



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:09 PM UTC

PDB ID : 8ZOF / pdb_00008zof
EMDB ID : EMD-60291
Title : Structure of the canthaxanthin mutant PSI-3VCPI supercomplex in Nan-
nochloropsis oceanica
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 3.06 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:

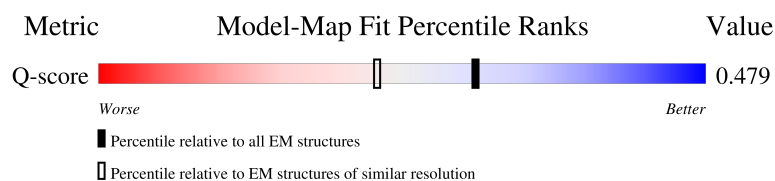
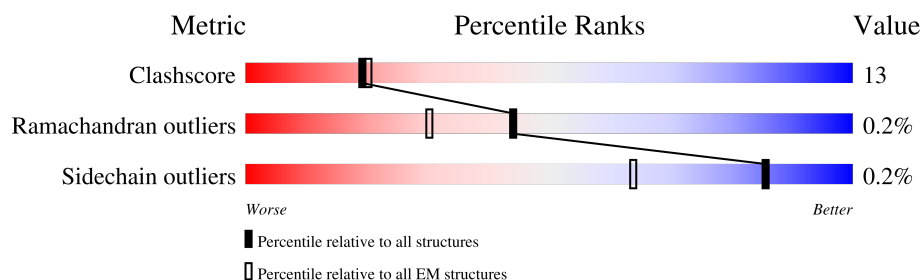
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.06 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.



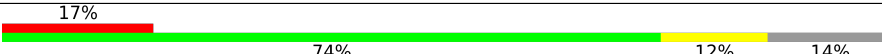
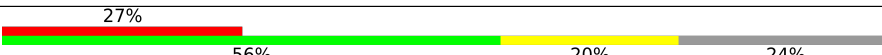
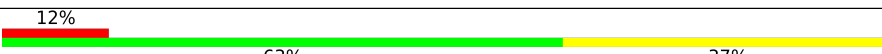
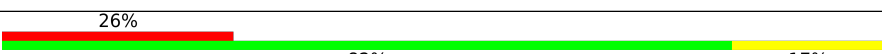
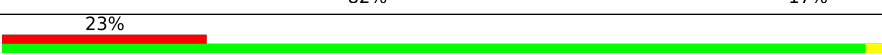
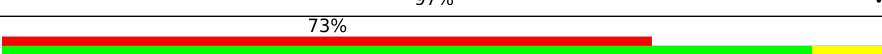
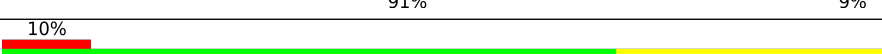
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13976 (2.56 - 3.56)

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	1	208	
4	a	745	

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Mol	Chain	Length	Quality of chain
5	b	737	
6	d	136	
7	e	67	
8	f	185	
9	i	45	
10	j	41	
11	l	172	
12	m	30	
13	g	55	
14	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
17	CLA	1	305	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	307	X	-	-	-
17	CLA	1	308	X	-	-	-
17	CLA	1	309	X	-	-	-
17	CLA	1	310	X	-	-	-
17	CLA	1	311	X	-	-	-
17	CLA	1	312	X	-	-	-
17	CLA	1	313	X	-	-	-
17	CLA	1	314	X	-	-	-
17	CLA	4	307	X	-	-	-
17	CLA	4	308	X	-	-	-
17	CLA	4	309	X	-	-	-
17	CLA	4	310	X	-	-	-
17	CLA	4	311	X	-	-	-
17	CLA	4	312	X	-	-	-
17	CLA	4	313	X	-	-	-
17	CLA	4	314	X	-	-	-
17	CLA	4	315	X	-	-	-
17	CLA	4	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	4	317	X	-	-	-
17	CLA	4	318	X	-	-	-
17	CLA	5	305	X	-	-	-
17	CLA	5	306	X	-	-	-
17	CLA	5	307	X	-	-	-
17	CLA	5	308	X	-	-	-
17	CLA	5	309	X	-	-	-
17	CLA	5	310	X	-	-	-
17	CLA	5	311	X	-	-	-
17	CLA	5	312	X	-	-	-
17	CLA	5	313	X	-	-	-
17	CLA	5	314	X	-	-	-
17	CLA	5	315	X	-	-	-
17	CLA	a	801	X	-	-	-
17	CLA	a	802	X	-	-	-
17	CLA	a	803	X	-	-	-
17	CLA	a	804	X	-	-	-
17	CLA	a	805	X	-	-	-
17	CLA	a	806	X	-	-	-
17	CLA	a	807	X	-	-	-
17	CLA	a	808	X	-	-	-
17	CLA	a	809	X	-	-	-
17	CLA	a	810	X	-	-	-
17	CLA	a	811	X	-	-	-
17	CLA	a	812	X	-	-	-
17	CLA	a	813	X	-	-	-
17	CLA	a	814	X	-	-	-
17	CLA	a	815	X	-	-	-
17	CLA	a	816	X	-	-	-
17	CLA	a	817	X	-	-	-
17	CLA	a	818	X	-	-	-
17	CLA	a	819	X	-	-	-
17	CLA	a	820	X	-	-	-
17	CLA	a	821	X	-	-	-
17	CLA	a	822	X	-	-	-
17	CLA	a	823	X	-	-	-
17	CLA	a	824	X	-	-	-
17	CLA	a	825	X	-	-	-
17	CLA	a	826	X	-	-	-
17	CLA	a	827	X	-	-	-
17	CLA	a	828	X	-	-	-
17	CLA	a	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	a	830	X	-	-	-
17	CLA	a	831	X	-	-	-
17	CLA	a	832	X	-	-	-
17	CLA	a	833	X	-	-	-
17	CLA	a	834	X	-	-	-
17	CLA	a	835	X	-	-	-
17	CLA	a	836	X	-	-	-
17	CLA	a	837	X	-	-	-
17	CLA	a	838	X	-	-	-
17	CLA	a	839	X	-	-	-
17	CLA	a	840	X	-	-	-
17	CLA	a	841	X	-	-	-
17	CLA	a	842	X	-	-	-
17	CLA	a	844	X	-	-	-
17	CLA	a	854	X	-	-	-
17	CLA	b	801	X	-	-	-
17	CLA	b	802	X	-	-	-
17	CLA	b	803	X	-	-	-
17	CLA	b	804	X	-	-	-
17	CLA	b	805	X	-	-	-
17	CLA	b	806	X	-	-	-
17	CLA	b	807	X	-	-	-
17	CLA	b	808	X	-	-	-
17	CLA	b	809	X	-	-	-
17	CLA	b	810	X	-	-	-
17	CLA	b	811	X	-	-	-
17	CLA	b	812	X	-	-	-
17	CLA	b	813	X	-	-	-
17	CLA	b	814	X	-	-	-
17	CLA	b	815	X	-	-	-
17	CLA	b	816	X	-	-	-
17	CLA	b	817	X	-	-	-
17	CLA	b	818	X	-	-	-
17	CLA	b	819	X	-	-	-
17	CLA	b	820	X	-	-	-
17	CLA	b	821	X	-	-	-
17	CLA	b	822	X	-	-	-
17	CLA	b	823	X	-	-	-
17	CLA	b	824	X	-	-	-
17	CLA	b	825	X	-	-	-
17	CLA	b	826	X	-	-	-
17	CLA	b	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	b	828	X	-	-	-
17	CLA	b	829	X	-	-	-
17	CLA	b	830	X	-	-	-
17	CLA	b	831	X	-	-	-
17	CLA	b	832	X	-	-	-
17	CLA	b	833	X	-	-	-
17	CLA	b	834	X	-	-	-
17	CLA	b	835	X	-	-	-
17	CLA	b	836	X	-	-	-
17	CLA	b	837	X	-	-	-
17	CLA	b	838	X	-	-	-
17	CLA	b	839	X	-	-	-
17	CLA	b	840	X	-	-	-
17	CLA	b	841	X	-	-	-
17	CLA	f	802	X	-	-	-
17	CLA	f	803	X	-	-	-
17	CLA	i	102	X	-	-	-
17	CLA	j	102	X	-	-	-
17	CLA	j	103	X	-	-	-
17	CLA	l	202	X	-	-	-
17	CLA	l	203	X	-	-	-
17	CLA	l	204	X	-	-	-
24	SF4	c	102	-	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 30455 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-1.

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

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

- Molecule 6 is a protein called Photosystem I reaction center subunit II.

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

- Molecule 7 is a protein called Photosystem I reaction center subunit IV.

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

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

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

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

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

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

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

- Molecule 11 is a protein called PSI subunit V.

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

- Molecule 12 is a protein called PsaM.

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

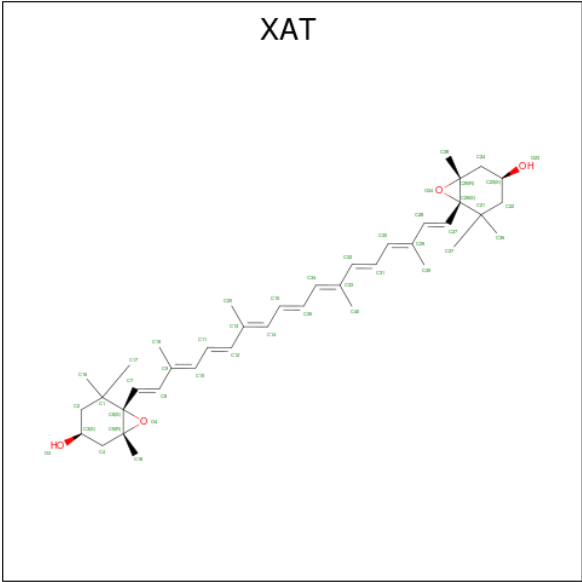
- Molecule 13 is a protein called PsaS.

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

- Molecule 14 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 15 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).



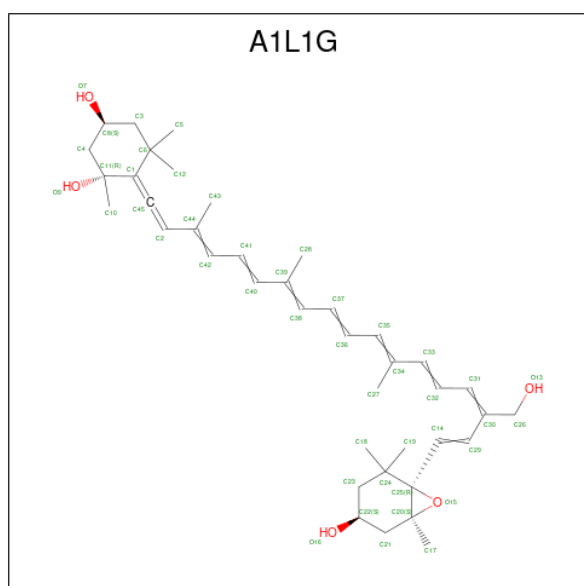
Mol	Chain	Residues	Atoms			AltConf
15	5	1	Total	C	O	0
			44	40	4	
15	5	1	Total	C	O	0
			44	40	4	
15	5	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	1	1	Total	C	O	0
			44	40	4	

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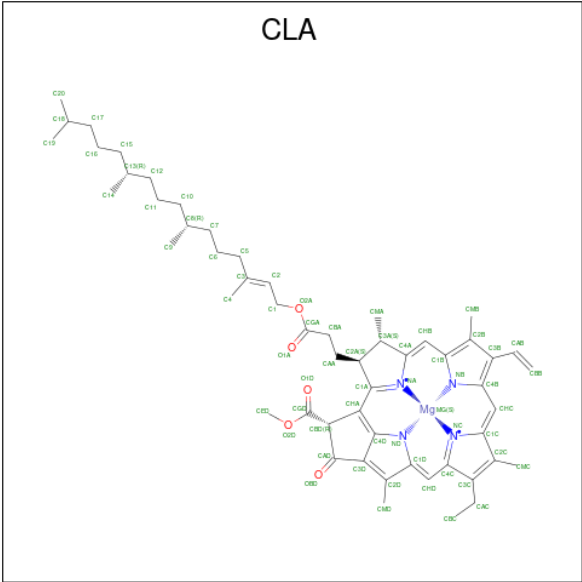
Mol	Chain	Residues	Atoms			AltConf
15	1	1	Total	C	O	0
			44	40	4	
15	a	1	Total	C	O	0
			44	40	4	
15	j	1	Total	C	O	0
			44	40	4	

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



Mol	Chain	Residues	Atoms			AltConf
16	5	1	Total	C	O	0
			45	40	5	
16	1	1	Total	C	O	0
			45	40	5	

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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

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

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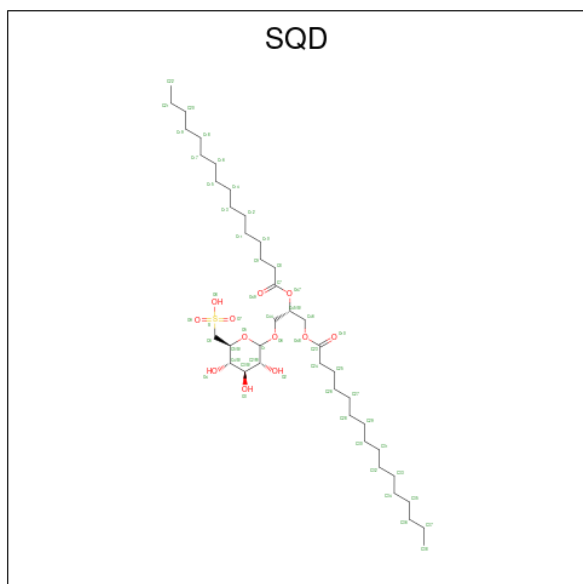
Mol	Chain	Residues	Atoms					AltConf
17	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0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

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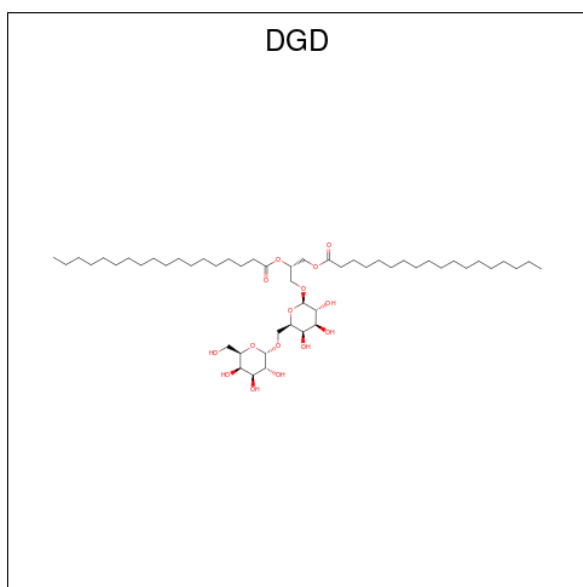
Mol	Chain	Residues	Atoms					AltConf
17	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	i	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



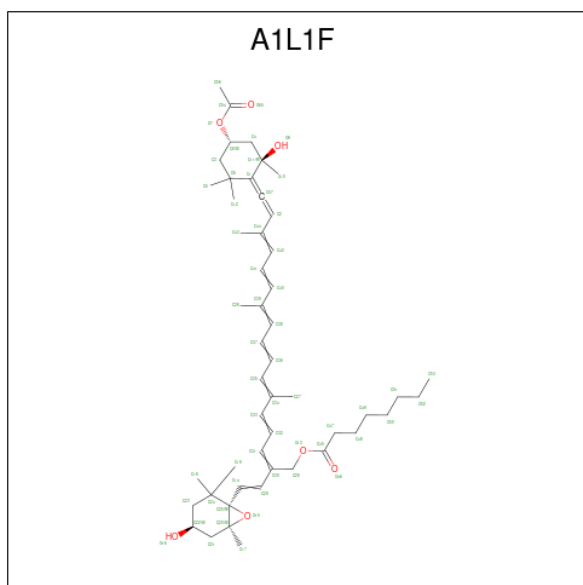
Mol	Chain	Residues	Atoms				AltConf
18	5	1	Total	C	O	S	0
			35	22	12	1	
18	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 19 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



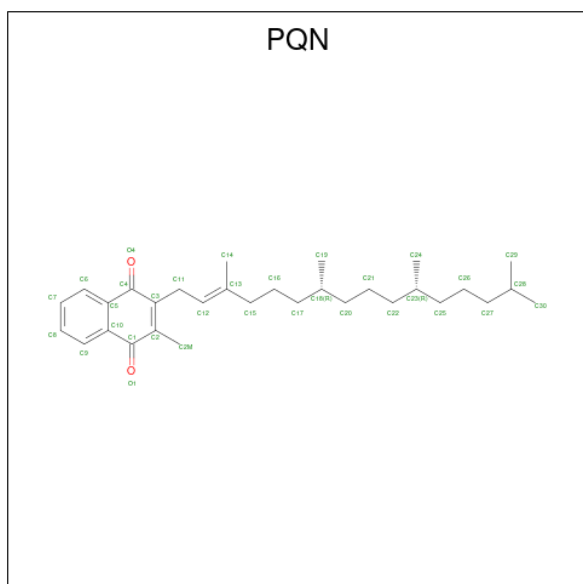
Mol	Chain	Residues	Atoms			AltConf
19	4	1	Total	C	O	0
			40	25	15	
19	b	1	Total	C	O	0
			57	42	15	

- Molecule 20 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyl oxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S}, 6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: C₅₀H₇₂O₇) (labeled as "Ligand of Interest" by depositor).



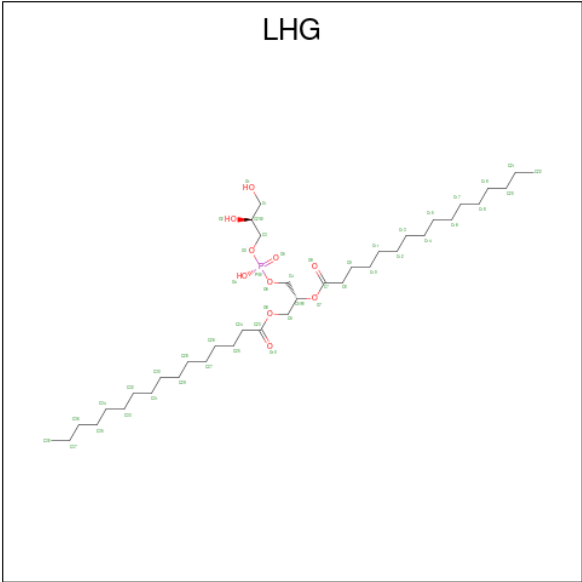
Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			57	50	7	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



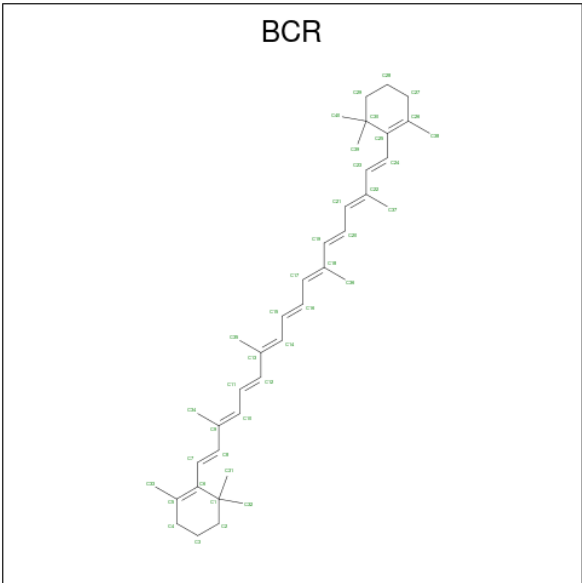
Mol	Chain	Residues	Atoms			AltConf
21	a	1	Total	C	O	0
			33	31	2	
21	b	1	Total	C	O	0
			33	31	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



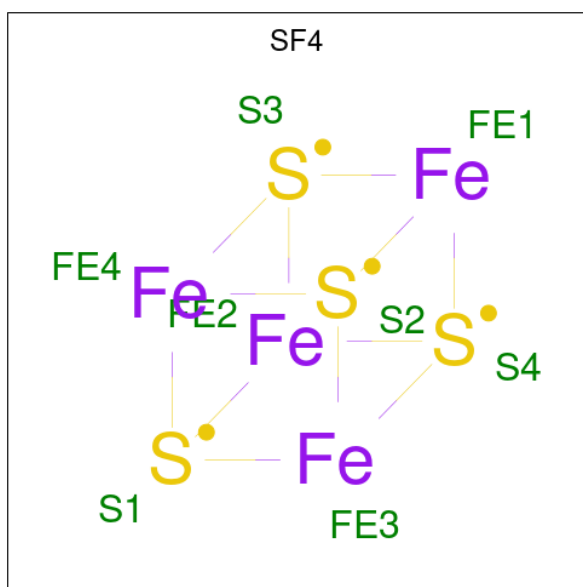
Mol	Chain	Residues	Atoms				AltConf
22	a	1	Total	C	O	P	0
			48	37	10	1	
22	a	1	Total	C	O	P	0
			27	16	10	1	
22	b	1	Total	C	O	P	0
			31	20	10	1	
22	m	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



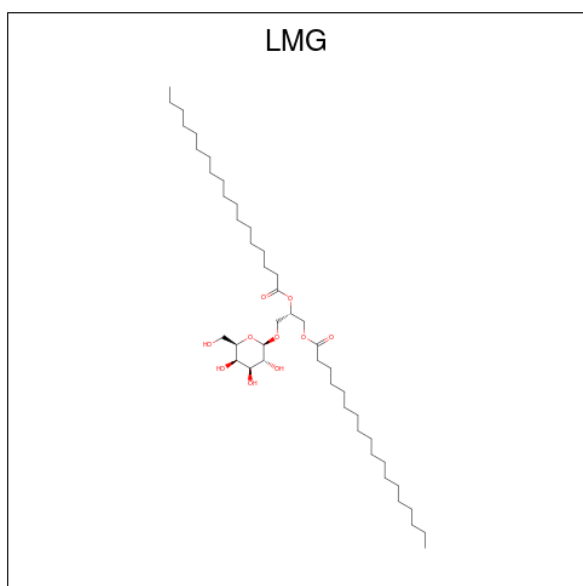
Mol	Chain	Residues	Atoms	AltConf
23	a	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C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

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

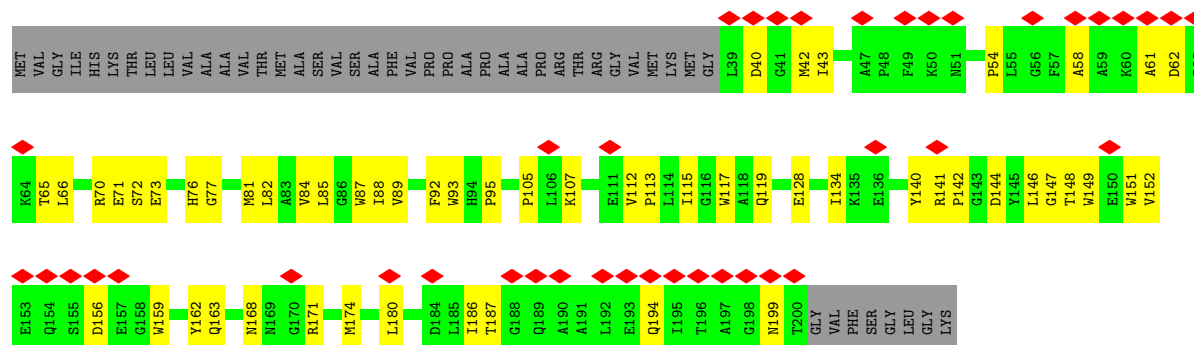
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



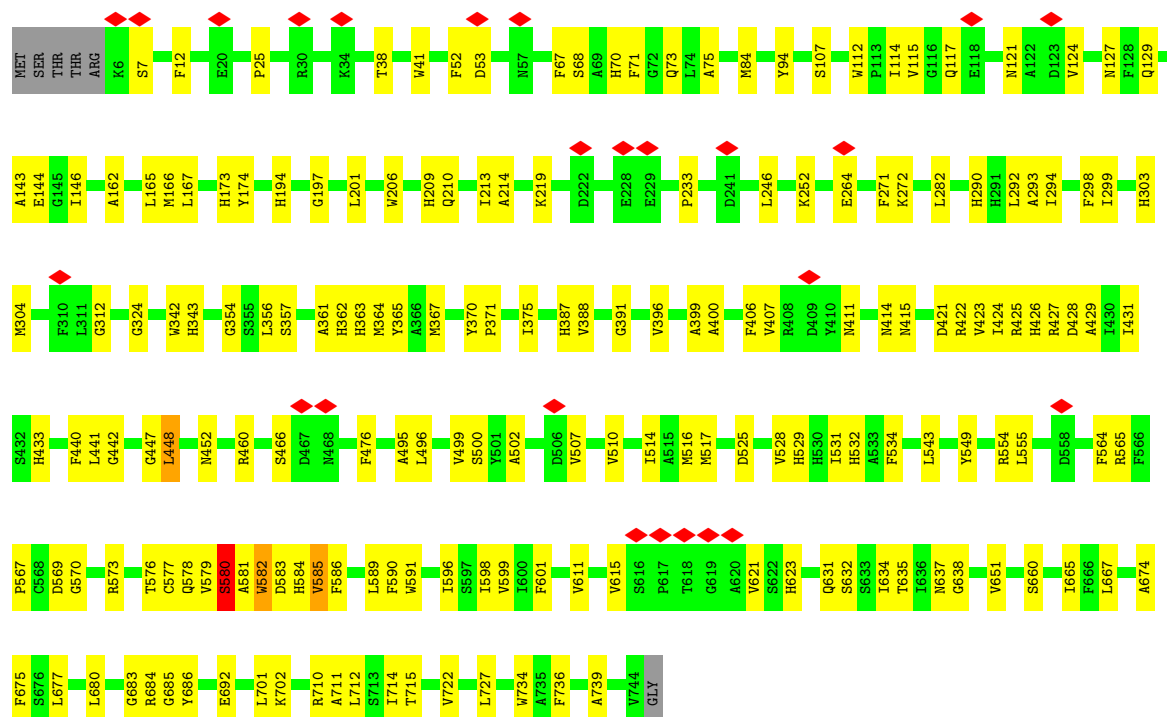
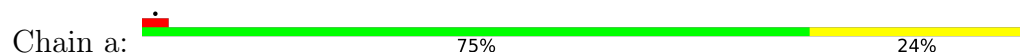
Mol	Chain	Residues	Atoms			AltConf
25	a	1	Total	C	O	0
			34	24	10	
25	j	1	Total	C	O	0
			32	22	10	



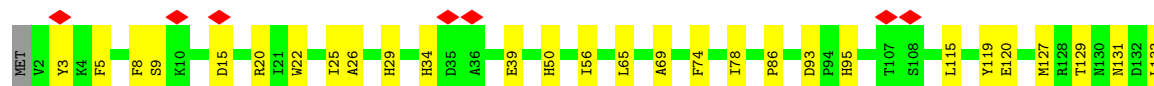
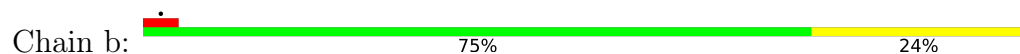
• Molecule 3: VCPI-1

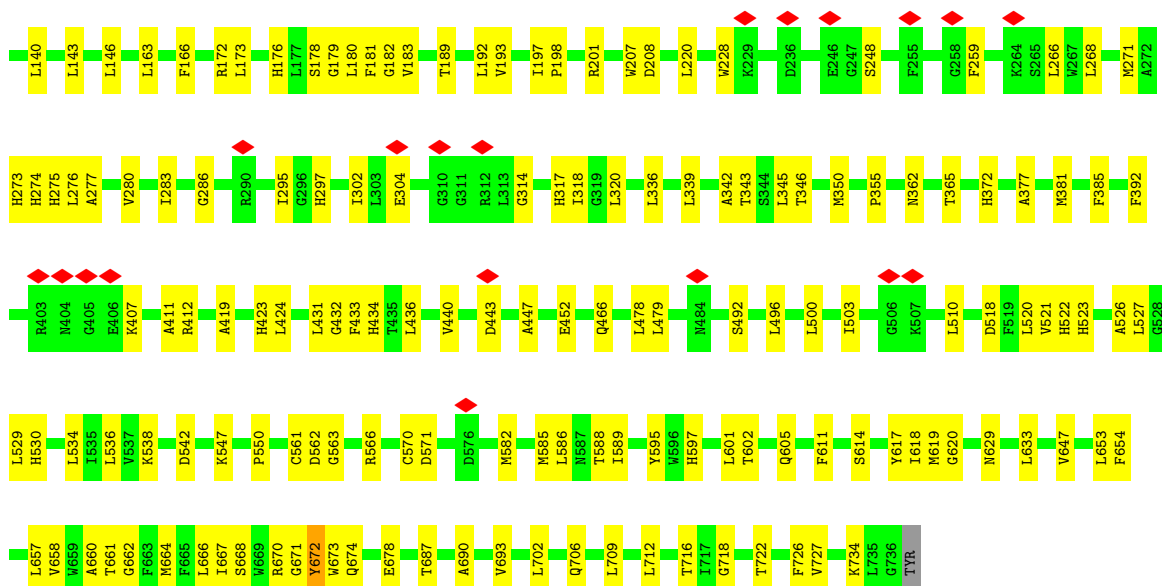


• Molecule 4: Photosystem I P700 chlorophyll a apoprotein A1

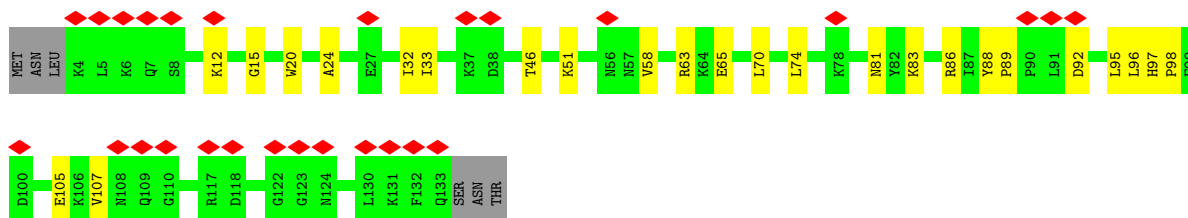
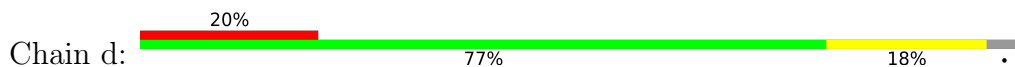


• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A2

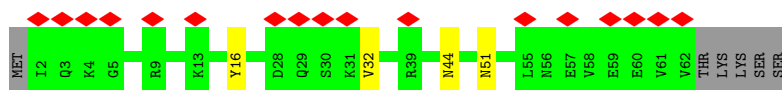
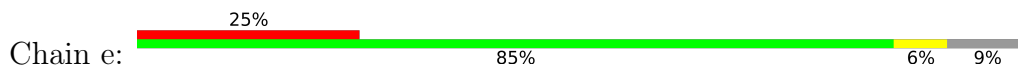




