	302	A1L1G	C32-C33-C34-C27
26	a	850	BCR	C37-C22-C23-C24
26	f	801	BCR	C37-C22-C23-C24
17	2	303	XAT	C7-C8-C9-C10
18	3	302	A1L1G	C32-C33-C34-C35
26	a	850	BCR	C21-C22-C23-C24
26	f	801	BCR	C21-C22-C23-C24
19	4	317	CLA	O1A-CGA-O2A-C1
19	a	816	CLA	O1A-CGA-O2A-C1
19	b	802	CLA	O1A-CGA-O2A-C1
19	b	824	CLA	O1D-CGD-O2D-CED
19	2	310	CLA	C2A-CAA-CBA-CGA
19	b	832	CLA	C2A-CAA-CBA-CGA
19	b	830	CLA	C10-C11-C12-C13
19	3	309	CLA	O1D-CGD-O2D-CED
19	a	806	CLA	O2A-C1-C2-C3
19	5	315	CLA	C2C-C3C-CAC-CBC
18	5	303	A1L1G	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
19	b	834	CLA	C16-C17-C18-C19
19	b	841	CLA	C16-C17-C18-C20
19	a	841	CLA	O1D-CGD-O2D-CED
19	b	828	CLA	O1A-CGA-O2A-C1
19	b	840	CLA	C5-C6-C7-C8
18	3	302	A1L1G	C37-C38-C39-C40
18	3	306	A1L1G	C33-C34-C35-C36
19	a	814	CLA	O1A-CGA-O2A-C1
19	a	835	CLA	O1D-CGD-O2D-CED
19	b	825	CLA	C5-C6-C7-C8
19	b	828	CLA	O1D-CGD-O2D-CED
19	a	818	CLA	C2-C1-O2A-CGA
19	4	308	CLA	C16-C17-C18-C20
19	b	811	CLA	C16-C17-C18-C19
19	a	854	CLA	C5-C6-C7-C8
21	b	851	DGD	C9B-CAB-CBB-CCB
19	a	836	CLA	CBD-CGD-O2D-CED
18	3	306	A1L1G	C35-C36-C37-C38
26	m	102	BCR	C14-C15-C16-C17
25	a	845	LHG	C11-C10-C9-C8
19	a	834	CLA	O1D-CGD-O2D-CED
19	b	828	CLA	C8-C10-C11-C12
24	a	843	PQN	C25-C26-C27-C28
19	b	832	CLA	O1A-CGA-O2A-C1
19	b	817	CLA	CBA-CGA-O2A-C1
25	a	845	LHG	O1-C1-C2-O2
25	a	846	LHG	O1-C1-C2-O2
25	b	849	LHG	O1-C1-C2-O2
25	a	845	LHG	C27-C28-C29-C30
19	4	312	CLA	C4B-C3B-CAB-CBB
19	2	307	CLA	C4B-C3B-CAB-CBB
19	a	801	CLA	C4B-C3B-CAB-CBB
19	a	841	CLA	C4B-C3B-CAB-CBB
19	b	841	CLA	C4B-C3B-CAB-CBB
25	m	101	LHG	C9-C10-C11-C12
19	b	812	CLA	C6-C7-C8-C9
19	b	834	CLA	C16-C17-C18-C20
19	f	802	CLA	C16-C17-C18-C19
19	f	802	CLA	C16-C17-C18-C20
19	1	314	CLA	C2A-CAA-CBA-CGA
19	b	829	CLA	C2A-CAA-CBA-CGA
19	a	814	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	a	827	CLA	C8-C10-C11-C12
19	a	841	CLA	C8-C10-C11-C12
19	b	806	CLA	C15-C16-C17-C18
19	b	836	CLA	C5-C6-C7-C8
19	b	841	CLA	O1D-CGD-O2D-CED
19	1	308	CLA	C11-C10-C8-C7
22	2	317	LMG	C28-C29-C30-C31
19	b	809	CLA	C10-C11-C12-C13
25	a	845	LHG	C13-C14-C15-C16
19	a	844	CLA	O1A-CGA-O2A-C1
19	4	310	CLA	C3A-C2A-CAA-CBA
19	3	312	CLA	C3A-C2A-CAA-CBA
19	3	314	CLA	C3A-C2A-CAA-CBA
19	2	306	CLA	C3A-C2A-CAA-CBA
19	a	807	CLA	C3A-C2A-CAA-CBA
19	a	838	CLA	C3A-C2A-CAA-CBA
19	a	854	CLA	C3A-C2A-CAA-CBA
19	b	810	CLA	C3A-C2A-CAA-CBA
19	b	813	CLA	C3A-C2A-CAA-CBA
19	b	815	CLA	C3A-C2A-CAA-CBA
19	f	803	CLA	C3A-C2A-CAA-CBA
19	b	812	CLA	C6-C7-C8-C10
19	a	833	CLA	O1A-CGA-O2A-C1
19	a	838	CLA	O1A-CGA-O2A-C1
20	1	315	SQD	O10-C23-O48-C46
25	m	101	LHG	C28-C29-C30-C31
19	a	814	CLA	C5-C6-C7-C8
19	a	823	CLA	CBA-CGA-O2A-C1
19	b	807	CLA	CBA-CGA-O2A-C1
19	b	836	CLA	CBA-CGA-O2A-C1
20	1	315	SQD	C11-C10-C9-C8
21	4	318	DGD	C2B-C3B-C4B-C5B
25	m	101	LHG	C14-C15-C16-C17
19	a	807	CLA	O1D-CGD-O2D-CED
19	4	308	CLA	O1D-CGD-O2D-CED
19	a	810	CLA	O1D-CGD-O2D-CED
21	b	851	DGD	C4A-C5A-C6A-C7A
19	b	801	CLA	C16-C17-C18-C20
19	4	311	CLA	C2B-C3B-CAB-CBB
19	4	312	CLA	C2B-C3B-CAB-CBB
19	4	314	CLA	C2B-C3B-CAB-CBB
19	2	307	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	a	808	CLA	C2B-C3B-CAB-CBB
19	a	836	CLA	C2B-C3B-CAB-CBB
19	b	820	CLA	C2B-C3B-CAB-CBB
19	b	839	CLA	C2B-C3B-CAB-CBB
26	a	850	BCR	C23-C24-C25-C30
26	l	205	BCR	C23-C24-C25-C26
26	l	205	BCR	C23-C24-C25-C30
19	3	314	CLA	CBD-CGD-O2D-CED
19	b	825	CLA	CBA-CGA-O2A-C1
19	b	808	CLA	C5-C6-C7-C8
19	b	808	CLA	C3-C5-C6-C7
19	5	306	CLA	C2A-CAA-CBA-CGA
19	a	814	CLA	C2A-CAA-CBA-CGA
21	b	851	DGD	C4B-C5B-C6B-C7B
25	m	101	LHG	C11-C12-C13-C14
19	a	811	CLA	C11-C10-C8-C7
19	1	308	CLA	C4-C3-C5-C6
19	1	310	CLA	C4-C3-C5-C6
18	5	303	A1L1G	C39-C40-C41-C42
21	b	851	DGD	C2B-C3B-C4B-C5B
19	a	825	CLA	CBA-CGA-O2A-C1
19	b	826	CLA	C11-C10-C8-C9
21	b	851	DGD	C3B-C4B-C5B-C6B
21	4	318	DGD	O6D-C1D-O3G-C3G
19	j	102	CLA	CBD-CGD-O2D-CED
19	a	840	CLA	C13-C15-C16-C17
19	b	817	CLA	O1A-CGA-O2A-C1
19	4	316	CLA	O1A-CGA-O2A-C1
21	b	851	DGD	C2B-C1B-O2G-C2G
25	a	846	LHG	C8-C7-O7-C5
19	b	839	CLA	C15-C16-C17-C18
19	a	809	CLA	C13-C15-C16-C17
19	b	804	CLA	C2C-C3C-CAC-CBC
19	a	810	CLA	C2A-CAA-CBA-CGA
19	b	833	CLA	C2A-CAA-CBA-CGA
19	2	314	CLA	C11-C10-C8-C9
19	a	806	CLA	C16-C17-C18-C19
19	b	801	CLA	C16-C17-C18-C19
19	4	310	CLA	C4-C3-C5-C6
19	b	835	CLA	C4-C3-C5-C6
19	b	840	CLA	C4-C3-C5-C6
23	1	304	A1L1F	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
19	b	830	CLA	C15-C16-C17-C18
19	j	102	CLA	C8-C10-C11-C12
25	a	845	LHG	C26-C27-C28-C29
19	a	823	CLA	O1A-CGA-O2A-C1
19	b	807	CLA	O1A-CGA-O2A-C1
19	4	307	CLA	C3-C5-C6-C7
19	b	805	CLA	C13-C15-C16-C17
19	b	810	CLA	C5-C6-C7-C8
22	2	317	LMG	C10-C11-C12-C13
25	b	849	LHG	O6-C4-C5-O7
19	b	833	CLA	C15-C16-C17-C18
19	b	841	CLA	C16-C17-C18-C19
20	1	315	SQD	C7-C8-C9-C10
19	4	308	CLA	C15-C16-C17-C18
19	2	308	CLA	C3-C5-C6-C7
21	4	318	DGD	O1G-C1G-C2G-O2G
19	b	836	CLA	O1A-CGA-O2A-C1
19	4	308	CLA	C13-C15-C16-C17
19	a	806	CLA	C13-C15-C16-C17
19	3	315	CLA	CBA-CGA-O2A-C1
19	a	801	CLA	C16-C17-C18-C19
19	a	820	CLA	C16-C17-C18-C20
19	4	310	CLA	C2-C3-C5-C6
19	1	308	CLA	C2-C3-C5-C6
19	b	840	CLA	C2-C3-C5-C6
25	a	846	LHG	O9-C7-O7-C5
19	b	810	CLA	C10-C11-C12-C13
19	a	822	CLA	C2A-CAA-CBA-CGA
19	a	808	CLA	CBD-CGD-O2D-CED
19	5	305	CLA	O1A-CGA-O2A-C1
19	1	305	CLA	C8-C10-C11-C12
19	a	844	CLA	C10-C11-C12-C13
19	5	311	CLA	O1D-CGD-O2D-CED
19	b	825	CLA	O1A-CGA-O2A-C1
19	5	306	CLA	C1A-C2A-CAA-CBA
19	4	313	CLA	C1A-C2A-CAA-CBA
19	3	314	CLA	C1A-C2A-CAA-CBA
19	2	306	CLA	C1A-C2A-CAA-CBA
19	1	306	CLA	C1A-C2A-CAA-CBA
19	a	807	CLA	C1A-C2A-CAA-CBA
19	a	817	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	a	825	CLA	C1A-C2A-CAA-CBA
19	b	817	CLA	C1A-C2A-CAA-CBA
19	b	818	CLA	C1A-C2A-CAA-CBA
19	b	838	CLA	C1A-C2A-CAA-CBA
19	f	803	CLA	C1A-C2A-CAA-CBA
19	b	809	CLA	C15-C16-C17-C18
25	a	845	LHG	O6-C4-C5-C6
19	a	839	CLA	C3-C5-C6-C7
19	b	801	CLA	C3-C5-C6-C7
19	b	814	CLA	C3-C5-C6-C7
19	a	807	CLA	C12-C13-C15-C16
19	a	810	CLA	C12-C13-C15-C16
19	a	822	CLA	C6-C7-C8-C10
19	a	830	CLA	C12-C13-C15-C16
19	a	841	CLA	C11-C10-C8-C7
19	a	844	CLA	C11-C12-C13-C15
19	b	807	CLA	C11-C10-C8-C7
19	b	807	CLA	C12-C13-C15-C16
19	b	811	CLA	C11-C12-C13-C15
19	b	819	CLA	C6-C7-C8-C10
19	b	823	CLA	C6-C7-C8-C10
19	b	825	CLA	C11-C10-C8-C7
19	b	826	CLA	C6-C7-C8-C10
19	b	828	CLA	C6-C7-C8-C10
19	b	834	CLA	C11-C12-C13-C15
19	b	839	CLA	C6-C7-C8-C10
19	f	802	CLA	C11-C12-C13-C15
19	b	815	CLA	C6-C7-C8-C10
19	b	839	CLA	C4-C3-C5-C6
19	b	811	CLA	C2-C3-C5-C6
21	b	851	DGD	CAB-CBB-CCB-CDB
19	b	830	CLA	C13-C15-C16-C17
19	b	836	CLA	C2C-C3C-CAC-CBC
25	b	849	LHG	C8-C7-O7-C5
19	a	806	CLA	C2A-CAA-CBA-CGA
19	4	308	CLA	C11-C12-C13-C14
19	2	310	CLA	C14-C13-C15-C16
19	1	308	CLA	C11-C10-C8-C9
19	a	807	CLA	C11-C12-C13-C14
19	a	809	CLA	C14-C13-C15-C16
19	a	814	CLA	C11-C10-C8-C9
19	a	822	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	a	827	CLA	C11-C10-C8-C9
19	a	842	CLA	C11-C12-C13-C14
19	a	844	CLA	C11-C10-C8-C9
19	a	844	CLA	C14-C13-C15-C16
19	b	801	CLA	C11-C12-C13-C14
19	b	803	CLA	C11-C10-C8-C9
19	b	807	CLA	C14-C13-C15-C16
19	b	808	CLA	C11-C10-C8-C9
19	b	823	CLA	C6-C7-C8-C9
19	b	825	CLA	C11-C10-C8-C9
19	b	826	CLA	C6-C7-C8-C9
19	b	837	CLA	C14-C13-C15-C16
21	b	851	DGD	CBB-CCB-CDB-CEB
19	a	812	CLA	C10-C11-C12-C13
21	b	851	DGD	C6A-C7A-C8A-C9A
21	4	318	DGD	O1G-C1G-C2G-C3G
25	a	845	LHG	C4-C5-C6-O8
25	b	849	LHG	C4-C5-C6-O8
19	5	315	CLA	C4C-C3C-CAC-CBC
19	b	807	CLA	O1D-CGD-O2D-CED
19	b	823	CLA	O1D-CGD-O2D-CED
19	a	835	CLA	CBA-CGA-O2A-C1
19	a	844	CLA	C16-C17-C18-C19
25	m	101	LHG	C29-C30-C31-C32
19	a	825	CLA	O1A-CGA-O2A-C1
19	4	315	CLA	O1D-CGD-O2D-CED
19	a	829	CLA	C10-C11-C12-C13
19	a	820	CLA	C8-C10-C11-C12
19	b	815	CLA	C6-C7-C8-C9
19	b	819	CLA	C11-C12-C13-C14
25	m	101	LHG	C11-C10-C9-C8
17	4	305	XAT	C27-C28-C29-C30
19	1	308	CLA	C13-C15-C16-C17
19	a	854	CLA	C10-C11-C12-C13
19	b	840	CLA	C13-C15-C16-C17
24	a	843	PQN	C23-C25-C26-C27
19	4	307	CLA	CBA-CGA-O2A-C1
19	a	841	CLA	CBA-CGA-O2A-C1
19	1	310	CLA	C5-C6-C7-C8
19	a	844	CLA	C16-C17-C18-C20
19	b	837	CLA	C2C-C3C-CAC-CBC
19	b	804	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	b	851	DGD	C2A-C1A-O1G-C1G
19	b	802	CLA	C4-C3-C5-C6
19	b	811	CLA	C4-C3-C5-C6
23	1	304	A1L1F	C50-C51-C52-C53
19	b	805	CLA	C16-C17-C18-C20
25	m	101	LHG	C12-C13-C14-C15
22	a	853	LMG	C14-C15-C16-C17
19	5	310	CLA	CAA-CBA-CGA-O2A
21	b	851	DGD	C3A-C4A-C5A-C6A
22	j	105	LMG	C13-C14-C15-C16
19	b	828	CLA	C15-C16-C17-C18
19	3	314	CLA	CBA-CGA-O2A-C1
19	1	306	CLA	CBA-CGA-O2A-C1
19	1	310	CLA	CBA-CGA-O2A-C1
19	b	829	CLA	CBA-CGA-O2A-C1
19	1	311	CLA	CBD-CGD-O2D-CED
19	4	317	CLA	C3-C5-C6-C7
19	f	802	CLA	O1D-CGD-O2D-CED
19	a	829	CLA	C8-C10-C11-C12
19	b	802	CLA	O1D-CGD-O2D-CED
19	a	811	CLA	C11-C10-C8-C9
19	a	805	CLA	C6-C7-C8-C9
19	a	824	CLA	O1A-CGA-O2A-C1
19	a	801	CLA	C4-C3-C5-C6
19	a	804	CLA	C2-C3-C5-C6
19	b	803	CLA	C2-C3-C5-C6
19	a	831	CLA	CBA-CGA-O2A-C1
19	b	812	CLA	CBA-CGA-O2A-C1
19	4	310	CLA	C11-C10-C8-C9
19	a	810	CLA	C14-C13-C15-C16
19	a	814	CLA	C11-C12-C13-C14
19	a	830	CLA	C14-C13-C15-C16
19	a	835	CLA	C6-C7-C8-C9
19	a	841	CLA	C11-C10-C8-C9
19	a	844	CLA	C11-C12-C13-C14
19	b	803	CLA	C6-C7-C8-C9
19	b	810	CLA	C6-C7-C8-C9
19	b	811	CLA	C11-C12-C13-C14
19	b	819	CLA	C6-C7-C8-C9
19	b	829	CLA	C11-C12-C13-C14
19	b	838	CLA	C14-C13-C15-C16
19	j	102	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	1	308	CLA	C15-C16-C17-C18
19	a	810	CLA	C5-C6-C7-C8
19	a	826	CLA	C15-C16-C17-C18
25	m	101	LHG	C2-C3-O3-P
19	5	308	CLA	C4B-C3B-CAB-CBB
19	4	311	CLA	C4B-C3B-CAB-CBB
19	4	314	CLA	C4B-C3B-CAB-CBB
19	3	307	CLA	C4B-C3B-CAB-CBB
19	3	308	CLA	C4B-C3B-CAB-CBB
19	1	305	CLA	C4B-C3B-CAB-CBB
19	1	309	CLA	C4B-C3B-CAB-CBB
19	1	313	CLA	C4B-C3B-CAB-CBB
19	1	314	CLA	C4B-C3B-CAB-CBB
19	a	808	CLA	C4B-C3B-CAB-CBB
19	a	825	CLA	C4B-C3B-CAB-CBB
19	a	836	CLA	C4B-C3B-CAB-CBB
19	a	837	CLA	C4B-C3B-CAB-CBB
19	b	818	CLA	C4B-C3B-CAB-CBB
19	b	819	CLA	C4B-C3B-CAB-CBB
19	j	102	CLA	C4B-C3B-CAB-CBB
19	3	315	CLA	CAA-CBA-CGA-O2A
19	a	844	CLA	C15-C16-C17-C18
19	b	807	CLA	C10-C11-C12-C13
19	a	819	CLA	C2A-CAA-CBA-CGA
21	b	851	DGD	CCB-CDB-CEB-CFB
21	4	318	DGD	C2D-C1D-O3G-C3G
19	b	833	CLA	C3-C5-C6-C7
19	b	834	CLA	C3-C5-C6-C7
25	b	849	LHG	C9-C10-C11-C12
25	b	849	LHG	O6-C4-C5-C6
19	4	308	CLA	C12-C13-C15-C16
19	4	310	CLA	C11-C10-C8-C7
19	1	308	CLA	C11-C12-C13-C15
19	a	807	CLA	C11-C12-C13-C15
19	a	809	CLA	C6-C7-C8-C10
19	a	812	CLA	C6-C7-C8-C10
19	a	814	CLA	C11-C12-C13-C15
19	a	827	CLA	C11-C10-C8-C7
19	a	829	CLA	C6-C7-C8-C10
19	a	835	CLA	C6-C7-C8-C10
19	a	842	CLA	C11-C12-C13-C15
19	a	844	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	b	801	CLA	C11-C12-C13-C15
19	b	803	CLA	C6-C7-C8-C10
19	b	803	CLA	C11-C10-C8-C7
19	b	803	CLA	C12-C13-C15-C16
19	b	808	CLA	C11-C10-C8-C7
19	b	810	CLA	C6-C7-C8-C10
19	b	829	CLA	C12-C13-C15-C16
19	b	830	CLA	C12-C13-C15-C16
19	b	837	CLA	C12-C13-C15-C16
19	b	838	CLA	C12-C13-C15-C16
19	b	839	CLA	C12-C13-C15-C16
19	j	102	CLA	C6-C7-C8-C10
19	a	812	CLA	C8-C10-C11-C12
25	a	845	LHG	C7-C8-C9-C10
19	4	311	CLA	C3A-C2A-CAA-CBA
19	3	315	CLA	C3A-C2A-CAA-CBA
19	2	314	CLA	C3A-C2A-CAA-CBA
19	a	804	CLA	C4-C3-C5-C6
19	a	820	CLA	C4-C3-C5-C6
19	a	829	CLA	C3A-C2A-CAA-CBA
19	a	840	CLA	C4-C3-C5-C6
19	b	803	CLA	C4-C3-C5-C6
19	j	102	CLA	C3A-C2A-CAA-CBA
19	a	828	CLA	C2-C3-C5-C6
19	a	835	CLA	O1A-CGA-O2A-C1
22	j	105	LMG	C28-C29-C30-C31
18	3	306	A1L1G	C40-C41-C42-C44
19	b	801	CLA	C5-C6-C7-C8
17	5	301	XAT	C7-C8-C9-C19
17	4	305	XAT	C27-C28-C29-C39
19	4	307	CLA	O1A-CGA-O2A-C1
19	a	826	CLA	O1D-CGD-O2D-CED
19	a	836	CLA	O1D-CGD-O2D-CED
19	a	809	CLA	C2A-CAA-CBA-CGA
20	1	315	SQD	O6-C44-C45-C46
22	2	317	LMG	O1-C7-C8-C9
25	a	846	LHG	C4-C5-C6-O8
19	b	813	CLA	C5-C6-C7-C8
19	b	836	CLA	C3-C5-C6-C7
19	a	805	CLA	C6-C7-C8-C10
19	b	819	CLA	C11-C12-C13-C15
19	a	828	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	b	814	CLA	C4-C3-C5-C6
19	a	801	CLA	C2-C3-C5-C6
19	b	807	CLA	C2-C3-C5-C6
19	a	827	CLA	C3-C5-C6-C7
19	4	308	CLA	C16-C17-C18-C19
19	1	310	CLA	C16-C17-C18-C20
21	b	851	DGD	O1B-C1B-O2G-C2G
19	j	102	CLA	C5-C6-C7-C8
19	3	307	CLA	C2B-C3B-CAB-CBB
19	1	309	CLA	C2B-C3B-CAB-CBB
19	a	825	CLA	C2B-C3B-CAB-CBB
19	a	837	CLA	C2B-C3B-CAB-CBB
19	a	841	CLA	C2B-C3B-CAB-CBB
19	b	818	CLA	C2B-C3B-CAB-CBB
19	j	102	CLA	C2B-C3B-CAB-CBB
26	b	844	BCR	C1-C6-C7-C8
26	m	102	BCR	C1-C6-C7-C8
19	b	823	CLA	C10-C11-C12-C13
19	a	830	CLA	C5-C6-C7-C8
19	a	806	CLA	C16-C17-C18-C20
25	a	845	LHG	C34-C35-C36-C37
19	b	807	CLA	C4-C3-C5-C6
19	5	309	CLA	C5-C6-C7-C8
19	4	317	CLA	C5-C6-C7-C8
19	a	803	CLA	C15-C16-C17-C18
19	a	820	CLA	C2-C3-C5-C6
19	b	814	CLA	C2-C3-C5-C6
19	a	820	CLA	C16-C17-C18-C19
21	b	851	DGD	C7A-C8A-C9A-CAA
19	1	308	CLA	C11-C12-C13-C14
19	1	310	CLA	C6-C7-C8-C9
19	1	310	CLA	C11-C10-C8-C9
19	a	807	CLA	C14-C13-C15-C16
19	a	829	CLA	C6-C7-C8-C9
19	b	802	CLA	C11-C10-C8-C9
19	b	825	CLA	C11-C12-C13-C14
19	b	833	CLA	C14-C13-C15-C16
19	3	314	CLA	O1D-CGD-O2D-CED
19	a	841	CLA	O1A-CGA-O2A-C1
19	2	315	CLA	C1A-C2A-CAA-CBA
19	j	103	CLA	C1A-C2A-CAA-CBA
19	b	803	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	b	806	CLA	C10-C11-C12-C13
17	2	304	XAT	C33-C34-C35-C15
23	1	304	A1L1F	C14-C29-C30-C31
19	b	812	CLA	O1A-CGA-O2A-C1
19	4	313	CLA	CBA-CGA-O2A-C1
25	a	846	LHG	O6-C4-C5-C6
25	m	101	LHG	O6-C4-C5-C6
18	3	306	A1L1G	C32-C33-C34-C27
19	1	306	CLA	C6-C7-C8-C10
19	a	801	CLA	C6-C7-C8-C10
19	a	802	CLA	C6-C7-C8-C10
19	a	814	CLA	C6-C7-C8-C10
19	a	820	CLA	C11-C12-C13-C15
19	a	829	CLA	C11-C10-C8-C7
19	b	814	CLA	C11-C10-C8-C7
19	b	825	CLA	C6-C7-C8-C10
19	b	833	CLA	C12-C13-C15-C16
19	i	102	CLA	C11-C10-C8-C7
19	a	806	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	C15-C16-C17-C18
19	a	854	CLA	C8-C10-C11-C12
19	b	839	CLA	C13-C15-C16-C17
21	b	851	DGD	O1A-C1A-O1G-C1G
19	b	828	CLA	C16-C17-C18-C20
25	b	849	LHG	O9-C7-O7-C5
19	a	807	CLA	C4-C3-C5-C6
19	b	810	CLA	CAA-CBA-CGA-O2A
19	3	314	CLA	O1A-CGA-O2A-C1
19	1	310	CLA	C2-C3-C5-C6
19	a	840	CLA	C2-C3-C5-C6
22	a	853	LMG	C12-C13-C14-C15
19	b	807	CLA	C5-C6-C7-C8
19	b	829	CLA	C5-C6-C7-C8
22	a	853	LMG	C9-C8-O7-C10
19	a	831	CLA	O1A-CGA-O2A-C1
19	b	829	CLA	O1A-CGA-O2A-C1
19	1	306	CLA	C16-C17-C18-C20
19	1	310	CLA	C16-C17-C18-C19
19	1	306	CLA	O1A-CGA-O2A-C1
19	1	310	CLA	O1A-CGA-O2A-C1
19	i	102	CLA	CBA-CGA-O2A-C1
20	1	315	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	a	842	CLA	C8-C10-C11-C12
19	2	310	CLA	C16-C17-C18-C20
19	b	805	CLA	C16-C17-C18-C19
19	a	827	CLA	C5-C6-C7-C8
19	2	314	CLA	C2A-CAA-CBA-CGA
19	b	835	CLA	C2-C3-C5-C6
19	1	306	CLA	C3-C5-C6-C7
19	1	306	CLA	C11-C10-C8-C9
19	a	801	CLA	C6-C7-C8-C9
19	a	802	CLA	C6-C7-C8-C9
19	a	820	CLA	C11-C12-C13-C14
19	a	840	CLA	C11-C10-C8-C9
19	b	802	CLA	C6-C7-C8-C9
19	b	802	CLA	C11-C12-C13-C14
19	b	804	CLA	C6-C7-C8-C9
19	b	806	CLA	C6-C7-C8-C9
19	b	814	CLA	C11-C10-C8-C9
19	b	839	CLA	C11-C12-C13-C14
19	b	839	CLA	C14-C13-C15-C16
22	2	317	LMG	C31-C32-C33-C34
19	4	313	CLA	O1A-CGA-O2A-C1
25	a	845	LHG	C9-C10-C11-C12
19	a	841	CLA	C13-C15-C16-C17
19	a	808	CLA	O1D-CGD-O2D-CED
19	2	310	CLA	C16-C17-C18-C19
19	b	808	CLA	C16-C17-C18-C20
19	2	314	CLA	C4-C3-C5-C6
19	2	307	CLA	C2A-CAA-CBA-CGA
19	b	810	CLA	C16-C17-C18-C19
19	b	818	CLA	C10-C11-C12-C13
22	2	317	LMG	C33-C34-C35-C36
19	5	305	CLA	C4B-C3B-CAB-CBB
19	5	306	CLA	C4B-C3B-CAB-CBB
19	5	310	CLA	C4B-C3B-CAB-CBB
19	4	306	CLA	C4B-C3B-CAB-CBB
19	4	307	CLA	C4B-C3B-CAB-CBB
19	4	315	CLA	C4B-C3B-CAB-CBB
19	4	317	CLA	C4B-C3B-CAB-CBB
19	3	311	CLA	C1A-C2A-CAA-CBA
19	3	312	CLA	C4B-C3B-CAB-CBB
19	2	306	CLA	C4B-C3B-CAB-CBB
19	2	311	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	2	314	CLA	C1A-C2A-CAA-CBA
19	2	314	CLA	C4B-C3B-CAB-CBB
19	2	315	CLA	C4B-C3B-CAB-CBB
19	2	316	CLA	C4B-C3B-CAB-CBB
19	a	807	CLA	C4B-C3B-CAB-CBB
19	a	813	CLA	C4B-C3B-CAB-CBB
19	a	817	CLA	C4B-C3B-CAB-CBB
19	a	819	CLA	C4B-C3B-CAB-CBB
19	a	824	CLA	C1A-C2A-CAA-CBA
19	a	824	CLA	C4B-C3B-CAB-CBB
19	b	801	CLA	C4B-C3B-CAB-CBB
19	b	809	CLA	C4B-C3B-CAB-CBB
19	b	814	CLA	C1A-C2A-CAA-CBA
19	b	824	CLA	C1A-C2A-CAA-CBA
19	b	829	CLA	C4B-C3B-CAB-CBB
19	b	835	CLA	C4B-C3B-CAB-CBB
19	b	838	CLA	C4B-C3B-CAB-CBB
19	f	803	CLA	C4B-C3B-CAB-CBB
19	i	102	CLA	C4B-C3B-CAB-CBB
19	j	103	CLA	C4B-C3B-CAB-CBB
19	j	102	CLA	O1D-CGD-O2D-CED
17	5	301	XAT	C7-C8-C9-C10
19	b	802	CLA	C2A-CAA-CBA-CGA
19	b	808	CLA	C2A-CAA-CBA-CGA
19	b	819	CLA	C8-C10-C11-C12
19	5	311	CLA	C2-C3-C5-C6
19	5	307	CLA	C11-C10-C8-C7
19	2	310	CLA	C11-C12-C13-C15
19	a	842	CLA	C12-C13-C15-C16
19	b	801	CLA	C11-C10-C8-C7
19	b	801	CLA	C12-C13-C15-C16
19	b	806	CLA	C11-C12-C13-C15
19	b	810	CLA	C11-C10-C8-C7
19	b	828	CLA	C11-C10-C8-C7
19	b	830	CLA	C11-C12-C13-C15
24	a	843	PQN	C22-C23-C25-C26
22	a	853	LMG	C31-C32-C33-C34
19	1	307	CLA	C5-C6-C7-C8
19	b	811	CLA	C3A-C2A-CAA-CBA
25	m	101	LHG	O6-C4-C5-O7
19	3	311	CLA	C2A-CAA-CBA-CGA
19	4	308	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	a	809	CLA	C6-C7-C8-C9
19	a	814	CLA	C6-C7-C8-C9
19	a	830	CLA	C8-C10-C11-C12
17	4	301	XAT	C29-C30-C31-C32
18	3	302	A1L1G	C36-C37-C38-C39
26	m	102	BCR	C13-C14-C15-C16
20	1	315	SQD	C13-C14-C15-C16
19	a	823	CLA	C1-C2-C3-C4
19	b	832	CLA	C1-C2-C3-C4
19	a	806	CLA	O1D-CGD-O2D-CED
19	b	815	CLA	C3-C5-C6-C7
19	i	102	CLA	O1A-CGA-O2A-C1
20	5	316	SQD	O47-C45-C46-O48
20	1	315	SQD	O6-C44-C45-O47
25	a	846	LHG	O7-C5-C6-O8
25	b	849	LHG	O7-C5-C6-O8
19	4	312	CLA	CBA-CGA-O2A-C1
19	a	809	CLA	C10-C11-C12-C13
19	b	841	CLA	C15-C16-C17-C18
20	5	316	SQD	C44-C45-C46-O48
19	1	313	CLA	CAD-CBD-CGD-O2D
19	a	814	CLA	CAD-CBD-CGD-O2D
19	a	839	CLA	CAD-CBD-CGD-O2D
19	a	844	CLA	CAD-CBD-CGD-O2D
19	b	833	CLA	CAD-CBD-CGD-O2D
19	b	837	CLA	CAD-CBD-CGD-O2D
19	1	311	CLA	CBA-CGA-O2A-C1
19	3	315	CLA	O1A-CGA-O2A-C1
19	b	825	CLA	C2A-CAA-CBA-CGA
25	a	846	LHG	C10-C11-C12-C13
17	j	101	XAT	C9-C10-C11-C12
18	3	302	A1L1G	C40-C41-C42-C44
18	1	301	A1L1G	C37-C38-C39-C28
19	5	313	CLA	CHA-CBD-CGD-O1D
19	5	313	CLA	CHA-CBD-CGD-O2D
19	4	314	CLA	CHA-CBD-CGD-O1D
19	4	314	CLA	CHA-CBD-CGD-O2D
19	4	315	CLA	CAD-CBD-CGD-O1D
19	2	307	CLA	CHA-CBD-CGD-O1D
19	1	313	CLA	CAD-CBD-CGD-O1D
19	a	806	CLA	CAD-CBD-CGD-O1D
19	a	814	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	a	828	CLA	CAD-CBD-CGD-O1D
19	a	839	CLA	CAD-CBD-CGD-O1D
19	a	844	CLA	CAD-CBD-CGD-O1D
19	b	822	CLA	CHA-CBD-CGD-O1D
19	b	833	CLA	CAD-CBD-CGD-O1D
19	b	836	CLA	CAD-CBD-CGD-O1D
19	b	837	CLA	CAD-CBD-CGD-O1D
19	f	802	CLA	CAD-CBD-CGD-O1D
19	f	803	CLA	CHA-CBD-CGD-O2D
19	j	102	CLA	CHA-CBD-CGD-O1D
19	j	102	CLA	CHA-CBD-CGD-O2D
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
25	m	101	LHG	C3-O3-P-O5
25	m	101	LHG	C3-O3-P-O6
25	m	101	LHG	C4-O6-P-O3
25	m	101	LHG	C4-O6-P-O5
19	b	808	CLA	C16-C17-C18-C19
19	a	841	CLA	C4-C3-C5-C6
19	5	306	CLA	C2B-C3B-CAB-CBB
19	5	310	CLA	C2B-C3B-CAB-CBB
19	4	317	CLA	C2B-C3B-CAB-CBB
19	2	311	CLA	C2B-C3B-CAB-CBB
19	2	315	CLA	C2B-C3B-CAB-CBB
19	2	316	CLA	C2B-C3B-CAB-CBB
19	1	314	CLA	C2B-C3B-CAB-CBB
19	a	819	CLA	C2B-C3B-CAB-CBB
19	b	801	CLA	C2B-C3B-CAB-CBB
19	b	835	CLA	C2B-C3B-CAB-CBB
19	b	838	CLA	C2B-C3B-CAB-CBB
19	b	841	CLA	C2B-C3B-CAB-CBB
19	i	102	CLA	C2B-C3B-CAB-CBB
26	l	201	BCR	C1-C6-C7-C8
19	1	308	CLA	CBD-CGD-O2D-CED
19	a	807	CLA	C2-C3-C5-C6
19	b	839	CLA	C2-C3-C5-C6
19	a	834	CLA	C5-C6-C7-C8
19	b	825	CLA	C8-C10-C11-C12
19	1	308	CLA	C16-C17-C18-C19
19	2	308	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	b	803	CLA	C3-C5-C6-C7
19	b	823	CLA	C3-C5-C6-C7
19	b	840	CLA	C2C-C3C-CAC-CBC
25	m	101	LHG	C10-C11-C12-C13
20	1	315	SQD	C46-C45-O47-C7
19	a	830	CLA	C16-C17-C18-C19
19	b	805	CLA	CBA-CGA-O2A-C1
19	a	839	CLA	C15-C16-C17-C18
19	5	309	CLA	C6-C7-C8-C9
19	3	312	CLA	C6-C7-C8-C9
19	a	807	CLA	C6-C7-C8-C9
19	a	812	CLA	C6-C7-C8-C9
19	b	803	CLA	C14-C13-C15-C16
19	b	804	CLA	C11-C12-C13-C14
19	b	807	CLA	C11-C12-C13-C14
19	b	810	CLA	C11-C10-C8-C9
19	b	829	CLA	C14-C13-C15-C16
19	3	312	CLA	C6-C7-C8-C10
19	b	802	CLA	C11-C12-C13-C15
19	a	821	CLA	C2A-CAA-CBA-CGA
19	1	311	CLA	O1A-CGA-O2A-C1
19	2	314	CLA	C2-C3-C5-C6
19	b	833	CLA	C2C-C3C-CAC-CBC
25	m	101	LHG	C13-C14-C15-C16
19	b	828	CLA	C10-C11-C12-C13
19	b	805	CLA	O1A-CGA-O2A-C1
19	b	818	CLA	CBA-CGA-O2A-C1
18	3	306	A1L1G	C30-C31-C32-C33
19	3	308	CLA	CAA-CBA-CGA-O2A
19	1	305	CLA	C2A-CAA-CBA-CGA
19	1	308	CLA	C2A-CAA-CBA-CGA
19	b	801	CLA	O1A-CGA-O2A-C1
19	b	818	CLA	O1A-CGA-O2A-C1
19	a	802	CLA	C4-C3-C5-C6
19	b	828	CLA	C16-C17-C18-C19
19	a	801	CLA	CAA-CBA-CGA-O2A
19	1	311	CLA	O1D-CGD-O2D-CED
25	b	849	LHG	C25-C26-C27-C28
19	4	317	CLA	C2A-CAA-CBA-CGA
19	a	813	CLA	C2A-CAA-CBA-CGA
19	b	828	CLA	C2A-CAA-CBA-CGA
18	1	301	A1L1G	C40-C41-C42-C44

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Mol	Chain	Res	Type	Atoms
20	5	316	SQD	C7-C8-C9-C10
19	a	854	CLA	CBD-CGD-O2D-CED
19	a	841	CLA	C2-C3-C5-C6
19	b	801	CLA	CBA-CGA-O2A-C1
19	1	308	CLA	O1D-CGD-O2D-CED
19	b	803	CLA	C16-C17-C18-C20
19	a	801	CLA	C14-C13-C15-C16
19	a	826	CLA	C11-C10-C8-C9
19	a	842	CLA	C14-C13-C15-C16
19	b	828	CLA	C11-C10-C8-C9
24	a	843	PQN	C24-C23-C25-C26
19	3	314	CLA	C4B-C3B-CAB-CBB
19	a	832	CLA	C4B-C3B-CAB-CBB
19	b	831	CLA	C4B-C3B-CAB-CBB
19	a	813	CLA	CBA-CGA-O2A-C1
19	5	307	CLA	C8-C10-C11-C12
19	a	830	CLA	C15-C16-C17-C18
19	a	854	CLA	C15-C16-C17-C18
19	a	813	CLA	O1A-CGA-O2A-C1
19	5	315	CLA	CAA-CBA-CGA-O2A
19	a	802	CLA	C2-C3-C5-C6
19	b	802	CLA	C2-C3-C5-C6
19	a	830	CLA	C16-C17-C18-C20
19	a	831	CLA	C11-C10-C8-C7
19	b	802	CLA	C12-C13-C15-C16
19	b	807	CLA	C11-C12-C13-C15
19	3	312	CLA	CBA-CGA-O2A-C1
19	1	308	CLA	C16-C17-C18-C20
19	b	840	CLA	C16-C17-C18-C20
19	5	310	CLA	CAA-CBA-CGA-O1A
21	b	851	DGD	O2G-C2G-C3G-O3G
19	2	310	CLA	C3A-C2A-CAA-CBA
19	a	830	CLA	C4-C3-C5-C6
19	b	814	CLA	C3A-C2A-CAA-CBA
19	b	832	CLA	C3A-C2A-CAA-CBA
19	2	309	CLA	C2A-CAA-CBA-CGA
26	b	845	BCR	C11-C10-C9-C34
26	b	845	BCR	C20-C21-C22-C37
26	f	804	BCR	C35-C13-C14-C15
26	l	201	BCR	C11-C10-C9-C34
19	a	812	CLA	C3-C5-C6-C7
19	a	820	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	b	814	CLA	C10-C11-C12-C13
19	5	306	CLA	CAA-CBA-CGA-O1A
19	5	311	CLA	C4-C3-C5-C6
25	a	846	LHG	C1-C2-C3-O3
19	a	854	CLA	O1D-CGD-O2D-CED
25	a	845	LHG	C25-C26-C27-C28
19	3	312	CLA	O1A-CGA-O2A-C1
19	5	307	CLA	C11-C10-C8-C9
19	1	310	CLA	C11-C12-C13-C14
19	a	822	CLA	C11-C10-C8-C9
19	a	829	CLA	C11-C12-C13-C14
19	a	831	CLA	C6-C7-C8-C9
19	a	831	CLA	C11-C10-C8-C9
19	a	844	CLA	C6-C7-C8-C9
19	a	854	CLA	C11-C10-C8-C9
19	b	808	CLA	C6-C7-C8-C9
19	4	310	CLA	CBD-CGD-O2D-CED
19	a	832	CLA	CBD-CGD-O2D-CED
19	4	314	CLA	CAA-CBA-CGA-O1A
19	a	839	CLA	C16-C17-C18-C20
19	a	832	CLA	O1D-CGD-O2D-CED
19	5	309	CLA	C2A-CAA-CBA-CGA
19	a	803	CLA	C2A-CAA-CBA-CGA
19	3	315	CLA	CAA-CBA-CGA-O1A
19	a	801	CLA	O1A-CGA-O2A-C1
19	4	311	CLA	C1A-C2A-CAA-CBA
19	4	316	CLA	C1A-C2A-CAA-CBA
19	2	310	CLA	C1A-C2A-CAA-CBA
19	2	316	CLA	C1A-C2A-CAA-CBA
19	b	816	CLA	C1A-C2A-CAA-CBA
19	b	823	CLA	C1A-C2A-CAA-CBA
19	b	835	CLA	C1A-C2A-CAA-CBA
26	b	845	BCR	C11-C10-C9-C8
26	b	845	BCR	C20-C21-C22-C23
26	f	804	BCR	C12-C13-C14-C15
26	1	201	BCR	C11-C10-C9-C8
19	4	314	CLA	CAA-CBA-CGA-O2A
19	5	305	CLA	C2B-C3B-CAB-CBB
19	5	308	CLA	C2B-C3B-CAB-CBB
19	4	306	CLA	C2B-C3B-CAB-CBB
19	4	307	CLA	C2B-C3B-CAB-CBB
19	4	315	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	3	308	CLA	C2B-C3B-CAB-CBB
19	3	312	CLA	C2B-C3B-CAB-CBB
19	3	314	CLA	C2B-C3B-CAB-CBB
19	2	306	CLA	C2B-C3B-CAB-CBB
19	2	314	CLA	C2B-C3B-CAB-CBB
19	1	305	CLA	C2B-C3B-CAB-CBB
19	1	313	CLA	C2B-C3B-CAB-CBB
19	a	801	CLA	C2B-C3B-CAB-CBB
19	a	807	CLA	C2B-C3B-CAB-CBB
19	a	810	CLA	C2B-C3B-CAB-CBB
19	a	813	CLA	C2B-C3B-CAB-CBB
19	a	817	CLA	C2B-C3B-CAB-CBB
19	a	824	CLA	C2B-C3B-CAB-CBB
19	a	832	CLA	C2B-C3B-CAB-CBB
19	b	809	CLA	C2B-C3B-CAB-CBB
19	b	829	CLA	C2B-C3B-CAB-CBB
19	b	831	CLA	C2B-C3B-CAB-CBB
19	f	803	CLA	C2B-C3B-CAB-CBB
19	j	103	CLA	C2B-C3B-CAB-CBB
26	b	844	BCR	C5-C6-C7-C8
26	b	852	BCR	C23-C24-C25-C30
26	l	205	BCR	C1-C6-C7-C8
26	m	102	BCR	C5-C6-C7-C8
19	5	306	CLA	CAA-CBA-CGA-O2A
19	5	313	CLA	CAA-CBA-CGA-O1A
19	a	801	CLA	CBA-CGA-O2A-C1
19	b	841	CLA	CBA-CGA-O2A-C1
19	b	841	CLA	O1A-CGA-O2A-C1
19	b	808	CLA	C4-C3-C5-C6
19	a	830	CLA	C2-C3-C5-C6
22	2	317	LMG	O9-C10-O7-C8
19	a	826	CLA	C11-C10-C8-C7
19	f	802	CLA	C6-C7-C8-C10
19	b	809	CLA	C2A-CAA-CBA-CGA
19	b	811	CLA	C2A-CAA-CBA-CGA
19	a	817	CLA	CAA-CBA-CGA-O1A
22	2	317	LMG	C11-C10-O7-C8
25	a	845	LHG	C14-C15-C16-C17
19	1	305	CLA	C3-C5-C6-C7
19	a	817	CLA	CAA-CBA-CGA-O2A
19	1	307	CLA	C6-C7-C8-C9
25	m	101	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	2	314	CLA	C11-C10-C8-C7
19	b	808	CLA	C2-C3-C5-C6
18	3	306	A1L1G	C32-C33-C34-C35
22	a	853	LMG	C11-C12-C13-C14
19	b	840	CLA	C4C-C3C-CAC-CBC
19	b	838	CLA	C11-C12-C13-C14
19	5	313	CLA	CAA-CBA-CGA-O2A
19	4	310	CLA	C13-C15-C16-C17
19	a	835	CLA	C4-C3-C5-C6
19	a	835	CLA	C2-C3-C5-C6
19	b	818	CLA	CBD-CGD-O2D-CED
19	5	307	CLA	C2A-CAA-CBA-CGA
19	5	314	CLA	C4-C3-C5-C6
19	b	834	CLA	C4-C3-C5-C6
20	1	315	SQD	C15-C16-C17-C18
19	a	819	CLA	CAA-CBA-CGA-O2A
19	a	826	CLA	C13-C15-C16-C17
19	4	310	CLA	C4B-C3B-CAB-CBB
19	a	810	CLA	C4B-C3B-CAB-CBB
19	4	310	CLA	O1D-CGD-O2D-CED
19	a	830	CLA	O1A-CGA-O2A-C1
19	a	842	CLA	O1A-CGA-O2A-C1
19	1	306	CLA	C16-C17-C18-C19
19	b	814	CLA	C16-C17-C18-C19
19	a	804	CLA	O1A-CGA-O2A-C1
19	4	306	CLA	C2A-CAA-CBA-CGA
19	1	314	CLA	CAA-CBA-CGA-O2A
19	5	307	CLA	C11-C12-C13-C14
19	b	818	CLA	O1D-CGD-O2D-CED
19	a	842	CLA	CBA-CGA-O2A-C1
19	5	310	CLA	CBA-CGA-O2A-C1
19	1	314	CLA	CAA-CBA-CGA-O1A
19	b	802	CLA	C10-C11-C12-C13
19	a	813	CLA	C6-C7-C8-C9
17	a	852	XAT	C31-C32-C33-C34
19	a	828	CLA	C14-C13-C15-C16
19	a	839	CLA	C6-C7-C8-C9
19	a	840	CLA	C14-C13-C15-C16
19	b	806	CLA	C11-C12-C13-C14
19	b	830	CLA	C11-C12-C13-C14
19	2	314	CLA	O1A-CGA-O2A-C1
19	a	839	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	a	830	CLA	CBA-CGA-O2A-C1
19	4	306	CLA	C3A-C2A-CAA-CBA
19	2	316	CLA	C3A-C2A-CAA-CBA
19	1	310	CLA	C3A-C2A-CAA-CBA
19	b	809	CLA	C3A-C2A-CAA-CBA
25	m	101	LHG	O1-C1-C2-C3
21	b	851	DGD	C1B-C2B-C3B-C4B
19	b	814	CLA	C13-C15-C16-C17
19	l	204	CLA	CAA-CBA-CGA-O2A
19	b	814	CLA	C5-C6-C7-C8
19	b	811	CLA	C8-C10-C11-C12
24	a	843	PQN	C18-C20-C21-C22
17	5	301	XAT	O4-C6-C7-C8
17	5	304	XAT	O24-C26-C27-C28
17	4	301	XAT	O4-C6-C7-C8
17	4	305	XAT	O4-C6-C7-C8
17	3	303	XAT	O4-C6-C7-C8
17	2	301	XAT	O4-C6-C7-C8
17	2	305	XAT	O24-C26-C27-C28
18	3	302	A1L1G	C29-C14-C25-O15
22	j	105	LMG	C11-C12-C13-C14
19	a	804	CLA	CBA-CGA-O2A-C1
19	b	834	CLA	C15-C16-C17-C18
19	4	308	CLA	C3-C5-C6-C7
19	a	804	CLA	C6-C7-C8-C9
25	m	101	LHG	C35-C36-C37-C38
19	4	306	CLA	CAA-CBA-CGA-O2A
19	4	308	CLA	C6-C7-C8-C9
19	4	309	CLA	CAA-CBA-CGA-O2A
19	b	803	CLA	CAA-CBA-CGA-O2A
19	b	803	CLA	C10-C11-C12-C13
17	2	304	XAT	C7-C8-C9-C10
19	4	312	CLA	O1A-CGA-O2A-C1
19	3	313	CLA	C4-C3-C5-C6
19	a	829	CLA	CAA-CBA-CGA-O2A
19	b	819	CLA	C2A-CAA-CBA-CGA
19	1	305	CLA	C11-C10-C8-C7
19	a	801	CLA	C11-C10-C8-C7
19	a	835	CLA	C11-C12-C13-C15
19	a	839	CLA	C6-C7-C8-C10
19	a	840	CLA	C12-C13-C15-C16
19	b	838	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	b	819	CLA	C2B-C3B-CAB-CBB
19	b	824	CLA	C2B-C3B-CAB-CBB
26	b	848	BCR	C1-C6-C7-C8
26	b	848	BCR	C5-C6-C7-C8
26	b	852	BCR	C23-C24-C25-C26
26	f	804	BCR	C23-C24-C25-C26
26	f	804	BCR	C23-C24-C25-C30
26	j	104	BCR	C1-C6-C7-C8
26	l	201	BCR	C5-C6-C7-C8
26	l	205	BCR	C5-C6-C7-C8
19	b	838	CLA	CAA-CBA-CGA-O2A
19	5	311	CLA	C2-C1-O2A-CGA
19	a	814	CLA	C2-C1-O2A-CGA
19	a	822	CLA	C2-C1-O2A-CGA
19	b	810	CLA	C2-C1-O2A-CGA
19	b	807	CLA	C16-C17-C18-C19
19	b	825	CLA	C10-C11-C12-C13
19	b	836	CLA	C4C-C3C-CAC-CBC
19	1	306	CLA	CAA-CBA-CGA-O2A
19	1	309	CLA	CAA-CBA-CGA-O2A
19	a	818	CLA	CAA-CBA-CGA-O2A
19	a	827	CLA	C10-C11-C12-C13
19	b	801	CLA	CAA-CBA-CGA-O2A
19	4	308	CLA	C2A-CAA-CBA-CGA
19	2	308	CLA	C2A-CAA-CBA-CGA
20	1	315	SQD	O47-C7-C8-C9
20	5	316	SQD	C4-C5-C6-S
19	2	314	CLA	CBA-CGA-O2A-C1
19	j	102	CLA	C3-C5-C6-C7
19	4	306	CLA	CAA-CBA-CGA-O1A
19	a	801	CLA	C11-C10-C8-C9
19	b	803	CLA	C5-C6-C7-C8
19	b	807	CLA	CAA-CBA-CGA-O2A
22	j	105	LMG	C7-C8-C9-O8
19	4	316	CLA	C4B-C3B-CAB-CBB
19	3	315	CLA	C4B-C3B-CAB-CBB
19	a	803	CLA	C1A-C2A-CAA-CBA
19	a	814	CLA	C1A-C2A-CAA-CBA
19	a	840	CLA	C4B-C3B-CAB-CBB
19	b	803	CLA	C4B-C3B-CAB-CBB
19	b	826	CLA	C1A-C2A-CAA-CBA
19	b	839	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	m	102	BCR	C22-C23-C24-C25
19	a	810	CLA	CAA-CBA-CGA-O2A
26	f	801	BCR	C17-C18-C19-C20
19	b	810	CLA	CAA-CBA-CGA-O1A
19	a	836	CLA	CAA-CBA-CGA-O2A
19	a	829	CLA	C2A-CAA-CBA-CGA
19	a	841	CLA	C2A-CAA-CBA-CGA
25	m	101	LHG	C27-C28-C29-C30
19	a	826	CLA	C10-C11-C12-C13
19	b	820	CLA	C6-C7-C8-C9
19	b	809	CLA	CAA-CBA-CGA-O2A
19	b	818	CLA	CAA-CBA-CGA-O2A
19	a	810	CLA	C2-C1-O2A-CGA
19	1	312	CLA	CAA-CBA-CGA-O2A
19	1	310	CLA	C12-C13-C15-C16
19	a	801	CLA	C11-C12-C13-C15
19	a	834	CLA	C11-C12-C13-C15
19	b	805	CLA	C11-C12-C13-C15
19	b	819	CLA	C11-C10-C8-C7
19	l	203	CLA	C6-C7-C8-C10
19	b	810	CLA	C16-C17-C18-C20
19	a	834	CLA	C10-C11-C12-C13
19	b	833	CLA	CAA-CBA-CGA-O2A
25	m	101	LHG	C30-C31-C32-C33
19	4	310	CLA	C8-C10-C11-C12
19	j	102	CLA	CAA-CBA-CGA-O2A
19	b	838	CLA	CAA-CBA-CGA-O1A
19	j	102	CLA	C10-C11-C12-C13
19	a	801	CLA	C5-C6-C7-C8
19	1	306	CLA	C3A-C2A-CAA-CBA
19	a	814	CLA	C3A-C2A-CAA-CBA
19	b	818	CLA	CAA-CBA-CGA-O1A
19	5	309	CLA	C15-C16-C17-C18
19	a	810	CLA	C16-C17-C18-C20
19	a	814	CLA	C16-C17-C18-C19
18	3	306	A1L1G	C14-C29-C30-C31
25	a	845	LHG	O8-C23-C24-C25
19	a	818	CLA	CAA-CBA-CGA-O1A
19	b	801	CLA	CAA-CBA-CGA-O1A
19	a	801	CLA	C11-C12-C13-C14
19	a	834	CLA	C11-C12-C13-C14
19	f	802	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	3	312	CLA	CAA-CBA-CGA-O2A
19	4	309	CLA	CAA-CBA-CGA-O1A
20	1	315	SQD	O49-C7-C8-C9
20	5	316	SQD	O5-C5-C6-S
23	1	304	A1L1F	C29-C14-C25-C24
26	i	101	BCR	C17-C18-C19-C20
19	b	807	CLA	CAA-CBA-CGA-O1A
19	b	825	CLA	C15-C16-C17-C18
19	3	309	CLA	C2A-CAA-CBA-CGA
20	5	316	SQD	C10-C11-C12-C13
19	b	809	CLA	CAA-CBA-CGA-O1A
19	b	833	CLA	CAA-CBA-CGA-O1A
19	a	813	CLA	CAA-CBA-CGA-O2A
19	1	312	CLA	CAA-CBA-CGA-O1A
18	3	306	A1L1G	O13-C26-C30-C31
19	5	314	CLA	CAD-CBD-CGD-O2D
19	3	310	CLA	CAD-CBD-CGD-O2D
19	a	810	CLA	CAD-CBD-CGD-O2D
19	a	816	CLA	CAD-CBD-CGD-O2D
19	a	828	CLA	CAD-CBD-CGD-O2D
19	a	832	CLA	CAD-CBD-CGD-O2D
19	a	854	CLA	CAD-CBD-CGD-O2D
19	b	836	CLA	CAD-CBD-CGD-O2D
19	a	836	CLA	CAA-CBA-CGA-O1A
19	a	816	CLA	C2-C1-O2A-CGA
19	a	839	CLA	C2-C1-O2A-CGA
19	b	825	CLA	C4-C3-C5-C6
19	b	804	CLA	CAA-CBA-CGA-O2A
19	a	826	CLA	C8-C10-C11-C12
20	1	315	SQD	C12-C13-C14-C15
19	a	813	CLA	CBD-CGD-O2D-CED
19	j	102	CLA	CAA-CBA-CGA-O1A
19	b	814	CLA	CBD-CGD-O2D-CED
19	a	835	CLA	CAA-CBA-CGA-O2A
19	b	830	CLA	O1A-CGA-O2A-C1
19	a	810	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

176 monomers are involved in 518 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	311	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	j	102	CLA	6	0
19	b	837	CLA	6	0
19	b	832	CLA	2	0
26	b	852	BCR	6	0
21	4	318	DGD	11	0
19	b	813	CLA	4	0
19	1	310	CLA	2	0
26	f	801	BCR	8	0
19	a	805	CLA	1	0
26	i	101	BCR	2	0
19	a	804	CLA	4	0
19	b	809	CLA	2	0
17	j	101	XAT	5	0
19	1	306	CLA	4	0
19	a	809	CLA	2	0
26	b	844	BCR	1	0
19	4	308	CLA	5	0
20	5	316	SQD	1	0
19	4	313	CLA	4	0
19	a	802	CLA	5	0
26	b	847	BCR	6	0
19	a	814	CLA	3	0
19	b	817	CLA	4	0
19	1	308	CLA	3	0
19	a	824	CLA	1	0
19	b	818	CLA	8	0
19	b	840	CLA	4	0
19	b	819	CLA	3	0
19	b	826	CLA	3	0
23	1	304	A1L1F	2	0
17	2	304	XAT	2	0
19	a	827	CLA	2	0
17	2	305	XAT	5	0
19	a	831	CLA	5	0
17	2	301	XAT	3	0
19	b	802	CLA	3	0
19	b	836	CLA	5	0
19	a	833	CLA	2	0
19	a	839	CLA	4	0
19	a	841	CLA	7	0
27	c	102	SF4	2	0
26	b	845	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	5	307	CLA	7	0
26	m	102	BCR	1	0
19	a	825	CLA	5	0
19	5	314	CLA	1	0
17	5	301	XAT	5	0
18	5	303	A1L1G	1	0
19	a	818	CLA	10	0
19	5	309	CLA	3	0
19	a	826	CLA	7	0
19	4	314	CLA	1	0
17	3	301	XAT	5	0
19	a	808	CLA	1	0
19	b	829	CLA	2	0
19	b	825	CLA	6	0
19	a	806	CLA	8	0
19	b	828	CLA	2	0
19	i	102	CLA	5	0
17	3	304	XAT	4	0
19	5	312	CLA	3	0
17	4	301	XAT	4	0
19	3	311	CLA	1	0
19	a	830	CLA	6	0
19	b	801	CLA	5	0
26	l	205	BCR	10	0
17	a	852	XAT	4	0
22	2	317	LMG	2	0
19	2	310	CLA	3	0
24	a	843	PQN	3	0
19	a	812	CLA	1	0
19	b	808	CLA	1	0
26	b	850	BCR	4	0
19	b	833	CLA	3	0
17	3	305	XAT	4	0
19	b	827	CLA	4	0
19	f	802	CLA	1	0
17	5	302	XAT	8	0
19	a	810	CLA	4	0
25	m	101	LHG	3	0
19	j	103	CLA	2	0
26	b	843	BCR	4	0
19	a	807	CLA	4	0
19	a	820	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	838	CLA	1	0
19	4	315	CLA	1	0
19	a	840	CLA	7	0
22	j	105	LMG	6	0
18	1	301	A1L1G	1	0
19	4	309	CLA	3	0
19	b	812	CLA	2	0
17	2	303	XAT	12	0
19	b	821	CLA	2	0
19	b	841	CLA	5	0
19	2	314	CLA	1	0
19	b	815	CLA	3	0
25	a	846	LHG	3	0
19	a	822	CLA	5	0
19	b	823	CLA	5	0
19	b	839	CLA	6	0
19	b	804	CLA	5	0
19	b	811	CLA	6	0
17	4	303	XAT	10	0
19	b	830	CLA	4	0
19	4	316	CLA	1	0
19	b	831	CLA	5	0
19	a	803	CLA	4	0
26	b	846	BCR	1	0
19	3	312	CLA	2	0
17	1	303	XAT	3	0
19	2	316	CLA	2	0
19	1	312	CLA	2	0
19	a	842	CLA	3	0
17	3	303	XAT	2	0
19	4	312	CLA	1	0
17	4	305	XAT	5	0
19	5	310	CLA	2	0
19	a	819	CLA	6	0
25	a	845	LHG	3	0
19	5	311	CLA	1	0
17	4	304	XAT	4	0
19	4	307	CLA	2	0
19	3	313	CLA	3	0
20	1	315	SQD	2	0
26	l	201	BCR	3	0
19	a	816	CLA	2	0

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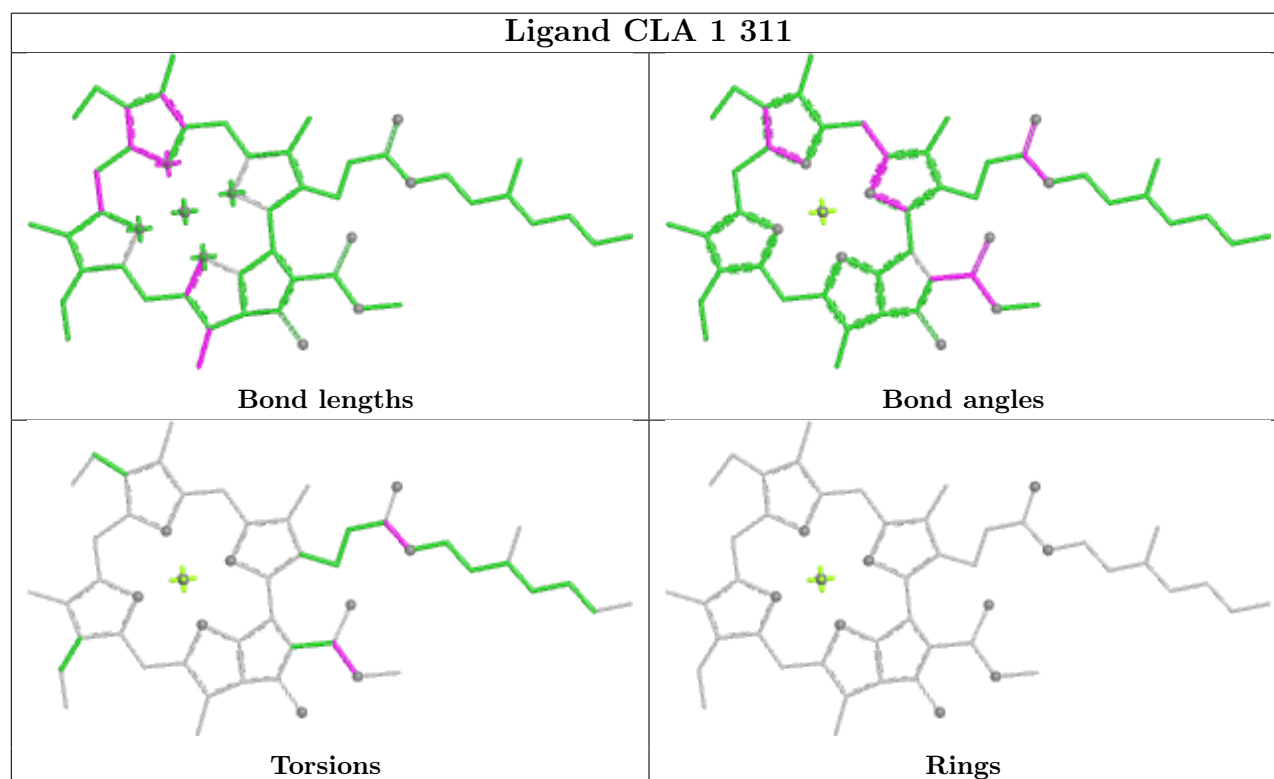
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	l	203	CLA	2	0
19	a	828	CLA	6	0
19	b	822	CLA	3	0
26	a	847	BCR	4	0
19	a	832	CLA	1	0
26	f	804	BCR	5	0
19	4	311	CLA	1	0
19	3	310	CLA	1	0
26	a	848	BCR	5	0
19	2	308	CLA	4	0
19	a	835	CLA	4	0
19	b	806	CLA	3	0
17	1	302	XAT	3	0
19	b	824	CLA	6	0
21	b	851	DGD	5	0
19	b	807	CLA	6	0
22	a	853	LMG	11	0
24	b	842	PQN	2	0
19	4	310	CLA	4	0
26	j	104	BCR	8	0
19	b	814	CLA	7	0
19	a	844	CLA	5	0
19	b	834	CLA	5	0
19	a	834	CLA	6	0
26	b	848	BCR	2	0
19	a	836	CLA	1	0
19	b	803	CLA	3	0
19	4	317	CLA	7	0
19	a	801	CLA	6	0
26	a	849	BCR	4	0
19	a	837	CLA	1	0
19	b	805	CLA	3	0
19	5	305	CLA	2	0
19	b	820	CLA	2	0
19	a	813	CLA	1	0
19	4	306	CLA	2	0
19	a	823	CLA	3	0
17	4	302	XAT	5	0
19	l	202	CLA	1	0
19	a	829	CLA	6	0
26	a	850	BCR	2	0
19	3	308	CLA	2	0

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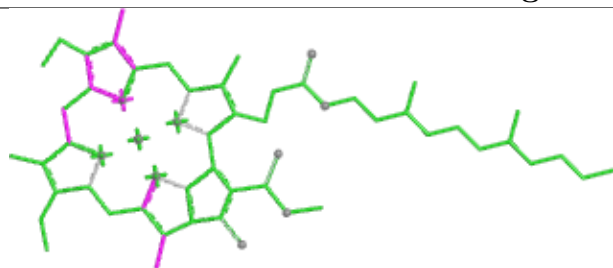
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	838	CLA	5	0
17	5	304	XAT	5	0
19	3	309	CLA	1	0
19	5	315	CLA	2	0
19	a	854	CLA	3	0
17	2	302	XAT	2	0
19	5	308	CLA	2	0

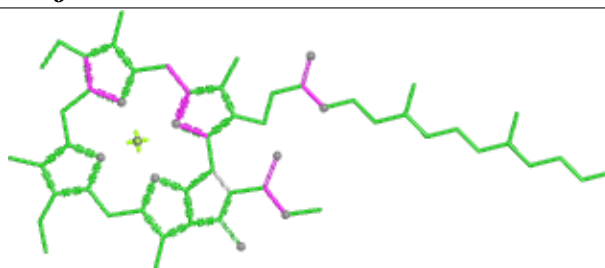
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



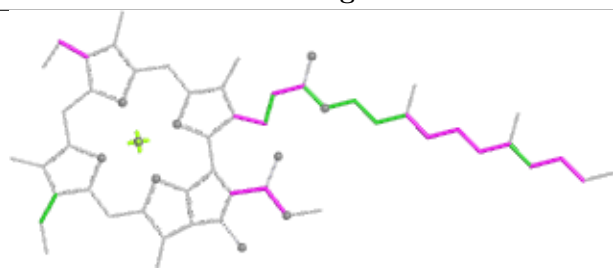
Ligand CLA j 102



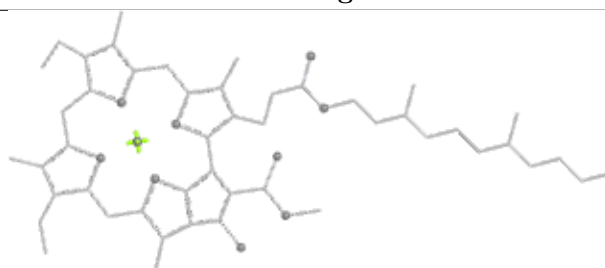
Bond lengths



Bond angles

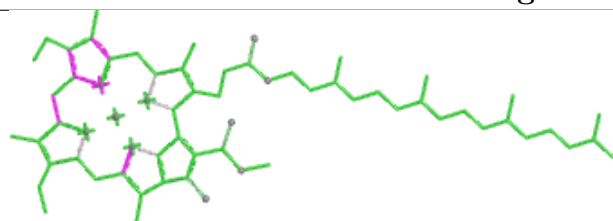


Torsions

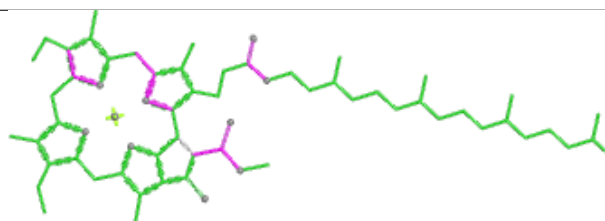


Rings

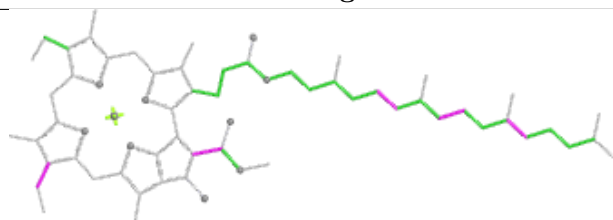
Ligand CLA b 837



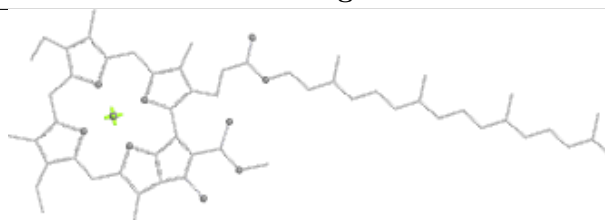
Bond lengths



Bond angles

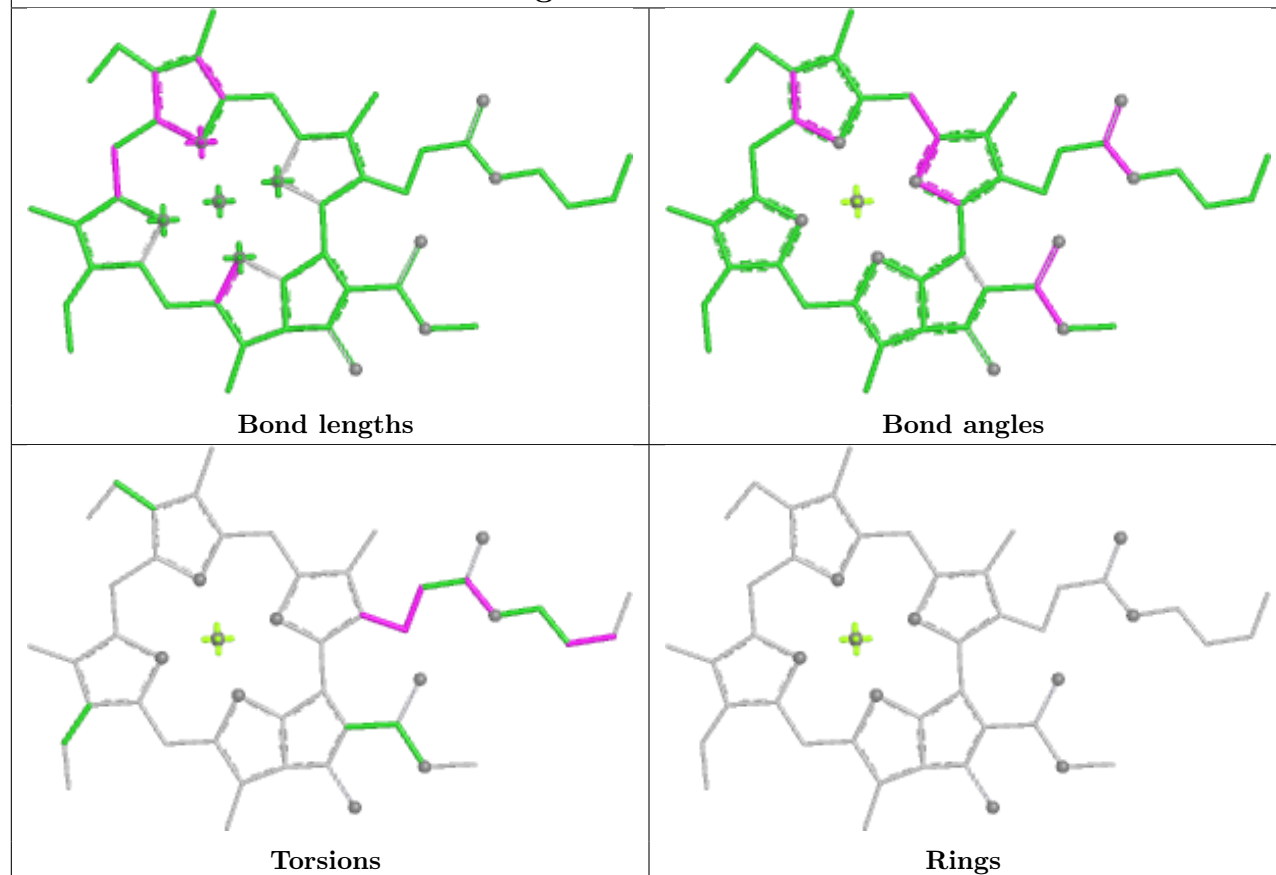


Torsions

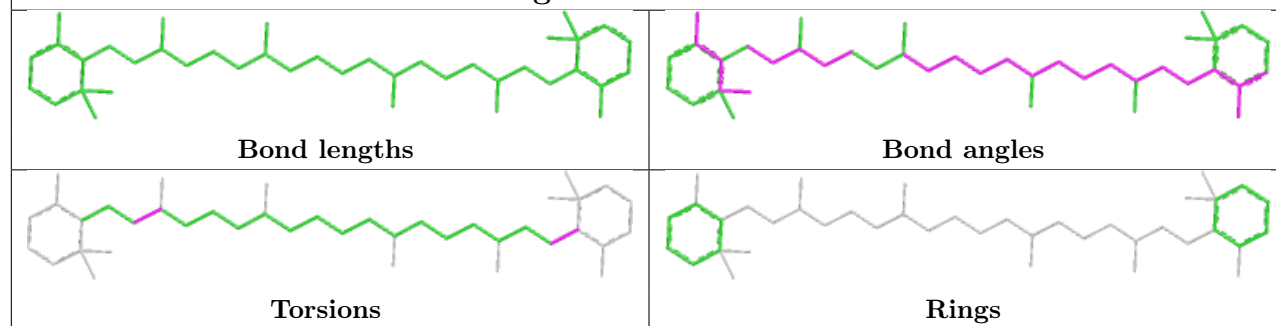


Rings

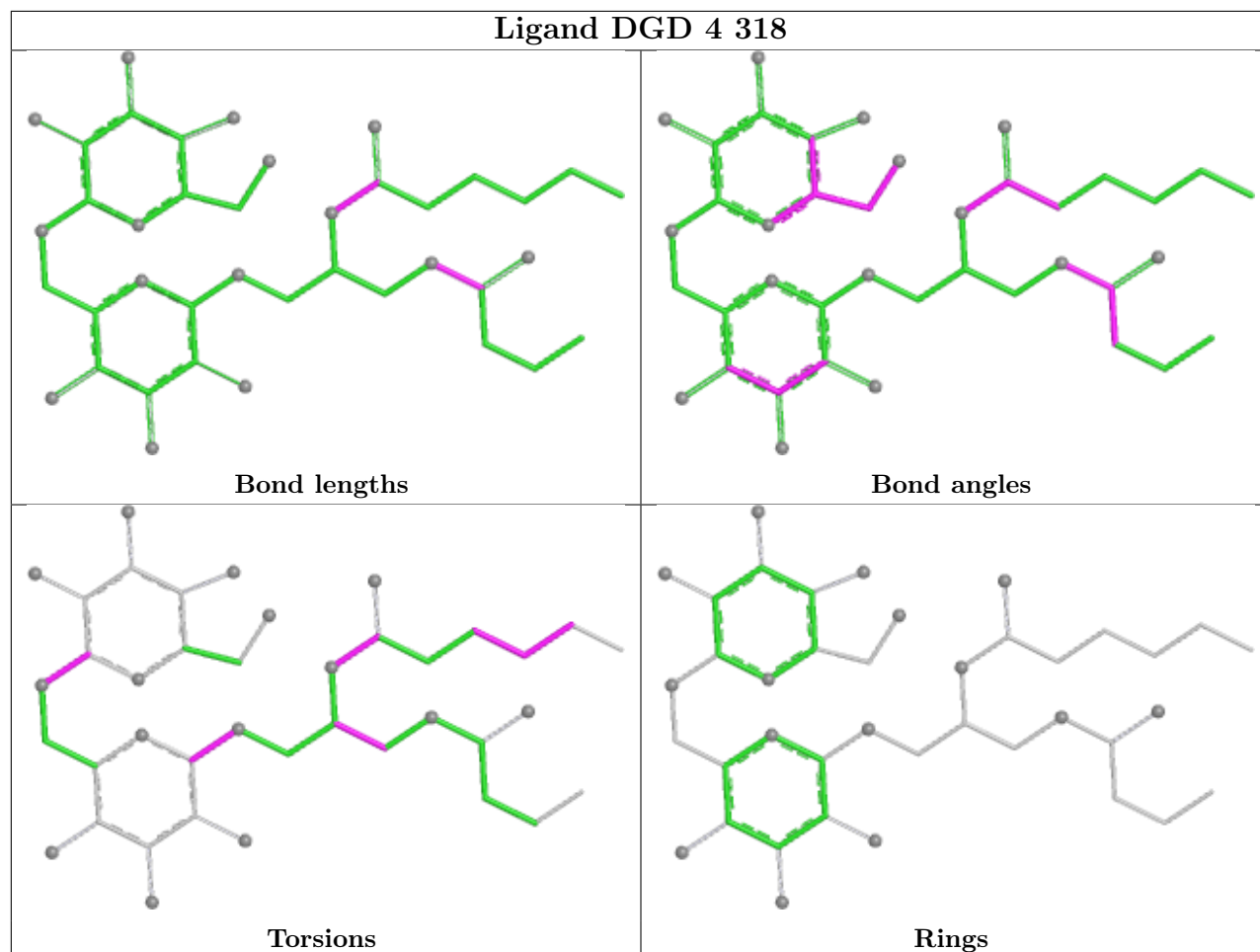
Ligand CLA b 832



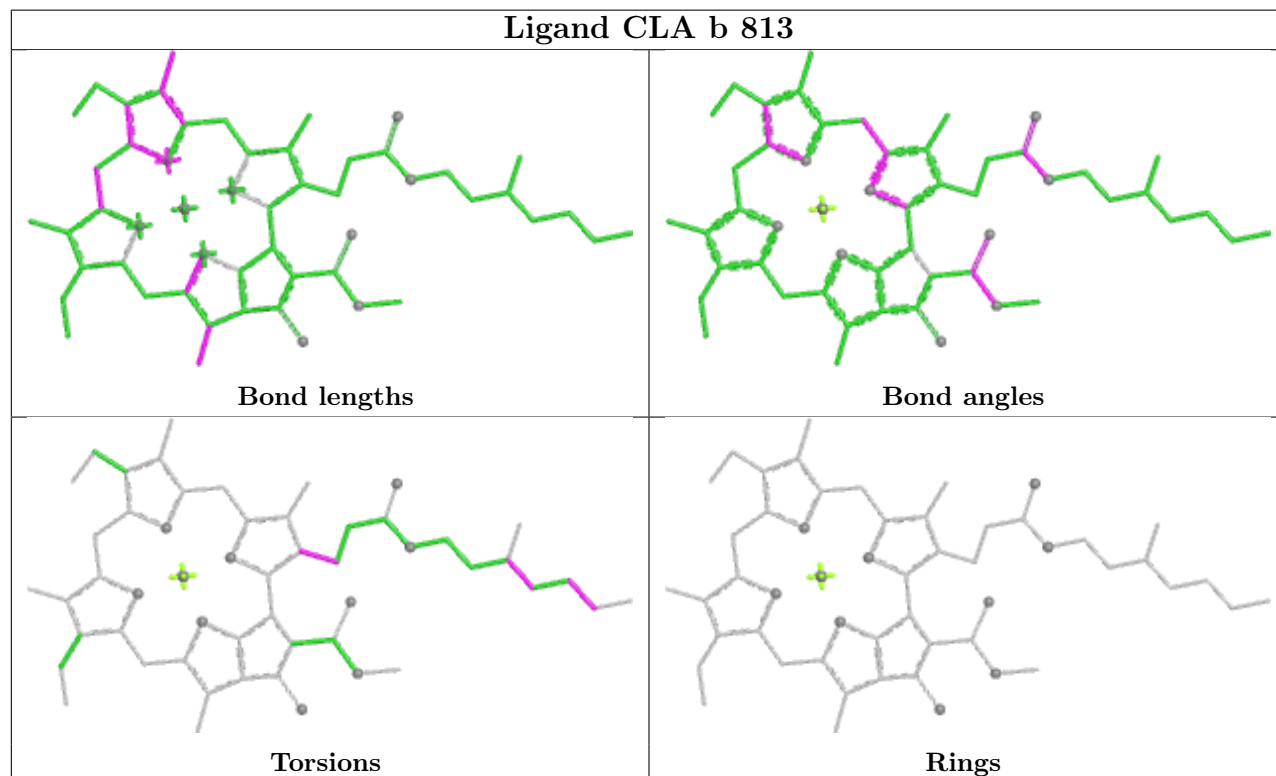
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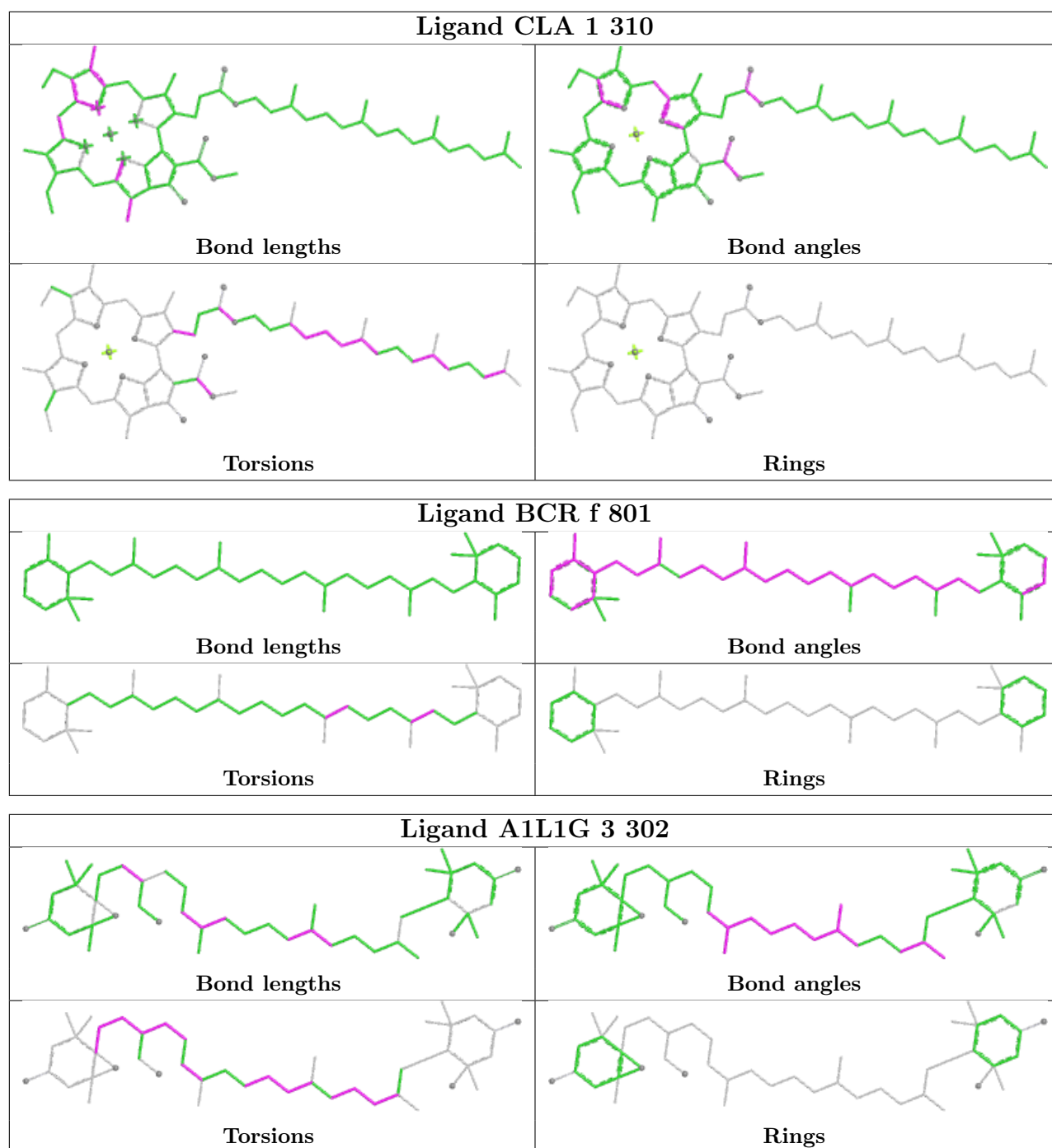


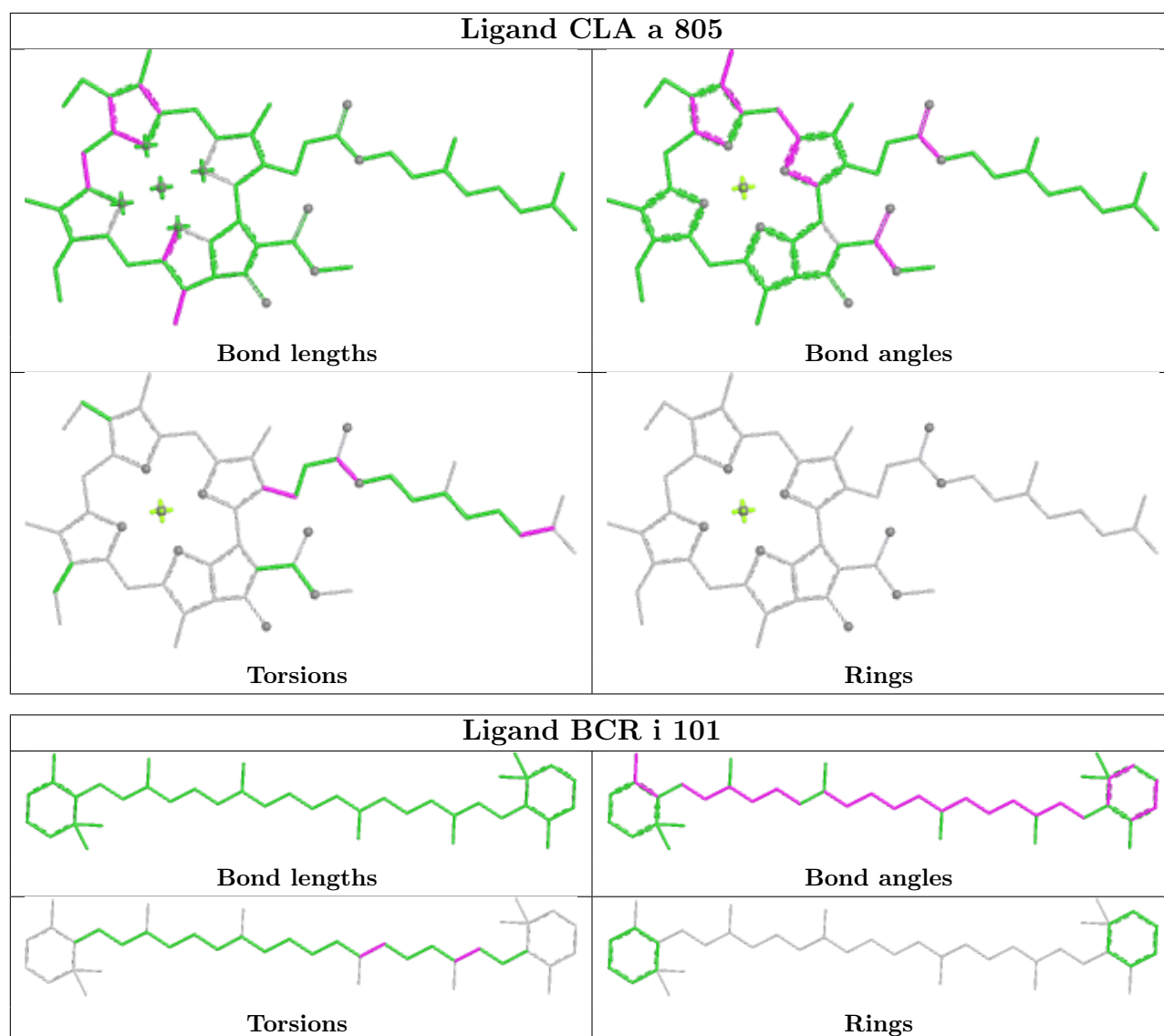
Ligand DGD 4 318



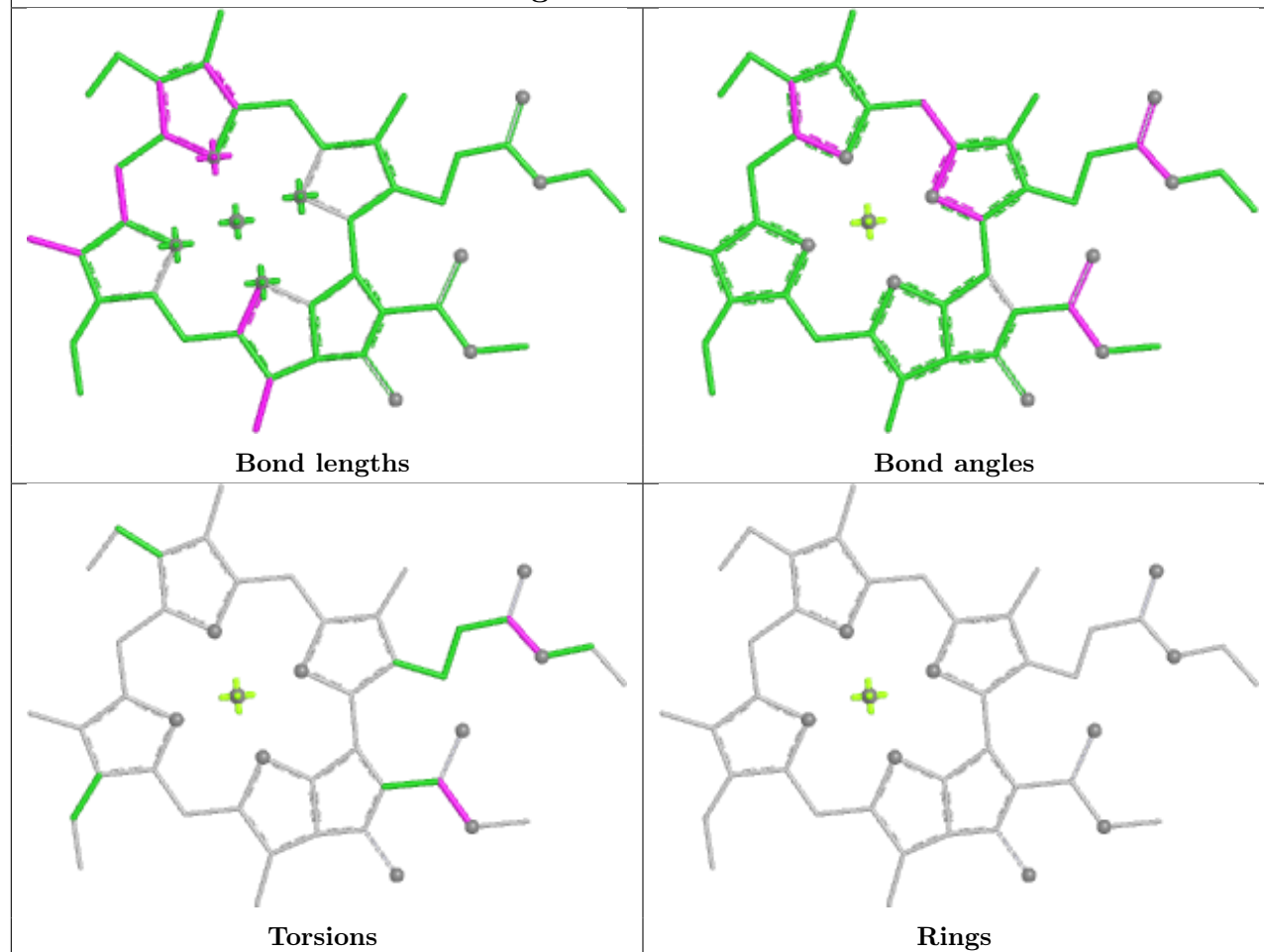
Ligand CLA b 813



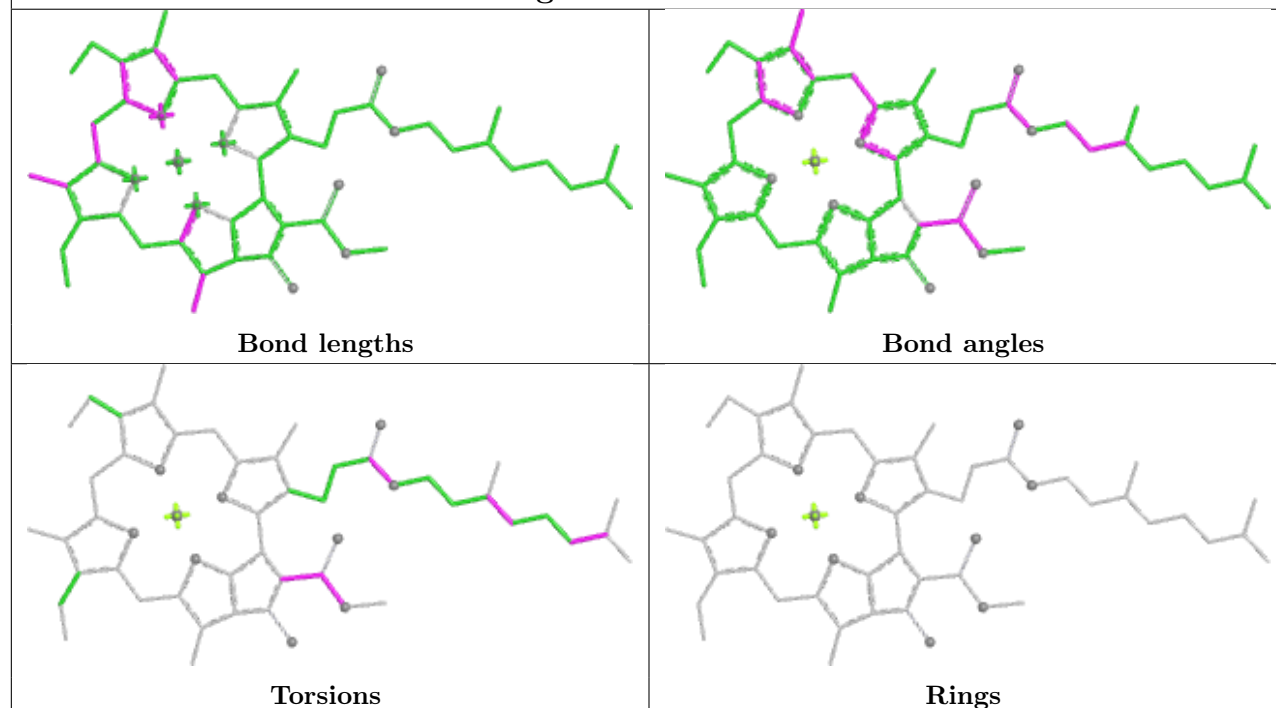


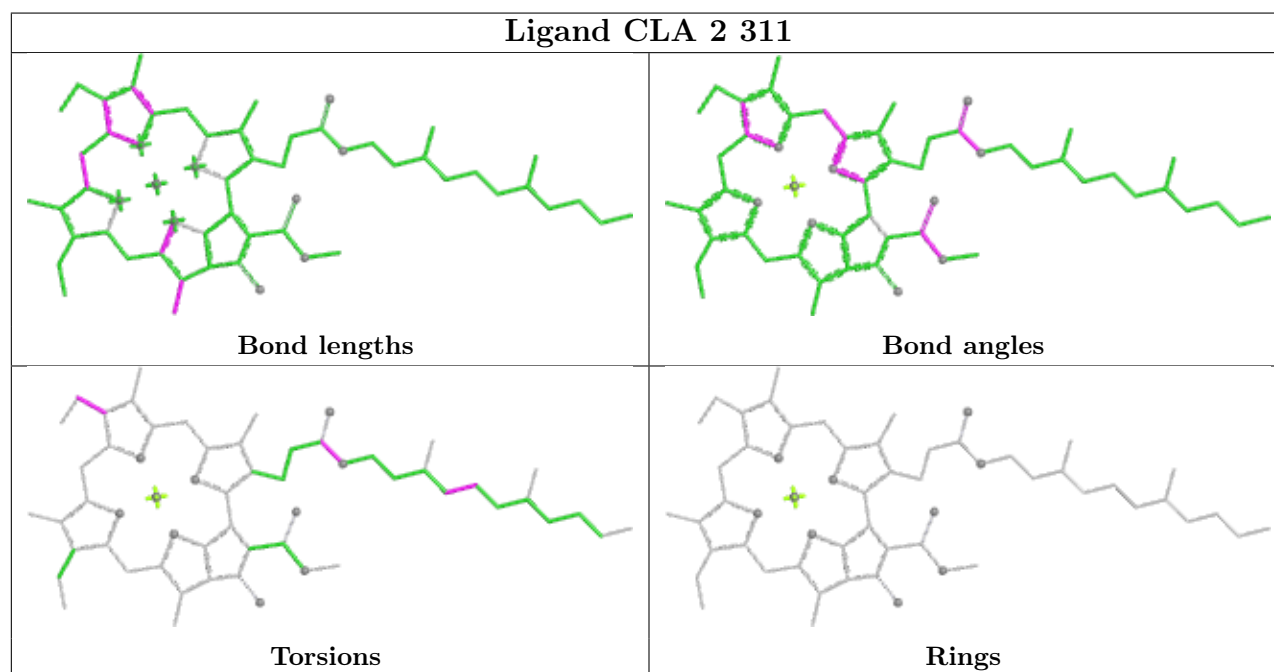
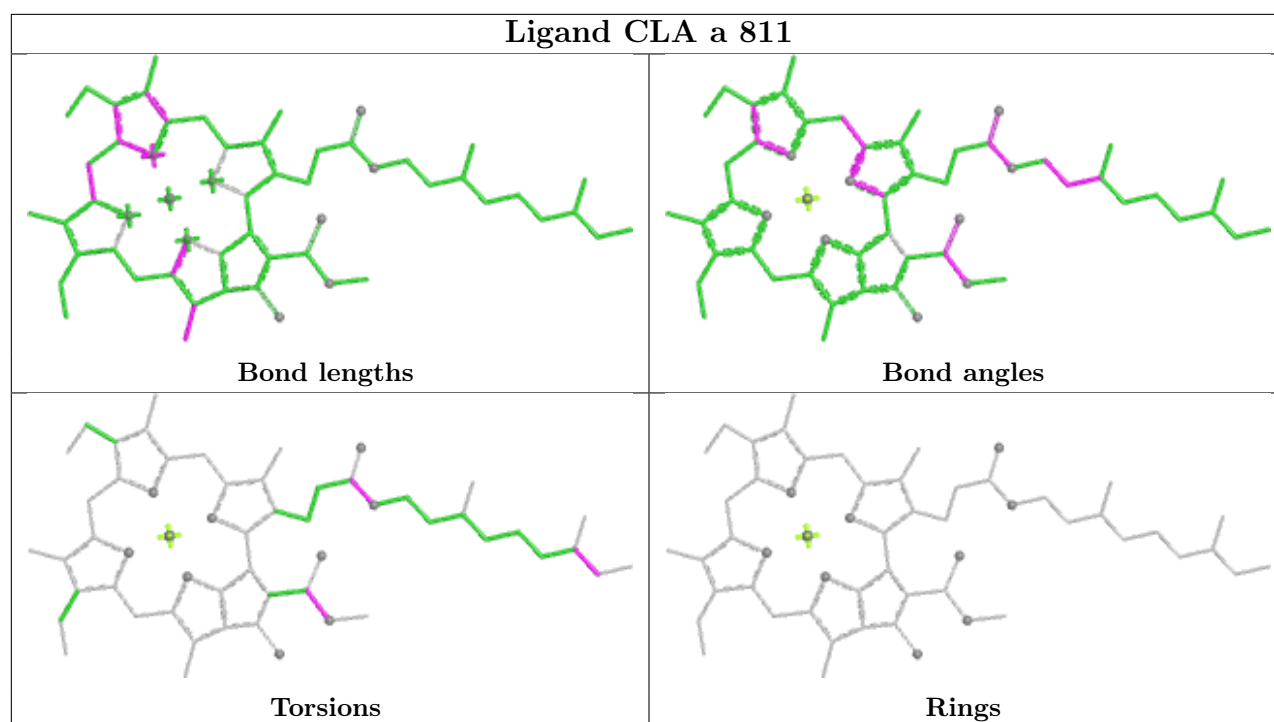


Ligand CLA 2 312

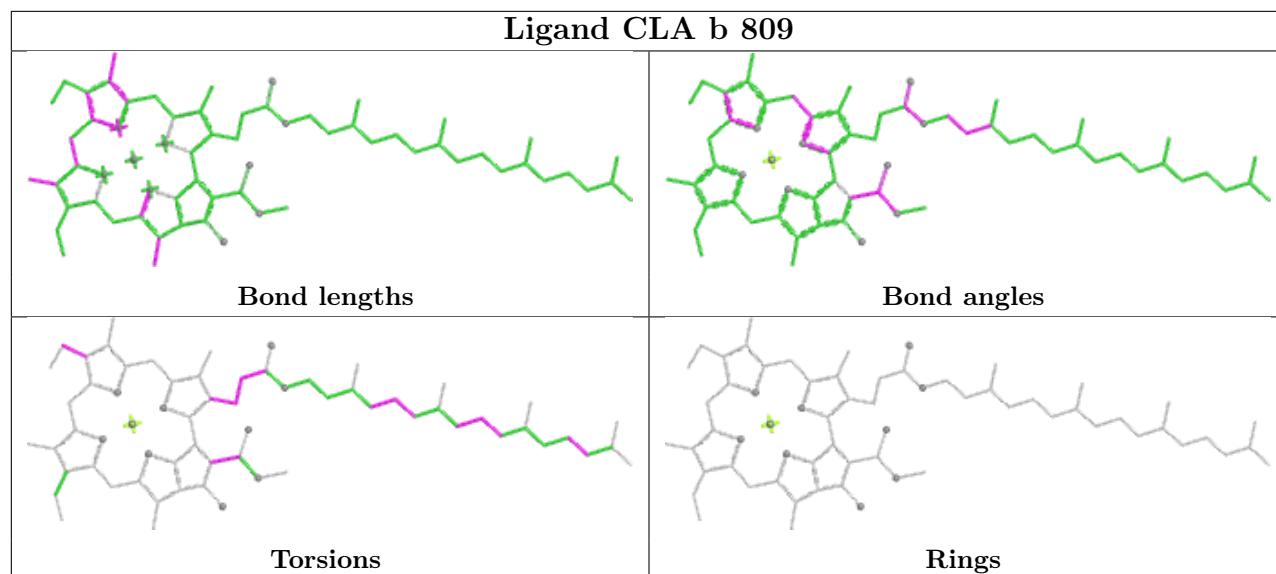


Ligand CLA a 804

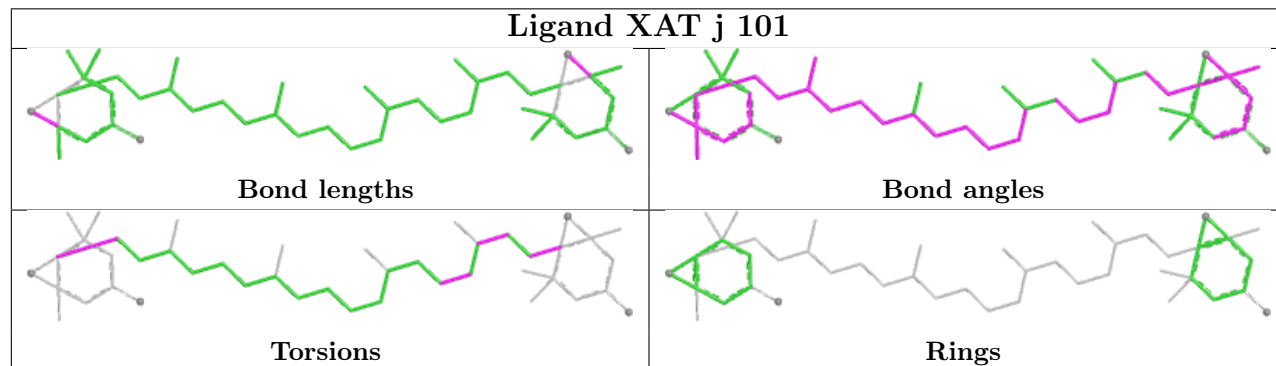




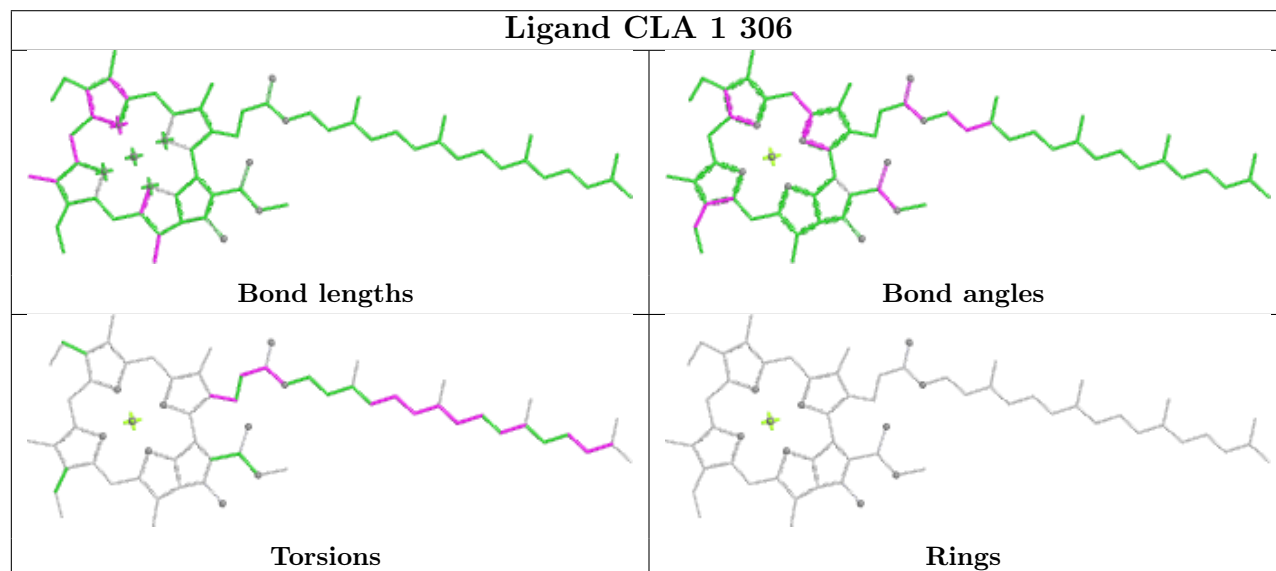
Ligand CLA b 809

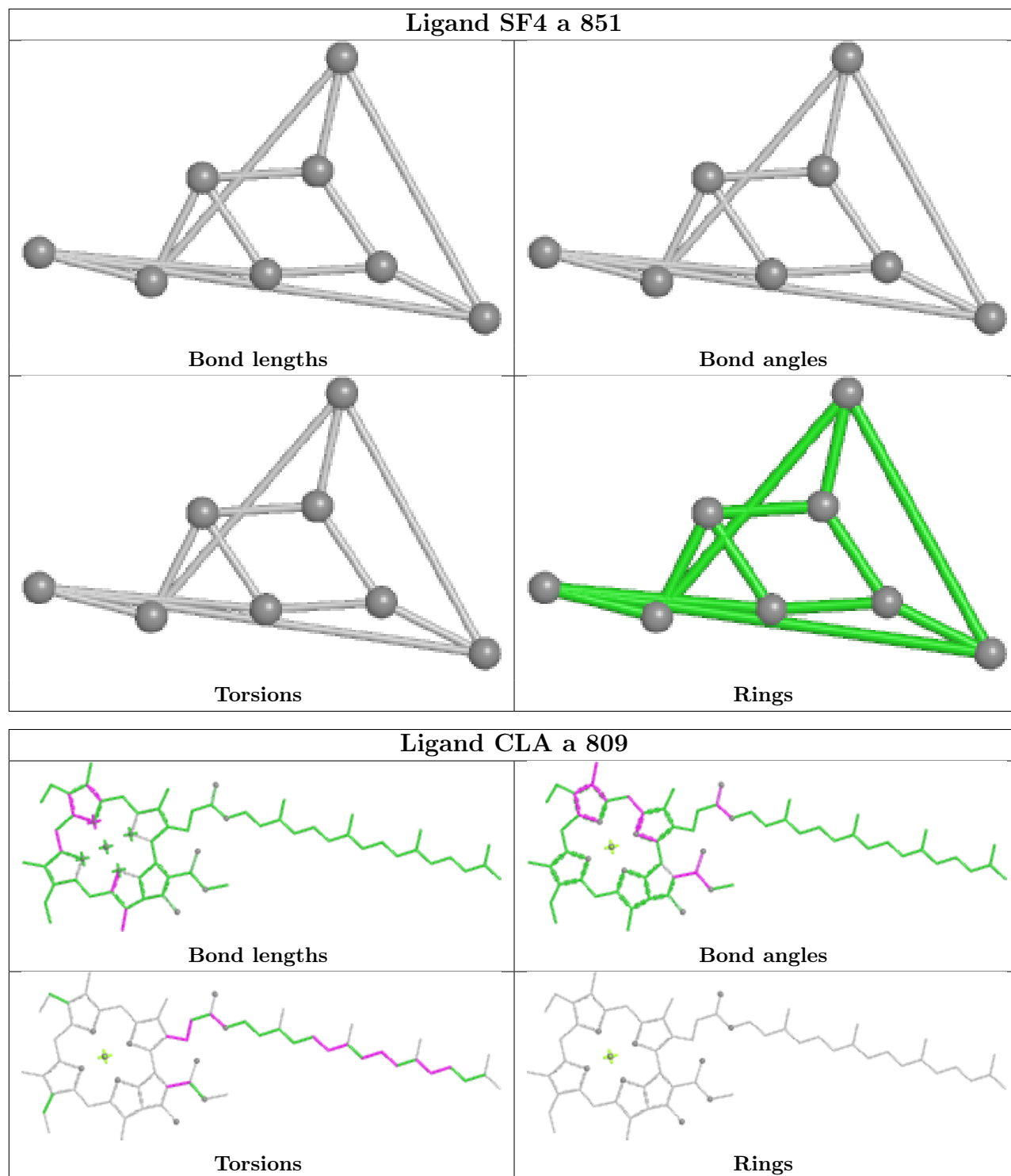


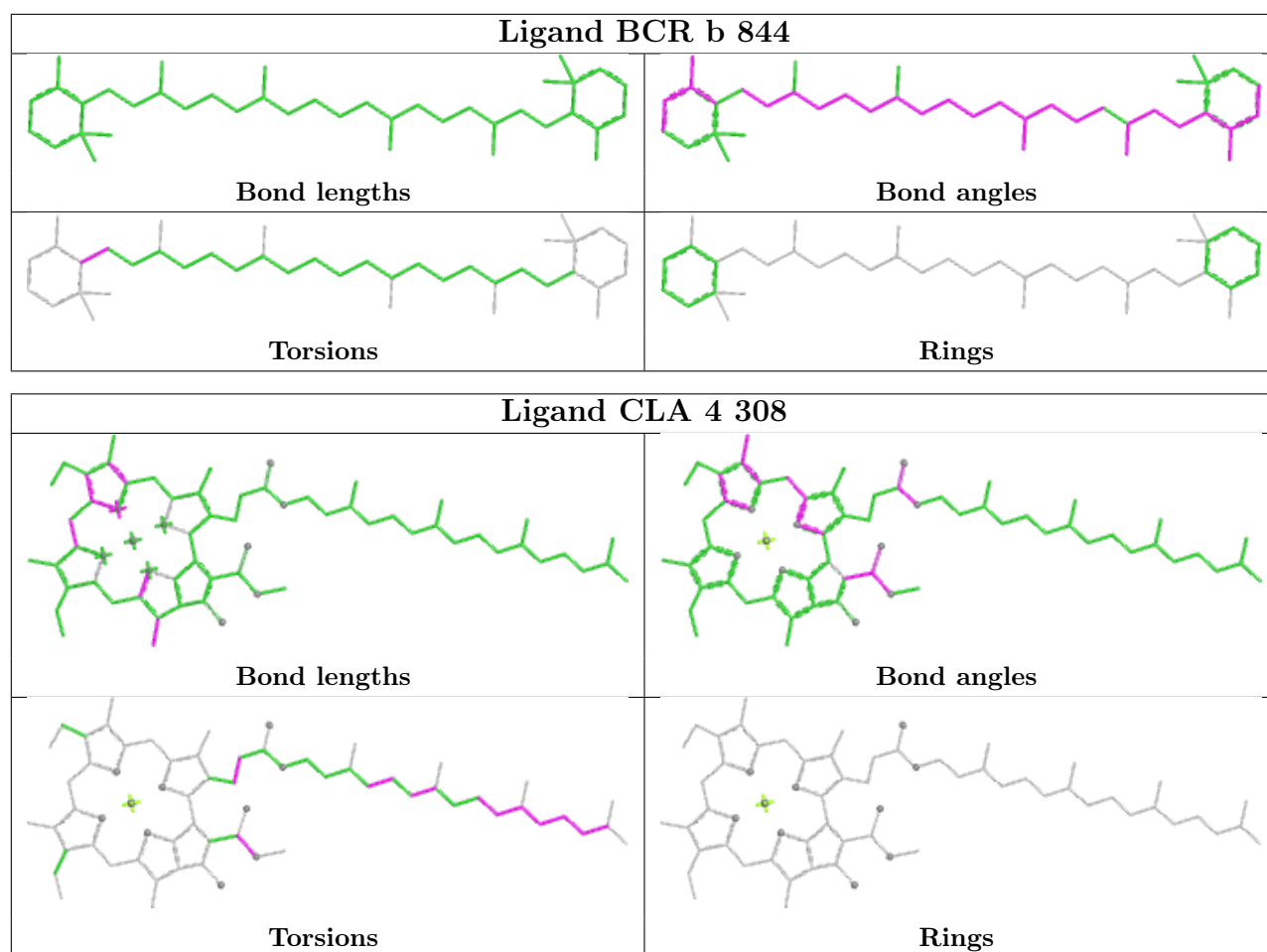
Ligand XAT j 101



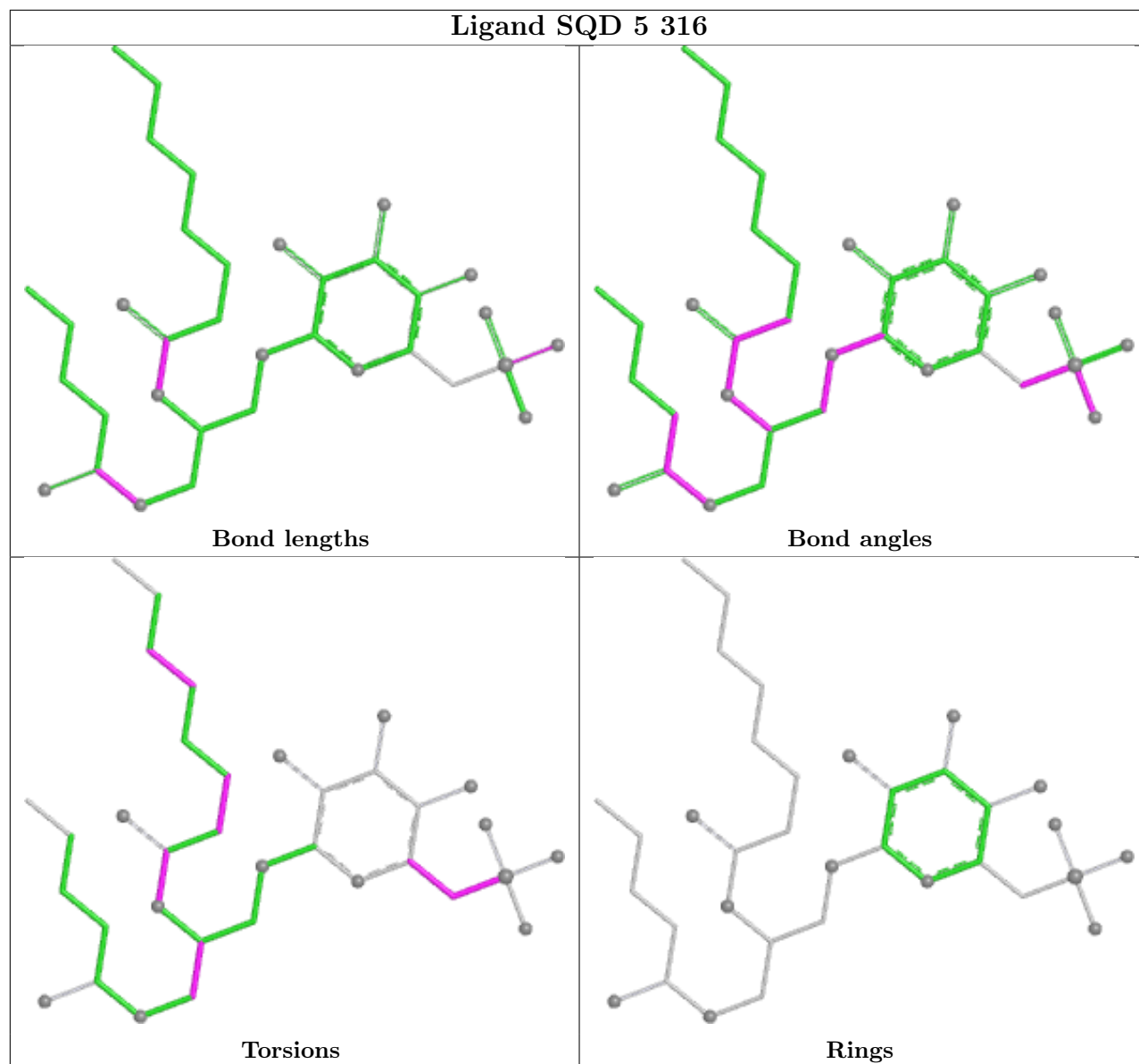
Ligand CLA 1 306

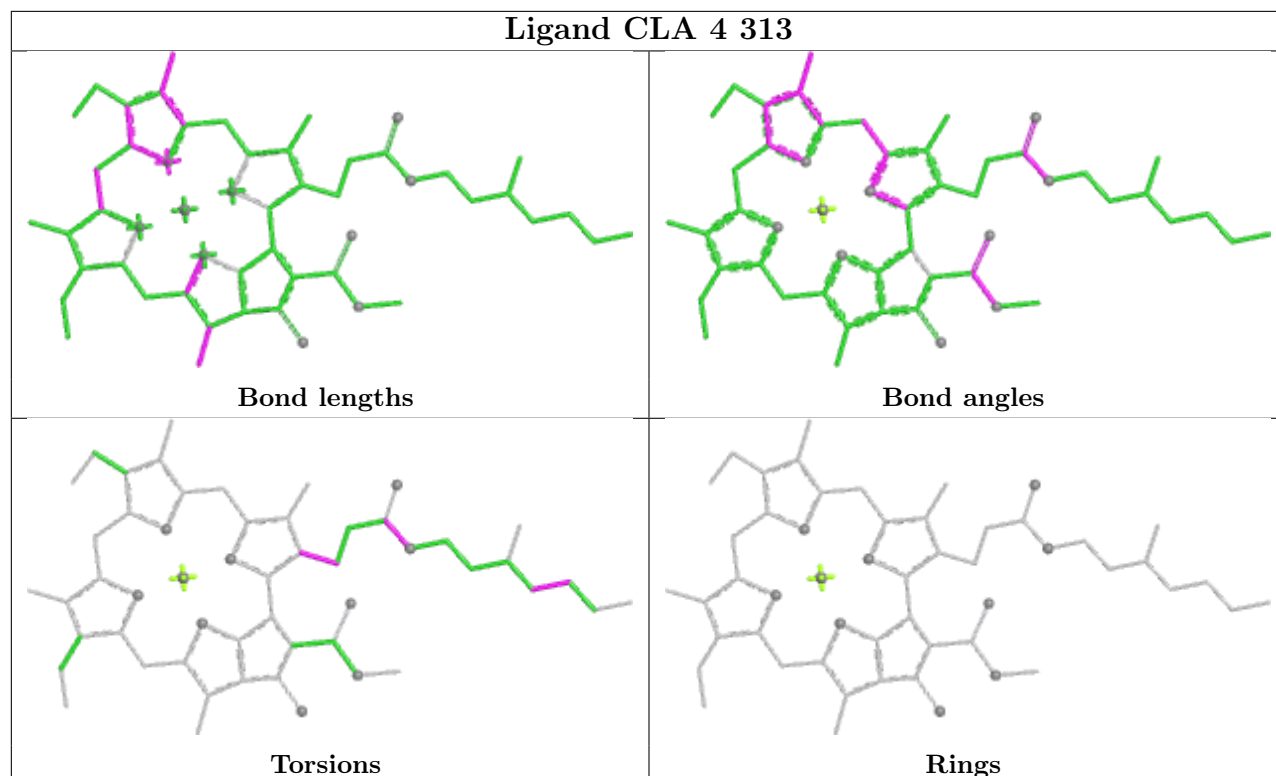
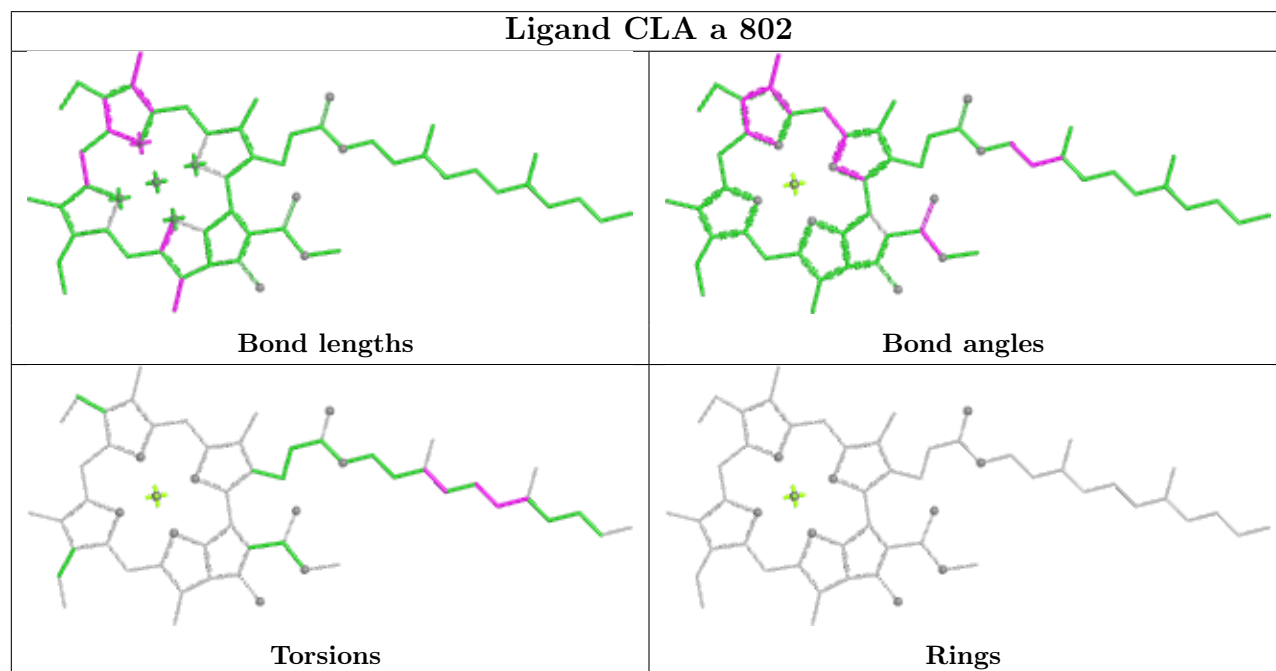


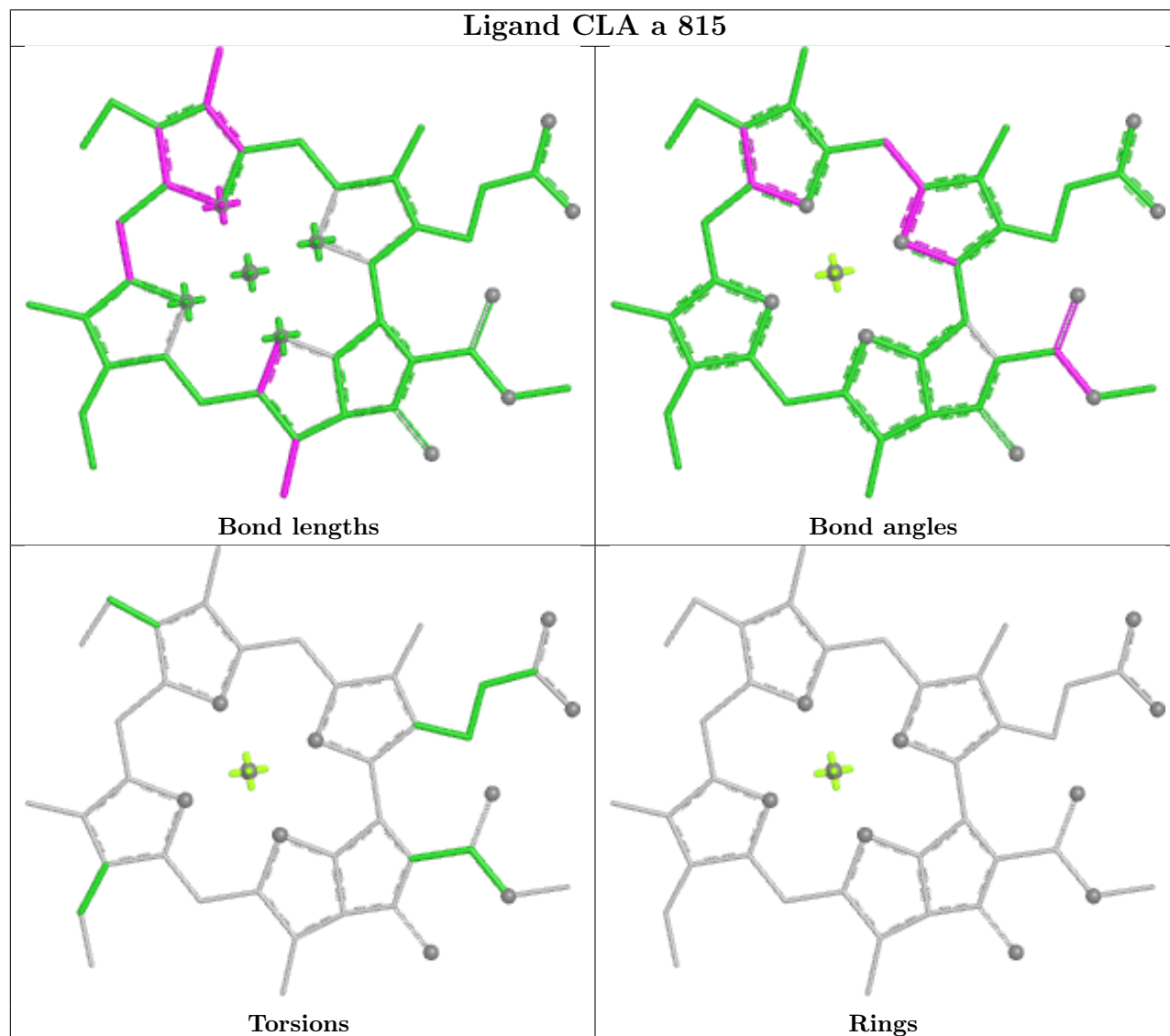
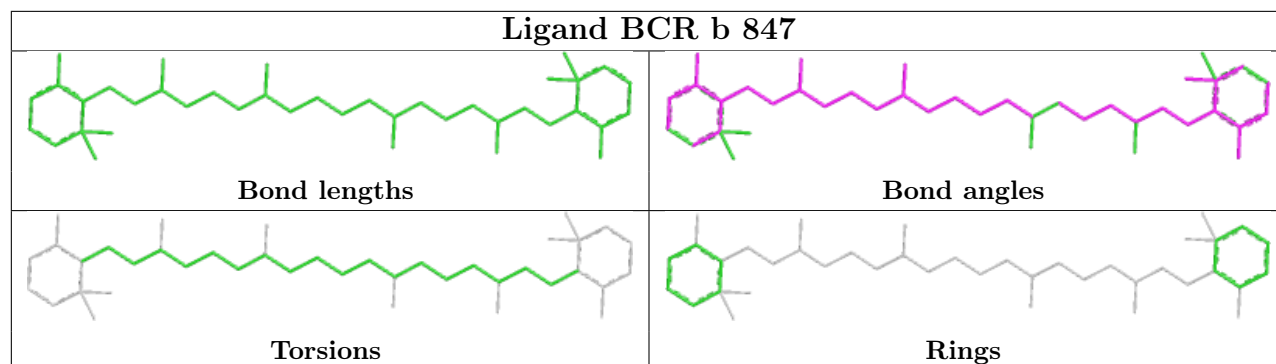




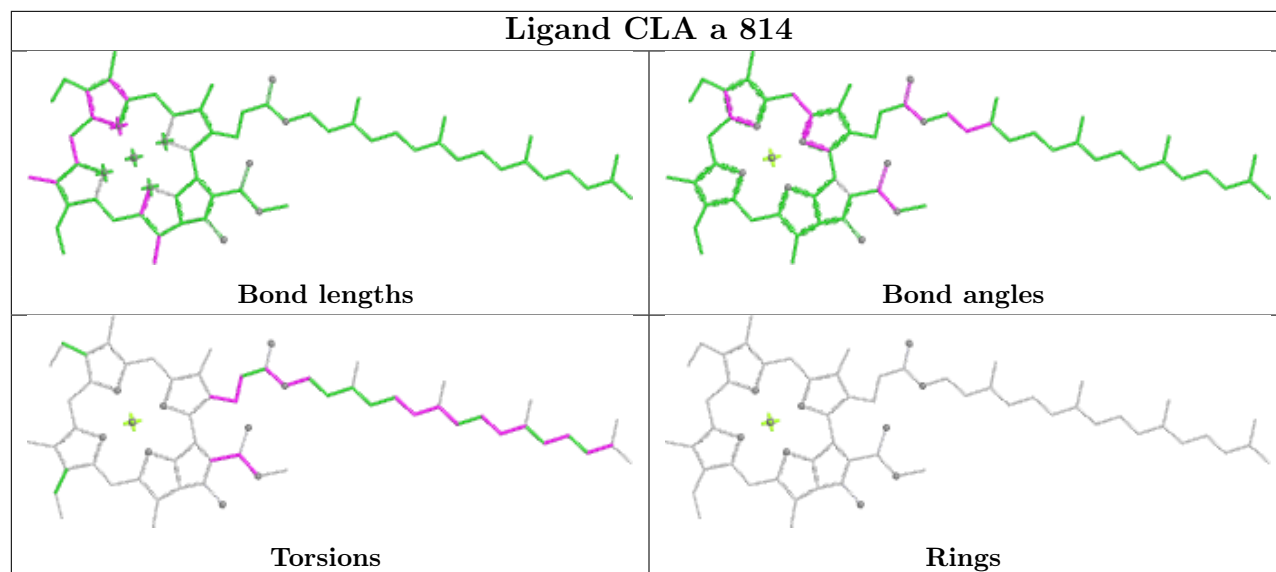
Ligand SQD 5 316



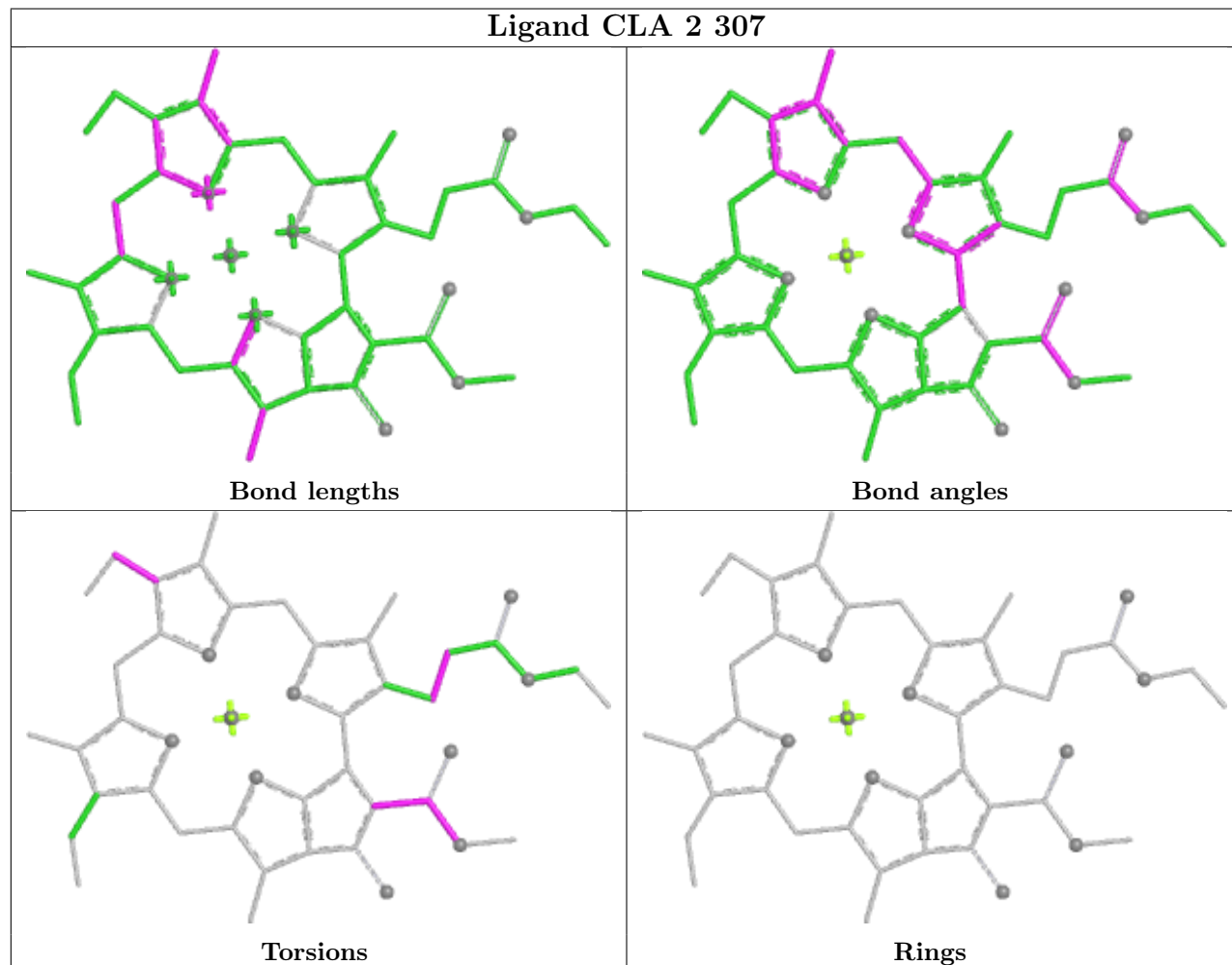
Ligand CLA 4 313**Ligand CLA a 802**



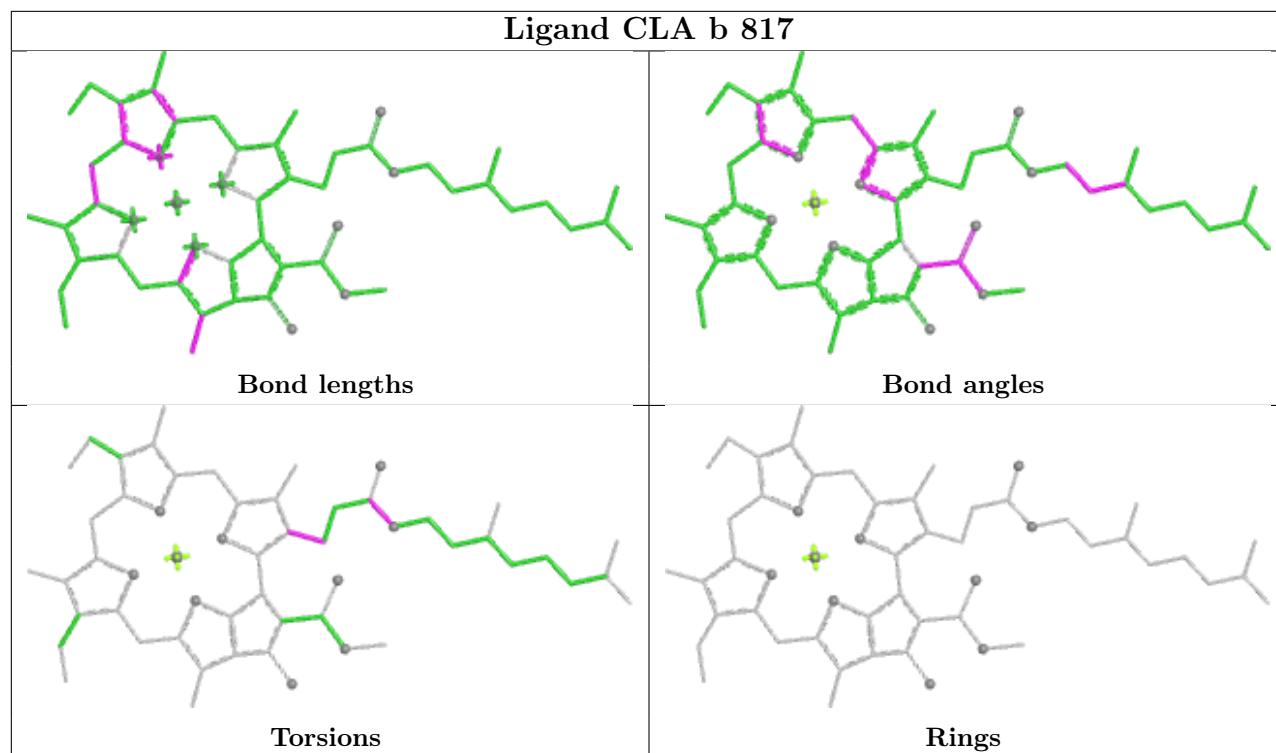
Ligand CLA a 814



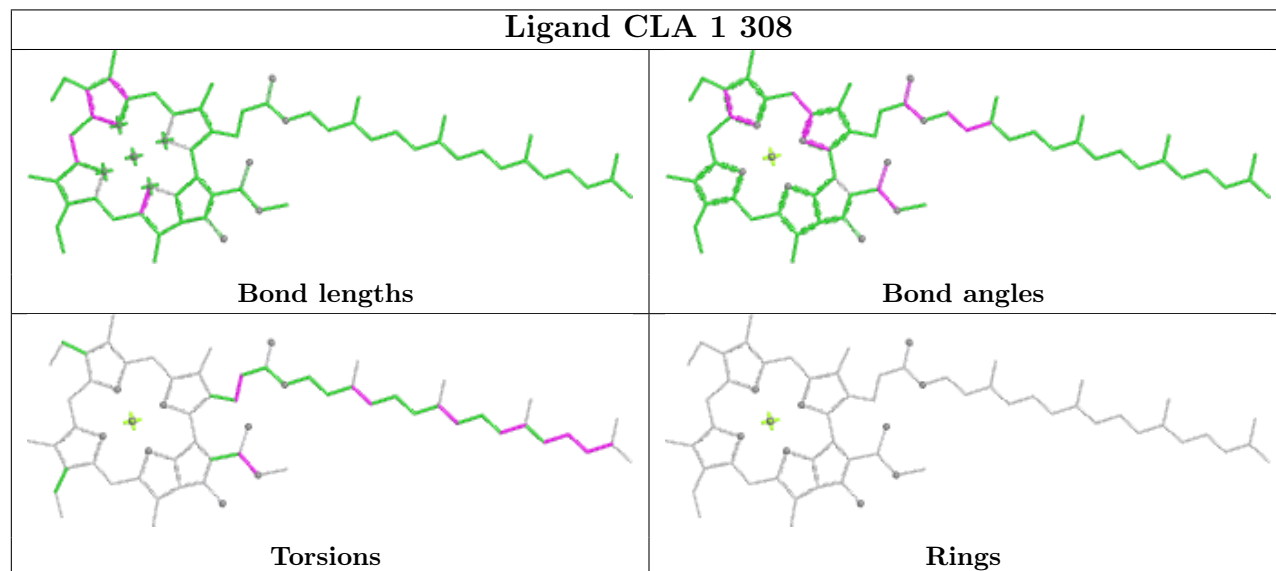
Ligand CLA 2 307



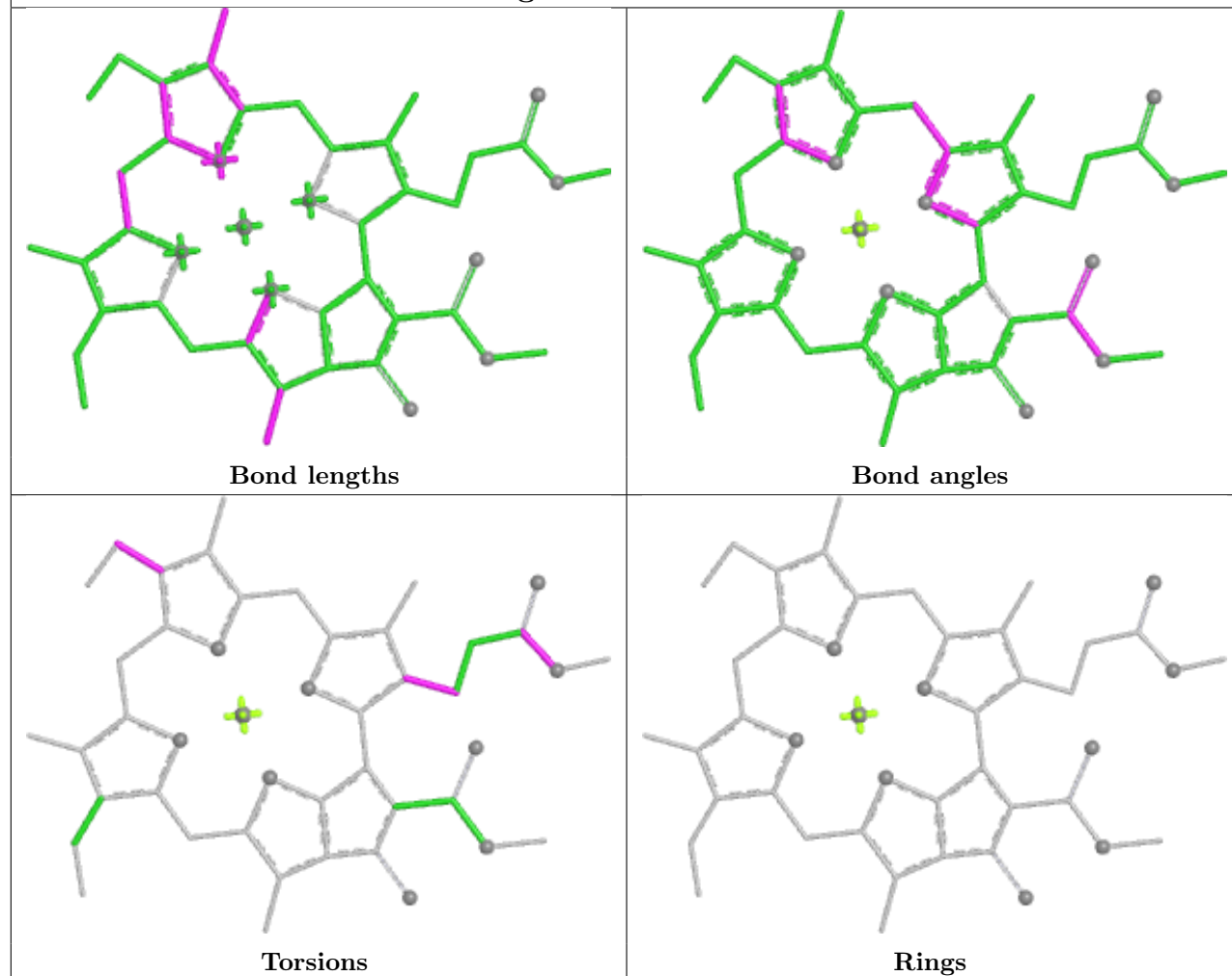
Ligand CLA b 817



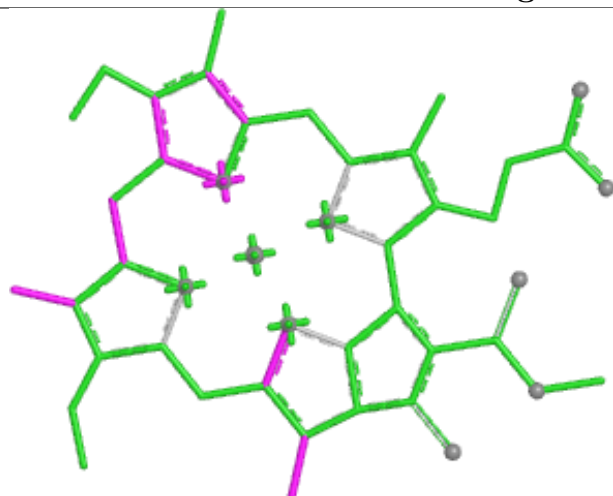
Ligand CLA 1 308



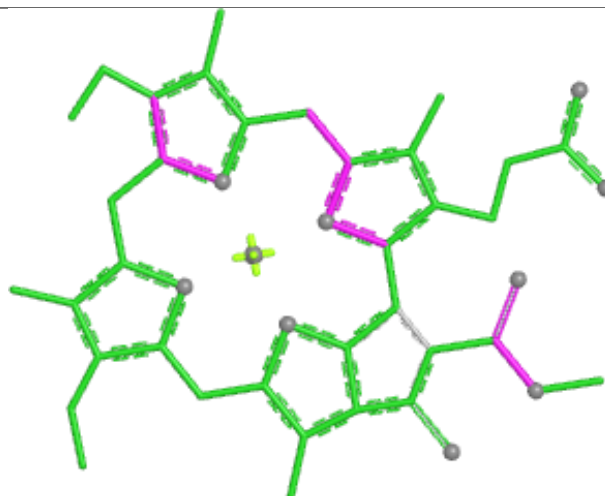
Ligand CLA a 824



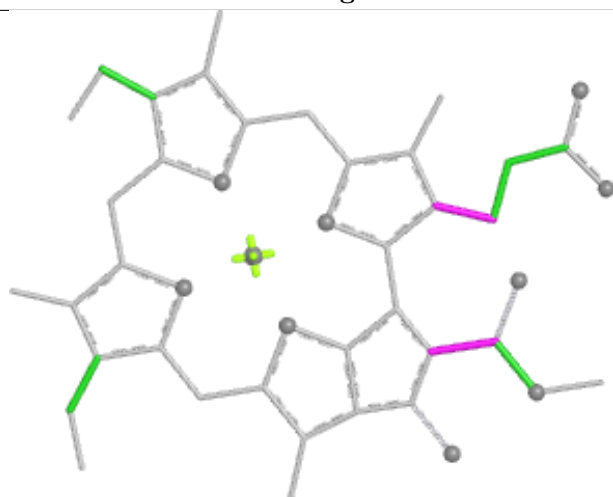
Ligand CLA b 816



Bond lengths



Bond angles

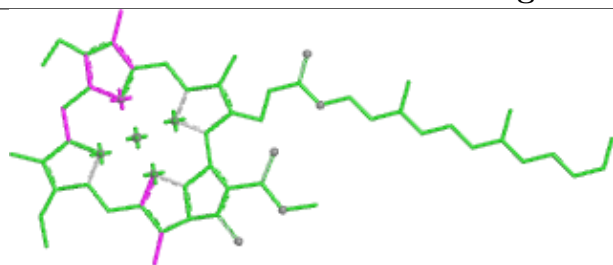


Torsions

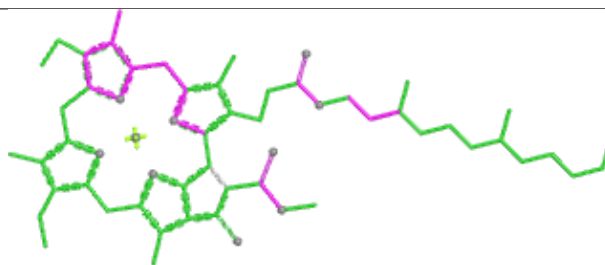


Rings

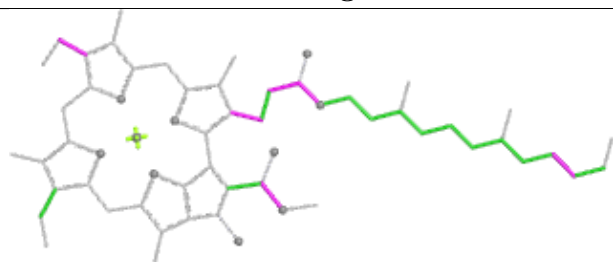
Ligand CLA b 818



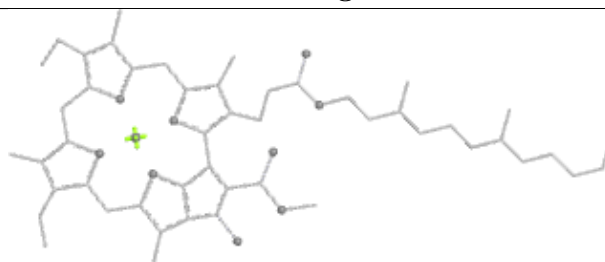
Bond lengths



Bond angles

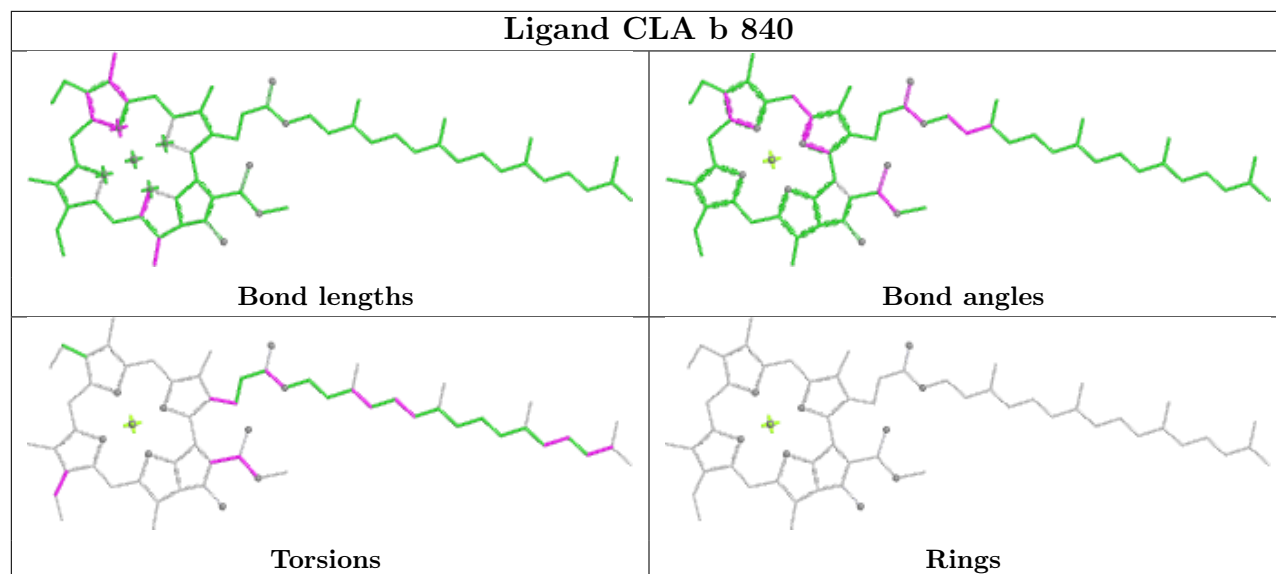


Torsions

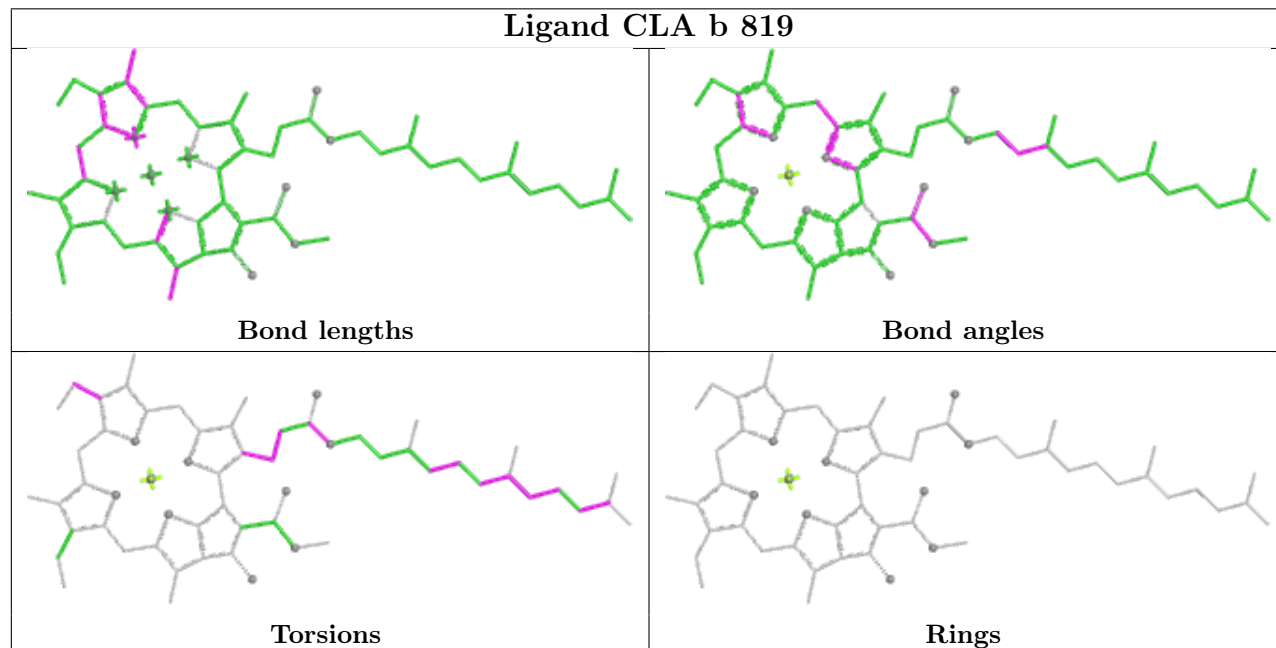


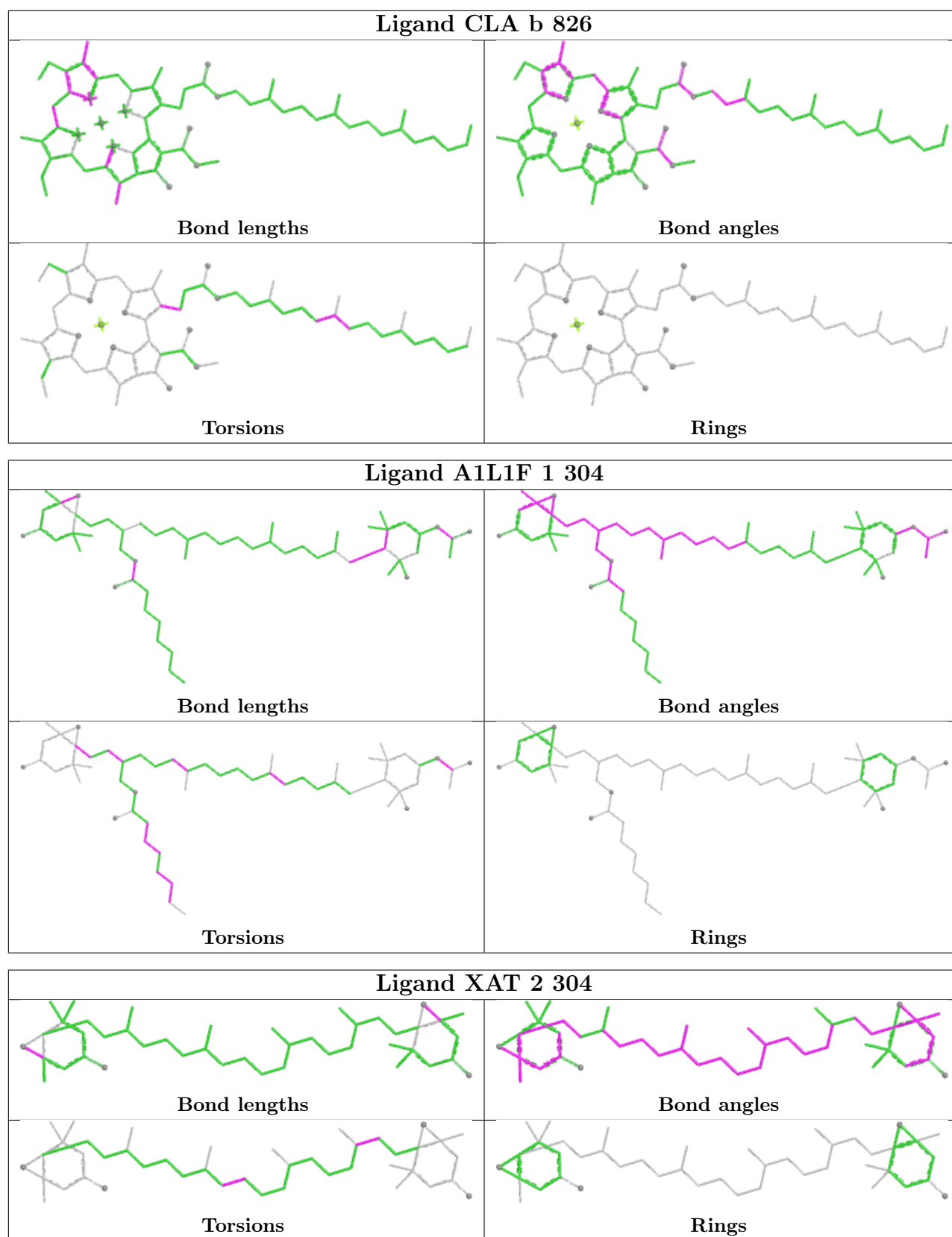
Rings

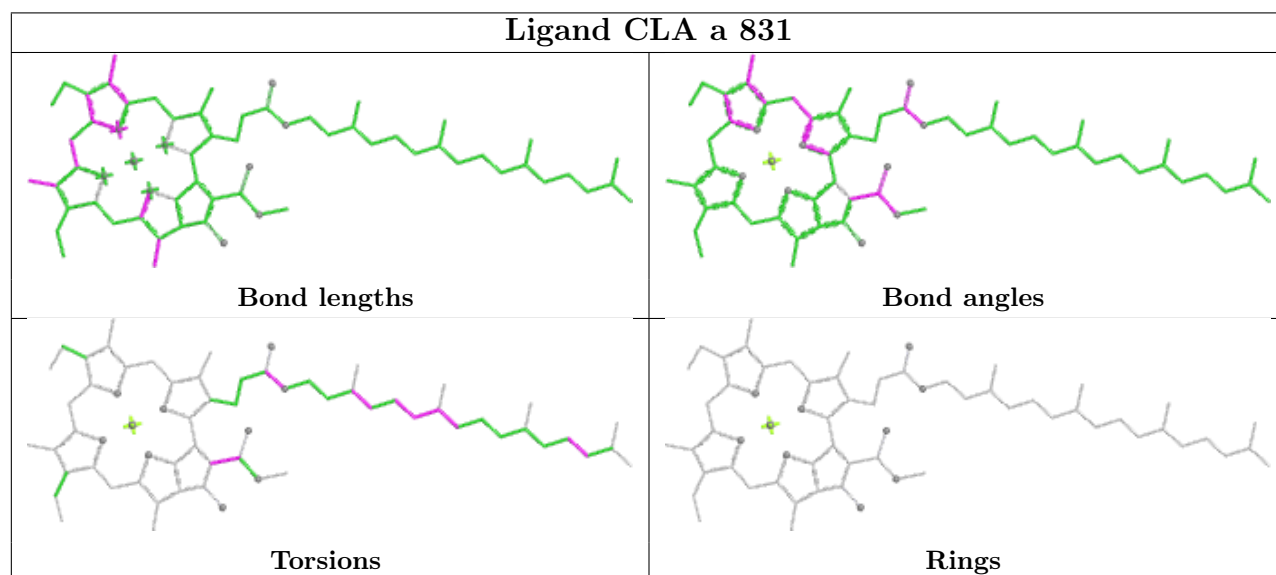
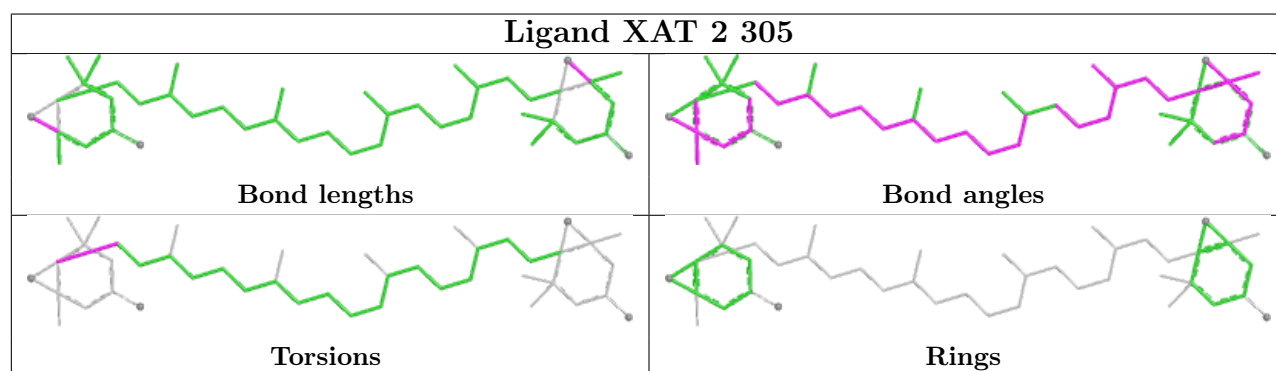
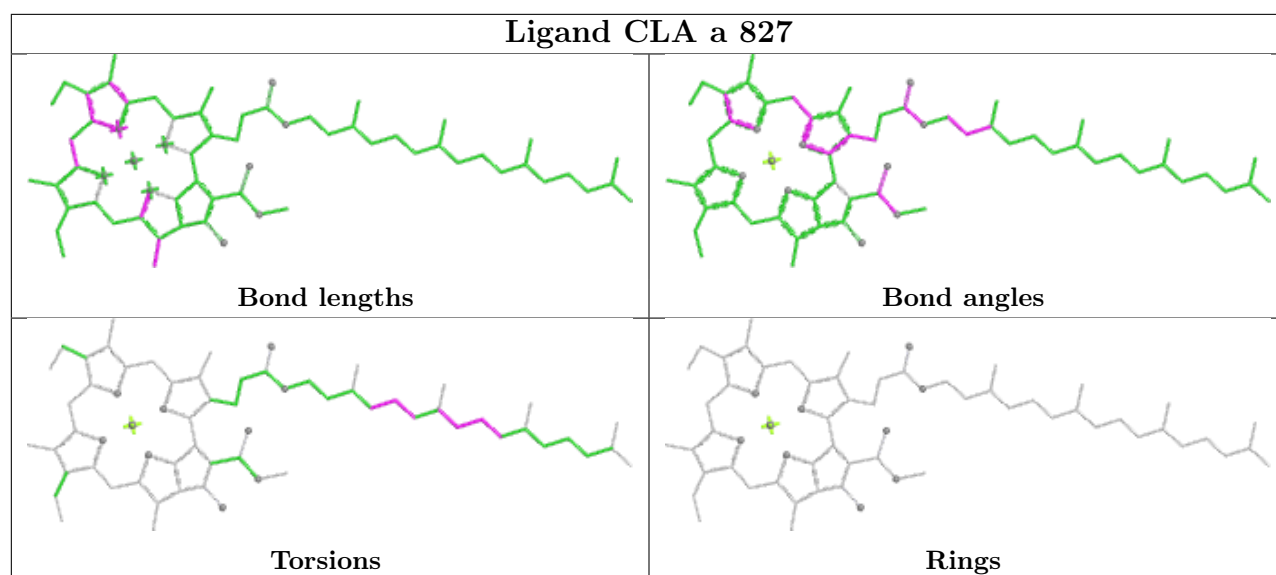
Ligand CLA b 840