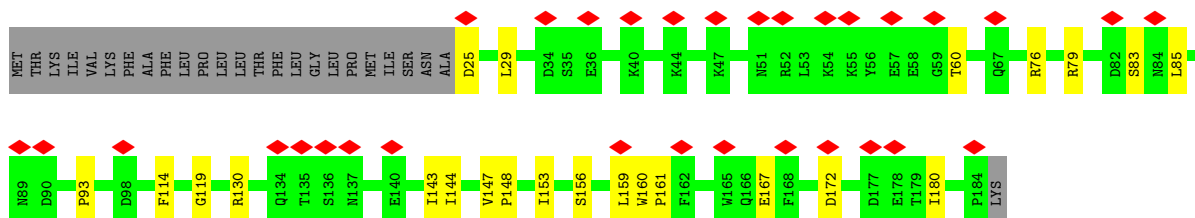
• Molecule 6: Photosystem I reaction center subunit II



• Molecule 7: Photosystem I reaction center subunit IV



• Molecule 8: Photosystem I reaction center subunit III



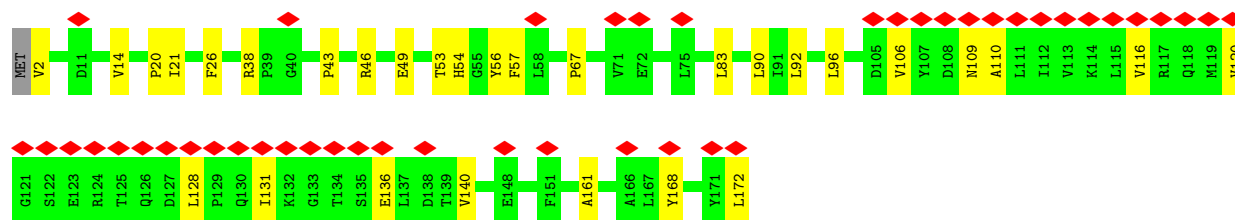
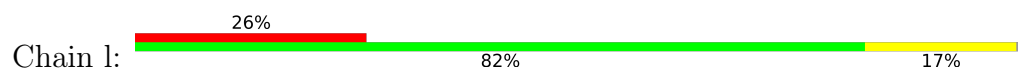
• Molecule 9: Photosystem I reaction center subunit VIII



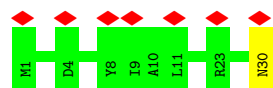
• Molecule 10: Photosystem I reaction center subunit IX



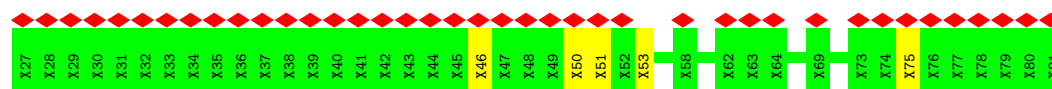
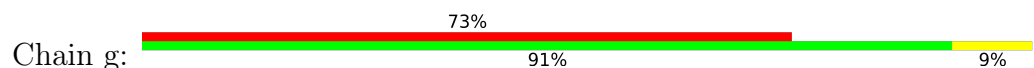
• Molecule 11: PSI subunit V