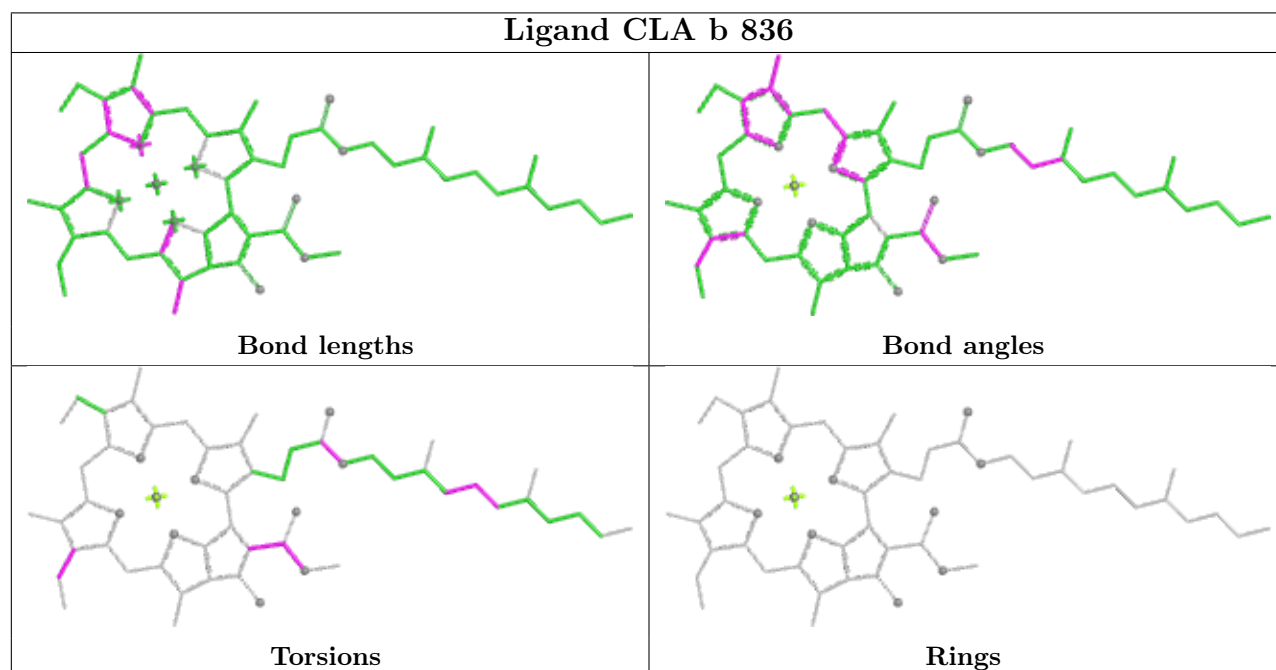
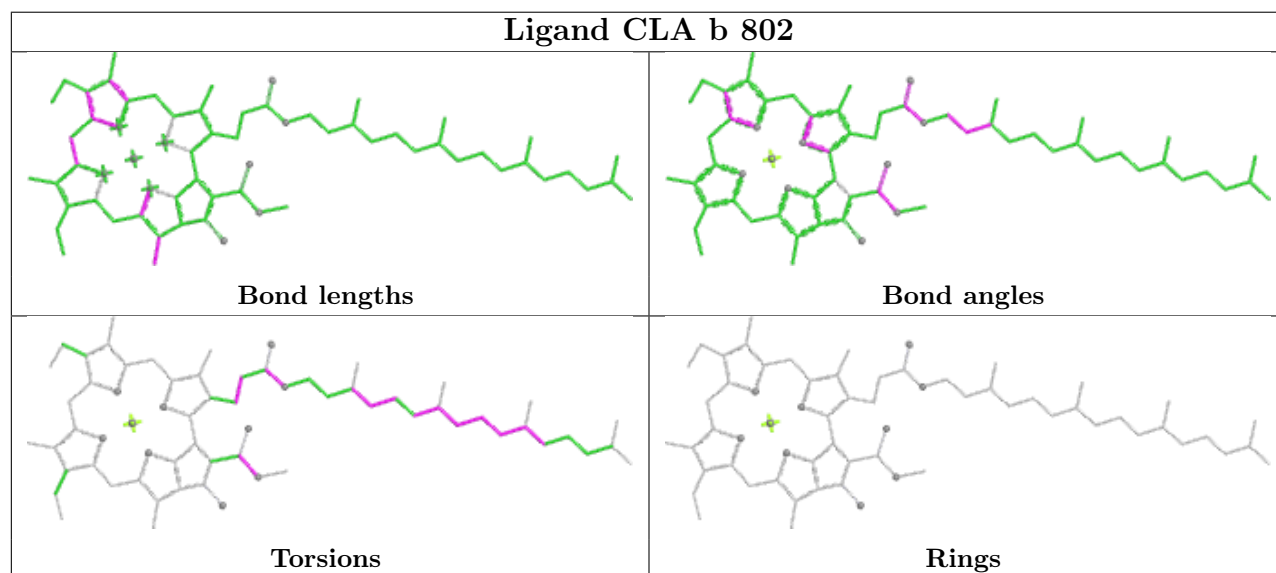
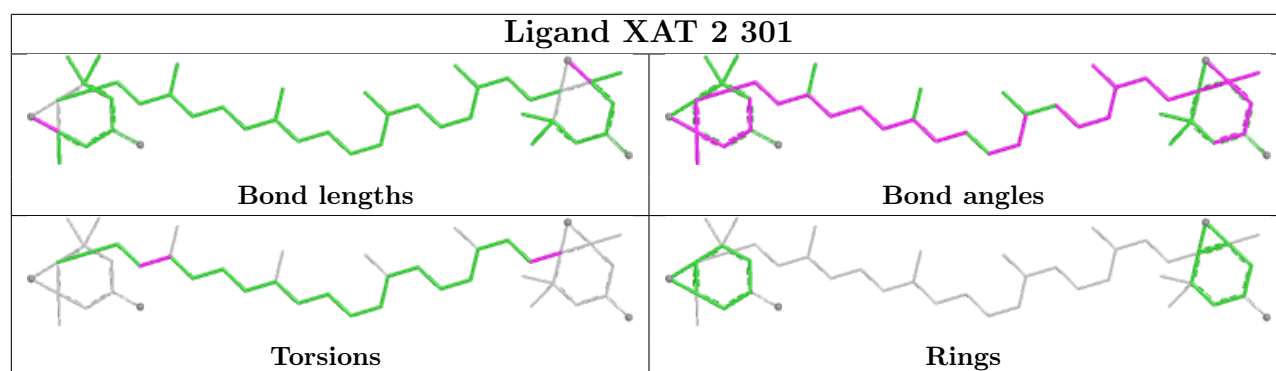


Ligand CLA b 819

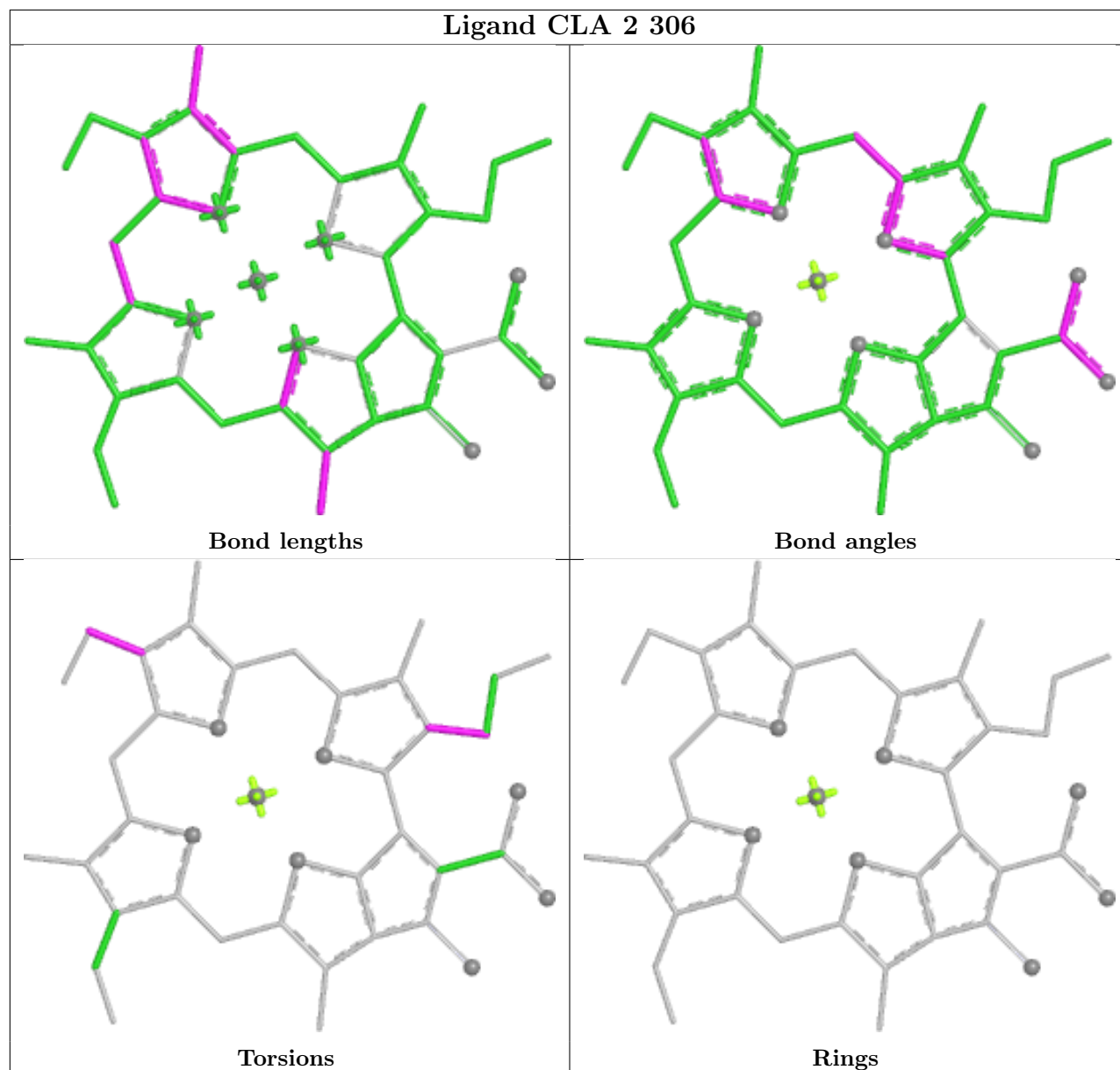


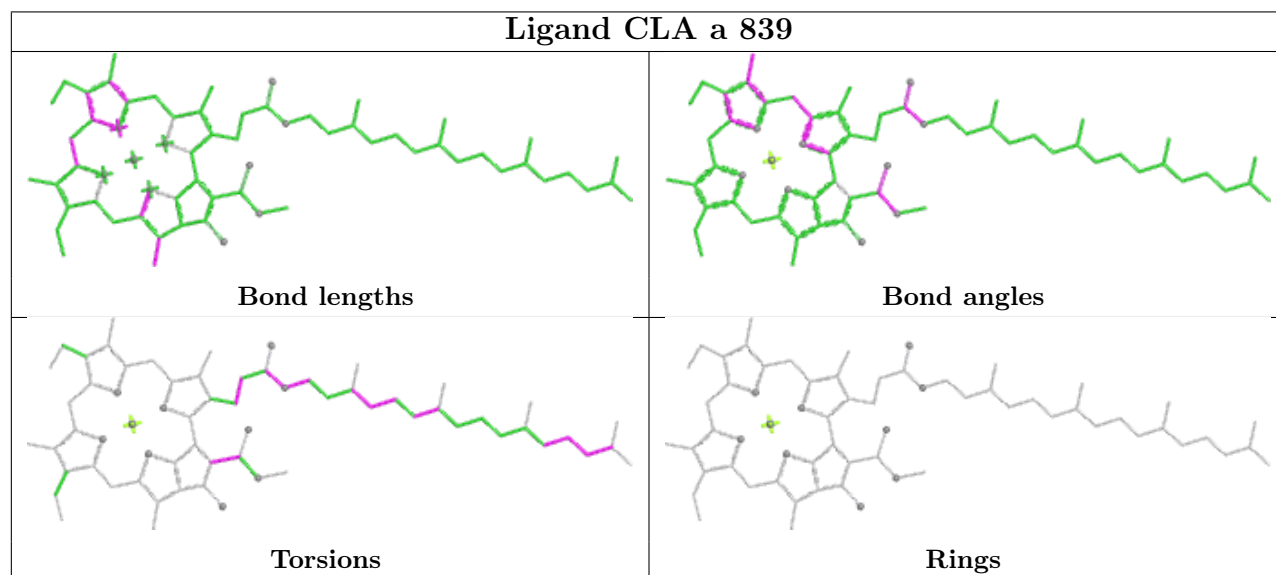
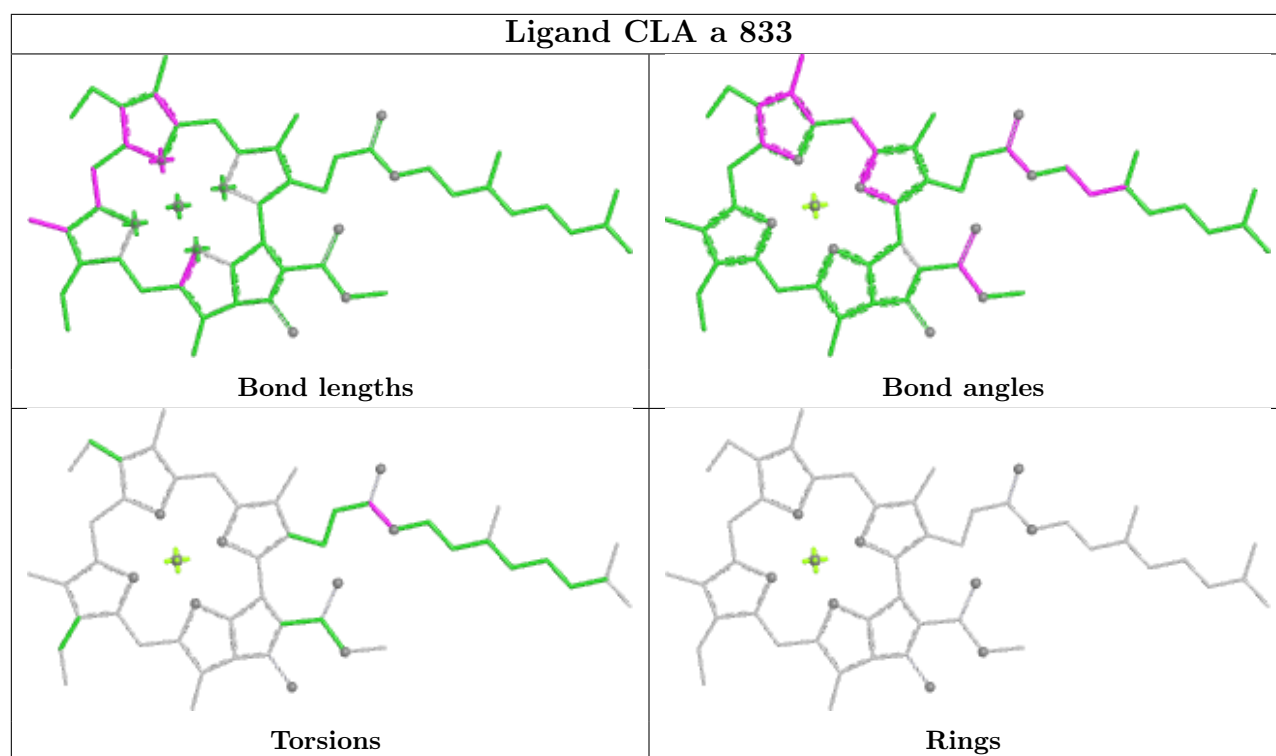


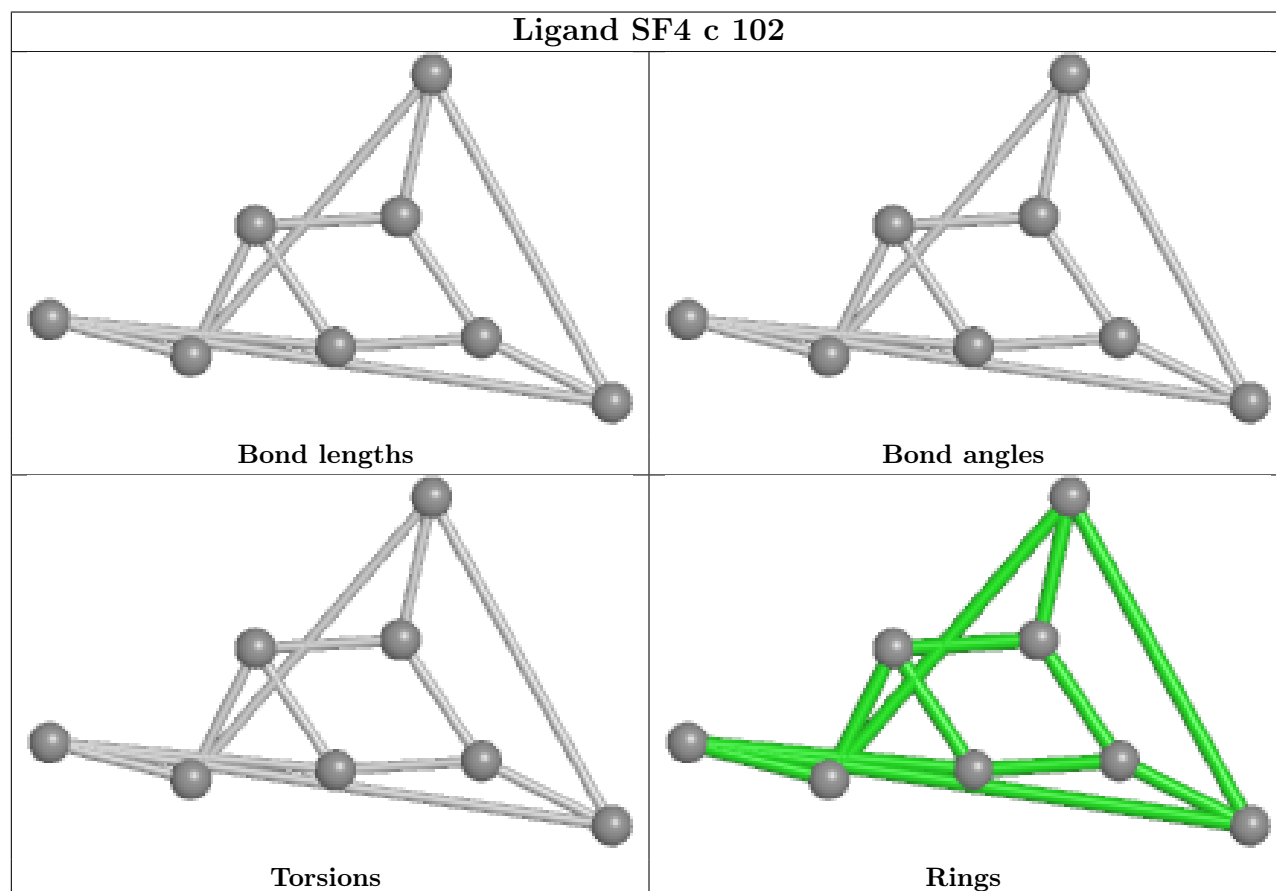
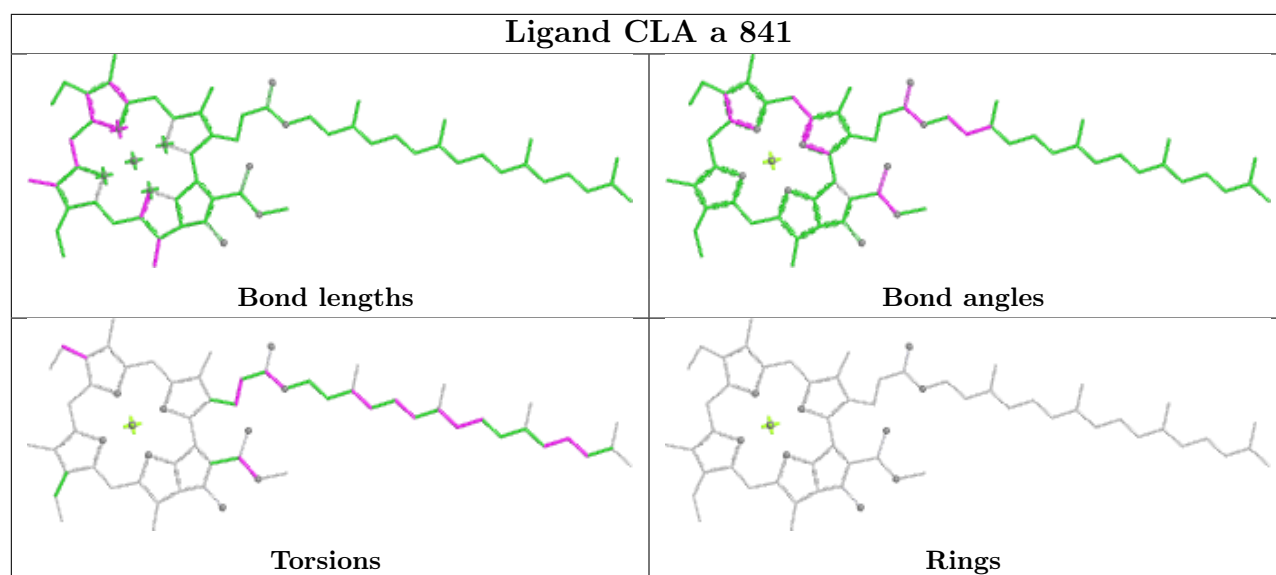


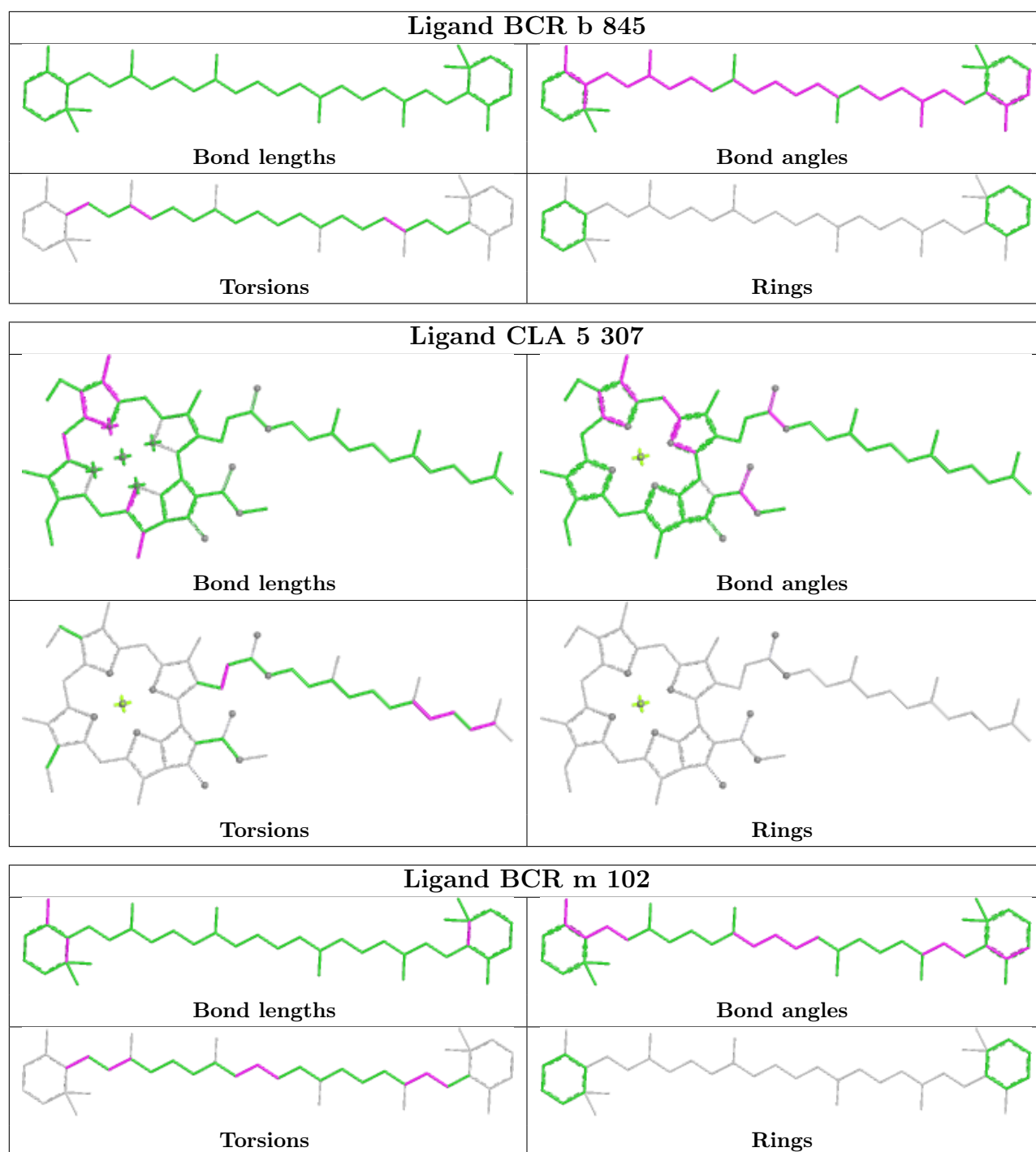


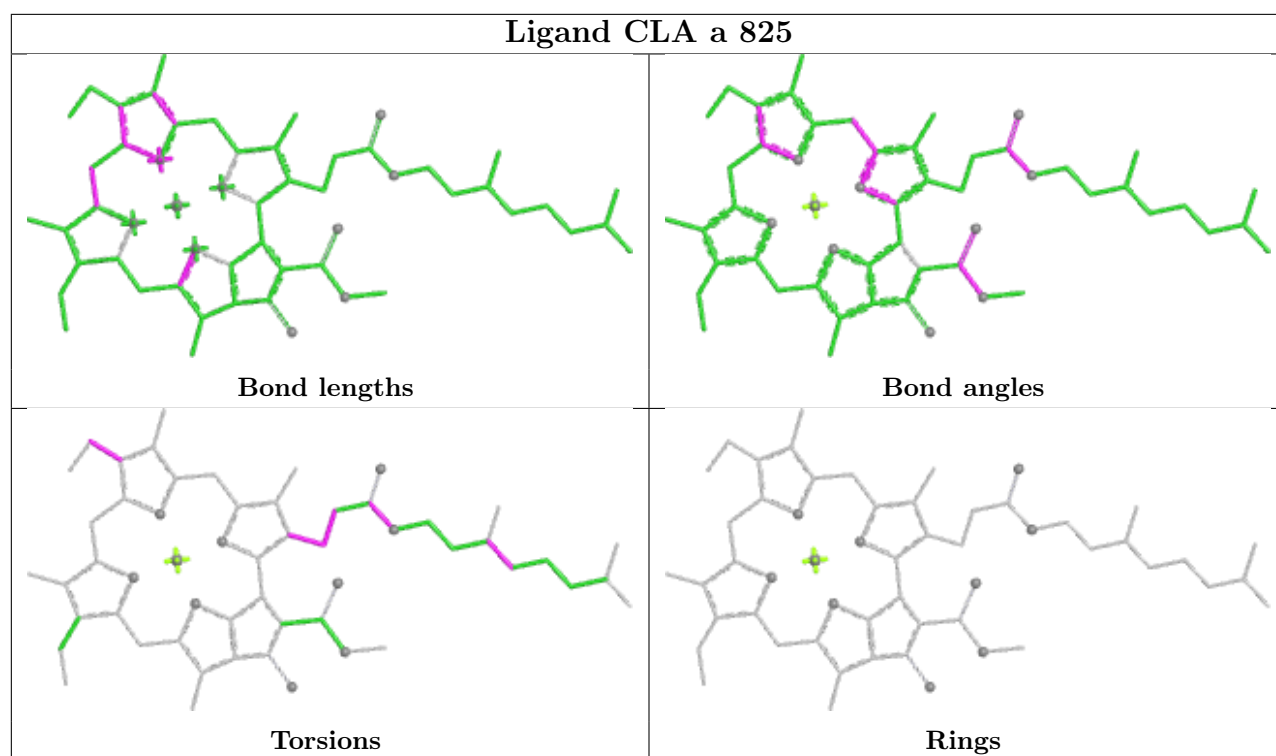
Ligand CLA 2 306



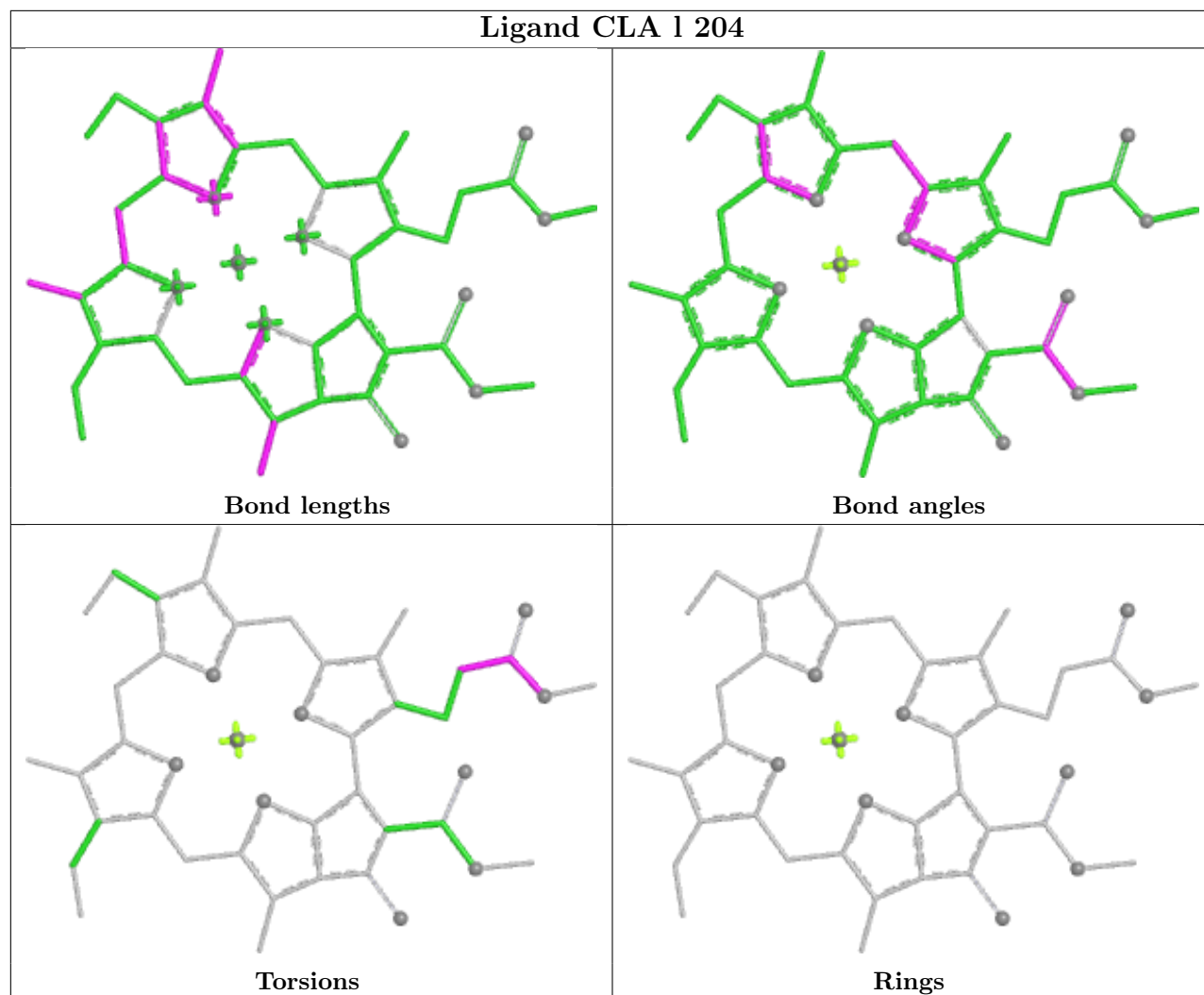




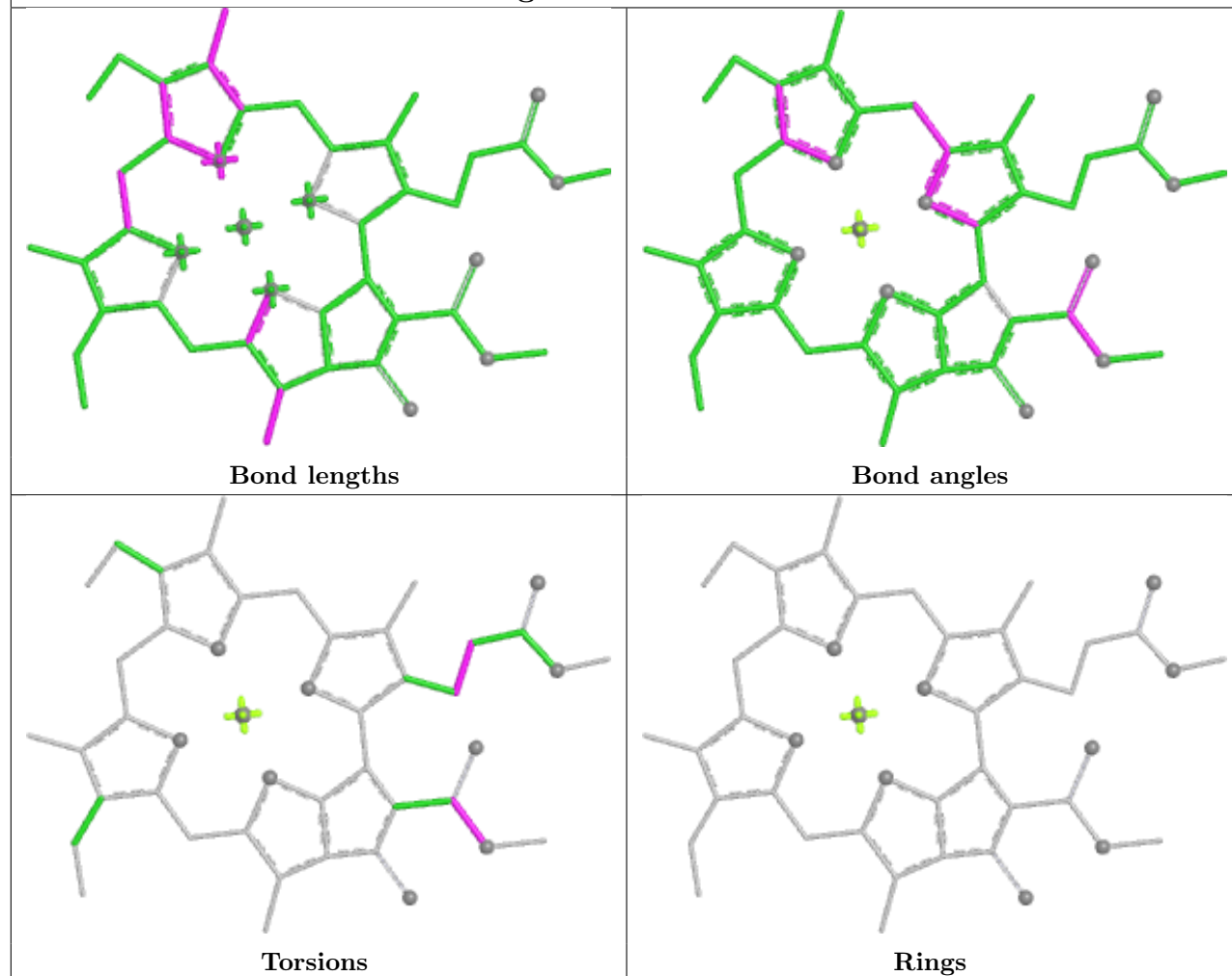




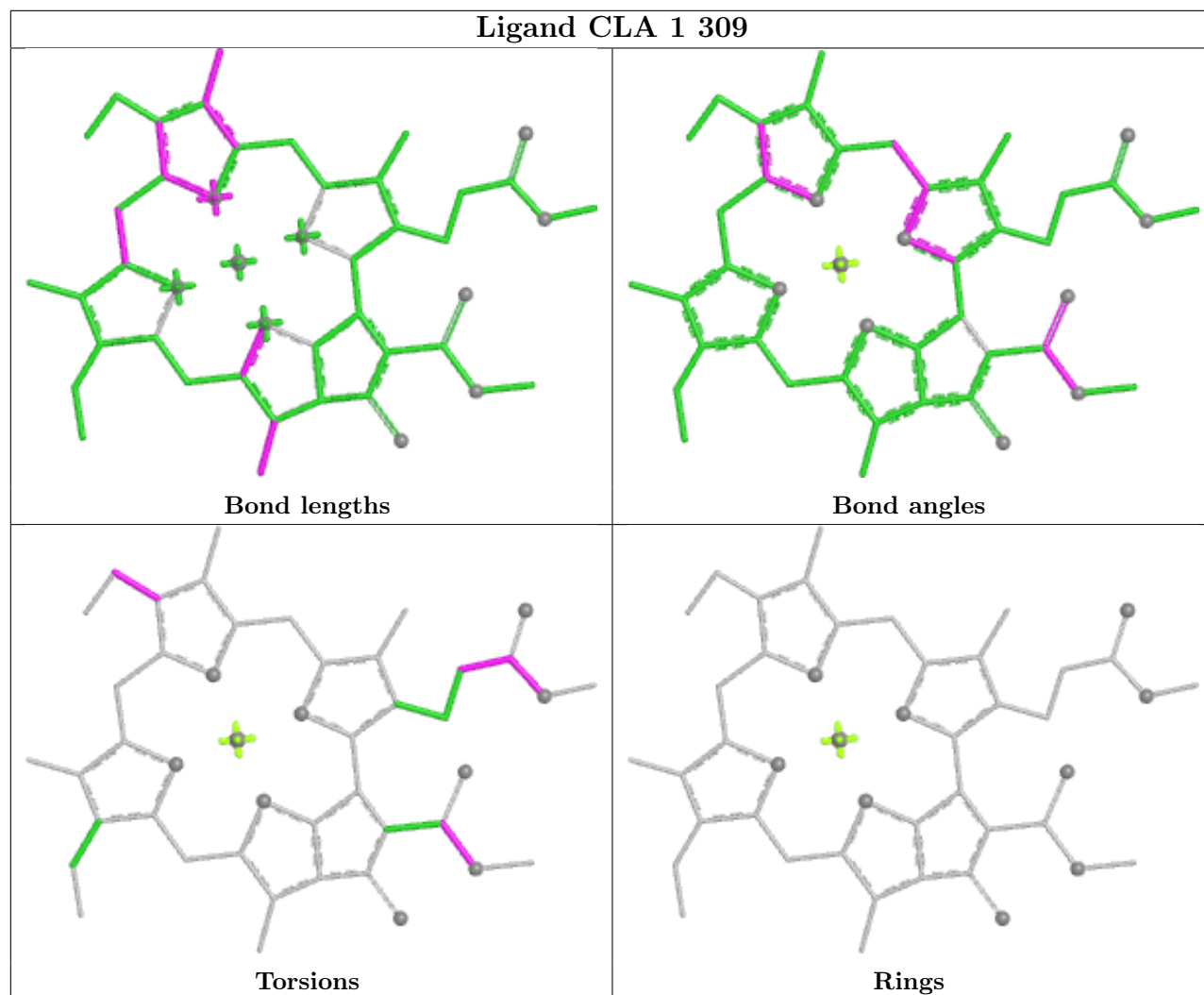
Ligand CLA 1 204



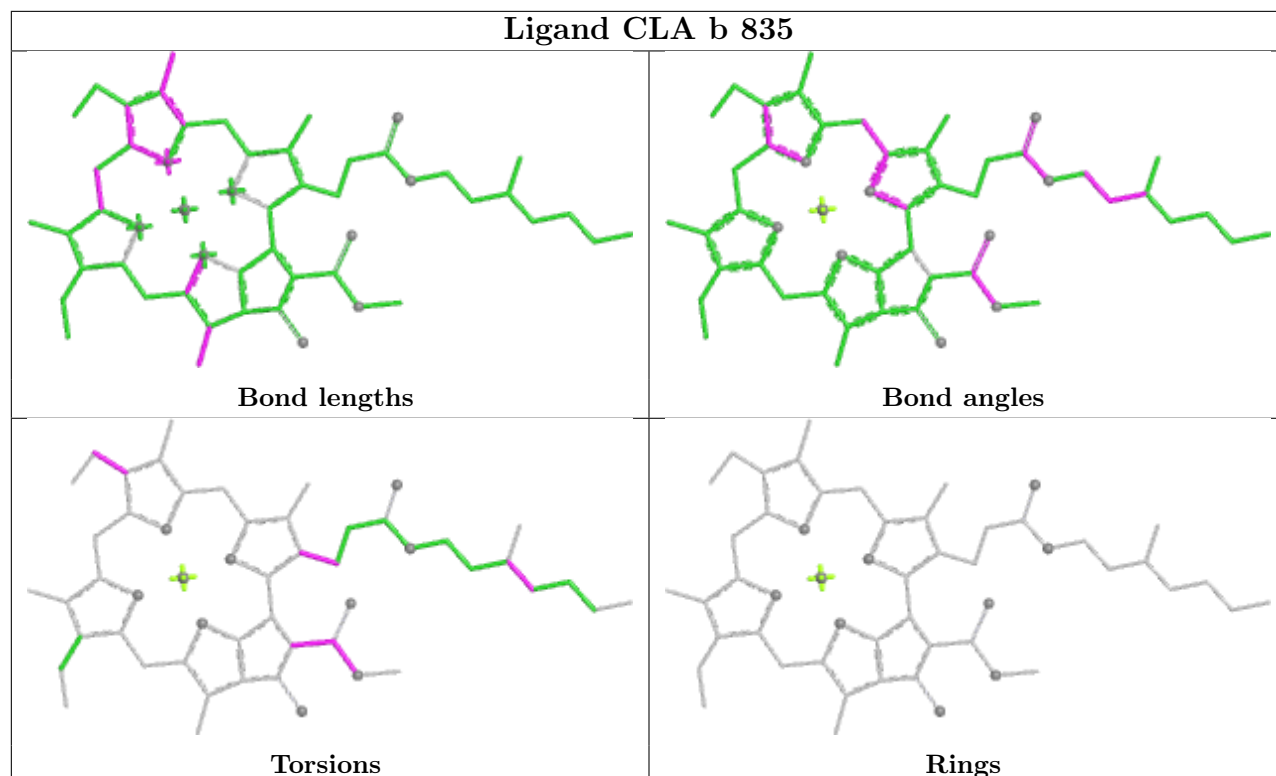
Ligand CLA 2 309



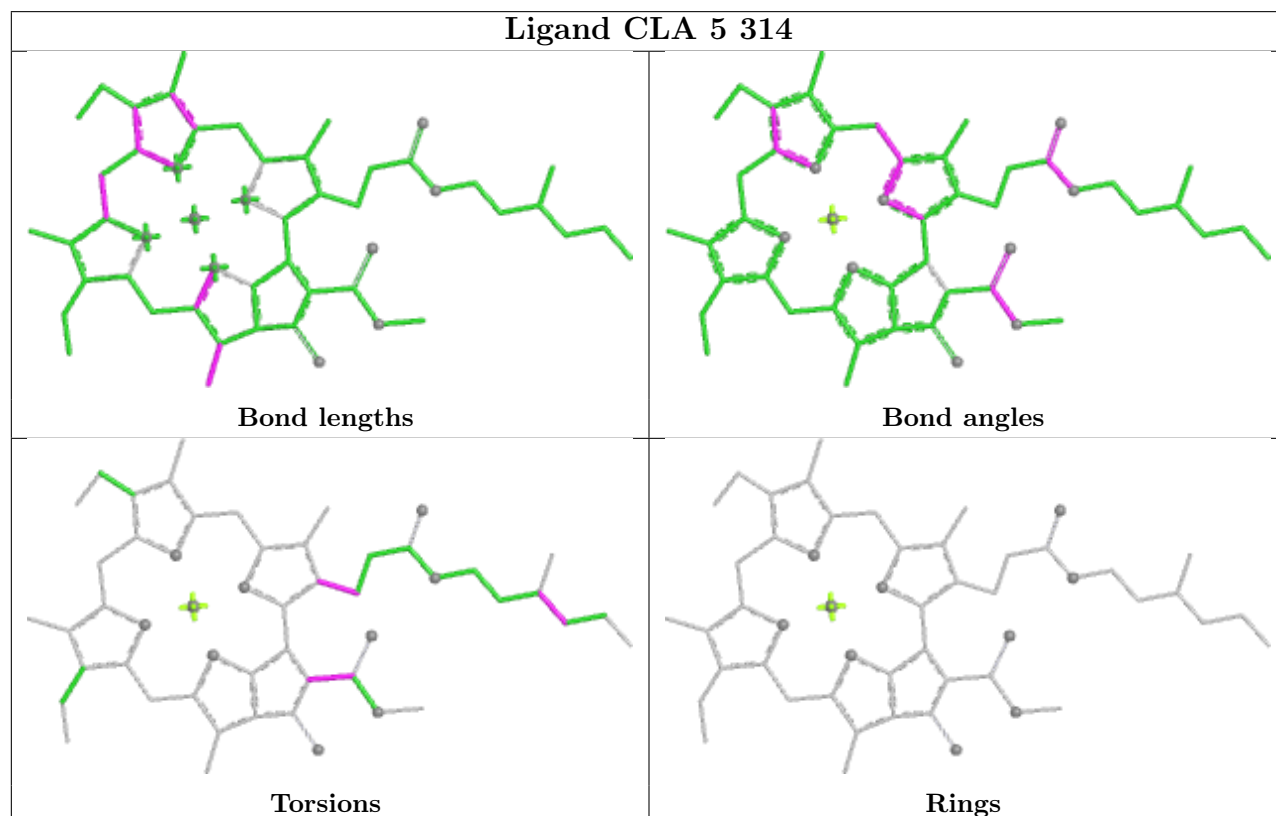
Ligand CLA 1 309

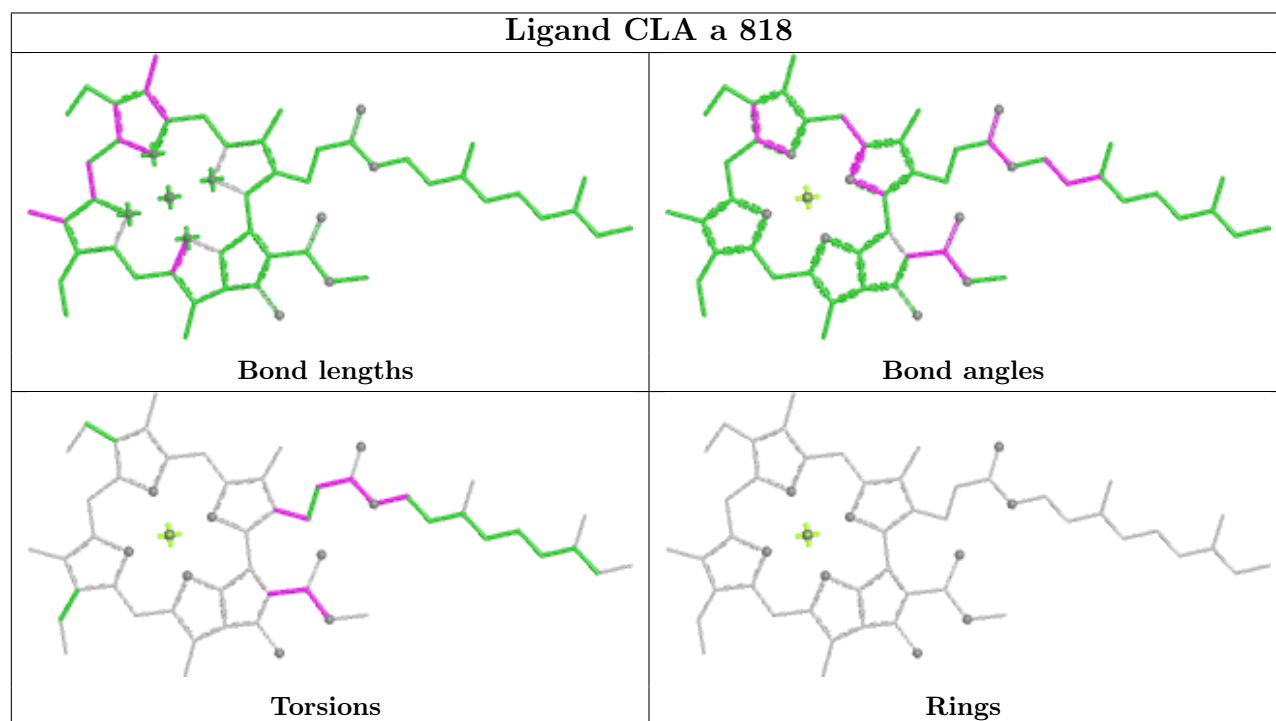
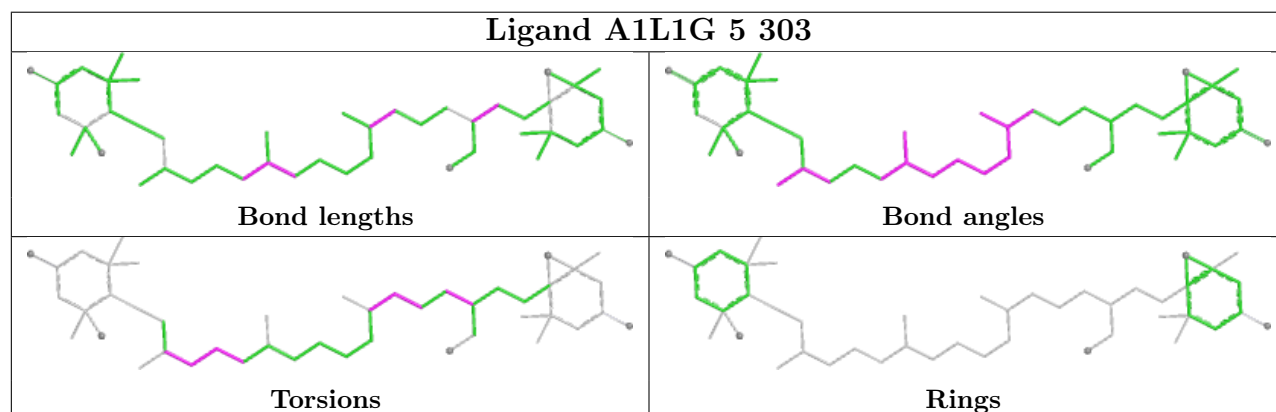
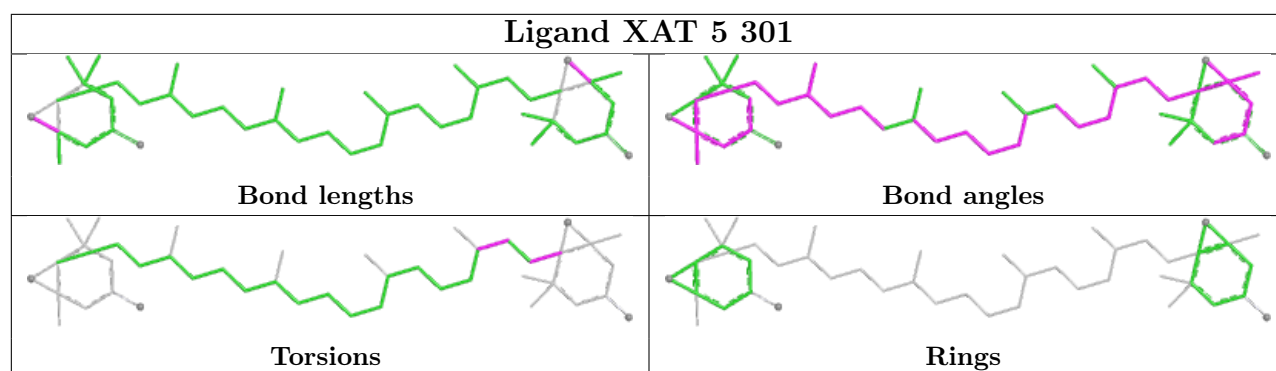


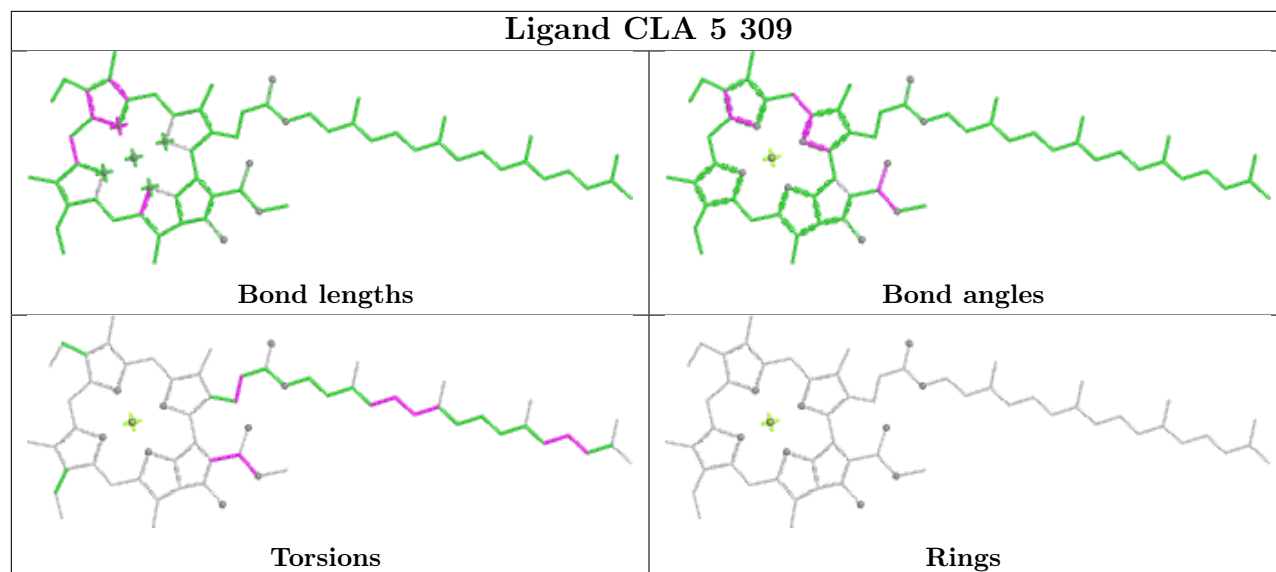
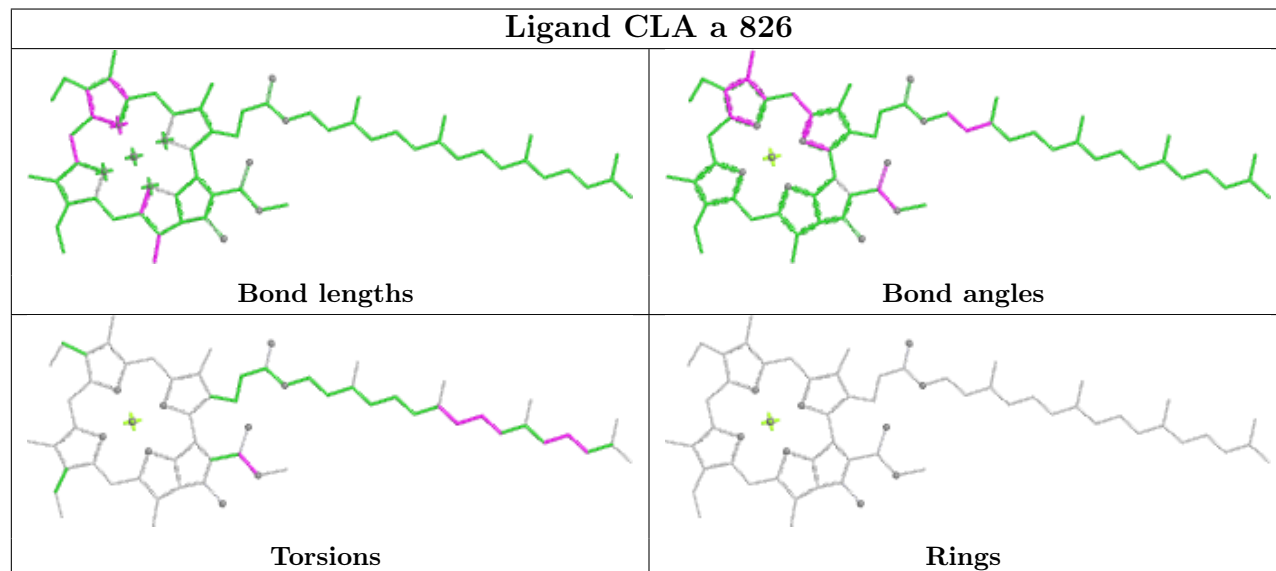
Ligand CLA b 835



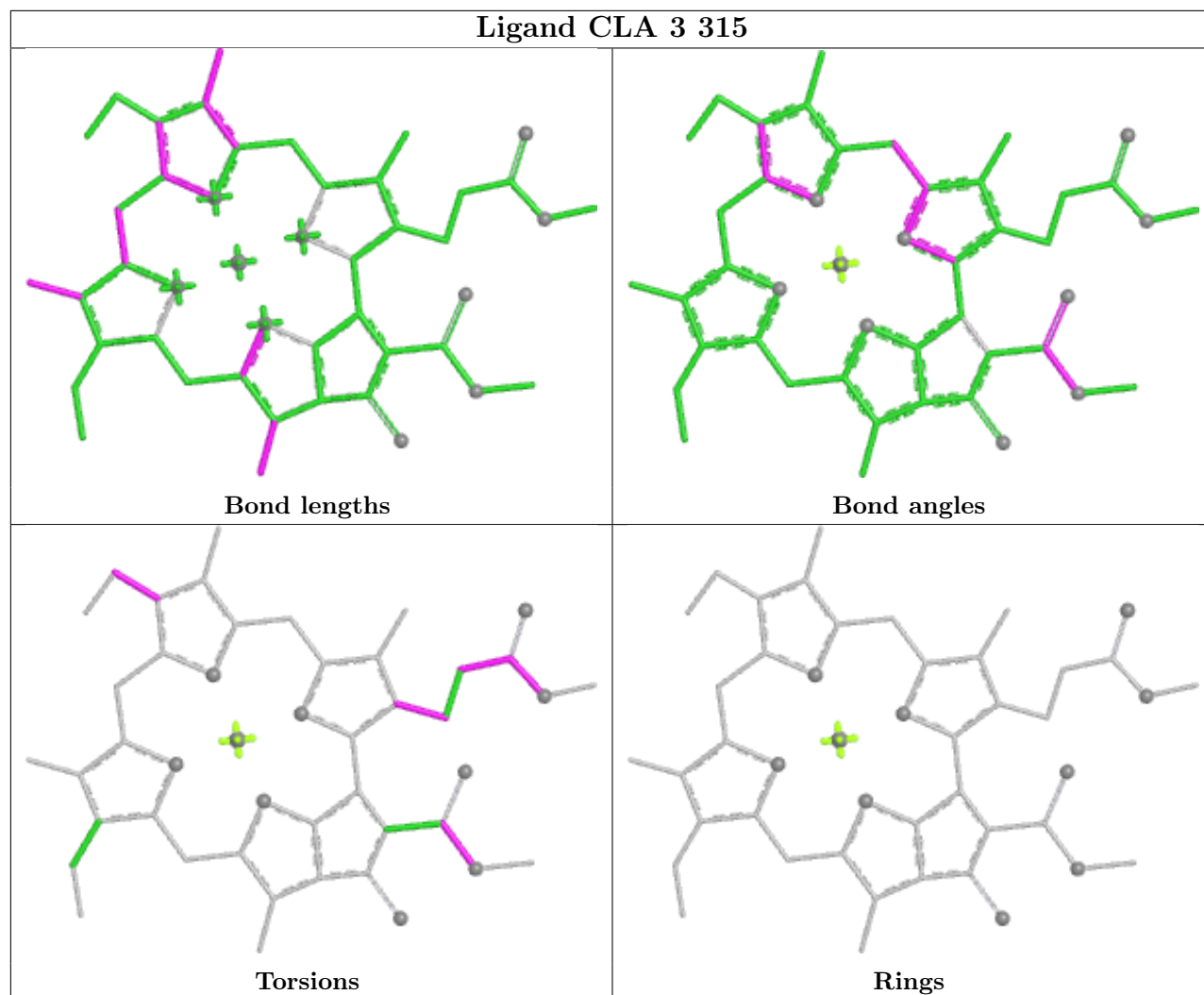
Ligand CLA 5 314



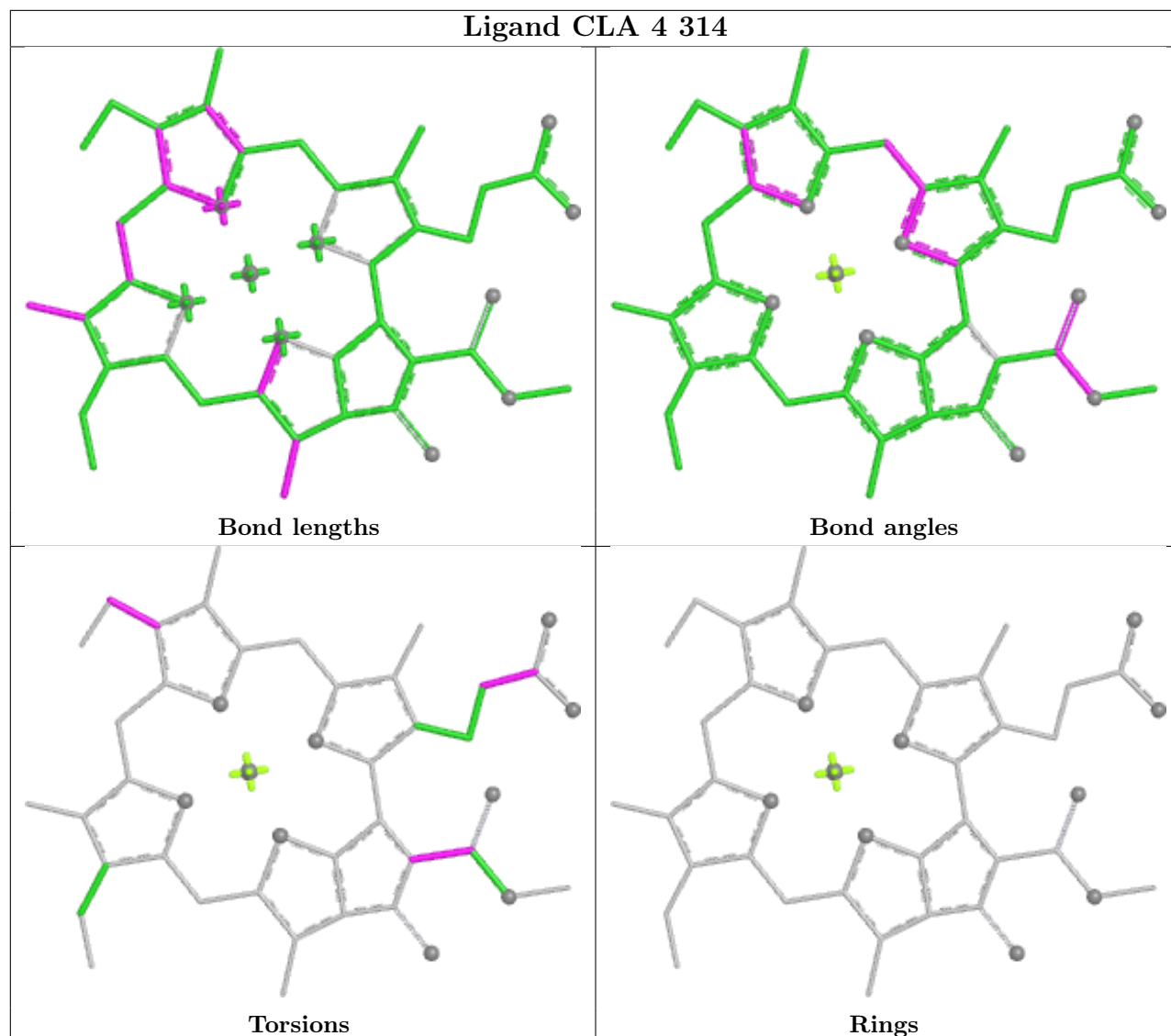


Ligand CLA 5 309**Ligand CLA a 826**

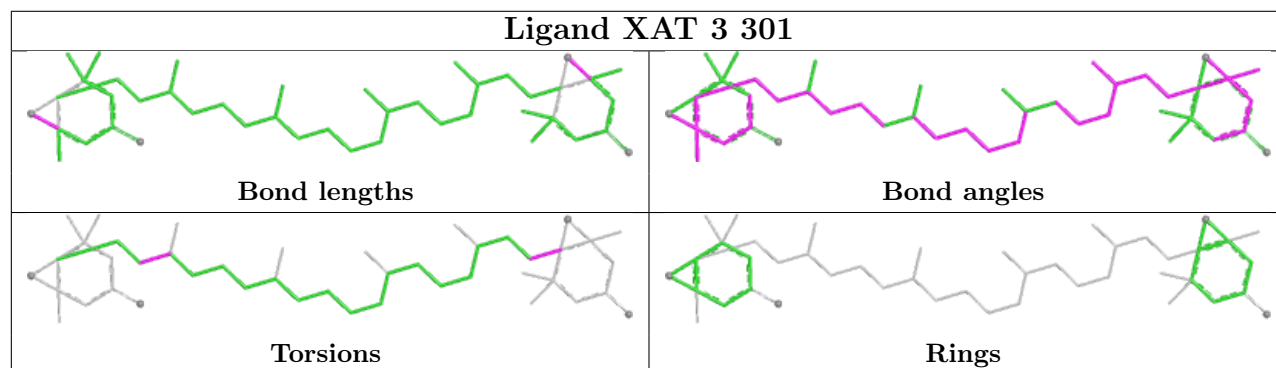
Ligand CLA 3 315

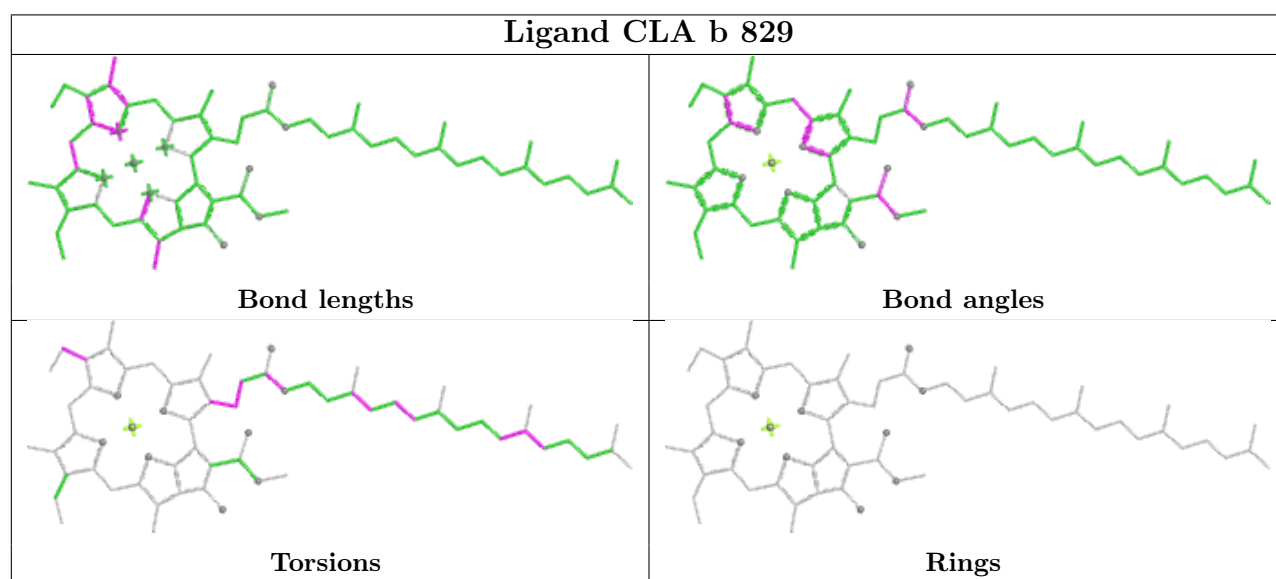
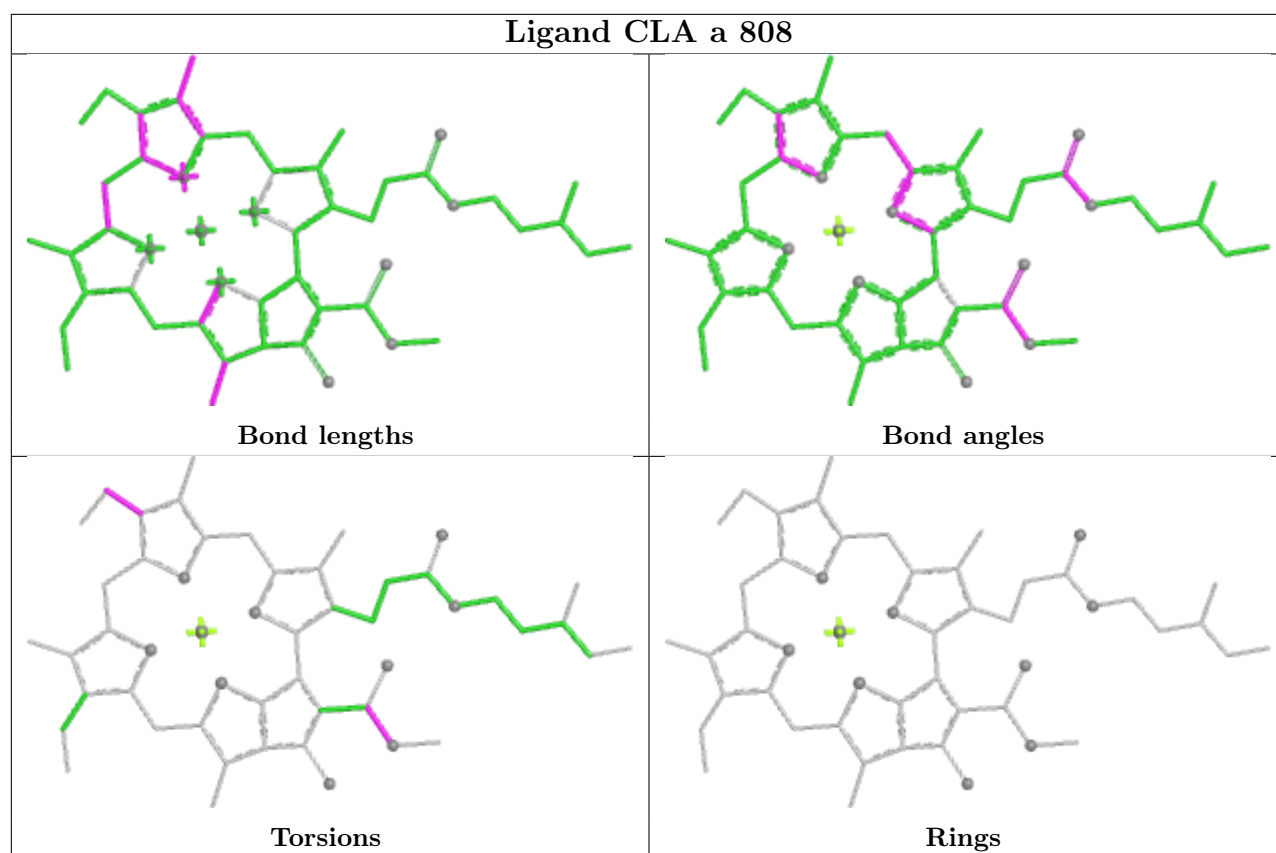