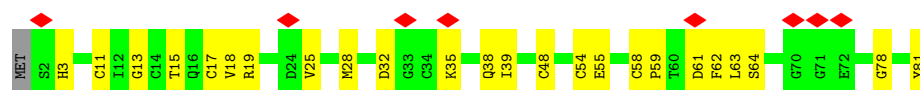
• Molecule 12: PsaM



• Molecule 13: PsaS



• Molecule 14: 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	35610	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	1.594	Depositor
Minimum map value	-0.417	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.345	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: PQN, LMG, XAT, BCR, SF4, A1L1G, SQD, LHG, A1L1F, DGD, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5	0.14	0/1353	0.29	0/1823
2	4	0.17	0/1298	0.32	0/1761
3	1	0.14	0/1293	0.33	0/1759
4	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
5	b	0.20	0/6080	0.32	1/8302 (0.0%)
6	d	0.12	0/1040	0.32	0/1402
7	e	0.09	0/502	0.20	0/681
8	f	0.14	0/1297	0.31	0/1762
9	i	0.14	0/278	0.33	0/378
10	j	0.16	0/351	0.36	0/478
11	l	0.14	0/1315	0.31	0/1796
12	m	0.09	0/210	0.28	0/288
14	c	0.13	0/606	0.34	0/822
All	All	0.21	3/21647 (0.0%)	0.32	5/29471 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	580	SER	CA-C	-7.08	1.43	1.52
4	a	581	ALA	CA-C	-5.48	1.45	1.52
4	a	582	TRP	CA-C	-5.05	1.45	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	581	ALA	N-CA-C	-8.63	102.50	113.72
4	a	448	LEU	N-CA-C	-6.10	104.19	111.69
4	a	584	HIS	N-CA-C	-5.83	106.51	113.97
5	b	672	TYR	N-CA-C	-5.56	106.33	113.23
4	a	585	VAL	N-CA-C	-5.07	105.45	112.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1317	0	1318	37	0
2	4	1268	0	1288	23	0
3	1	1262	0	1237	41	0
4	a	5827	0	5697	141	0
5	b	5865	0	5710	145	0
6	d	1014	0	1015	19	0
7	e	494	0	495	4	0
8	f	1266	0	1262	20	0
9	i	271	0	292	11	0
10	j	339	0	342	21	0
11	l	1283	0	1278	21	0
12	m	210	0	226	1	0
13	g	275	0	62	3	0
14	c	596	0	583	20	0
15	1	88	0	112	7	0
15	4	264	0	336	27	0
15	5	132	0	168	20	0
15	a	44	0	56	5	0
15	j	44	0	56	5	0
16	1	45	0	0	1	0
16	5	45	0	0	1	0
17	1	547	0	508	15	0
17	4	613	0	522	33	0
17	5	563	0	472	23	0
17	a	2579	0	2562	144	0
17	b	2475	0	2536	126	0
17	f	117	0	115	1	0
17	i	62	0	63	4	0
17	j	100	0	86	7	0
17	l	148	0	123	3	0
18	1	45	0	54	3	0
18	5	35	0	34	1	0
19	4	40	0	38	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	b	57	0	72	6	0
20	l	57	0	0	2	0
21	a	33	0	46	3	0
21	b	33	0	46	2	0
22	a	75	0	93	6	0
22	b	31	0	32	0	0
22	m	46	0	65	1	0
23	a	160	0	224	12	0
23	b	320	0	448	29	0
23	f	80	0	112	14	0
23	i	40	0	56	2	0
23	j	40	0	56	8	0
23	l	80	0	112	16	0
23	m	40	0	56	3	0
24	a	8	0	0	0	0
24	c	16	0	0	3	0
25	a	34	0	38	11	0
25	j	32	0	34	7	0
All	All	30455	0	30136	767	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (767) 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	19:4:319:DGD:HE62	1.13	1.12
2:4:193:ALA:HB1	19:4:319:DGD:C6E	1.85	1.07
19:4:319:DGD:O5E	19:4:319:DGD:O4E	1.61	0.95
15:5:302:XAT:H12	17:5:307:CLA:HAB	1.53	0.90
17:a:806:CLA:O1A	17:a:814:CLA:HBA1	1.81	0.81
4:a:531:ILE:HD12	17:a:801:CLA:H172	1.63	0.80
17:b:826:CLA:HMA1	23:b:847:BCR:H17C	1.66	0.78
15:4:304:XAT:H12	17:4:309:CLA:HAB	1.67	0.76
17:1:312:CLA:HHC	17:1:312:CLA:HBB1	1.69	0.75
2:4:193:ALA:CB	19:4:319:DGD:HE62	2.07	0.74
23:a:847:BCR:H362	23:a:848:BCR:H21C	1.73	0.70
17:b:834:CLA:H72	23:b:847:BCR:H391	1.72	0.70
17:b:807:CLA:H151	17:b:829:CLA:HBB2	1.74	0.70
17:4:318:CLA:H2A	19:4:319:DGD:HE62	1.73	0.69
8:f:167:GLU:HG3	8:f:172:ASP:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:43:ILE:O	3:1:70:ARG:NH2	2.25	0.69
5:b:273:HIS:HD1	17:b:818:CLA:HAB	1.58	0.69
10:j:22:THR:HA	10:j:25:PHE:CE1	2.28	0.68
4:a:363:HIS:ND1	17:a:819:CLA:OBD	2.26	0.67
4:a:569:ASP:OD2	4:a:573:ARG:NH2	2.27	0.67
15:4:303:XAT:H14	17:4:311:CLA:H12	1.76	0.67
17:4:318:CLA:HAA2	19:4:319:DGD:HE5	1.77	0.67
3:1:194:GLN:HG3	3:1:199:ASN:HB3	1.77	0.67
3:1:70:ARG:NH1	3:1:73:GLU:OE1	2.28	0.66
1:5:179:LEU:HD12	8:f:159:LEU:HD11	1.75	0.66
17:a:804:CLA:HED1	10:j:15:LEU:HD22	1.76	0.66
10:j:31:ARG:HD3	15:j:101:XAT:H222	1.77	0.66
1:5:113:ARG:NH1	1:5:116:GLU:OE1	2.29	0.66
5:b:304:GLU:HG2	5:b:318:ILE:HG13	1.78	0.66
5:b:336:LEU:HD21	17:b:830:CLA:HAB	1.78	0.65
5:b:9:SER:HB2	19:b:851:DGD:HE62	1.78	0.65
5:b:295:ILE:HG13	17:b:821:CLA:HED1	1.77	0.65
17:b:814:CLA:H121	17:b:819:CLA:H72	1.79	0.65
17:a:808:CLA:HMB2	23:j:104:BCR:HC8	1.79	0.65
17:b:824:CLA:HBB1	17:b:838:CLA:H151	1.79	0.65
4:a:112:TRP:HB3	15:j:101:XAT:H373	1.77	0.65
3:1:146:LEU:HD13	17:a:844:CLA:H91	1.77	0.64
4:a:356:LEU:HD11	17:a:820:CLA:H71	1.78	0.64
15:4:304:XAT:H193	17:4:309:CLA:H142	1.78	0.64
5:b:115:LEU:HA	5:b:365:THR:HG22	1.80	0.64
9:i:29:TYR:HA	9:i:32:LYS:HE2	1.78	0.64
8:f:25:ASP:N	8:f:29:LEU:O	2.30	0.64
4:a:197:GLY:O	4:a:201:LEU:HB2	1.97	0.64
1:5:120:GLY:O	1:5:124:MET:HG3	1.98	0.64
8:f:79:ARG:NH1	10:j:35:ASP:O	2.30	0.64
4:a:429:ALA:O	4:a:433:HIS:ND1	2.31	0.63
5:b:29:HIS:ND1	17:b:807:CLA:O1A	2.28	0.63
5:b:424:LEU:HD13	5:b:534:LEU:HA	1.81	0.63
4:a:684:ARG:H	5:b:570:CYS:HB2	1.64	0.63
17:a:834:CLA:H142	23:b:848:BCR:H15C	1.79	0.63
5:b:129:THR:HG22	5:b:131:ASN:H	1.63	0.63
1:5:130:PHE:CE1	15:5:302:XAT:O24	2.52	0.63
4:a:362:HIS:HA	4:a:365:TYR:CE1	2.33	0.63
10:j:21:PHE:HA	17:j:103:CLA:HBB2	1.80	0.62
15:4:302:XAT:H10	15:4:306:XAT:H363	1.80	0.62
15:4:305:XAT:H32	17:4:314:CLA:HAB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:298:PHE:CE1	17:a:822:CLA:HAB	2.35	0.62
18:5:316:SQD:H2	15:4:301:XAT:H373	1.82	0.62
4:a:589:LEU:HD21	17:a:831:CLA:HBC1	1.81	0.62
5:b:15:ASP:HB3	5:b:20:ARG:HB2	1.82	0.62
17:a:818:CLA:C3D	25:a:853:LMG:HC91	2.30	0.61
6:d:86:ARG:HB2	6:d:96:LEU:HD11	1.82	0.61
6:d:88:TYR:HB2	6:d:92:ASP:HB2	1.81	0.61
10:j:26:VAL:HG11	23:j:104:BCR:H24C	1.81	0.61
4:a:114:ILE:HB	15:j:101:XAT:H372	1.81	0.61
4:a:298:PHE:HE1	17:a:822:CLA:HAB	1.64	0.61
17:4:318:CLA:H2A	19:4:319:DGD:C6E	2.30	0.61
4:a:121:ASN:HB3	4:a:129:GLN:HB3	1.83	0.61
4:a:167:LEU:HD11	17:a:810:CLA:H193	1.83	0.60
17:a:833:CLA:HBC2	17:a:840:CLA:HMC2	1.83	0.60
15:5:302:XAT:H162	17:5:307:CLA:H2	1.82	0.60
4:a:162:ALA:O	4:a:166:MET:HG2	2.00	0.60
1:5:225:ILE:HG22	17:5:314:CLA:HAB	1.82	0.60
17:b:831:CLA:HAB	17:b:838:CLA:HBB2	1.82	0.60
1:5:190:ARG:NH1	1:5:191:GLU:O	2.34	0.60
2:4:185:PHE:CZ	15:4:304:XAT:H30	2.37	0.60
17:b:832:CLA:HBC3	23:f:804:BCR:H362	1.82	0.60
3:1:186:ILE:HG13	3:1:187:THR:HG23	1.83	0.60
20:1:304:A1L1F:C2	17:a:844:CLA:H11	2.31	0.60
6:d:12:LYS:HB2	6:d:51:LYS:HB3	1.82	0.60
5:b:412:ARG:NH2	17:b:831:CLA:O1D	2.35	0.59
5:b:660:ALA:HB3	17:b:804:CLA:HBB2	1.83	0.59
17:a:804:CLA:ND	10:j:12:PRO:HG3	2.17	0.59
17:a:820:CLA:H92	17:a:830:CLA:H91	1.84	0.59
11:l:38:ARG:O	11:l:46:ARG:NH2	2.35	0.59
2:4:170:MET:HE1	17:4:314:CLA:H43	1.84	0.59
4:a:507:VAL:HG22	4:a:517:MET:HG3	1.85	0.59
1:5:190:ARG:HH12	1:5:194:ASN:H	1.51	0.58
4:a:107:SER:HB2	4:a:124:VAL:HG11	1.85	0.58
16:1:301:A1L1G:C18	17:1:306:CLA:HAC2	2.32	0.58
4:a:598:ILE:HG13	17:a:801:CLA:H192	1.86	0.58
5:b:561:CYS:SG	5:b:563:GLY:N	2.71	0.58
1:5:155:VAL:HG21	17:5:309:CLA:HAA2	1.86	0.58
4:a:292:LEU:HD21	17:a:818:CLA:CAB	2.34	0.58
5:b:69:ALA:HB2	5:b:133:LEU:HB2	1.86	0.58
17:b:804:CLA:CGA	17:b:804:CLA:H3A	2.34	0.58
4:a:53:ASP:OD2	4:a:343:HIS:NE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:f:801:BCR:HC32	17:j:102:CLA:H43	1.86	0.57
1:5:112:LEU:HD22	17:5:307:CLA:H12	1.86	0.57
17:a:802:CLA:CGA	17:a:802:CLA:H3A	2.35	0.57
5:b:39:GLU:HB3	5:b:163:LEU:HD11	1.87	0.57
5:b:178:SER:HB3	5:b:286:GLY:HA3	1.86	0.57
1:5:220:GLY:O	1:5:224:MET:HG3	2.04	0.57
4:a:324:GLY:HA3	22:a:846:LHG:HC32	1.87	0.57
17:a:826:CLA:HBA1	17:a:830:CLA:H193	1.86	0.57
17:a:818:CLA:C1D	25:a:853:LMG:H291	2.34	0.57
23:b:843:BCR:H23C	23:b:850:BCR:H323	1.86	0.57
9:i:26:LEU:HD13	23:l:205:BCR:HC8	1.86	0.57
1:5:224:MET:O	1:5:227:ILE:HG22	2.04	0.57
5:b:74:PHE:O	5:b:78:ILE:HG12	2.04	0.57
4:a:114:ILE:HG13	4:a:115:VAL:HG13	1.86	0.57
4:a:517:MET:HE1	4:a:623:HIS:NE2	2.19	0.57
4:a:7:SER:H	4:a:12:PHE:HE2	1.53	0.56
4:a:651:VAL:HG22	4:a:739:ALA:HB3	1.87	0.56
1:5:111:TRP:NE1	17:5:308:CLA:O1A	2.33	0.56
2:4:136:VAL:HG22	17:4:313:CLA:HMA1	1.87	0.56
4:a:70:HIS:ND1	17:a:814:CLA:OBD	2.31	0.56
5:b:582:MET:HG3	5:b:712:LEU:HD21	1.87	0.56
5:b:693:VAL:HG11	17:b:801:CLA:HAB	1.87	0.56
1:5:170:LEU:O	1:5:174:MET:HG3	2.05	0.56
17:a:822:CLA:HBC3	17:a:828:CLA:H172	1.87	0.56
17:a:841:CLA:H72	23:f:801:BCR:H17C	1.88	0.56
25:a:853:LMG:H112	25:a:853:LMG:C9	2.35	0.56
6:d:105:GLU:HG2	14:c:19:ARG:HB3	1.88	0.56
17:b:805:CLA:H18	9:i:14:VAL:HG22	1.86	0.56
6:d:97:HIS:HB3	6:d:98:PRO:HD3	1.86	0.56
15:5:301:XAT:H14	17:5:309:CLA:H12	1.86	0.56
4:a:213:ILE:HG23	4:a:233:PRO:HB3	1.87	0.56
3:1:88:ILE:HG22	3:1:92:PHE:HE1	1.71	0.56
4:a:651:VAL:HG21	4:a:736:PHE:HA	1.88	0.56
11:l:54:HIS:HA	11:l:57:PHE:CE2	2.41	0.56
4:a:734:TRP:NE1	17:a:829:CLA:O1A	2.36	0.55
4:a:290:HIS:HB2	17:a:819:CLA:C1B	2.37	0.55
4:a:441:LEU:HB3	4:a:534:PHE:HB2	1.88	0.55
4:a:660:SER:HB2	5:b:447:ALA:HB1	1.88	0.55
17:a:841:CLA:H92	23:f:801:BCR:H15C	1.88	0.55
25:a:853:LMG:H112	25:a:853:LMG:O8	2.05	0.55
17:b:806:CLA:HBA1	17:b:814:CLA:HBA1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:92:LEU:HB3	23:l:205:BCR:H401	1.89	0.55
17:a:818:CLA:CHD	25:a:853:LMG:H291	2.36	0.55
17:a:825:CLA:H12	23:a:849:BCR:H14C	1.88	0.55
17:a:854:CLA:H112	10:j:14:LEU:HD22	1.88	0.55
5:b:521:VAL:HG21	5:b:595:TYR:HB2	1.89	0.55
7:e:32:VAL:HG11	14:c:35:LYS:HD3	1.89	0.55
2:4:185:PHE:CE2	15:4:304:XAT:H30	2.42	0.55
4:a:197:GLY:HA3	17:a:814:CLA:HBB1	1.89	0.55
17:a:829:CLA:H101	23:j:104:BCR:H341	1.89	0.55
3:1:115:ILE:O	3:1:119:GLN:NE2	2.40	0.54
4:a:388:VAL:HG12	4:a:596:ILE:HG23	1.89	0.54
16:5:303:A1L1G:C41	17:5:312:CLA:HMC1	2.37	0.54
4:a:702:LYS:HB3	8:f:130:ARG:HD3	1.89	0.54
4:a:667:LEU:HD11	5:b:619:MET:HB2	1.89	0.54
17:a:831:CLA:H42	22:a:845:LHG:H251	1.90	0.54
4:a:219:LYS:HD3	4:a:246:LEU:HB3	1.90	0.54
4:a:573:ARG:HG3	14:c:78:GLY:HA3	1.90	0.54
5:b:22:TRP:CG	5:b:706:GLN:HE22	2.26	0.54
6:d:63:ARG:NH2	6:d:65:GLU:OE1	2.41	0.54
10:j:14:LEU:HD21	25:j:105:LMG:H141	1.89	0.54
3:1:61:ALA:HB1	3:1:65:THR:HB	1.90	0.54
2:4:121:LEU:HD23	2:4:124:ILE:HD12	1.90	0.53
2:4:140:SER:OG	10:j:1:MET:SD	2.57	0.53
17:b:822:CLA:HHB	17:b:823:CLA:H2	1.88	0.53
4:a:591:TRP:HE1	17:b:804:CLA:C1D	2.20	0.53
5:b:5:PHE:HB2	9:i:30:ILE:HA	1.89	0.53
17:b:824:CLA:HBB2	17:b:841:CLA:H52	1.89	0.53
1:5:175:HIS:HB2	1:5:179:LEU:HD23	1.89	0.53
17:a:835:CLA:O2D	17:a:835:CLA:H2A	2.09	0.53
17:b:830:CLA:H42	19:b:851:DGD:HB42	1.91	0.53
14:c:15:THR:HG22	14:c:28:MET:HG3	1.89	0.53
5:b:355:PRO:HG3	17:b:819:CLA:HBA1	1.90	0.53
2:4:83:ILE:HD11	15:4:303:XAT:H362	1.90	0.53
3:1:77:GLY:O	3:1:81:MET:HG3	2.09	0.53
4:a:210:GLN:HA	4:a:214:ALA:HB3	1.89	0.53
5:b:443:ASP:OD1	5:b:617:TYR:HB2	2.08	0.53
3:1:72:SER:O	3:1:76:HIS:ND1	2.28	0.53
5:b:317:HIS:HB3	5:b:320:LEU:HD12	1.90	0.53
5:b:633:LEU:HD22	5:b:726:PHE:HA	1.89	0.53
5:b:709:LEU:HD11	19:b:851:DGD:HB41	1.90	0.53
17:a:825:CLA:HMA3	17:a:844:CLA:HAB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:193:ALA:O	19:4:319:DGD:O6E	2.28	0.52
17:4:318:CLA:O2D	19:4:319:DGD:HE61	2.09	0.52
3:1:85:LEU:HB3	17:1:308:CLA:HMC2	1.92	0.52
17:a:810:CLA:HAB	17:j:102:CLA:HMD2	1.91	0.52
5:b:661:THR:O	5:b:664:MET:HB3	2.08	0.52
17:b:837:CLA:HBC3	23:f:804:BCR:H292	1.91	0.52
17:b:837:CLA:HBC3	23:f:804:BCR:H401	1.91	0.52
1:5:155:VAL:HG22	1:5:159:PRO:HG2	1.92	0.52
1:5:236:VAL:HG23	1:5:237:THR:HG23	1.92	0.52
5:b:718:GLY:O	5:b:722:THR:HG22	2.08	0.52
17:b:801:CLA:H101	17:b:801:CLA:HBB1	1.92	0.52
13:g:51:UNK:O	13:g:53:UNK:N	2.42	0.52
15:5:302:XAT:C16	17:5:307:CLA:H2	2.39	0.52
14:c:11:CYS:SG	14:c:39:ILE:HG13	2.50	0.52
6:d:95:LEU:HD22	13:g:75:UNK:HA	1.91	0.52
17:a:809:CLA:CHC	17:a:810:CLA:HMD2	2.39	0.52
5:b:140:LEU:HG	23:b:845:BCR:H382	1.90	0.52
17:a:834:CLA:H151	21:b:842:PQN:H202	1.91	0.52
5:b:189:THR:HG21	5:b:276:LEU:HB2	1.91	0.51
8:f:85:LEU:HD13	8:f:93:PRO:HB3	1.92	0.51
4:a:396:VAL:HG11	4:a:589:LEU:HG	1.91	0.51
2:4:81:CYS:HB3	2:4:178:GLY:HA3	1.91	0.51
17:a:820:CLA:HAB	17:a:820:CLA:H8	1.90	0.51
17:a:827:CLA:H93	17:a:840:CLA:H52	1.92	0.51
5:b:179:GLY:O	5:b:183:VAL:HB	2.10	0.51
5:b:342:ALA:O	5:b:346:THR:HG23	2.10	0.51
1:5:178:LYS:HD2	1:5:183:ASP:HB3	1.92	0.51
4:a:422:ARG:O	4:a:426:HIS:ND1	2.41	0.51
6:d:33:ILE:HG22	6:d:58:VAL:HG22	1.92	0.51
14:c:58:CYS:SG	14:c:63:LEU:HA	2.51	0.51
17:b:812:CLA:H72	17:b:813:CLA:HBC3	1.93	0.51
4:a:431:ILE:HG13	4:a:549:TYR:HE1	1.74	0.51
5:b:602:THR:HG21	5:b:611:PHE:HB2	1.93	0.51
20:1:304:A1L1F:C56	22:a:846:LHG:H241	2.41	0.51
17:a:818:CLA:HHC	17:a:818:CLA:HBB1	1.93	0.51
5:b:93:ASP:OD1	5:b:95:HIS:ND1	2.33	0.51
5:b:662:GLY:O	5:b:666:LEU:HG	2.10	0.51
11:l:109:ASN:OD1	11:l:110:ALA:N	2.35	0.51
4:a:460:ARG:NH2	17:a:835:CLA:O1D	2.44	0.51
4:a:686:TYR:OH	17:a:802:CLA:OBD	2.22	0.51
5:b:274:HIS:HB2	17:b:818:CLA:C1B	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:434:HIS:CD2	23:b:852:BCR:H333	2.46	0.51
8:f:143:ILE:HG13	8:f:144:ILE:HG13	1.92	0.51
15:4:304:XAT:C16	17:4:309:CLA:H2	2.41	0.51
5:b:478:LEU:HG	5:b:479:LEU:HG	1.93	0.51
4:a:425:ARG:NH2	6:d:15:GLY:O	2.44	0.50
4:a:577:CYS:O	5:b:671:GLY:HA3	2.11	0.50
25:a:853:LMG:C11	25:a:853:LMG:HC92	2.41	0.50
25:a:853:LMG:H131	25:a:853:LMG:H292	1.93	0.50
17:b:807:CLA:H52	19:b:851:DGD:HB72	1.92	0.50
8:f:160:TRP:CD1	8:f:161:PRO:HD3	2.46	0.50
14:c:13:GLY:O	14:c:38:GLN:NE2	2.44	0.50
4:a:565:ARG:HG2	4:a:715:THR:HG21	1.93	0.50
17:a:818:CLA:O1A	25:a:853:LMG:O10	2.30	0.50
14:c:17:CYS:SG	14:c:18:VAL:N	2.85	0.50
5:b:26:ALA:HA	17:b:830:CLA:H43	1.93	0.50
9:i:26:LEU:HD22	23:l:205:BCR:H323	1.94	0.50
11:l:106:VAL:H	11:l:140:VAL:HG23	1.77	0.50
4:a:712:LEU:N	21:a:843:PQN:O4	2.45	0.50
5:b:419:ALA:O	5:b:423:HIS:ND1	2.40	0.50
17:b:824:CLA:HAB	17:b:831:CLA:HMD1	1.93	0.50
4:a:674:ALA:HB3	17:a:802:CLA:HBB2	1.94	0.49
14:c:17:CYS:HB3	24:c:102:SF4:S4	2.52	0.49
3:1:144:ASP:OD2	3:1:148:THR:OG1	2.23	0.49
5:b:526:ALA:O	5:b:530:HIS:ND1	2.37	0.49
4:a:292:LEU:HD12	17:a:816:CLA:HMC3	1.95	0.49
5:b:722:THR:HG23	17:b:803:CLA:O1D	2.11	0.49
23:b:852:BCR:H23C	10:j:33:TYR:CD2	2.47	0.49
17:5:312:CLA:CGA	17:5:312:CLA:H3A	2.41	0.49
17:4:310:CLA:HAC1	17:4:317:CLA:HAB	1.95	0.49
1:5:190:ARG:HH12	1:5:194:ASN:N	2.10	0.49
4:a:440:PHE:HE2	17:a:839:CLA:HAB	1.76	0.49
5:b:466:GLN:NE2	17:b:836:CLA:OBD	2.34	0.49
4:a:554:ARG:HB2	5:b:678:GLU:OE1	2.13	0.49
5:b:407:LYS:HB3	5:b:411:ALA:HB3	1.95	0.49
11:l:43:PRO:HD3	11:l:136:GLU:CD	2.38	0.49
1:5:130:PHE:HE1	15:5:302:XAT:O24	1.94	0.49
1:5:171:GLU:HG3	17:5:311:CLA:NB	2.28	0.49
3:1:112:VAL:HB	3:1:117:TRP:NE1	2.27	0.49
4:a:712:LEU:HD21	21:a:843:PQN:H151	1.95	0.49
5:b:166:PHE:O	5:b:172:ARG:NH2	2.46	0.49
4:a:290:HIS:HB2	17:a:819:CLA:CHB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:423:VAL:HA	4:a:426:HIS:CE1	2.47	0.48
5:b:25:ILE:HG12	23:l:205:BCR:H312	1.94	0.48
5:b:271:MET:O	5:b:275:HIS:ND1	2.47	0.48
3:1:42:MET:HE1	3:1:66:LEU:HD22	1.96	0.48
4:a:400:ALA:HB2	4:a:585:VAL:HG11	1.96	0.48
5:b:273:HIS:ND1	17:b:818:CLA:HAB	2.25	0.48
17:b:833:CLA:HBB2	23:f:801:BCR:HC41	1.94	0.48
23:b:852:BCR:H23C	10:j:33:TYR:HD2	1.78	0.48
11:l:38:ARG:NH1	11:l:49:GLU:OE1	2.40	0.48
13:g:46:UNK:O	13:g:50:UNK:N	2.45	0.48
17:a:841:CLA:H61	17:b:833:CLA:H42	1.95	0.48
5:b:492:SER:HA	5:b:496:LEU:HD12	1.94	0.48
5:b:597:HIS:CE1	5:b:601:LEU:HD11	2.48	0.48
17:b:825:CLA:H193	17:b:825:CLA:H141	1.95	0.48
15:5:304:XAT:C10	17:5:315:CLA:HBC3	2.44	0.48
4:a:615:VAL:HG22	4:a:621:VAL:HG22	1.95	0.48
17:a:803:CLA:H2	5:b:657:LEU:HD22	1.95	0.48
5:b:8:PHE:HB2	5:b:34:HIS:CG	2.49	0.48
5:b:181:PHE:HE2	17:b:820:CLA:HAB	1.78	0.48
5:b:266:LEU:HD22	17:b:818:CLA:HBA1	1.95	0.48
5:b:412:ARG:HH21	17:b:831:CLA:CGD	2.27	0.48
17:b:824:CLA:H2A	17:b:824:CLA:HED3	1.95	0.48
17:a:818:CLA:CHD	17:a:819:CLA:HBB2	2.43	0.48
17:a:825:CLA:H71	17:a:840:CLA:H62	1.96	0.48
17:b:808:CLA:H93	17:b:808:CLA:H61	1.71	0.48
7:e:51:ASN:CG	14:c:61:ASP:HB2	2.39	0.48
15:5:301:XAT:H193	17:5:310:CLA:HBA2	1.94	0.48
5:b:65:LEU:HD11	23:b:845:BCR:H281	1.96	0.48
2:4:159:ASN:C	2:4:161:ALA:H	2.20	0.48
5:b:452:GLU:OE2	8:f:76:ARG:NE	2.42	0.48
17:a:802:CLA:H41	5:b:436:LEU:HD22	1.95	0.48
5:b:277:ALA:HA	17:b:817:CLA:HMC2	1.95	0.48
17:b:811:CLA:H202	11:l:90:LEU:HD22	1.96	0.48
1:5:102:GLY:O	1:5:105:THR:OG1	2.29	0.48
4:a:68:SER:OG	4:a:174:TYR:HB2	2.14	0.48
4:a:114:ILE:HG23	4:a:115:VAL:HG22	1.96	0.48
5:b:443:ASP:OD1	5:b:618:ILE:N	2.46	0.48
5:b:595:TYR:CZ	17:b:836:CLA:HBC3	2.49	0.48
5:b:670:ARG:C	5:b:672:TYR:H	2.22	0.48
17:b:822:CLA:CHB	17:b:823:CLA:H2	2.44	0.48
9:i:26:LEU:HB3	23:l:205:BCR:H323	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:127:ASN:HD21	8:f:60:THR:HG21	1.79	0.47
5:b:3:TYR:HB2	9:i:33:GLU:HA	1.95	0.47
17:b:813:CLA:H62	17:b:813:CLA:H41	1.62	0.47
17:b:825:CLA:H92	17:b:825:CLA:H61	1.72	0.47
17:b:839:CLA:HAB	21:b:842:PQN:H172	1.96	0.47
3:1:84:VAL:O	3:1:88:ILE:HG12	2.14	0.47
17:b:840:CLA:H13	23:i:101:BCR:H19C	1.95	0.47
4:a:637:ASN:HB2	5:b:653:LEU:HD11	1.94	0.47
5:b:518:ASP:O	5:b:522:HIS:ND1	2.38	0.47
6:d:95:LEU:HD11	6:d:98:PRO:HD2	1.95	0.47
4:a:375:ILE:HG21	4:a:510:VAL:HB	1.97	0.47
17:b:809:CLA:H142	17:b:809:CLA:H111	1.70	0.47
1:5:130:PHE:HD2	1:5:230:LEU:HD12	1.79	0.47
5:b:385:PHE:HB3	5:b:536:LEU:HB3	1.97	0.47
2:4:184:ALA:HA	17:4:316:CLA:HBB1	1.96	0.47
17:4:318:CLA:CGD	19:4:319:DGD:HE61	2.45	0.47
3:1:88:ILE:HG22	3:1:92:PHE:CE1	2.49	0.47
17:a:832:CLA:HAB	17:a:840:CLA:HBB2	1.96	0.47
5:b:208:ASP:OD1	5:b:208:ASP:N	2.43	0.47
5:b:538:LYS:O	5:b:542:ASP:HB2	2.15	0.47
17:b:811:CLA:HBA2	11:l:67:PRO:HG3	1.97	0.47
17:b:831:CLA:HAB	17:b:838:CLA:CBB	2.44	0.47
23:b:844:BCR:H351	23:b:844:BCR:H15C	1.78	0.47
23:b:852:BCR:H11C	23:b:852:BCR:H341	1.73	0.47
10:j:2:LYS:O	25:j:105:LMG:HC61	2.13	0.47
5:b:120:GLU:OE2	5:b:362:ASN:ND2	2.39	0.47
5:b:176:HIS:O	5:b:180:LEU:HB3	2.14	0.47
10:j:5:LEU:HB3	25:j:105:LMG:HC72	1.96	0.47
4:a:476:PHE:HB3	17:a:838:CLA:H11	1.96	0.47
4:a:677:LEU:HB2	17:a:802:CLA:HMC2	1.97	0.47
5:b:586:LEU:HD21	5:b:716:THR:HG23	1.96	0.47
3:1:40:ASP:HB2	3:1:42:MET:HG3	1.97	0.47
3:1:73:GLU:HB2	17:1:306:CLA:C1B	2.45	0.47
17:1:306:CLA:H93	17:1:306:CLA:H61	1.70	0.47
5:b:687:THR:HG23	5:b:690:ALA:HB3	1.97	0.47
23:b:845:BCR:H311	23:b:845:BCR:HC8	1.97	0.47
15:4:306:XAT:H35	15:4:306:XAT:H401	1.77	0.46
3:1:62:ASP:OD1	3:1:62:ASP:N	2.49	0.46
5:b:50:HIS:ND1	17:b:814:CLA:OBD	2.38	0.46
5:b:432:GLY:HA2	5:b:527:LEU:HD22	1.96	0.46
5:b:433:PHE:HZ	23:f:801:BCR:H372	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:f:153:ILE:O	8:f:156:SER:OG	2.31	0.46
10:j:30:ASN:ND2	17:j:102:CLA:O1A	2.47	0.46
1:5:96:VAL:HG12	17:5:307:CLA:OBD	2.15	0.46
17:a:820:CLA:H203	17:a:828:CLA:H3A	1.96	0.46
17:a:834:CLA:CAD	23:l:201:BCR:H10C	2.45	0.46
5:b:297:HIS:HB3	5:b:302:ILE:HD11	1.96	0.46
17:b:811:CLA:H71	11:l:83:LEU:HG	1.97	0.46
6:d:83:LYS:HG2	6:d:98:PRO:HG2	1.97	0.46
2:4:193:ALA:HB1	19:4:319:DGD:O5E	2.16	0.46
15:4:301:XAT:H35	15:4:301:XAT:H401	1.66	0.46
17:b:818:CLA:H41	17:b:834:CLA:HAA2	1.98	0.46
17:b:839:CLA:H12	23:l:205:BCR:H15C	1.97	0.46
11:l:168:TYR:O	11:l:172:LEU:HB2	2.16	0.46
4:a:144:GLU:HG2	4:a:206:TRP:HH2	1.80	0.46
4:a:354:GLY:HA2	4:a:391:GLY:HA2	1.97	0.46
4:a:514:ILE:HD11	4:a:621:VAL:HG13	1.96	0.46
17:j:102:CLA:NB	23:j:104:BCR:H281	2.30	0.46
23:l:205:BCR:H11C	23:l:205:BCR:H341	1.84	0.46
17:a:806:CLA:H72	23:a:848:BCR:HC8	1.98	0.46
25:a:853:LMG:H112	25:a:853:LMG:HC92	1.98	0.46
5:b:143:LEU:HD23	5:b:146:LEU:HD12	1.97	0.46
17:b:812:CLA:H51	17:b:813:CLA:H43	1.97	0.46
9:i:28:LEU:O	9:i:32:LYS:HG3	2.15	0.46
17:a:801:CLA:HBD	17:a:801:CLA:HED2	1.48	0.46
17:a:818:CLA:NC	25:a:853:LMG:H302	2.31	0.46
5:b:280:VAL:HG21	17:b:817:CLA:HAB	1.98	0.46
17:b:823:CLA:HHC	17:b:841:CLA:HED1	1.98	0.46
1:5:124:MET:HE3	17:5:312:CLA:HMC2	1.98	0.46
15:4:303:XAT:H30	17:4:311:CLA:H151	1.98	0.46
17:a:834:CLA:H201	23:l:205:BCR:H343	1.98	0.46
17:a:854:CLA:H143	25:j:105:LMG:H142	1.98	0.46
5:b:127:MET:HE1	23:b:845:BCR:H282	1.97	0.46
5:b:372:HIS:HB2	17:b:828:CLA:C1B	2.45	0.46
15:5:301:XAT:H35	15:5:301:XAT:H401	1.77	0.46
2:4:185:PHE:CZ	15:4:304:XAT:H28	2.50	0.46
17:b:824:CLA:HBA1	23:b:846:BCR:H16C	1.98	0.46
17:b:826:CLA:HAA2	17:b:827:CLA:OBD	2.16	0.46
6:d:20:TRP:CZ2	11:l:14:VAL:HG12	2.50	0.46
22:m:101:LHG:H321	22:m:101:LHG:H291	1.66	0.46
17:a:801:CLA:CED	17:a:801:CLA:HAA2	2.46	0.46
17:a:801:CLA:H61	17:a:803:CLA:O1D	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:853:LMG:C9	25:a:853:LMG:C11	2.91	0.46
4:a:38:THR:HB	4:a:710:ARG:HG3	1.97	0.45
4:a:114:ILE:O	4:a:117:GLN:HG2	2.16	0.45
15:5:302:XAT:H11	15:5:302:XAT:H191	1.65	0.45
17:4:309:CLA:H143	17:4:309:CLA:H112	1.66	0.45
1:5:164:PHE:HE1	17:f:802:CLA:H121	1.82	0.45
2:4:37:SER:HB3	2:4:45:ARG:HA	1.98	0.45
17:4:312:CLA:O2D	17:4:312:CLA:H2A	2.17	0.45
4:a:342:TRP:CD1	17:a:826:CLA:H192	2.51	0.45
4:a:686:TYR:CE1	5:b:538:LYS:HD2	2.52	0.45
17:a:827:CLA:H13	17:a:827:CLA:H172	1.76	0.45
17:a:835:CLA:H61	23:l:201:BCR:H363	1.99	0.45
5:b:339:LEU:O	5:b:343:THR:HG22	2.16	0.45
5:b:518:ASP:OD2	5:b:595:TYR:OH	2.23	0.45
9:i:14:VAL:O	9:i:19:PRO:HD2	2.17	0.45
5:b:228:TRP:HZ3	23:b:850:BCR:H363	1.81	0.45
8:f:119:GLY:HA3	8:f:160:TRP:CE2	2.51	0.45
1:5:116:GLU:HB2	17:5:307:CLA:C1B	2.46	0.45
15:1:303:XAT:H183	17:1:308:CLA:C2B	2.47	0.45
4:a:502:ALA:HB2	4:a:516:MET:HE2	1.97	0.45
17:a:829:CLA:HBB1	17:a:829:CLA:HMB1	1.97	0.45
23:a:848:BCR:H15C	23:a:848:BCR:H351	1.78	0.45
5:b:392:PHE:CE2	23:b:847:BCR:HC42	2.51	0.45
1:5:232:HIS:HE1	15:5:304:XAT:H14	1.81	0.45
15:5:302:XAT:H15	15:5:302:XAT:H201	1.74	0.45
3:1:141:ARG:HD3	3:1:149:TRP:HB3	1.99	0.45
5:b:678:GLU:HG2	14:c:81:TYR:HE1	1.81	0.45
4:a:282:LEU:HD21	4:a:367:MET:HB3	1.98	0.45
4:a:312:GLY:HA2	17:a:823:CLA:HMD2	1.99	0.45
4:a:411:ASN:ND2	4:a:414:ASN:OD1	2.37	0.45
4:a:665:ILE:HG23	17:a:809:CLA:H171	1.98	0.45
5:b:26:ALA:HB1	19:b:851:DGD:O1B	2.17	0.45
5:b:50:HIS:HE1	17:b:806:CLA:H171	1.81	0.45
17:b:833:CLA:H18	23:f:804:BCR:H17C	1.97	0.45
1:5:92:MET:HE3	1:5:113:ARG:HE	1.82	0.45
17:a:803:CLA:H151	17:b:811:CLA:HBC3	1.97	0.45
17:a:831:CLA:H61	17:a:831:CLA:H92	1.70	0.45
25:j:105:LMG:H292	25:j:105:LMG:H111	1.98	0.45
14:c:3:HIS:HB2	14:c:48:CYS:SG	2.56	0.45
2:4:170:MET:CE	17:4:314:CLA:H12	2.47	0.45
15:1:302:XAT:H31	15:1:302:XAT:H391	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:312:CLA:HMA2	18:1:315:SQD:H141	1.99	0.45
4:a:407:VAL:HG11	4:a:564:PHE:N	2.32	0.45
17:a:826:CLA:HMB3	17:a:826:CLA:HBB1	1.99	0.45
5:b:562:ASP:OD2	5:b:566:ARG:NH2	2.38	0.45
17:b:837:CLA:H62	17:b:837:CLA:H102	1.77	0.45
4:a:683:GLY:HA3	5:b:571:ASP:HB2	1.99	0.45
17:a:831:CLA:H62	17:a:831:CLA:H41	1.76	0.45
17:a:839:CLA:H62	17:a:839:CLA:H41	1.54	0.45
5:b:605:GLN:HE21	5:b:734:LYS:HB3	1.82	0.45
17:b:824:CLA:HHB	17:b:841:CLA:O1D	2.16	0.45
15:4:301:XAT:H31	15:4:301:XAT:H391	1.73	0.44
5:b:268:LEU:HD23	5:b:271:MET:HE3	1.98	0.44
1:5:158:GLN:HB3	1:5:159:PRO:HD3	1.99	0.44
3:1:89:VAL:O	3:1:93:TRP:N	2.49	0.44
4:a:304:MET:HG3	17:a:823:CLA:C3C	2.47	0.44
17:a:804:CLA:H41	17:a:841:CLA:HMC1	1.98	0.44
17:a:822:CLA:H12	17:a:825:CLA:HBA2	1.98	0.44
5:b:201:ARG:HG2	5:b:248:SER:HB2	1.99	0.44
17:b:805:CLA:H2	17:b:805:CLA:H61	1.62	0.44
14:c:25:VAL:HG21	14:c:48:CYS:HA	1.99	0.44
4:a:25:PRO:HB2	4:a:41:TRP:HH2	1.81	0.44
25:j:105:LMG:H122	25:j:105:LMG:H151	1.56	0.44
1:5:106:PHE:HB2	8:f:148:PRO:HG3	1.99	0.44
15:4:302:XAT:H15	15:4:302:XAT:H201	1.79	0.44
15:4:302:XAT:H391	15:4:302:XAT:H31	1.83	0.44
15:1:303:XAT:H15	15:1:303:XAT:H201	1.85	0.44
4:a:565:ARG:HD2	22:a:845:LHG:HC61	2.00	0.44
17:b:825:CLA:H52	17:b:825:CLA:H12	1.85	0.44
15:4:302:XAT:H35	15:4:302:XAT:H401	1.81	0.44
4:a:367:MET:HG2	4:a:500:SER:HB2	1.99	0.44
4:a:415:ASN:O	4:a:421:ASP:HB2	2.18	0.44
5:b:343:THR:HG23	5:b:377:ALA:HB2	2.00	0.44
17:4:311:CLA:CGA	17:4:311:CLA:C1A	2.96	0.44
3:1:105:PRO:C	3:1:107:LYS:H	2.24	0.44
3:1:152:VAL:HG11	3:1:159:TRP:CD1	2.53	0.44
4:a:532:HIS:CE1	4:a:599:VAL:HA	2.53	0.44
17:a:807:CLA:H43	22:a:845:LHG:H252	2.00	0.44
17:a:829:CLA:H91	17:a:831:CLA:H192	2.00	0.44
5:b:654:PHE:O	5:b:658:VAL:HG23	2.17	0.44
17:b:821:CLA:HBA2	17:b:821:CLA:H3A	1.33	0.44
15:5:302:XAT:H383	17:5:309:CLA:C2B	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:95:PRO:HD2	17:1:308:CLA:HMD3	1.99	0.44
3:1:156:ASP:OD2	11:l:2:VAL:N	2.51	0.44
4:a:73:GLN:HG2	17:a:806:CLA:H3A	2.00	0.44
4:a:447:GLY:HA3	17:a:835:CLA:HAB	1.98	0.44
4:a:466:SER:HG	4:a:631:GLN:HE22	1.63	0.44
17:b:814:CLA:H143	17:b:825:CLA:H51	1.99	0.44
8:f:79:ARG:O	8:f:83:SER:HB2	2.17	0.44
11:l:116:VAL:HG11	11:l:128:LEU:C	2.42	0.44
23:l:205:BCR:H15C	23:l:205:BCR:H351	1.75	0.44
15:1:302:XAT:H35	15:1:302:XAT:H401	1.72	0.44
4:a:71:PHE:HD1	4:a:166:MET:HE3	1.82	0.44
4:a:578:GLN:HA	4:a:583:ASP:OD2	2.18	0.44
5:b:172:ARG:HD2	17:b:825:CLA:OBD	2.18	0.44
6:d:81:ASN:H	6:d:81:ASN:ND2	2.16	0.44
8:f:160:TRP:CG	8:f:161:PRO:HD3	2.52	0.44
10:j:26:VAL:CG1	23:j:104:BCR:H403	2.47	0.44
14:c:59:PRO:HD2	24:c:102:SF4:S2	2.58	0.44
4:a:194:HIS:HE1	17:a:826:CLA:H72	1.83	0.44
17:a:820:CLA:CAD	17:a:830:CLA:H41	2.48	0.44
5:b:259:PHE:CZ	5:b:510:LEU:HD12	2.52	0.44
17:b:802:CLA:H112	17:b:802:CLA:H93	1.70	0.44
17:b:802:CLA:H162	17:b:802:CLA:H122	1.61	0.44
17:b:811:CLA:H112	17:i:102:CLA:HAB	1.99	0.44
15:5:302:XAT:H35	15:5:302:XAT:H401	1.87	0.43
2:4:85:MET:HE3	2:4:177:ASN:HB3	2.00	0.43
4:a:84:MET:SD	17:a:829:CLA:HED1	2.58	0.43
4:a:567:PRO:HB3	4:a:714:ILE:HB	2.00	0.43
4:a:580:SER:HB2	4:a:582:TRP:H	1.82	0.43
4:a:701:LEU:HD12	17:a:841:CLA:HMA2	2.00	0.43
17:a:844:CLA:C1C	22:a:846:LHG:HC31	2.48	0.43
5:b:424:LEU:HG	17:b:838:CLA:CBB	2.48	0.43
8:f:143:ILE:O	10:j:11:ALA:N	2.48	0.43
18:1:315:SQD:H282	18:1:315:SQD:H311	1.84	0.43
14:c:54:CYS:SG	14:c:55:GLU:N	2.91	0.43
17:4:310:CLA:HED2	17:4:310:CLA:HBD	1.83	0.43
15:1:302:XAT:H15	15:1:302:XAT:H201	1.87	0.43
4:a:143:ALA:HB2	4:a:371:PRO:HD2	2.01	0.43
5:b:529:LEU:HD23	5:b:588:THR:HG21	2.00	0.43
17:b:815:CLA:H61	17:b:815:CLA:H2	1.77	0.43
17:b:817:CLA:CHD	17:b:818:CLA:HBB2	2.49	0.43
17:b:839:CLA:H161	11:l:92:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:252:LYS:NZ	4:a:264:GLU:OE1	2.41	0.43
23:b:845:BCR:H371	23:b:845:BCR:H24C	1.70	0.43
17:j:103:CLA:O1D	17:j:103:CLA:H2A	2.18	0.43
17:4:311:CLA:H162	17:4:311:CLA:H141	1.70	0.43
17:1:306:CLA:H162	17:1:306:CLA:H202	1.69	0.43
17:1:310:CLA:H92	17:1:310:CLA:H61	1.73	0.43
17:a:809:CLA:HBA2	17:a:809:CLA:H3A	1.67	0.43
17:b:814:CLA:H161	17:b:814:CLA:H141	1.77	0.43
17:b:836:CLA:H12	17:b:837:CLA:O1A	2.18	0.43
2:4:59:PHE:HE1	17:4:307:CLA:HBC3	1.83	0.43
17:4:308:CLA:H41	17:4:308:CLA:H61	1.86	0.43
4:a:75:ALA:HB2	4:a:166:MET:HB2	2.01	0.43
4:a:94:TYR:OH	4:a:146:ILE:O	2.23	0.43
17:a:807:CLA:H102	17:a:807:CLA:H161	2.00	0.43
17:a:807:CLA:H161	17:a:807:CLA:H192	1.83	0.43
17:a:819:CLA:HBA2	17:a:819:CLA:H3A	1.53	0.43
17:a:833:CLA:H72	17:l:203:CLA:H12	2.00	0.43
17:a:840:CLA:H72	23:a:850:BCR:H373	2.01	0.43
15:a:852:XAT:H15	15:a:852:XAT:H201	1.67	0.43
10:j:14:LEU:CD2	25:j:105:LMG:H141	2.49	0.43
3:1:140:TYR:OH	3:1:142:PRO:O	2.25	0.43
5:b:207:TRP:HE1	17:b:815:CLA:H11	1.84	0.43
17:b:813:CLA:HBA2	17:b:813:CLA:H3A	1.61	0.43
17:b:826:CLA:H3A	17:b:826:CLA:HBA2	1.73	0.43
6:d:20:TRP:HB2	6:d:24:ALA:HB3	1.99	0.43
1:5:98:PHE:HE1	17:5:305:CLA:HBC3	1.84	0.43
2:4:183:LEU:HD11	17:4:309:CLA:HAC1	2.00	0.43
3:1:171:ARG:HA	3:1:174:MET:CE	2.49	0.43
4:a:442:GLY:HA3	17:b:804:CLA:O1A	2.18	0.43
17:a:832:CLA:HBA1	17:a:832:CLA:H3A	1.80	0.43
5:b:140:LEU:HD23	5:b:143:LEU:HD12	2.01	0.43
5:b:526:ALA:HB2	17:b:837:CLA:HMA1	2.00	0.43
17:b:811:CLA:H141	17:b:811:CLA:H162	1.75	0.43
17:b:819:CLA:H3A	17:b:819:CLA:HBA2	1.37	0.43
3:1:171:ARG:HA	3:1:174:MET:HE3	2.00	0.43
17:a:854:CLA:H142	17:a:854:CLA:H111	1.80	0.43
5:b:172:ARG:HB2	17:b:814:CLA:HBC2	2.00	0.43
5:b:440:VAL:HG12	17:j:102:CLA:HAC1	2.01	0.43
17:b:829:CLA:H61	17:b:829:CLA:H41	1.75	0.43
17:4:307:CLA:CHA	17:4:307:CLA:HBA1	2.48	0.43
17:a:803:CLA:O1A	17:a:803:CLA:H3A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:831:CLA:H93	17:a:842:CLA:HED3	2.01	0.43
17:a:834:CLA:H202	17:a:834:CLA:H162	1.78	0.43
17:b:809:CLA:H143	17:b:809:CLA:H161	1.83	0.43
17:b:838:CLA:H101	17:b:838:CLA:H13	1.78	0.43
6:d:70:LEU:O	6:d:74:LEU:HG	2.19	0.43
7:e:16:TYR:CD2	7:e:44:ASN:HA	2.54	0.43
3:1:128:GLU:HG3	15:1:302:XAT:H372	2.01	0.42
4:a:364:MET:HE1	17:a:830:CLA:CAD	2.49	0.42
4:a:517:MET:HE2	4:a:611:VAL:HA	2.00	0.42
4:a:525:ASP:HA	4:a:528:VAL:HG12	2.01	0.42
5:b:345:LEU:CD1	17:b:827:CLA:HAA1	2.49	0.42
17:b:814:CLA:H161	17:b:814:CLA:H192	1.76	0.42
23:b:850:BCR:H15C	23:b:850:BCR:H351	1.90	0.42
8:f:114:PHE:HB2	23:f:801:BCR:C32	2.49	0.42
4:a:52:PHE:CD2	17:a:806:CLA:HMC2	2.53	0.42
4:a:440:PHE:CE2	17:a:839:CLA:HAB	2.55	0.42
17:a:807:CLA:H92	17:a:807:CLA:H61	1.69	0.42
17:a:826:CLA:H141	17:a:826:CLA:H161	1.81	0.42
5:b:302:ILE:HD13	17:b:823:CLA:HMD2	1.99	0.42
17:b:801:CLA:H12	17:b:801:CLA:H52	1.85	0.42
6:d:88:TYR:HB3	6:d:89:PRO:HD2	2.01	0.42
15:5:301:XAT:H31	15:5:301:XAT:H391	1.88	0.42
17:1:306:CLA:H91	17:1:306:CLA:H112	1.69	0.42
5:b:520:LEU:HD23	5:b:520:LEU:HA	1.88	0.42
23:i:101:BCR:H11C	23:i:101:BCR:H341	1.86	0.42
4:a:555:LEU:HD11	5:b:674:GLN:HB3	2.01	0.42
17:a:834:CLA:H142	23:b:848:BCR:H17C	2.01	0.42
5:b:274:HIS:HB2	17:b:818:CLA:CHB	2.48	0.42
1:5:149:VAL:HG22	15:5:304:XAT:H182	2.02	0.42
2:4:75:GLU:OE1	2:4:148:ARG:NH2	2.47	0.42
4:a:271:PHE:HE2	4:a:495:ALA:HB2	1.84	0.42
4:a:727:LEU:HD22	17:a:842:CLA:HMA3	2.01	0.42
17:a:805:CLA:H52	17:a:805:CLA:H12	1.77	0.42
17:b:839:CLA:H162	17:b:839:CLA:H192	1.73	0.42
6:d:107:VAL:HG21	14:c:38:GLN:HB3	2.01	0.42
1:5:137:ARG:HD2	1:5:144:SER:HA	2.00	0.42
15:5:304:XAT:H35	15:5:304:XAT:H401	1.79	0.42
15:4:306:XAT:H31	15:4:306:XAT:H391	1.62	0.42
3:1:58:ALA:HB1	3:1:66:LEU:HD21	2.00	0.42
23:a:847:BCR:H20C	23:a:847:BCR:H361	1.80	0.42
5:b:647:VAL:HG21	17:b:809:CLA:HAC1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:807:CLA:H102	17:b:807:CLA:H161	2.01	0.42
6:d:32:ILE:HG21	6:d:70:LEU:HD23	2.00	0.42
17:4:308:CLA:HBD	17:4:315:CLA:OBD	2.20	0.42
3:1:54:PRO:HD2	15:1:303:XAT:H242	2.02	0.42
3:1:151:TRP:CH2	11:l:20:PRO:HA	2.54	0.42
4:a:399:ALA:HB1	4:a:543:LEU:HB3	2.02	0.42
17:a:810:CLA:HBB1	23:j:104:BCR:H23C	2.00	0.42
17:a:813:CLA:H62	17:a:813:CLA:H41	1.85	0.42
5:b:500:LEU:HA	5:b:503:ILE:HG22	2.02	0.42
17:b:827:CLA:HED1	23:b:847:BCR:H21C	2.02	0.42
15:5:301:XAT:H15	15:5:301:XAT:H201	1.85	0.42
4:a:692:GLU:CD	5:b:547:LYS:HB2	2.44	0.42
17:a:806:CLA:H72	23:a:848:BCR:C8	2.50	0.42
17:a:820:CLA:H3A	17:a:820:CLA:HBA2	1.48	0.42
17:a:822:CLA:OBD	17:a:824:CLA:HMD3	2.19	0.42
9:i:17:VAL:HG21	17:i:102:CLA:HMC2	2.01	0.42
23:m:102:BCR:H20C	23:m:102:BCR:H361	1.85	0.42
3:1:147:GLY:HA2	3:1:149:TRP:CZ3	2.55	0.42
17:1:306:CLA:H3A	17:1:306:CLA:O2A	2.20	0.42
4:a:684:ARG:NH1	4:a:711:ALA:O	2.52	0.42
17:a:804:CLA:C4D	10:j:12:PRO:HG3	2.50	0.42
5:b:629:ASN:HA	5:b:734:LYS:HE2	2.02	0.42
17:b:801:CLA:H51	17:b:839:CLA:H102	2.01	0.42
17:b:815:CLA:CHA	17:b:815:CLA:HBA1	2.49	0.42
10:j:12:PRO:HB2	15:j:101:XAT:H21	2.01	0.42
11:l:96:LEU:HG	23:l:205:BCR:H24C	2.01	0.42
23:l:201:BCR:H352	17:l:203:CLA:HAB	2.02	0.42
4:a:685:GLY:N	5:b:570:CYS:O	2.48	0.42
23:a:849:BCR:H15C	23:a:849:BCR:H351	1.79	0.42
5:b:193:VAL:O	5:b:198:PRO:HD3	2.20	0.42
5:b:597:HIS:CE1	5:b:727:VAL:HG23	2.54	0.42
17:b:828:CLA:H161	17:b:828:CLA:H143	1.78	0.42
9:i:29:TYR:HE1	12:m:30:ASN:HD21	1.67	0.42
1:5:145:GLU:HB2	1:5:154:GLN:OE1	2.20	0.41
15:4:305:XAT:H30	17:4:314:CLA:H71	2.02	0.41
4:a:427:ARG:NH2	6:d:46:THR:O	2.53	0.41
17:a:823:CLA:CHD	15:a:852:XAT:H183	2.49	0.41
17:a:842:CLA:H12	21:a:843:PQN:H301	2.02	0.41
15:a:852:XAT:H31	15:a:852:XAT:H391	1.82	0.41
5:b:220:LEU:HD21	23:b:843:BCR:H391	2.01	0.41
5:b:381:MET:HE1	23:b:847:BCR:H352	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:585:MET:O	5:b:589:ILE:HG12	2.20	0.41
17:5:307:CLA:HBC1	15:4:301:XAT:H383	2.01	0.41
4:a:201:LEU:HD23	4:a:201:LEU:HA	1.89	0.41
4:a:370:TYR:OH	17:a:830:CLA:OBD	2.27	0.41
4:a:452:ASN:HD22	4:a:634:ILE:HB	1.85	0.41
4:a:570:GLY:O	4:a:576:THR:OG1	2.32	0.41
23:a:850:BCR:H15C	23:a:850:BCR:H351	1.77	0.41
23:a:850:BCR:H20C	23:a:850:BCR:H361	1.80	0.41
5:b:702:LEU:HD22	5:b:706:GLN:NE2	2.35	0.41
17:b:807:CLA:H2	17:b:807:CLA:H62	1.79	0.41
23:b:844:BCR:H11C	23:b:844:BCR:H341	1.76	0.41
3:1:71:GLU:HG2	3:1:142:PRO:O	2.20	0.41
3:1:162:TYR:CE2	17:a:844:CLA:HBD	2.56	0.41
3:1:168:ASN:HA	3:1:171:ARG:HD2	2.01	0.41
18:1:315:SQD:H132	18:1:315:SQD:H161	1.72	0.41
4:a:67:PHE:HE2	4:a:173:HIS:CG	2.38	0.41
4:a:361:ALA:HB2	4:a:387:HIS:HB2	2.01	0.41
17:b:835:CLA:H62	17:b:835:CLA:H41	1.86	0.41
11:l:53:THR:HG22	17:l:202:CLA:C1B	2.49	0.41
23:l:205:BCR:H20C	23:l:205:BCR:H361	1.91	0.41
17:5:309:CLA:H93	17:5:309:CLA:H111	1.84	0.41
4:a:601:PHE:CZ	17:a:801:CLA:HED3	2.55	0.41
23:a:850:BCR:H11C	23:a:850:BCR:H341	1.88	0.41
17:b:809:CLA:C4A	17:b:809:CLA:HBA2	2.51	0.41
17:b:817:CLA:CBB	23:b:850:BCR:H14C	2.50	0.41
23:b:843:BCR:H341	23:b:843:BCR:H11C	1.74	0.41
7:e:51:ASN:ND2	14:c:61:ASP:HB2	2.35	0.41
23:f:804:BCR:H12C	23:f:804:BCR:H15C	1.82	0.41
15:j:101:XAT:H15	15:j:101:XAT:H201	1.82	0.41
14:c:32:ASP:N	14:c:32:ASP:OD1	2.53	0.41
1:5:143:TYR:OH	17:5:310:CLA:OBD	2.23	0.41
15:4:302:XAT:C10	15:4:306:XAT:H363	2.49	0.41
3:1:82:LEU:HD11	17:1:311:CLA:HBC1	2.01	0.41
4:a:356:LEU:HB2	17:a:828:CLA:H41	2.02	0.41
4:a:680:LEU:HB3	5:b:667:ILE:HG12	2.02	0.41
17:a:841:CLA:HED3	17:a:841:CLA:H2A	2.01	0.41
5:b:314:GLY:HA3	5:b:412:ARG:HD2	2.02	0.41
17:b:802:CLA:HMA1	17:b:803:CLA:H161	2.02	0.41
17:1:308:CLA:H121	17:1:308:CLA:H8	1.97	0.41
4:a:406:PHE:HE2	4:a:424:ILE:HD11	1.86	0.41
17:a:841:CLA:HAA2	17:b:832:CLA:HMB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:192:LEU:HD23	5:b:192:LEU:HA	1.84	0.41
17:i:102:CLA:H142	17:i:102:CLA:H111	1.61	0.41
17:5:305:CLA:HAB	2:4:153:PHE:O	2.21	0.41
15:4:305:XAT:H31	15:4:305:XAT:H391	1.92	0.41
4:a:299:ILE:O	4:a:303:HIS:ND1	2.53	0.41
17:a:839:CLA:H161	17:a:839:CLA:H141	1.68	0.41
5:b:350:MET:HE2	5:b:350:MET:HB3	1.89	0.41
5:b:668:SER:OG	5:b:673:TRP:NE1	2.52	0.41
1:5:83:LEU:HD23	1:5:83:LEU:HA	1.93	0.41
4:a:499:VAL:HG12	17:a:819:CLA:H11	2.03	0.41
4:a:632:SER:O	4:a:638:GLY:HA3	2.21	0.41
17:a:816:CLA:C4B	15:a:852:XAT:H242	2.50	0.41
17:a:828:CLA:H61	17:a:828:CLA:H2	1.78	0.41
17:b:834:CLA:H161	17:b:834:CLA:H141	1.85	0.41
17:b:840:CLA:H92	17:b:840:CLA:H61	1.73	0.41
23:j:104:BCR:H351	23:j:104:BCR:H15C	1.78	0.41
23:l:201:BCR:H351	23:l:201:BCR:H15C	1.82	0.41
17:5:308:CLA:CBB	17:5:315:CLA:HAB	2.51	0.41
15:4:304:XAT:H383	17:4:311:CLA:C2B	2.51	0.41
15:4:305:XAT:H35	15:4:305:XAT:H401	1.80	0.41
17:4:310:CLA:HBA1	17:4:310:CLA:H3A	1.77	0.41
3:1:87:TRP:CG	3:1:180:LEU:HD13	2.56	0.41
4:a:194:HIS:ND1	17:a:826:CLA:OBD	2.48	0.41
17:a:818:CLA:OBD	17:a:837:CLA:HED2	2.21	0.41
17:a:828:CLA:H152	17:a:840:CLA:H191	2.03	0.41
5:b:173:LEU:HD23	5:b:173:LEU:HA	1.89	0.41
5:b:342:ALA:HB2	17:b:825:CLA:H43	2.02	0.41
5:b:433:PHE:CZ	23:f:801:BCR:H372	2.56	0.41
17:b:810:CLA:H142	17:b:810:CLA:H111	1.83	0.41
17:b:822:CLA:H12	17:b:823:CLA:H52	2.03	0.41
17:b:834:CLA:HBA2	17:b:834:CLA:H3A	1.52	0.41
23:b:846:BCR:H15C	23:b:846:BCR:H351	1.83	0.41
23:b:847:BCR:H24C	23:b:847:BCR:H371	1.83	0.41
23:j:104:BCR:H341	23:j:104:BCR:H11C	1.72	0.41
3:1:134:ILE:HD11	11:l:26:PHE:HA	2.03	0.41
4:a:342:TRP:HB3	17:a:806:CLA:HAC1	2.02	0.41
17:a:805:CLA:H41	17:a:805:CLA:H61	1.91	0.41
17:a:805:CLA:HBA1	17:a:805:CLA:H3A	1.89	0.41
5:b:197:ILE:HB	5:b:198:PRO:HD3	2.02	0.41
17:b:805:CLA:HHC	17:b:807:CLA:OBD	2.21	0.41
17:b:827:CLA:HMB2	17:b:834:CLA:HBA1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:828:CLA:H13	17:b:830:CLA:H141	2.02	0.41
17:b:829:CLA:H3A	17:b:829:CLA:HBA2	1.76	0.41
17:b:836:CLA:HMB1	17:b:836:CLA:HBB1	2.02	0.41
15:5:304:XAT:H15	15:5:304:XAT:H201	1.76	0.40
15:4:304:XAT:H163	17:4:309:CLA:H2	2.02	0.40
4:a:293:ALA:HB1	17:a:818:CLA:HBC2	2.03	0.40
4:a:357:SER:HB2	17:a:830:CLA:HMC2	2.01	0.40
4:a:586:PHE:CE1	4:a:722:VAL:HB	2.57	0.40
4:a:701:LEU:HD23	4:a:701:LEU:HA	1.94	0.40
17:a:806:CLA:H52	23:a:848:BCR:HC8	2.03	0.40
5:b:56:ILE:HD11	23:m:102:BCR:HC7	2.02	0.40
17:b:841:CLA:H91	17:b:841:CLA:H112	1.87	0.40
17:l:311:CLA:H72	11:l:21:ILE:HG12	2.02	0.40
4:a:290:HIS:O	4:a:294:ILE:HG12	2.20	0.40
4:a:675:PHE:HZ	17:a:842:CLA:HBC2	1.86	0.40
17:a:834:CLA:H143	17:a:834:CLA:H161	1.94	0.40
5:b:86:PRO:HB3	5:b:119:TYR:CD2	2.56	0.40
5:b:614:SER:O	5:b:620:GLY:HA3	2.21	0.40
17:b:840:CLA:H141	17:b:840:CLA:H161	1.91	0.40
8:f:114:PHE:HB2	23:f:801:BCR:H321	2.02	0.40
23:m:102:BCR:H15C	23:m:102:BCR:H351	1.98	0.40
14:c:64:SER:HB2	24:c:102:SF4:S3	2.62	0.40
4:a:165:LEU:HD23	4:a:165:LEU:HA	1.90	0.40
4:a:586:PHE:CE1	4:a:590:PHE:HE2	2.39	0.40
17:a:827:CLA:HBA2	17:a:827:CLA:H3A	1.79	0.40
17:a:829:CLA:O1D	17:a:830:CLA:HMA1	2.21	0.40
17:a:835:CLA:H141	17:a:835:CLA:H161	1.84	0.40
17:a:842:CLA:H101	17:a:842:CLA:H62	1.90	0.40
5:b:182:GLY:HA3	5:b:283:ILE:HG13	2.03	0.40
17:b:807:CLA:H201	17:b:828:CLA:H143	2.03	0.40
17:i:102:CLA:H41	17:i:102:CLA:H62	1.88	0.40
23:l:201:BCR:H20C	23:l:201:BCR:H361	1.96	0.40
15:4:304:XAT:H162	17:4:309:CLA:H2	2.04	0.40
4:a:272:LYS:HG2	4:a:496:LEU:HD12	2.02	0.40
4:a:529:HIS:CG	17:a:839:CLA:HED2	2.56	0.40
17:a:839:CLA:H203	17:a:839:CLA:H162	1.80	0.40
15:a:852:XAT:H35	15:a:852:XAT:H401	1.85	0.40
5:b:431:LEU:HD11	17:b:837:CLA:HMB1	2.03	0.40
5:b:547:LYS:HE2	8:f:180:ILE:HD11	2.03	0.40
5:b:709:LEU:CD1	19:b:851:DGD:HB41	2.51	0.40
8:f:147:VAL:HG22	10:j:14:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:f:801:BCR:H20C	23:f:801:BCR:H361	1.86	0.40
1:5:221:ARG:HA	1:5:224:MET:HE3	2.04	0.40
15:5:302:XAT:H3	15:5:302:XAT:H173	1.86	0.40
17:4:309:CLA:H192	17:4:309:CLA:H161	1.77	0.40
17:4:311:CLA:H142	17:4:311:CLA:H112	1.78	0.40
3:1:43:ILE:HG21	3:1:163:GLN:HB2	2.04	0.40
3:1:113:PRO:C	3:1:115:ILE:H	2.30	0.40
4:a:209:HIS:HB2	17:a:815:CLA:C1C	2.52	0.40
4:a:452:ASN:HB3	4:a:635:THR:HG22	2.04	0.40
5:b:181:PHE:CE2	17:b:820:CLA:HAB	2.56	0.40
5:b:523:HIS:CE1	23:b:852:BCR:H322	2.56	0.40
5:b:550:PRO:HD2	14:c:62:PHE:CE1	2.57	0.40
23:b:847:BCR:H15C	23:b:847:BCR:H351	1.85	0.40
11:l:56:TYR:CD2	11:l:161:ALA:HB2	2.56	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	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
4	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	75
5	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
6	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
7	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
8	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
9	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	j	39/41 (95%)	39 (100%)	0	0	100	100
11	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	10	32
12	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	2654/2893 (92%)	2513 (95%)	137 (5%)	4 (0%)	44	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	l	120	VAL
4	a	580	SER
11	l	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	1	128/165 (78%)	128 (100%)	0	100	100
4	a	607/613 (99%)	603 (99%)	4 (1%)	76	80
5	b	599/602 (100%)	599 (100%)	0	100	100
6	d	107/113 (95%)	107 (100%)	0	100	100
7	e	56/62 (90%)	56 (100%)	0	100	100
8	f	138/162 (85%)	138 (100%)	0	100	100
9	i	32/43 (74%)	32 (100%)	0	100	100
10	j	36/36 (100%)	36 (100%)	0	100	100
11	l	130/141 (92%)	130 (100%)	0	100	100
12	m	21/24 (88%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2187/2370 (92%)	2183 (100%)	4 (0%)	85	87

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	133	GLN
3	1	63	GLN
3	1	119	GLN
3	1	132	ASN
3	1	194	GLN
4	a	127	ASN
4	a	186	ASN
4	a	435	ASN
5	b	80	ASN
5	b	112	ASN
5	b	169	ASN
5	b	326	ASN
5	b	373	HIS
5	b	605	GLN
5	b	629	ASN
6	d	7	GLN
8	f	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

176 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$
15	XAT	4	304	-	41,47,47	0.90	2 (4%)	54,74,74	2.59	17 (31%)
17	CLA	b	830	-	69,73,73	1.20	8 (11%)	82,113,113	1.30	9 (10%)
17	CLA	a	804	-	59,63,73	1.27	8 (13%)	70,101,113	1.41	8 (11%)
17	CLA	4	307	2	49,53,73	1.38	5 (10%)	58,89,113	1.41	4 (6%)
17	CLA	1	312	3	56,60,73	1.32	7 (12%)	65,97,113	1.35	5 (7%)
17	CLA	a	824	-	50,54,73	1.36	8 (16%)	59,90,113	1.36	4 (6%)
17	CLA	4	312	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	5 (8%)
17	CLA	a	841	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	6 (7%)
17	CLA	a	811	-	60,64,73	1.26	7 (11%)	71,102,113	1.34	6 (8%)
17	CLA	1	311	-	57,61,73	1.29	7 (12%)	67,98,113	1.36	7 (10%)
17	CLA	b	834	-	69,73,73	1.18	6 (8%)	82,113,113	1.23	4 (4%)
17	CLA	a	803	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	6 (7%)
17	CLA	4	311	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	5 (6%)
17	CLA	a	830	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
15	XAT	5	302	-	41,47,47	0.96	2 (4%)	54,74,74	2.59	19 (35%)
17	CLA	b	813	-	57,61,73	1.30	9 (15%)	67,98,113	1.35	5 (7%)
17	CLA	b	829	-	69,73,73	1.18	8 (11%)	82,113,113	1.20	5 (6%)
17	CLA	a	810	4	69,73,73	1.18	8 (11%)	82,113,113	1.32	6 (7%)
17	CLA	a	813	-	58,62,73	1.28	7 (12%)	68,99,113	1.31	5 (7%)
17	CLA	a	835	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)
16	A1L1G	1	301	-	40,47,47	1.15	5 (12%)	49,71,71	1.46	10 (20%)
17	CLA	4	314	-	57,61,73	1.29	8 (14%)	67,98,113	1.32	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	l	205	-	41,41,41	0.65	0	56,56,56	2.04	14 (25%)
17	CLA	5	315	-	50,54,73	1.36	6 (12%)	59,90,113	1.39	4 (6%)
17	CLA	a	818	-	60,64,73	1.27	8 (13%)	71,102,113	1.32	7 (9%)
17	CLA	a	825	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	5 (7%)
24	SF4	c	101	-	0,12,12	-	-	-		
17	CLA	a	838	-	55,59,73	1.30	7 (12%)	64,96,113	1.41	6 (9%)
17	CLA	b	801	-	69,73,73	1.19	8 (11%)	82,113,113	1.26	5 (6%)
25	LMG	j	105	-	32,32,55	1.13	2 (6%)	40,40,63	1.15	4 (10%)
17	CLA	b	802	-	69,73,73	1.16	6 (8%)	82,113,113	1.18	5 (6%)
17	CLA	b	818	-	63,67,73	1.23	8 (12%)	74,105,113	1.36	9 (12%)
17	CLA	b	812	-	58,62,73	1.36	9 (15%)	71,100,113	1.34	7 (9%)
17	CLA	a	806	-	69,73,73	1.21	10 (14%)	82,113,113	1.57	12 (14%)
17	CLA	b	827	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
17	CLA	4	315	2	49,53,73	1.40	9 (18%)	58,89,113	1.41	4 (6%)
15	XAT	a	852	-	41,47,47	0.92	2 (4%)	54,74,74	2.70	19 (35%)
17	CLA	5	307	1	64,68,73	1.21	7 (10%)	76,107,113	1.27	6 (7%)
17	CLA	a	854	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
17	CLA	1	313	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	5 (9%)
17	CLA	a	844	22	69,73,73	1.17	7 (10%)	82,113,113	1.26	8 (9%)
17	CLA	b	831	-	45,49,73	1.40	8 (17%)	54,84,113	1.47	6 (11%)
23	BCR	i	101	-	41,41,41	0.73	0	56,56,56	2.14	13 (23%)
19	DGD	4	319	-	41,41,67	1.08	2 (4%)	55,55,81	1.79	6 (10%)
17	CLA	a	833	-	59,63,73	1.25	6 (10%)	70,101,113	1.39	8 (11%)
17	CLA	b	817	-	59,63,73	1.26	7 (11%)	70,101,113	1.32	6 (8%)
17	CLA	b	823	-	64,68,73	1.21	7 (10%)	76,107,113	1.26	5 (6%)
17	CLA	1	305	-	65,69,73	1.21	7 (10%)	77,108,113	1.27	5 (6%)
17	CLA	1	310	3	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
17	CLA	a	821	-	49,53,73	1.39	9 (18%)	58,89,113	1.47	4 (6%)
17	CLA	j	102	-	62,66,73	1.24	7 (11%)	73,104,113	1.30	5 (6%)
21	PQN	b	842	-	34,34,34	1.59	2 (5%)	43,45,45	1.24	5 (11%)
24	SF4	a	851	-	0,12,12	-	-	-		
17	CLA	b	804	-	69,73,73	1.14	7 (10%)	82,113,113	1.44	8 (9%)
15	XAT	5	304	-	41,47,47	0.87	2 (4%)	54,74,74	2.85	20 (37%)
17	CLA	b	816	-	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
15	XAT	1	303	-	41,47,47	0.90	2 (4%)	54,74,74	2.54	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	1	307	-	58,62,73	1.28	8 (13%)	68,99,113	1.36	6 (8%)
17	CLA	a	802	-	62,66,73	1.22	9 (14%)	73,104,113	1.34	7 (9%)
17	CLA	b	839	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
17	CLA	a	817	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
17	CLA	a	823	-	53,57,73	1.32	7 (13%)	61,93,113	1.42	6 (9%)
17	CLA	b	811	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	7 (8%)
17	CLA	a	837	4	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
17	CLA	a	819	-	58,62,73	1.27	9 (15%)	68,99,113	1.33	5 (7%)
17	CLA	a	842	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
15	XAT	4	301	-	41,47,47	0.95	2 (4%)	54,74,74	2.63	19 (35%)
17	CLA	1	308	3	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
15	XAT	5	301	-	41,47,47	0.93	2 (4%)	54,74,74	2.59	19 (35%)
17	CLA	b	815	-	59,63,73	1.27	6 (10%)	70,101,113	1.40	7 (10%)
17	CLA	l	202	-	46,50,73	1.41	8 (17%)	53,85,113	1.44	4 (7%)
17	CLA	a	839	-	69,73,73	1.16	6 (8%)	82,113,113	1.29	6 (7%)
17	CLA	b	822	-	55,59,73	1.30	7 (12%)	64,96,113	1.41	7 (10%)
17	CLA	b	841	22	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
17	CLA	4	310	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	5 (7%)
25	LMG	a	853	-	34,34,55	1.14	2 (5%)	42,42,63	1.17	3 (7%)
17	CLA	b	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
17	CLA	4	317	-	50,54,73	1.36	5 (10%)	59,90,113	1.43	4 (6%)
19	DGD	b	851	-	58,58,67	1.13	5 (8%)	72,72,81	1.50	10 (13%)
23	BCR	b	845	-	41,41,41	0.66	0	56,56,56	2.09	15 (26%)
17	CLA	1	306	-	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
23	BCR	b	848	-	41,41,41	0.69	0	56,56,56	1.80	14 (25%)
17	CLA	a	815	-	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
23	BCR	j	104	-	41,41,41	0.68	0	56,56,56	2.09	17 (30%)
23	BCR	f	801	-	41,41,41	0.66	0	56,56,56	2.16	15 (26%)
17	CLA	a	834	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
17	CLA	a	816	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	7 (10%)
15	XAT	4	302	-	41,47,47	0.91	2 (4%)	54,74,74	2.56	19 (35%)
17	CLA	a	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
17	CLA	b	806	-	69,73,73	1.16	6 (8%)	82,113,113	1.30	5 (6%)
23	BCR	f	804	-	41,41,41	0.69	0	56,56,56	2.05	14 (25%)
17	CLA	4	313	-	50,54,73	1.37	7 (14%)	59,90,113	1.38	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	a	846	17	26,26,48	1.30	5 (19%)	29,32,54	1.18	2 (6%)
17	CLA	b	805	-	69,73,73	1.17	5 (7%)	82,113,113	1.28	6 (7%)
17	CLA	j	103	10	46,50,73	1.41	6 (13%)	53,85,113	1.48	4 (7%)
17	CLA	a	812	17	66,70,73	1.19	7 (10%)	78,109,113	1.30	5 (6%)
17	CLA	b	835	-	57,61,73	1.31	8 (14%)	67,98,113	1.37	6 (8%)
15	XAT	4	303	-	41,47,47	0.90	2 (4%)	54,74,74	2.59	19 (35%)
17	CLA	b	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.28	7 (8%)
23	BCR	b	844	-	41,41,41	0.68	0	56,56,56	1.93	16 (28%)
17	CLA	5	309	1	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
17	CLA	5	313	1	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
17	CLA	b	814	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
17	CLA	b	825	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
17	CLA	5	311	-	55,59,73	1.30	6 (10%)	64,96,113	1.37	7 (10%)
17	CLA	l	204	-	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
23	BCR	b	843	-	41,41,41	0.64	0	56,56,56	2.30	21 (37%)
23	BCR	b	847	-	41,41,41	0.66	0	56,56,56	2.22	22 (39%)
17	CLA	4	309	-	69,73,73	1.16	7 (10%)	82,113,113	1.22	6 (7%)
17	CLA	f	802	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
17	CLA	a	826	-	69,73,73	1.18	7 (10%)	82,113,113	1.31	7 (8%)
17	CLA	4	308	-	60,64,73	1.26	6 (10%)	71,102,113	1.32	6 (8%)
17	CLA	b	809	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
17	CLA	b	824	-	57,61,73	1.29	8 (14%)	67,98,113	1.35	6 (8%)
17	CLA	1	314	-	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)
17	CLA	a	809	4	69,73,73	1.15	7 (10%)	82,113,113	1.29	9 (10%)
17	CLA	a	807	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	5 (6%)
17	CLA	5	310	-	50,54,73	1.37	8 (16%)	59,90,113	1.39	4 (6%)
17	CLA	b	808	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
17	CLA	a	814	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
23	BCR	a	848	-	41,41,41	0.68	0	56,56,56	1.96	18 (32%)
23	BCR	b	846	-	41,41,41	0.66	0	56,56,56	1.99	21 (37%)
17	CLA	1	309	3	50,54,73	1.37	8 (16%)	59,90,113	1.34	4 (6%)
17	CLA	5	312	-	56,60,73	1.30	8 (14%)	65,97,113	1.40	6 (9%)
23	BCR	a	847	-	41,41,41	0.67	0	56,56,56	1.95	16 (28%)
17	CLA	b	803	-	69,73,73	1.16	7 (10%)	82,113,113	1.25	5 (6%)
15	XAT	4	306	-	41,47,47	0.91	2 (4%)	54,74,74	2.75	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	XAT	j	101	-	41,47,47	0.87	2 (4%)	54,74,74	2.73	18 (33%)
22	LHG	m	101	-	45,45,48	1.19	6 (13%)	48,51,54	0.96	2 (4%)
17	CLA	b	837	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
17	CLA	a	831	-	69,73,73	1.18	9 (13%)	82,113,113	1.34	8 (9%)
17	CLA	f	803	8	56,60,73	1.30	7 (12%)	65,97,113	1.38	5 (7%)
23	BCR	l	201	-	41,41,41	0.67	0	56,56,56	1.97	17 (30%)
17	CLA	b	821	-	54,58,73	1.32	7 (12%)	64,95,113	1.44	7 (10%)
23	BCR	b	852	-	41,41,41	0.71	0	56,56,56	2.06	13 (23%)
17	CLA	b	836	-	62,66,73	1.24	6 (9%)	73,104,113	1.37	8 (10%)
17	CLA	a	828	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	5 (6%)
17	CLA	b	810	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
18	SQD	1	315	-	43,45,54	1.22	3 (6%)	53,56,65	1.12	2 (3%)
22	LHG	b	849	17	30,30,48	1.38	6 (20%)	33,36,54	1.17	2 (6%)
17	CLA	a	829	-	66,70,73	1.20	6 (9%)	78,109,113	1.25	7 (8%)
15	XAT	1	302	-	41,47,47	0.91	2 (4%)	54,74,74	2.60	18 (33%)
17	CLA	a	836	-	54,58,73	1.31	6 (11%)	64,95,113	1.38	6 (9%)
18	SQD	5	316	17	33,35,54	1.39	3 (9%)	43,46,65	1.31	5 (11%)
20	A1L1F	1	304	-	52,59,59	1.41	6 (11%)	63,85,85	2.27	17 (26%)
23	BCR	m	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	6 (10%)
17	CLA	b	833	-	69,73,73	1.16	7 (10%)	82,113,113	1.27	6 (7%)
22	LHG	a	845	-	47,47,48	1.16	6 (12%)	50,53,54	0.98	2 (4%)
23	BCR	b	850	-	41,41,41	0.67	0	56,56,56	1.90	17 (30%)
17	CLA	b	832	-	53,57,73	1.33	6 (11%)	61,93,113	1.38	5 (8%)
17	CLA	b	838	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	6 (7%)
17	CLA	b	820	-	59,63,73	1.26	8 (13%)	70,101,113	1.31	6 (8%)
17	CLA	b	840	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
17	CLA	5	306	18	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
17	CLA	a	808	-	55,59,73	1.33	8 (14%)	64,96,113	1.38	5 (7%)
23	BCR	a	850	-	41,41,41	0.69	0	56,56,56	2.18	15 (26%)
17	CLA	a	832	-	54,58,73	1.33	8 (14%)	64,95,113	1.40	6 (9%)
17	CLA	a	820	-	69,73,73	1.18	7 (10%)	82,113,113	1.31	7 (8%)
17	CLA	l	203	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	5 (6%)
17	CLA	a	840	-	69,73,73	1.19	8 (11%)	82,113,113	1.26	5 (6%)
17	CLA	a	827	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
17	CLA	5	305	1	50,54,73	1.38	7 (14%)	59,90,113	1.38	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	a	805	17	59,63,73	1.26	6 (10%)	70,101,113	1.36	6 (8%)
17	CLA	5	314	-	56,60,73	1.30	7 (12%)	65,97,113	1.40	5 (7%)
17	CLA	4	318	-	59,63,73	1.28	8 (13%)	70,101,113	1.34	5 (7%)
17	CLA	5	308	-	59,63,73	1.28	7 (11%)	70,101,113	1.35	6 (8%)
16	A1L1G	5	303	-	40,47,47	1.15	4 (10%)	49,71,71	1.38	7 (14%)
17	CLA	b	826	-	68,72,73	1.17	8 (11%)	80,111,113	1.30	7 (8%)
17	CLA	b	819	-	64,68,73	1.22	8 (12%)	76,107,113	1.28	5 (6%)
17	CLA	4	316	2	45,49,73	1.42	6 (13%)	54,84,113	1.47	5 (9%)
17	CLA	i	102	-	66,70,73	1.20	7 (10%)	78,109,113	1.27	6 (7%)
17	CLA	a	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.28	5 (6%)
24	SF4	c	102	-	0,12,12	-	-	-	-	-
15	XAT	4	305	-	41,47,47	0.90	2 (4%)	54,74,74	2.57	19 (35%)
21	PQN	a	843	-	34,34,34	1.61	2 (5%)	43,45,45	1.15	4 (9%)
23	BCR	a	849	-	41,41,41	0.67	0	56,56,56	2.19	22 (39%)