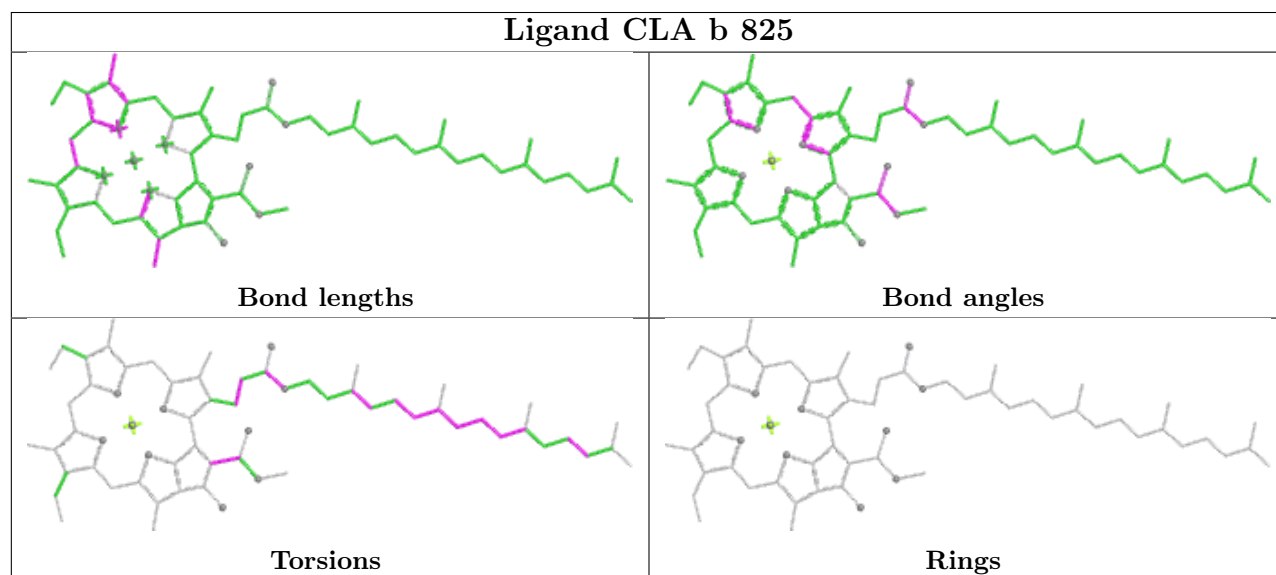
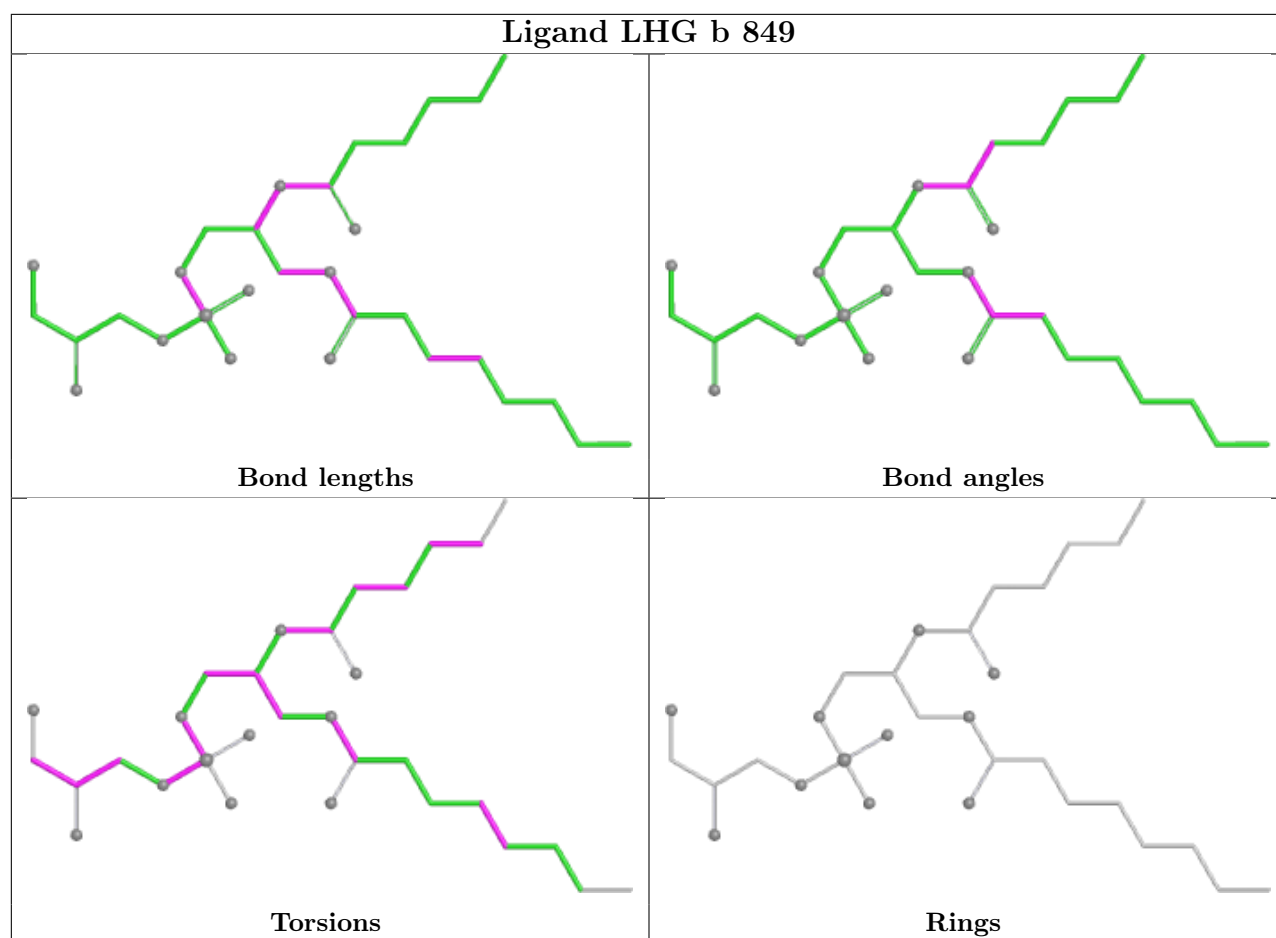
Ligand CLA 4 314

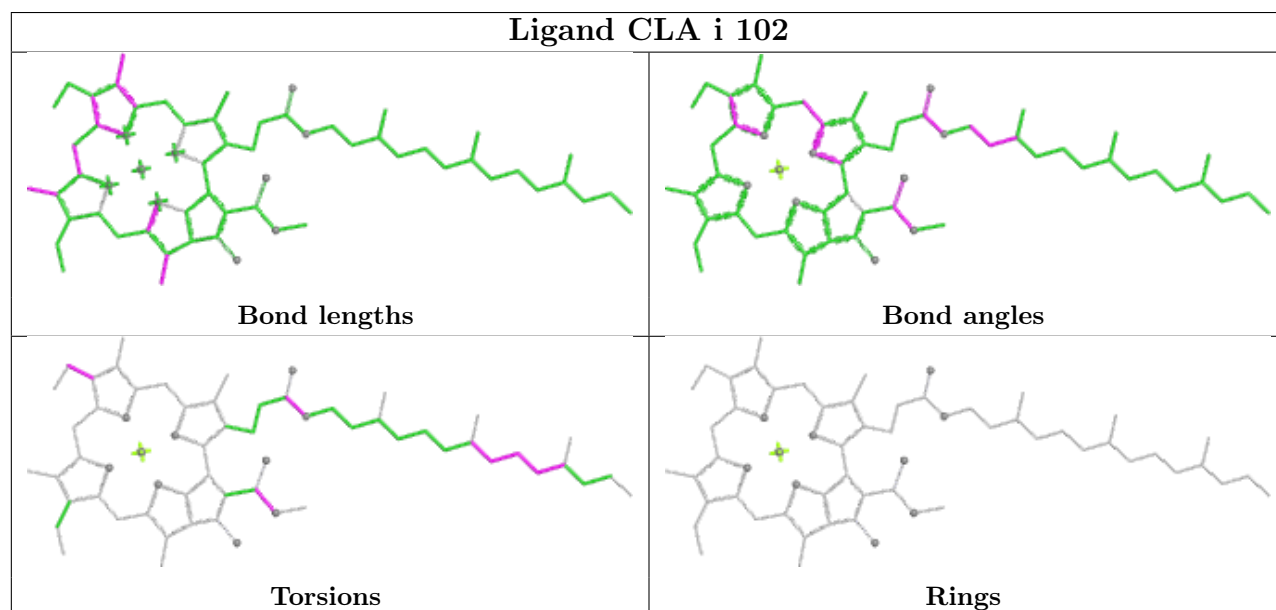
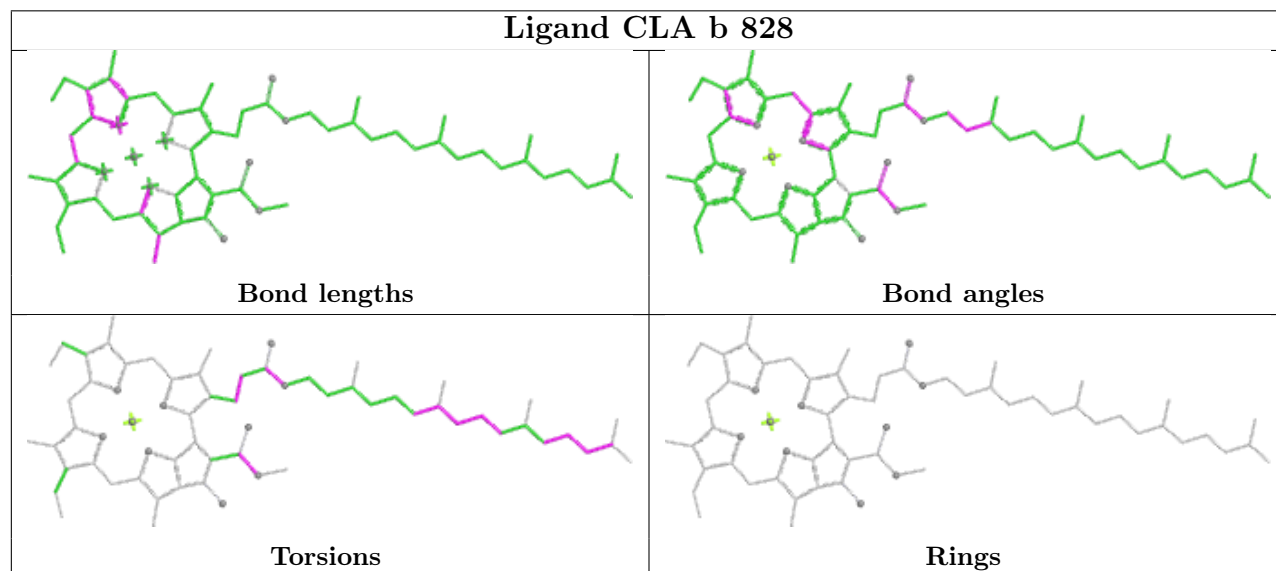
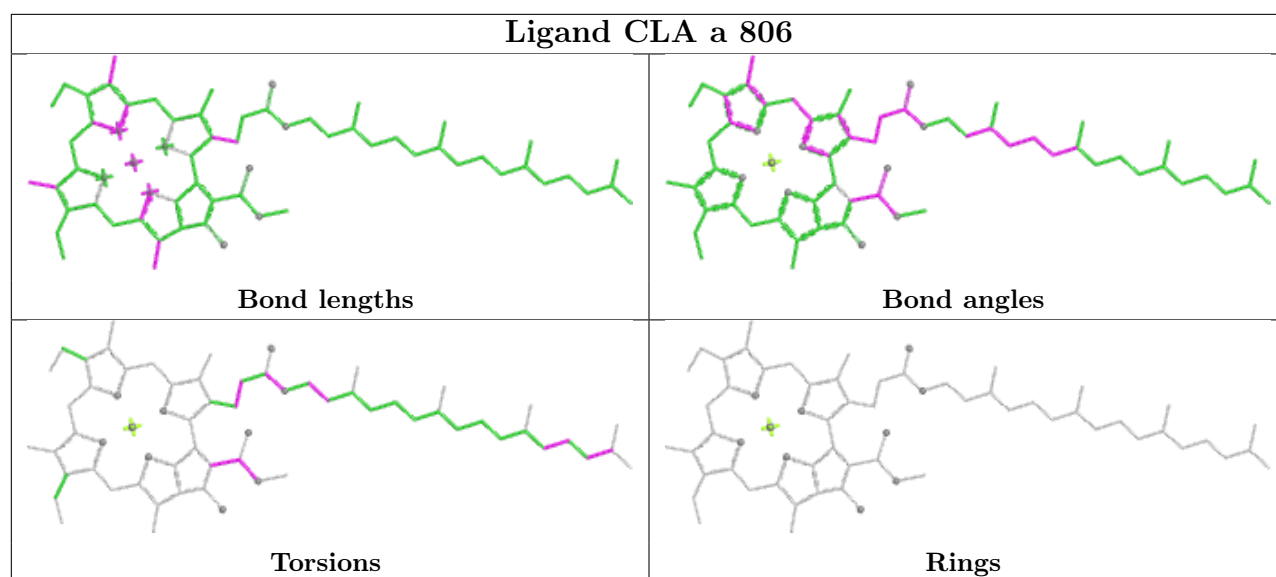


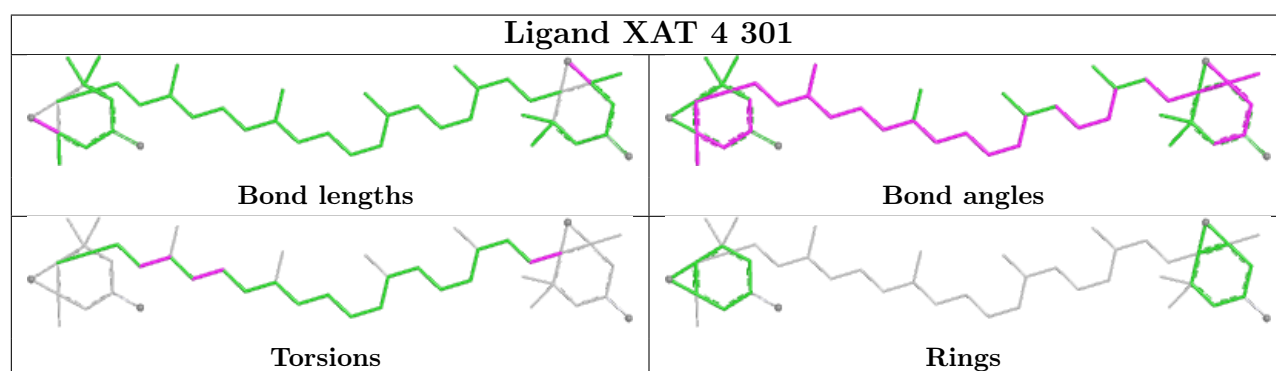
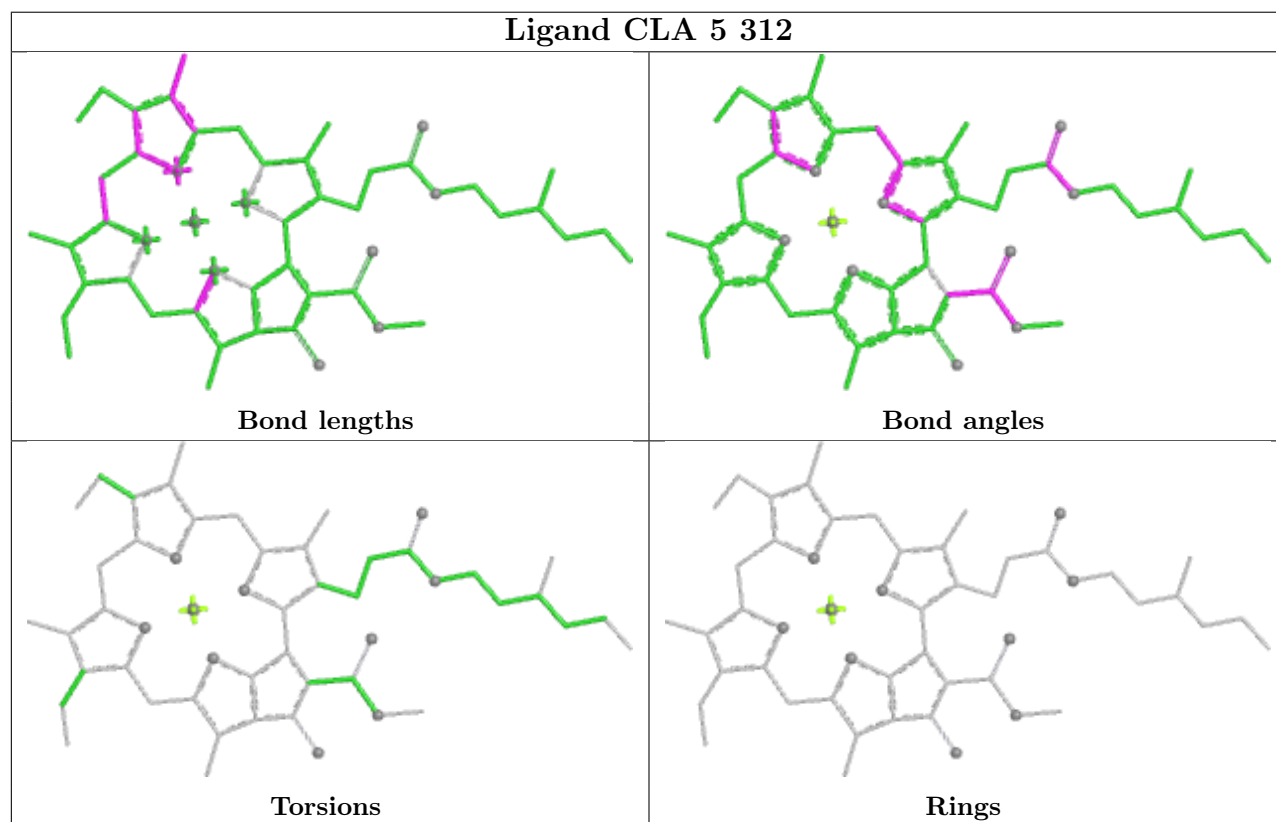
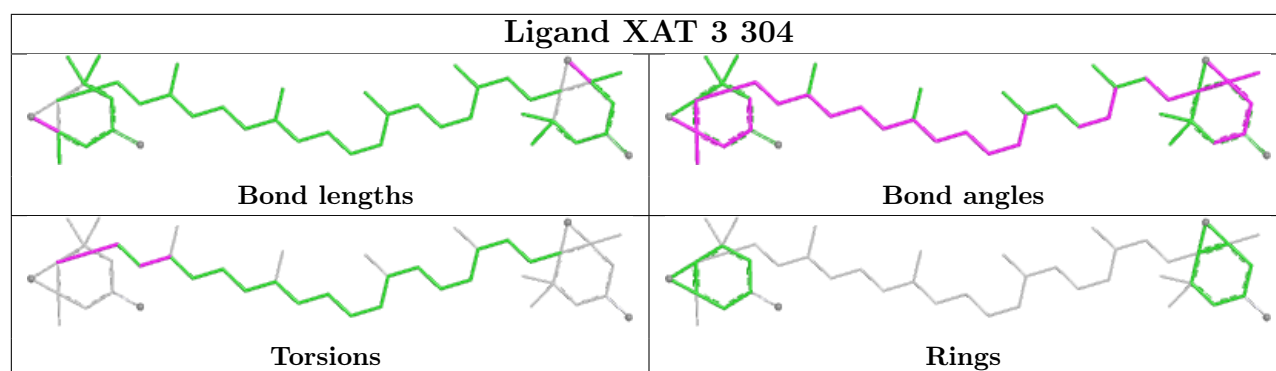
Ligand XAT 3 301



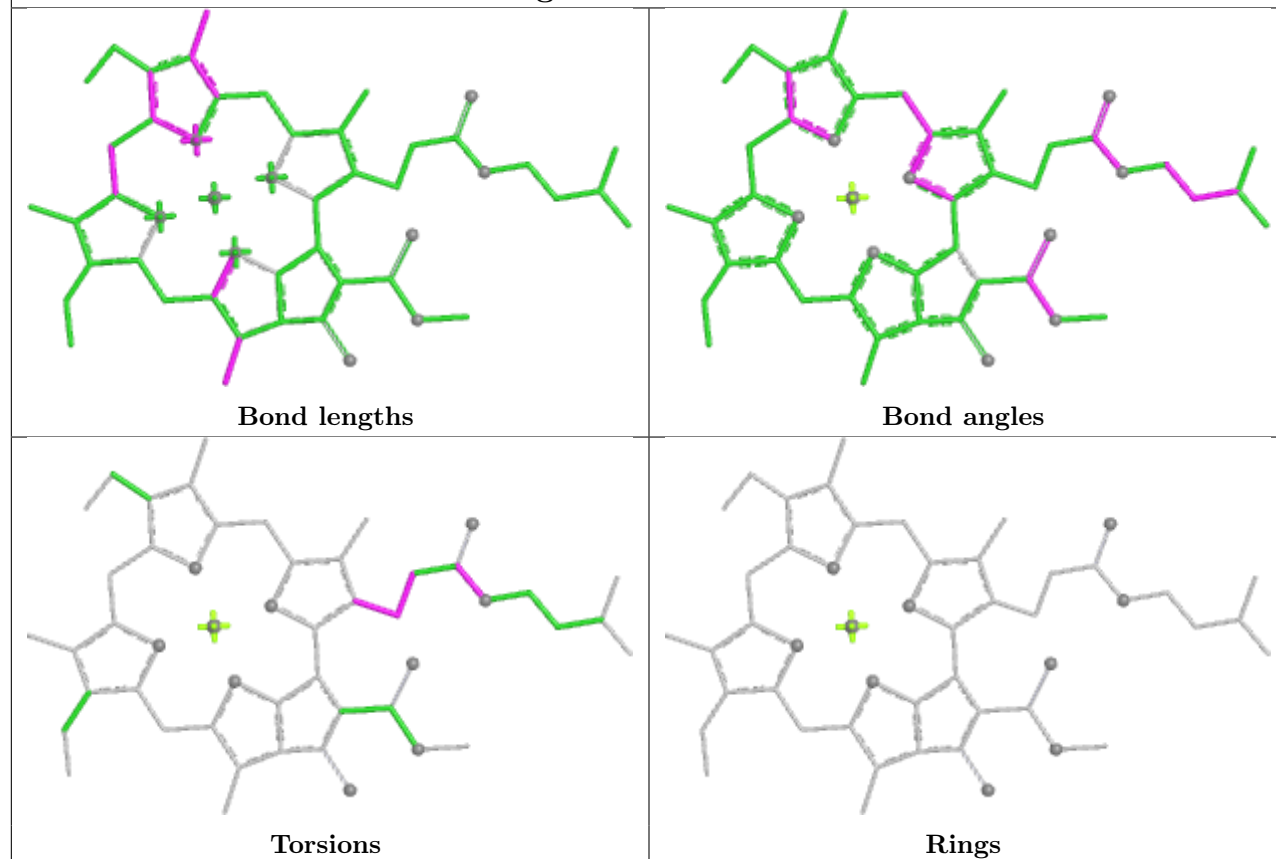




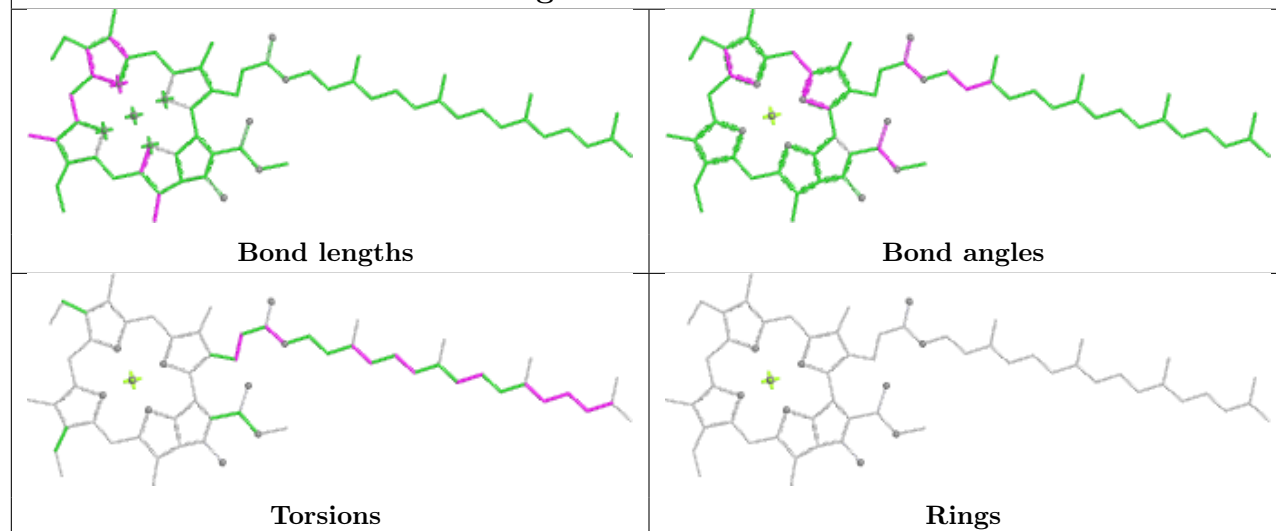


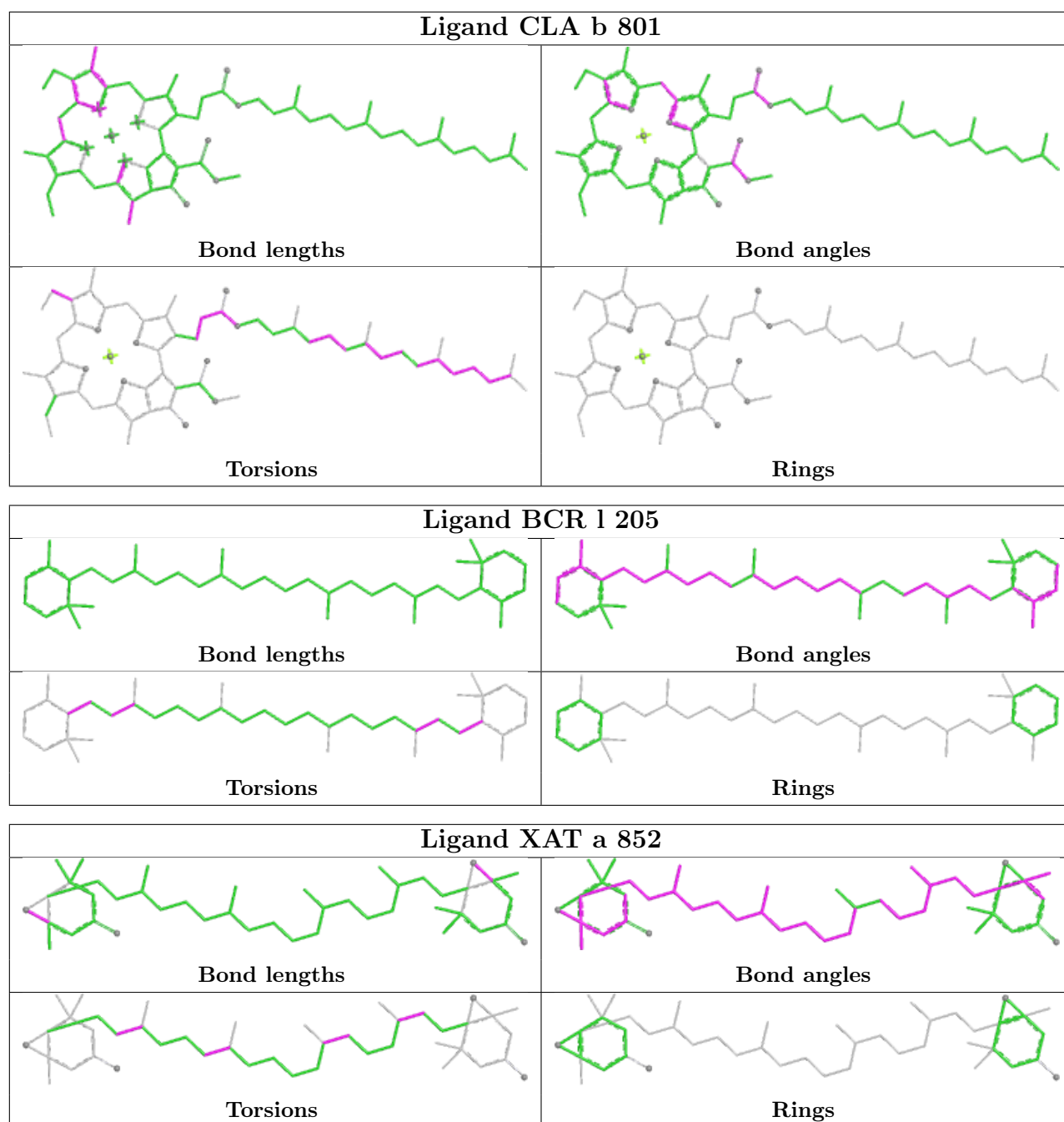


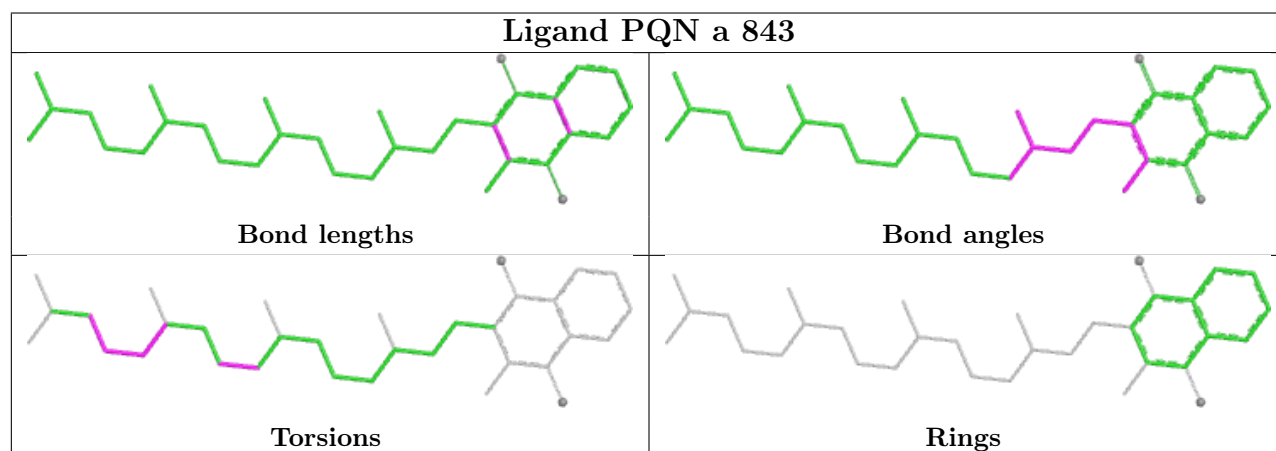
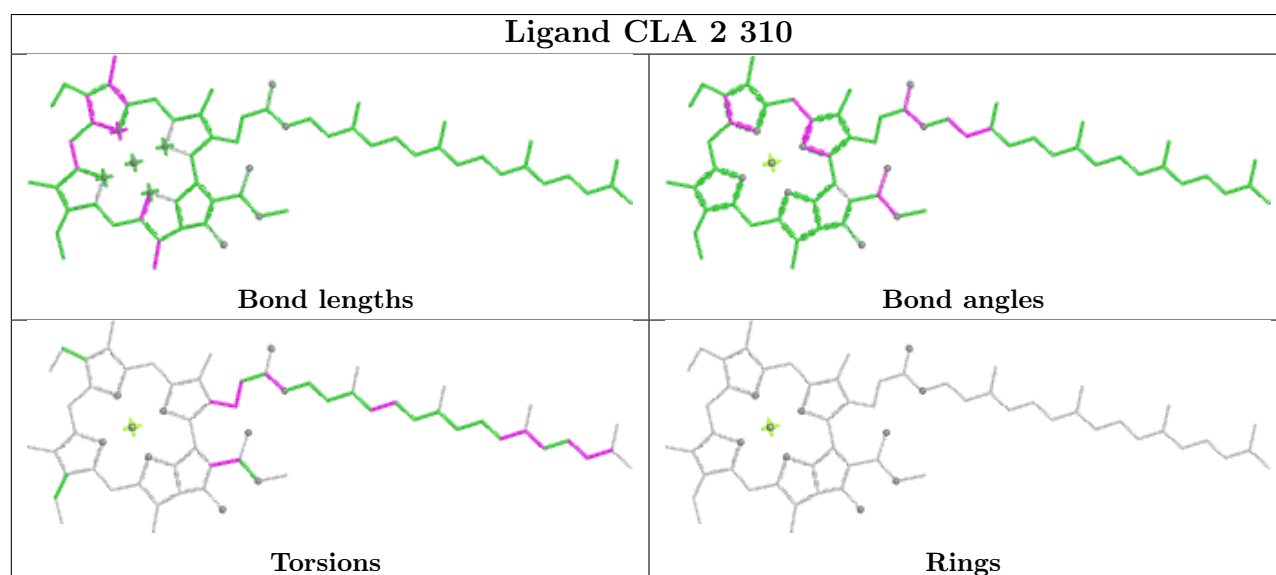
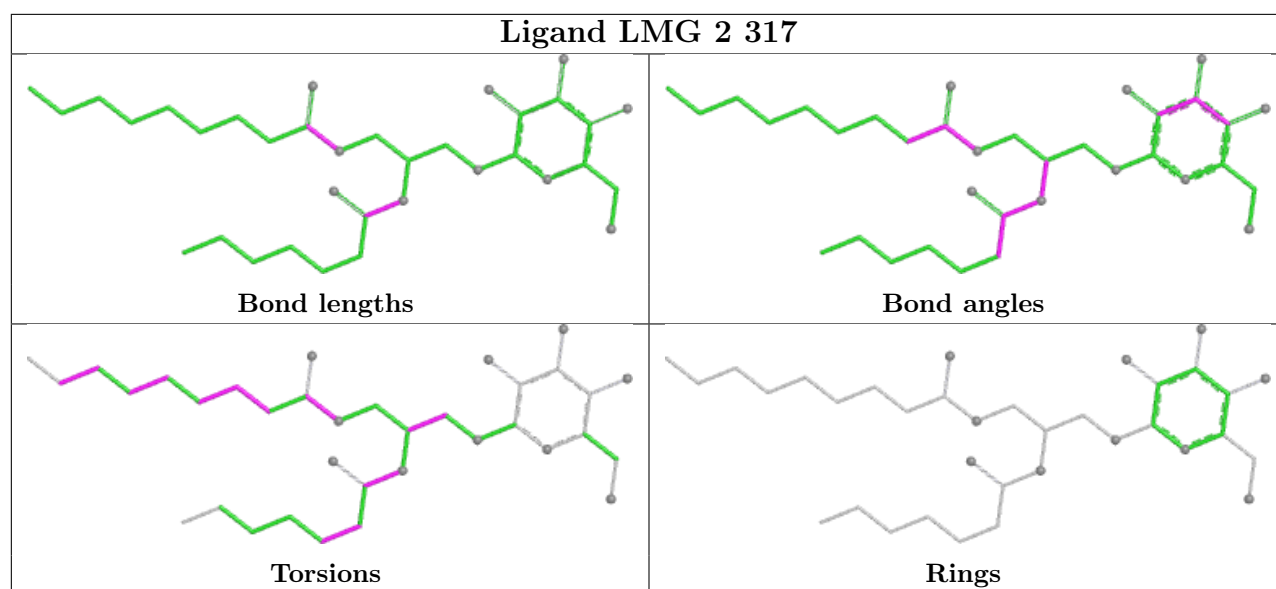
Ligand CLA 3 311

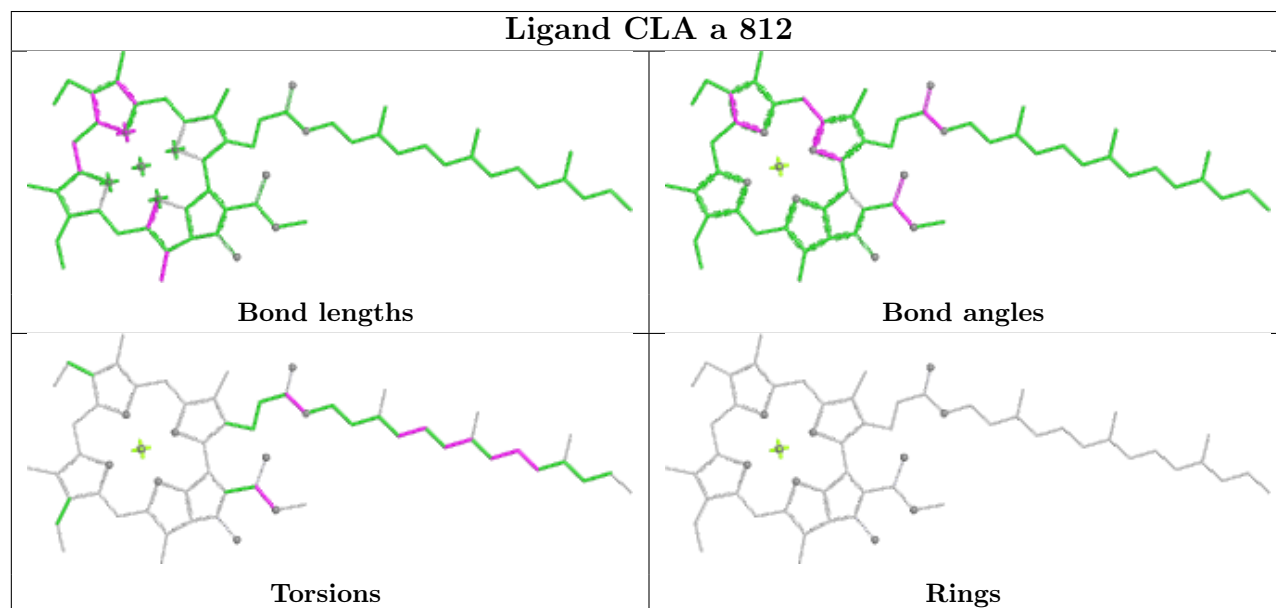
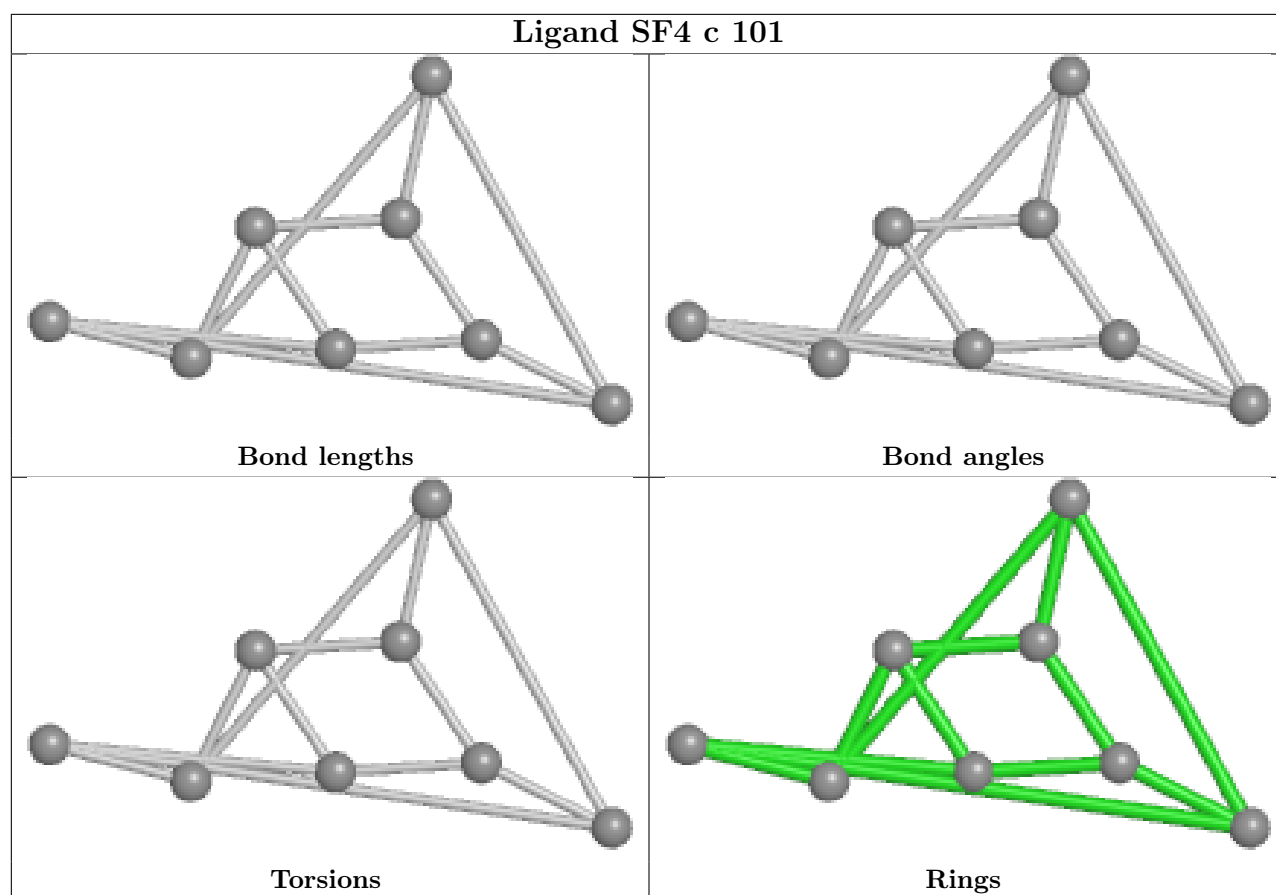


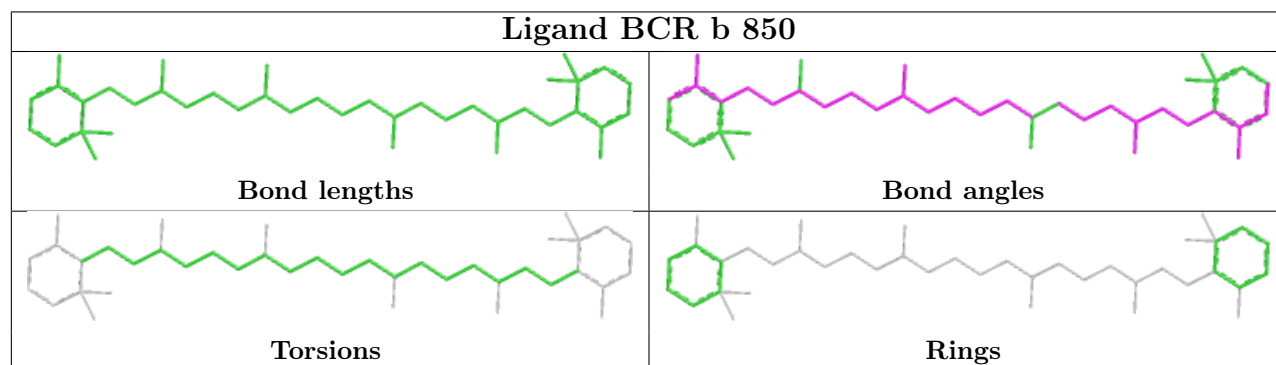
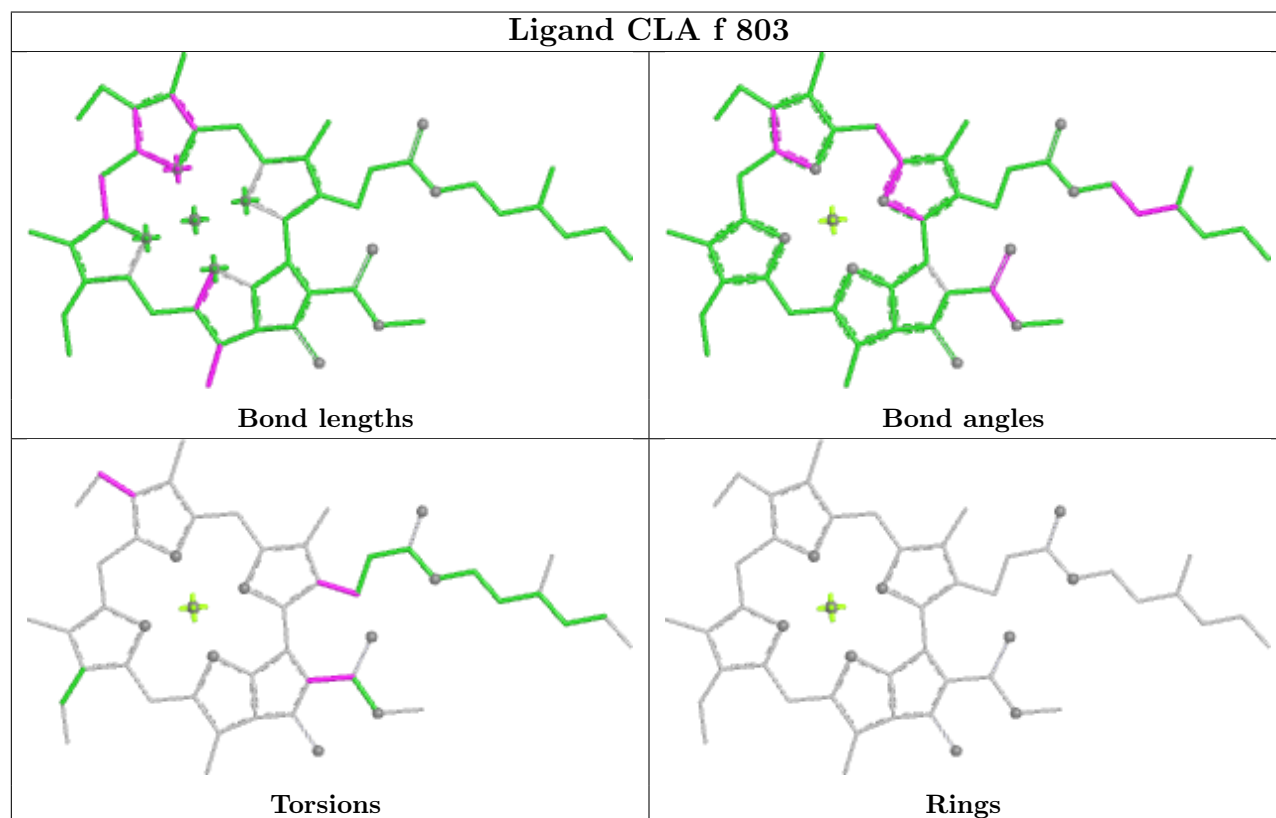
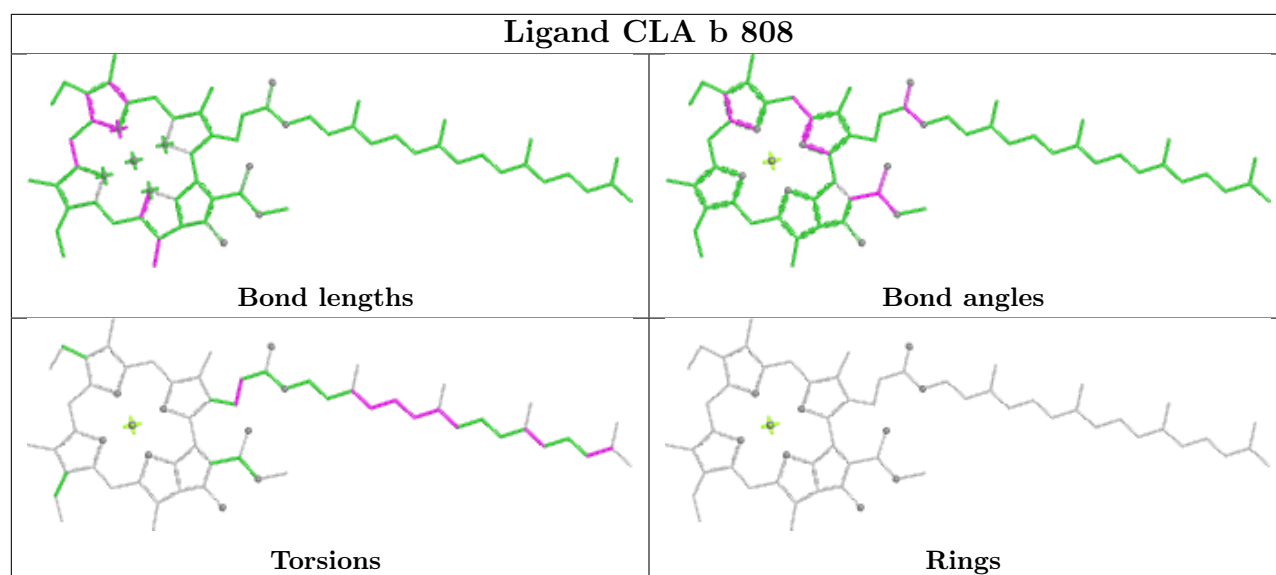
Ligand CLA a 830



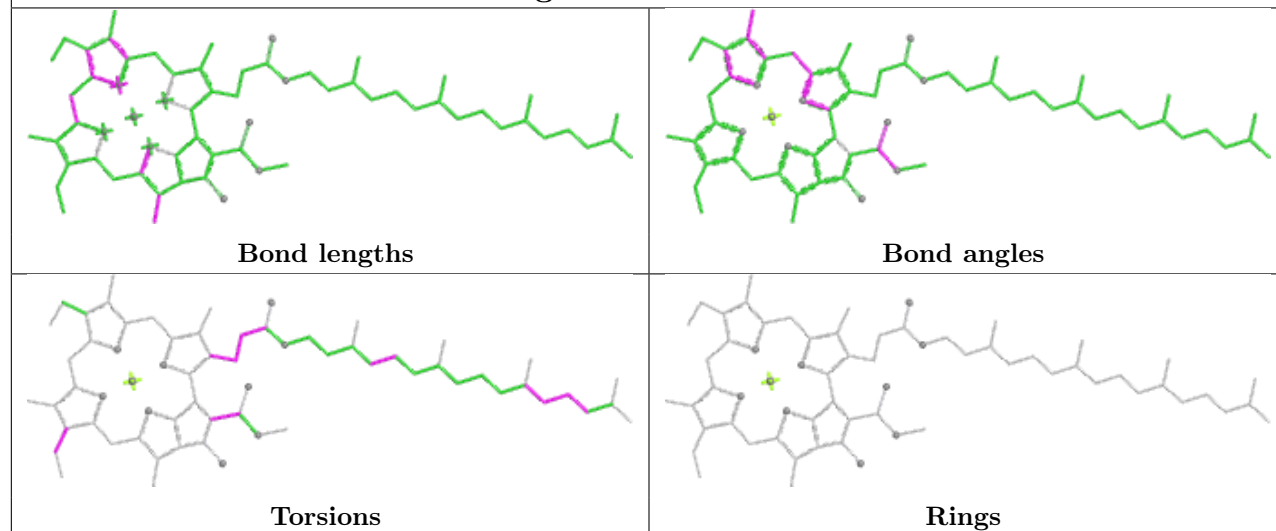




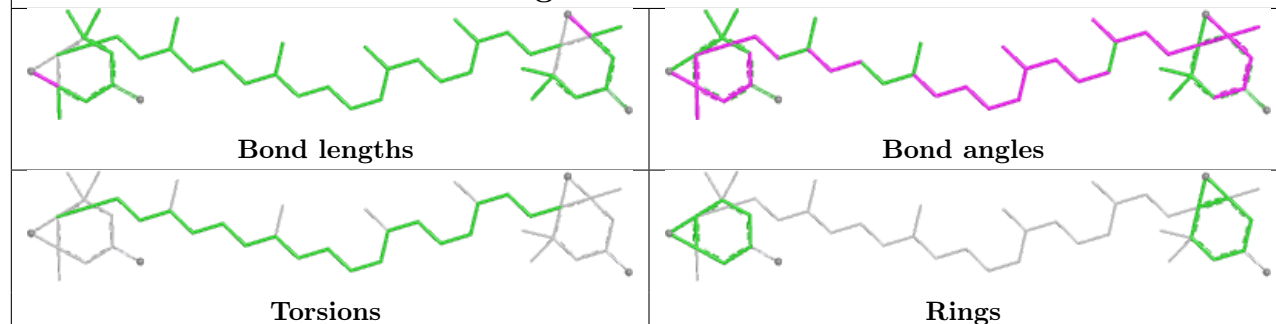




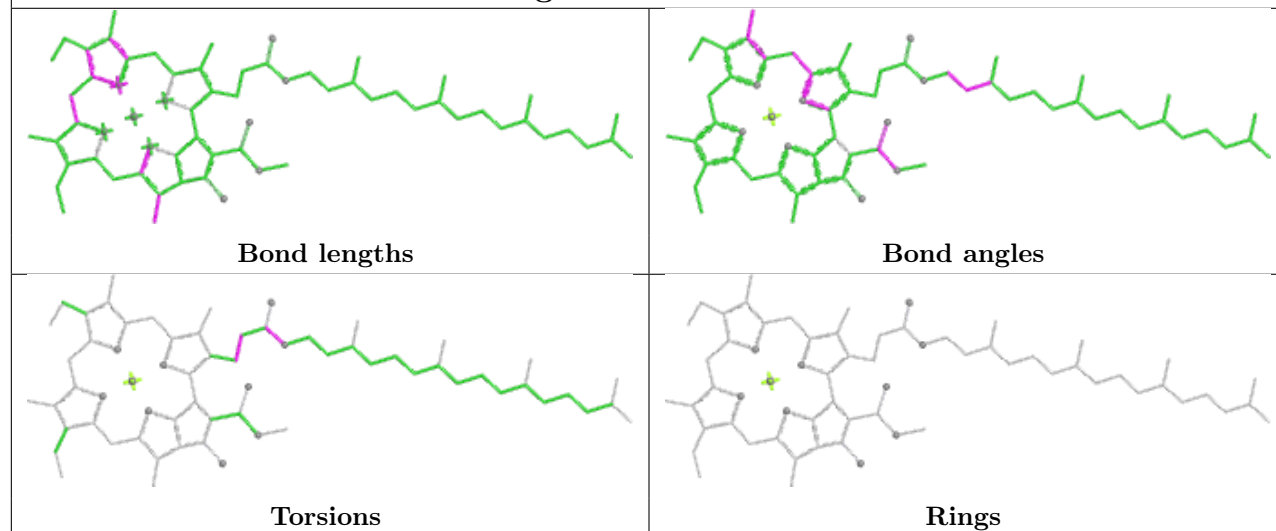
Ligand CLA b 833

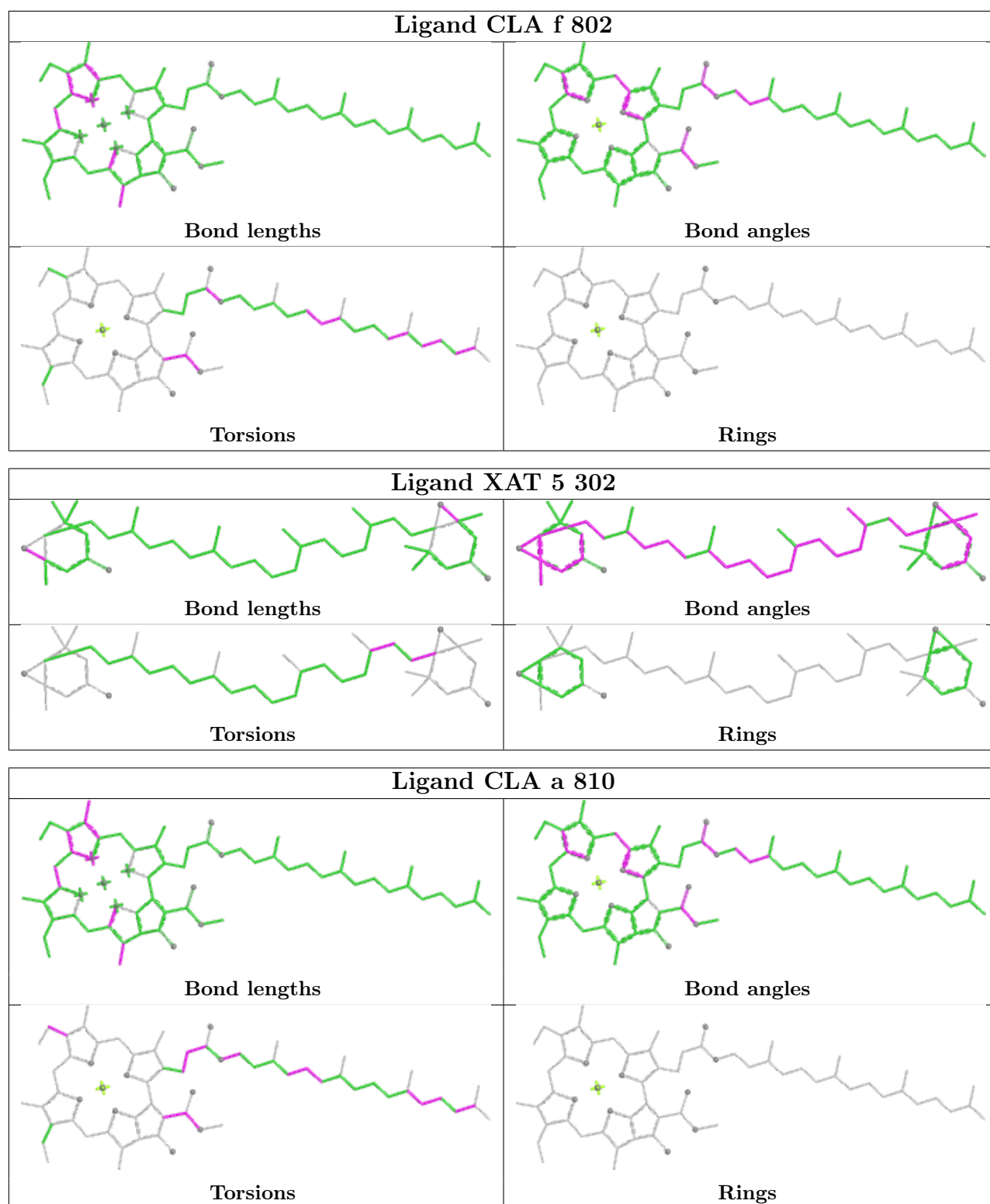


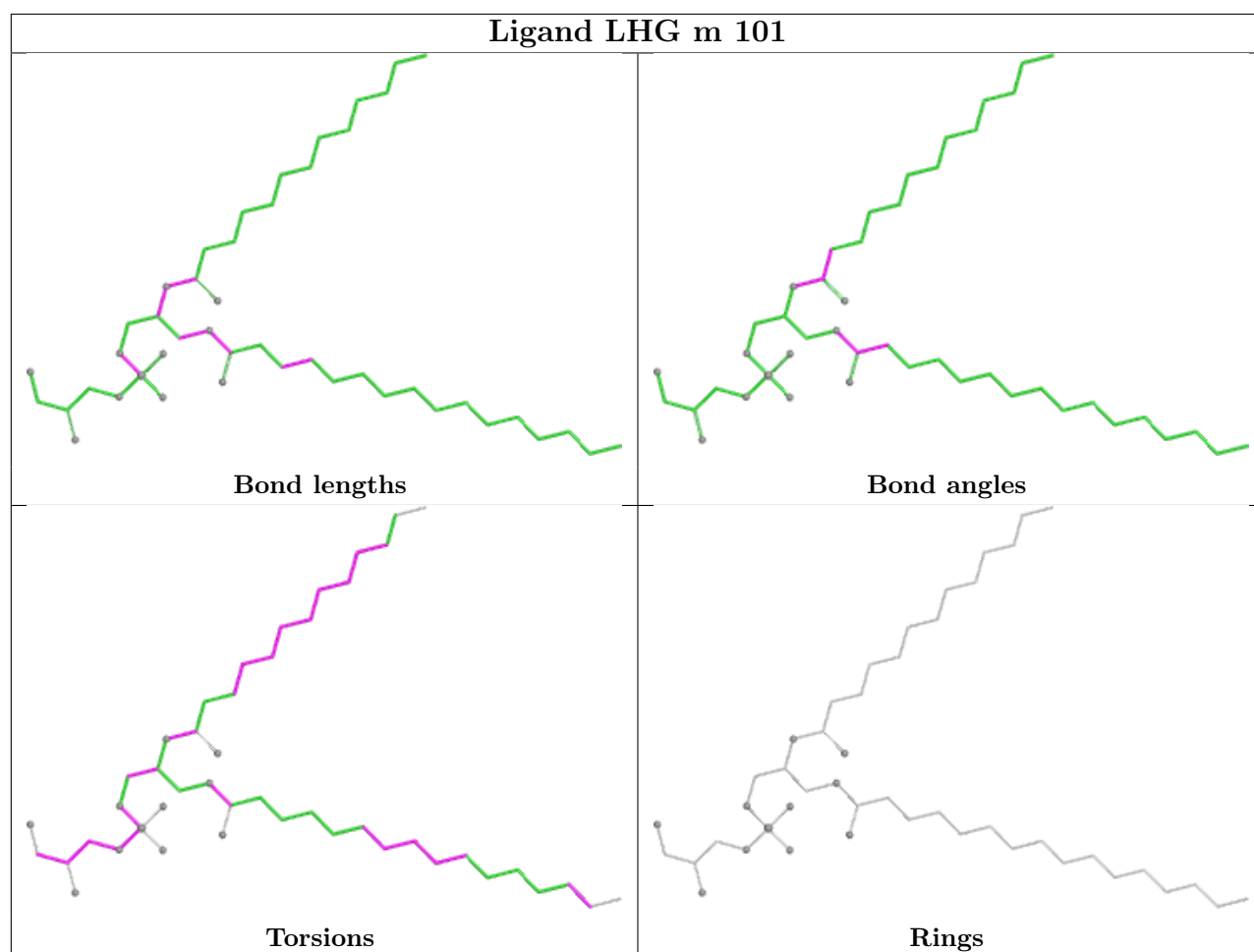
Ligand XAT 3 305



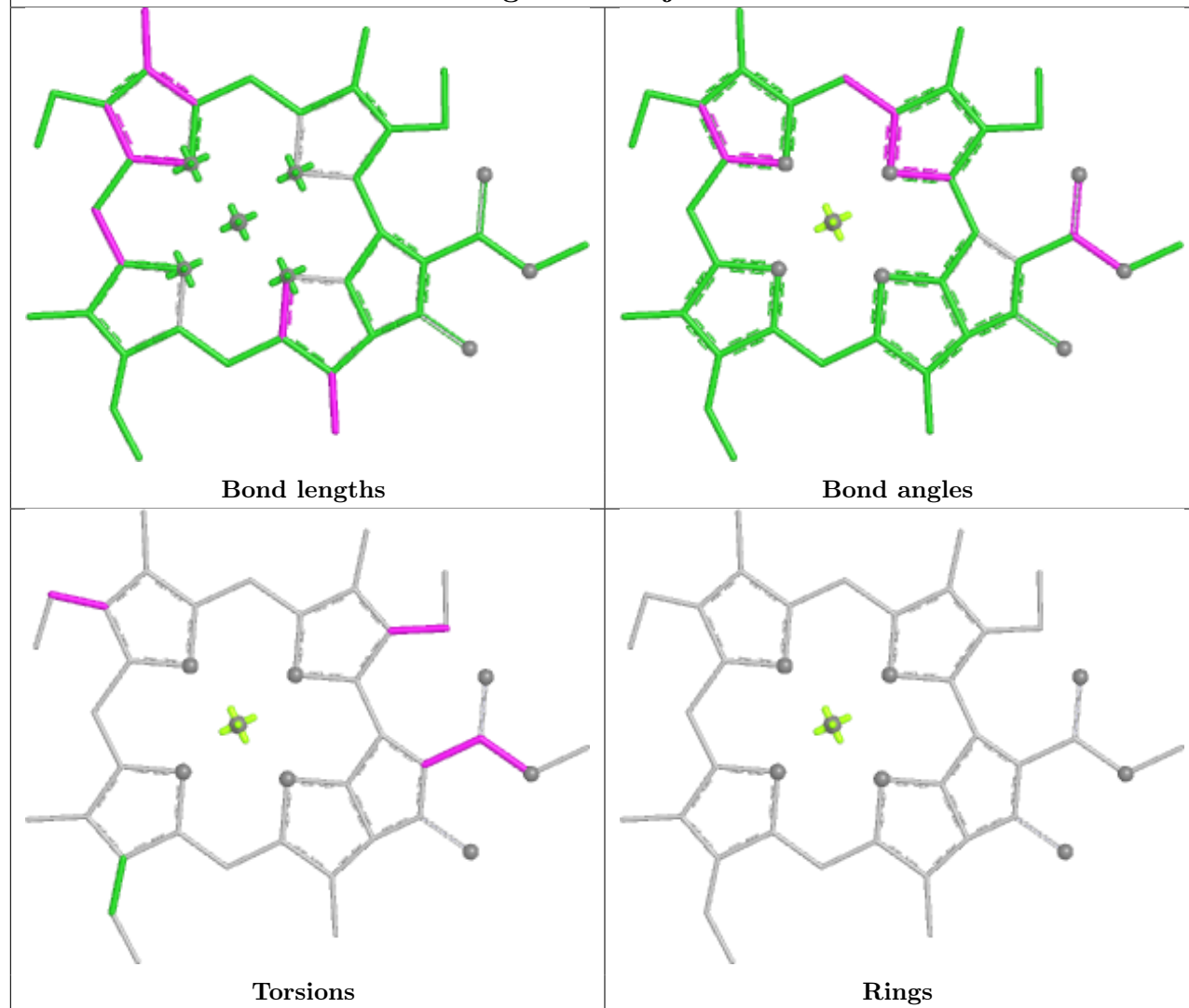
Ligand CLA b 827



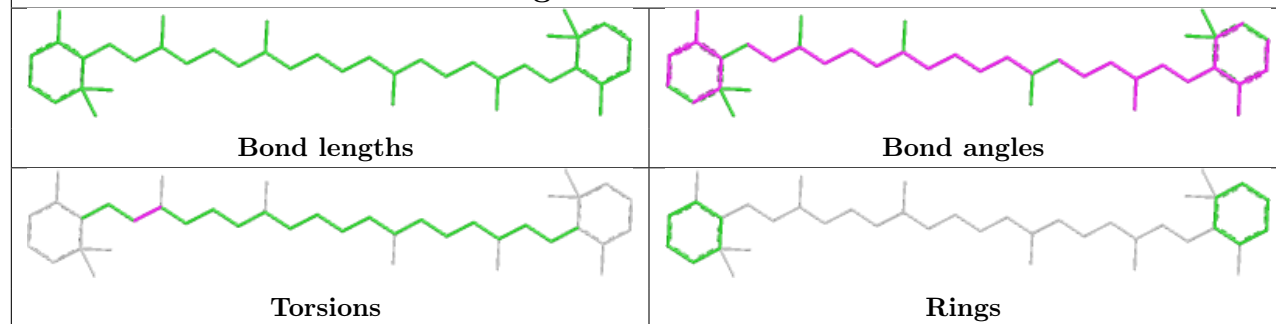


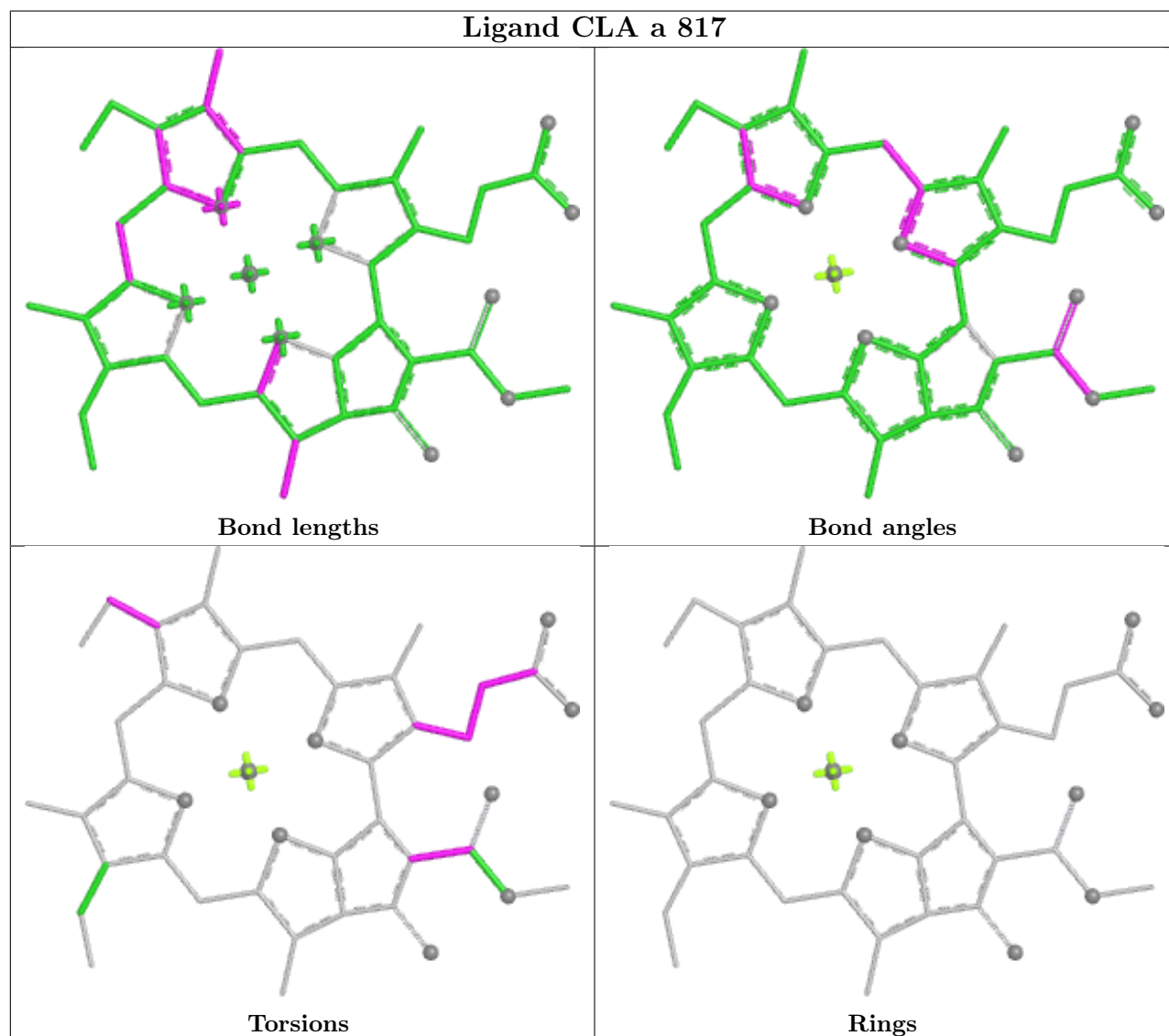
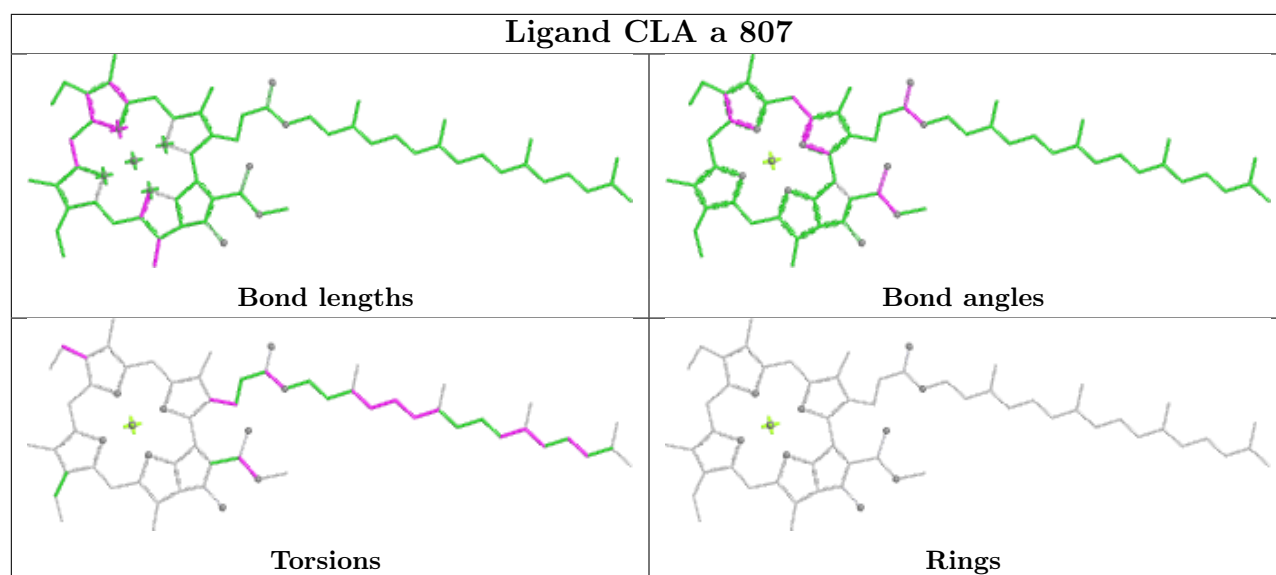