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
15	XAT	4	304	-	-	3/31/93/93	0/4/4/4
17	CLA	b	830	-	1/1/15/20	11/39/115/115	-
17	CLA	a	804	-	1/1/13/20	9/27/103/115	-
17	CLA	4	307	2	1/1/11/20	9/15/91/115	-
17	CLA	1	312	3	1/1/12/20	3/24/100/115	-
17	CLA	a	824	-	1/1/11/20	5/17/93/115	-
17	CLA	4	312	-	1/1/11/20	9/17/93/115	-
17	CLA	a	841	-	1/1/15/20	15/39/115/115	-
17	CLA	a	811	-	1/1/13/20	6/29/105/115	-
17	CLA	1	311	-	1/1/12/20	4/25/101/115	-
17	CLA	b	834	-	1/1/15/20	13/39/115/115	-
17	CLA	a	803	-	1/1/15/20	3/39/115/115	-
17	CLA	4	311	-	1/1/15/20	14/39/115/115	-
17	CLA	a	830	-	1/1/15/20	13/39/115/115	-
15	XAT	5	302	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	813	-	1/1/12/20	5/25/101/115	-
17	CLA	b	829	-	1/1/15/20	13/39/115/115	-
17	CLA	a	810	4	1/1/15/20	15/39/115/115	-
17	CLA	a	813	-	1/1/12/20	10/26/102/115	-
17	CLA	a	835	-	1/1/15/20	11/39/115/115	-
16	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
17	CLA	4	314	-	1/1/12/20	4/25/101/115	-
23	BCR	l	205	-	-	8/29/63/63	0/2/2/2
17	CLA	5	315	-	1/1/11/20	5/17/93/115	-
17	CLA	a	818	-	1/1/13/20	11/29/105/115	-
17	CLA	a	825	-	1/1/13/20	8/27/103/115	-
24	SF4	c	101	-	-	-	0/6/5/5
17	CLA	a	838	-	1/1/12/20	6/23/99/115	-
17	CLA	b	801	-	1/1/15/20	20/39/115/115	-
25	LMG	j	105	-	-	11/27/47/70	0/1/1/1
17	CLA	b	802	-	1/1/15/20	15/39/115/115	-
17	CLA	b	818	-	1/1/13/20	11/32/108/115	-
17	CLA	b	812	-	1/1/13/20	4/25/101/115	-
17	CLA	a	806	-	1/1/15/20	11/39/115/115	-
17	CLA	b	827	-	1/1/15/20	3/39/115/115	-
17	CLA	4	315	2	1/1/11/20	6/15/91/115	-
15	XAT	a	852	-	-	7/31/93/93	0/4/4/4
17	CLA	5	307	1	1/1/14/20	5/33/109/115	-
17	CLA	a	854	-	1/1/15/20	14/39/115/115	-
17	CLA	1	313	-	1/1/10/20	6/10/86/115	-
17	CLA	a	844	22	1/1/15/20	15/39/115/115	-
17	CLA	b	831	-	1/1/10/20	2/10/86/115	-
23	BCR	i	101	-	-	3/29/63/63	0/2/2/2
19	DGD	4	319	-	-	10/29/69/95	0/2/2/2
17	CLA	a	833	-	1/1/13/20	2/27/103/115	-
17	CLA	b	817	-	1/1/13/20	3/27/103/115	-
17	CLA	b	823	-	1/1/14/20	7/33/109/115	-
17	CLA	1	305	-	1/1/14/20	9/35/111/115	-
17	CLA	1	310	3	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	821	-	1/1/11/20	1/15/91/115	-
17	CLA	j	102	-	1/1/13/20	18/31/107/115	-
21	PQN	b	842	-	-	1/23/43/43	0/2/2/2
24	SF4	a	851	-	-	-	0/6/5/5
17	CLA	b	804	-	1/1/15/20	7/39/115/115	-
17	CLA	b	816	-	1/1/11/20	3/15/91/115	-
15	XAT	5	304	-	-	1/31/93/93	0/4/4/4
15	XAT	1	303	-	-	0/31/93/93	0/4/4/4
17	CLA	1	307	-	1/1/12/20	5/26/102/115	-
17	CLA	a	802	-	1/1/13/20	5/31/107/115	-
17	CLA	b	839	-	1/1/15/20	15/39/115/115	-
17	CLA	a	817	-	1/1/11/20	8/15/91/115	-
17	CLA	a	823	-	1/1/11/20	7/20/96/115	-
17	CLA	b	811	-	1/1/15/20	16/39/115/115	-
17	CLA	a	837	4	1/1/11/20	4/15/91/115	-
17	CLA	a	819	-	1/1/12/20	6/26/102/115	-
17	CLA	a	842	-	1/1/15/20	8/39/115/115	-
15	XAT	4	301	-	-	4/31/93/93	0/4/4/4
17	CLA	1	308	3	1/1/15/20	13/39/115/115	-
15	XAT	5	301	-	-	3/31/93/93	0/4/4/4
17	CLA	b	815	-	1/1/13/20	10/27/103/115	-
17	CLA	l	202	-	1/1/10/20	0/12/88/115	-
17	CLA	a	839	-	1/1/15/20	14/39/115/115	-
17	CLA	b	822	-	1/1/12/20	4/23/99/115	-
17	CLA	b	841	22	1/1/15/20	11/39/115/115	-
17	CLA	4	310	-	1/1/12/20	4/21/97/115	-
25	LMG	a	853	-	-	13/29/49/70	0/1/1/1
17	CLA	b	828	-	1/1/15/20	14/39/115/115	-
17	CLA	4	317	-	1/1/11/20	7/17/93/115	-
19	DGD	b	851	-	-	20/46/86/95	0/2/2/2
23	BCR	b	845	-	-	6/29/63/63	0/2/2/2
17	CLA	1	306	-	1/1/15/20	15/39/115/115	-
23	BCR	b	848	-	-	2/29/63/63	0/2/2/2
17	CLA	a	815	-	1/1/11/20	0/15/91/115	-
23	BCR	j	104	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	f	801	-	-	3/29/63/63	0/2/2/2
17	CLA	a	834	-	1/1/15/20	9/39/115/115	-
17	CLA	a	816	-	1/1/12/20	4/21/97/115	-
15	XAT	4	302	-	-	3/31/93/93	0/4/4/4
17	CLA	a	822	-	1/1/15/20	5/39/115/115	-
17	CLA	b	806	-	1/1/15/20	13/39/115/115	-
23	BCR	f	804	-	-	4/29/63/63	0/2/2/2
17	CLA	4	313	-	1/1/11/20	6/17/93/115	-
22	LHG	a	846	17	-	15/31/31/53	-
17	CLA	b	805	-	1/1/15/20	11/39/115/115	-
17	CLA	j	103	10	1/1/10/20	7/12/88/115	-
17	CLA	a	812	17	1/1/14/20	9/36/112/115	-
17	CLA	b	835	-	1/1/12/20	9/25/101/115	-
17	CLA	b	807	-	1/1/15/20	18/39/115/115	-
15	XAT	4	303	-	-	0/31/93/93	0/4/4/4
23	BCR	b	844	-	-	2/29/63/63	0/2/2/2
17	CLA	5	309	1	1/1/15/20	10/39/115/115	-
17	CLA	5	313	1	1/1/11/20	6/15/91/115	-
17	CLA	b	814	-	1/1/15/20	13/39/115/115	-
17	CLA	b	825	-	1/1/15/20	14/39/115/115	-
17	CLA	5	311	-	1/1/12/20	7/23/99/115	-
17	CLA	l	204	-	1/1/11/20	3/17/93/115	-
23	BCR	b	843	-	-	2/29/63/63	0/2/2/2
23	BCR	b	847	-	-	0/29/63/63	0/2/2/2
17	CLA	4	309	-	1/1/15/20	13/39/115/115	-
17	CLA	f	802	-	1/1/15/20	13/39/115/115	-
17	CLA	a	826	-	1/1/15/20	8/39/115/115	-
17	CLA	4	308	-	1/1/13/20	9/29/105/115	-
17	CLA	b	809	-	1/1/15/20	13/39/115/115	-
17	CLA	b	824	-	1/1/12/20	6/25/101/115	-
17	CLA	1	314	-	1/1/11/20	7/15/91/115	-
17	CLA	a	809	4	1/1/15/20	15/39/115/115	-
17	CLA	a	807	-	1/1/15/20	18/39/115/115	-
17	CLA	5	310	-	1/1/11/20	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	808	-	1/1/15/20	11/39/115/115	-
17	CLA	a	814	-	1/1/15/20	19/39/115/115	-
23	BCR	a	848	-	-	0/29/63/63	0/2/2/2
23	BCR	b	846	-	-	0/29/63/63	0/2/2/2
17	CLA	1	309	3	1/1/11/20	7/17/93/115	-
17	CLA	5	312	-	1/1/12/20	0/24/100/115	-
23	BCR	a	847	-	-	0/29/63/63	0/2/2/2
17	CLA	b	803	-	1/1/15/20	17/39/115/115	-
15	XAT	4	306	-	-	4/31/93/93	0/4/4/4
15	XAT	j	101	-	-	5/31/93/93	0/4/4/4
22	LHG	m	101	-	-	28/50/50/53	-
17	CLA	b	837	-	1/1/15/20	7/39/115/115	-
17	CLA	a	831	-	1/1/15/20	11/39/115/115	-
17	CLA	f	803	8	1/1/12/20	5/24/100/115	-
23	BCR	l	201	-	-	4/29/63/63	0/2/2/2
17	CLA	b	821	-	1/1/12/20	5/21/97/115	-
23	BCR	b	852	-	-	4/29/63/63	0/2/2/2
17	CLA	b	836	-	1/1/13/20	10/31/107/115	-
17	CLA	a	828	-	1/1/15/20	8/39/115/115	-
17	CLA	b	810	-	1/1/15/20	14/39/115/115	-
18	SQD	1	315	-	-	19/40/60/69	0/1/1/1
22	LHG	b	849	17	-	20/35/35/53	-
17	CLA	a	829	-	1/1/14/20	13/36/112/115	-
17	CLA	a	836	-	1/1/12/20	8/21/97/115	-
15	XAT	1	302	-	-	0/31/93/93	0/4/4/4
18	SQD	5	316	17	-	11/30/50/69	0/1/1/1
20	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
23	BCR	m	102	-	-	8/29/63/63	0/2/2/2
17	CLA	b	833	-	1/1/15/20	13/39/115/115	-
22	LHG	a	845	-	-	26/52/52/53	-
23	BCR	b	850	-	-	0/29/63/63	0/2/2/2
17	CLA	b	832	-	1/1/11/20	5/20/96/115	-
17	CLA	b	838	-	1/1/15/20	9/39/115/115	-
17	CLA	b	820	-	1/1/13/20	5/27/103/115	-
17	CLA	b	840	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	5	306	18	1/1/11/20	8/15/91/115	-
17	CLA	a	808	-	1/1/12/20	4/23/99/115	-
23	BCR	a	850	-	-	4/29/63/63	0/2/2/2
17	CLA	a	832	-	1/1/12/20	7/21/97/115	-
17	CLA	a	820	-	1/1/15/20	13/39/115/115	-
17	CLA	l	203	-	1/1/14/20	4/33/109/115	-
17	CLA	a	840	-	1/1/15/20	8/39/115/115	-
17	CLA	a	827	-	1/1/15/20	6/39/115/115	-
17	CLA	5	305	1	1/1/11/20	6/17/93/115	-
17	CLA	a	805	17	1/1/13/20	6/27/103/115	-
17	CLA	5	314	-	1/1/12/20	4/24/100/115	-
17	CLA	4	318	-	1/1/13/20	9/27/103/115	-
17	CLA	5	308	-	1/1/13/20	6/27/103/115	-
17	CLA	b	826	-	1/1/14/20	4/38/114/115	-
16	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
17	CLA	b	819	-	1/1/14/20	15/33/109/115	-
17	CLA	4	316	2	1/1/10/20	6/10/86/115	-
17	CLA	i	102	-	1/1/14/20	11/36/112/115	-
17	CLA	a	801	-	1/1/15/20	22/39/115/115	-
24	SF4	c	102	-	-	-	0/6/5/5
15	XAT	4	305	-	-	0/31/93/93	0/4/4/4
21	PQN	a	843	-	-	5/23/43/43	0/2/2/2
23	BCR	a	849	-	-	0/29/63/63	0/2/2/2

All (1017) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	843	PQN	C3-C2	7.71	1.49	1.35
21	b	842	PQN	C3-C2	7.52	1.48	1.35
21	a	843	PQN	C10-C5	4.93	1.48	1.40
21	b	842	PQN	C10-C5	4.92	1.48	1.40
20	1	304	A1L1F	O7-C54	4.60	1.45	1.35
18	5	316	SQD	O8-S	4.45	1.63	1.47
18	1	315	SQD	O8-S	4.40	1.63	1.47
18	1	315	SQD	O48-C23	4.30	1.45	1.33
18	5	316	SQD	O48-C23	4.23	1.45	1.33
25	a	853	LMG	O8-C28	4.22	1.45	1.33
20	1	304	A1L1F	O13-C45	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	315	SQD	O47-C7	4.22	1.46	1.34
20	1	304	A1L1F	C57-C1	-4.22	1.25	1.30
25	a	853	LMG	O7-C10	4.14	1.46	1.34
18	5	316	SQD	O47-C7	4.09	1.45	1.34
19	4	319	DGD	O1G-C1A	4.08	1.45	1.33
25	j	105	LMG	O8-C28	4.08	1.45	1.33
19	b	851	DGD	O2G-C1B	4.00	1.45	1.34
19	b	851	DGD	O1G-C1A	3.96	1.44	1.33
23	m	102	BCR	C1-C6	-3.91	1.48	1.53
25	j	105	LMG	O7-C10	3.89	1.45	1.34
19	4	319	DGD	O2G-C1B	3.87	1.45	1.34
20	1	304	A1L1F	C57-C2	-3.64	1.26	1.31
17	b	827	CLA	C1D-ND	3.63	1.42	1.37
17	4	315	CLA	C1D-ND	3.62	1.42	1.37
17	a	804	CLA	C1D-ND	3.61	1.42	1.37
17	1	312	CLA	C1D-ND	3.61	1.42	1.37
17	5	311	CLA	C1D-ND	3.61	1.42	1.37
17	b	841	CLA	C1D-ND	3.60	1.42	1.37
17	5	310	CLA	C1D-ND	3.59	1.42	1.37
17	5	313	CLA	C1D-ND	3.59	1.42	1.37
17	1	310	CLA	C1D-ND	3.59	1.42	1.37
17	a	811	CLA	C1D-ND	3.58	1.42	1.37
17	a	837	CLA	C1D-ND	3.58	1.42	1.37
17	a	840	CLA	C1D-ND	3.58	1.42	1.37
17	a	828	CLA	C1D-ND	3.57	1.42	1.37
17	b	813	CLA	C1D-ND	3.57	1.42	1.37
17	4	308	CLA	C1D-ND	3.57	1.42	1.37
17	b	819	CLA	C1D-ND	3.57	1.42	1.37
17	a	829	CLA	C1D-ND	3.57	1.42	1.37
17	b	825	CLA	C1D-ND	3.57	1.42	1.37
17	b	807	CLA	C1D-ND	3.56	1.42	1.37
17	5	308	CLA	C1D-ND	3.56	1.42	1.37
17	1	314	CLA	C1D-ND	3.55	1.42	1.37
17	5	306	CLA	C1D-ND	3.55	1.42	1.37
17	1	311	CLA	C1D-ND	3.54	1.42	1.37
17	b	818	CLA	C1D-ND	3.53	1.42	1.37
17	5	305	CLA	C1D-ND	3.53	1.42	1.37
17	j	103	CLA	C1D-ND	3.53	1.42	1.37
17	a	844	CLA	C1D-ND	3.53	1.42	1.37
17	f	802	CLA	C1D-ND	3.53	1.42	1.37
17	l	204	CLA	C1D-ND	3.53	1.42	1.37
17	a	814	CLA	C1D-ND	3.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	820	CLA	C1D-ND	3.52	1.42	1.37
17	a	826	CLA	C1D-ND	3.52	1.42	1.37
17	a	822	CLA	C1D-ND	3.51	1.42	1.37
17	b	817	CLA	C1D-ND	3.51	1.42	1.37
17	4	317	CLA	C1D-ND	3.51	1.42	1.37
17	b	834	CLA	C1D-ND	3.51	1.42	1.37
17	5	315	CLA	C1D-ND	3.51	1.42	1.37
17	a	809	CLA	C1D-ND	3.51	1.42	1.37
17	b	836	CLA	C1D-ND	3.51	1.42	1.37
17	b	832	CLA	C1D-ND	3.51	1.42	1.37
17	a	839	CLA	C1D-ND	3.51	1.42	1.37
17	b	805	CLA	C1D-ND	3.51	1.42	1.37
17	5	312	CLA	C1D-ND	3.50	1.42	1.37
17	4	318	CLA	C1D-ND	3.50	1.42	1.37
17	a	825	CLA	C1D-ND	3.50	1.42	1.37
17	4	316	CLA	C1D-ND	3.50	1.42	1.37
17	a	821	CLA	C1D-ND	3.50	1.42	1.37
17	5	309	CLA	C1D-ND	3.50	1.42	1.37
17	a	819	CLA	C1D-ND	3.50	1.42	1.37
17	a	823	CLA	C1D-ND	3.49	1.42	1.37
17	b	801	CLA	C1D-ND	3.49	1.42	1.37
17	a	807	CLA	C1D-ND	3.49	1.42	1.37
17	b	814	CLA	C1D-ND	3.49	1.42	1.37
17	5	314	CLA	C1D-ND	3.49	1.42	1.37
17	a	854	CLA	C1D-ND	3.48	1.42	1.37
17	a	813	CLA	C1D-ND	3.48	1.42	1.37
17	a	838	CLA	C1D-ND	3.48	1.42	1.37
17	l	202	CLA	C1D-ND	3.48	1.42	1.37
17	b	835	CLA	C1D-ND	3.48	1.42	1.37
17	4	309	CLA	C1D-ND	3.48	1.42	1.37
17	1	309	CLA	C1D-ND	3.48	1.42	1.37
17	b	821	CLA	C1D-ND	3.48	1.42	1.37
17	1	306	CLA	C1D-ND	3.48	1.42	1.37
17	a	834	CLA	C1D-ND	3.47	1.42	1.37
17	b	829	CLA	C1D-ND	3.47	1.42	1.37
17	a	835	CLA	C1D-ND	3.47	1.42	1.37
17	1	305	CLA	C1D-ND	3.47	1.42	1.37
17	a	842	CLA	C1D-ND	3.47	1.42	1.37
17	a	841	CLA	C1D-ND	3.47	1.42	1.37
17	a	816	CLA	C1D-ND	3.47	1.42	1.37
17	i	102	CLA	C1D-ND	3.47	1.42	1.37
17	j	102	CLA	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	840	CLA	C1D-ND	3.47	1.42	1.37
17	b	816	CLA	C1D-ND	3.46	1.42	1.37
17	4	311	CLA	C1D-ND	3.46	1.42	1.37
17	a	836	CLA	C1D-ND	3.46	1.42	1.37
17	1	308	CLA	C1D-ND	3.46	1.42	1.37
17	4	307	CLA	C1D-ND	3.45	1.42	1.37
17	f	803	CLA	C1D-ND	3.45	1.42	1.37
17	4	313	CLA	C1D-ND	3.45	1.42	1.37
17	a	820	CLA	C1D-ND	3.45	1.42	1.37
17	b	822	CLA	C1D-ND	3.44	1.42	1.37
17	a	808	CLA	C1D-ND	3.44	1.42	1.37
17	b	823	CLA	C1D-ND	3.44	1.42	1.37
17	b	815	CLA	C1D-ND	3.44	1.42	1.37
17	a	815	CLA	C1D-ND	3.43	1.42	1.37
17	1	307	CLA	C1D-ND	3.43	1.42	1.37
17	a	817	CLA	C1D-ND	3.43	1.42	1.37
17	a	832	CLA	C1D-ND	3.43	1.42	1.37
17	a	831	CLA	C1D-ND	3.42	1.42	1.37
17	b	808	CLA	C1D-ND	3.42	1.42	1.37
17	4	310	CLA	C1D-ND	3.42	1.42	1.37
17	a	818	CLA	C1D-ND	3.42	1.42	1.37
17	b	830	CLA	C1D-ND	3.41	1.42	1.37
17	b	838	CLA	C1D-ND	3.41	1.42	1.37
17	b	811	CLA	C1D-ND	3.41	1.42	1.37
17	b	824	CLA	C1D-ND	3.41	1.42	1.37
17	a	805	CLA	C1D-ND	3.40	1.42	1.37
17	b	828	CLA	C1D-ND	3.40	1.42	1.37
17	4	312	CLA	C1D-ND	3.40	1.42	1.37
17	b	837	CLA	C1D-ND	3.40	1.42	1.37
17	b	839	CLA	C1D-ND	3.40	1.42	1.37
23	m	102	BCR	C30-C25	-3.39	1.49	1.53
17	a	824	CLA	C1D-ND	3.39	1.42	1.37
17	b	826	CLA	C1D-ND	3.38	1.42	1.37
17	b	809	CLA	C1D-ND	3.38	1.42	1.37
17	a	827	CLA	C1D-ND	3.38	1.42	1.37
17	a	812	CLA	C1D-ND	3.38	1.42	1.37
17	5	307	CLA	C1D-ND	3.38	1.42	1.37
17	b	833	CLA	C1D-ND	3.37	1.42	1.37
17	4	314	CLA	C1D-ND	3.37	1.42	1.37
17	a	830	CLA	C1D-ND	3.37	1.42	1.37
17	a	810	CLA	C1D-ND	3.37	1.42	1.37
17	b	810	CLA	C1D-ND	3.37	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	l	203	CLA	C1D-ND	3.36	1.42	1.37
17	b	803	CLA	C1D-ND	3.36	1.42	1.37
17	1	313	CLA	C1D-ND	3.35	1.42	1.37
17	1	312	CLA	C4B-NB	3.35	1.42	1.37
17	a	803	CLA	C1D-ND	3.35	1.42	1.37
17	b	806	CLA	C1D-ND	3.34	1.42	1.37
17	b	812	CLA	C1D-ND	3.32	1.42	1.37
17	b	802	CLA	C1D-ND	3.31	1.42	1.37
17	a	818	CLA	C4B-NB	3.27	1.42	1.37
17	a	802	CLA	C1D-ND	3.27	1.42	1.37
17	a	801	CLA	C1D-ND	3.27	1.42	1.37
22	a	845	LHG	C26-C25	-3.26	1.35	1.51
17	a	840	CLA	C4B-NB	3.25	1.42	1.37
17	b	838	CLA	C4B-NB	3.24	1.42	1.37
22	m	101	LHG	C26-C25	-3.23	1.35	1.51
17	a	833	CLA	C1D-ND	3.22	1.42	1.37
17	b	831	CLA	C1D-ND	3.21	1.42	1.37
22	b	849	LHG	C26-C25	-3.20	1.35	1.51
17	a	842	CLA	C4B-NB	3.19	1.42	1.37
17	a	808	CLA	C4B-NB	3.19	1.42	1.37
17	4	312	CLA	C4B-NB	3.17	1.42	1.37
17	b	835	CLA	C4B-NB	3.16	1.42	1.37
17	b	821	CLA	C4B-NB	3.16	1.42	1.37
17	5	313	CLA	C4B-NB	3.15	1.42	1.37
17	4	315	CLA	C4B-NB	3.15	1.42	1.37
17	b	830	CLA	C4B-NB	3.15	1.42	1.37
17	b	819	CLA	C4B-NB	3.15	1.42	1.37
17	1	305	CLA	C4B-NB	3.15	1.42	1.37
17	4	316	CLA	C4B-NB	3.15	1.42	1.37
17	5	305	CLA	C4B-NB	3.14	1.42	1.37
17	b	812	CLA	CAB-C3B	-3.13	1.44	1.50
17	1	314	CLA	C4B-NB	3.13	1.42	1.37
17	a	817	CLA	C4B-NB	3.13	1.42	1.37
17	a	804	CLA	C4B-NB	3.13	1.42	1.37
17	1	309	CLA	C4B-NB	3.12	1.42	1.37
17	j	102	CLA	C4B-NB	3.12	1.42	1.37
17	b	827	CLA	C4B-NB	3.12	1.42	1.37
17	4	313	CLA	C4B-NB	3.12	1.42	1.37
17	b	801	CLA	C4B-NB	3.10	1.41	1.37
17	i	102	CLA	C4B-NB	3.10	1.41	1.37
17	a	824	CLA	C4B-NB	3.10	1.41	1.37
17	b	829	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	310	CLA	C4B-NB	3.09	1.41	1.37
17	4	317	CLA	C4B-NB	3.09	1.41	1.37
17	4	318	CLA	C4B-NB	3.09	1.41	1.37
17	b	832	CLA	C4B-NB	3.08	1.41	1.37
17	4	307	CLA	C4B-NB	3.08	1.41	1.37
17	f	803	CLA	C4B-NB	3.07	1.41	1.37
17	a	805	CLA	C4B-NB	3.07	1.41	1.37
17	a	813	CLA	C4B-NB	3.07	1.41	1.37
17	4	308	CLA	C4B-NB	3.07	1.41	1.37
17	1	313	CLA	C4B-NB	3.07	1.41	1.37
17	a	854	CLA	C4B-NB	3.07	1.41	1.37
17	b	841	CLA	C4B-NB	3.06	1.41	1.37
17	4	310	CLA	C4B-NB	3.06	1.41	1.37
17	a	810	CLA	C4B-NB	3.06	1.41	1.37
17	a	837	CLA	C4B-NB	3.06	1.41	1.37
17	l	202	CLA	C4B-NB	3.05	1.41	1.37
17	b	840	CLA	C4B-NB	3.05	1.41	1.37
17	j	103	CLA	C4B-NB	3.05	1.41	1.37
17	a	831	CLA	C4B-NB	3.05	1.41	1.37
17	1	310	CLA	C4B-NB	3.05	1.41	1.37
17	a	830	CLA	C4B-NB	3.04	1.41	1.37
17	a	825	CLA	C4B-NB	3.04	1.41	1.37
17	a	820	CLA	C4B-NB	3.04	1.41	1.37
17	4	314	CLA	C4B-NB	3.04	1.41	1.37
17	b	805	CLA	C4B-NB	3.04	1.41	1.37
17	b	817	CLA	C4B-NB	3.03	1.41	1.37
17	a	832	CLA	C4B-NB	3.03	1.41	1.37
17	b	802	CLA	C4B-NB	3.03	1.41	1.37
17	b	825	CLA	C4B-NB	3.03	1.41	1.37
17	5	309	CLA	C4B-NB	3.03	1.41	1.37
17	a	841	CLA	C4B-NB	3.03	1.41	1.37
17	5	307	CLA	C4B-NB	3.03	1.41	1.37
17	a	822	CLA	C4B-NB	3.03	1.41	1.37
17	4	311	CLA	C4B-NB	3.02	1.41	1.37
17	a	836	CLA	C4B-NB	3.02	1.41	1.37
17	b	834	CLA	C4B-NB	3.02	1.41	1.37
17	b	804	CLA	C1D-ND	3.02	1.41	1.37
17	5	306	CLA	C4B-NB	3.01	1.41	1.37
17	a	812	CLA	C4B-NB	3.01	1.41	1.37
17	a	826	CLA	C4B-NB	3.00	1.41	1.37
17	b	804	CLA	C4B-NB	3.00	1.41	1.37
17	b	812	CLA	C4B-NB	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	828	CLA	C4B-NB	3.00	1.41	1.37
17	b	823	CLA	C4B-NB	3.00	1.41	1.37
17	a	816	CLA	C4B-NB	3.00	1.41	1.37
17	b	815	CLA	C4B-NB	2.99	1.41	1.37
17	5	312	CLA	C4B-NB	2.99	1.41	1.37
17	5	314	CLA	C4B-NB	2.98	1.41	1.37
17	1	307	CLA	C4B-NB	2.98	1.41	1.37
17	a	821	CLA	C4B-NB	2.98	1.41	1.37
17	5	308	CLA	C4B-NB	2.98	1.41	1.37
17	a	811	CLA	C4B-NB	2.98	1.41	1.37
17	b	803	CLA	C1B-C2B	2.98	1.50	1.43
17	1	311	CLA	C4B-NB	2.97	1.41	1.37
17	l	203	CLA	C4B-NB	2.97	1.41	1.37
17	a	834	CLA	C4B-NB	2.97	1.41	1.37
17	5	315	CLA	C4B-NB	2.97	1.41	1.37
17	a	823	CLA	C4B-NB	2.97	1.41	1.37
17	1	306	CLA	C4B-NB	2.97	1.41	1.37
17	f	802	CLA	C4B-NB	2.97	1.41	1.37
17	1	308	CLA	C4B-NB	2.96	1.41	1.37
17	b	808	CLA	C4B-NB	2.96	1.41	1.37
17	a	835	CLA	C4B-NB	2.96	1.41	1.37
17	b	809	CLA	C4B-NB	2.96	1.41	1.37
17	b	810	CLA	C4B-NB	2.96	1.41	1.37
17	b	839	CLA	C4B-NB	2.96	1.41	1.37
17	a	839	CLA	C4B-NB	2.95	1.41	1.37
17	b	837	CLA	C4B-NB	2.95	1.41	1.37
17	a	829	CLA	C4B-NB	2.95	1.41	1.37
17	b	816	CLA	C4B-NB	2.95	1.41	1.37
17	a	833	CLA	C4B-NB	2.95	1.41	1.37
17	a	844	CLA	C4B-NB	2.94	1.41	1.37
17	b	803	CLA	C4B-NB	2.94	1.41	1.37
17	a	814	CLA	C4B-NB	2.94	1.41	1.37
17	b	833	CLA	C4B-NB	2.93	1.41	1.37
17	a	827	CLA	C4B-NB	2.93	1.41	1.37
17	b	811	CLA	C4B-NB	2.93	1.41	1.37
17	b	813	CLA	C4B-NB	2.93	1.41	1.37
17	a	819	CLA	C4B-NB	2.92	1.41	1.37
17	a	803	CLA	C4B-NB	2.92	1.41	1.37
17	b	836	CLA	C4B-NB	2.92	1.41	1.37
17	a	815	CLA	C4B-NB	2.92	1.41	1.37
17	b	820	CLA	C4B-NB	2.91	1.41	1.37
17	l	204	CLA	C4B-NB	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	818	CLA	C4B-NB	2.90	1.41	1.37
17	b	806	CLA	C4B-NB	2.90	1.41	1.37
17	a	801	CLA	C4B-NB	2.90	1.41	1.37
17	b	814	CLA	C4B-NB	2.89	1.41	1.37
17	a	807	CLA	C4B-NB	2.89	1.41	1.37
17	b	807	CLA	C4B-NB	2.89	1.41	1.37
17	a	802	CLA	C4B-NB	2.89	1.41	1.37
17	b	822	CLA	C4B-NB	2.89	1.41	1.37
17	b	824	CLA	C4B-NB	2.88	1.41	1.37
17	b	831	CLA	C4B-NB	2.88	1.41	1.37
17	a	838	CLA	C4B-NB	2.87	1.41	1.37
17	b	826	CLA	C4B-NB	2.85	1.41	1.37
17	5	311	CLA	C4B-NB	2.84	1.41	1.37
17	4	309	CLA	C4B-NB	2.84	1.41	1.37
17	b	821	CLA	C1B-C2B	2.82	1.49	1.43
17	1	305	CLA	C1B-C2B	2.82	1.49	1.43
17	b	811	CLA	C1B-C2B	2.82	1.49	1.43
17	a	823	CLA	C1B-C2B	2.81	1.49	1.43
17	b	807	CLA	C1B-C2B	2.81	1.49	1.43
17	b	828	CLA	C1B-C2B	2.81	1.49	1.43
17	b	840	CLA	C1B-C2B	2.80	1.49	1.43
17	a	830	CLA	C1B-C2B	2.80	1.49	1.43
17	b	824	CLA	C1B-C2B	2.79	1.49	1.43
17	1	306	CLA	C1B-C2B	2.79	1.49	1.43
17	1	311	CLA	C1B-C2B	2.79	1.49	1.43
17	b	833	CLA	C1B-C2B	2.78	1.49	1.43
17	a	809	CLA	C4B-NB	2.78	1.41	1.37
17	a	817	CLA	C1B-C2B	2.78	1.49	1.43
17	1	313	CLA	C1B-C2B	2.77	1.49	1.43
17	a	844	CLA	C1B-C2B	2.77	1.49	1.43
17	a	821	CLA	C1B-C2B	2.77	1.49	1.43
17	b	834	CLA	C1B-C2B	2.77	1.49	1.43
17	a	810	CLA	C1B-C2B	2.76	1.49	1.43
17	1	308	CLA	C1B-C2B	2.76	1.49	1.43
17	l	204	CLA	C1B-C2B	2.76	1.49	1.43
17	5	309	CLA	C1B-C2B	2.76	1.49	1.43
17	j	103	CLA	C1B-C2B	2.75	1.49	1.43
17	a	812	CLA	C1B-C2B	2.75	1.49	1.43
17	a	829	CLA	C1B-C2B	2.75	1.49	1.43
17	f	802	CLA	C1B-C2B	2.75	1.49	1.43
17	b	808	CLA	C1B-C2B	2.75	1.49	1.43
17	a	818	CLA	C3B-C4B	2.74	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	828	CLA	C4B-NB	2.74	1.41	1.37
17	a	826	CLA	C1B-C2B	2.74	1.49	1.43
17	4	311	CLA	C1B-C2B	2.74	1.49	1.43
17	a	835	CLA	C1B-C2B	2.74	1.49	1.43
17	5	310	CLA	C1B-C2B	2.74	1.49	1.43
17	b	837	CLA	C1B-C2B	2.74	1.49	1.43
17	4	308	CLA	C1B-C2B	2.74	1.49	1.43
17	b	812	CLA	C4B-C3B	2.74	1.49	1.43
17	b	822	CLA	C1B-C2B	2.74	1.49	1.43
17	j	102	CLA	C1B-C2B	2.74	1.49	1.43
17	a	811	CLA	C1B-C2B	2.74	1.49	1.43
17	4	315	CLA	C1B-C2B	2.74	1.49	1.43
17	b	809	CLA	C1B-C2B	2.73	1.49	1.43
17	a	804	CLA	C1B-C2B	2.72	1.49	1.43
17	a	828	CLA	C1B-C2B	2.72	1.49	1.43
17	4	317	CLA	C1B-C2B	2.72	1.49	1.43
17	a	824	CLA	C1B-C2B	2.72	1.49	1.43
17	4	310	CLA	C1B-C2B	2.72	1.49	1.43
17	a	806	CLA	MG-NB	-2.72	2.00	2.05
17	4	309	CLA	C1B-C2B	2.72	1.49	1.43
17	a	838	CLA	C1B-C2B	2.72	1.49	1.43
17	b	813	CLA	C1B-C2B	2.72	1.49	1.43
17	4	318	CLA	C1B-C2B	2.72	1.49	1.43
17	b	802	CLA	C1B-C2B	2.72	1.49	1.43
17	5	306	CLA	C1B-C2B	2.72	1.49	1.43
17	l	202	CLA	C1B-C2B	2.72	1.49	1.43
17	a	813	CLA	C1B-C2B	2.72	1.49	1.43
17	5	311	CLA	C1B-C2B	2.72	1.49	1.43
17	b	830	CLA	CMB-C2B	-2.71	1.45	1.50
17	5	315	CLA	C1B-C2B	2.71	1.49	1.43
17	i	102	CLA	C1B-C2B	2.71	1.49	1.43
17	5	314	CLA	C1B-C2B	2.71	1.49	1.43
17	a	842	CLA	C1B-C2B	2.71	1.49	1.43
17	a	834	CLA	C1B-C2B	2.71	1.49	1.43
17	b	805	CLA	C1B-C2B	2.71	1.49	1.43
17	a	809	CLA	C1B-C2B	2.71	1.49	1.43
17	a	825	CLA	C1B-C2B	2.71	1.49	1.43
17	1	309	CLA	C1B-C2B	2.71	1.49	1.43
17	1	307	CLA	C1B-C2B	2.71	1.49	1.43
17	b	801	CLA	C1B-C2B	2.71	1.49	1.43
17	4	313	CLA	C1B-C2B	2.70	1.49	1.43
17	b	806	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	838	CLA	C1B-C2B	2.70	1.49	1.43
17	1	314	CLA	C1B-C2B	2.70	1.49	1.43
17	5	313	CLA	C1B-C2B	2.70	1.49	1.43
17	a	814	CLA	C1B-C2B	2.70	1.49	1.43
17	4	307	CLA	C1B-C2B	2.70	1.49	1.43
17	b	816	CLA	C1B-C2B	2.70	1.49	1.43
17	b	841	CLA	C1B-C2B	2.69	1.49	1.43
17	a	839	CLA	C1B-C2B	2.69	1.49	1.43
17	a	807	CLA	C1B-C2B	2.69	1.49	1.43
17	5	312	CLA	C1B-C2B	2.69	1.49	1.43
17	b	812	CLA	C1B-C2B	2.69	1.49	1.43
17	b	832	CLA	C1B-C2B	2.69	1.49	1.43
17	4	312	CLA	C1B-C2B	2.68	1.49	1.43
17	a	816	CLA	C1B-C2B	2.68	1.49	1.43
17	a	854	CLA	C1B-C2B	2.68	1.49	1.43
17	1	312	CLA	C3B-C4B	2.68	1.50	1.42
17	a	840	CLA	C1B-C2B	2.67	1.49	1.43
17	5	307	CLA	C1B-C2B	2.67	1.49	1.43
17	f	803	CLA	C1B-C2B	2.67	1.49	1.43
17	a	815	CLA	C1B-C2B	2.67	1.49	1.43
17	a	837	CLA	C1B-C2B	2.67	1.49	1.43
17	b	814	CLA	C1B-C2B	2.67	1.49	1.43
17	a	805	CLA	C1B-C2B	2.67	1.49	1.43
17	b	815	CLA	C1B-C2B	2.67	1.49	1.43
17	a	808	CLA	C1B-C2B	2.67	1.49	1.43
17	b	810	CLA	C1B-C2B	2.67	1.49	1.43
17	b	827	CLA	C1B-C2B	2.67	1.49	1.43
17	b	839	CLA	C1B-C2B	2.66	1.49	1.43
17	b	823	CLA	C1B-C2B	2.66	1.49	1.43
17	4	316	CLA	C1B-C2B	2.66	1.49	1.43
17	5	305	CLA	C1B-C2B	2.66	1.49	1.43
17	a	819	CLA	C1B-C2B	2.65	1.49	1.43
17	b	825	CLA	C1B-C2B	2.65	1.49	1.43
17	a	801	CLA	C1B-C2B	2.65	1.49	1.43
17	l	203	CLA	C1B-C2B	2.64	1.49	1.43
17	b	836	CLA	C1B-C2B	2.64	1.49	1.43
17	a	832	CLA	C1B-C2B	2.64	1.49	1.43
16	5	303	A1L1G	C33-C34	-2.64	1.40	1.46
17	a	831	CLA	CMB-C2B	-2.63	1.45	1.50
17	a	836	CLA	C1B-C2B	2.62	1.49	1.43
17	b	817	CLA	C1B-C2B	2.62	1.49	1.43
17	a	822	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	310	CLA	C1B-C2B	2.61	1.49	1.43
17	a	827	CLA	C1B-C2B	2.61	1.49	1.43
17	1	312	CLA	C1B-C2B	2.61	1.49	1.43
17	5	308	CLA	C1B-C2B	2.61	1.49	1.43
17	b	819	CLA	C1B-C2B	2.60	1.49	1.43
17	a	833	CLA	C1B-C2B	2.60	1.49	1.43
17	b	820	CLA	C1B-C2B	2.60	1.49	1.43
17	b	829	CLA	C1B-C2B	2.60	1.49	1.43
17	b	826	CLA	C1B-C2B	2.57	1.49	1.43
17	b	835	CLA	C1B-C2B	2.56	1.49	1.43
16	5	303	A1L1G	C40-C39	-2.56	1.40	1.46
17	4	314	CLA	C3B-C4B	2.56	1.50	1.42
17	a	841	CLA	C1B-C2B	2.55	1.49	1.43
20	1	304	A1L1F	O15-C20	-2.54	1.42	1.46
17	b	831	CLA	C1B-C2B	2.53	1.49	1.43
17	a	818	CLA	C1B-C2B	2.53	1.49	1.43
17	b	830	CLA	CMD-C2D	-2.52	1.45	1.50
17	4	314	CLA	CHC-C1C	2.52	1.43	1.38
17	a	806	CLA	CMD-C2D	-2.51	1.45	1.50
17	a	831	CLA	C1B-C2B	2.50	1.49	1.43
17	a	803	CLA	C1B-C2B	2.49	1.49	1.43
17	b	815	CLA	C3B-C4B	2.49	1.50	1.42
17	5	313	CLA	C3B-C4B	2.49	1.50	1.42
17	a	801	CLA	CMD-C2D	-2.47	1.45	1.50
17	a	842	CLA	C3B-C4B	2.47	1.49	1.42
17	a	802	CLA	C1B-C2B	2.47	1.48	1.43
16	1	301	A1L1G	C33-C34	-2.46	1.40	1.46
17	4	314	CLA	C1B-C2B	2.46	1.48	1.43
17	b	830	CLA	C1B-C2B	2.46	1.48	1.43
17	a	806	CLA	CMB-C2B	-2.46	1.45	1.50
17	a	820	CLA	C1B-C2B	2.46	1.48	1.43
17	b	814	CLA	C3B-C4B	2.46	1.49	1.42
17	a	830	CLA	CMC-C2C	-2.46	1.45	1.50
17	4	316	CLA	C3B-C4B	2.46	1.49	1.42
17	a	827	CLA	C3B-C4B	2.44	1.49	1.42
17	a	813	CLA	C3B-C4B	2.44	1.49	1.42
17	a	841	CLA	C3B-C4B	2.44	1.49	1.42
17	5	306	CLA	C3B-C4B	2.44	1.49	1.42
17	4	313	CLA	CHC-C1C	2.44	1.43	1.38
17	a	840	CLA	C3B-C4B	2.44	1.49	1.42
17	a	819	CLA	C3B-C4B	2.43	1.49	1.42
17	a	814	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	804	CLA	C3B-C4B	2.43	1.49	1.42
17	b	836	CLA	C3B-C4B	2.43	1.49	1.42
17	a	802	CLA	CHC-C1C	2.43	1.43	1.38
17	a	806	CLA	CMC-C2C	-2.43	1.45	1.50
17	a	817	CLA	C3B-C4B	2.43	1.49	1.42
17	4	309	CLA	C3B-C4B	2.43	1.49	1.42
17	b	817	CLA	C3B-C4B	2.43	1.49	1.42
22	a	846	LHG	O7-C5	-2.43	1.40	1.46
17	4	308	CLA	C3B-C4B	2.42	1.49	1.42
17	b	829	CLA	C3B-C4B	2.42	1.49	1.42
22	b	849	LHG	O8-C6	-2.42	1.39	1.45
17	b	806	CLA	C3B-C4B	2.42	1.49	1.42
17	a	829	CLA	C3B-C4B	2.41	1.49	1.42
17	b	835	CLA	C3B-C4B	2.41	1.49	1.42
17	b	809	CLA	C3B-C4B	2.41	1.49	1.42
17	1	309	CLA	C3B-C4B	2.41	1.49	1.42
17	a	819	CLA	CHC-C1C	2.41	1.43	1.38
17	a	802	CLA	C3B-C4B	2.41	1.49	1.42
17	f	803	CLA	C3B-C4B	2.41	1.49	1.42
17	a	822	CLA	CHC-C1C	2.41	1.43	1.38
17	a	816	CLA	C3B-C4B	2.40	1.49	1.42
17	5	305	CLA	C3B-C4B	2.40	1.49	1.42
15	1	302	XAT	O4-C5	-2.40	1.43	1.46
17	b	839	CLA	CHC-C1C	2.40	1.43	1.38
22	a	846	LHG	O8-C6	-2.40	1.39	1.45
22	m	101	LHG	O8-C6	-2.40	1.39	1.45
17	i	102	CLA	C3B-C4B	2.39	1.49	1.42
17	a	801	CLA	CMB-C2B	-2.39	1.45	1.50
15	5	302	XAT	O4-C5	-2.39	1.43	1.46
17	4	317	CLA	C3B-C4B	2.39	1.49	1.42
17	j	102	CLA	C3B-C4B	2.39	1.49	1.42
17	1	314	CLA	C3B-C4B	2.39	1.49	1.42
22	a	845	LHG	O8-C6	-2.39	1.39	1.45
17	b	812	CLA	CHC-C1C	2.39	1.43	1.38
22	b	849	LHG	O7-C5	-2.39	1.41	1.46
17	a	818	CLA	CHC-C1C	2.39	1.43	1.38
17	a	822	CLA	C3B-C4B	2.38	1.49	1.42
17	b	802	CLA	C3B-C4B	2.38	1.49	1.42
17	b	807	CLA	C3B-C4B	2.38	1.49	1.42
17	a	805	CLA	C3B-C4B	2.38	1.49	1.42
17	a	804	CLA	C3B-C4B	2.38	1.49	1.42
17	b	816	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	809	CLA	C3B-C4B	2.37	1.49	1.42
17	4	313	CLA	C3B-C4B	2.37	1.49	1.42
17	5	312	CLA	C3B-C4B	2.37	1.49	1.42
17	5	314	CLA	C3B-C4B	2.37	1.49	1.42
17	b	837	CLA	C3B-C4B	2.37	1.49	1.42
17	a	828	CLA	C3B-C4B	2.37	1.49	1.42
17	b	838	CLA	C3B-C4B	2.37	1.49	1.42
17	5	315	CLA	C3B-C4B	2.37	1.49	1.42
17	a	826	CLA	C3B-C4B	2.37	1.49	1.42
17	b	832	CLA	C3B-C4B	2.37	1.49	1.42
17	4	312	CLA	CMD-C2D	-2.37	1.45	1.50
17	a	808	CLA	C3B-C4B	2.37	1.49	1.42
17	a	811	CLA	C3B-C4B	2.37	1.49	1.42
17	a	806	CLA	C1D-ND	2.37	1.41	1.37
17	a	820	CLA	C3B-C4B	2.37	1.49	1.42
17	b	822	CLA	C3B-C4B	2.37	1.49	1.42
17	5	307	CLA	C3B-C4B	2.37	1.49	1.42
17	a	837	CLA	C3B-C4B	2.36	1.49	1.42
17	a	833	CLA	C3B-C4B	2.36	1.49	1.42
17	a	825	CLA	C3B-C4B	2.36	1.49	1.42
17	b	839	CLA	C3B-C4B	2.36	1.49	1.42
17	a	834	CLA	C3B-C4B	2.36	1.49	1.42
17	a	839	CLA	C3B-C4B	2.36	1.49	1.42
17	5	310	CLA	C3B-C4B	2.36	1.49	1.42
17	a	854	CLA	CHC-C1C	2.36	1.43	1.38
17	b	818	CLA	C1B-C2B	2.36	1.48	1.43
17	1	310	CLA	CHC-C1C	2.36	1.43	1.38
17	b	805	CLA	C3B-C4B	2.36	1.49	1.42
17	b	836	CLA	CHC-C1C	2.36	1.43	1.38
17	1	308	CLA	C3B-C4B	2.35	1.49	1.42
17	a	823	CLA	C3B-C4B	2.35	1.49	1.42
17	4	307	CLA	C3B-C4B	2.35	1.49	1.42
17	j	103	CLA	C3B-C4B	2.35	1.49	1.42
17	i	102	CLA	CHC-C1C	2.35	1.43	1.38
17	b	823	CLA	C3B-C4B	2.35	1.49	1.42
17	b	804	CLA	C1B-C2B	2.35	1.48	1.43
17	a	815	CLA	C3B-C4B	2.35	1.49	1.42
17	b	817	CLA	CHC-C1C	2.35	1.43	1.38
17	4	315	CLA	C3B-C4B	2.35	1.49	1.42