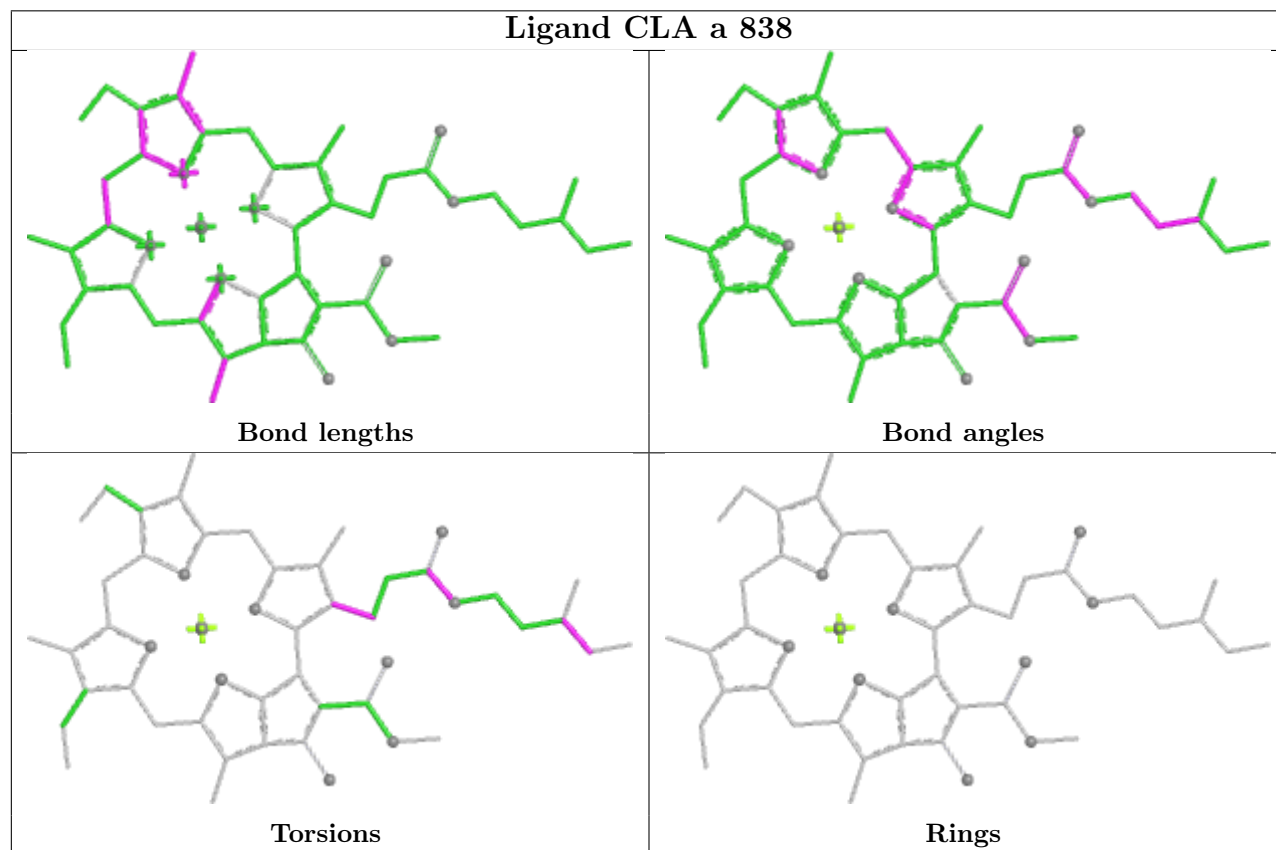
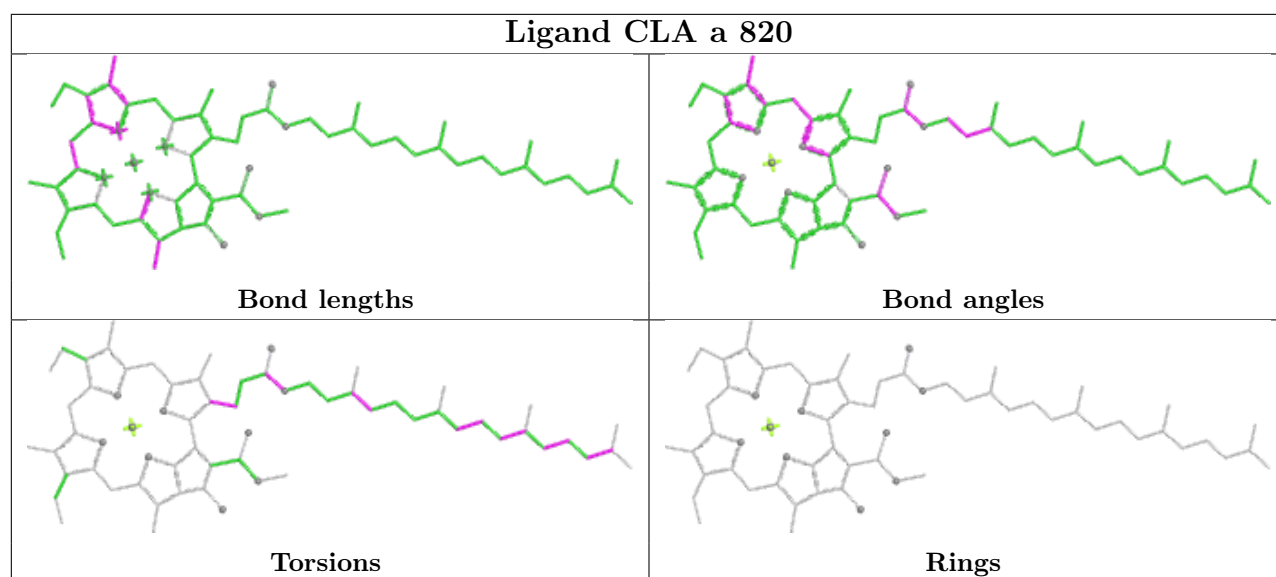
Ligand CLA j 103



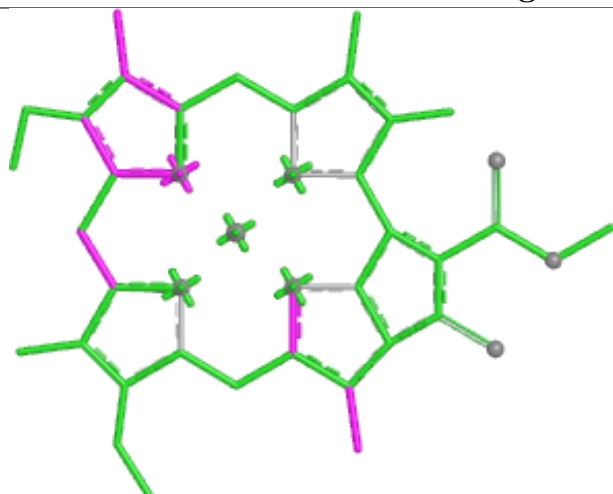
Ligand BCR b 843



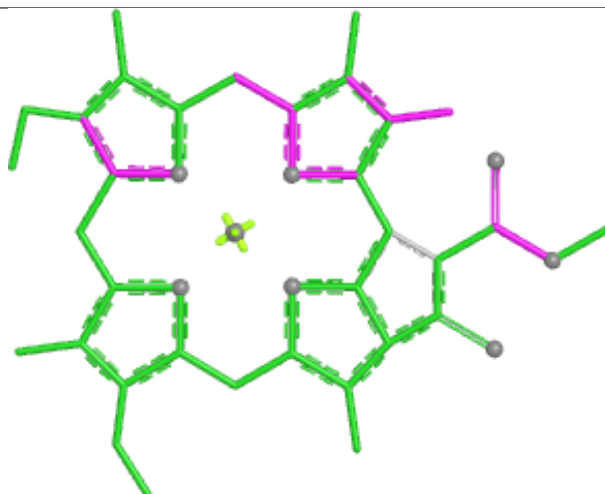




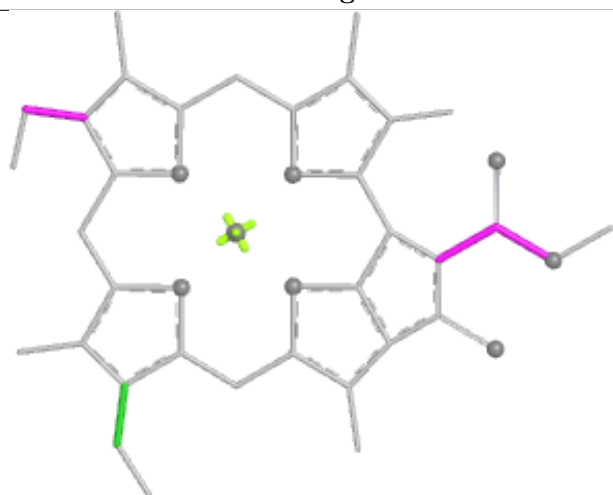
Ligand CLA 4 315



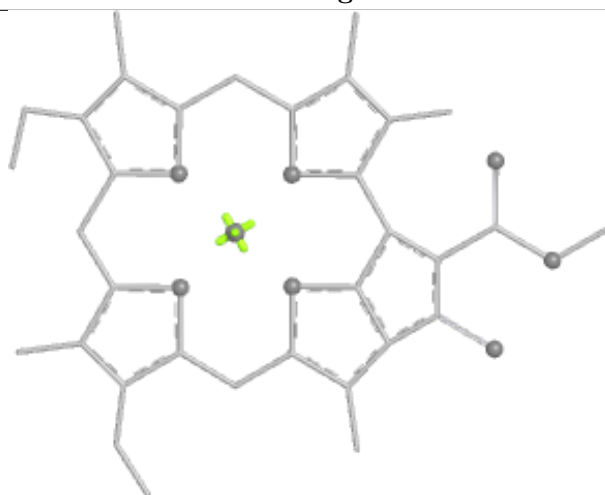
Bond lengths



Bond angles

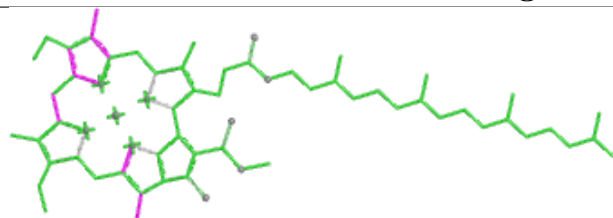


Torsions

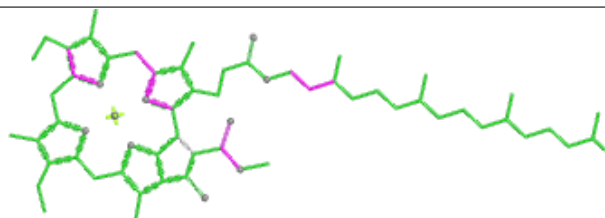


Rings

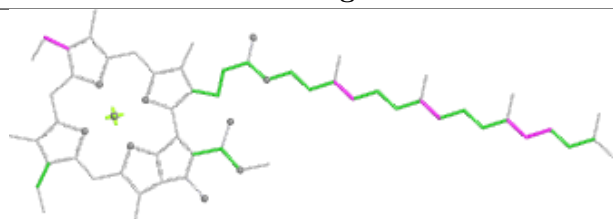
Ligand CLA a 840



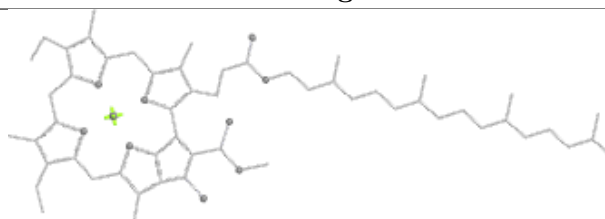
Bond lengths



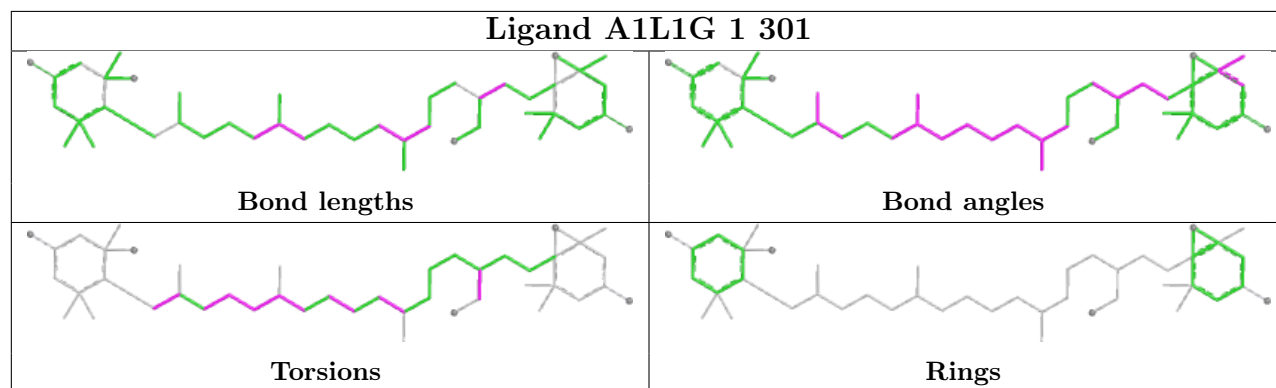
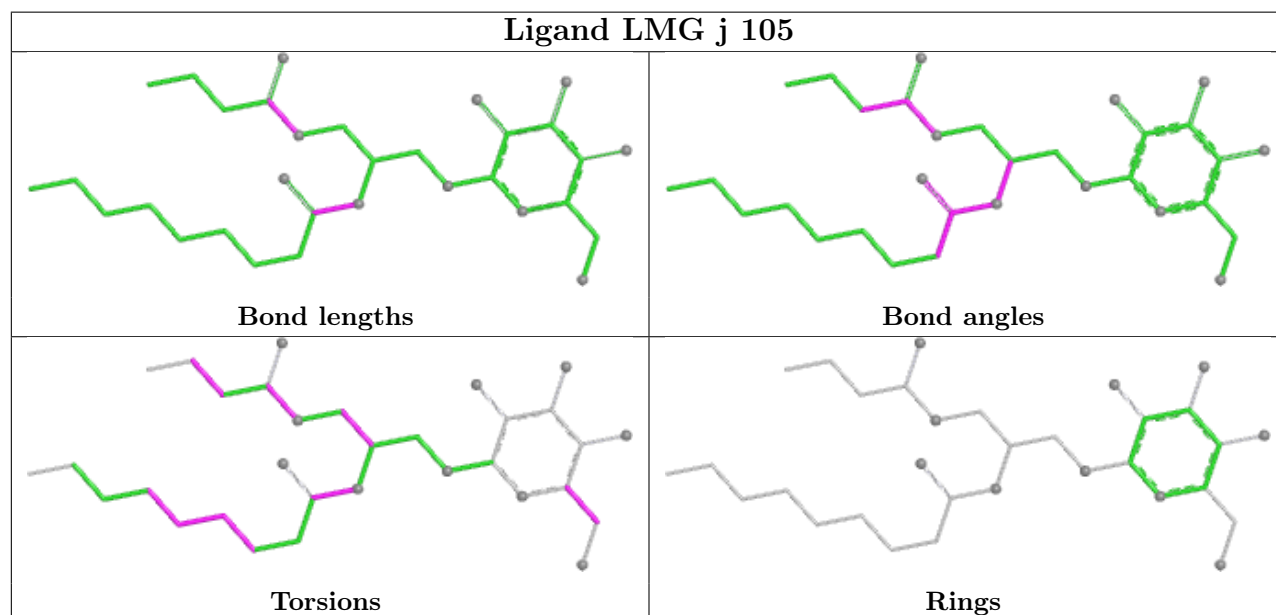
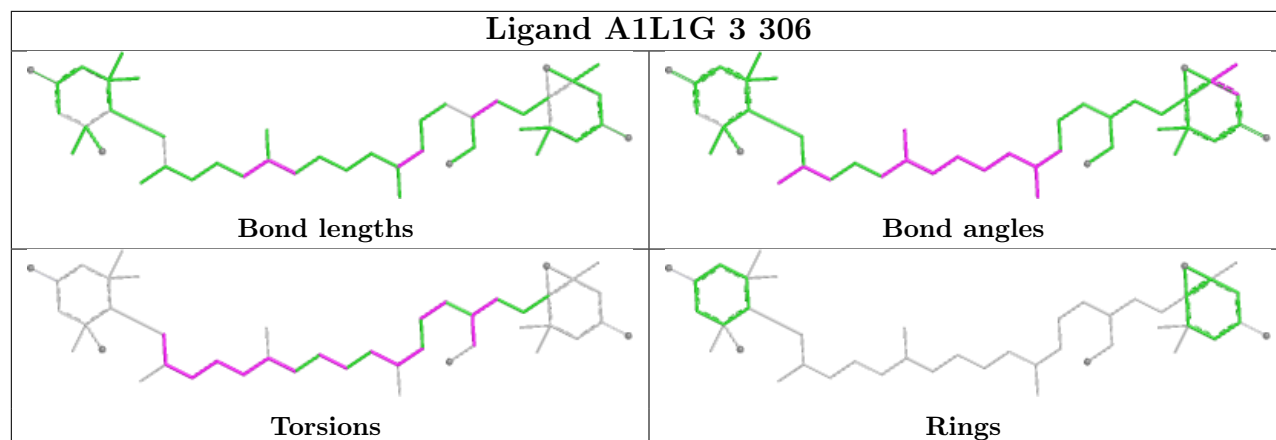
Bond angles



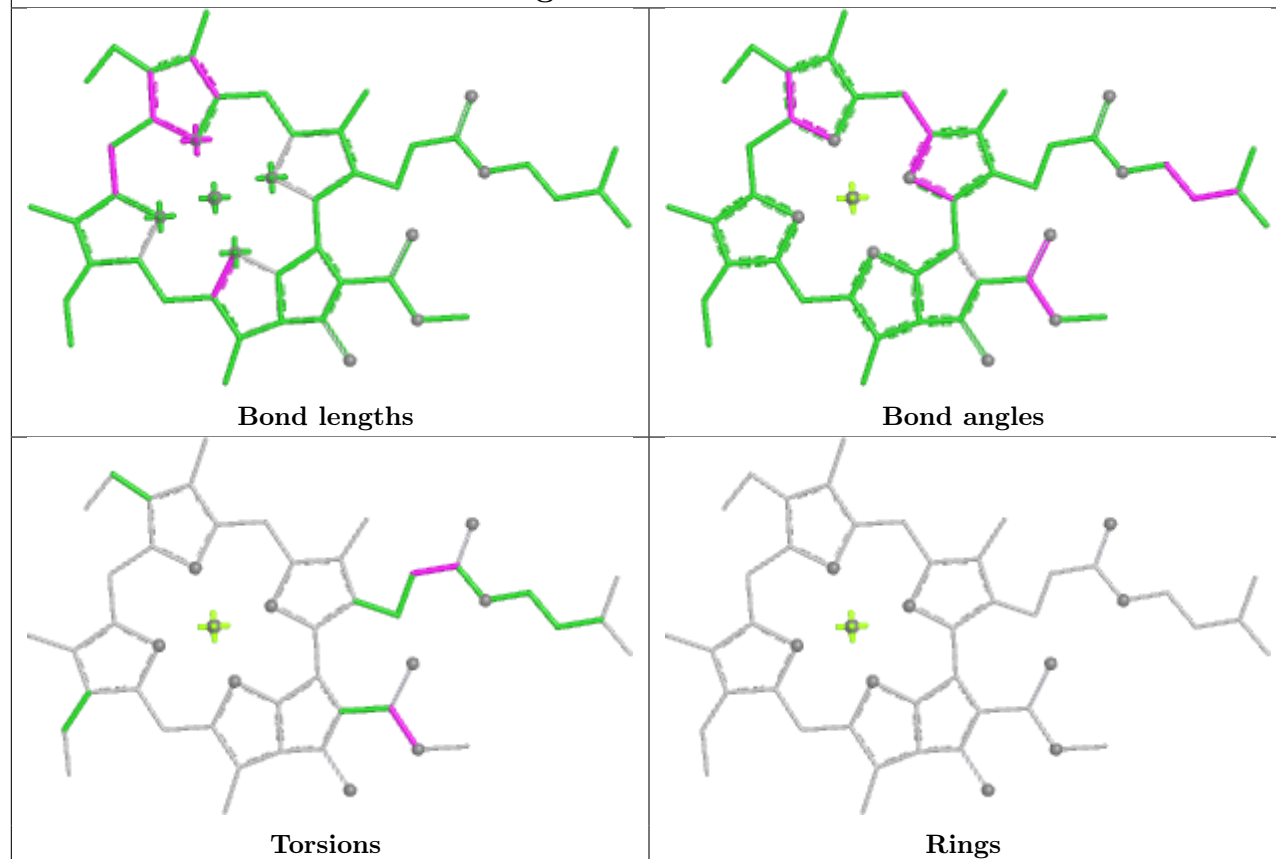
Torsions



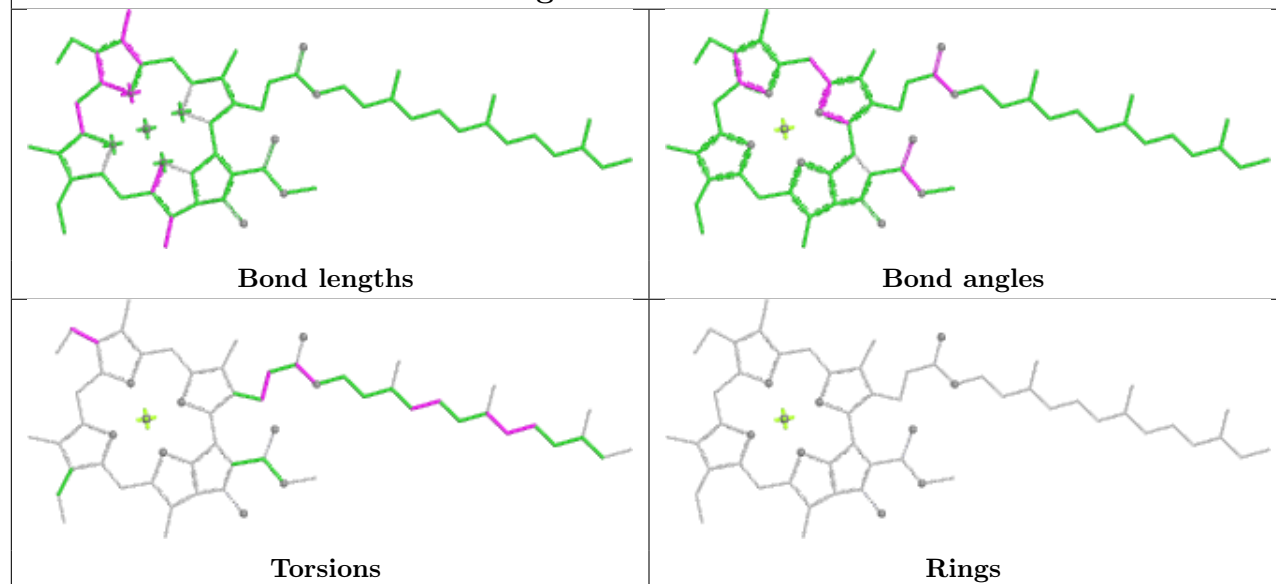
Rings



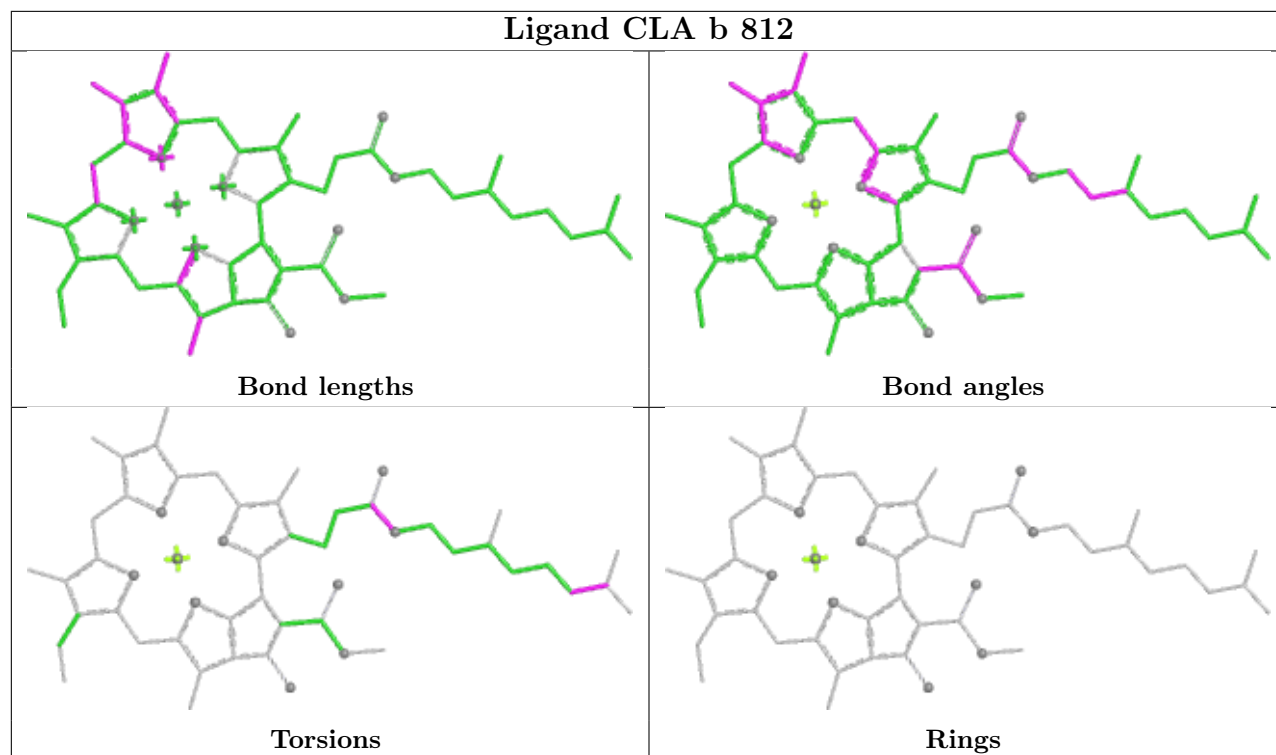
Ligand CLA 4 309



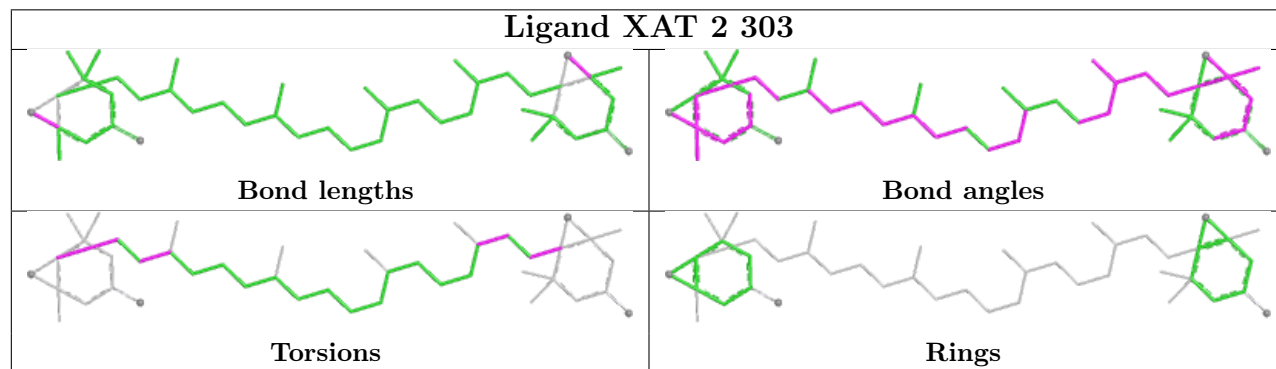
Ligand CLA 1 305



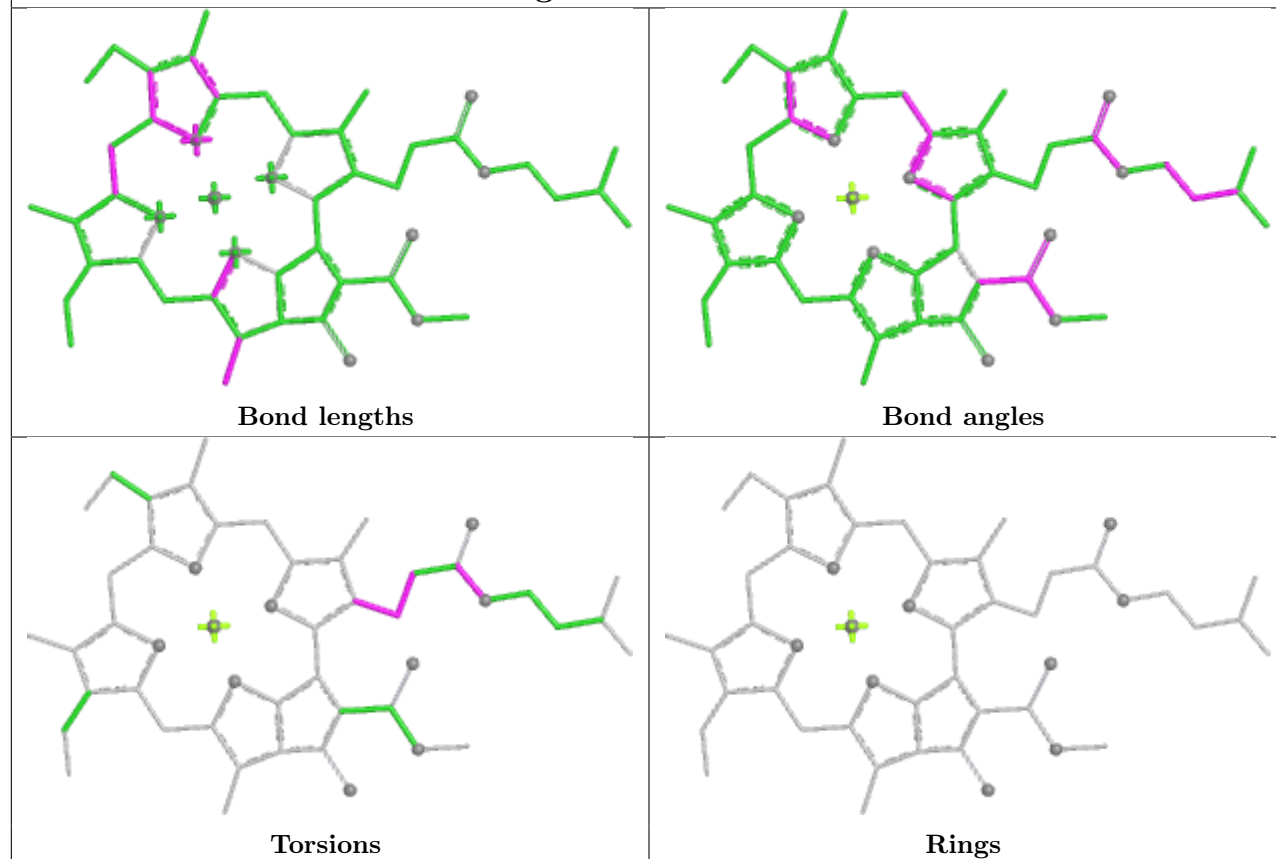
Ligand CLA b 812



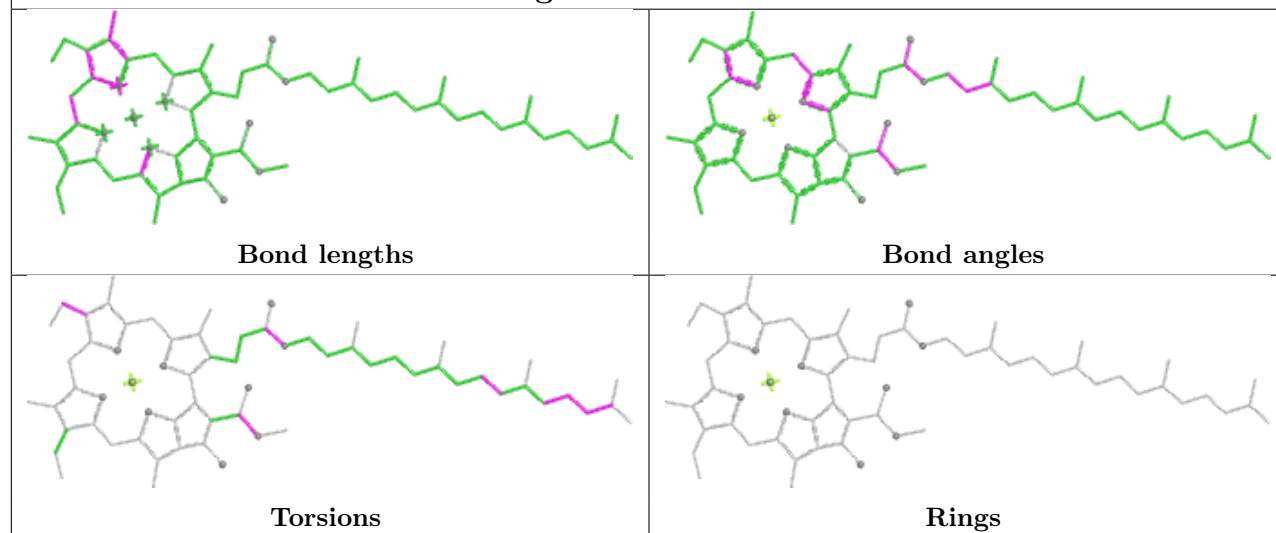
Ligand XAT 2 303



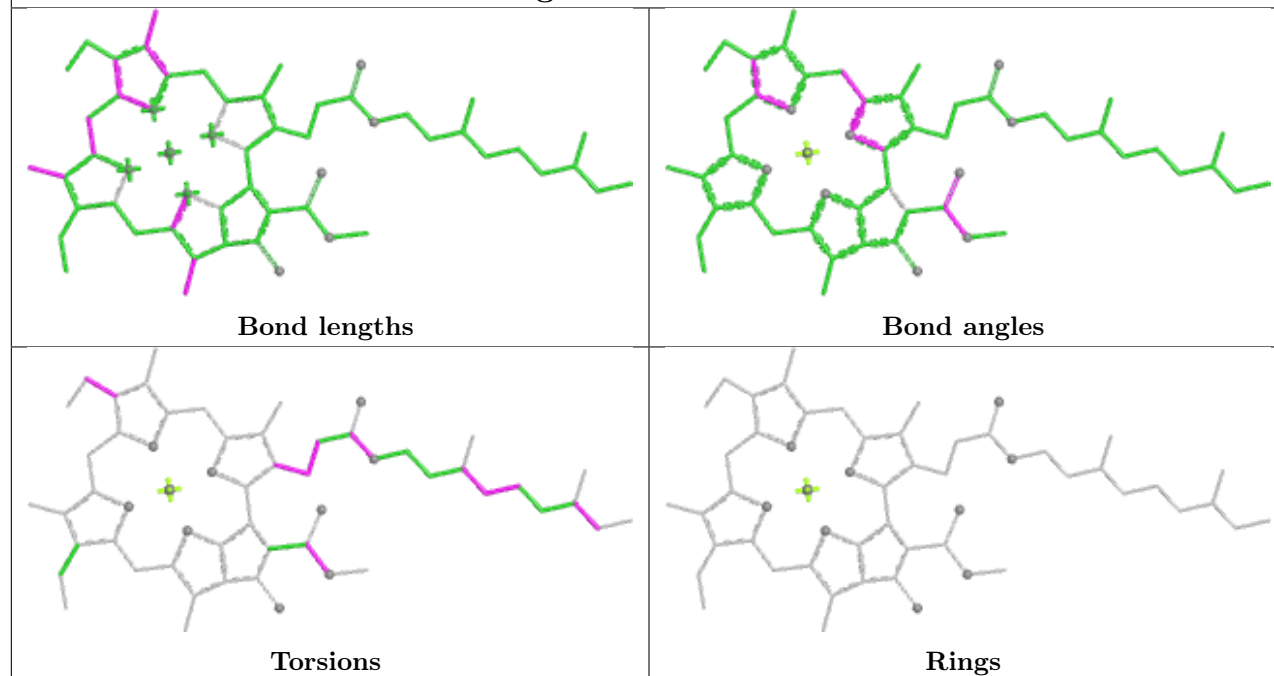
Ligand CLA b 821



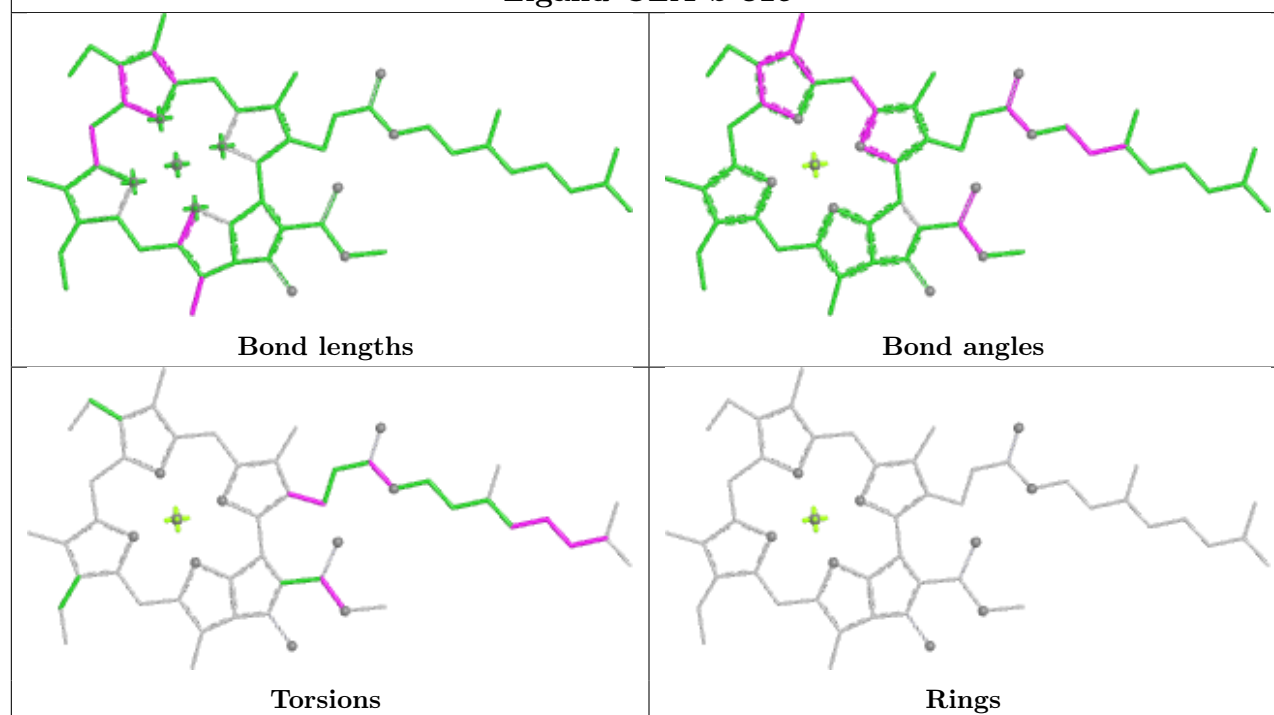
Ligand CLA b 841

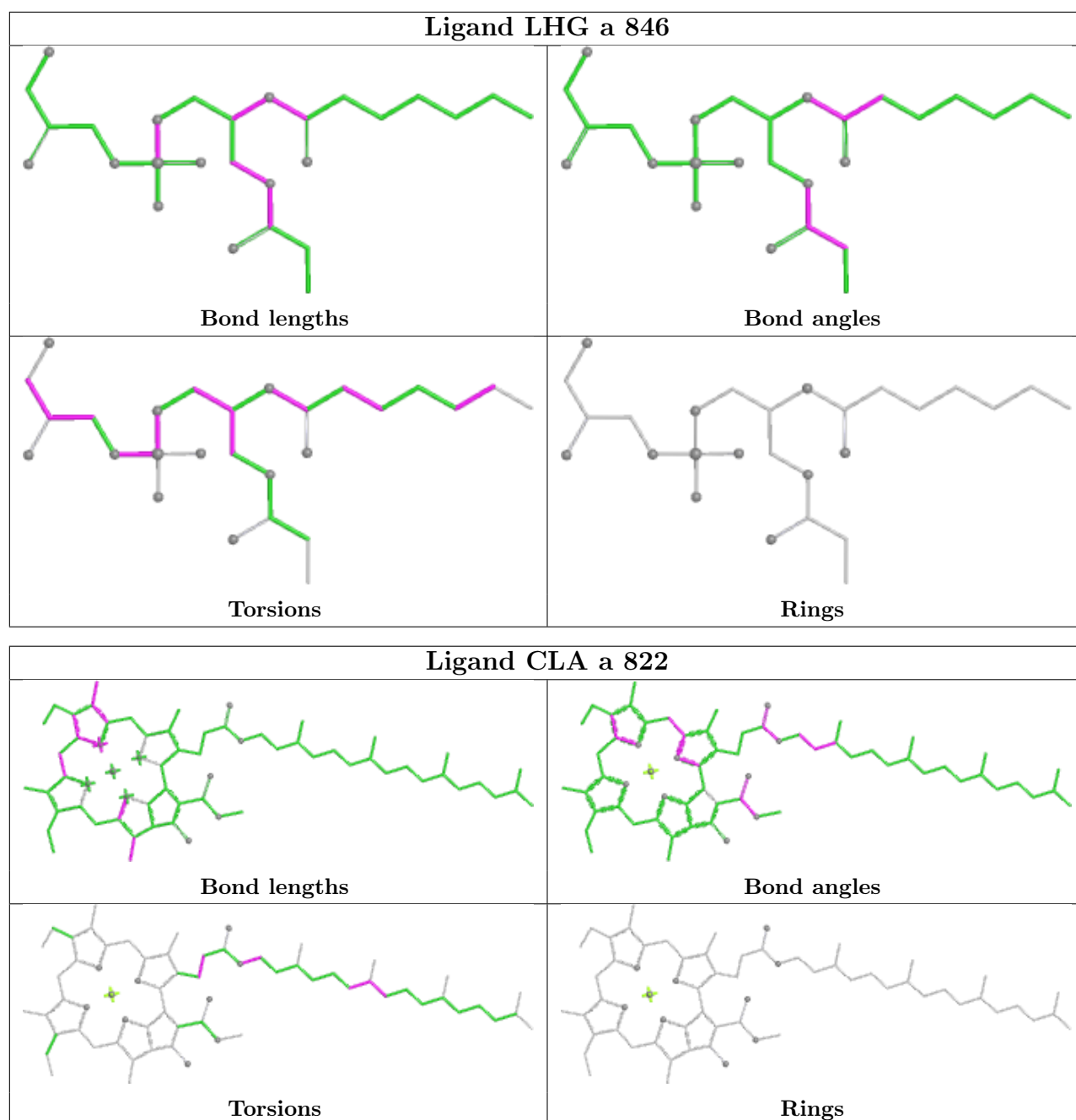


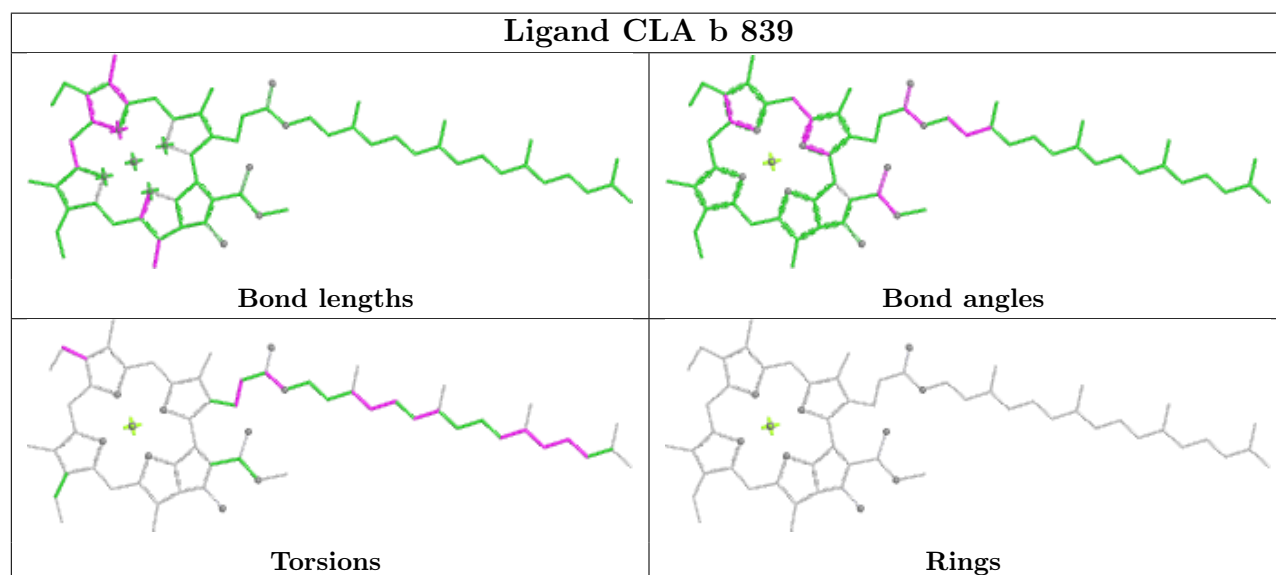
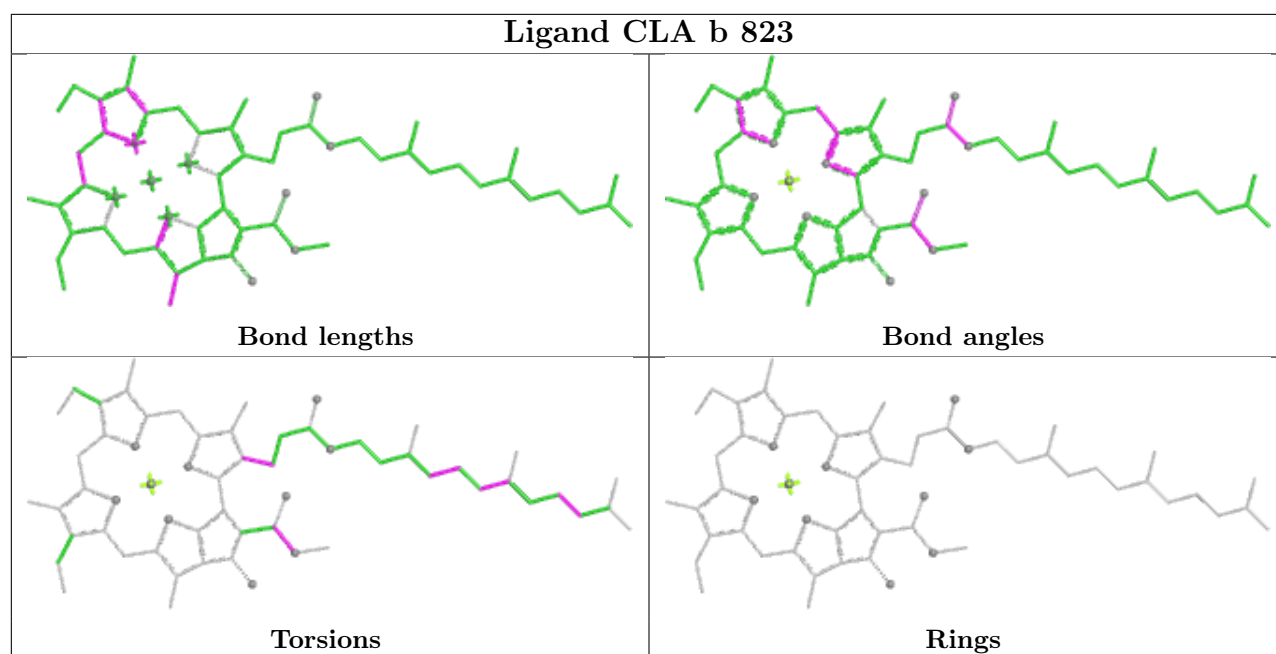
Ligand CLA 2 314

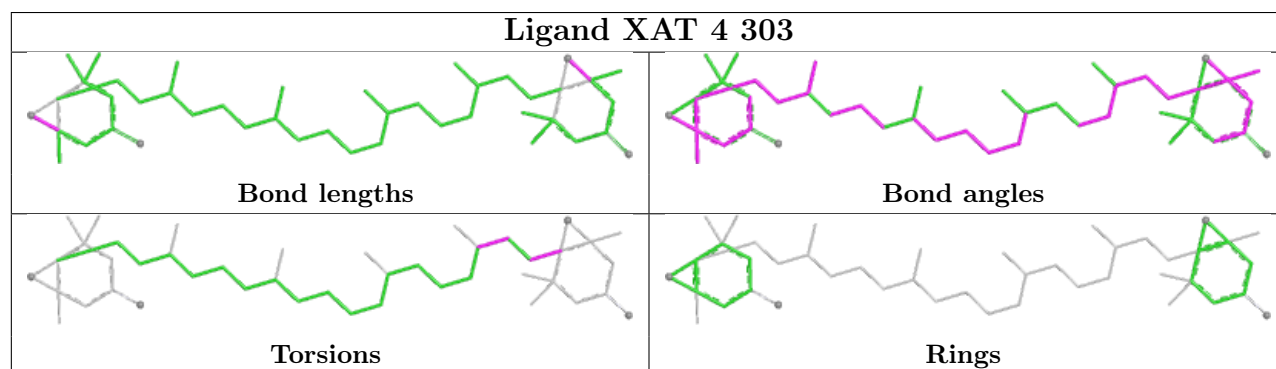
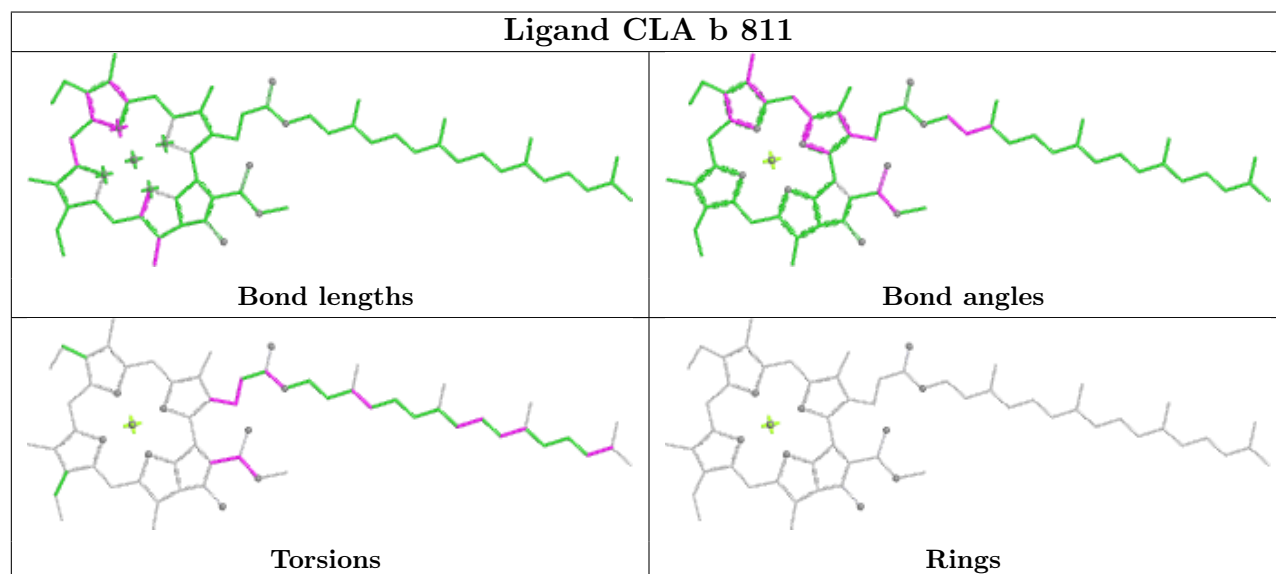
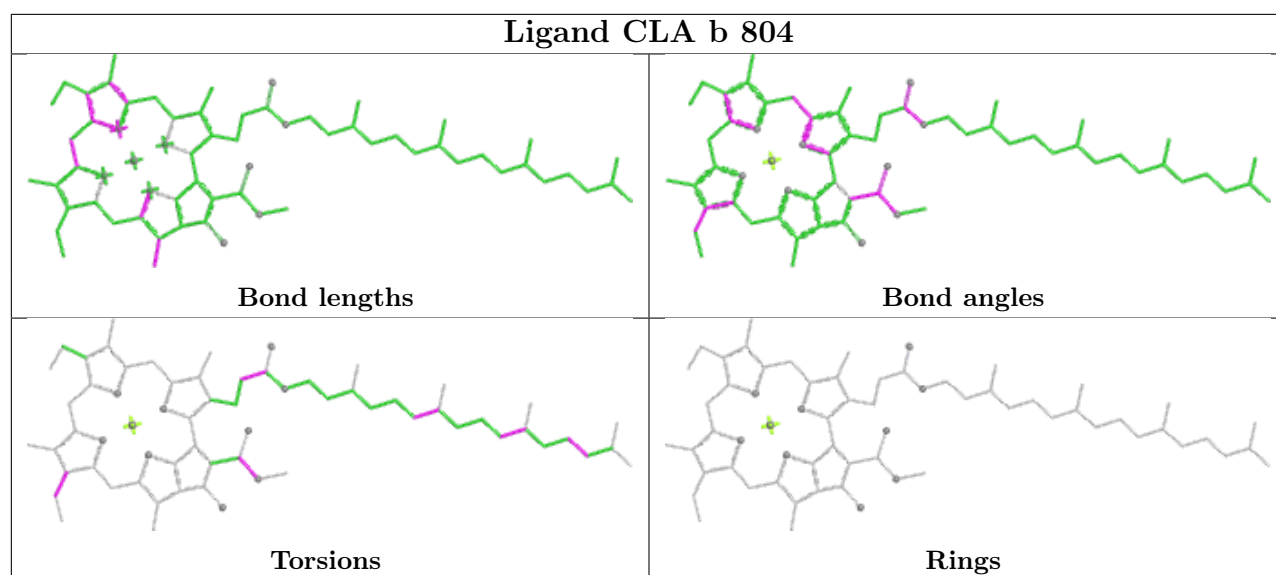