17	l	203	CLA	C3B-C4B	2.35	1.49	1.42
17	b	801	CLA	C3B-C4B	2.35	1.49	1.42
17	5	309	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	m	101	LHG	O8-C23	2.35	1.40	1.33
17	1	313	CLA	C3B-C4B	2.35	1.49	1.42
17	b	818	CLA	C3B-C4B	2.35	1.49	1.42
15	4	301	XAT	O24-C25	-2.35	1.43	1.46
17	5	308	CLA	C3B-C4B	2.34	1.49	1.42
17	b	837	CLA	CHC-C1C	2.34	1.43	1.38
17	5	309	CLA	CHC-C1C	2.34	1.43	1.38
15	4	305	XAT	O24-C25	-2.34	1.43	1.46
17	a	820	CLA	CHC-C1C	2.34	1.43	1.38
16	1	301	A1L1G	C40-C39	-2.34	1.40	1.46
22	a	845	LHG	O7-C5	-2.34	1.41	1.46
22	b	849	LHG	O8-C23	2.34	1.40	1.33
17	1	310	CLA	C3B-C4B	2.34	1.49	1.42
17	l	204	CLA	C3B-C4B	2.34	1.49	1.42
17	a	829	CLA	CHC-C1C	2.34	1.43	1.38
17	a	844	CLA	CHC-C1C	2.34	1.43	1.38
17	b	826	CLA	C3B-C4B	2.34	1.49	1.42
17	a	844	CLA	C3B-C4B	2.34	1.49	1.42
17	4	318	CLA	C3B-C4B	2.34	1.49	1.42
17	a	841	CLA	CHC-C1C	2.33	1.43	1.38
22	m	101	LHG	O7-C5	-2.33	1.41	1.46
17	5	311	CLA	C3B-C4B	2.33	1.49	1.42
17	5	312	CLA	CHC-C1C	2.33	1.43	1.38
17	b	815	CLA	CHC-C1C	2.33	1.43	1.38
17	f	802	CLA	C3B-C4B	2.33	1.49	1.42
17	4	318	CLA	CHC-C1C	2.33	1.43	1.38
17	b	802	CLA	CHC-C1C	2.33	1.43	1.38
17	4	311	CLA	C3B-C4B	2.33	1.49	1.42
17	a	827	CLA	CHC-C1C	2.33	1.43	1.38
17	b	816	CLA	CHC-C1C	2.33	1.43	1.38
17	4	312	CLA	C3B-C4B	2.33	1.49	1.42
17	b	825	CLA	C3B-C4B	2.33	1.49	1.42
17	a	832	CLA	CHC-C1C	2.33	1.43	1.38
17	a	830	CLA	C3B-C4B	2.33	1.49	1.42
15	a	852	XAT	O4-C5	-2.33	1.43	1.46
17	l	202	CLA	C3B-C4B	2.33	1.49	1.42
17	b	820	CLA	CMB-C2B	-2.32	1.46	1.50
17	a	821	CLA	C3B-C4B	2.32	1.49	1.42
17	b	833	CLA	C3B-C4B	2.32	1.49	1.42
17	1	306	CLA	C3B-C4B	2.32	1.49	1.42
17	a	824	CLA	C3B-C4B	2.32	1.49	1.42
17	a	836	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	854	CLA	C3B-C4B	2.32	1.49	1.42
17	a	826	CLA	CHC-C1C	2.32	1.43	1.38
17	b	829	CLA	CHC-C1C	2.32	1.43	1.38
17	b	835	CLA	CHC-C1C	2.32	1.43	1.38
17	b	834	CLA	C3B-C4B	2.32	1.49	1.42
17	a	812	CLA	C3B-C4B	2.32	1.49	1.42
17	b	806	CLA	CHC-C1C	2.32	1.43	1.38
17	5	314	CLA	CHC-C1C	2.32	1.43	1.38
17	1	311	CLA	C3B-C4B	2.32	1.49	1.42
17	1	312	CLA	CHC-C1C	2.32	1.43	1.38
17	b	840	CLA	C3B-C4B	2.31	1.49	1.42
17	a	816	CLA	CHC-C1C	2.31	1.43	1.38
17	b	828	CLA	C3B-C4B	2.31	1.49	1.42
17	4	310	CLA	C3B-C4B	2.31	1.49	1.42
17	4	310	CLA	CHC-C1C	2.31	1.43	1.38
17	1	314	CLA	CHC-C1C	2.31	1.43	1.38
17	a	813	CLA	CHC-C1C	2.31	1.43	1.38
17	1	308	CLA	CHC-C1C	2.31	1.43	1.38
17	5	315	CLA	CHC-C1C	2.31	1.43	1.38
17	a	835	CLA	C3B-C4B	2.31	1.49	1.42
17	a	828	CLA	CHC-C1C	2.31	1.43	1.38
17	a	808	CLA	CHC-C1C	2.31	1.43	1.38
17	b	813	CLA	C3B-C4B	2.30	1.49	1.42
17	b	832	CLA	CHC-C1C	2.30	1.43	1.38
17	b	827	CLA	C3B-C4B	2.30	1.49	1.42
22	a	845	LHG	O7-C7	2.30	1.40	1.34
17	b	833	CLA	CHC-C1C	2.30	1.43	1.38
17	l	203	CLA	CHC-C1C	2.30	1.43	1.38
17	a	809	CLA	CHC-C1C	2.30	1.43	1.38
17	a	833	CLA	CHC-C1C	2.30	1.43	1.38
17	b	824	CLA	C3B-C4B	2.30	1.49	1.42
15	5	301	XAT	O4-C5	-2.30	1.43	1.46
17	b	821	CLA	C3B-C4B	2.30	1.49	1.42
15	4	302	XAT	O24-C25	-2.30	1.43	1.46
17	1	311	CLA	CHC-C1C	2.30	1.43	1.38
17	b	809	CLA	CHC-C1C	2.30	1.43	1.38
17	b	831	CLA	MG-NB	-2.30	2.01	2.05
17	b	814	CLA	CHC-C1C	2.30	1.43	1.38
17	b	834	CLA	CHC-C1C	2.30	1.43	1.38
17	f	803	CLA	CHC-C1C	2.29	1.43	1.38
17	1	307	CLA	C3B-C4B	2.29	1.49	1.42
22	m	101	LHG	O7-C7	2.29	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	315	CLA	CHC-C1C	2.29	1.43	1.38
17	1	204	CLA	CHC-C1C	2.29	1.43	1.38
17	5	307	CLA	CHC-C1C	2.29	1.43	1.38
17	b	805	CLA	CHC-C1C	2.29	1.43	1.38
17	a	832	CLA	C3B-C4B	2.29	1.49	1.42
17	5	311	CLA	CHC-C1C	2.29	1.43	1.38
17	a	814	CLA	CHC-C1C	2.29	1.43	1.38
17	b	824	CLA	CHC-C1C	2.29	1.43	1.38
17	b	818	CLA	MG-NB	-2.29	2.01	2.05
17	b	808	CLA	C3B-C4B	2.29	1.49	1.42
17	b	819	CLA	C3B-C4B	2.28	1.49	1.42
17	5	306	CLA	CHC-C1C	2.28	1.43	1.38
17	a	824	CLA	CHC-C1C	2.28	1.43	1.38
17	a	804	CLA	CHC-C1C	2.28	1.43	1.38
17	4	309	CLA	CHC-C1C	2.28	1.43	1.38
17	a	805	CLA	CHC-C1C	2.28	1.43	1.38
17	b	831	CLA	C3B-C4B	2.28	1.49	1.42
17	b	823	CLA	CHC-C1C	2.27	1.43	1.38
17	b	828	CLA	CHC-C1C	2.27	1.43	1.38
17	1	309	CLA	CHC-C1C	2.27	1.43	1.38
17	b	826	CLA	CHC-C1C	2.27	1.43	1.38
17	a	824	CLA	CMD-C2D	-2.27	1.46	1.50
17	a	810	CLA	C3B-C4B	2.27	1.49	1.42
17	4	311	CLA	CHC-C1C	2.27	1.43	1.38
17	a	836	CLA	CHC-C1C	2.27	1.43	1.38
17	a	842	CLA	CHC-C1C	2.27	1.43	1.38
17	b	838	CLA	CHC-C1C	2.27	1.43	1.38
22	a	845	LHG	O8-C23	2.27	1.40	1.33
17	a	837	CLA	CHC-C1C	2.26	1.43	1.38
22	a	846	LHG	O7-C7	2.26	1.40	1.34
17	b	811	CLA	C3B-C4B	2.26	1.49	1.42
17	b	823	CLA	CMD-C2D	-2.26	1.46	1.50
17	b	810	CLA	CMB-C2B	-2.26	1.46	1.50
17	a	810	CLA	CMD-C2D	-2.26	1.46	1.50
15	4	306	XAT	O4-C5	-2.26	1.43	1.46
17	b	803	CLA	C3B-C4B	2.26	1.49	1.42
17	b	818	CLA	CHC-C1C	2.26	1.43	1.38
17	b	841	CLA	CHC-C1C	2.26	1.43	1.38
17	b	809	CLA	CMD-C2D	-2.26	1.46	1.50
17	5	310	CLA	CHC-C1C	2.26	1.43	1.38
22	a	846	LHG	O8-C23	2.26	1.39	1.33
17	4	308	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	801	CLA	CHC-C1C	2.25	1.43	1.38
17	b	801	CLA	CMB-C2B	-2.25	1.46	1.50
17	a	812	CLA	CHC-C1C	2.25	1.43	1.38
17	a	830	CLA	CMD-C2D	-2.25	1.46	1.50
17	5	313	CLA	CHC-C1C	2.25	1.43	1.38
17	1	307	CLA	CHC-C1C	2.25	1.43	1.38
17	b	831	CLA	CHC-C1C	2.25	1.43	1.38
17	4	307	CLA	CHC-C1C	2.25	1.43	1.38
17	1	305	CLA	C3B-C4B	2.25	1.49	1.42
17	a	838	CLA	C3B-C4B	2.25	1.49	1.42
17	a	804	CLA	CMC-C2C	-2.25	1.46	1.50
17	a	823	CLA	CHC-C1C	2.25	1.43	1.38
17	a	803	CLA	CHC-C1C	2.25	1.43	1.38
22	b	849	LHG	O7-C7	2.25	1.40	1.34
17	b	813	CLA	CHC-C1C	2.25	1.43	1.38
17	b	840	CLA	CMB-C2B	-2.25	1.46	1.50
17	4	312	CLA	CHC-C1C	2.24	1.43	1.38
20	1	304	A1L1F	C6-C1	-2.24	1.50	1.54
15	a	852	XAT	O24-C25	-2.24	1.43	1.46
17	l	202	CLA	CHC-C1C	2.24	1.43	1.38
17	a	828	CLA	CMC-C2C	-2.24	1.46	1.50
17	1	313	CLA	CHC-C1C	2.24	1.43	1.38
17	a	815	CLA	CHC-C1C	2.24	1.43	1.38
17	a	834	CLA	CHC-C1C	2.24	1.43	1.38
17	b	825	CLA	CHC-C1C	2.24	1.43	1.38
15	4	301	XAT	O4-C5	-2.24	1.43	1.46
17	a	835	CLA	CHC-C1C	2.24	1.43	1.38
17	a	839	CLA	CHC-C1C	2.24	1.43	1.38
17	b	824	CLA	CMD-C2D	-2.24	1.46	1.50
17	b	831	CLA	CMD-C2D	-2.23	1.46	1.50
17	f	802	CLA	CHC-C1C	2.23	1.43	1.38
17	a	838	CLA	CHC-C1C	2.23	1.43	1.38
17	a	803	CLA	C3B-C4B	2.23	1.49	1.42
17	b	807	CLA	CHC-C1C	2.23	1.43	1.38
17	b	841	CLA	C3B-C4B	2.23	1.49	1.42
17	5	305	CLA	CHC-C1C	2.23	1.43	1.38
17	1	305	CLA	CHC-C1C	2.23	1.43	1.38
17	b	821	CLA	CHC-C1C	2.23	1.43	1.38
17	b	804	CLA	CHC-C1C	2.23	1.43	1.38
17	b	820	CLA	C3B-C4B	2.23	1.49	1.42
17	5	305	CLA	CMD-C2D	-2.23	1.46	1.50
17	b	810	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	830	CLA	CHC-C1C	2.22	1.42	1.38
17	a	832	CLA	CMB-C2B	-2.22	1.46	1.50
15	4	302	XAT	O4-C5	-2.22	1.43	1.46
17	4	316	CLA	CHC-C1C	2.22	1.42	1.38
17	a	831	CLA	C3B-C4B	2.22	1.49	1.42
17	b	820	CLA	CHC-C1C	2.22	1.42	1.38
17	4	317	CLA	CHC-C1C	2.22	1.42	1.38
17	a	833	CLA	MG-NB	-2.22	2.01	2.05
17	5	308	CLA	CHC-C1C	2.22	1.42	1.38
16	1	301	A1L1G	C38-C39	2.21	1.40	1.35
17	a	801	CLA	CMC-C2C	-2.21	1.46	1.50
17	a	811	CLA	CHC-C1C	2.21	1.42	1.38
17	b	811	CLA	CHC-C1C	2.21	1.42	1.38
17	b	822	CLA	CHC-C1C	2.21	1.42	1.38
15	5	304	XAT	O4-C5	-2.21	1.43	1.46
17	b	804	CLA	MG-NB	-2.21	2.01	2.05
17	a	825	CLA	CHC-C1C	2.21	1.42	1.38
17	a	832	CLA	MG-NB	-2.21	2.01	2.05
17	b	803	CLA	CMD-C2D	-2.21	1.46	1.50
15	5	302	XAT	O24-C25	-2.20	1.43	1.46
17	1	306	CLA	CHC-C1C	2.20	1.42	1.38
17	a	807	CLA	C3B-C4B	2.20	1.49	1.42
17	a	817	CLA	CHC-C1C	2.20	1.42	1.38
17	4	312	CLA	CMB-C2B	-2.20	1.46	1.50
17	b	803	CLA	CHC-C1C	2.20	1.42	1.38
17	a	806	CLA	CAA-C2A	-2.20	1.50	1.54
17	b	829	CLA	CMD-C2D	-2.20	1.46	1.50
15	4	305	XAT	O4-C5	-2.20	1.43	1.46
17	b	830	CLA	MG-NB	-2.20	2.01	2.05
17	5	312	CLA	MG-NB	-2.19	2.01	2.05
17	j	103	CLA	CHC-C1C	2.19	1.42	1.38
15	1	303	XAT	O4-C5	-2.19	1.43	1.46
17	a	810	CLA	CHC-C1C	2.19	1.42	1.38
17	a	840	CLA	CHC-C1C	2.19	1.42	1.38
17	b	827	CLA	CHC-C1C	2.19	1.42	1.38
17	a	821	CLA	CHC-C1C	2.18	1.42	1.38
15	j	101	XAT	O24-C25	-2.18	1.43	1.46
17	a	820	CLA	CMB-C2B	-2.18	1.46	1.50
17	j	102	CLA	CHC-C1C	2.18	1.42	1.38
17	a	810	CLA	MG-NB	-2.18	2.01	2.05
17	b	808	CLA	CHC-C1C	2.18	1.42	1.38
17	a	807	CLA	MG-NB	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	1	301	A1L1G	C29-C30	-2.18	1.40	1.45
17	a	807	CLA	CHC-C1C	2.18	1.42	1.38
17	a	802	CLA	CMB-C2B	-2.18	1.46	1.50
17	b	818	CLA	CMB-C2B	-2.17	1.46	1.50
17	a	801	CLA	C3B-C4B	2.17	1.49	1.42
17	b	819	CLA	CHC-C1C	2.17	1.42	1.38
15	4	304	XAT	O4-C5	-2.17	1.43	1.46
17	b	821	CLA	CMD-C2D	-2.17	1.46	1.50
17	b	835	CLA	CMB-C2B	-2.16	1.46	1.50
17	a	806	CLA	C4B-NB	2.16	1.40	1.37
17	b	812	CLA	CMD-C2D	-2.16	1.46	1.50
17	b	830	CLA	C3B-C4B	2.16	1.49	1.42
17	b	809	CLA	CMC-C2C	-2.16	1.46	1.50
17	b	833	CLA	MG-NB	-2.16	2.01	2.05
17	a	836	CLA	CMB-C2B	-2.16	1.46	1.50
17	a	806	CLA	C1B-NB	-2.16	1.35	1.37
17	b	801	CLA	CMD-C2D	-2.16	1.46	1.50
17	5	308	CLA	CMD-C2D	-2.15	1.46	1.50
17	b	814	CLA	MG-NB	-2.15	2.01	2.05
16	1	301	A1L1G	C35-C34	2.15	1.40	1.35
17	4	310	CLA	MG-NB	-2.15	2.01	2.05
17	b	838	CLA	CMD-C2D	-2.15	1.46	1.50
17	1	307	CLA	MG-NB	-2.15	2.01	2.05
17	b	839	CLA	CMD-C2D	-2.15	1.46	1.50
17	b	831	CLA	CMB-C2B	-2.15	1.46	1.50
17	5	308	CLA	MG-NB	-2.14	2.01	2.05
17	a	831	CLA	MG-NB	-2.14	2.01	2.05
17	a	821	CLA	CMD-C2D	-2.14	1.46	1.50
17	a	803	CLA	MG-NB	-2.14	2.01	2.05
17	b	815	CLA	CMD-C2D	-2.14	1.46	1.50
17	a	808	CLA	CMB-C2B	-2.14	1.46	1.50
15	5	304	XAT	O24-C25	-2.14	1.43	1.46
15	j	101	XAT	O4-C5	-2.14	1.43	1.46
17	a	801	CLA	CHC-C1C	2.14	1.42	1.38
17	4	318	CLA	CMB-C2B	-2.14	1.46	1.50
17	b	825	CLA	MG-NB	-2.14	2.01	2.05
17	a	834	CLA	CMD-C2D	-2.14	1.46	1.50
17	b	824	CLA	MG-NB	-2.13	2.01	2.05
17	b	819	CLA	CMB-C2B	-2.13	1.46	1.50
17	a	824	CLA	CMB-C2B	-2.13	1.46	1.50
22	m	101	LHG	P-O6	2.13	1.67	1.59
17	a	806	CLA	MG-ND	-2.13	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	832	CLA	CMD-C2D	-2.13	1.46	1.50
17	b	836	CLA	MG-NB	-2.13	2.01	2.05
17	l	202	CLA	MG-NB	-2.13	2.01	2.05
17	a	837	CLA	CMB-C2B	-2.13	1.46	1.50
15	1	302	XAT	O24-C25	-2.13	1.43	1.46
17	a	820	CLA	MG-NB	-2.13	2.01	2.05
17	a	842	CLA	CMD-C2D	-2.13	1.46	1.50
17	1	310	CLA	MG-NB	-2.13	2.01	2.05
17	b	810	CLA	MG-NB	-2.12	2.01	2.05
17	j	102	CLA	CMD-C2D	-2.12	1.46	1.50
17	b	829	CLA	MG-NB	-2.12	2.01	2.05
17	a	827	CLA	CMD-C2D	-2.12	1.46	1.50
17	b	827	CLA	MG-NB	-2.12	2.01	2.05
15	1	303	XAT	O24-C25	-2.12	1.43	1.46
15	4	303	XAT	O24-C25	-2.12	1.43	1.46
15	4	303	XAT	O4-C5	-2.12	1.43	1.46
22	a	845	LHG	P-O6	2.12	1.67	1.59
17	a	802	CLA	MG-NB	-2.12	2.01	2.05
17	b	823	CLA	MG-NB	-2.11	2.01	2.05
17	b	820	CLA	CMD-C2D	-2.11	1.46	1.50
17	b	820	CLA	MG-NB	-2.11	2.01	2.05
17	a	831	CLA	CHC-C1C	2.11	1.42	1.38
17	a	816	CLA	CMD-C2D	-2.11	1.46	1.50
17	a	803	CLA	CMB-C2B	-2.11	1.46	1.50
17	b	807	CLA	MG-NB	-2.11	2.01	2.05
17	b	826	CLA	CMD-C2D	-2.11	1.46	1.50
17	a	812	CLA	CMD-C2D	-2.11	1.46	1.50
17	4	312	CLA	MG-NB	-2.11	2.01	2.05
17	b	835	CLA	MG-NB	-2.11	2.01	2.05
16	5	303	A1L1G	C29-C30	-2.11	1.40	1.45
15	5	301	XAT	O24-C25	-2.11	1.43	1.46
17	a	822	CLA	CMB-C2B	-2.11	1.46	1.50
17	a	826	CLA	MG-NB	-2.10	2.01	2.05
22	b	849	LHG	P-O6	2.10	1.67	1.59
17	a	854	CLA	MG-NB	-2.10	2.01	2.05
17	b	829	CLA	CMB-C2B	-2.10	1.46	1.50
17	a	801	CLA	MG-NB	-2.10	2.01	2.05
17	i	102	CLA	CMD-C2D	-2.10	1.46	1.50
17	a	814	CLA	MG-NB	-2.10	2.01	2.05
17	b	810	CLA	CHC-C1C	2.10	1.42	1.38
17	5	307	CLA	MG-NB	-2.10	2.01	2.05
17	5	311	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	l	202	CLA	CMD-C2D	-2.10	1.46	1.50
17	b	801	CLA	MG-NB	-2.10	2.01	2.05
17	b	841	CLA	MG-NB	-2.10	2.01	2.05
17	b	838	CLA	MG-NB	-2.09	2.01	2.05
17	a	838	CLA	MG-NB	-2.09	2.01	2.05
17	b	808	CLA	MG-NB	-2.09	2.01	2.05
15	4	304	XAT	O24-C25	-2.09	1.43	1.46
17	l	309	CLA	CMD-C2D	-2.09	1.46	1.50
17	a	828	CLA	MG-NB	-2.09	2.01	2.05
17	a	822	CLA	MG-NB	-2.09	2.01	2.05
17	a	817	CLA	CMB-C2B	-2.09	1.46	1.50
17	a	826	CLA	CMD-C2D	-2.09	1.46	1.50
17	4	309	CLA	MG-NB	-2.09	2.01	2.05
17	a	837	CLA	CMD-C2D	-2.09	1.46	1.50
17	b	835	CLA	CMD-C2D	-2.09	1.46	1.50
17	l	202	CLA	CMB-C2B	-2.09	1.46	1.50
17	b	803	CLA	CMC-C2C	-2.09	1.46	1.50
17	b	802	CLA	CMD-C2D	-2.09	1.46	1.50
17	l	314	CLA	CMB-C2B	-2.09	1.46	1.50
17	a	830	CLA	MG-NB	-2.08	2.01	2.05
17	4	309	CLA	CMD-C2D	-2.08	1.46	1.50
17	b	832	CLA	MG-NB	-2.08	2.01	2.05
17	b	834	CLA	CMD-C2D	-2.08	1.46	1.50
17	4	308	CLA	CMD-C2D	-2.08	1.46	1.50
17	l	204	CLA	CMC-C2C	-2.08	1.46	1.50
17	a	844	CLA	MG-NB	-2.08	2.01	2.05
17	b	818	CLA	CMD-C2D	-2.08	1.46	1.50
17	l	203	CLA	MG-NB	-2.08	2.01	2.05
17	j	103	CLA	CMB-C2B	-2.08	1.46	1.50
17	b	826	CLA	MG-NB	-2.07	2.01	2.05
17	a	829	CLA	CMD-C2D	-2.07	1.46	1.50
17	a	810	CLA	CMB-C2B	-2.07	1.46	1.50
17	a	838	CLA	CMD-C2D	-2.07	1.46	1.50
17	a	802	CLA	CMD-C2D	-2.07	1.46	1.50
17	a	803	CLA	CMD-C2D	-2.07	1.46	1.50
17	b	808	CLA	CMD-C2D	-2.07	1.46	1.50
17	a	811	CLA	MG-NB	-2.07	2.01	2.05
17	f	802	CLA	MG-NB	-2.07	2.01	2.05
17	a	827	CLA	MG-NB	-2.07	2.01	2.05
17	a	818	CLA	CMB-C2B	-2.07	1.46	1.50
17	a	835	CLA	CMB-C2B	-2.07	1.46	1.50
17	b	816	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	846	LHG	P-O6	2.07	1.67	1.59
17	a	840	CLA	CMD-C2D	-2.06	1.46	1.50
17	a	823	CLA	CMD-C2D	-2.06	1.46	1.50
17	l	203	CLA	CMB-C2B	-2.06	1.46	1.50
17	b	809	CLA	CMB-C2B	-2.06	1.46	1.50
17	a	823	CLA	MG-NB	-2.06	2.01	2.05
17	a	807	CLA	CMD-C2D	-2.06	1.46	1.50
17	a	816	CLA	MG-NB	-2.06	2.01	2.05
17	b	839	CLA	CMB-C2B	-2.06	1.46	1.50
17	5	315	CLA	MG-NB	-2.06	2.01	2.05
17	a	818	CLA	CMC-C2C	-2.06	1.46	1.50
17	1	311	CLA	MG-NB	-2.06	2.01	2.05
17	a	825	CLA	MG-NB	-2.06	2.01	2.05
17	4	314	CLA	CMB-C2B	-2.06	1.46	1.50
17	a	815	CLA	MG-NB	-2.06	2.01	2.05
17	4	315	CLA	MG-NB	-2.06	2.01	2.05
17	1	306	CLA	MG-NB	-2.06	2.01	2.05
17	1	312	CLA	CMD-C2D	-2.06	1.46	1.50
17	b	812	CLA	MG-NB	-2.06	2.01	2.05
17	b	828	CLA	CMD-C2D	-2.06	1.46	1.50
17	a	839	CLA	CMD-C2D	-2.06	1.46	1.50
17	a	808	CLA	MG-NB	-2.06	2.01	2.05
17	i	102	CLA	MG-NB	-2.06	2.01	2.05
17	a	817	CLA	CMD-C2D	-2.06	1.46	1.50
17	l	203	CLA	CMC-C2C	-2.06	1.46	1.50
17	b	839	CLA	MG-NB	-2.06	2.01	2.05
17	a	814	CLA	CMD-C2D	-2.05	1.46	1.50
17	b	813	CLA	MG-NB	-2.05	2.01	2.05
17	4	315	CLA	CMB-C2B	-2.05	1.46	1.50
17	5	313	CLA	CMD-C2D	-2.05	1.46	1.50
17	4	311	CLA	CMD-C2D	-2.05	1.46	1.50
17	f	802	CLA	CMD-C2D	-2.05	1.46	1.50
17	b	812	CLA	CMB-C2B	-2.05	1.46	1.50
19	b	851	DGD	C1E-C2E	2.05	1.58	1.52
17	5	306	CLA	CMB-C2B	-2.05	1.46	1.50
17	5	314	CLA	CMD-C2D	-2.05	1.46	1.50
17	1	309	CLA	CMB-C2B	-2.05	1.46	1.50
17	b	825	CLA	CMB-C2B	-2.05	1.46	1.50
17	a	824	CLA	MG-NB	-2.05	2.01	2.05
17	a	815	CLA	CMB-C2B	-2.05	1.46	1.50
17	b	833	CLA	CMD-C2D	-2.05	1.46	1.50
17	4	316	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	814	CLA	CMC-C2C	-2.05	1.46	1.50
17	b	837	CLA	MG-NB	-2.05	2.01	2.05
17	5	312	CLA	CMB-C2B	-2.05	1.46	1.50
17	b	811	CLA	CMD-C2D	-2.05	1.46	1.50
16	5	303	A1L1G	C38-C39	2.05	1.40	1.35
17	b	817	CLA	MG-NB	-2.05	2.01	2.05
17	b	840	CLA	CMD-C2D	-2.05	1.46	1.50
17	b	827	CLA	CMD-C2D	-2.05	1.46	1.50
17	b	804	CLA	CMD-C2D	-2.05	1.46	1.50
17	b	821	CLA	MG-NB	-2.05	2.01	2.05
17	b	819	CLA	CMD-C2D	-2.05	1.46	1.50
17	b	819	CLA	MG-NB	-2.04	2.01	2.05
17	1	313	CLA	CMD-C2D	-2.04	1.46	1.50
17	a	825	CLA	CMB-C2B	-2.04	1.46	1.50
17	b	809	CLA	MG-NB	-2.04	2.01	2.05
17	a	802	CLA	CMC-C2C	-2.04	1.46	1.50
17	b	806	CLA	MG-NB	-2.04	2.01	2.05
17	a	806	CLA	C1B-C2B	2.04	1.47	1.43
17	5	309	CLA	MG-NB	-2.04	2.01	2.05
17	b	840	CLA	MG-NB	-2.04	2.01	2.05
17	a	819	CLA	CMC-C2C	-2.04	1.46	1.50
19	b	851	DGD	O3D-C3D	-2.04	1.37	1.43
17	a	842	CLA	CMB-C2B	-2.04	1.46	1.50
17	4	318	CLA	MG-NB	-2.04	2.01	2.05
17	1	309	CLA	MG-NB	-2.04	2.01	2.05
17	a	831	CLA	CMC-C2C	-2.04	1.46	1.50
15	4	306	XAT	O24-C25	-2.04	1.43	1.46
17	b	807	CLA	CMD-C2D	-2.04	1.46	1.50
17	5	312	CLA	CMD-C2D	-2.04	1.46	1.50
17	b	837	CLA	CMD-C2D	-2.04	1.46	1.50
17	1	311	CLA	CMB-C2B	-2.04	1.46	1.50
17	1	204	CLA	CMB-C2B	-2.04	1.46	1.50
17	a	809	CLA	MG-NB	-2.04	2.01	2.05
17	1	204	CLA	MG-NB	-2.04	2.01	2.05
17	b	816	CLA	CMB-C2B	-2.04	1.46	1.50
17	1	307	CLA	CMB-C2B	-2.03	1.46	1.50
17	5	310	CLA	MG-NB	-2.03	2.01	2.05
17	a	808	CLA	CMD-C2D	-2.03	1.46	1.50
17	a	813	CLA	CMB-C2B	-2.03	1.46	1.50
17	a	805	CLA	CMD-C2D	-2.03	1.46	1.50
17	a	854	CLA	CMD-C2D	-2.03	1.46	1.50
17	a	835	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	308	CLA	MG-NB	-2.03	2.01	2.05
17	a	831	CLA	CMD-C2D	-2.03	1.46	1.50
17	1	312	CLA	CMB-C2B	-2.03	1.46	1.50
17	a	834	CLA	CMB-C2B	-2.03	1.46	1.50
17	a	813	CLA	CMD-C2D	-2.03	1.46	1.50
17	a	804	CLA	MG-NB	-2.03	2.01	2.05
17	4	313	CLA	MG-NB	-2.03	2.01	2.05
17	a	837	CLA	MG-NB	-2.03	2.01	2.05
17	5	307	CLA	CMD-C2D	-2.03	1.46	1.50
17	b	813	CLA	CMD-C2D	-2.03	1.46	1.50
17	a	812	CLA	MG-NB	-2.03	2.01	2.05
17	b	814	CLA	CMC-C2C	-2.03	1.46	1.50
17	1	313	CLA	MG-NB	-2.03	2.01	2.05
17	1	307	CLA	CMD-C2D	-2.03	1.46	1.50
17	a	854	CLA	CMB-C2B	-2.03	1.46	1.50
19	b	851	DGD	O4D-C4D	-2.03	1.37	1.43
17	b	826	CLA	CMB-C2B	-2.03	1.46	1.50
17	5	310	CLA	CMB-C2B	-2.03	1.46	1.50
17	1	313	CLA	CMB-C2B	-2.03	1.46	1.50
17	a	821	CLA	MG-NB	-2.02	2.01	2.05
17	b	822	CLA	CMD-C2D	-2.02	1.46	1.50
17	5	314	CLA	MG-NB	-2.02	2.01	2.05
17	b	841	CLA	CMB-C2B	-2.02	1.46	1.50
17	f	803	CLA	MG-NB	-2.02	2.01	2.05
17	4	315	CLA	CMD-C2D	-2.02	1.46	1.50
17	a	841	CLA	CMD-C2D	-2.02	1.46	1.50
17	b	837	CLA	CMB-C2B	-2.02	1.46	1.50
17	1	305	CLA	MG-NB	-2.02	2.01	2.05
17	b	816	CLA	CMD-C2D	-2.02	1.46	1.50
17	b	828	CLA	CMB-C2B	-2.02	1.46	1.50
17	b	811	CLA	MG-NB	-2.02	2.01	2.05
17	b	822	CLA	MG-NB	-2.02	2.01	2.05
17	a	818	CLA	CMD-C2D	-2.02	1.46	1.50
17	b	816	CLA	MG-NB	-2.02	2.01	2.05
17	4	313	CLA	CMB-C2B	-2.02	1.46	1.50
17	1	308	CLA	CMD-C2D	-2.02	1.46	1.50
17	a	816	CLA	CMC-C2C	-2.02	1.46	1.50
17	a	819	CLA	CMD-C2D	-2.02	1.46	1.50
17	b	813	CLA	CMB-C2B	-2.02	1.46	1.50
17	b	814	CLA	CMD-C2D	-2.02	1.46	1.50
17	5	309	CLA	CMB-C2B	-2.02	1.46	1.50
17	4	318	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	817	CLA	CMD-C2D	-2.02	1.46	1.50
17	a	819	CLA	MG-NB	-2.02	2.01	2.05
17	l	203	CLA	CMD-C2D	-2.02	1.46	1.50
17	j	102	CLA	CMB-C2B	-2.02	1.46	1.50
17	l	204	CLA	CMD-C2D	-2.02	1.46	1.50
17	a	835	CLA	MG-NB	-2.02	2.01	2.05
17	1	305	CLA	CMB-C2B	-2.02	1.46	1.50
17	1	310	CLA	CMB-C2B	-2.02	1.46	1.50
17	5	313	CLA	CMB-C2B	-2.01	1.46	1.50
17	4	310	CLA	CMD-C2D	-2.01	1.46	1.50
17	a	809	CLA	CMD-C2D	-2.01	1.46	1.50
17	a	822	CLA	CMD-C2D	-2.01	1.46	1.50
17	a	841	CLA	CMC-C2C	-2.01	1.46	1.50
17	b	824	CLA	CMC-C2C	-2.01	1.46	1.50
17	b	825	CLA	CMD-C2D	-2.01	1.46	1.50
17	b	828	CLA	MG-NB	-2.01	2.01	2.05
17	a	819	CLA	CMB-C2B	-2.01	1.46	1.50
17	5	306	CLA	CMD-C2D	-2.01	1.46	1.50
17	a	827	CLA	CMB-C2B	-2.01	1.46	1.50
17	4	314	CLA	MG-NB	-2.01	2.01	2.05
17	a	804	CLA	CMD-C2D	-2.01	1.46	1.50
17	a	840	CLA	CMB-C2B	-2.01	1.46	1.50
17	f	803	CLA	CMD-C2D	-2.01	1.46	1.50
17	4	310	CLA	CMC-C2C	-2.01	1.46	1.50
17	a	821	CLA	CMC-C2C	-2.01	1.46	1.50
17	b	830	CLA	CHC-C1C	2.01	1.42	1.38
17	5	305	CLA	MG-NB	-2.01	2.01	2.05
17	a	840	CLA	MG-NB	-2.01	2.01	2.05
17	4	314	CLA	CMD-C2D	-2.01	1.46	1.50
17	1	306	CLA	CMC-C2C	-2.01	1.46	1.50
17	a	842	CLA	MG-NB	-2.01	2.01	2.05
17	b	813	CLA	CMC-C2C	-2.00	1.46	1.50
17	b	814	CLA	CMB-C2B	-2.00	1.46	1.50
17	4	311	CLA	MG-NB	-2.00	2.01	2.05
17	4	315	CLA	CMC-C2C	-2.00	1.46	1.50
17	a	821	CLA	CMB-C2B	-2.00	1.46	1.50
17	a	844	CLA	CMD-C2D	-2.00	1.46	1.50
17	a	815	CLA	CMC-C2C	-2.00	1.46	1.50
17	5	310	CLA	CMD-C2D	-2.00	1.46	1.50
17	a	811	CLA	CMB-C2B	-2.00	1.46	1.50