Ligand CLA b 815

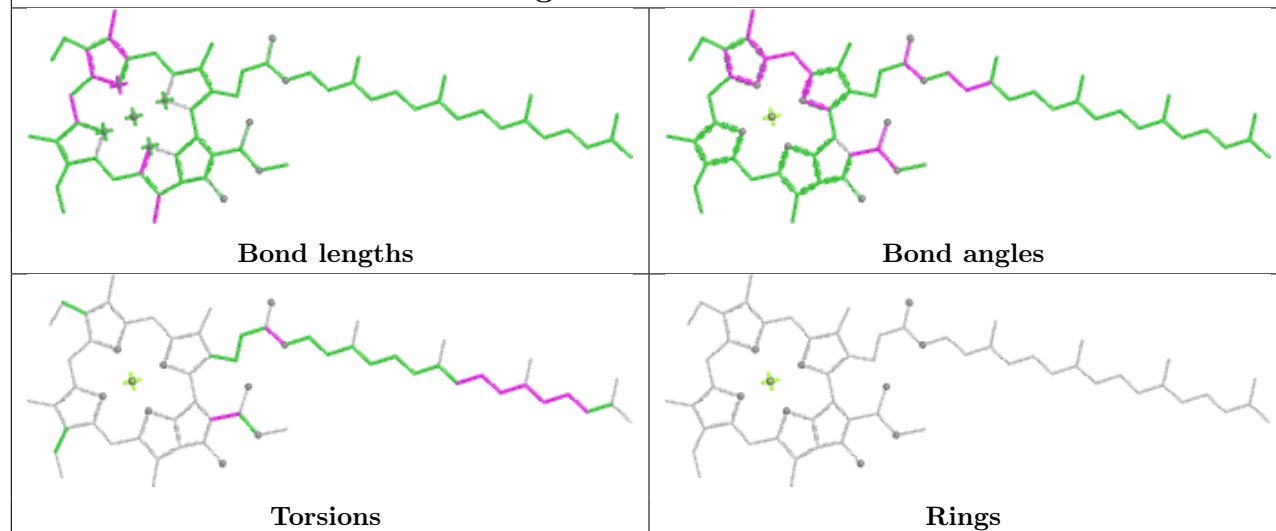




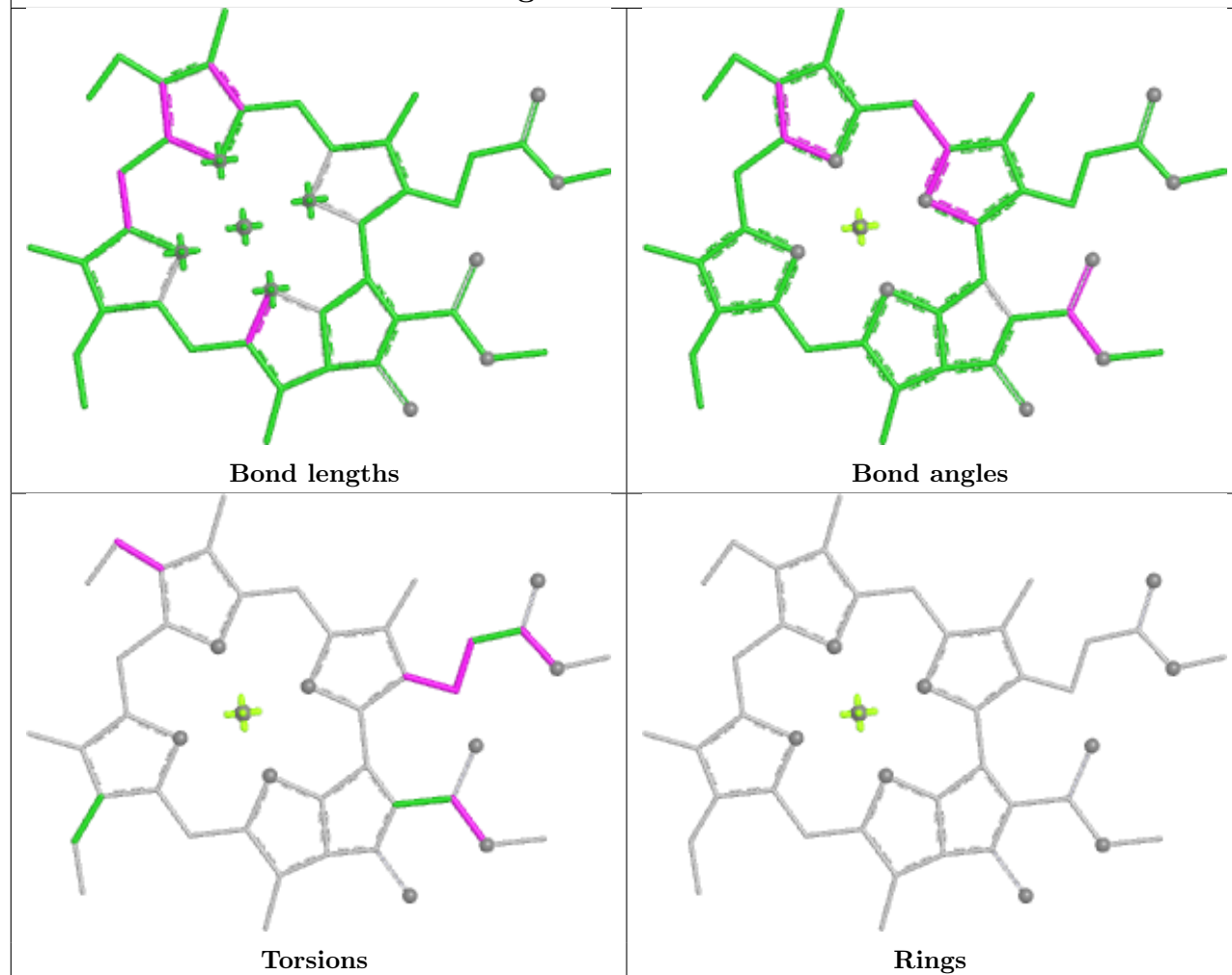




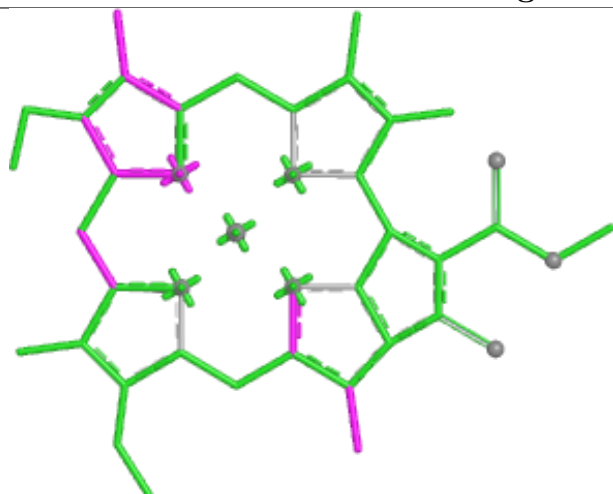
Ligand CLA b 830



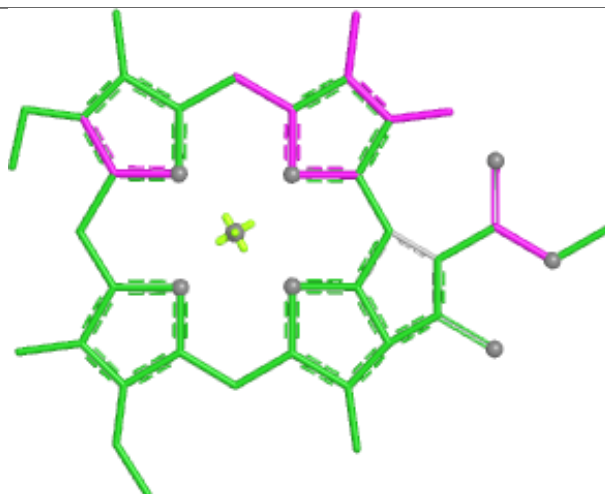
Ligand CLA 4 316



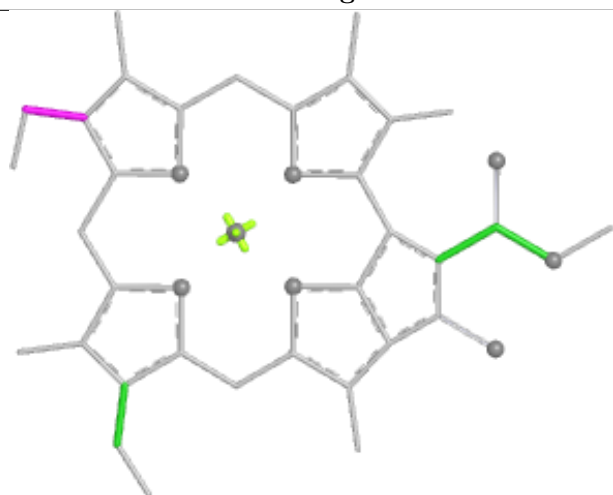
Ligand CLA b 831



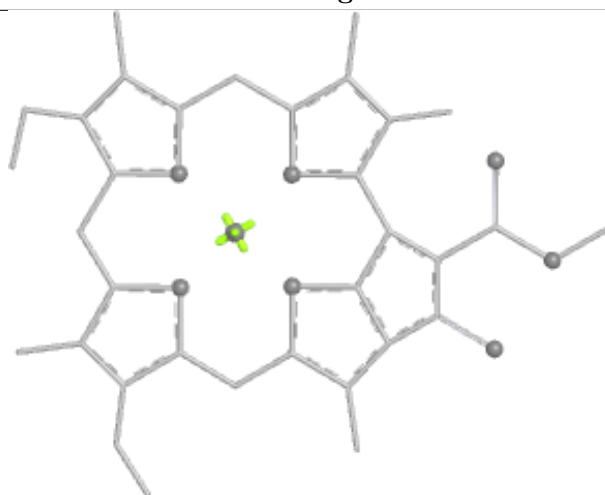
Bond lengths



Bond angles

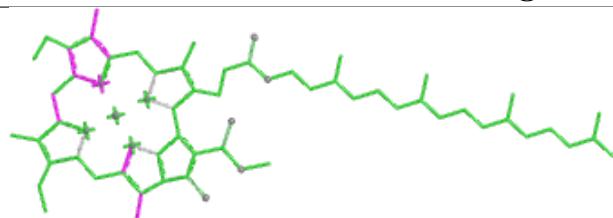


Torsions

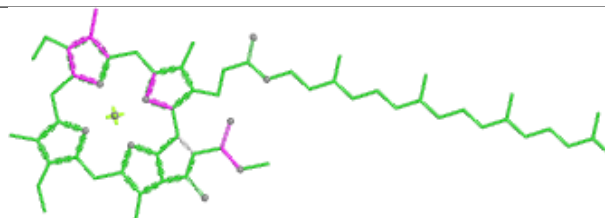


Rings

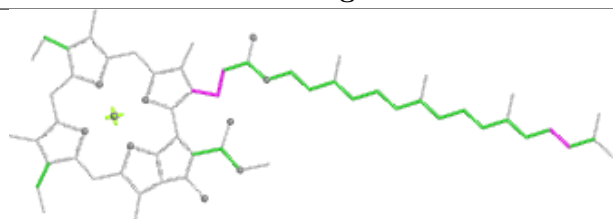
Ligand CLA a 803



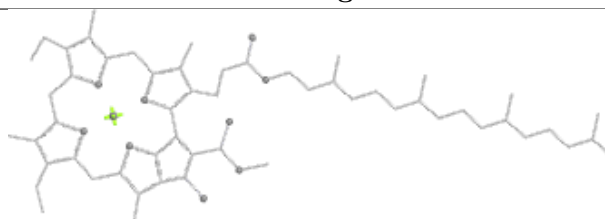
Bond lengths



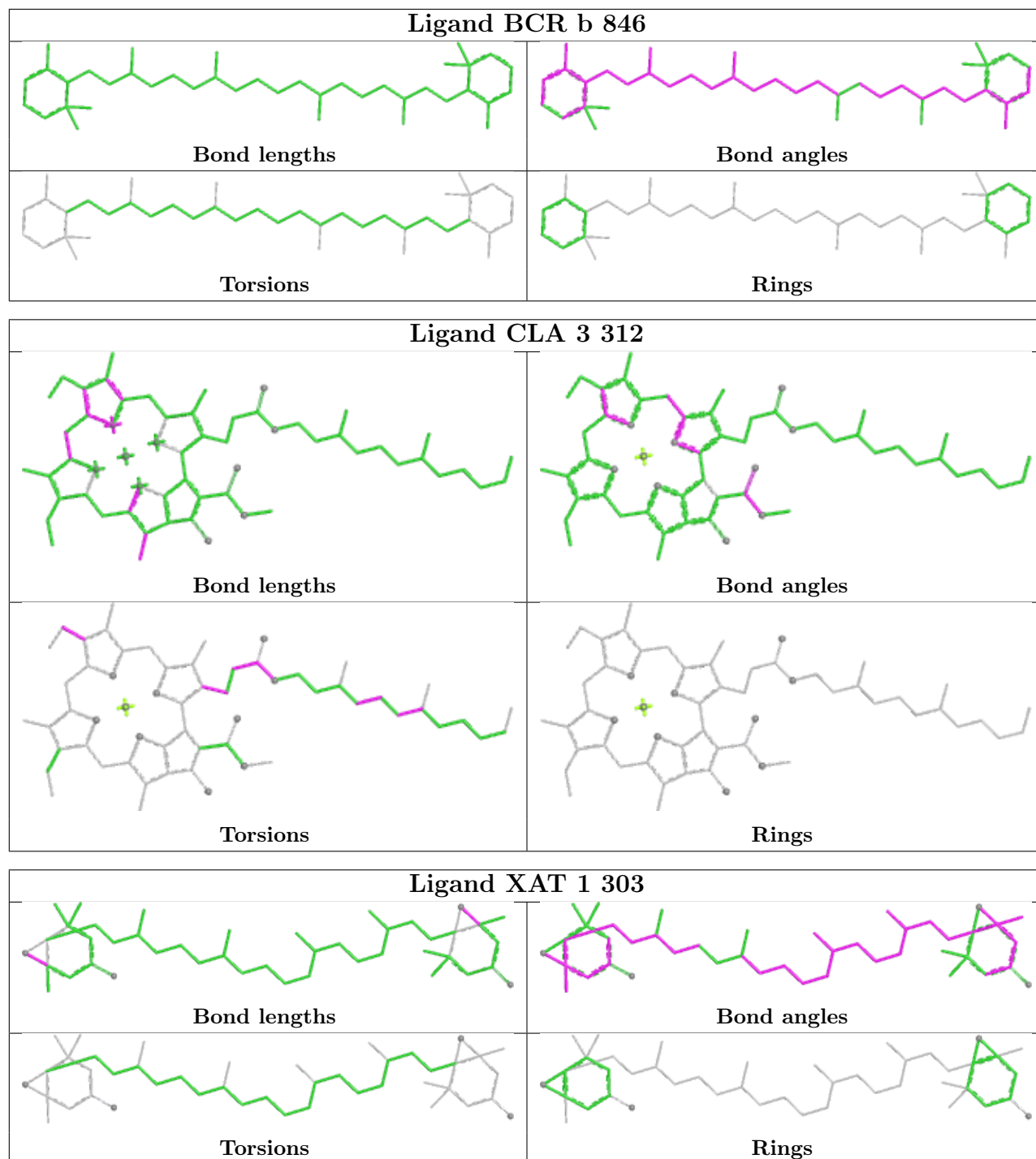
Bond angles



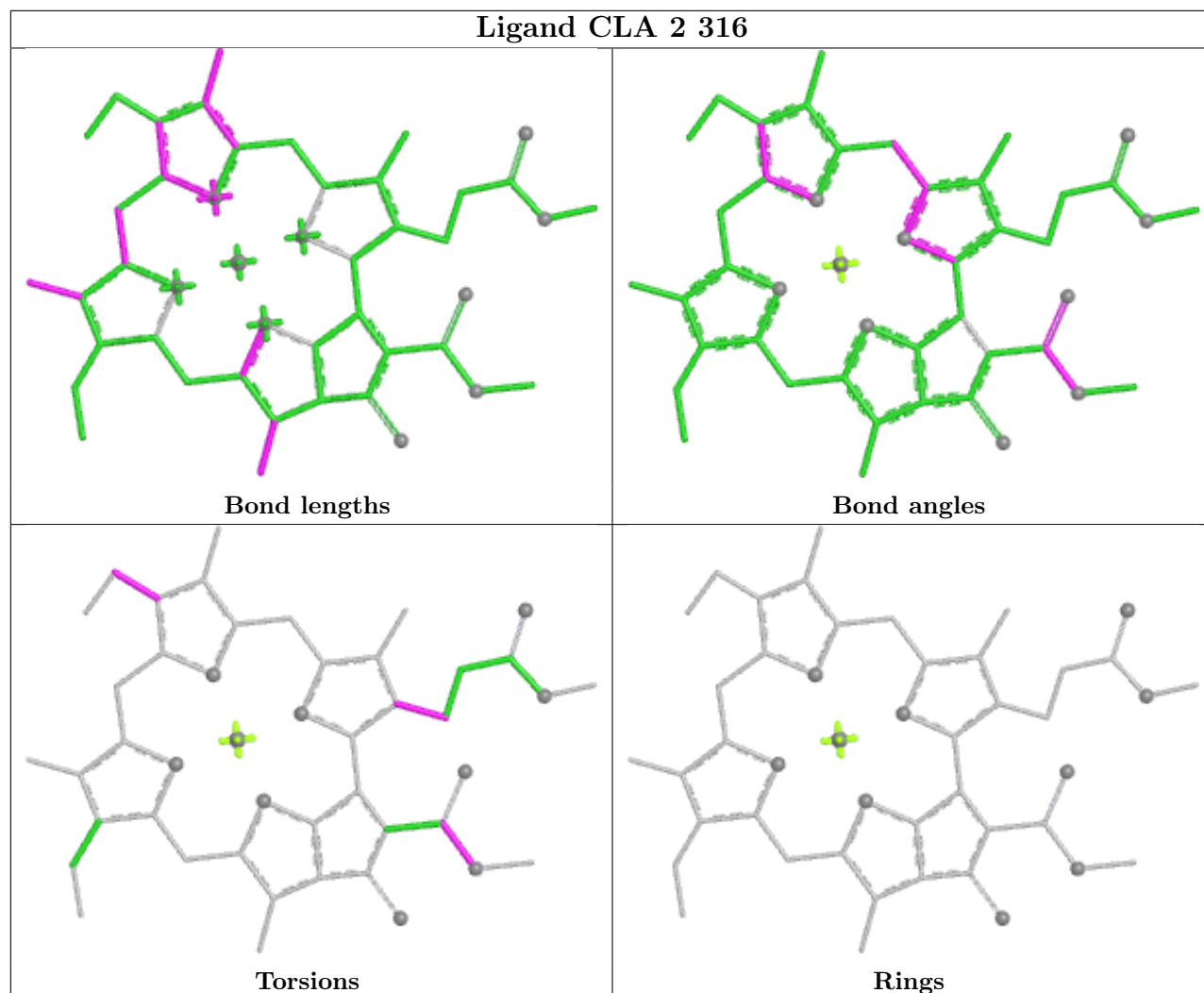
Torsions



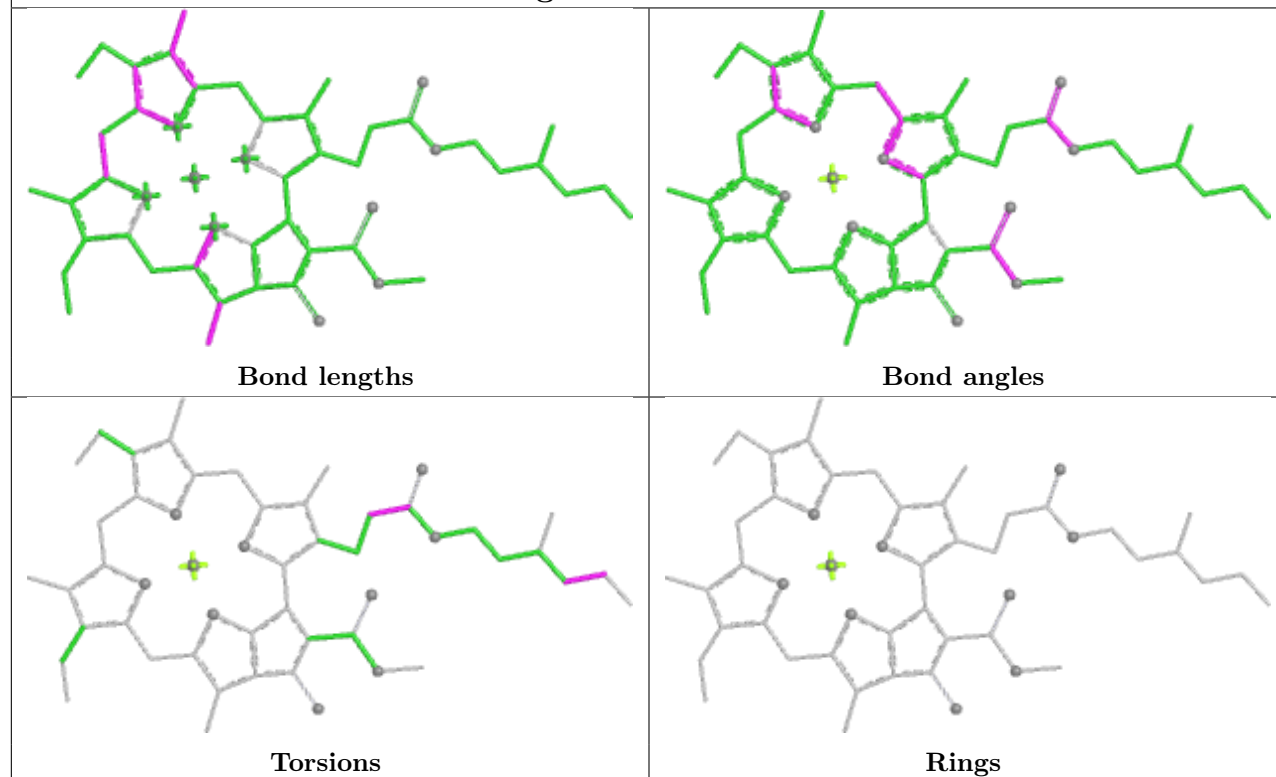
Rings



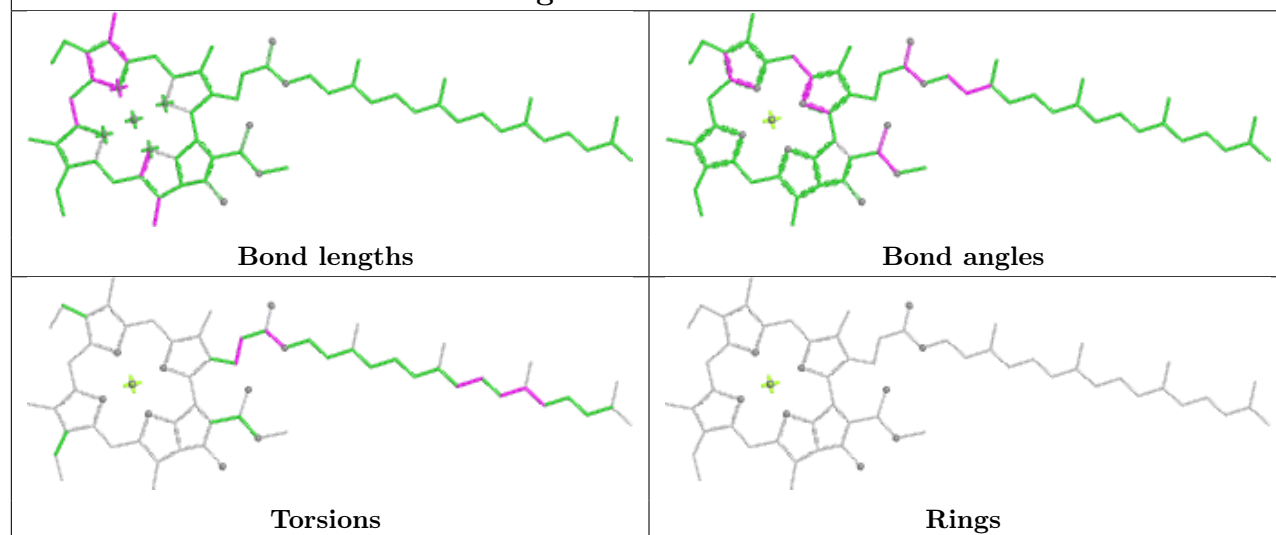
Ligand CLA 2 316



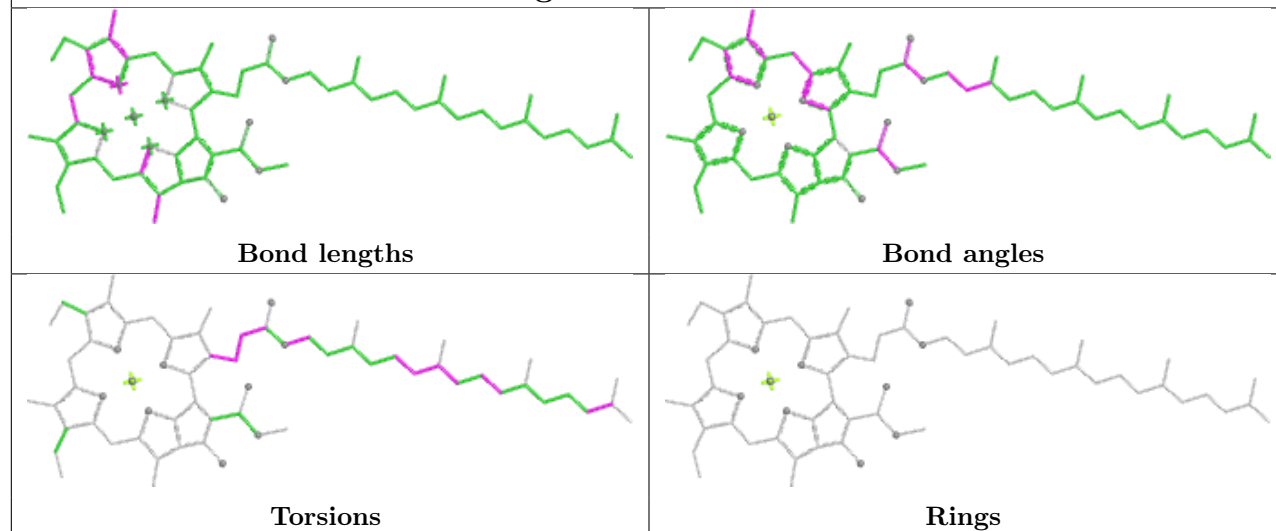
Ligand CLA 1 312



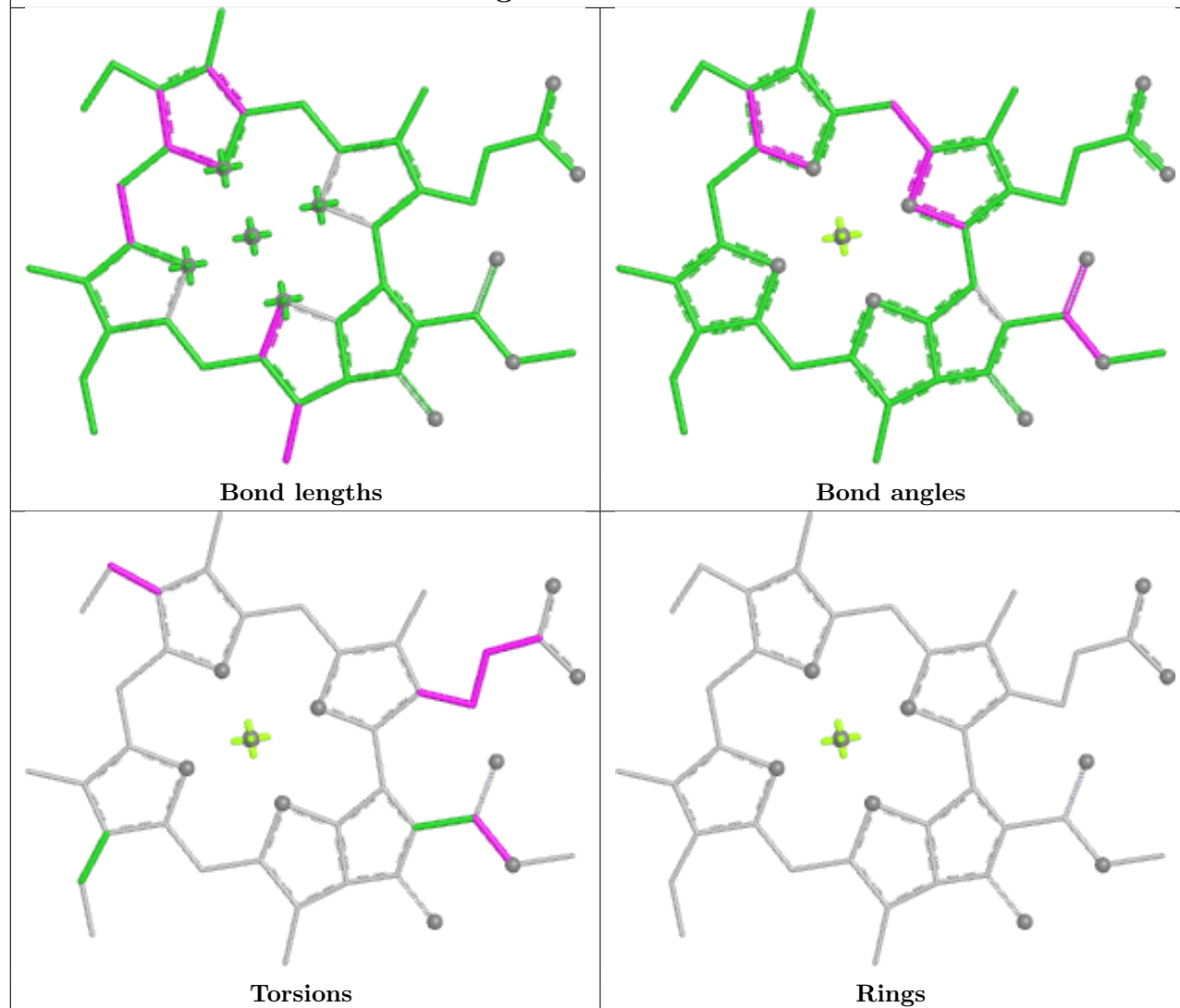
Ligand CLA a 842



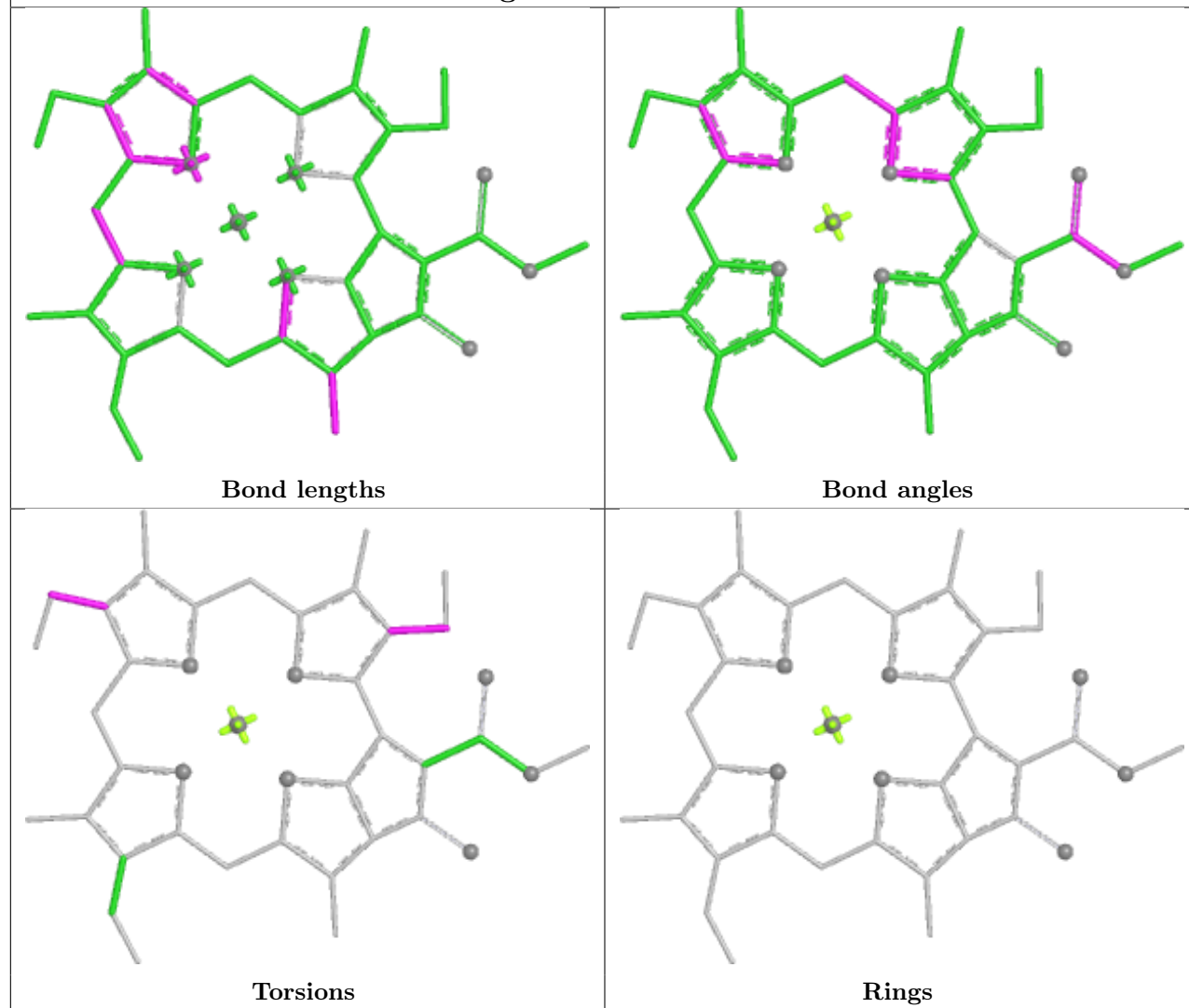
Ligand CLA b 810



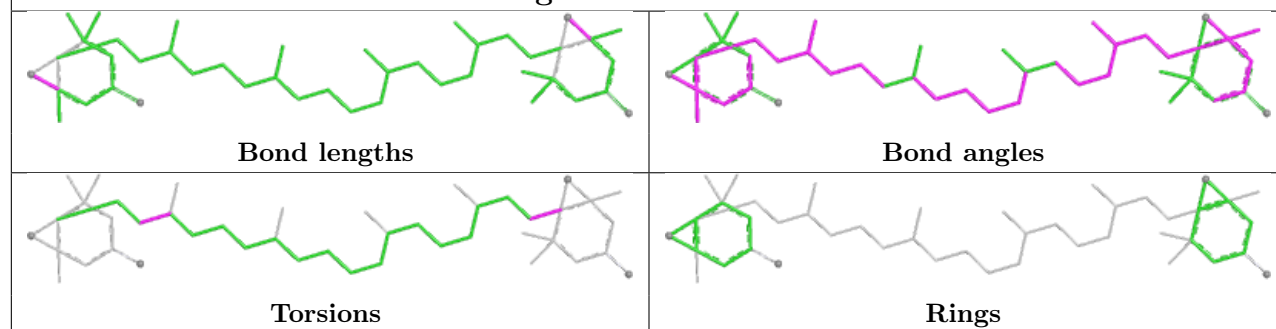
Ligand CLA 5 306



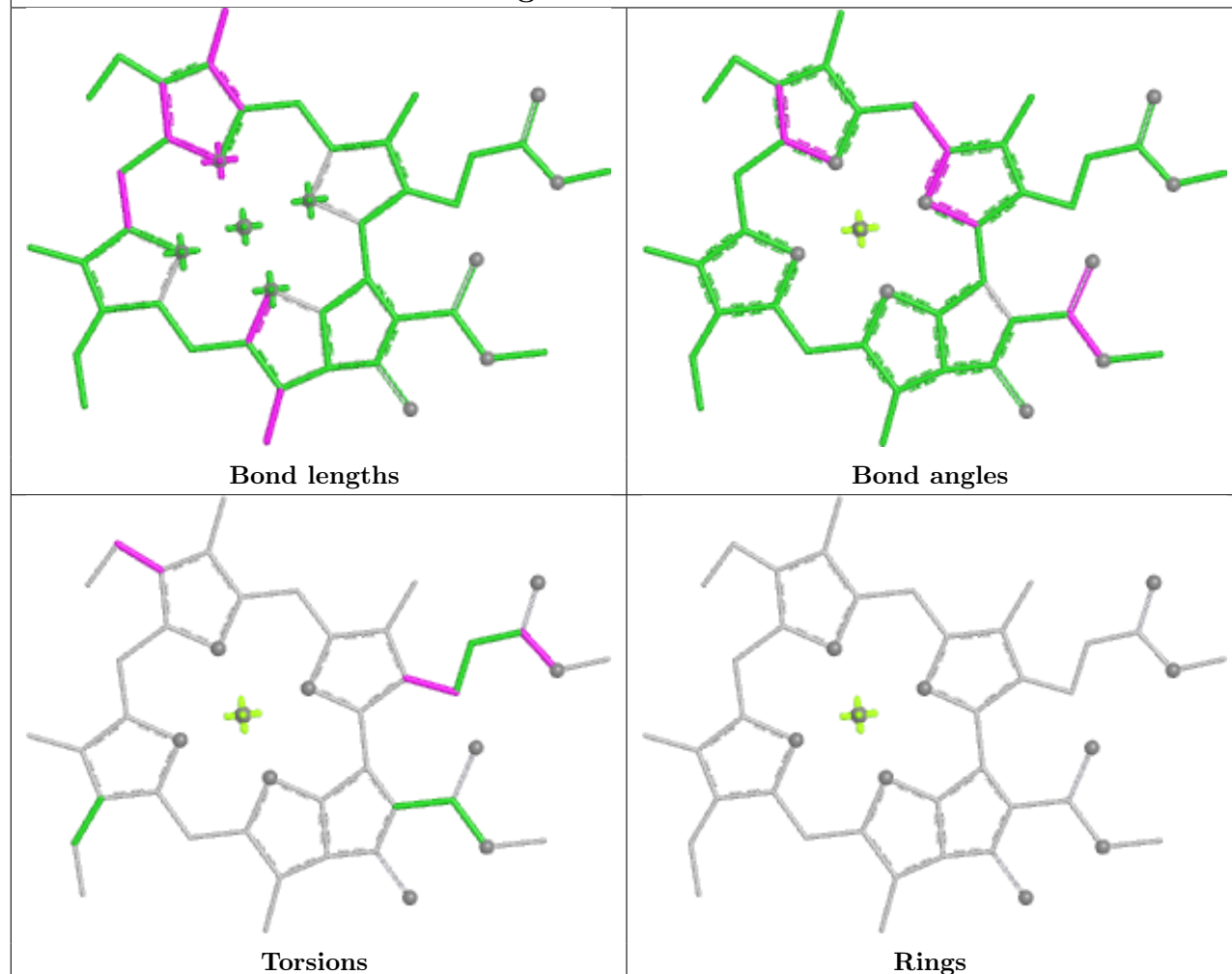
Ligand CLA 2 315



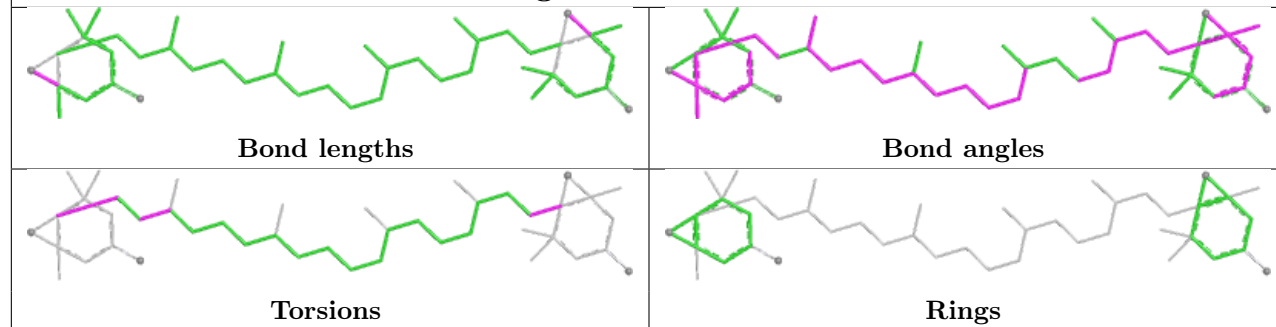
Ligand XAT 3 303



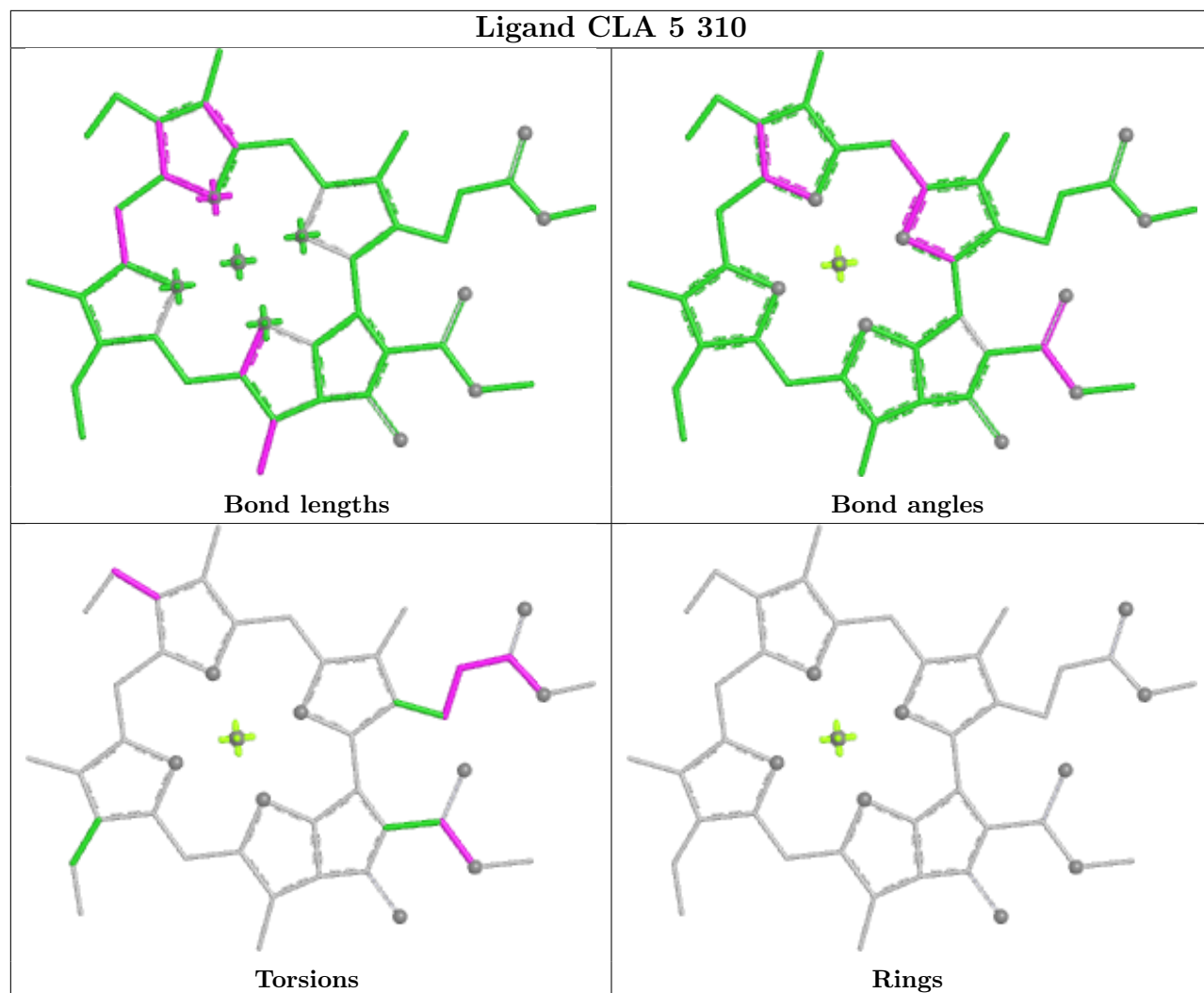
Ligand CLA 4 312

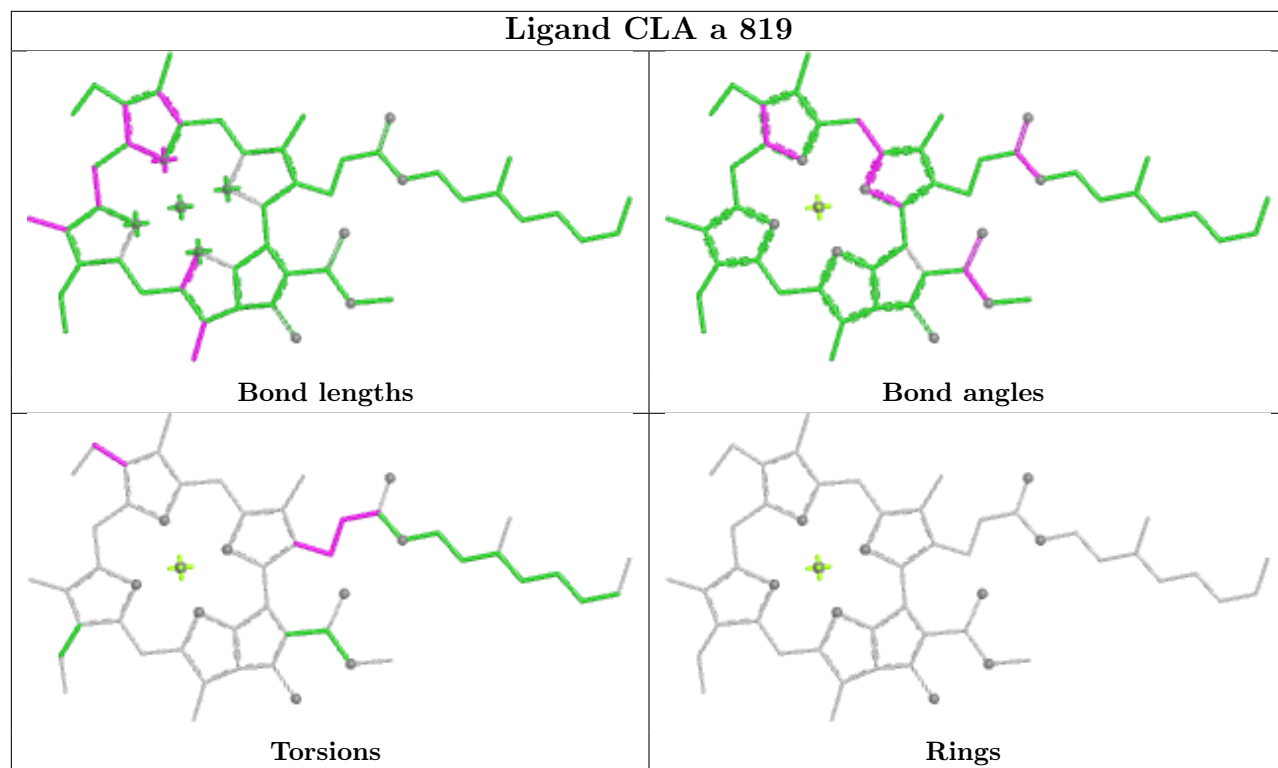


Ligand XAT 4 305

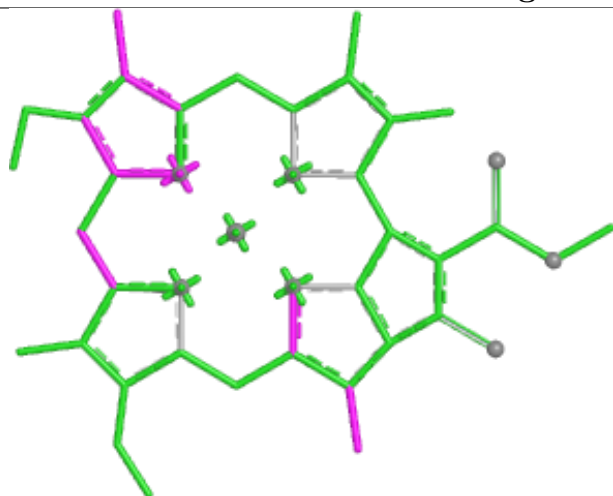


Ligand CLA 5 310

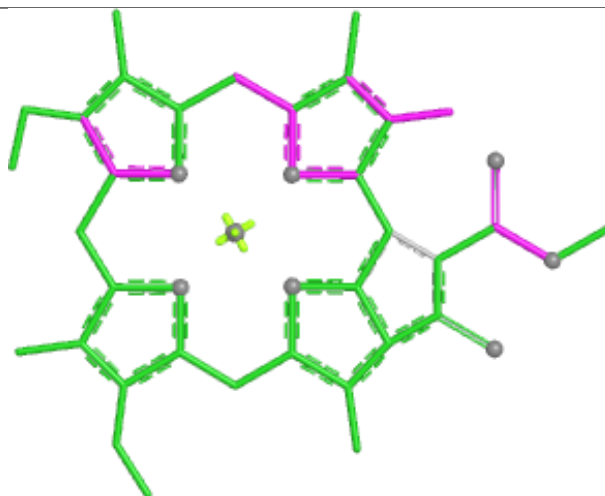




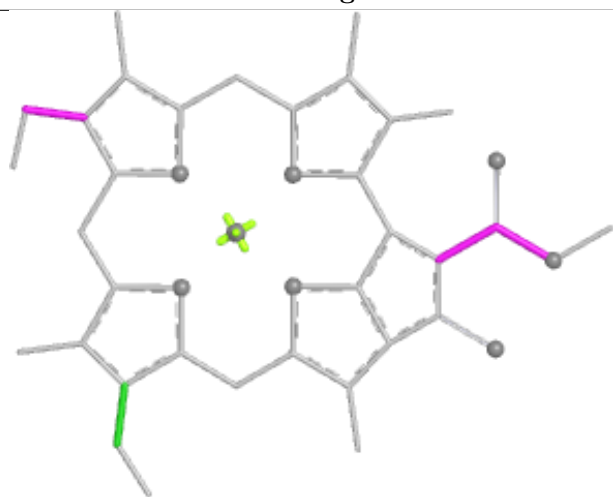
Ligand CLA 1 313



Bond lengths



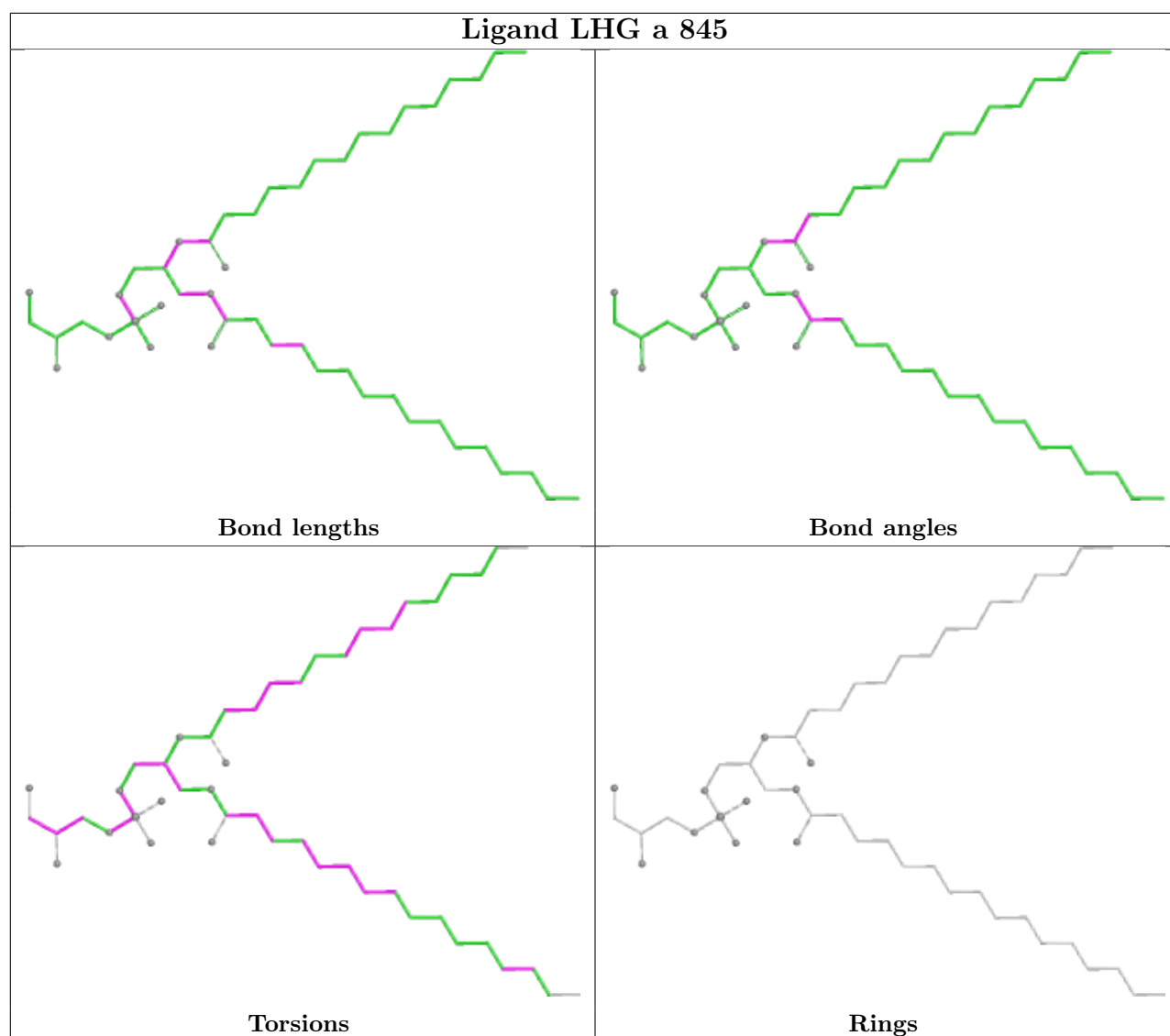
Bond angles

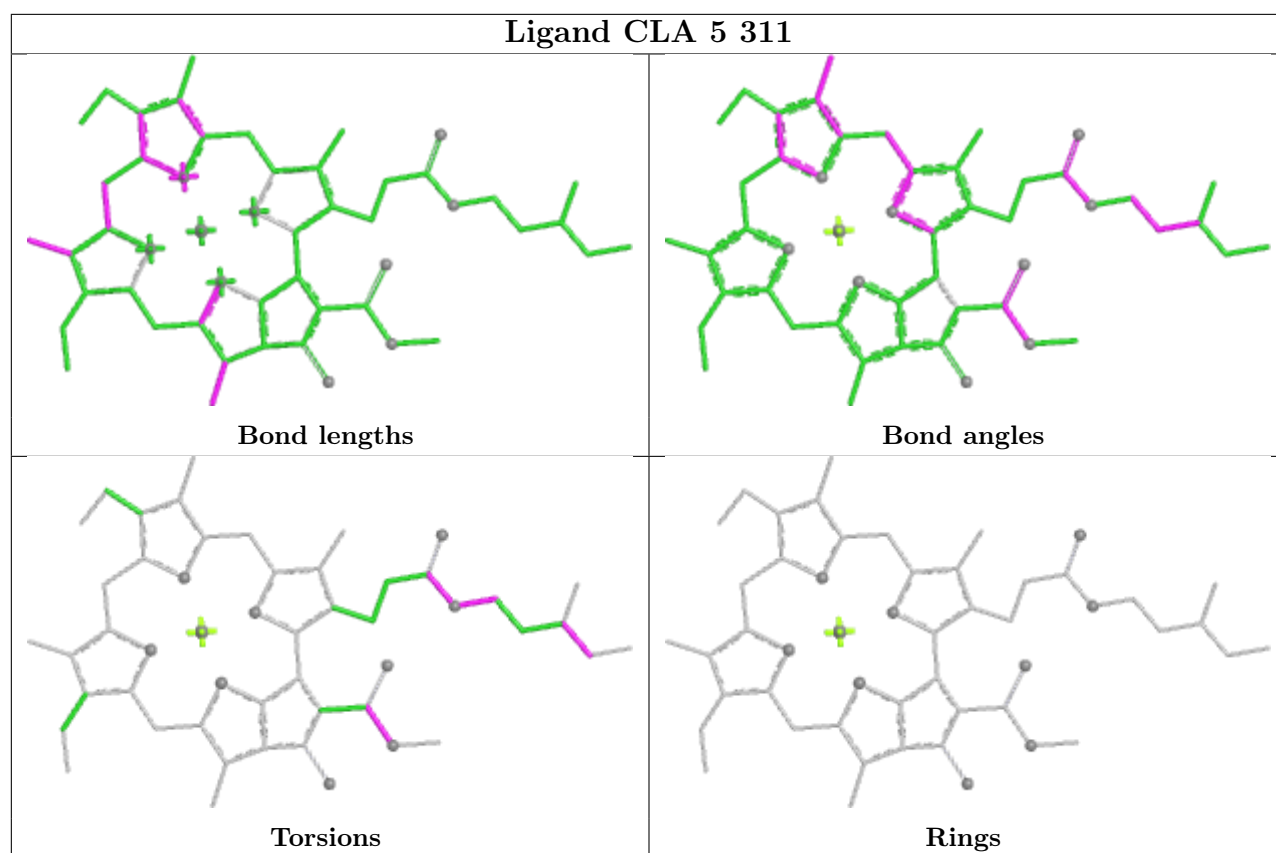


Torsions

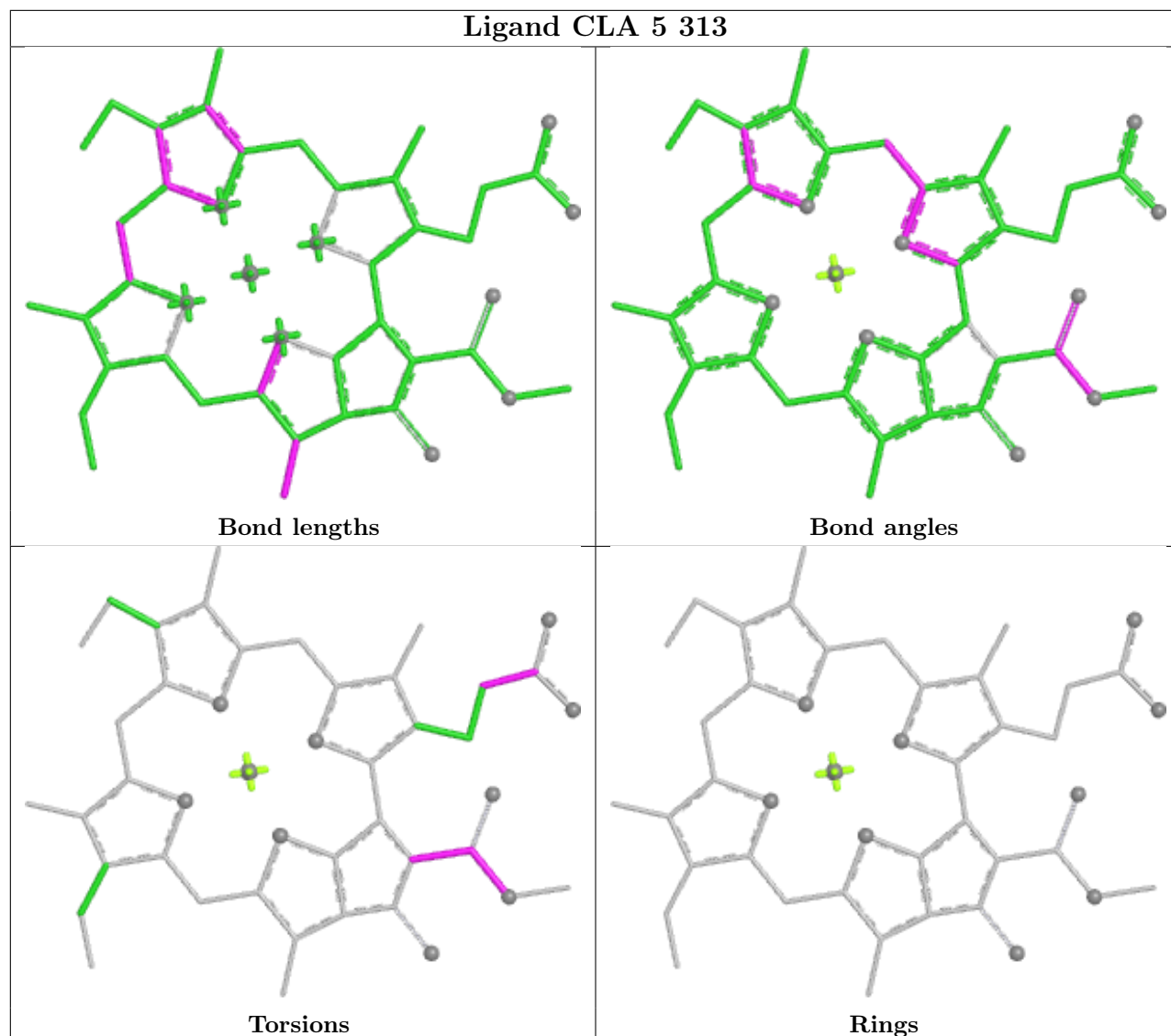


Rings

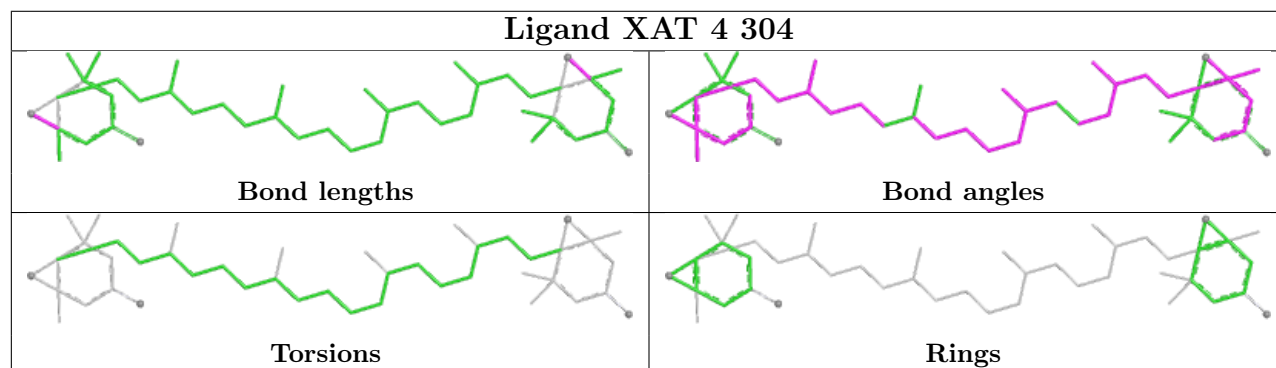




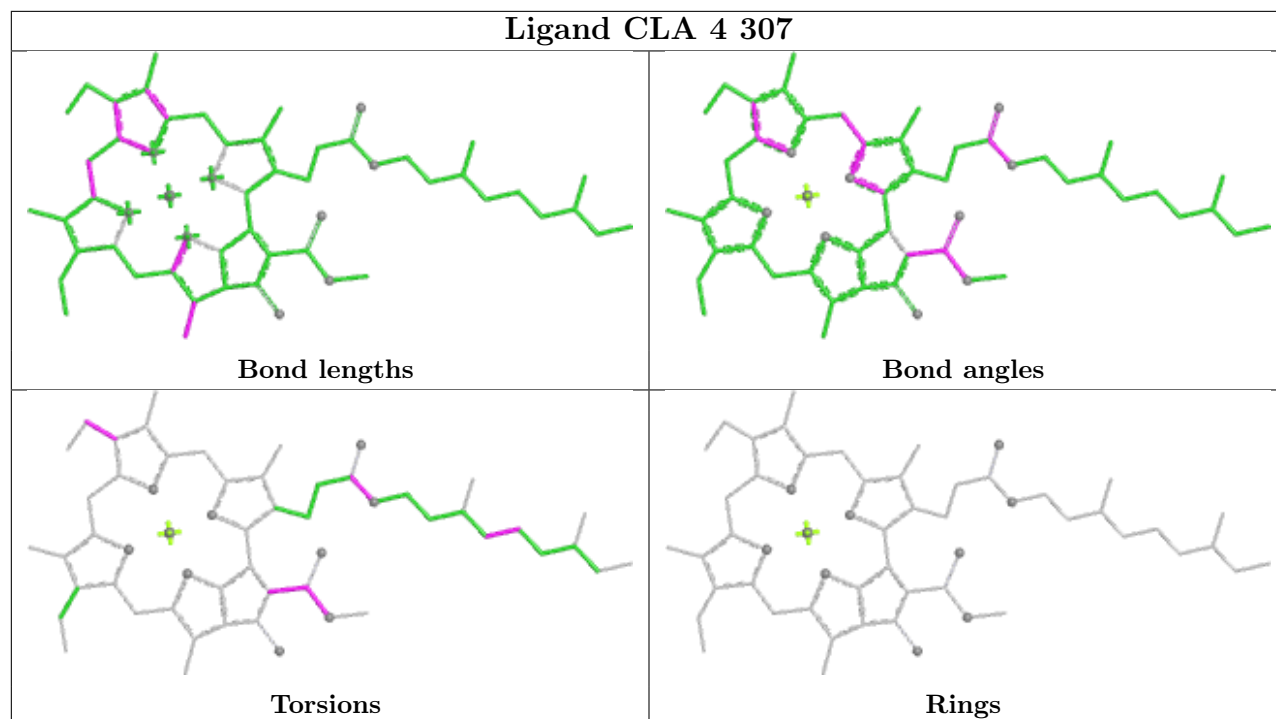
Ligand CLA 5 313



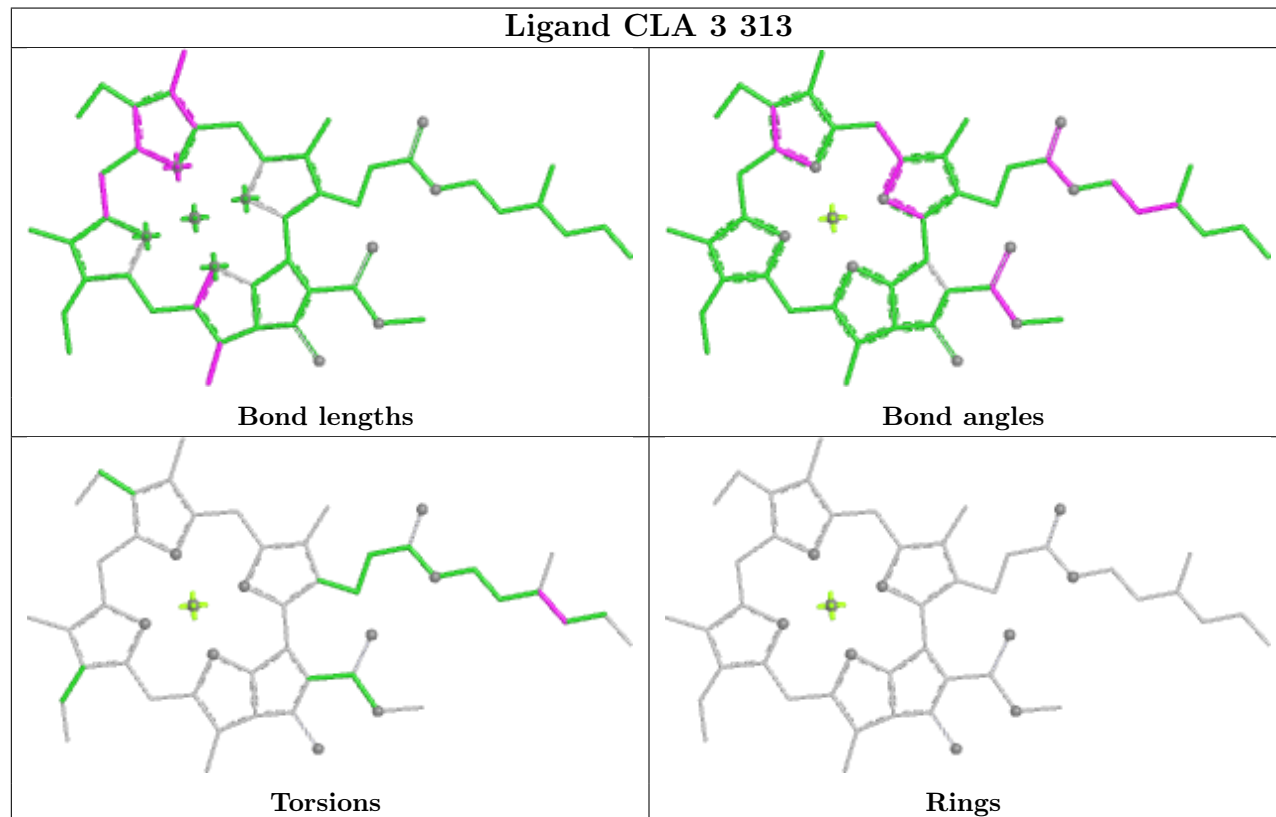
Ligand XAT 4 304

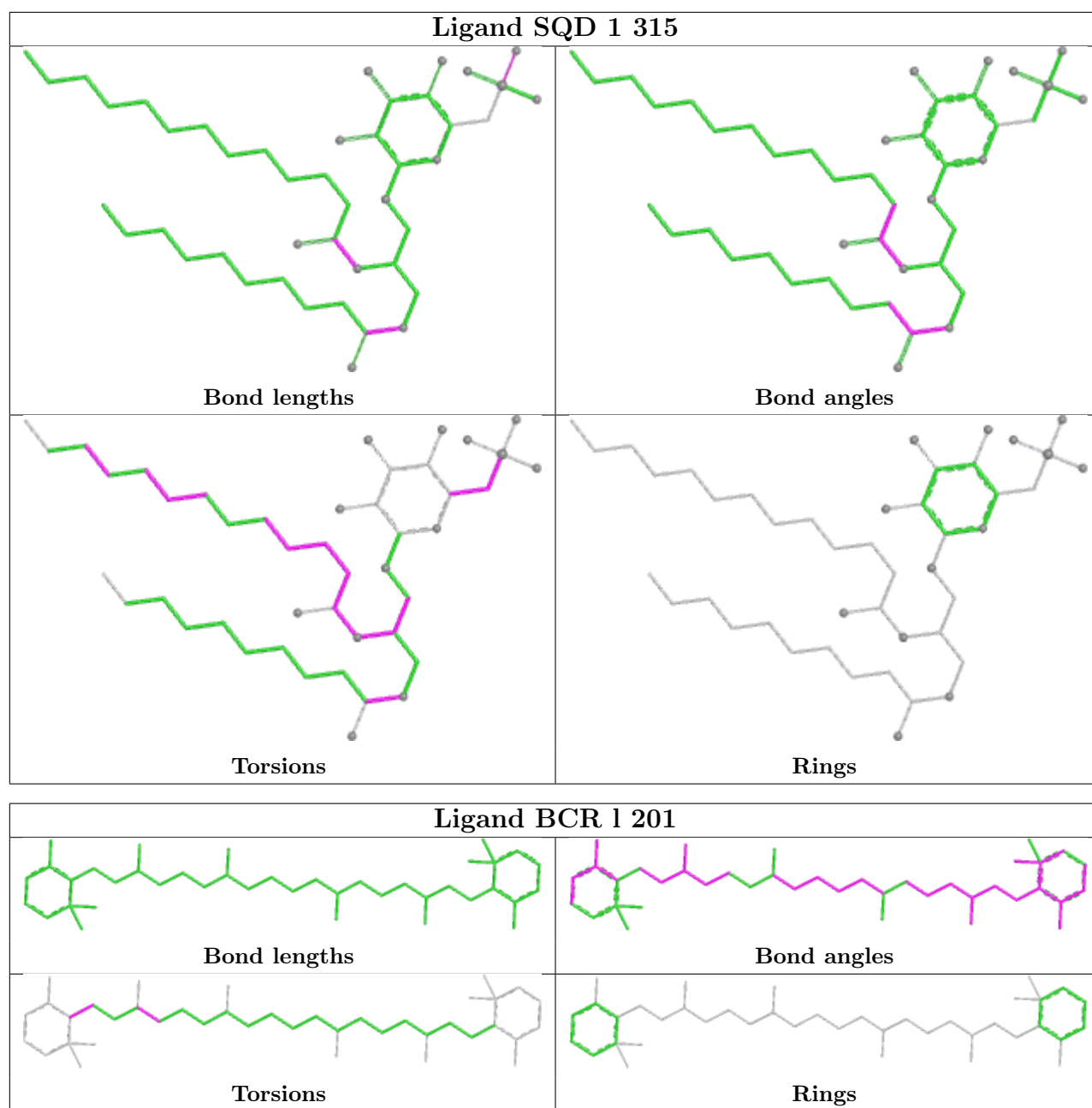


Ligand CLA 4 307

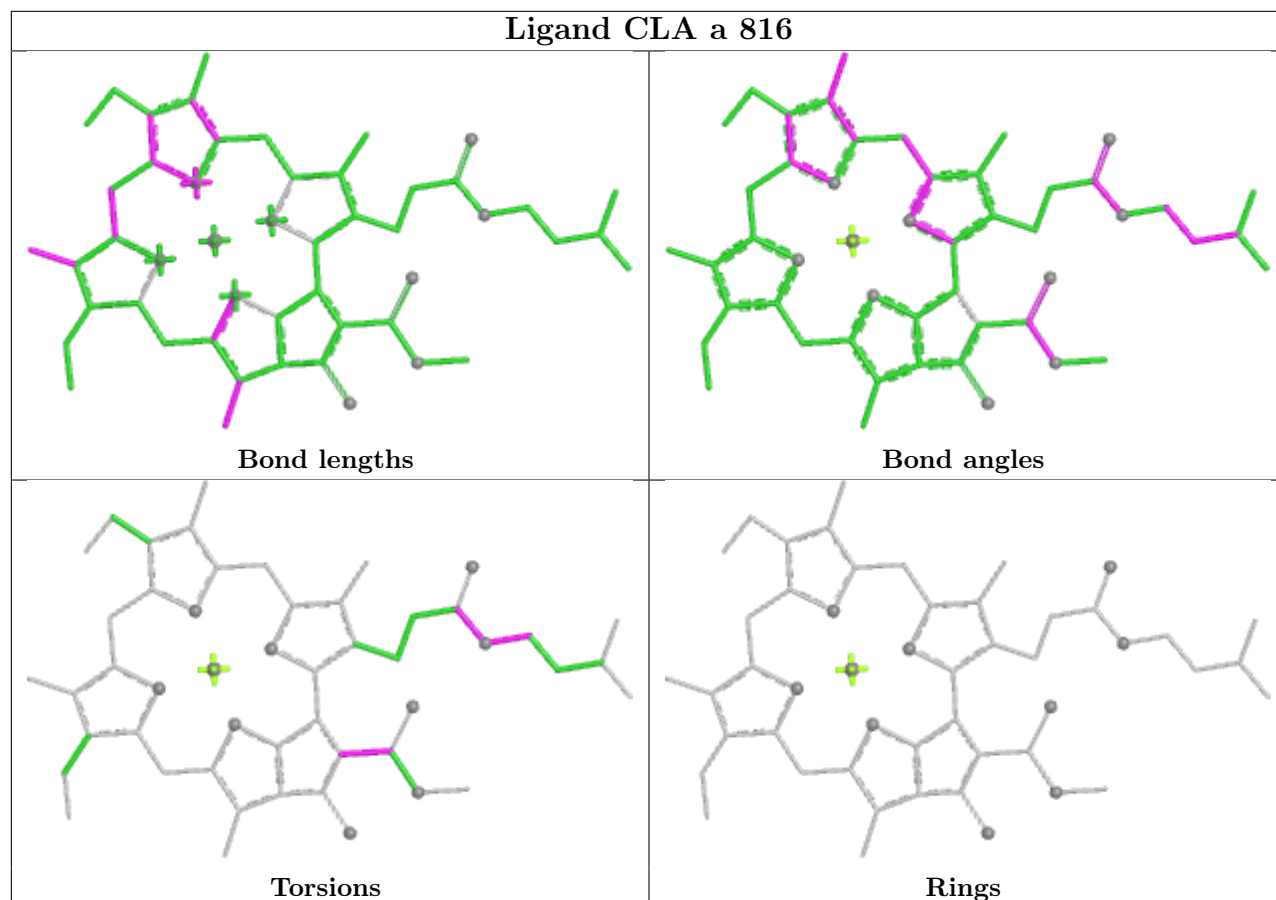


Ligand CLA 3 313

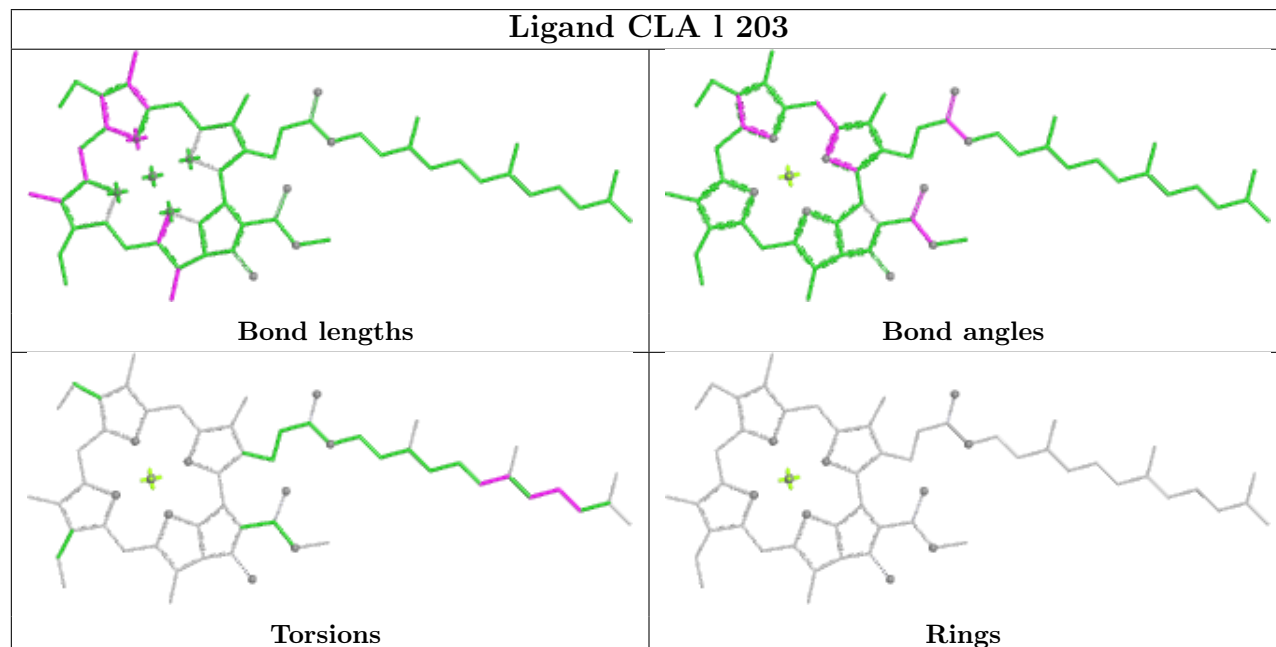


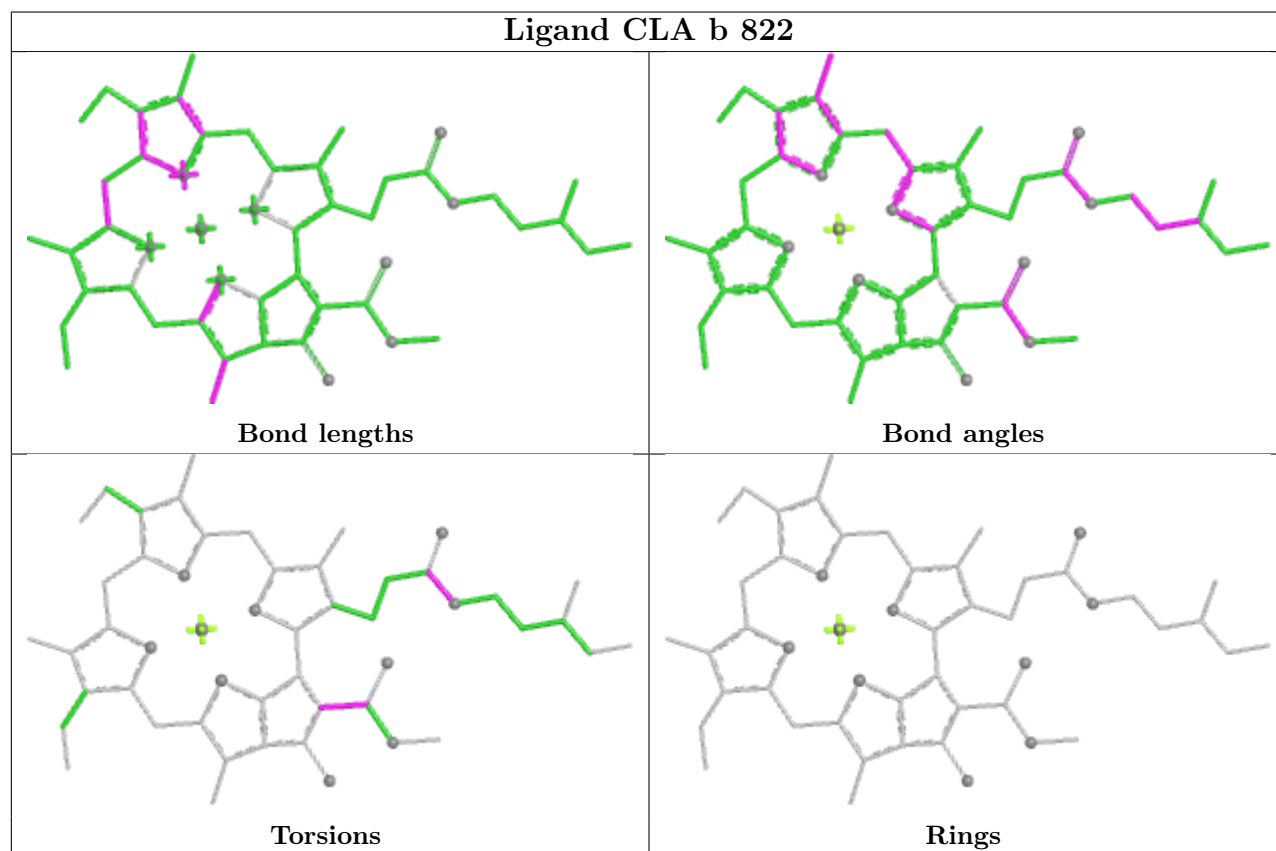
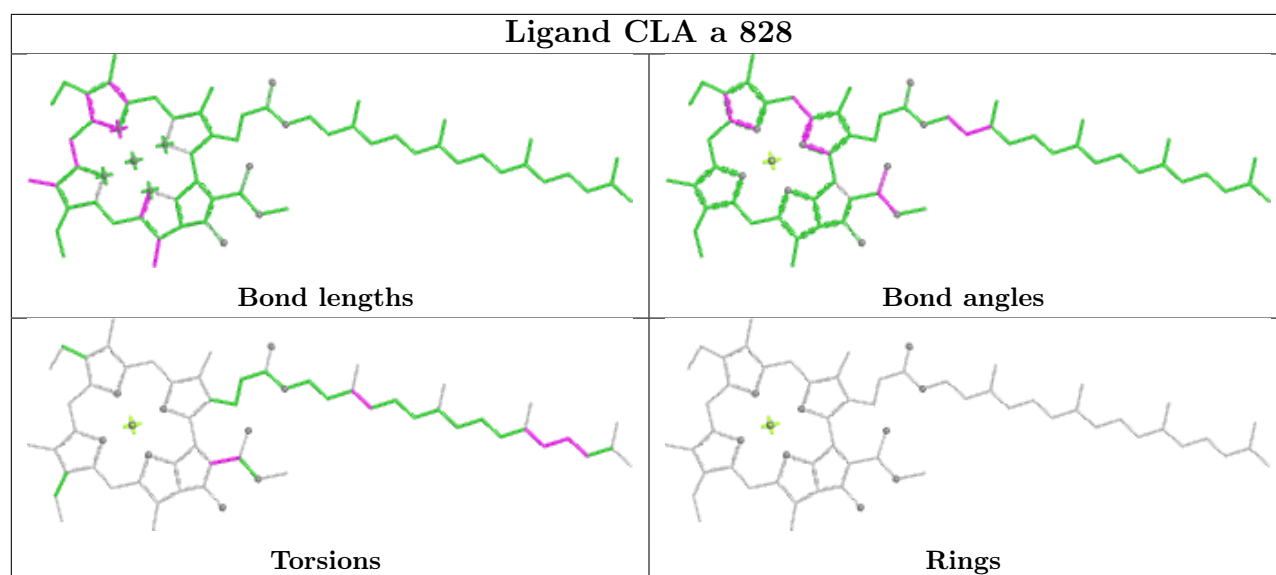


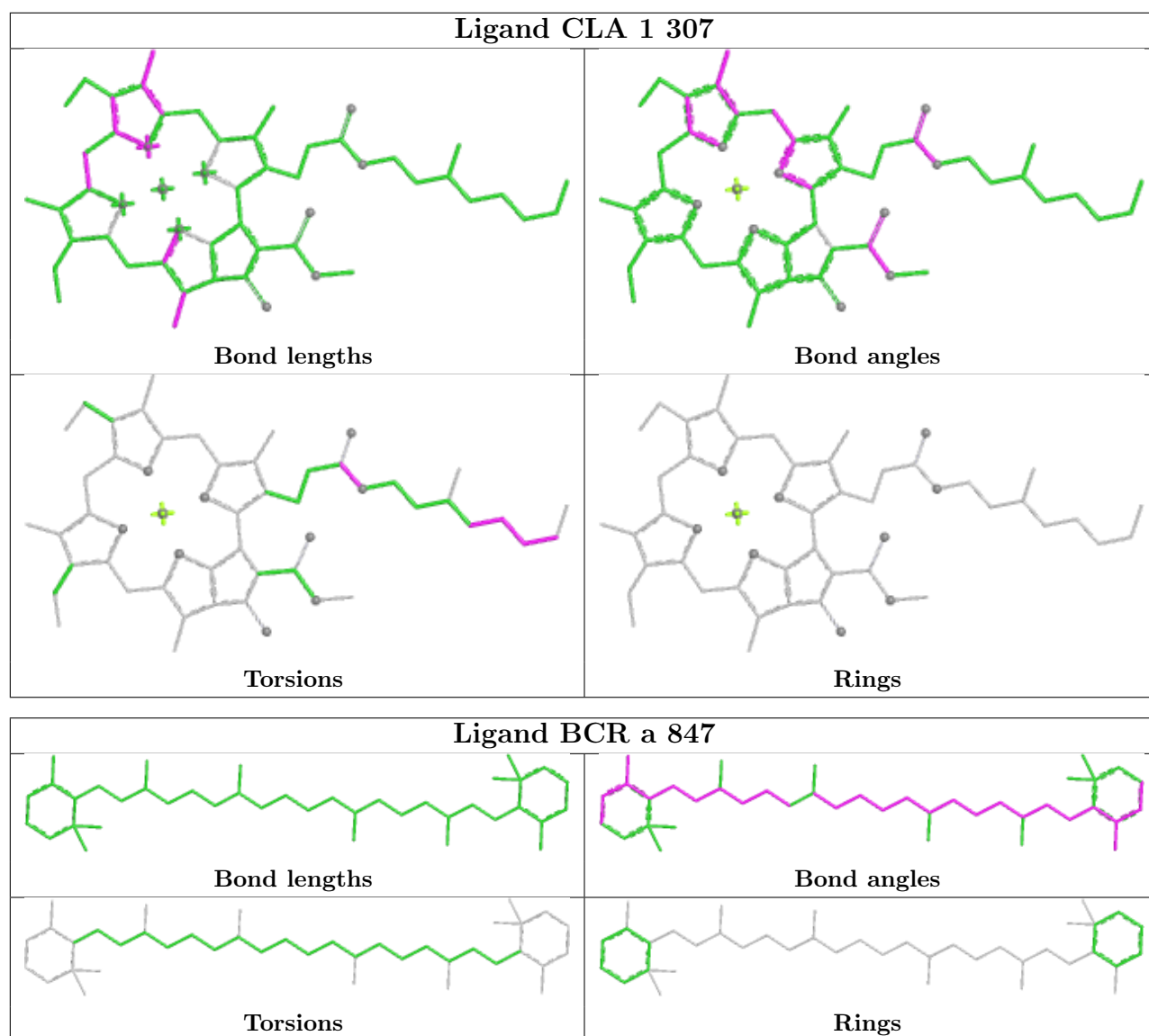
Ligand CLA a 816

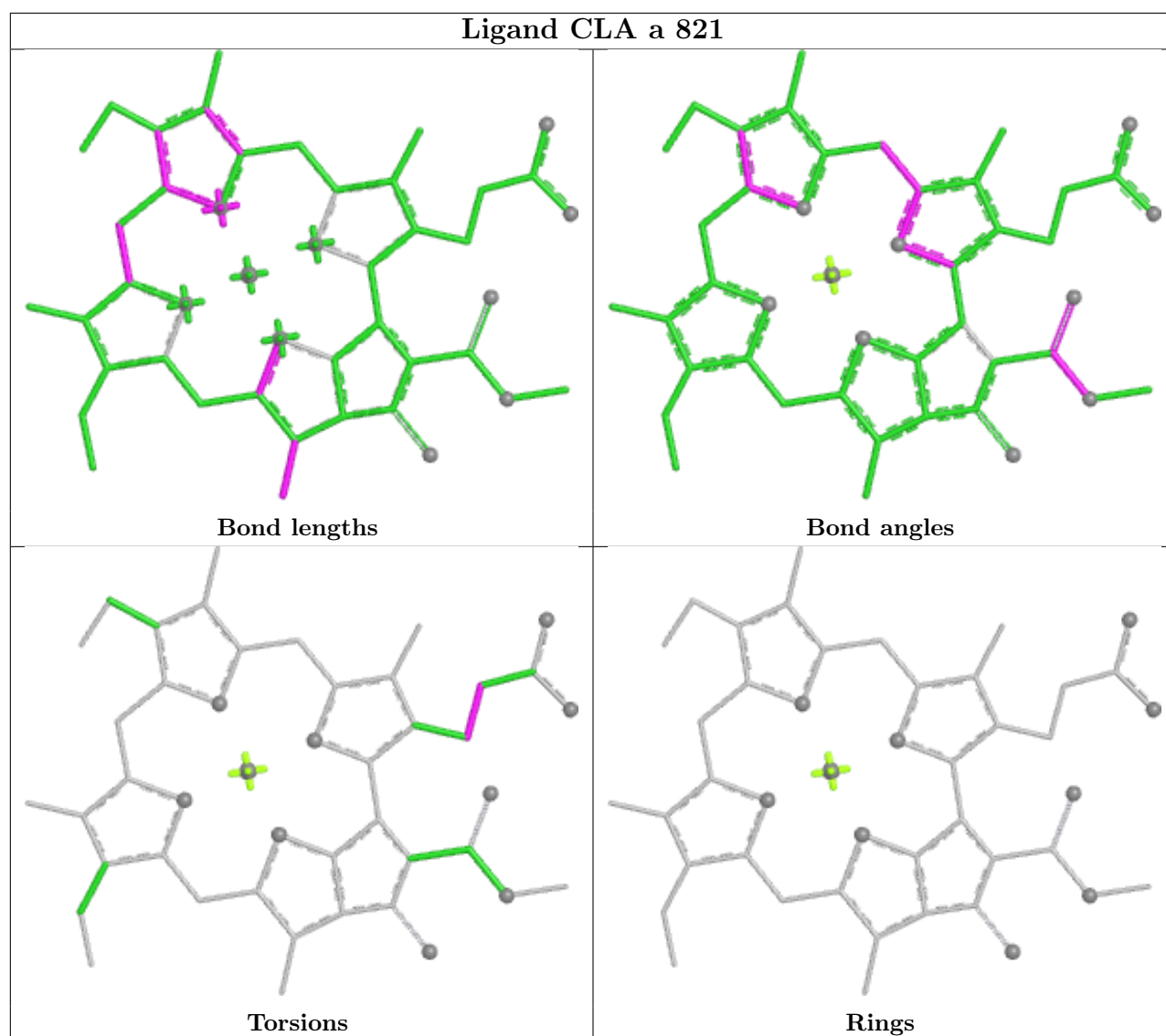


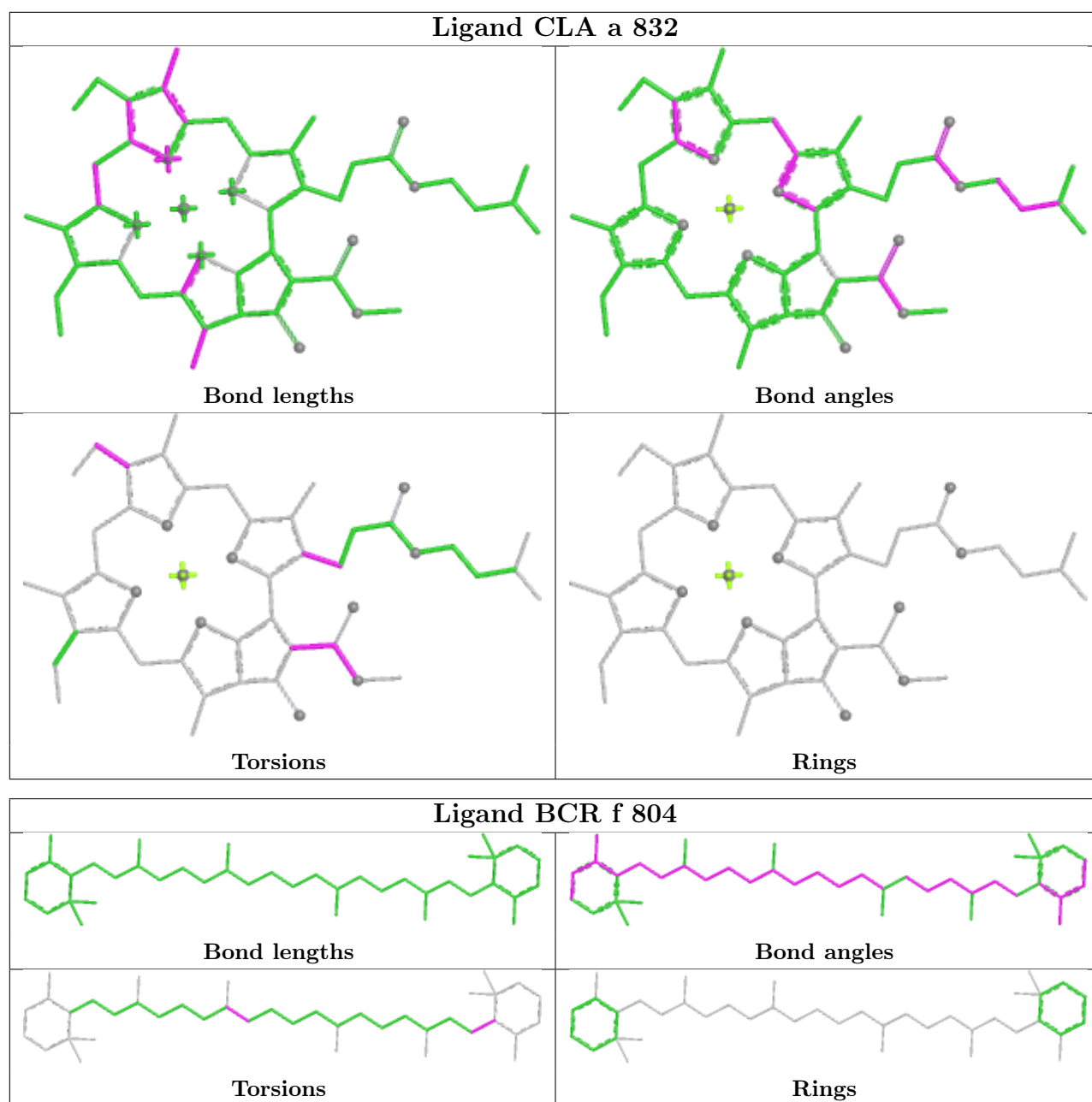
Ligand CLA l 203



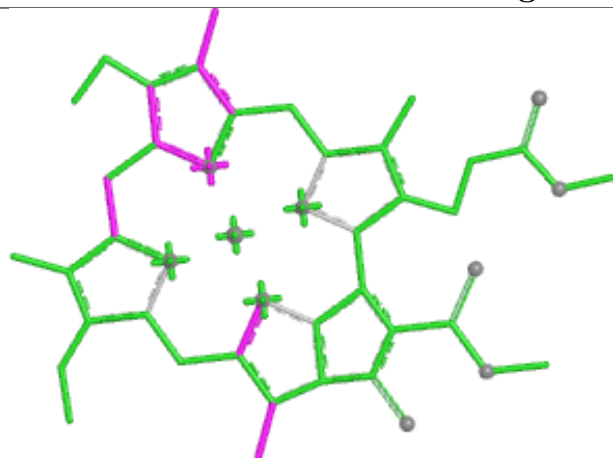




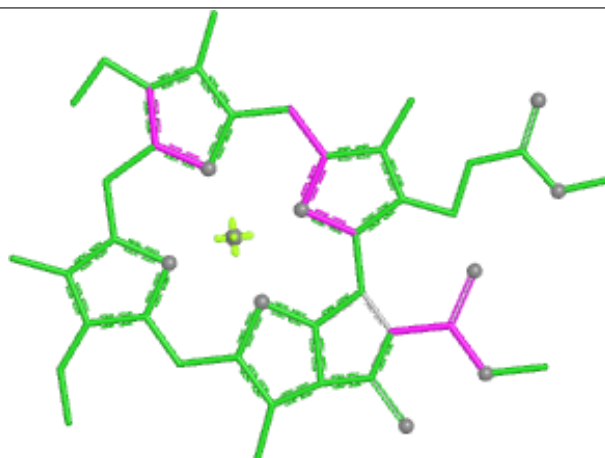




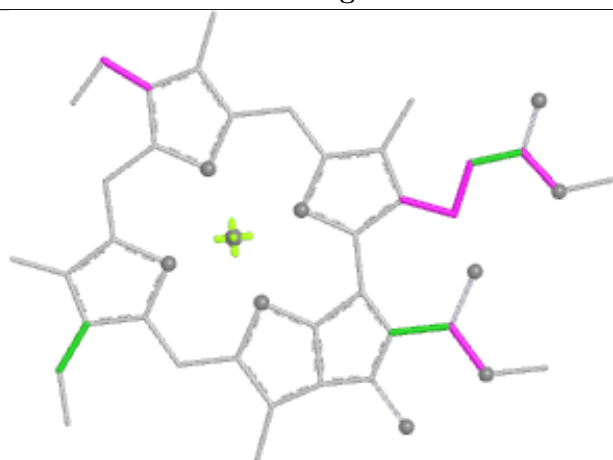
Ligand CLA 4 311



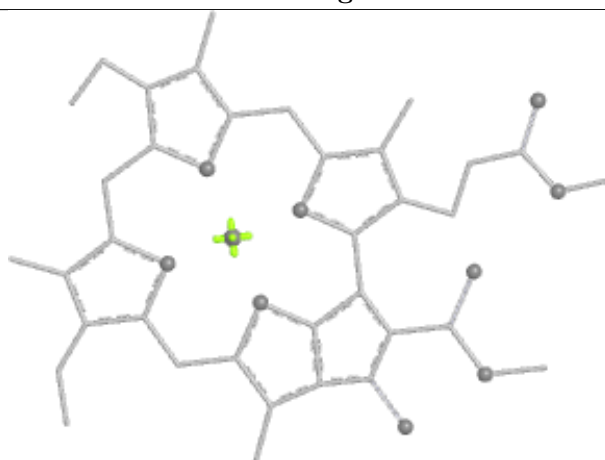
Bond lengths



Bond angles

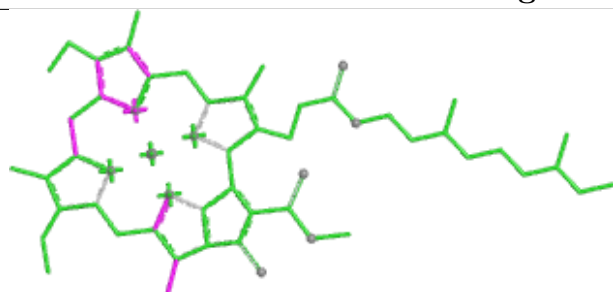


Torsions

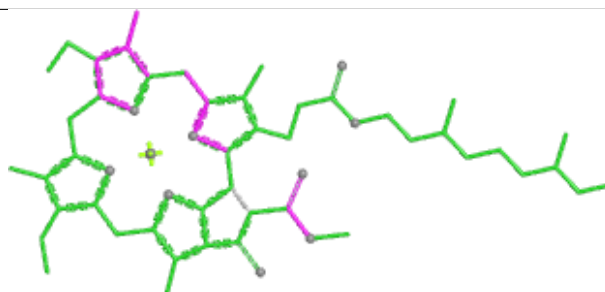


Rings

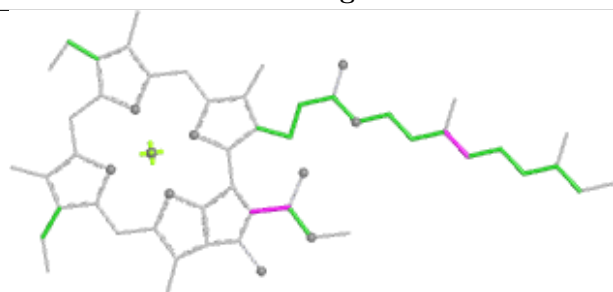
Ligand CLA 3 310



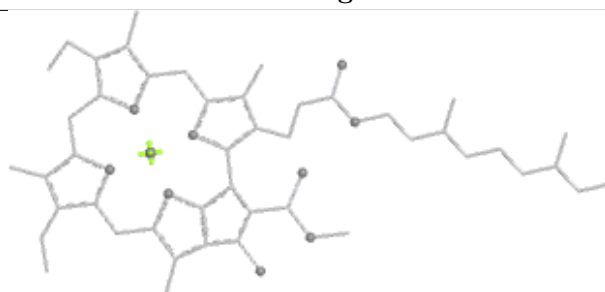
Bond lengths



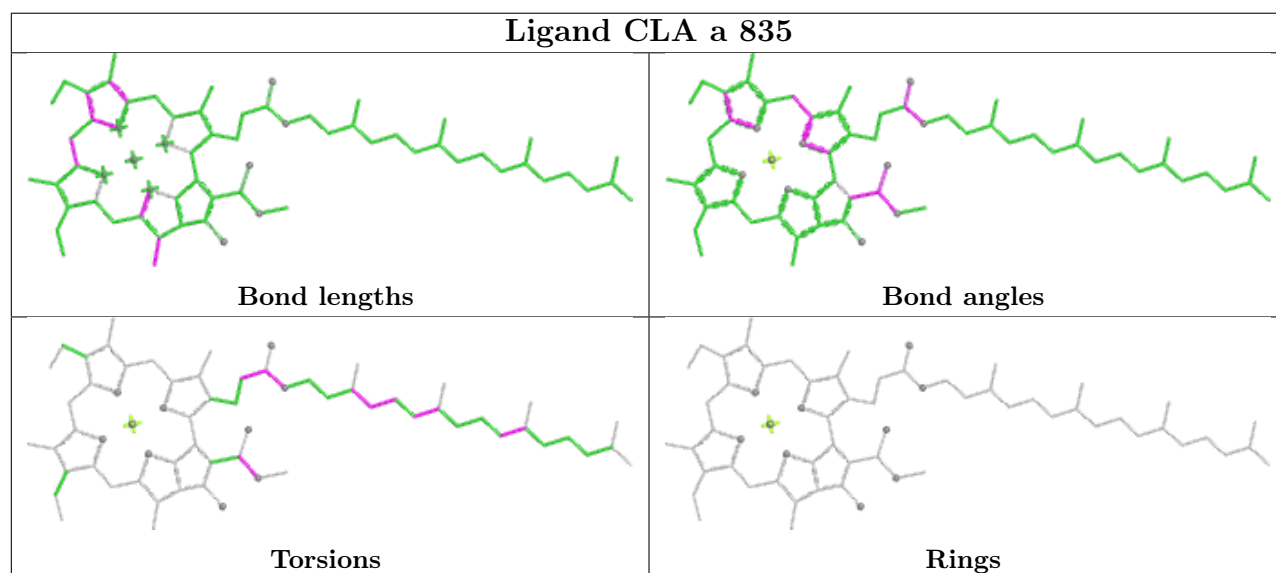
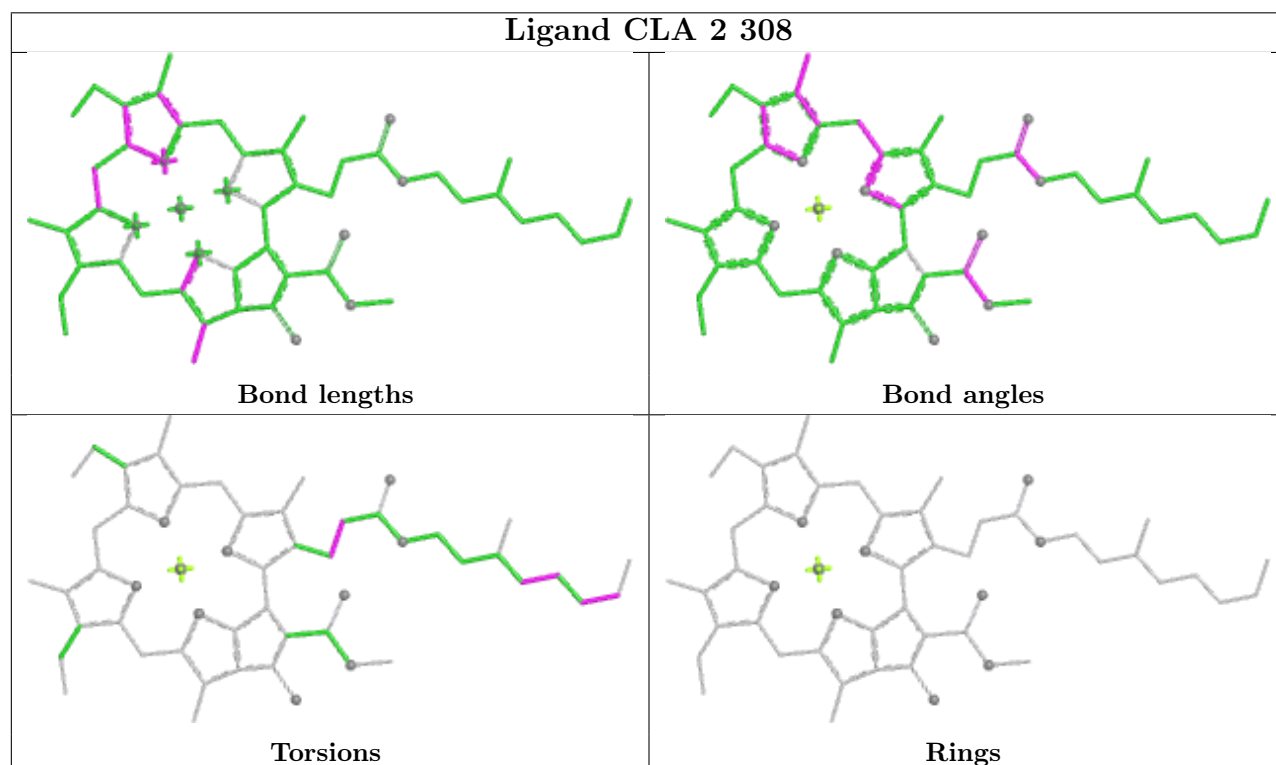
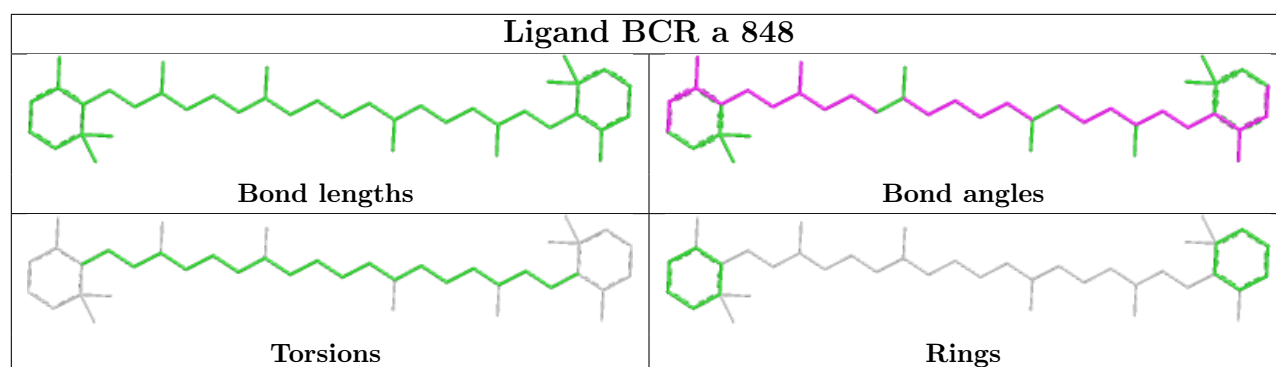
Bond angles

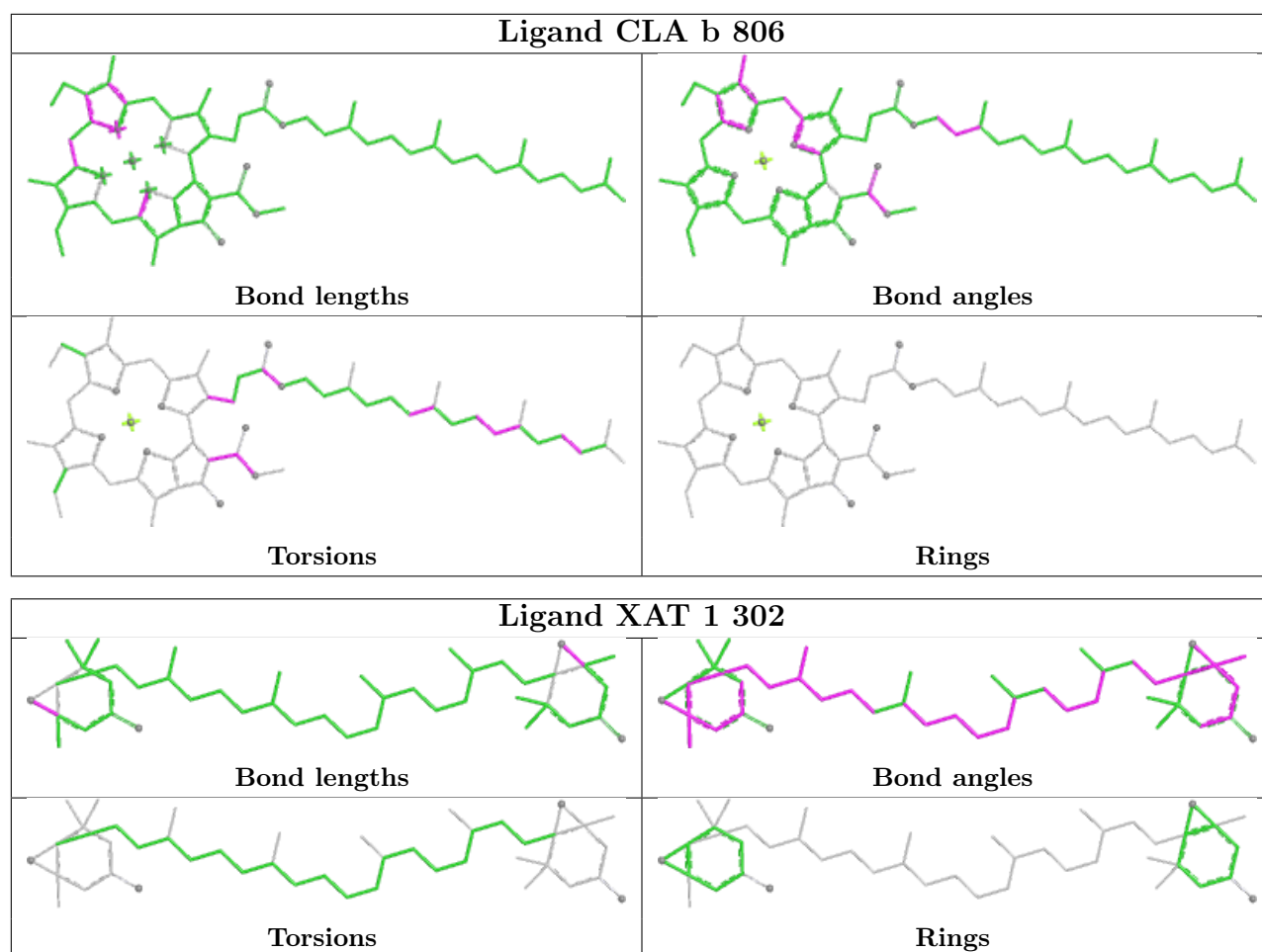


Torsions

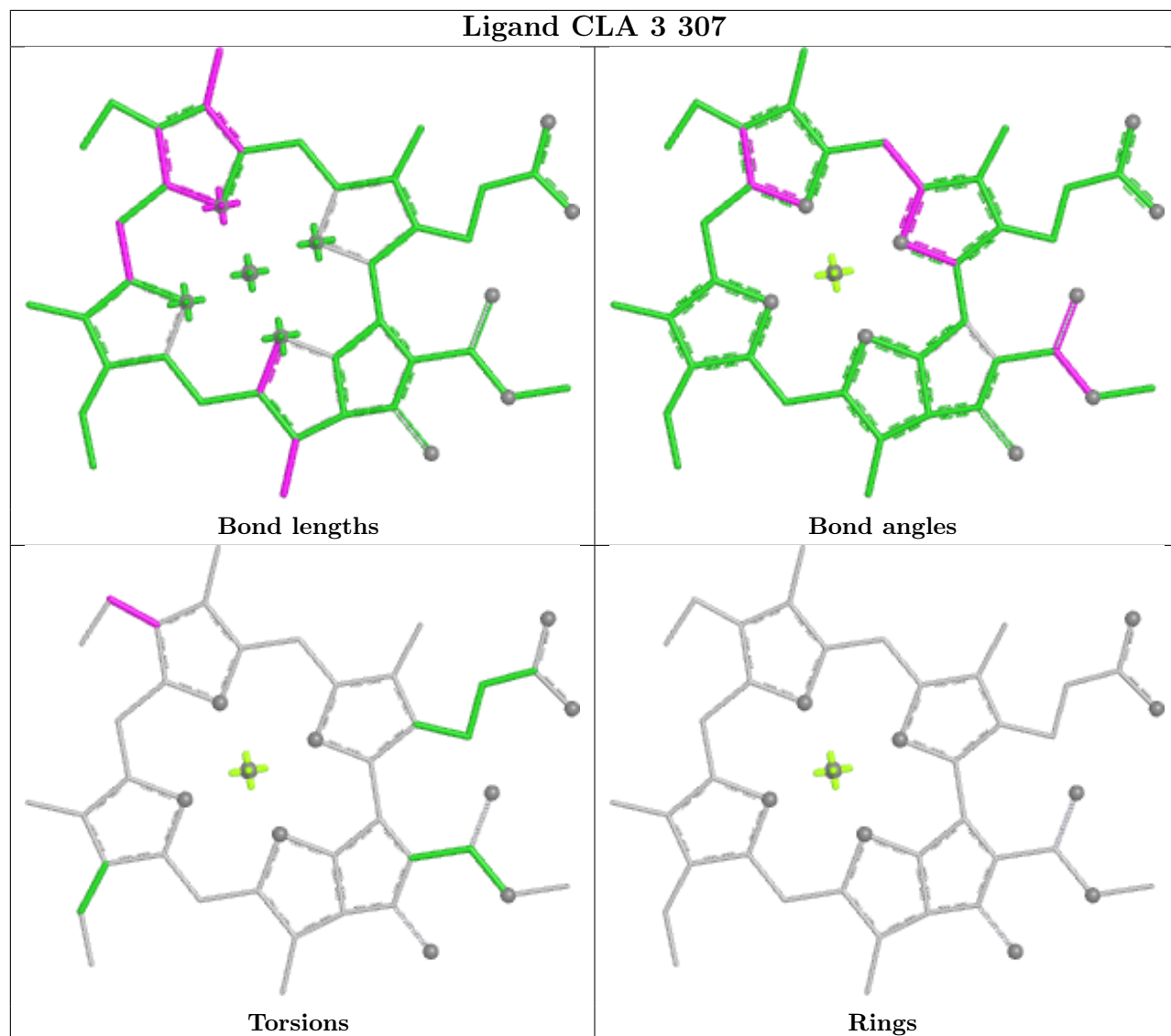


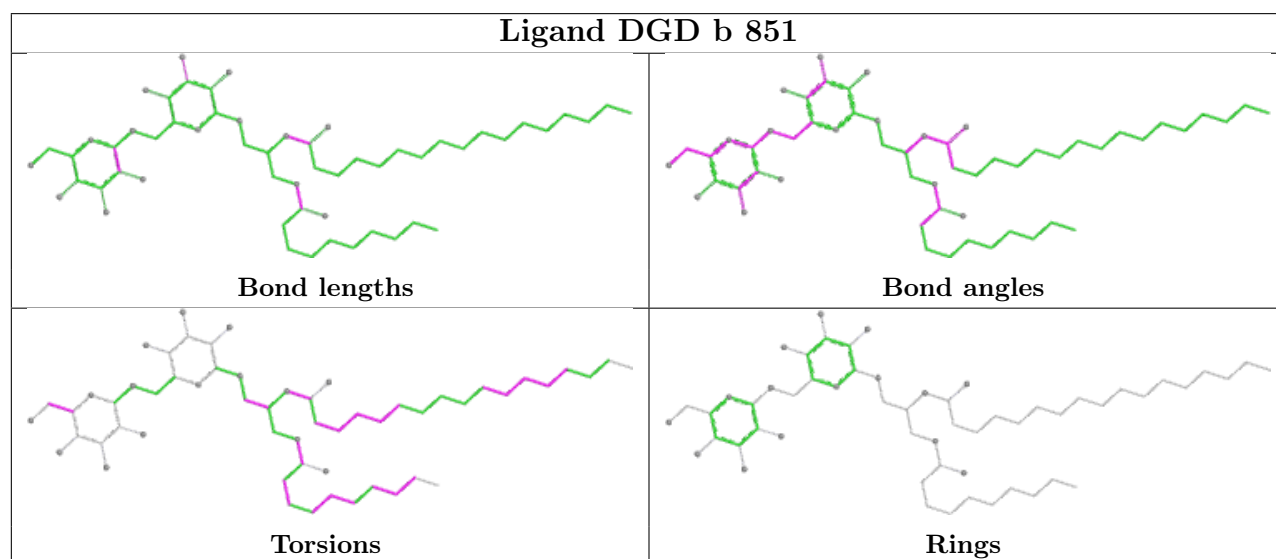
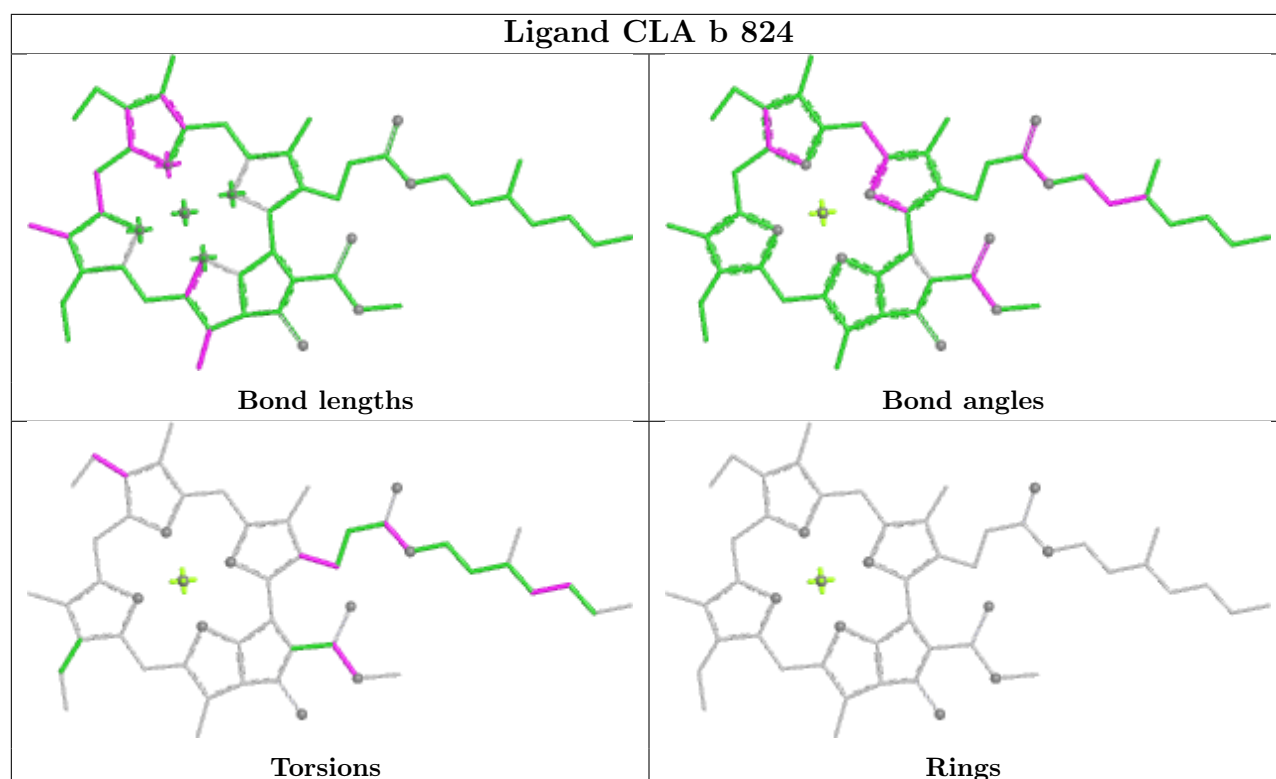
Rings



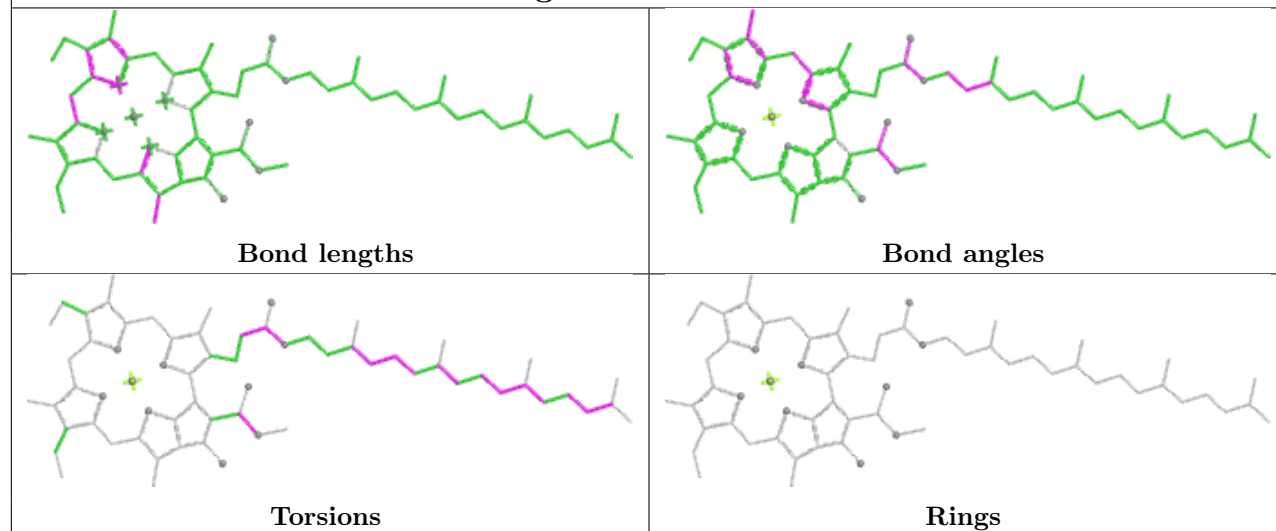


Ligand CLA 3 307

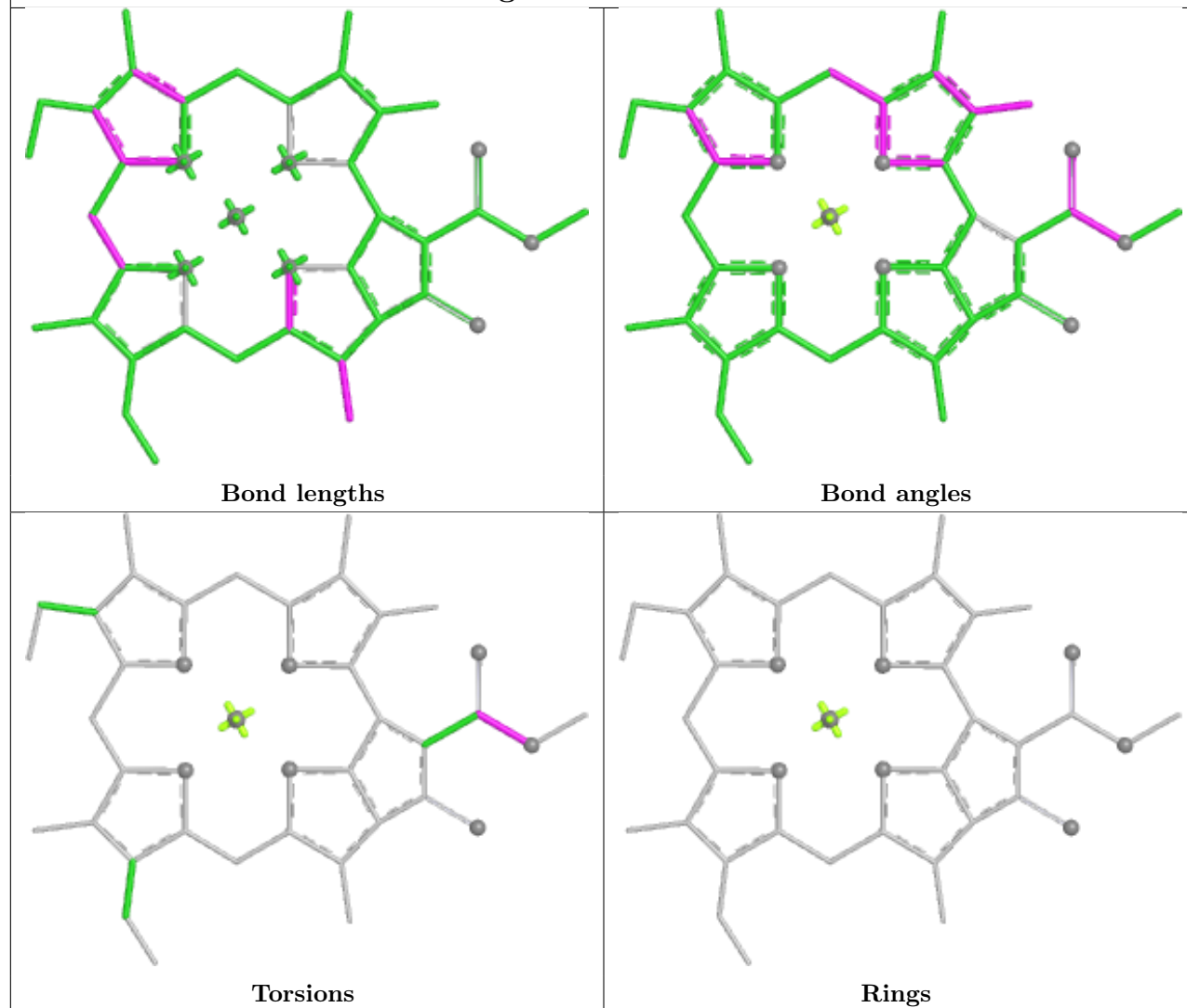


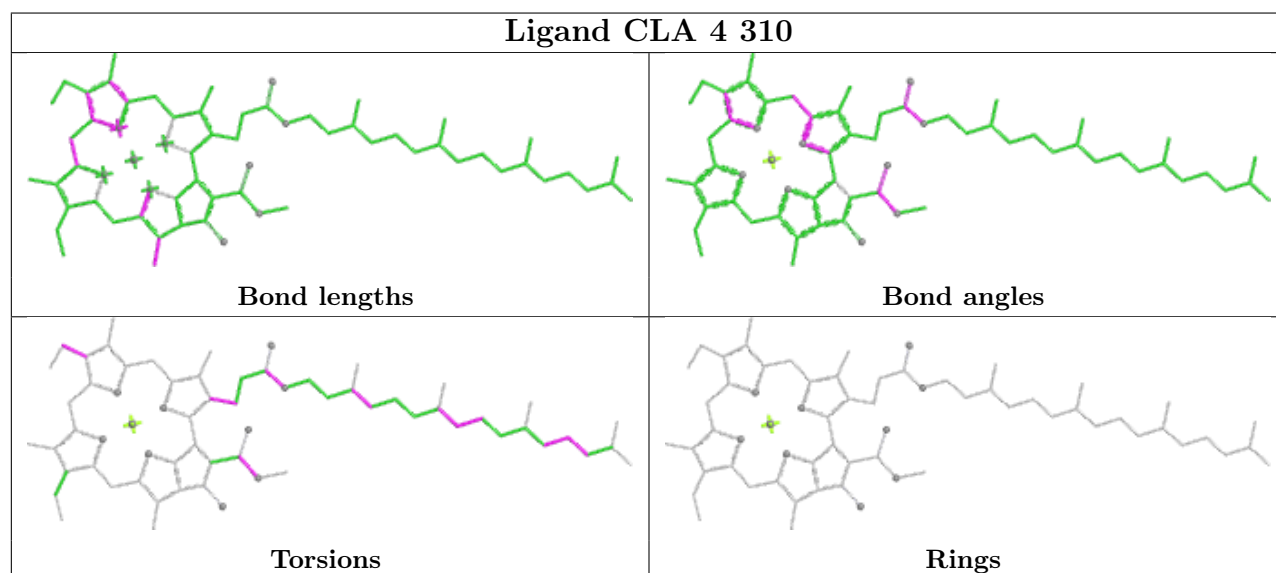
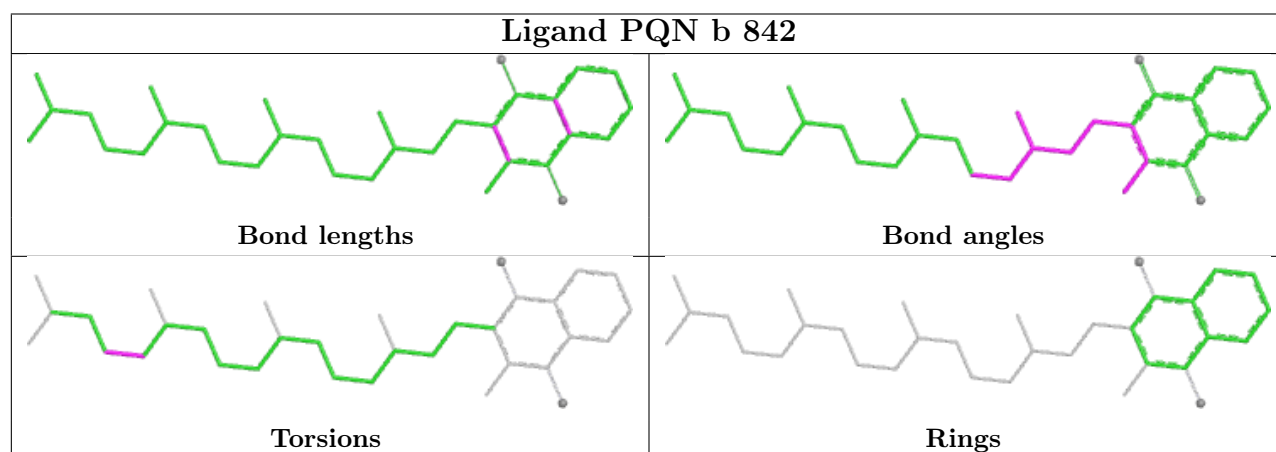
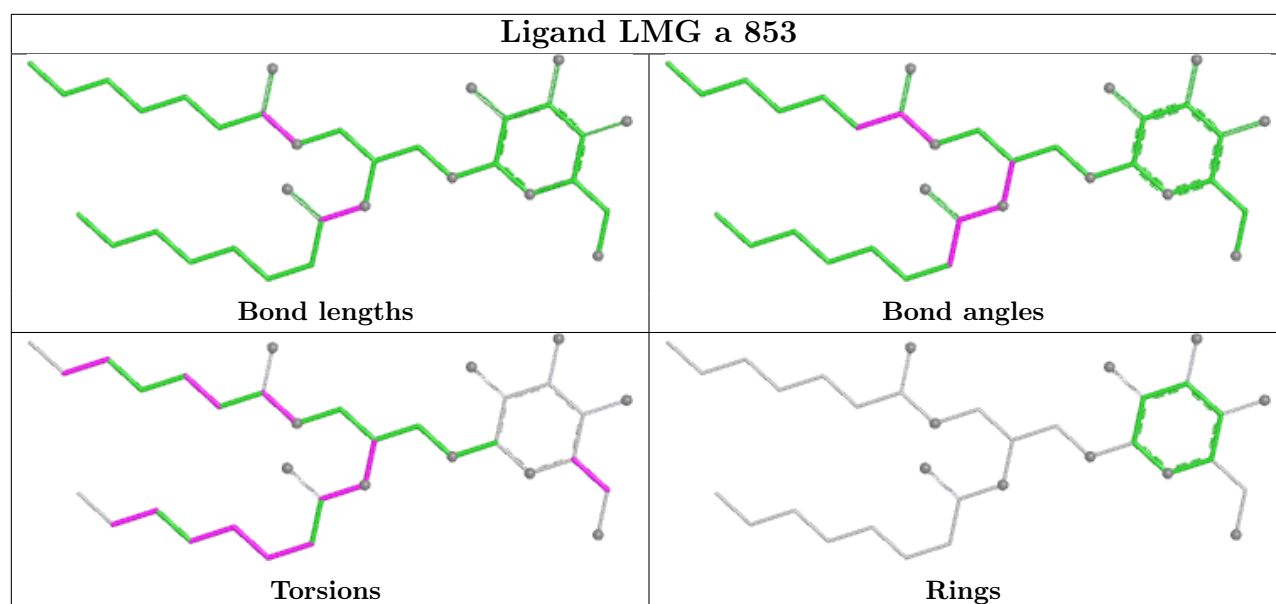


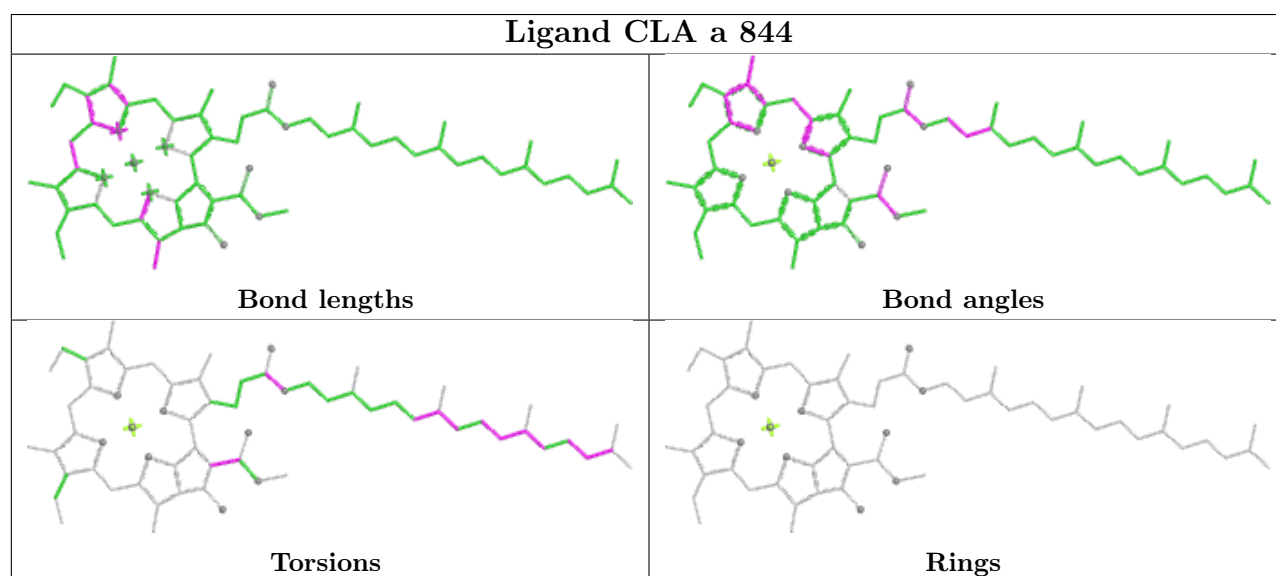
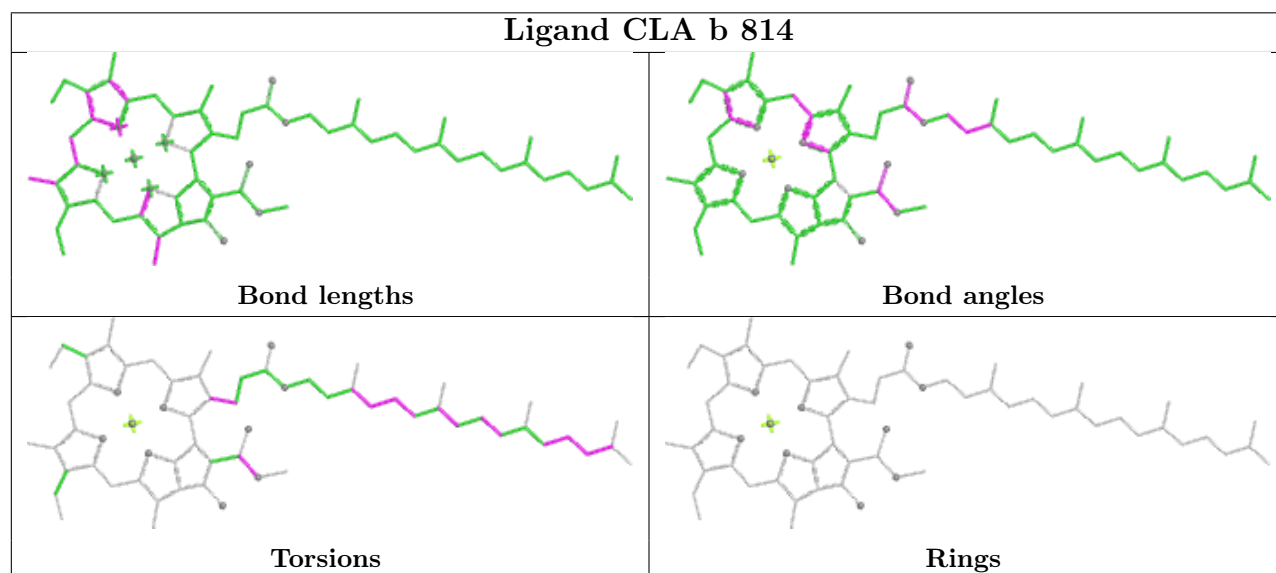
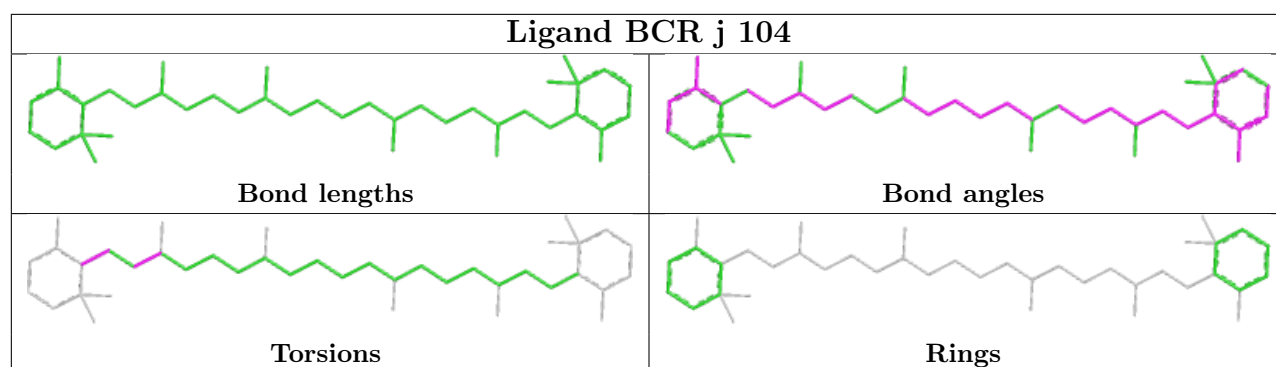
Ligand CLA b 807

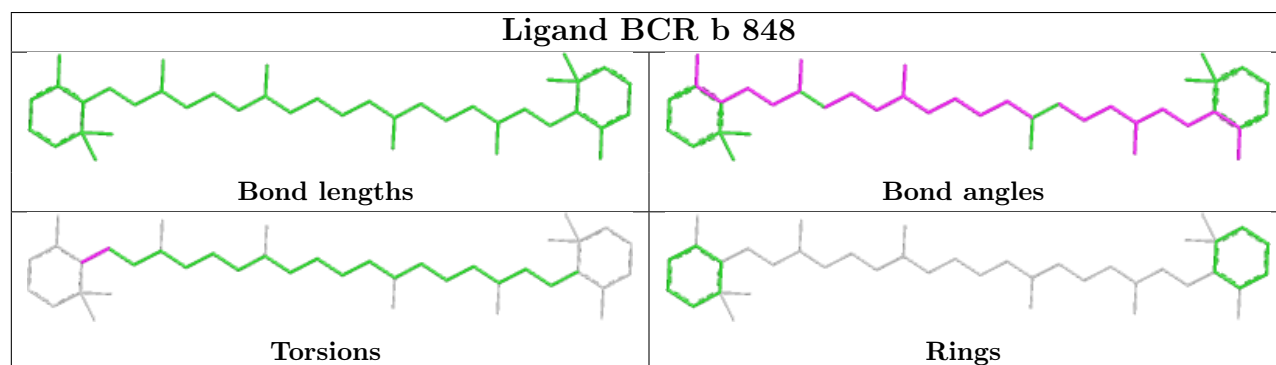
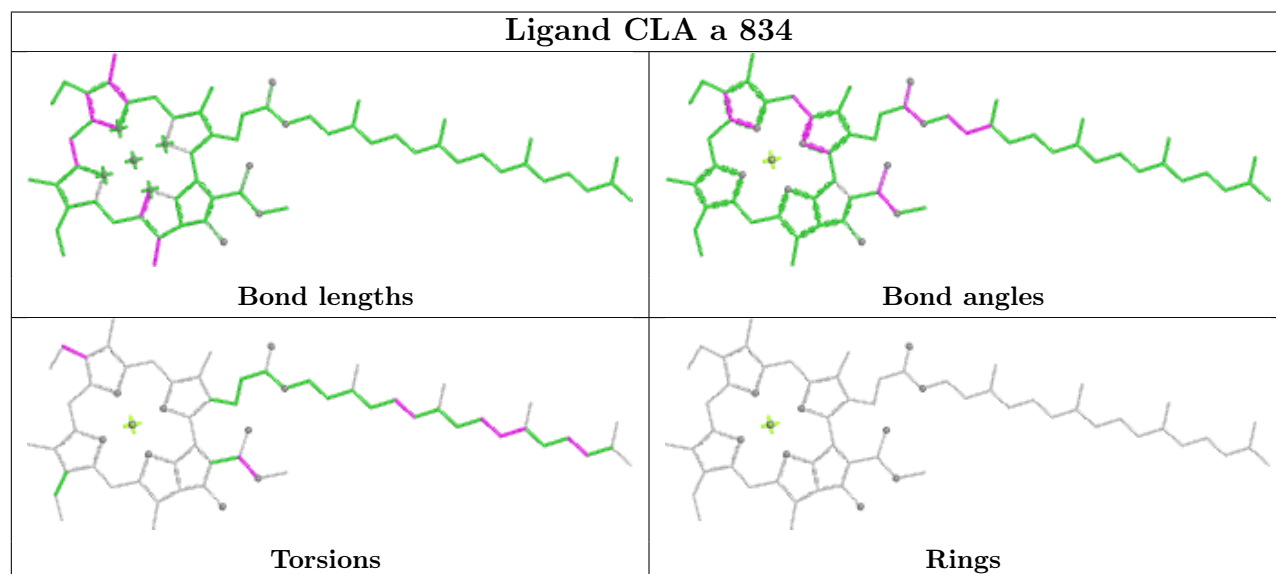
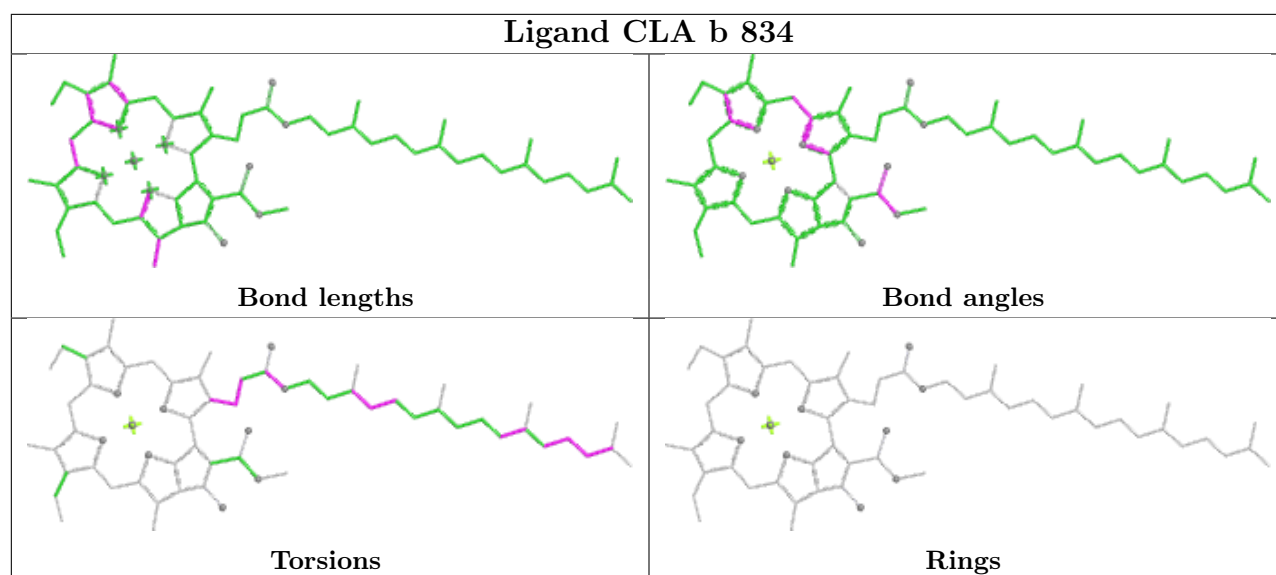


Ligand CLA 2 313

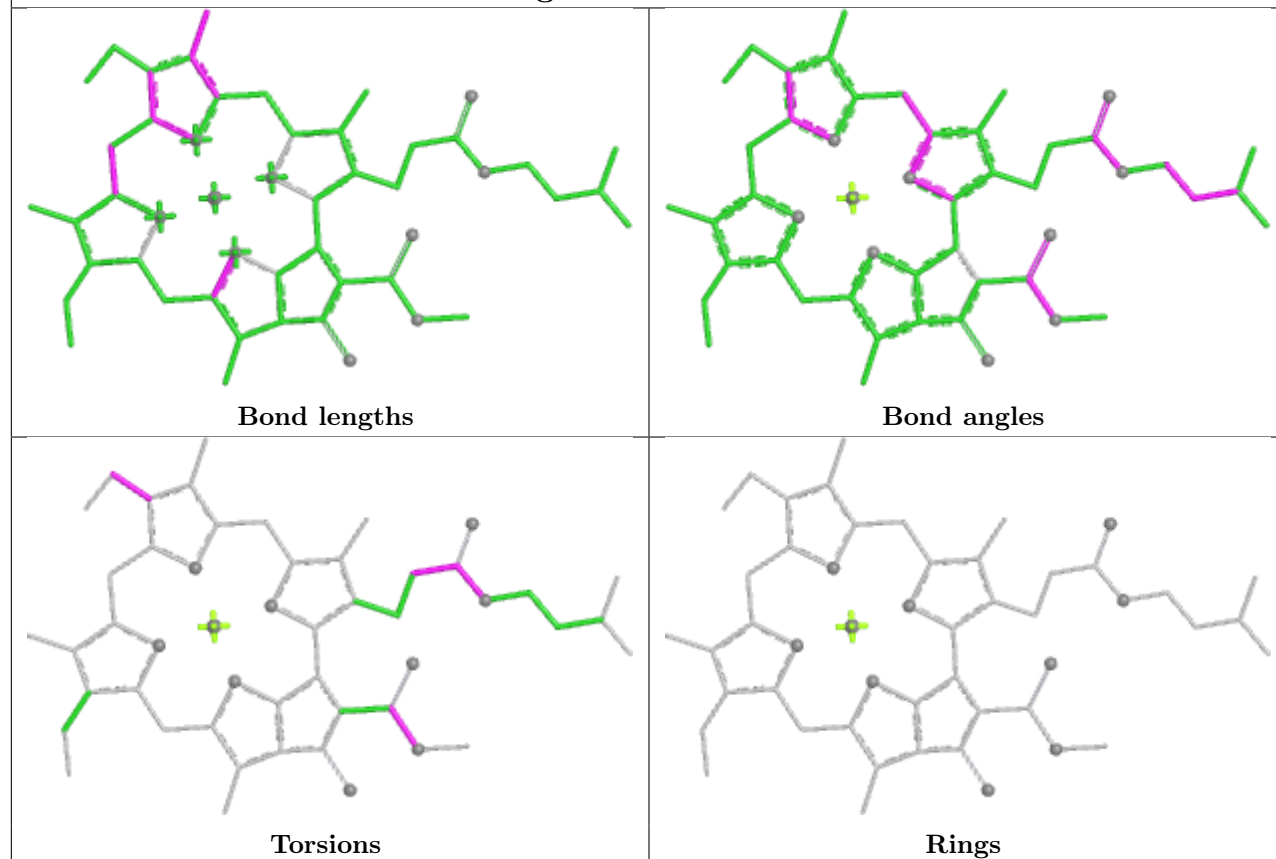




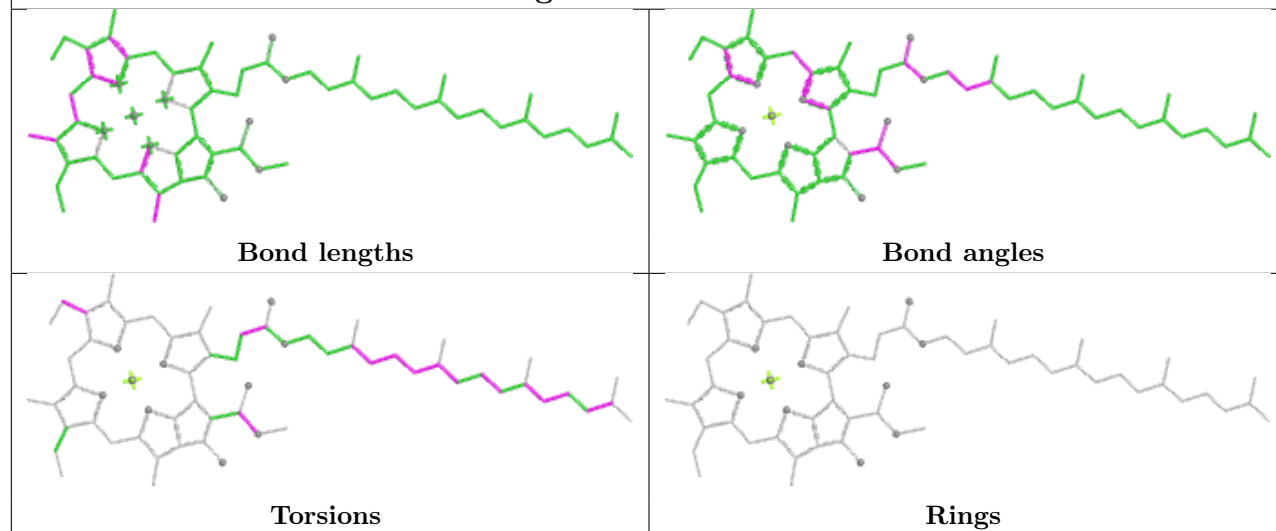




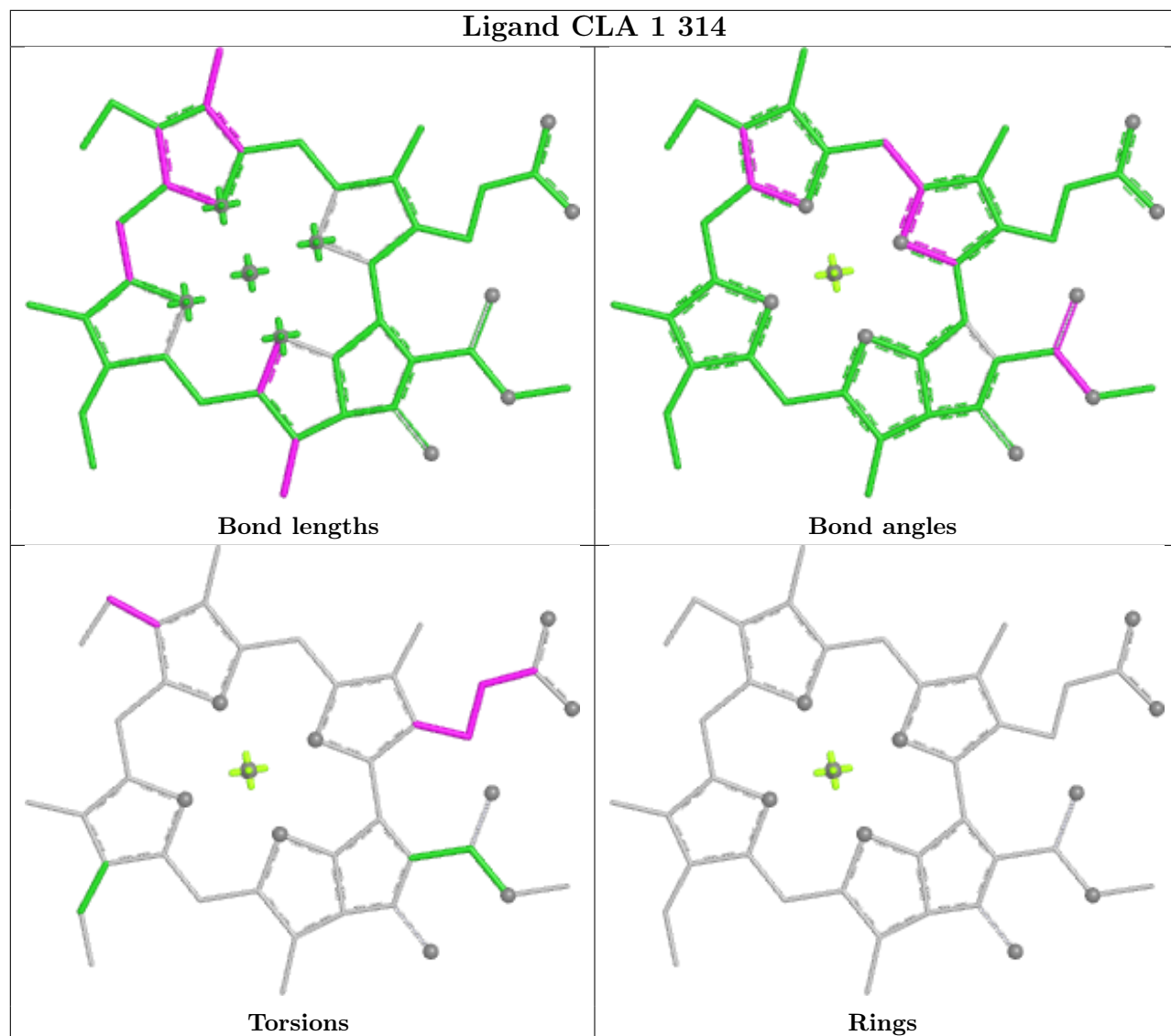
Ligand CLA a 836



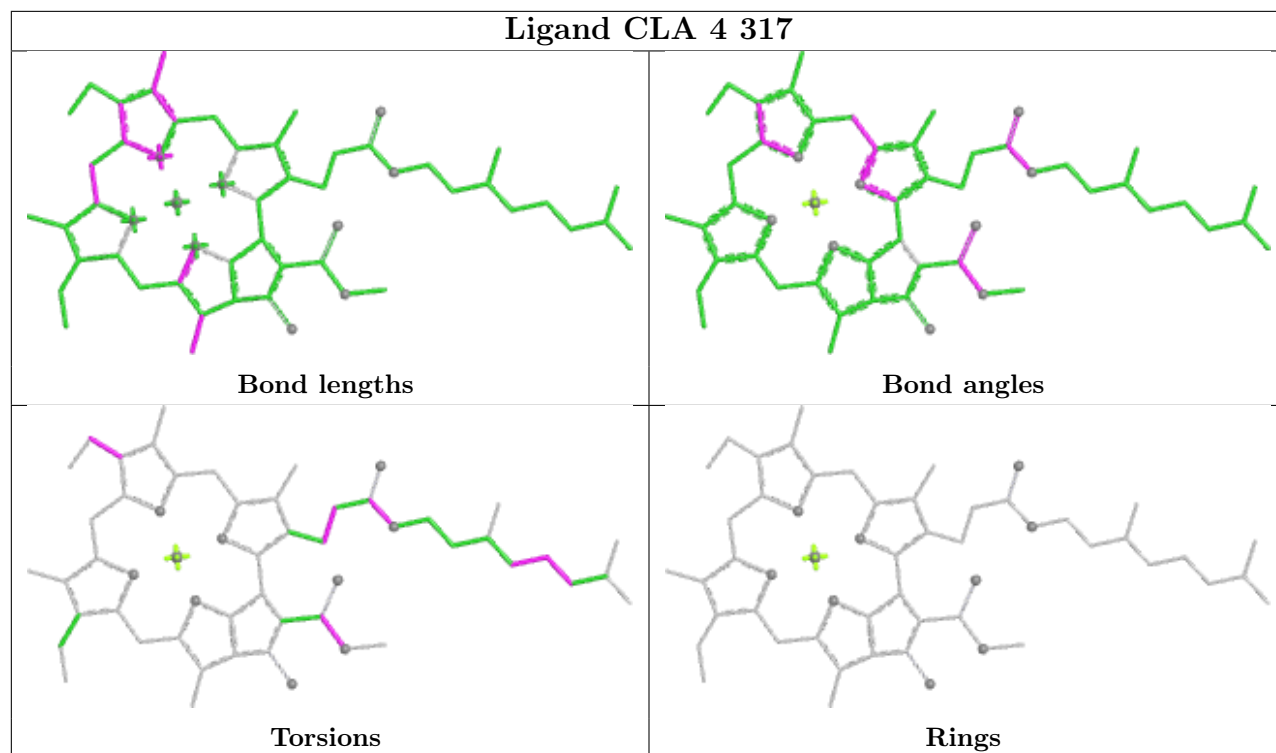
Ligand CLA b 803



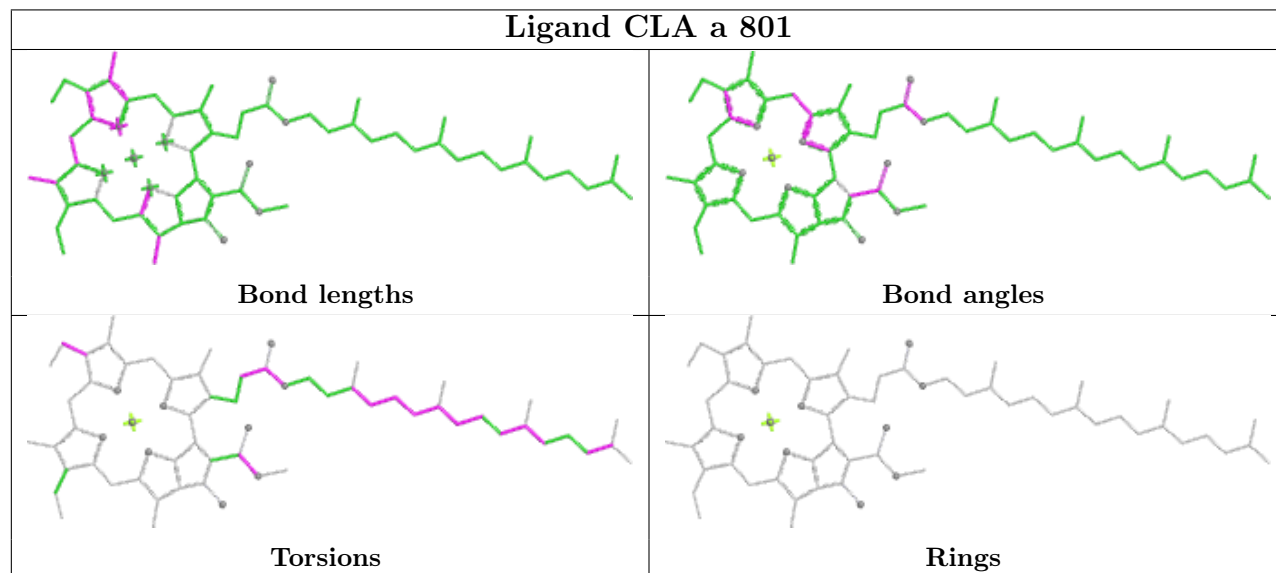
Ligand CLA 1 314



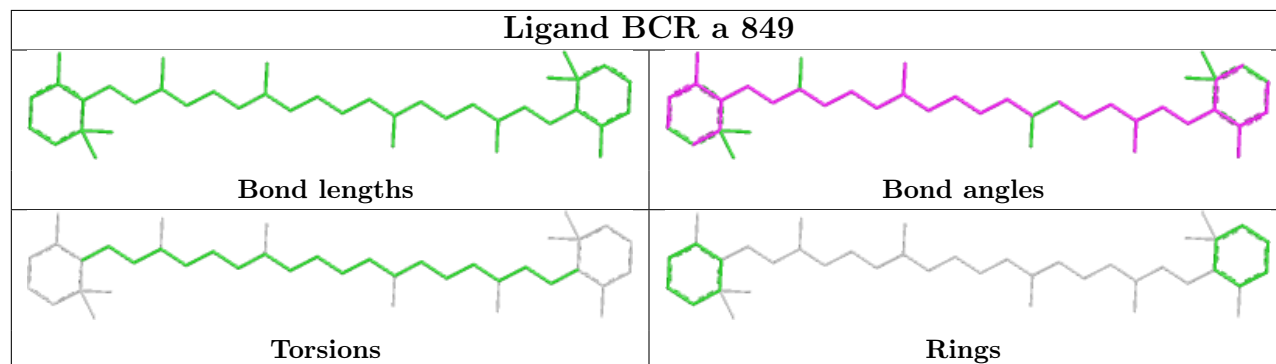
Ligand CLA 4 317



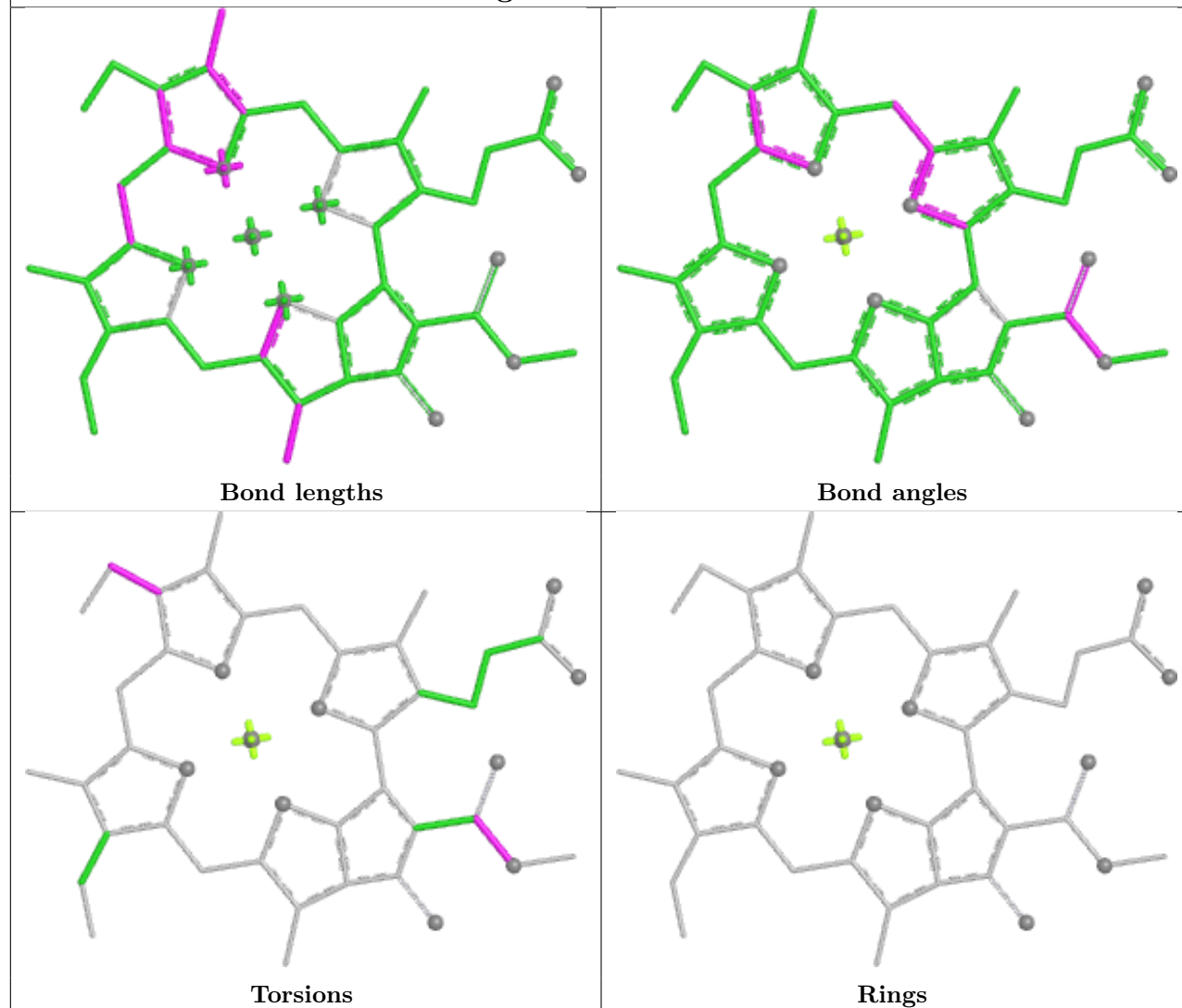
Ligand CLA a 801



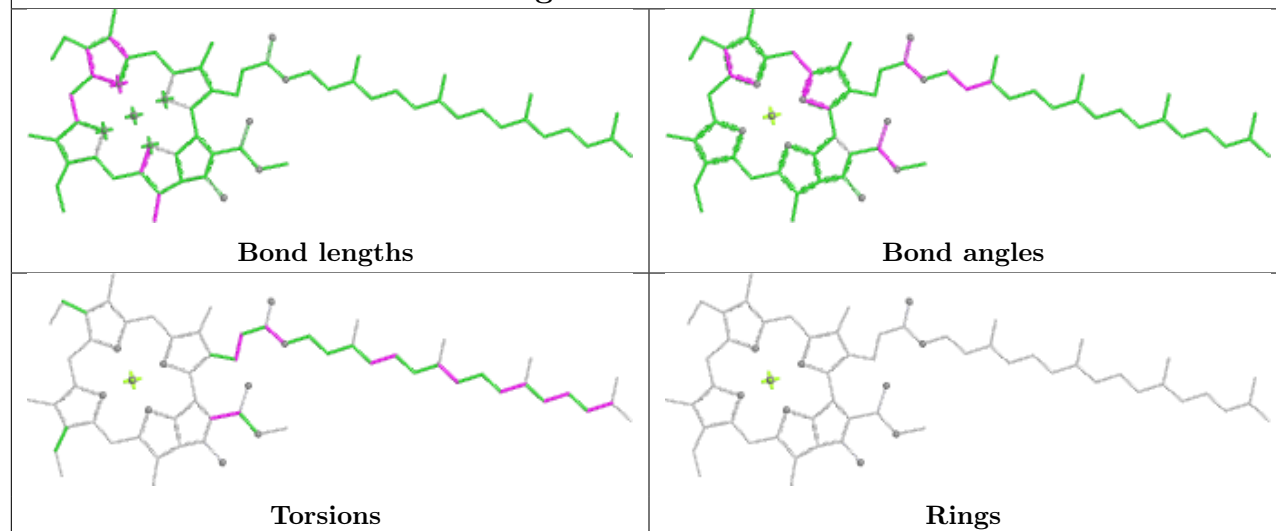
Ligand BCR a 849



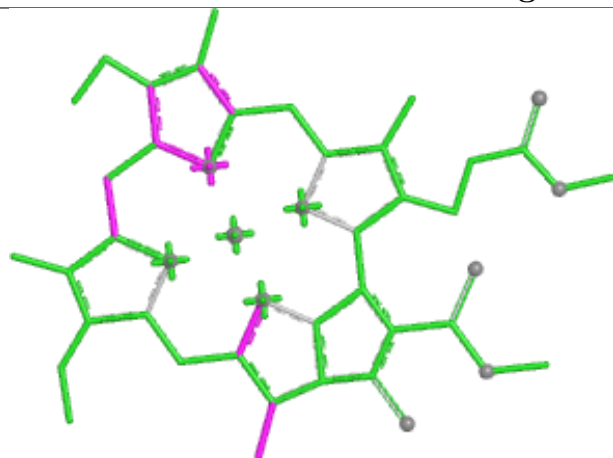
Ligand CLA a 837



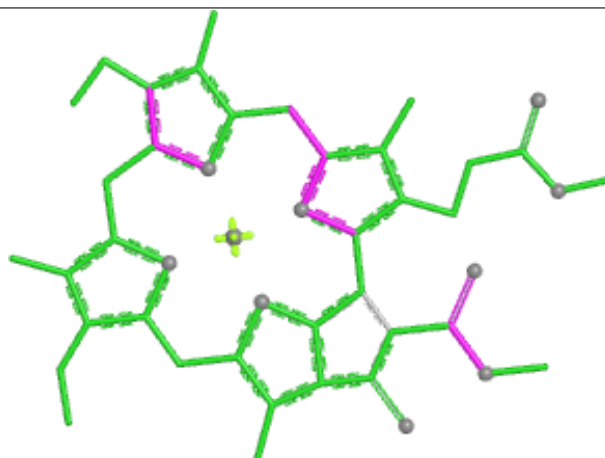
Ligand CLA b 805



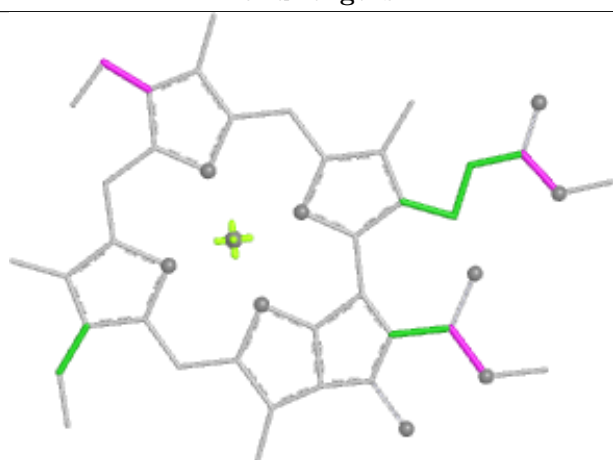
Ligand CLA 5 305



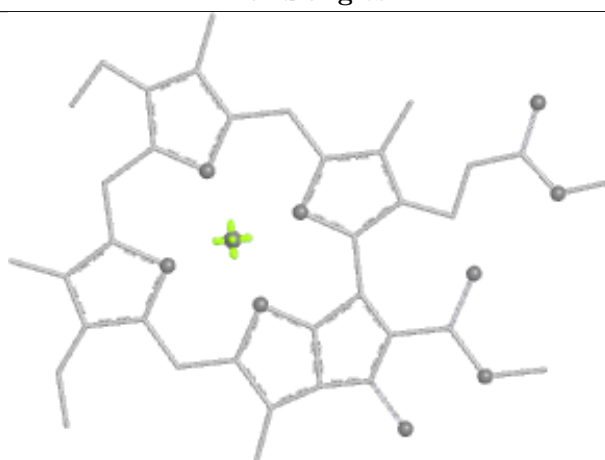
Bond lengths



Bond angles

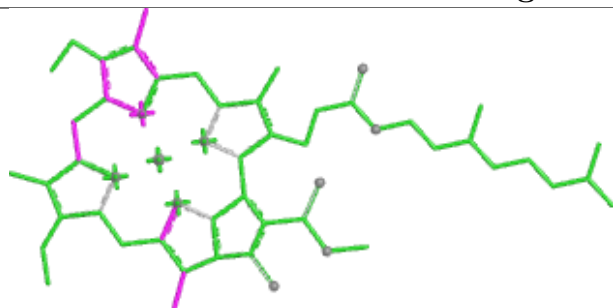


Torsions

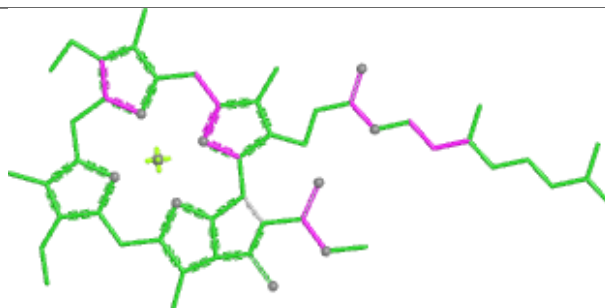


Rings

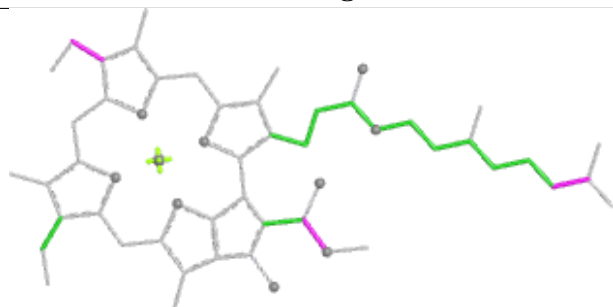
Ligand CLA b 820



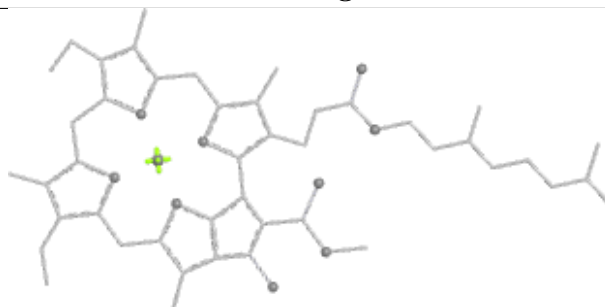
Bond lengths



Bond angles

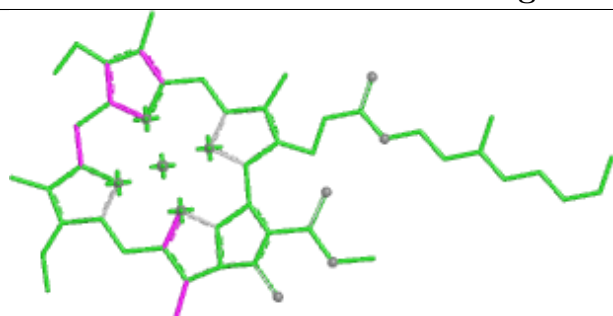


Torsions

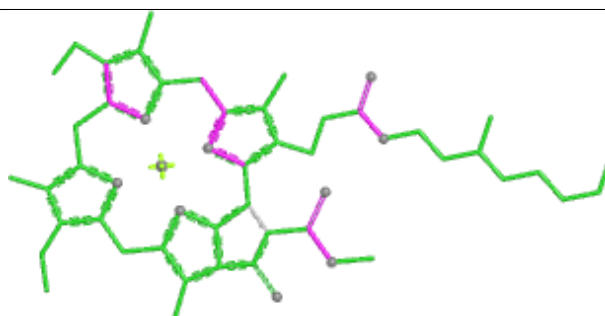


Rings

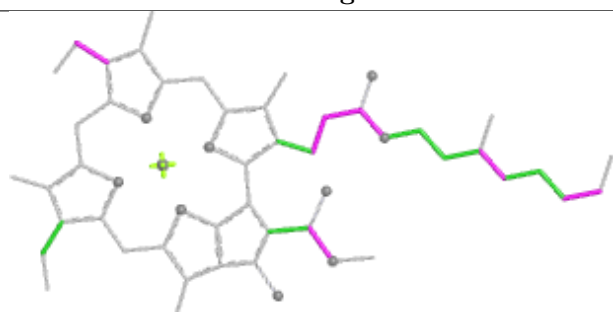
Ligand CLA a 813



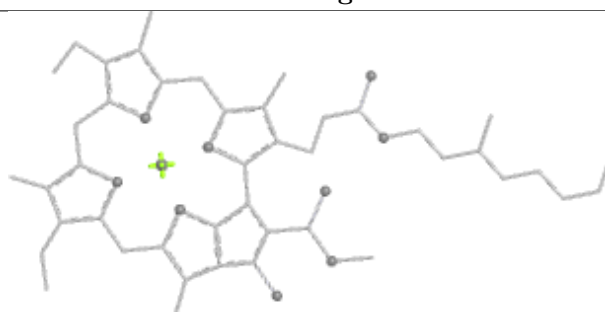
Bond lengths



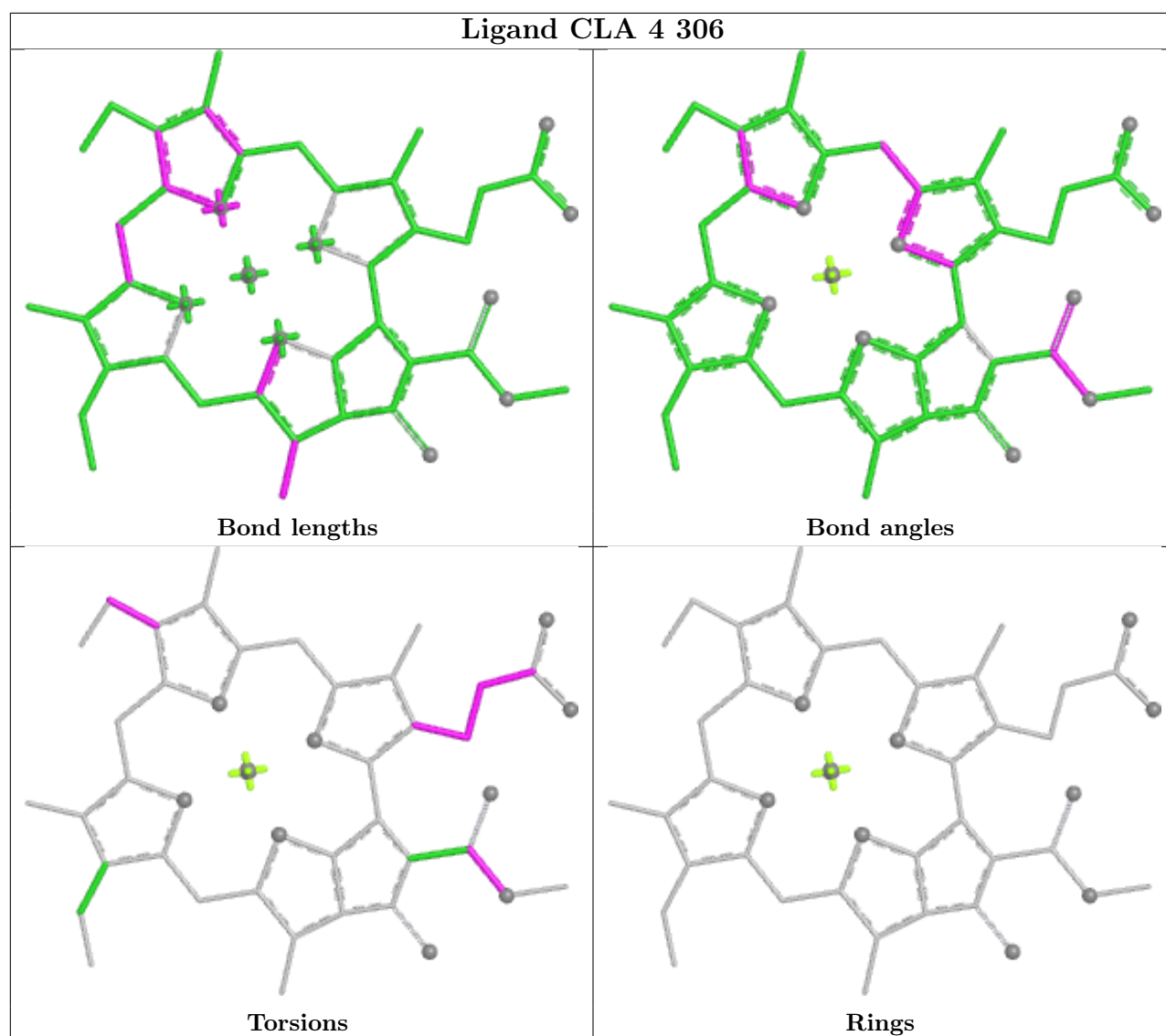
Bond angles



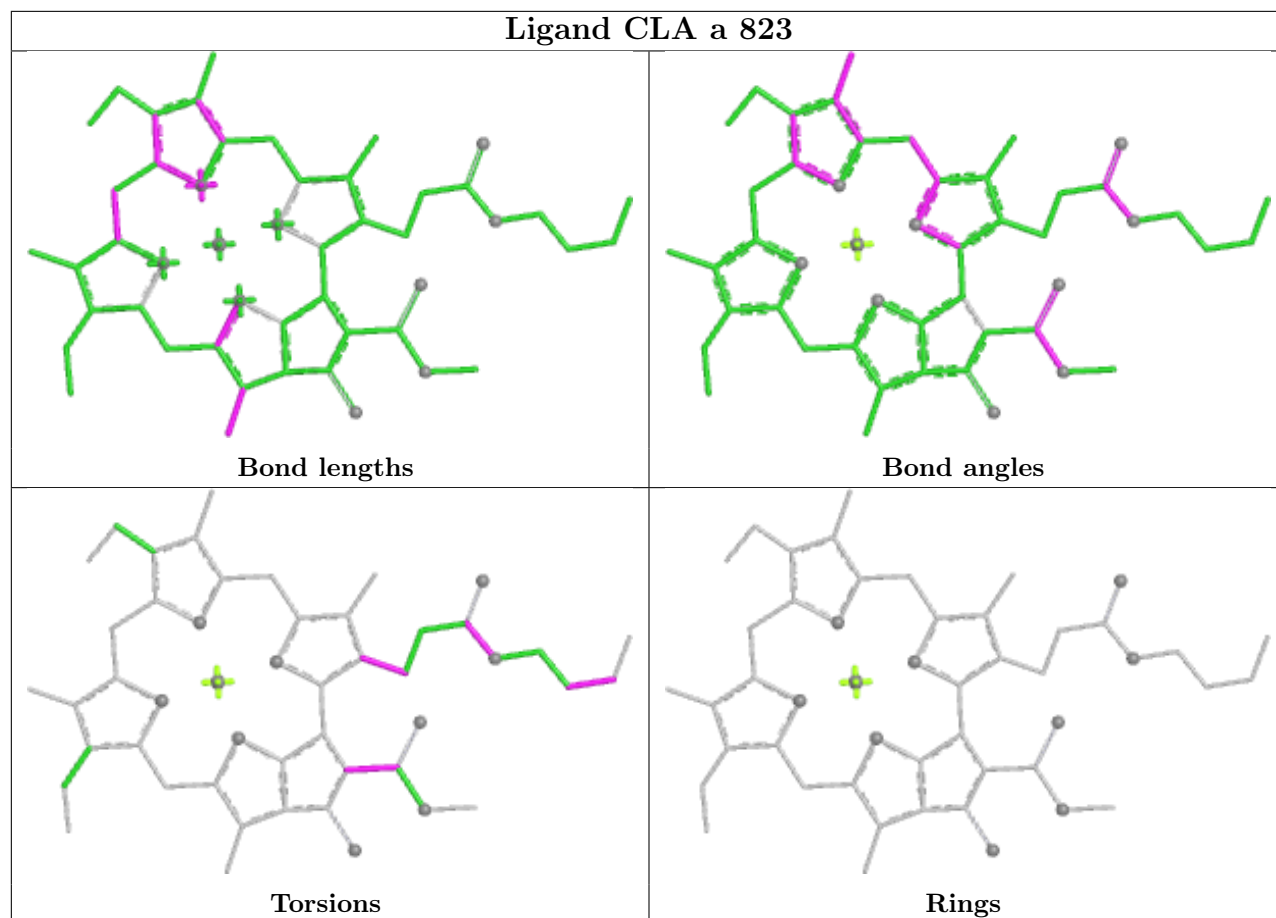
Torsions



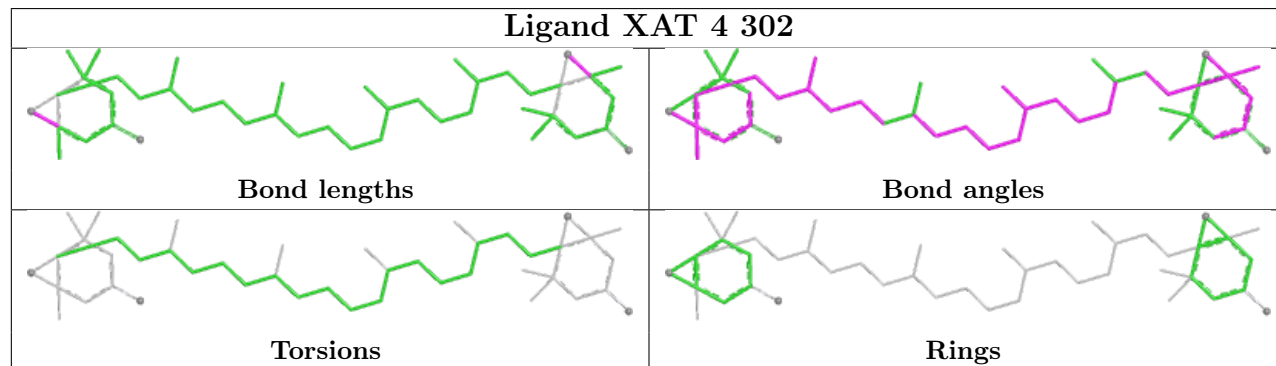
Rings



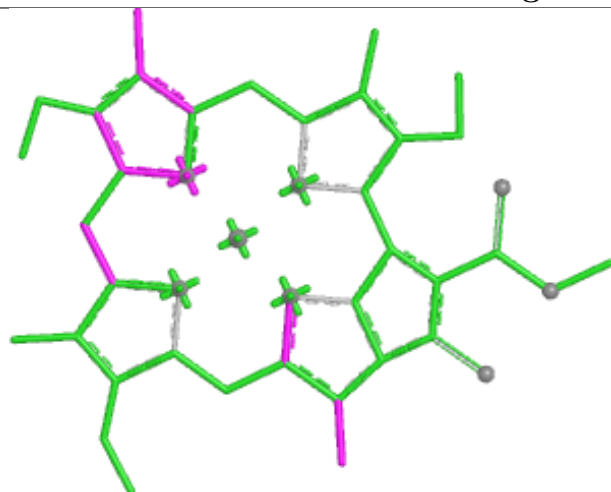
Ligand CLA a 823



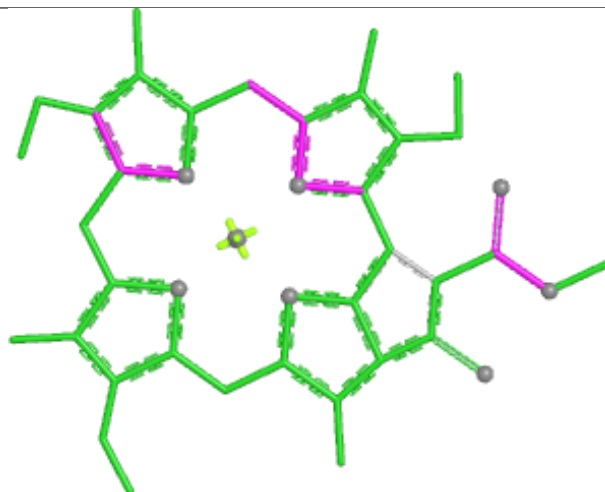
Ligand XAT 4 302



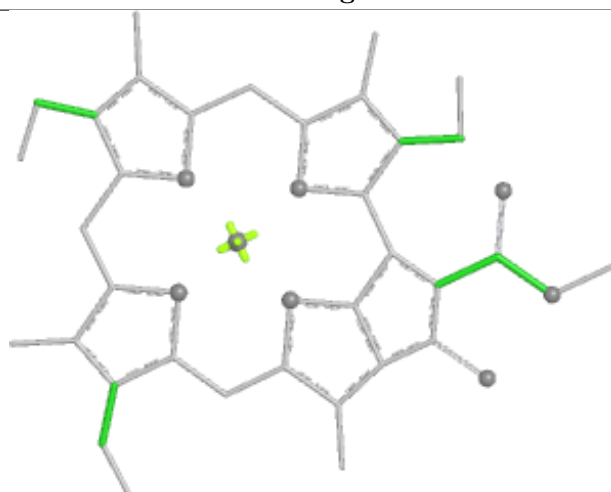
Ligand CLA 1 202



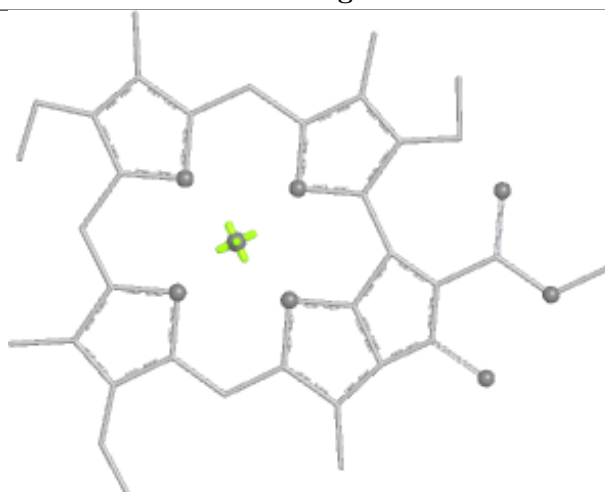
Bond lengths



Bond angles

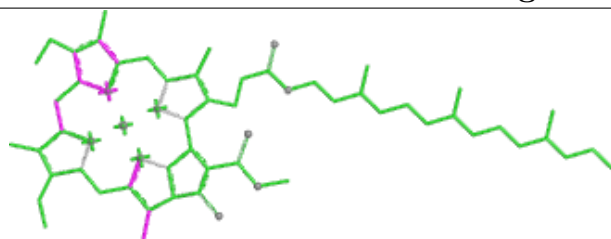


Torsions

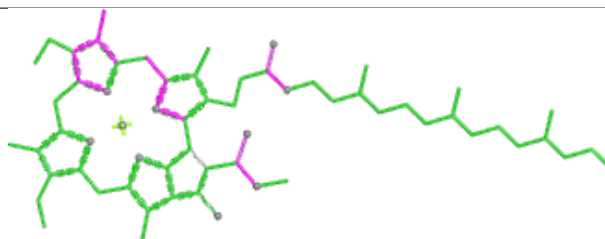


Rings

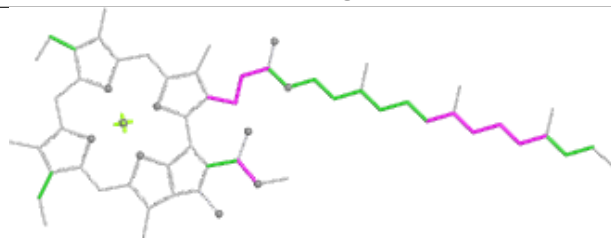
Ligand CLA a 829



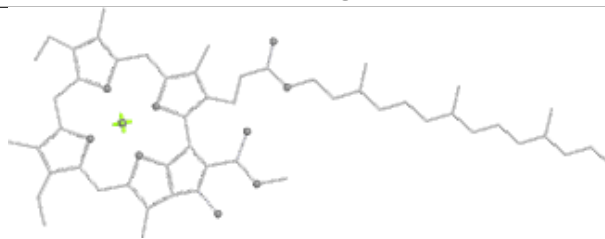
Bond lengths



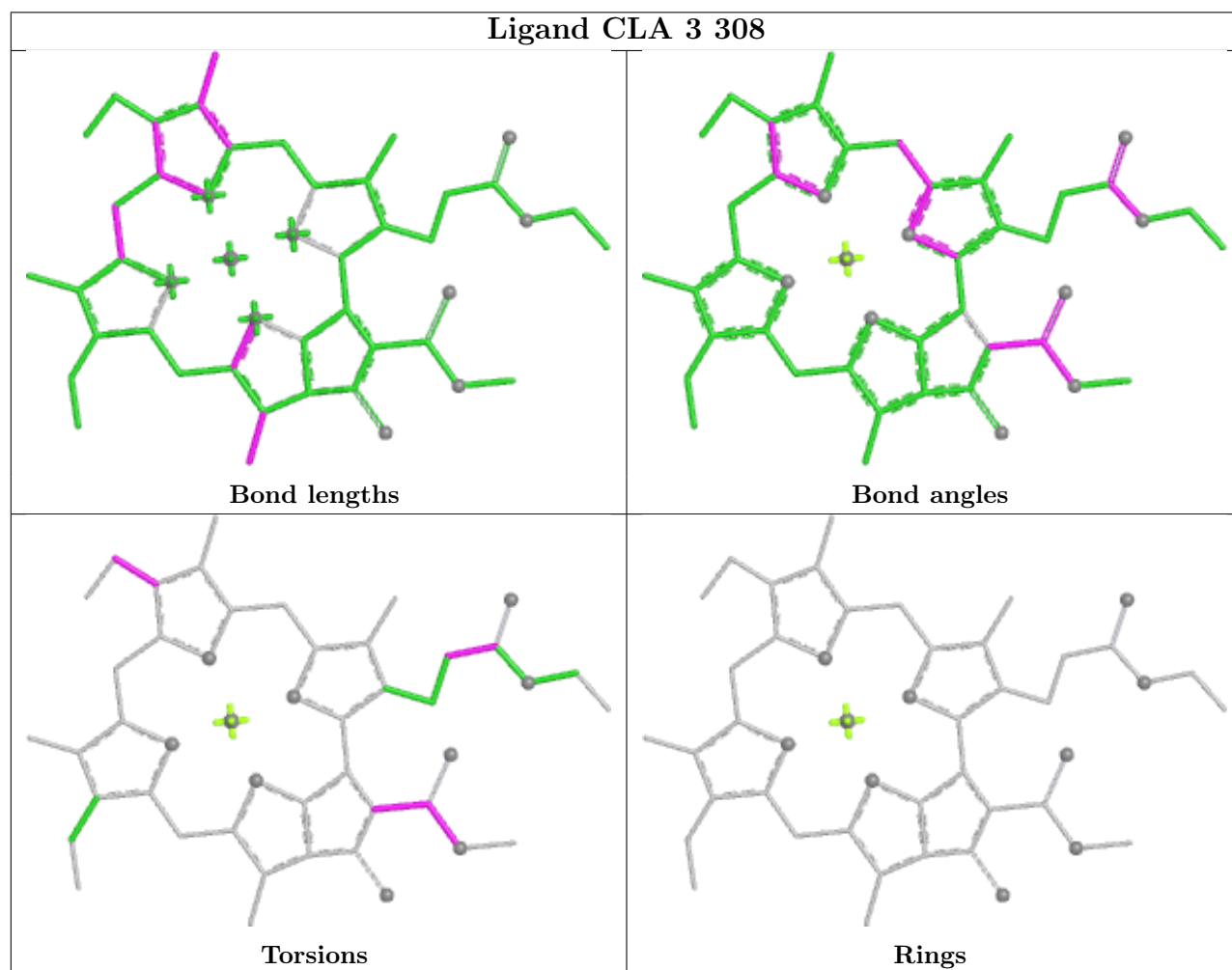
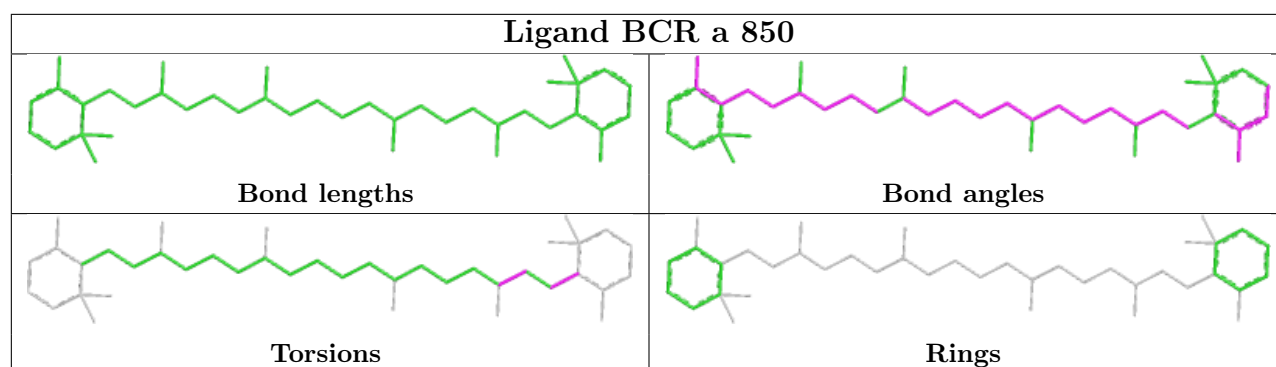
Bond angles



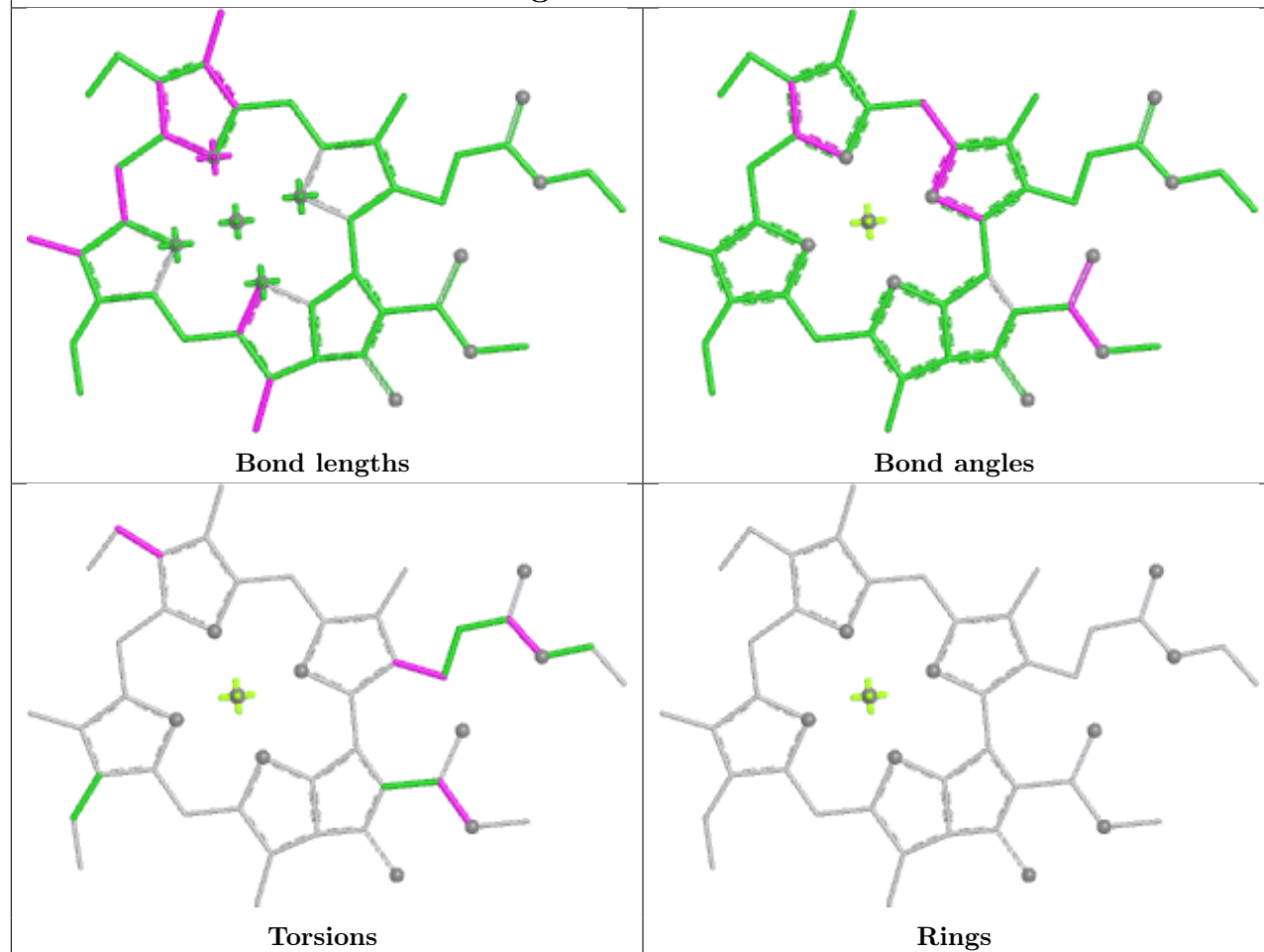
Torsions



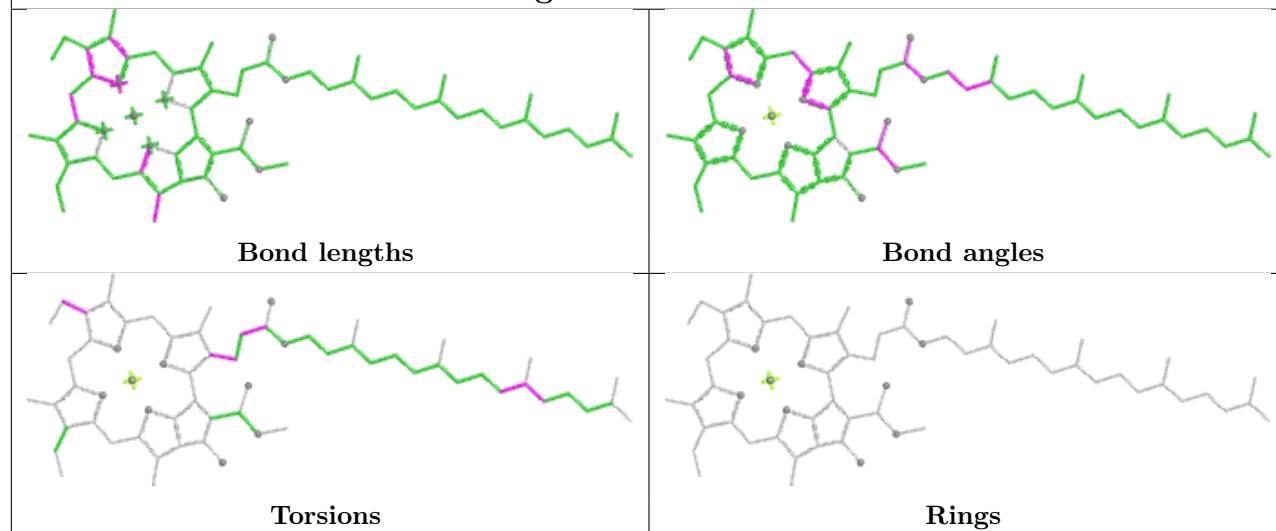
Rings

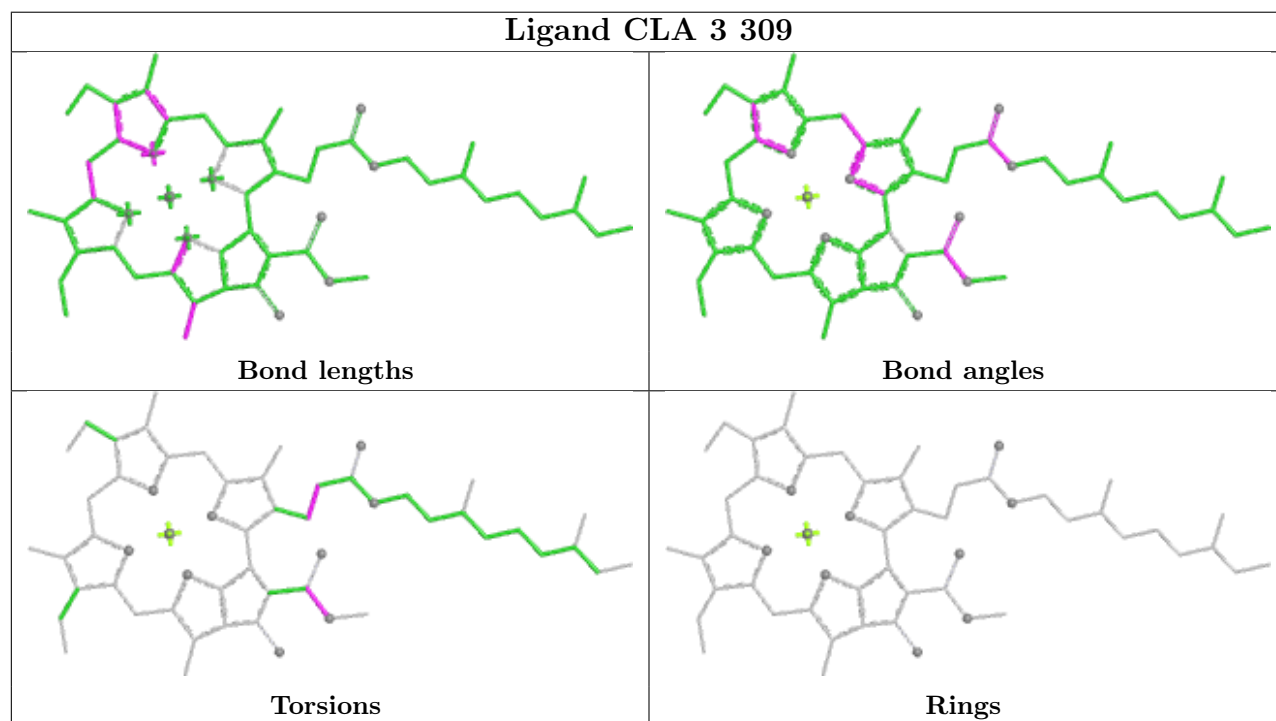
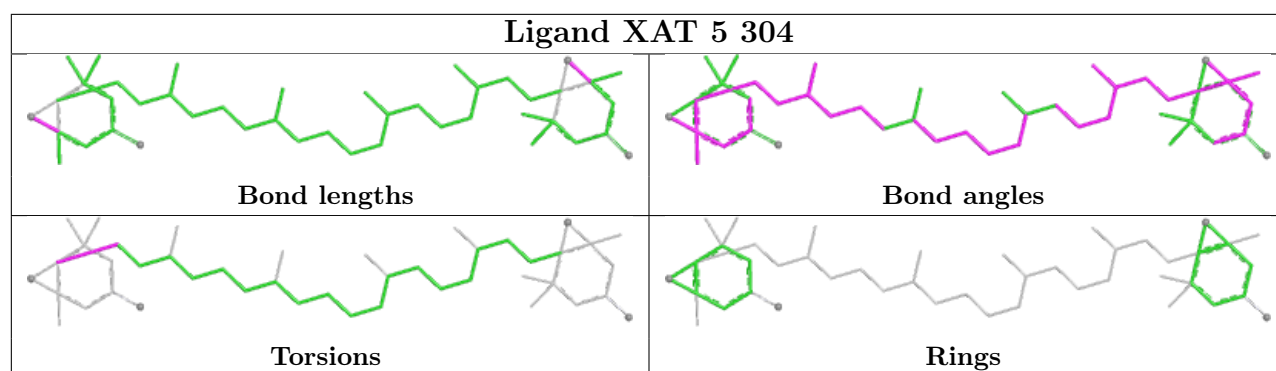


Ligand CLA 3 314

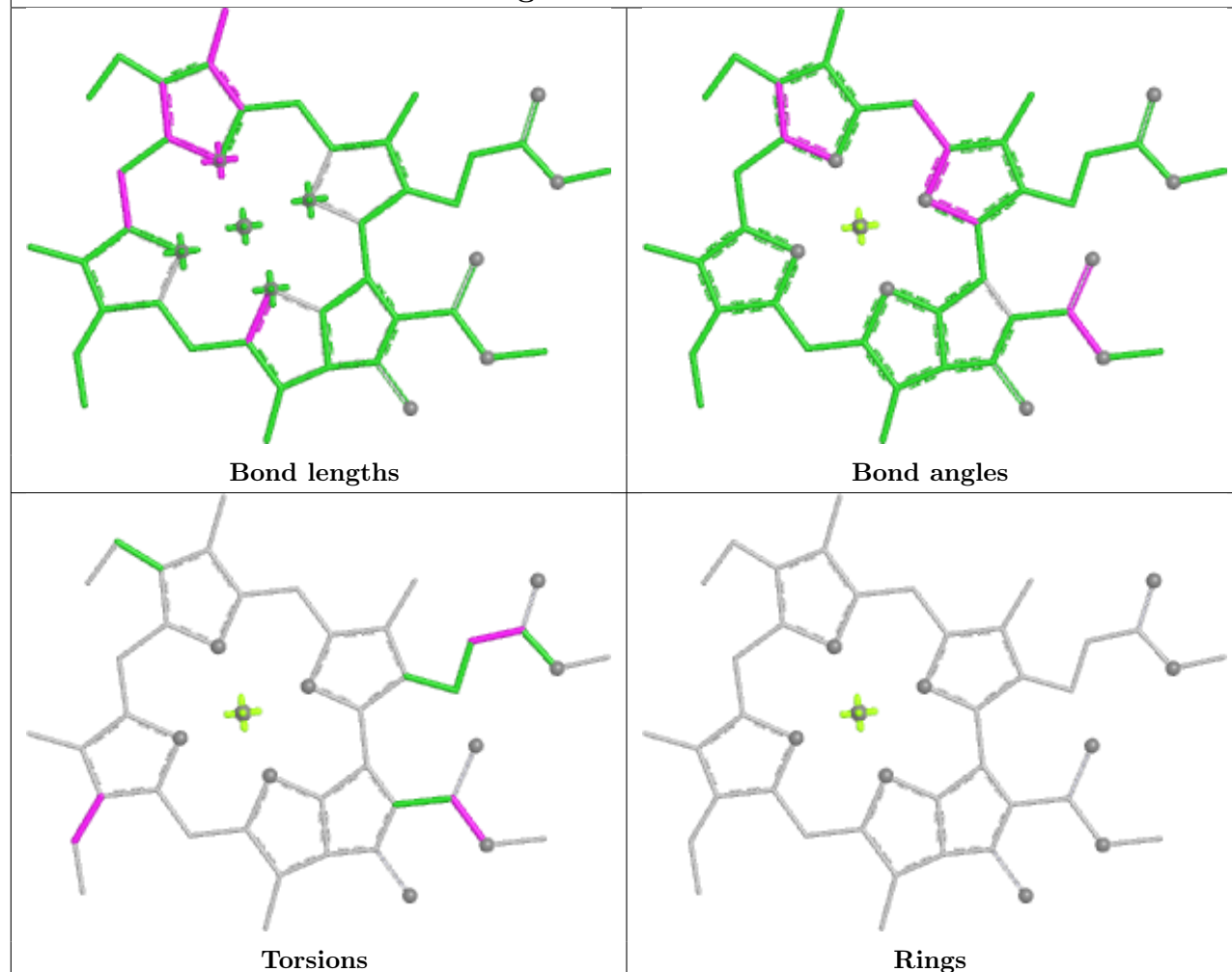


Ligand CLA b 838

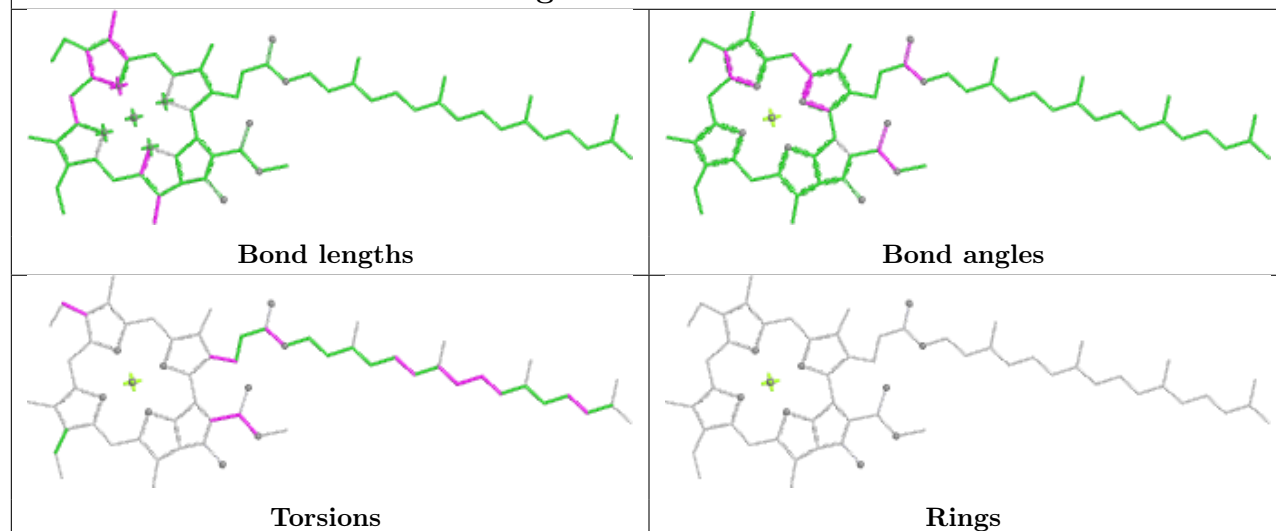


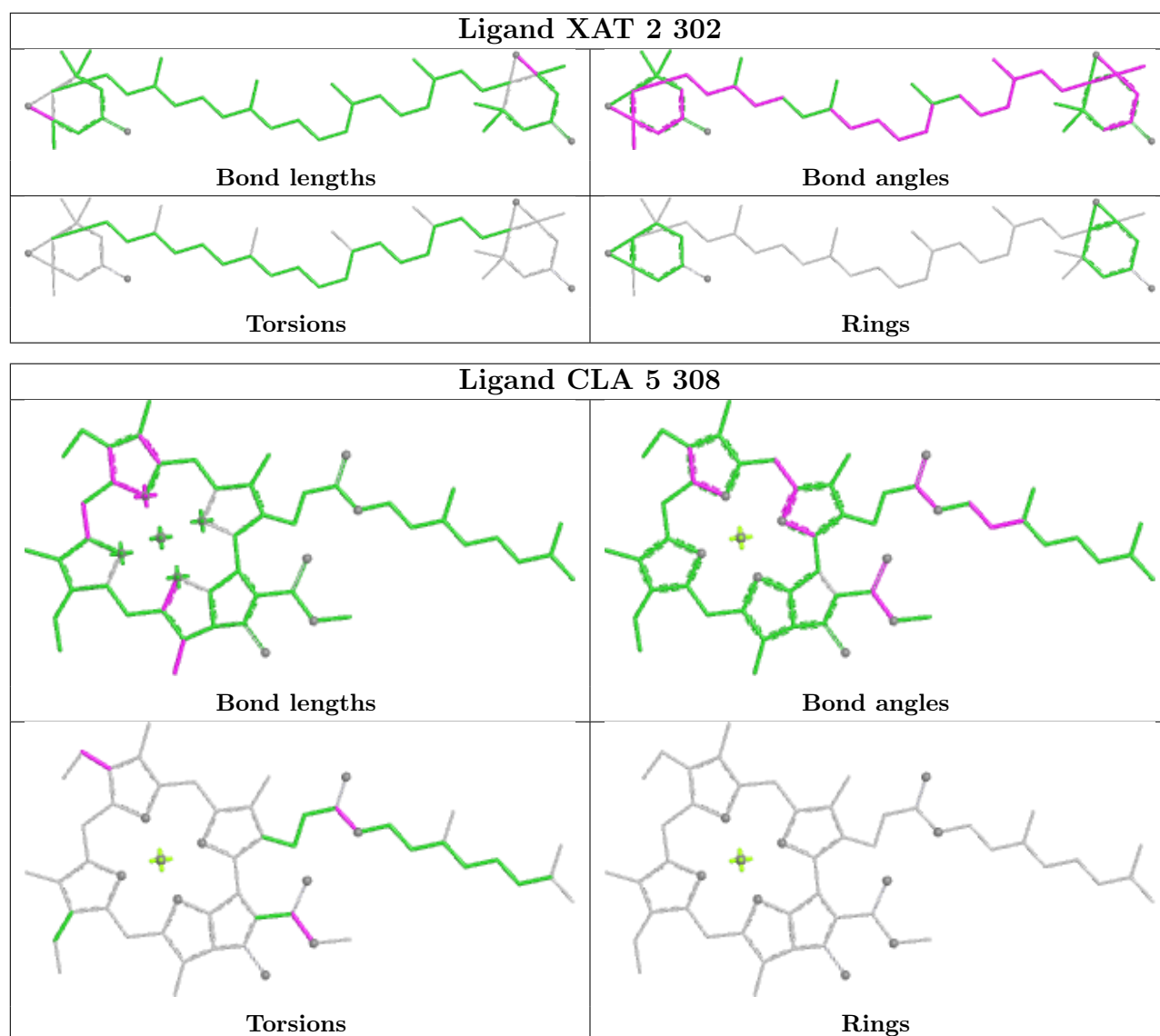


Ligand CLA 5 315



Ligand CLA a 854





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.

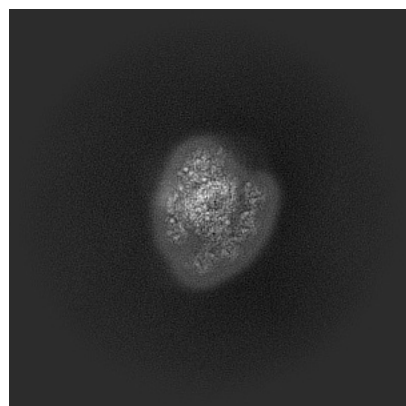
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60289. These allow visual inspection of the internal detail of the map and identification of artifacts.

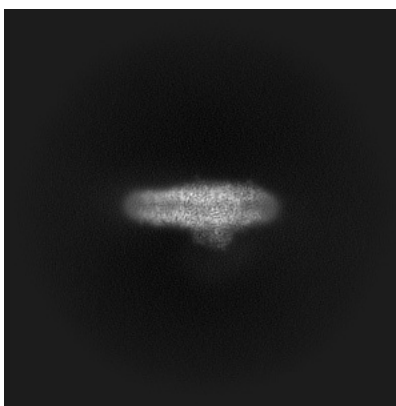
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

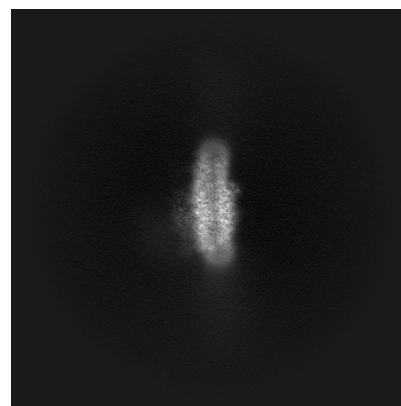
6.1.1 Primary map



X

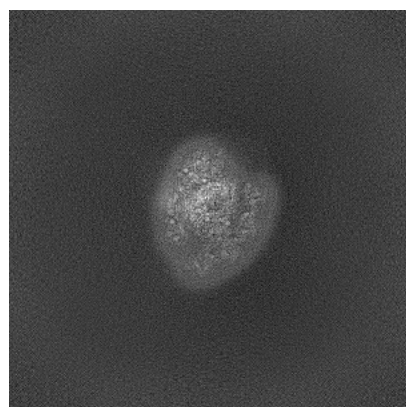


Y

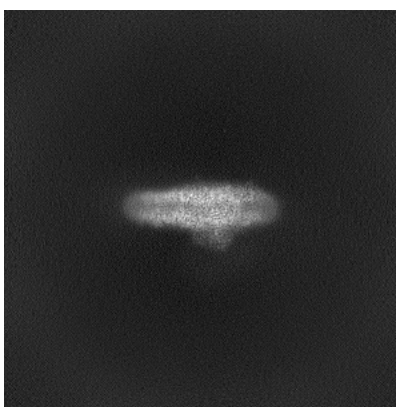


Z

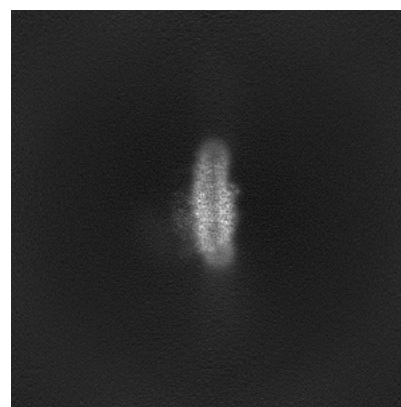
6.1.2 Raw map



X



Y

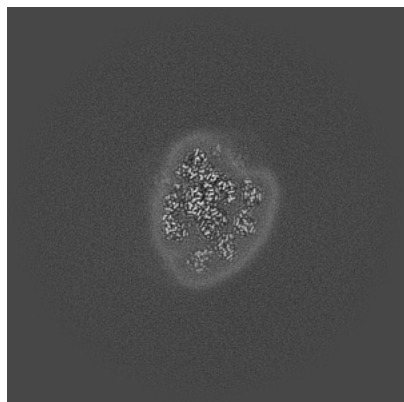


Z

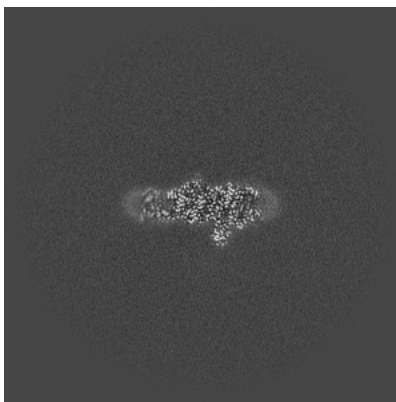
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

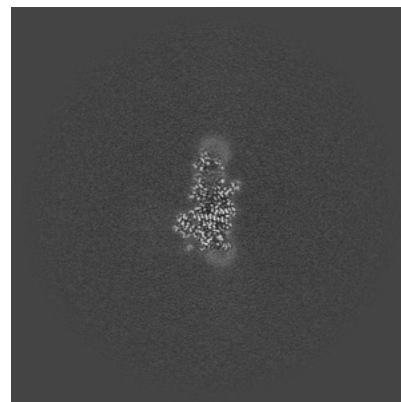
6.2.1 Primary map



X Index: 256

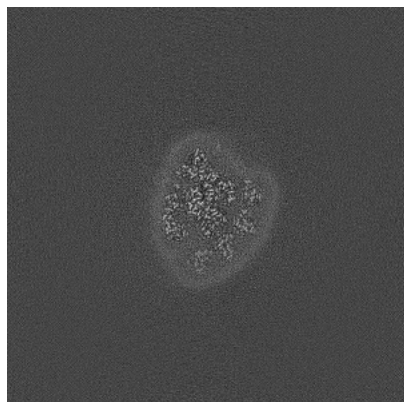


Y Index: 256

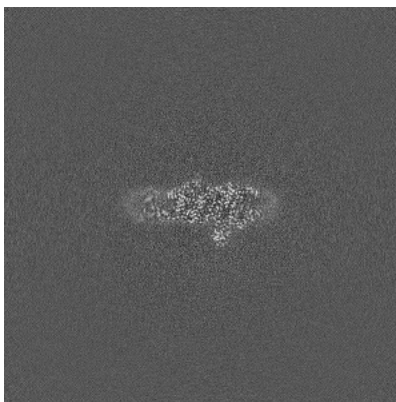


Z Index: 256

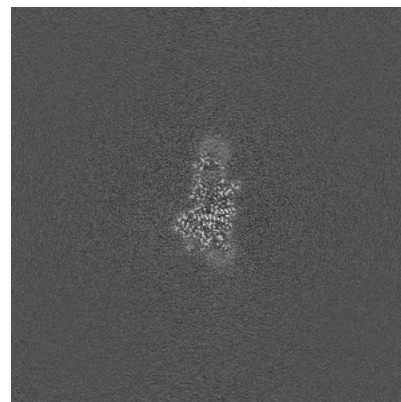
6.2.2 Raw map



X Index: 256



Y Index: 256

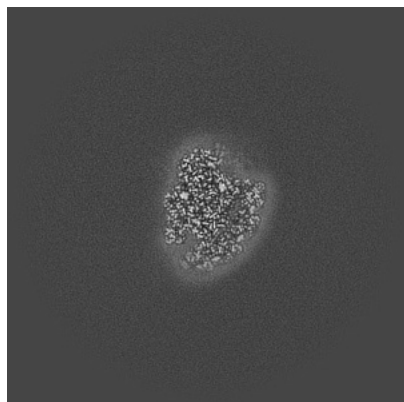


Z Index: 256

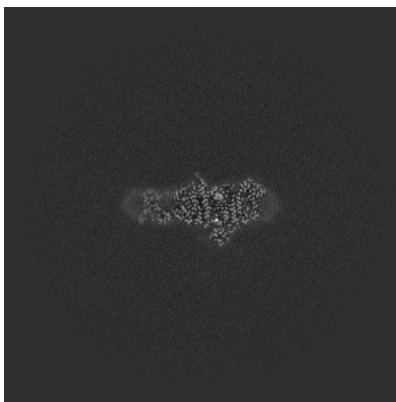
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

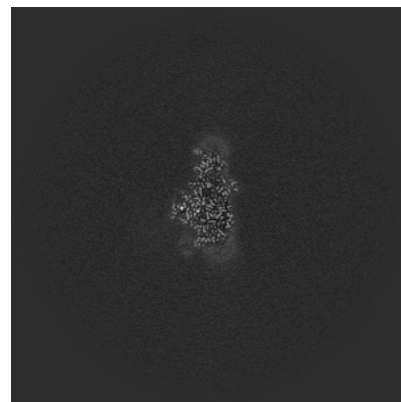
6.3.1 Primary map



X Index: 246

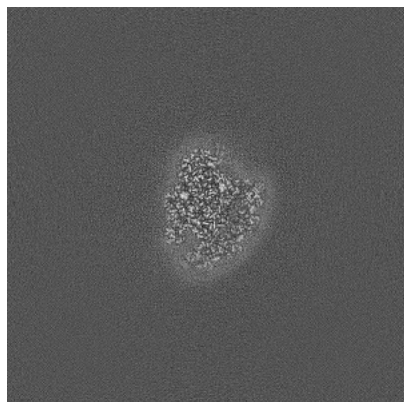


Y Index: 251



Z Index: 273

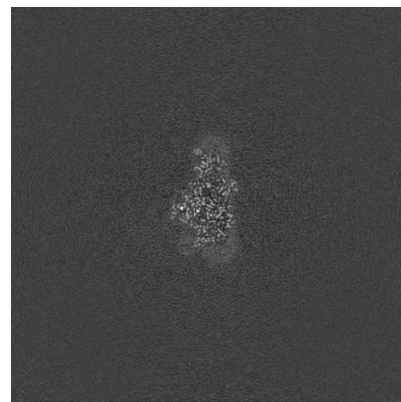
6.3.2 Raw map



X Index: 246



Y Index: 251

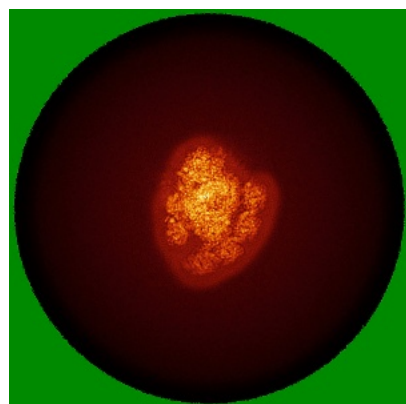


Z Index: 273

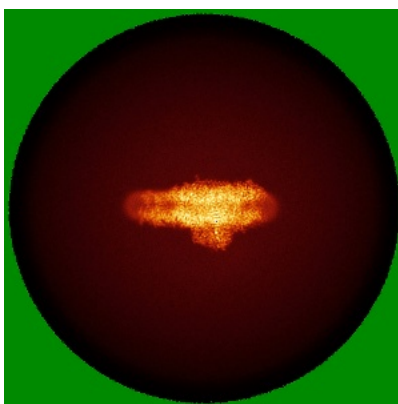
The images above show the largest variance slices of the map in three orthogonal directions.

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

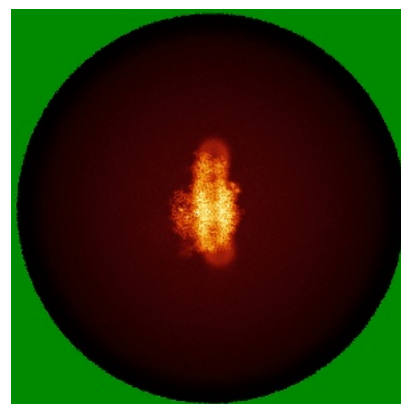
6.4.1 Primary map



X

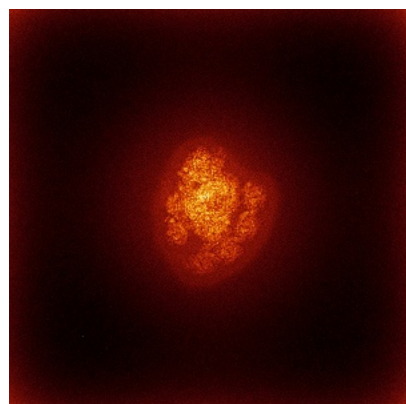


Y

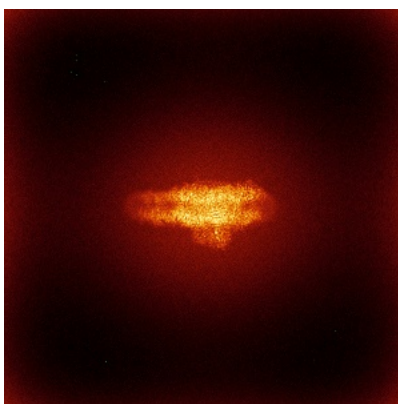


Z

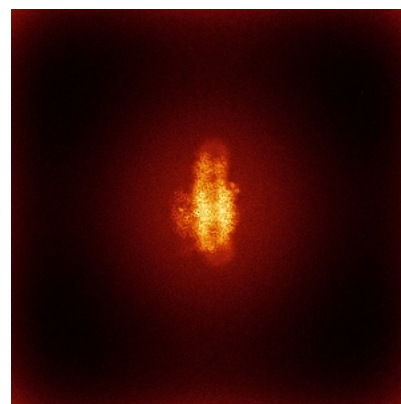
6.4.2 Raw map



X



Y

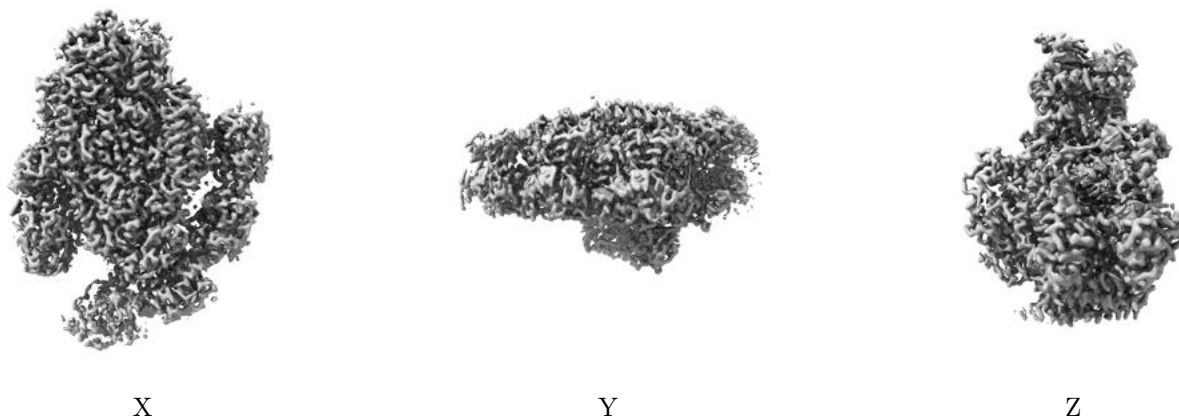


Z

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

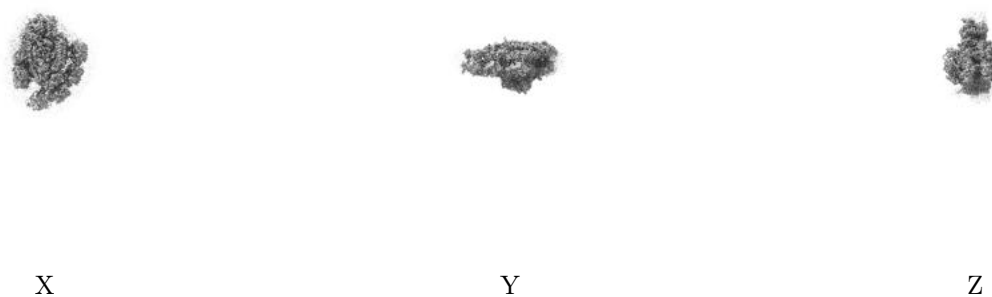
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.333. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

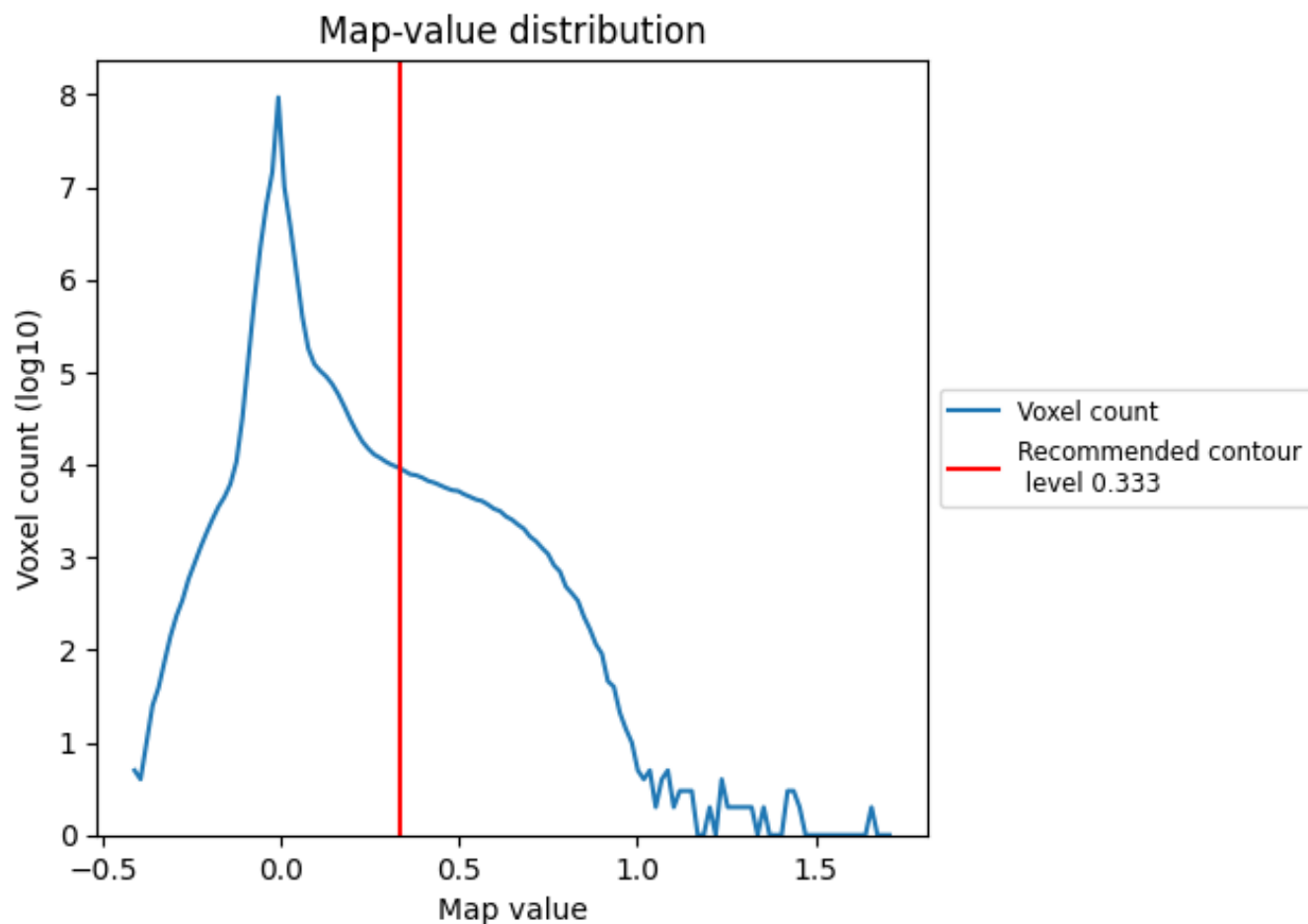
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

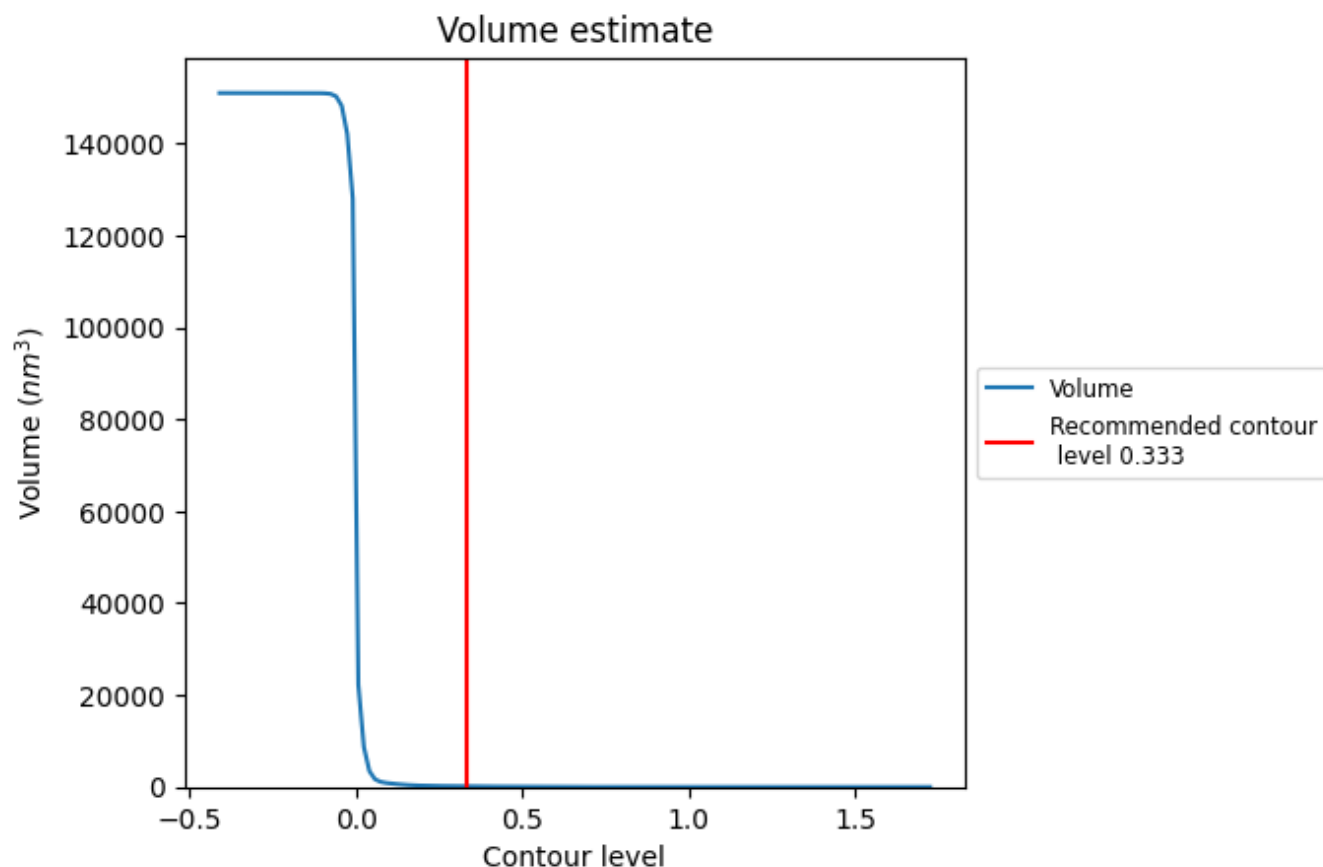
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

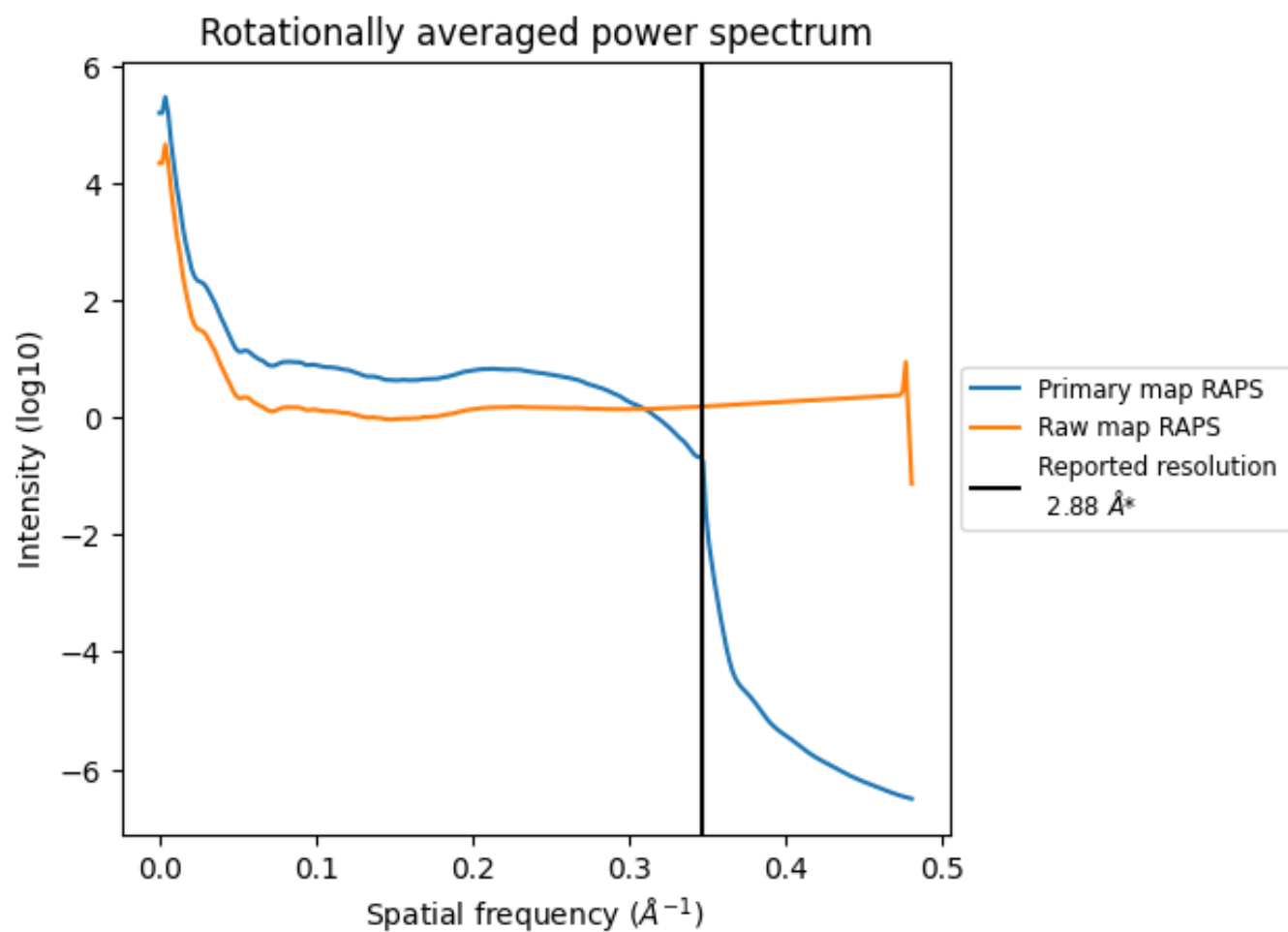
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm^3 ; this corresponds to an approximate mass of 123 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

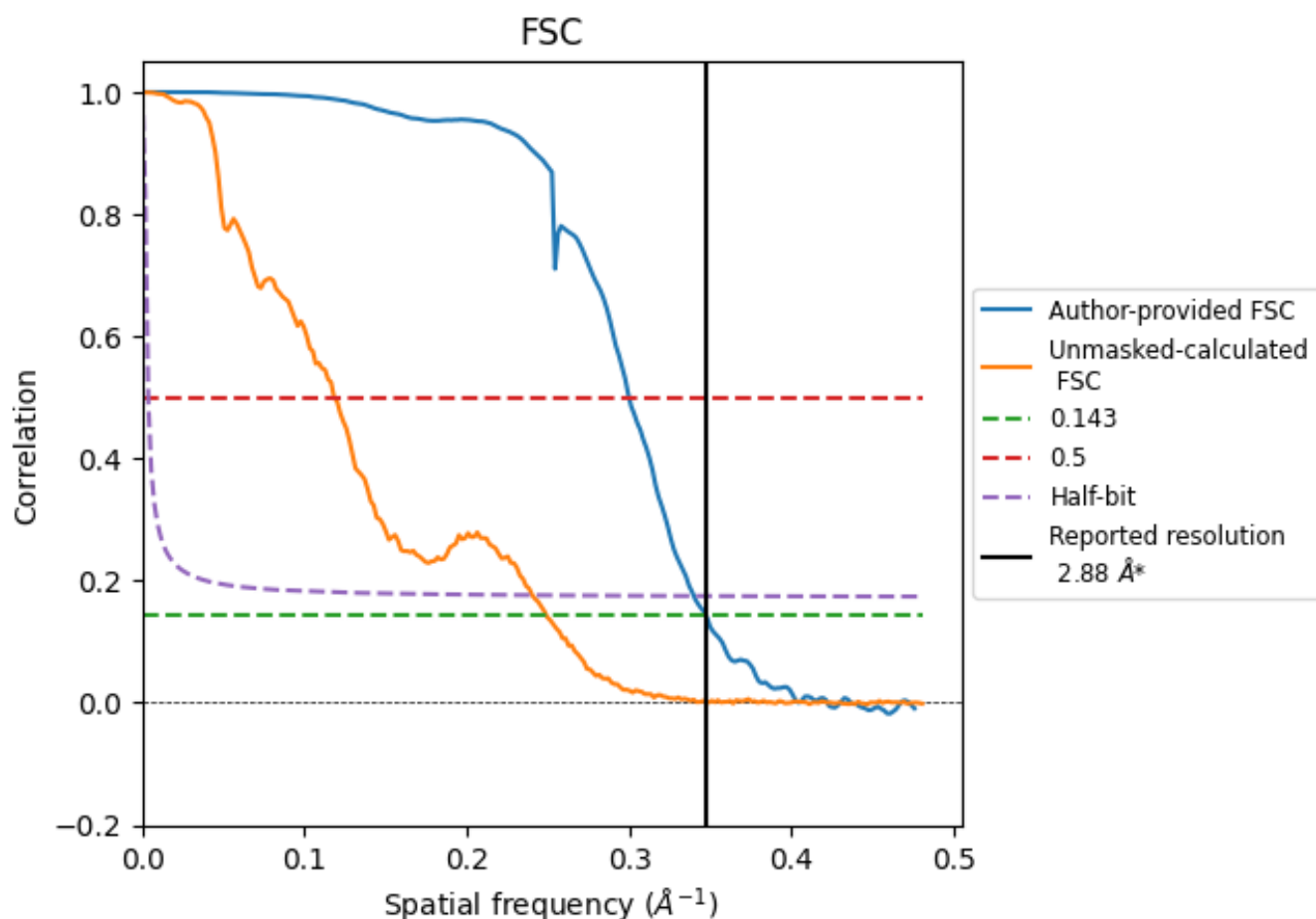


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.347 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

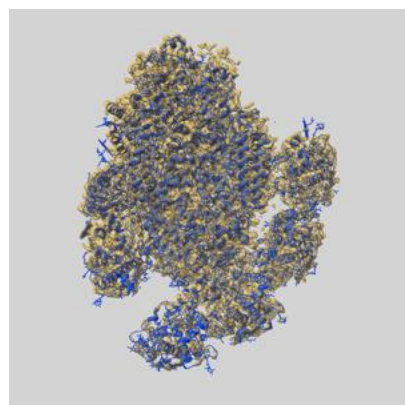
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.33	2.94
Unmasked-calculated*	4.01	8.45	4.16

*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 4.01 differs from the reported value 2.88 by more than 10 %

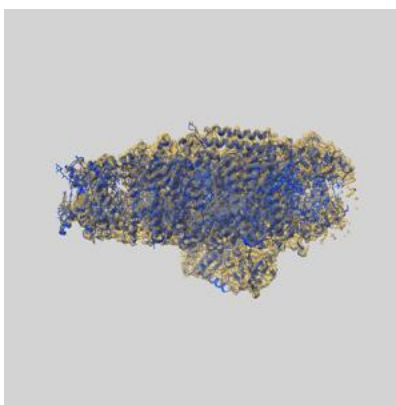
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60289 and PDB model 8ZOD. Per-residue inclusion information can be found in section 3 on page 26.

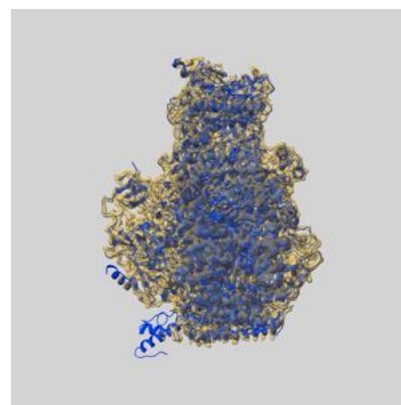
9.1 Map-model overlay [i](#)



X



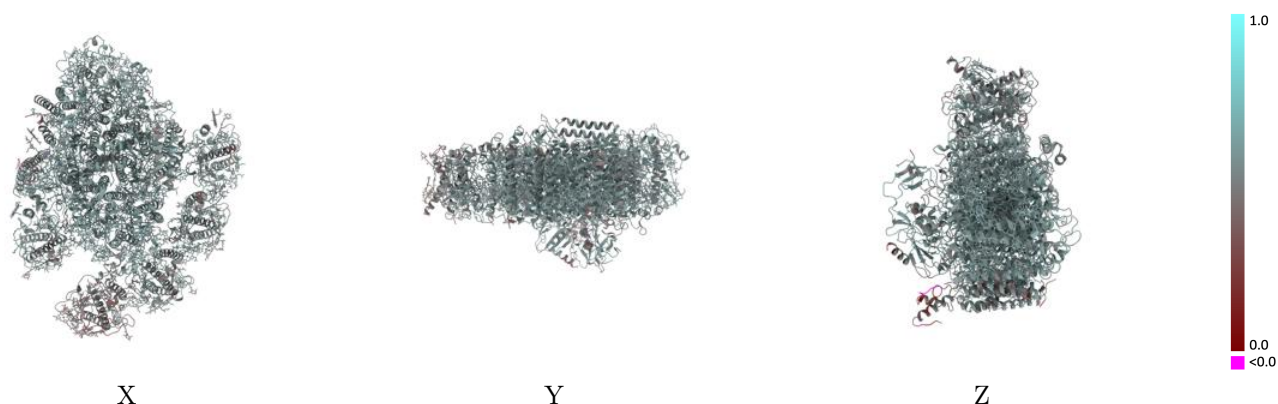
Y



Z

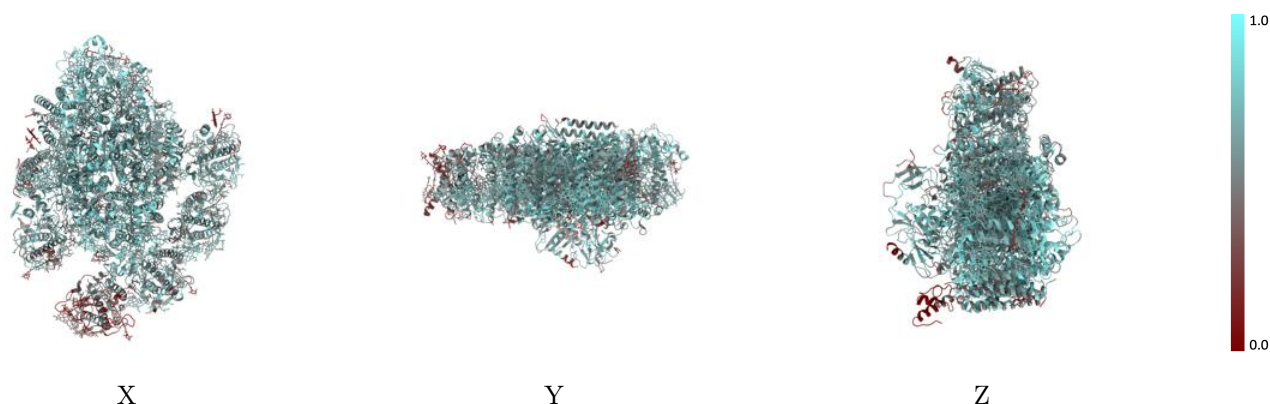
The images above show the 3D surface view of the map at the recommended contour level 0.333 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



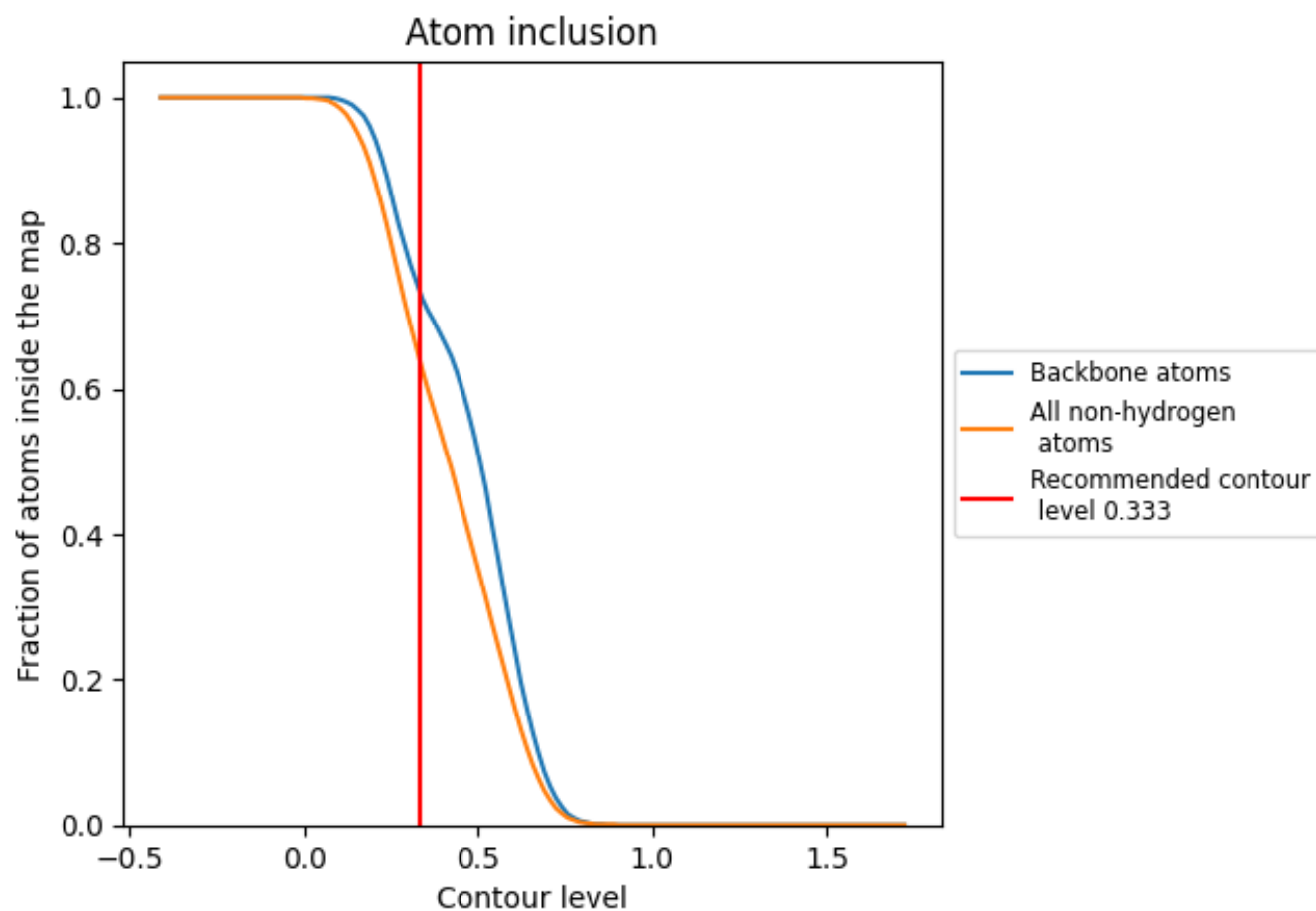
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.333).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 64% 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 (0.333) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6390	0.5470
1	0.5870	0.5340
2	0.3690	0.4550
3	0.5770	0.5300
4	0.5980	0.5290
5	0.5930	0.5250
a	0.7120	0.5780
b	0.7010	0.5680
c	0.7260	0.5600
d	0.6320	0.5540
e	0.6180	0.5490
f	0.6440	0.5420
g	0.3270	0.4330
i	0.5140	0.4990
j	0.6220	0.5630
l	0.6000	0.5130
m	0.5630	0.4950