All (1354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	319	DGD	C6E-C5E-C4E	-8.97	91.00	113.02
20	1	304	A1L1F	C17-C20-C25	-8.29	108.66	122.30
17	a	806	CLA	C4A-NA-C1A	7.36	110.04	106.68
15	1	303	XAT	C38-C25-C24	7.25	122.38	114.24
17	b	840	CLA	C4A-NA-C1A	7.25	109.98	106.68
15	4	306	XAT	C38-C25-C24	7.24	122.38	114.24
15	5	304	XAT	C38-C25-C24	7.24	122.38	114.24
17	4	311	CLA	C4A-NA-C1A	7.23	109.98	106.68
15	a	852	XAT	C15-C14-C13	-7.20	117.18	127.28
17	l	203	CLA	C4A-NA-C1A	7.16	109.95	106.68
23	f	801	BCR	C24-C23-C22	-7.16	115.65	126.23
17	a	810	CLA	C4A-NA-C1A	7.08	109.91	106.68
17	a	835	CLA	C4A-NA-C1A	7.08	109.91	106.68
17	b	803	CLA	C4A-NA-C1A	7.08	109.91	106.68
17	a	821	CLA	C4A-NA-C1A	7.07	109.91	106.68
15	4	305	XAT	C38-C25-C24	7.07	122.18	114.24
15	j	101	XAT	C38-C25-C24	7.07	122.18	114.24
17	b	809	CLA	C4A-NA-C1A	7.06	109.90	106.68
17	b	821	CLA	C4A-NA-C1A	7.05	109.89	106.68
17	a	833	CLA	C4A-NA-C1A	7.04	109.89	106.68
15	5	304	XAT	C18-C5-C4	7.04	122.15	114.24
17	a	826	CLA	C4A-NA-C1A	7.00	109.87	106.68
15	5	301	XAT	C38-C25-C26	-6.99	110.80	122.30
17	j	103	CLA	C4A-NA-C1A	6.97	109.86	106.68
15	4	306	XAT	C38-C25-C26	-6.96	110.84	122.30
17	a	823	CLA	C4A-NA-C1A	6.94	109.85	106.68
17	b	805	CLA	C4A-NA-C1A	6.94	109.84	106.68
15	4	304	XAT	C38-C25-C24	6.91	122.00	114.24
15	1	302	XAT	C38-C25-C24	6.91	122.00	114.24
15	5	304	XAT	C6-C7-C8	-6.84	111.52	125.99
15	a	852	XAT	C38-C25-C24	6.84	121.92	114.24
17	a	801	CLA	C4A-NA-C1A	6.84	109.80	106.68
15	5	304	XAT	C18-C5-C6	-6.83	111.07	122.30
17	a	828	CLA	C4A-NA-C1A	6.81	109.79	106.68
17	1	306	CLA	C4A-NA-C1A	6.81	109.79	106.68
17	4	317	CLA	C4A-NA-C1A	6.81	109.78	106.68
17	4	318	CLA	C4A-NA-C1A	6.81	109.78	106.68
17	b	810	CLA	C4A-NA-C1A	6.79	109.78	106.68
17	f	802	CLA	C4A-NA-C1A	6.79	109.78	106.68
17	a	805	CLA	C4A-NA-C1A	6.78	109.77	106.68
17	b	825	CLA	C4A-NA-C1A	6.78	109.77	106.68
17	b	822	CLA	C4A-NA-C1A	6.77	109.77	106.68
15	j	101	XAT	C38-C25-C26	-6.76	111.17	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	815	CLA	C4A-NA-C1A	6.76	109.76	106.68
17	b	828	CLA	C4A-NA-C1A	6.76	109.76	106.68
17	b	806	CLA	C4A-NA-C1A	6.75	109.76	106.68
17	a	842	CLA	C4A-NA-C1A	6.75	109.76	106.68
15	4	303	XAT	C38-C25-C24	6.75	121.82	114.24
17	a	817	CLA	C4A-NA-C1A	6.74	109.75	106.68
23	i	101	BCR	C24-C23-C22	-6.74	116.27	126.23
17	a	809	CLA	C4A-NA-C1A	6.72	109.75	106.68
15	5	302	XAT	C18-C5-C6	-6.71	111.26	122.30
17	b	811	CLA	C4A-NA-C1A	6.69	109.73	106.68
17	l	202	CLA	C4A-NA-C1A	6.69	109.73	106.68
17	a	831	CLA	C4A-NA-C1A	6.69	109.73	106.68
23	a	850	BCR	C24-C23-C22	-6.69	116.34	126.23
17	5	306	CLA	C4A-NA-C1A	6.68	109.73	106.68
17	a	839	CLA	C4A-NA-C1A	6.68	109.73	106.68
17	b	833	CLA	C4A-NA-C1A	6.68	109.73	106.68
15	4	304	XAT	C18-C5-C6	-6.67	111.32	122.30
17	5	310	CLA	C4A-NA-C1A	6.67	109.72	106.68
17	b	807	CLA	C4A-NA-C1A	6.67	109.72	106.68
17	b	813	CLA	C4A-NA-C1A	6.67	109.72	106.68
15	4	301	XAT	C18-C5-C6	-6.67	111.33	122.30
17	b	837	CLA	C4A-NA-C1A	6.66	109.72	106.68
15	4	302	XAT	C18-C5-C4	6.66	121.72	114.24
17	a	807	CLA	C4A-NA-C1A	6.66	109.72	106.68
15	5	304	XAT	C38-C25-C26	-6.65	111.35	122.30
17	b	801	CLA	C4A-NA-C1A	6.65	109.72	106.68
17	b	819	CLA	C4A-NA-C1A	6.65	109.72	106.68
17	5	311	CLA	C4A-NA-C1A	6.65	109.71	106.68
17	1	308	CLA	C4A-NA-C1A	6.65	109.71	106.68
15	4	304	XAT	C38-C25-C26	-6.64	111.37	122.30
17	a	825	CLA	C4A-NA-C1A	6.64	109.71	106.68
17	4	312	CLA	C4A-NA-C1A	6.64	109.71	106.68
17	f	803	CLA	C4A-NA-C1A	6.63	109.70	106.68
17	a	854	CLA	C4A-NA-C1A	6.63	109.70	106.68
15	4	301	XAT	C31-C30-C29	-6.62	117.99	127.28
17	4	308	CLA	C4A-NA-C1A	6.62	109.70	106.68
17	a	838	CLA	C4A-NA-C1A	6.61	109.70	106.68
17	a	811	CLA	C4A-NA-C1A	6.60	109.69	106.68
15	5	301	XAT	C38-C25-C24	6.60	121.66	114.24
17	5	313	CLA	C4A-NA-C1A	6.60	109.69	106.68
17	a	829	CLA	C4A-NA-C1A	6.60	109.69	106.68
17	a	841	CLA	C4A-NA-C1A	6.60	109.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	837	CLA	C4A-NA-C1A	6.59	109.69	106.68
17	4	316	CLA	C4A-NA-C1A	6.59	109.69	106.68
17	a	834	CLA	C4A-NA-C1A	6.58	109.68	106.68
17	a	840	CLA	C4A-NA-C1A	6.58	109.68	106.68
17	j	102	CLA	C4A-NA-C1A	6.58	109.68	106.68
15	4	301	XAT	C18-C5-C4	6.58	121.63	114.24
17	5	308	CLA	C4A-NA-C1A	6.57	109.68	106.68
17	a	804	CLA	C4A-NA-C1A	6.57	109.67	106.68
17	b	816	CLA	C4A-NA-C1A	6.57	109.67	106.68
17	l	204	CLA	C4A-NA-C1A	6.56	109.67	106.68
17	a	827	CLA	C4A-NA-C1A	6.56	109.67	106.68
15	1	302	XAT	C38-C25-C26	-6.55	111.52	122.30
17	b	808	CLA	C4A-NA-C1A	6.55	109.67	106.68
17	5	312	CLA	C4A-NA-C1A	6.55	109.67	106.68
15	j	101	XAT	C18-C5-C6	-6.54	111.53	122.30
17	5	314	CLA	C4A-NA-C1A	6.54	109.66	106.68
15	4	303	XAT	C18-C5-C4	6.54	121.59	114.24
17	a	812	CLA	C4A-NA-C1A	6.53	109.66	106.68
17	4	315	CLA	C4A-NA-C1A	6.53	109.66	106.68
15	4	302	XAT	C18-C5-C6	-6.52	111.56	122.30
17	1	305	CLA	C4A-NA-C1A	6.51	109.65	106.68
17	a	844	CLA	C4A-NA-C1A	6.51	109.65	106.68
17	b	839	CLA	C4A-NA-C1A	6.50	109.64	106.68
17	a	830	CLA	C4A-NA-C1A	6.50	109.64	106.68
17	b	836	CLA	C4A-NA-C1A	6.50	109.64	106.68
15	4	303	XAT	C18-C5-C6	-6.50	111.61	122.30
17	b	827	CLA	C4A-NA-C1A	6.49	109.64	106.68
17	a	832	CLA	C4A-NA-C1A	6.48	109.64	106.68
17	b	823	CLA	C4A-NA-C1A	6.47	109.63	106.68
17	1	307	CLA	C4A-NA-C1A	6.47	109.63	106.68
17	a	814	CLA	C4A-NA-C1A	6.47	109.63	106.68
17	a	836	CLA	C4A-NA-C1A	6.46	109.63	106.68
17	a	808	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	1	302	XAT	C18-C5-C6	-6.45	111.69	122.30
17	i	102	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	4	305	XAT	C18-C5-C6	-6.44	111.69	122.30
15	4	302	XAT	C38-C25-C26	-6.43	111.71	122.30
17	4	313	CLA	C4A-NA-C1A	6.43	109.61	106.68
17	a	824	CLA	C4A-NA-C1A	6.43	109.61	106.68
15	4	306	XAT	C18-C5-C6	-6.42	111.73	122.30
17	b	824	CLA	C4A-NA-C1A	6.42	109.61	106.68
17	4	307	CLA	C4A-NA-C1A	6.42	109.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	303	XAT	C18-C5-C6	-6.42	111.74	122.30
15	j	101	XAT	C18-C5-C4	6.41	121.44	114.24
15	4	303	XAT	C38-C25-C26	-6.40	111.77	122.30
17	1	313	CLA	C4A-NA-C1A	6.40	109.60	106.68
15	4	306	XAT	C31-C30-C29	-6.39	118.31	127.28
15	5	302	XAT	C26-C27-C28	-6.39	112.48	125.99
17	b	834	CLA	C4A-NA-C1A	6.39	109.59	106.68
15	4	305	XAT	C38-C25-C26	-6.39	111.78	122.30
15	a	852	XAT	C38-C25-C26	-6.39	111.79	122.30
17	b	832	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	1	303	XAT	C38-C25-C26	-6.38	111.80	122.30
17	b	835	CLA	C4A-NA-C1A	6.38	109.59	106.68
15	5	301	XAT	C18-C5-C6	-6.37	111.82	122.30
17	1	312	CLA	C4A-NA-C1A	6.37	109.58	106.68
17	a	822	CLA	C4A-NA-C1A	6.37	109.58	106.68
17	b	814	CLA	C4A-NA-C1A	6.37	109.58	106.68
17	5	315	CLA	C4A-NA-C1A	6.35	109.58	106.68
23	i	101	BCR	C20-C21-C22	-6.35	118.38	127.28
17	1	310	CLA	C4A-NA-C1A	6.34	109.57	106.68
17	b	826	CLA	C4A-NA-C1A	6.34	109.57	106.68
17	a	816	CLA	C4A-NA-C1A	6.34	109.57	106.68
17	4	310	CLA	C4A-NA-C1A	6.33	109.57	106.68
17	a	818	CLA	C4A-NA-C1A	6.33	109.57	106.68
15	4	304	XAT	C18-C5-C4	6.33	121.35	114.24
15	1	302	XAT	C18-C5-C4	6.33	121.35	114.24
17	a	815	CLA	C4A-NA-C1A	6.31	109.56	106.68
17	1	311	CLA	C4A-NA-C1A	6.31	109.56	106.68
17	4	309	CLA	C4A-NA-C1A	6.30	109.56	106.68
17	a	813	CLA	C4A-NA-C1A	6.30	109.55	106.68
17	5	309	CLA	C4A-NA-C1A	6.29	109.55	106.68
17	a	819	CLA	C4A-NA-C1A	6.28	109.55	106.68
17	5	307	CLA	C4A-NA-C1A	6.26	109.53	106.68
15	4	305	XAT	C18-C5-C4	6.25	121.26	114.24
17	b	820	CLA	C4A-NA-C1A	6.25	109.53	106.68
17	5	305	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	1	303	XAT	C18-C5-C4	6.23	121.24	114.24
17	1	314	CLA	C4A-NA-C1A	6.23	109.52	106.68
15	5	302	XAT	C38-C25-C24	6.22	121.23	114.24
15	4	302	XAT	C38-C25-C24	6.22	121.22	114.24
17	a	820	CLA	C4A-NA-C1A	6.21	109.51	106.68
17	1	309	CLA	C4A-NA-C1A	6.20	109.51	106.68
17	b	804	CLA	C4A-NA-C1A	6.19	109.50	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	802	CLA	C4A-NA-C1A	6.19	109.50	106.68
17	b	812	CLA	C4A-NA-C1A	6.14	109.48	106.68
17	b	841	CLA	C4A-NA-C1A	6.10	109.46	106.68
17	b	838	CLA	C4A-NA-C1A	6.09	109.46	106.68
15	a	852	XAT	C26-C27-C28	-6.09	113.11	125.99
15	4	306	XAT	C18-C5-C4	6.08	121.07	114.24
17	b	830	CLA	C4A-NA-C1A	6.08	109.45	106.68
17	4	314	CLA	C4A-NA-C1A	6.06	109.44	106.68
17	b	818	CLA	C4A-NA-C1A	6.06	109.44	106.68
20	1	304	A1L1F	O15-C20-C17	6.06	121.82	115.05
23	b	843	BCR	C7-C8-C9	-6.03	117.31	126.23
17	b	817	CLA	C4A-NA-C1A	6.02	109.43	106.68
17	b	829	CLA	C4A-NA-C1A	6.00	109.42	106.68
15	5	302	XAT	C38-C25-C26	-5.93	112.54	122.30
15	5	304	XAT	C26-C27-C28	-5.93	113.46	125.99
15	5	302	XAT	C18-C5-C4	5.92	120.89	114.24
17	b	802	CLA	C4A-NA-C1A	5.91	109.37	106.68
23	b	852	BCR	C16-C17-C18	-5.90	119.00	127.28
15	5	301	XAT	C18-C5-C4	5.89	120.86	114.24
15	j	101	XAT	C6-C7-C8	-5.86	113.61	125.99
17	b	831	CLA	C4A-NA-C1A	5.82	109.34	106.68
23	a	850	BCR	C20-C21-C22	-5.80	119.14	127.28
15	4	301	XAT	C35-C34-C33	-5.79	119.16	127.28
15	4	301	XAT	C38-C25-C24	5.77	120.72	114.24
15	5	302	XAT	C11-C10-C9	-5.75	119.22	127.28
23	b	843	BCR	C11-C10-C9	-5.73	119.24	127.28
20	1	304	A1L1F	O15-C20-C21	5.73	118.86	113.49
23	b	845	BCR	C24-C23-C22	-5.72	117.78	126.23
23	f	801	BCR	C16-C17-C18	-5.71	119.27	127.28
23	b	845	BCR	C7-C8-C9	-5.66	117.86	126.23
23	b	847	BCR	C16-C17-C18	-5.54	119.51	127.28
23	f	801	BCR	C20-C21-C22	-5.49	119.58	127.28
23	f	804	BCR	C15-C14-C13	-5.47	119.61	127.28
23	j	104	BCR	C28-C27-C26	-5.47	104.31	114.06
15	4	301	XAT	C38-C25-C26	-5.46	113.31	122.30
23	b	845	BCR	C33-C5-C6	-5.45	118.53	124.48
15	4	302	XAT	C6-C7-C8	-5.44	114.50	125.99
15	a	852	XAT	C18-C5-C6	-5.40	113.41	122.30
17	a	803	CLA	C4A-NA-C1A	5.38	109.13	106.68
23	b	843	BCR	C15-C14-C13	-5.35	119.78	127.28
15	4	306	XAT	C15-C14-C13	-5.35	119.78	127.28
23	l	201	BCR	C7-C8-C9	-5.32	118.37	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	304	XAT	C26-C27-C28	-5.29	114.80	125.99
19	b	851	DGD	O2G-C1B-C2B	5.29	122.93	111.48
23	a	849	BCR	C3-C4-C5	-5.29	104.62	114.06
23	b	843	BCR	C3-C4-C5	-5.29	104.63	114.06
23	l	205	BCR	C24-C23-C22	-5.28	118.42	126.23
15	a	852	XAT	C6-C7-C8	-5.26	114.88	125.99
15	4	305	XAT	C26-C27-C28	-5.24	114.91	125.99
15	a	852	XAT	C18-C5-C4	5.23	120.12	114.24
15	j	101	XAT	C26-C27-C28	-5.17	115.06	125.99
15	l	302	XAT	C35-C34-C33	-5.13	120.08	127.28
23	b	846	BCR	C3-C4-C5	-5.10	104.95	114.06
23	a	847	BCR	C16-C17-C18	-5.05	120.19	127.28
23	b	852	BCR	C11-C10-C9	-5.05	120.19	127.28
23	f	804	BCR	C11-C10-C9	-5.01	120.25	127.28
23	b	852	BCR	C20-C21-C22	-5.01	120.25	127.28
15	5	301	XAT	C26-C27-C28	-5.00	115.41	125.99
23	a	850	BCR	C16-C17-C18	-5.00	120.27	127.28
15	4	305	XAT	C6-C7-C8	-4.99	115.44	125.99
15	l	302	XAT	C26-C27-C28	-4.97	115.49	125.99
23	a	849	BCR	C16-C17-C18	-4.96	120.31	127.28
15	4	304	XAT	C11-C10-C9	-4.94	120.36	127.28
23	j	104	BCR	C11-C10-C9	-4.91	120.40	127.28
15	l	303	XAT	C6-C7-C8	-4.90	115.62	125.99
23	b	852	BCR	C38-C26-C25	-4.89	119.14	124.48
23	l	205	BCR	C15-C14-C13	-4.89	120.42	127.28
15	j	101	XAT	C11-C10-C9	-4.87	120.44	127.28
15	5	302	XAT	C15-C14-C13	-4.87	120.45	127.28
23	i	101	BCR	C16-C17-C18	-4.86	120.46	127.28
15	5	304	XAT	C15-C14-C13	-4.85	120.47	127.28
23	b	852	BCR	C7-C8-C9	-4.78	119.17	126.23
15	l	302	XAT	C6-C7-C8	-4.78	115.89	125.99
23	b	850	BCR	C16-C17-C18	-4.77	120.59	127.28
15	4	303	XAT	C26-C27-C28	-4.74	115.98	125.99
15	4	303	XAT	C6-C7-C8	-4.69	116.08	125.99
15	4	303	XAT	C35-C34-C33	-4.67	120.73	127.28
23	b	848	BCR	C16-C17-C18	-4.66	120.75	127.28
23	b	844	BCR	C11-C10-C9	-4.65	120.76	127.28
15	5	301	XAT	C35-C34-C33	-4.58	120.86	127.28
23	b	844	BCR	C7-C8-C9	-4.57	119.47	126.23
15	4	306	XAT	C26-C27-C28	-4.53	116.42	125.99
23	a	848	BCR	C16-C17-C18	-4.50	120.97	127.28
23	b	845	BCR	C16-C17-C18	-4.45	121.03	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	848	BCR	C15-C14-C13	-4.45	121.04	127.28
23	a	849	BCR	C15-C14-C13	-4.45	121.04	127.28
23	a	850	BCR	C15-C14-C13	-4.44	121.05	127.28
23	j	104	BCR	C15-C14-C13	-4.43	121.07	127.28
23	b	848	BCR	C33-C5-C6	-4.42	119.66	124.48
23	j	104	BCR	C16-C17-C18	-4.40	121.11	127.28
19	4	319	DGD	O6E-C5E-C6E	4.39	117.31	106.44
15	j	101	XAT	C35-C34-C33	-4.39	121.13	127.28
15	5	304	XAT	C35-C34-C33	-4.38	121.13	127.28
23	b	843	BCR	C16-C17-C18	-4.37	121.14	127.28
15	4	302	XAT	C15-C14-C13	-4.33	121.21	127.28
20	1	304	A1L1F	O7-C54-C56	4.32	118.79	111.09
23	j	104	BCR	C7-C8-C9	-4.30	119.87	126.23
23	f	804	BCR	C24-C23-C22	-4.28	119.90	126.23
15	4	305	XAT	C35-C34-C33	-4.27	121.28	127.28
15	4	301	XAT	C6-C7-C8	-4.27	116.96	125.99
23	a	850	BCR	C38-C26-C25	-4.26	119.83	124.48
23	b	845	BCR	C15-C14-C13	-4.26	121.31	127.28
20	1	304	A1L1F	C37-C38-C39	-4.25	121.32	127.28
23	b	847	BCR	C24-C23-C22	-4.24	119.96	126.23
19	4	319	DGD	O2G-C1B-C2B	4.24	120.65	111.48
23	b	850	BCR	C33-C5-C6	-4.24	119.86	124.48
23	l	201	BCR	C33-C5-C6	-4.23	119.87	124.48
15	4	306	XAT	C35-C34-C33	-4.23	121.35	127.28
23	b	844	BCR	C15-C14-C13	-4.23	121.35	127.28
23	b	846	BCR	C16-C17-C18	-4.22	121.36	127.28
23	l	201	BCR	C15-C14-C13	-4.22	121.36	127.28
23	l	205	BCR	C20-C21-C22	-4.20	121.39	127.28
22	a	845	LHG	O7-C7-C8	4.19	120.55	111.48
23	f	804	BCR	C7-C8-C9	-4.18	120.04	126.23
23	b	847	BCR	C20-C21-C22	-4.18	121.41	127.28
23	a	848	BCR	C11-C10-C9	-4.18	121.42	127.28
23	b	847	BCR	C7-C8-C9	-4.17	120.07	126.23
23	a	847	BCR	C38-C26-C25	-4.16	119.94	124.48
20	1	304	A1L1F	C17-C20-C21	4.15	118.91	114.24
15	5	301	XAT	C11-C10-C9	-4.13	121.49	127.28
21	b	842	PQN	C11-C12-C13	-4.12	119.72	126.83
23	l	205	BCR	C38-C26-C25	-4.12	119.98	124.48
22	b	849	LHG	O7-C7-C8	4.11	120.38	111.48
25	a	853	LMG	O7-C10-C11	4.10	120.36	111.48
15	4	301	XAT	C15-C14-C13	-4.10	121.53	127.28
23	b	847	BCR	C16-C15-C14	-4.09	115.16	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	f	801	BCR	C3-C4-C5	-4.07	106.79	114.06
23	b	843	BCR	C28-C27-C26	-4.04	106.84	114.06
15	4	302	XAT	C35-C34-C33	-4.03	121.63	127.28
15	4	306	XAT	C6-C7-C8	-4.02	117.50	125.99
23	b	847	BCR	C15-C14-C13	-4.02	121.65	127.28
23	f	804	BCR	C33-C5-C6	-4.01	120.11	124.48
15	4	306	XAT	C11-C10-C9	-4.00	121.66	127.28
23	f	804	BCR	C38-C26-C25	-4.00	120.12	124.48
23	b	847	BCR	C28-C27-C26	-3.99	106.93	114.06
23	i	101	BCR	C7-C8-C9	-3.99	120.33	126.23
23	l	201	BCR	C11-C10-C9	-3.99	121.69	127.28
17	b	804	CLA	O2D-CGD-O1D	-3.97	116.13	123.85
22	a	846	LHG	O7-C7-C8	3.97	120.06	111.48
15	a	852	XAT	C31-C30-C29	-3.96	121.73	127.28
25	j	105	LMG	O7-C10-C11	3.95	120.04	111.48
22	m	101	LHG	O7-C7-C8	3.95	120.03	111.48
15	4	304	XAT	C15-C14-C13	-3.94	121.75	127.28
23	a	847	BCR	C20-C21-C22	-3.92	121.77	127.28
15	1	303	XAT	C26-C27-C28	-3.92	117.72	125.99
15	j	101	XAT	C15-C14-C13	-3.90	121.81	127.28
23	b	848	BCR	C15-C14-C13	-3.89	121.82	127.28
23	l	201	BCR	C16-C17-C18	-3.88	121.83	127.28
23	l	205	BCR	C33-C5-C6	-3.87	120.26	124.48
23	f	804	BCR	C20-C21-C22	-3.87	121.85	127.28
23	l	205	BCR	C16-C17-C18	-3.86	121.87	127.28
16	1	301	A1L1G	C37-C36-C35	3.83	131.36	123.52
23	f	804	BCR	C16-C17-C18	-3.83	121.91	127.28
23	a	850	BCR	C33-C5-C6	-3.82	120.31	124.48
15	5	301	XAT	C15-C14-C13	-3.82	121.92	127.28
23	j	104	BCR	C20-C21-C22	-3.81	121.93	127.28
23	f	801	BCR	C16-C15-C14	-3.81	115.72	123.52
19	b	851	DGD	O5D-C6D-C5D	-3.80	100.85	109.42
15	1	303	XAT	C35-C34-C33	-3.79	121.97	127.28
23	b	846	BCR	C15-C14-C13	-3.78	121.98	127.28
23	a	849	BCR	C28-C27-C26	-3.76	107.35	114.06
15	4	302	XAT	C31-C30-C29	-3.76	122.01	127.28
23	a	849	BCR	C20-C21-C22	-3.74	122.03	127.28
18	1	315	SQD	O47-C7-C8	3.74	119.57	111.48
17	a	806	CLA	O2D-CGD-O1D	-3.74	116.57	123.85
23	a	849	BCR	C4-C5-C6	-3.74	117.65	122.70
16	5	303	A1L1G	C36-C37-C38	3.73	131.15	123.52
15	a	852	XAT	C35-C34-C33	-3.73	122.05	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	302	XAT	C26-C27-C28	-3.71	118.16	125.99
23	b	844	BCR	C3-C4-C5	-3.69	107.47	114.06
23	a	847	BCR	C33-C5-C6	-3.69	120.45	124.48
23	b	850	BCR	C7-C8-C9	-3.67	120.81	126.23
23	b	847	BCR	C3-C4-C5	-3.64	107.57	114.06
15	4	303	XAT	C35-C15-C14	-3.64	116.08	123.52
23	a	847	BCR	C7-C8-C9	-3.63	120.87	126.23
23	b	847	BCR	C10-C11-C12	-3.61	112.74	123.20
23	a	849	BCR	C11-C10-C9	-3.60	122.22	127.28
23	b	844	BCR	C33-C5-C6	-3.60	120.56	124.48
15	j	101	XAT	C10-C11-C12	-3.59	112.80	123.20
17	a	806	CLA	CAA-CBA-CGA	-3.59	103.01	113.21
15	1	302	XAT	C11-C10-C9	-3.58	122.25	127.28
15	4	303	XAT	C11-C10-C9	-3.57	122.27	127.28
23	b	846	BCR	C24-C23-C22	-3.57	120.96	126.23
23	i	101	BCR	C33-C5-C6	-3.57	120.59	124.48
23	a	847	BCR	C15-C14-C13	-3.56	122.29	127.28
15	4	304	XAT	C35-C34-C33	-3.56	122.29	127.28
23	l	205	BCR	C11-C10-C9	-3.55	122.30	127.28
23	b	850	BCR	C38-C26-C25	-3.55	120.61	124.48
23	a	848	BCR	C24-C23-C22	-3.54	121.00	126.23
23	l	205	BCR	C3-C4-C5	-3.54	107.74	114.06
20	1	304	AIL1F	C8-O7-C54	-3.54	111.60	117.85
17	a	806	CLA	C3B-C4B-NB	-3.54	107.37	110.53
23	a	849	BCR	C7-C8-C9	-3.52	121.03	126.23
18	5	316	SQD	O47-C7-C8	3.51	119.07	111.48
15	1	303	XAT	C15-C14-C13	-3.50	122.37	127.28
23	a	848	BCR	C20-C21-C22	-3.50	122.37	127.28
15	1	303	XAT	C24-C23-C22	-3.50	104.25	110.79
23	a	847	BCR	C24-C23-C22	-3.48	121.09	126.23
17	b	804	CLA	CHB-C4A-NA	3.47	129.41	124.40
15	a	852	XAT	C10-C11-C12	-3.46	113.17	123.20
23	a	849	BCR	C24-C23-C22	-3.46	121.11	126.23
23	i	101	BCR	C28-C27-C26	-3.46	107.89	114.06
23	a	847	BCR	C11-C10-C9	-3.43	122.47	127.28
15	5	302	XAT	C6-C7-C8	-3.42	118.76	125.99
15	5	301	XAT	C7-C8-C9	-3.40	120.26	125.53
19	b	851	DGD	C2G-O2G-C1B	-3.38	109.71	117.80
15	5	304	XAT	C24-C23-C22	-3.37	104.48	110.79
23	i	101	BCR	C15-C14-C13	-3.37	122.55	127.28
15	5	304	XAT	C4-C3-C2	-3.37	104.49	110.79
23	b	848	BCR	C10-C11-C12	-3.37	113.43	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	850	BCR	C11-C10-C9	-3.36	122.56	127.28
16	5	303	A1L1G	C37-C36-C35	3.36	130.39	123.52
15	5	301	XAT	C24-C23-C22	-3.36	104.52	110.79
15	5	301	XAT	C6-C7-C8	-3.35	118.91	125.99
17	5	312	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
23	a	847	BCR	C3-C4-C5	-3.35	108.09	114.06
15	4	301	XAT	C11-C10-C9	-3.34	122.59	127.28
15	1	303	XAT	C31-C30-C29	-3.34	122.60	127.28
23	j	104	BCR	C24-C23-C22	-3.32	121.32	126.23
20	1	304	A1L1F	C14-C29-C30	-3.32	119.82	125.47
23	i	101	BCR	C11-C10-C9	-3.30	122.65	127.28
23	a	850	BCR	C7-C8-C9	-3.30	121.36	126.23
16	1	301	A1L1G	C36-C37-C38	3.29	130.25	123.52
15	4	304	XAT	C6-C7-C8	-3.29	119.04	125.99
23	a	848	BCR	C33-C5-C6	-3.27	120.91	124.48
17	b	809	CLA	O2A-CGA-O1A	-3.27	115.45	123.63
15	a	852	XAT	C11-C10-C9	-3.27	122.69	127.28
15	4	304	XAT	C24-C23-C22	-3.26	104.69	110.79
23	b	852	BCR	C24-C23-C22	-3.25	121.42	126.23
15	4	305	XAT	C24-C23-C22	-3.25	104.72	110.79
17	j	103	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
15	1	302	XAT	C15-C14-C13	-3.24	122.74	127.28
23	b	846	BCR	C20-C21-C22	-3.24	122.74	127.28
23	l	201	BCR	C24-C23-C22	-3.23	121.45	126.23
15	4	305	XAT	C15-C14-C13	-3.23	122.74	127.28
17	b	821	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
17	b	804	CLA	C3B-C4B-NB	-3.23	107.65	110.53
23	l	201	BCR	C38-C26-C25	-3.23	120.97	124.48
23	a	848	BCR	C38-C26-C25	-3.22	120.97	124.48
21	a	843	PQN	C14-C13-C15	3.22	120.82	115.23
19	4	319	DGD	O1G-C1A-C2A	3.22	121.65	111.83
23	a	850	BCR	C11-C10-C9	-3.22	122.77	127.28
17	b	831	CLA	C3B-C4B-NB	-3.21	107.66	110.53
23	a	849	BCR	C38-C26-C25	-3.21	120.98	124.48
17	1	313	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
17	a	835	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
17	a	804	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
17	b	818	CLA	C3B-C4B-NB	-3.16	107.71	110.53
23	a	848	BCR	C3-C4-C5	-3.15	108.44	114.06
17	a	818	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
15	4	306	XAT	C24-C23-C22	-3.15	104.91	110.79
23	b	846	BCR	C38-C26-C25	-3.13	121.07	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	852	BCR	C33-C5-C6	-3.13	121.07	124.48
23	l	205	BCR	C8-C7-C6	-3.13	118.63	127.00
15	4	304	XAT	C30-C31-C32	-3.13	114.13	123.20
23	b	844	BCR	C16-C17-C18	-3.13	122.89	127.28
17	b	833	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
23	a	848	BCR	C8-C7-C6	-3.12	118.66	127.00
15	5	301	XAT	C31-C30-C29	-3.12	122.91	127.28
23	f	801	BCR	C8-C7-C6	-3.11	118.68	127.00
17	4	317	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
23	b	847	BCR	C11-C10-C9	-3.11	122.92	127.28
17	4	312	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
15	4	305	XAT	C35-C15-C14	-3.09	117.19	123.52
15	a	852	XAT	C35-C15-C14	-3.09	117.20	123.52
15	a	852	XAT	C31-C32-C33	-3.08	117.91	126.36
17	b	809	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
16	5	303	A1L1G	C40-C39-C38	3.08	123.85	119.01
15	1	302	XAT	C31-C30-C29	-3.07	122.97	127.28
17	a	819	CLA	C3B-C4B-NB	-3.07	107.79	110.53
17	a	807	CLA	C3B-C4B-NB	-3.07	107.79	110.53
17	i	102	CLA	C3B-C4B-NB	-3.07	107.79	110.53
16	1	301	A1L1G	C33-C34-C35	3.06	123.83	119.01
23	b	846	BCR	C4-C5-C6	-3.06	118.56	122.70
17	a	809	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	b	843	BCR	C20-C21-C22	-3.06	122.99	127.28
23	b	850	BCR	C15-C14-C13	-3.05	123.00	127.28
17	4	313	CLA	C3B-C4B-NB	-3.05	107.81	110.53
17	a	832	CLA	C3B-C4B-NB	-3.05	107.81	110.53
17	a	831	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
16	1	301	A1L1G	C40-C39-C38	3.05	123.80	119.01
22	a	846	LHG	O8-C23-C24	3.05	120.39	111.15
17	4	308	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
17	b	817	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
15	4	305	XAT	C4-C3-C2	-3.04	105.10	110.79
15	5	302	XAT	C24-C23-C22	-3.04	105.10	110.79
15	4	302	XAT	C4-C3-C2	-3.04	105.11	110.79
23	b	850	BCR	C16-C15-C14	-3.04	117.31	123.52
17	a	818	CLA	C3B-C4B-NB	-3.03	107.82	110.53
23	b	848	BCR	C8-C7-C6	-3.02	118.94	127.00
17	4	310	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
23	b	844	BCR	C38-C26-C25	-3.01	121.20	124.48
17	b	837	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
23	b	846	BCR	C8-C7-C6	-3.00	118.97	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	848	BCR	C21-C20-C19	-3.00	114.50	123.20
17	a	830	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
17	b	812	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
17	b	825	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
17	b	808	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
17	a	813	CLA	C3B-C4B-NB	-2.99	107.86	110.53
21	b	842	PQN	C16-C15-C13	-2.99	106.19	113.47
17	a	854	CLA	C3B-C4B-NB	-2.99	107.86	110.53
17	b	835	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
17	1	314	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	4	303	XAT	C24-C23-C22	-2.99	105.21	110.79
17	a	820	CLA	C1-C2-C3	-2.99	121.31	126.20
17	f	803	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	a	802	CLA	C3B-C4B-NB	-2.98	107.87	110.53
15	1	302	XAT	C4-C3-C2	-2.98	105.22	110.79
15	4	301	XAT	C31-C32-C33	-2.97	118.21	126.36
17	a	840	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
17	a	839	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
17	a	822	CLA	C3B-C4B-NB	-2.97	107.88	110.53
16	5	303	A1L1G	C28-C39-C38	-2.97	118.00	122.82
17	b	818	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
23	b	844	BCR	C21-C20-C19	-2.97	114.60	123.20
17	1	311	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
17	b	815	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
17	b	830	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
17	4	316	CLA	C3B-C4B-NB	-2.97	107.88	110.53
23	a	850	BCR	C28-C27-C26	-2.96	108.77	114.06
15	1	302	XAT	C35-C15-C14	-2.96	117.46	123.52
17	b	840	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
23	b	843	BCR	C4-C5-C6	-2.95	118.71	122.70
15	4	301	XAT	C4-C3-C2	-2.95	105.26	110.79
17	b	815	CLA	CHB-C4A-NA	2.95	128.66	124.40
17	a	841	CLA	C3B-C4B-NB	-2.95	107.90	110.53
23	f	801	BCR	C20-C19-C18	-2.95	118.28	126.36
17	a	808	CLA	C3B-C4B-NB	-2.95	107.90	110.53
23	b	852	BCR	C16-C15-C14	-2.95	117.49	123.52
23	b	850	BCR	C23-C24-C25	-2.95	119.13	127.00
15	a	852	XAT	C24-C23-C22	-2.94	105.28	110.79
17	a	812	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	1	302	XAT	C24-C23-C22	-2.94	105.29	110.79
17	a	842	CLA	C3B-C4B-NB	-2.94	107.91	110.53
17	b	819	CLA	O2D-CGD-O1D	-2.94	118.12	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	302	XAT	C10-C11-C12	-2.94	114.68	123.20
19	b	851	DGD	O3E-C3E-C2E	-2.94	103.45	110.38
17	1	314	CLA	C3B-C4B-NB	-2.94	107.91	110.53
23	a	848	BCR	C7-C8-C9	-2.94	121.89	126.23
15	4	303	XAT	C4-C3-C2	-2.93	105.30	110.79
23	b	847	BCR	C33-C5-C6	-2.93	121.28	124.48
23	f	801	BCR	C33-C5-C6	-2.93	121.28	124.48
17	a	804	CLA	C1-C2-C3	-2.93	121.39	126.20
17	4	318	CLA	C3B-C4B-NB	-2.93	107.92	110.53
23	a	849	BCR	C2-C1-C6	2.93	114.69	110.44
17	b	839	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	4	315	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	a	836	CLA	C3B-C4B-NB	-2.92	107.92	110.53
15	j	101	XAT	C4-C3-C2	-2.92	105.33	110.79
17	4	309	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	5	312	CLA	O2D-CGD-CBD	2.92	116.33	111.23
17	1	310	CLA	C3B-C4B-NB	-2.92	107.93	110.53
17	j	102	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	a	817	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
16	5	303	A1L1G	C33-C34-C35	2.91	123.59	119.01
15	1	303	XAT	C4-C3-C2	-2.91	105.34	110.79
15	5	304	XAT	C19-C9-C8	2.91	122.54	118.09
17	1	312	CLA	C3B-C4B-NB	-2.91	107.93	110.53
17	a	828	CLA	C3B-C4B-NB	-2.91	107.93	110.53
15	1	303	XAT	C10-C11-C12	-2.91	114.77	123.20
20	1	304	A1L1F	C26-O13-C45	2.91	121.74	115.64
17	b	806	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
17	a	813	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
17	b	827	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
17	b	809	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	b	805	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
16	1	301	A1L1G	C28-C39-C38	-2.90	118.12	122.82
23	b	845	BCR	C38-C26-C25	-2.89	121.33	124.48
17	5	315	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
17	a	820	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
17	j	102	CLA	C3B-C4B-NB	-2.89	107.95	110.53
15	5	302	XAT	C35-C34-C33	-2.89	123.23	127.28
16	1	301	A1L1G	C27-C34-C35	-2.89	118.14	122.82
17	a	837	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
17	a	833	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	l	202	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
17	a	827	CLA	O2D-CGD-O1D	-2.88	118.24	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	307	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
17	5	307	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	5	305	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	5	309	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	b	824	CLA	C3B-C4B-NB	-2.88	107.96	110.53
23	b	848	BCR	C15-C16-C17	-2.88	117.63	123.52
23	i	101	BCR	C29-C30-C25	2.88	114.62	110.44
17	a	825	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
17	4	313	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
17	a	811	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
17	a	833	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
19	b	851	DGD	O1G-C1A-C2A	2.87	120.59	111.83
17	1	312	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
17	a	834	CLA	C3B-C4B-NB	-2.87	107.97	110.53
17	5	309	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
17	b	838	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
17	b	820	CLA	C3B-C4B-NB	-2.87	107.97	110.53
17	4	317	CLA	C3B-C4B-NB	-2.87	107.97	110.53
17	a	817	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	b	846	BCR	C10-C11-C12	-2.86	114.90	123.20
17	4	312	CLA	C3B-C4B-NB	-2.86	107.97	110.53
15	5	304	XAT	C10-C11-C12	-2.86	114.91	123.20
17	b	817	CLA	C3B-C4B-NB	-2.86	107.98	110.53
19	4	319	DGD	O5E-C6E-C5E	-2.86	101.61	111.33
17	a	823	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
17	a	825	CLA	C3B-C4B-NB	-2.85	107.98	110.53
17	1	305	CLA	C3B-C4B-NB	-2.85	107.98	110.53
17	b	814	CLA	C3B-C4B-NB	-2.85	107.98	110.53
17	5	310	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	4	306	XAT	C4-C3-C2	-2.85	105.46	110.79
17	b	839	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	a	831	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
17	a	815	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
17	4	308	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	b	829	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
25	a	853	LMG	O8-C28-C29	2.84	120.48	111.83
17	a	832	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
17	a	826	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
23	f	801	BCR	C10-C11-C12	-2.83	114.99	123.20
17	1	313	CLA	C3B-C4B-NB	-2.83	108.00	110.53
23	b	843	BCR	C2-C1-C6	2.83	114.55	110.44
17	1	310	CLA	O2D-CGD-O1D	-2.83	118.35	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	304	A1L1F	C36-C35-C34	-2.83	123.31	127.28
16	5	303	A1L1G	C27-C34-C35	-2.83	118.24	122.82
17	a	816	CLA	C3B-C4B-NB	-2.82	108.01	110.53
17	b	801	CLA	C3B-C4B-NB	-2.82	108.01	110.53
15	4	305	XAT	C11-C10-C9	-2.82	123.32	127.28
17	b	813	CLA	C3B-C4B-NB	-2.82	108.01	110.53
17	a	816	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	4	303	XAT	C31-C30-C29	-2.82	123.33	127.28
17	b	835	CLA	C3B-C4B-NB	-2.82	108.02	110.53
17	b	805	CLA	C3B-C4B-NB	-2.81	108.02	110.53
17	b	816	CLA	C3B-C4B-NB	-2.81	108.02	110.53
17	4	314	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
23	b	846	BCR	C33-C5-C4	2.81	119.58	113.60
23	a	849	BCR	C33-C5-C4	2.81	119.58	113.60
17	5	306	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	b	843	BCR	C38-C26-C25	-2.81	121.42	124.48
17	l	203	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
23	b	845	BCR	C20-C21-C22	-2.81	123.34	127.28
15	j	101	XAT	C24-C23-C22	-2.80	105.55	110.79
17	a	805	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
17	b	832	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
21	a	843	PQN	C11-C3-C2	-2.80	120.09	124.89
17	1	308	CLA	C1-C2-C3	-2.80	121.61	126.20
17	a	802	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
23	b	850	BCR	C21-C20-C19	-2.80	115.08	123.20
17	5	313	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
18	1	315	SQD	O48-C23-C24	2.80	120.38	111.83
17	5	308	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
17	1	306	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
17	b	816	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
23	b	846	BCR	C2-C1-C6	2.80	114.50	110.44
17	b	841	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
17	b	822	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
17	1	305	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
17	a	811	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	a	839	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	b	828	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
17	a	821	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
17	b	801	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	b	850	BCR	C24-C23-C22	-2.79	122.11	126.23
23	b	847	BCR	C35-C13-C12	2.79	122.34	118.09
17	a	841	CLA	CHB-C4A-NA	2.78	128.42	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	m	102	BCR	C27-C26-C25	2.78	126.47	122.70
17	5	314	CLA	C3B-C4B-NB	-2.78	108.05	110.53
17	b	841	CLA	C3B-C4B-NB	-2.78	108.05	110.53
17	a	828	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	a	819	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
23	j	104	BCR	C23-C24-C25	-2.78	119.58	127.00
17	b	829	CLA	C3B-C4B-NB	-2.78	108.05	110.53
15	4	302	XAT	C19-C9-C8	2.78	122.33	118.09
17	a	803	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	a	836	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	a	838	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	4	307	CLA	C3B-C4B-NB	-2.78	108.05	110.53
15	4	304	XAT	C4-C3-C2	-2.78	105.60	110.79
17	5	314	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
17	5	315	CLA	C3B-C4B-NB	-2.77	108.05	110.53
23	i	101	BCR	C20-C19-C18	-2.77	118.76	126.36
15	5	302	XAT	C4-C3-C2	-2.77	105.61	110.79
22	m	101	LHG	O8-C23-C24	2.77	120.28	111.83
17	a	841	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
17	b	811	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
17	1	308	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	b	843	BCR	C24-C23-C22	-2.77	122.14	126.23
17	b	824	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
17	a	820	CLA	C3B-C4B-NB	-2.77	108.06	110.53
17	5	313	CLA	C3B-C4B-NB	-2.76	108.06	110.53
23	b	843	BCR	C23-C24-C25	-2.76	119.61	127.00
17	a	807	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
17	a	844	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
18	5	316	SQD	O48-C23-C24	2.76	120.26	111.83
15	4	301	XAT	C26-C27-C28	-2.76	120.15	125.99
16	1	301	A1L1G	C43-C44-C42	-2.76	118.34	122.82
23	b	852	BCR	C20-C19-C18	-2.76	118.79	126.36
17	l	204	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
17	f	802	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	5	305	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	a	837	CLA	C3B-C4B-NB	-2.76	108.07	110.53
17	4	307	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
15	4	302	XAT	C24-C23-C22	-2.75	105.64	110.79
17	b	820	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
17	5	310	CLA	C3B-C4B-NB	-2.75	108.08	110.53
17	4	311	CLA	C3B-C4B-NB	-2.75	108.08	110.53
17	j	103	CLA	C3B-C4B-NB	-2.75	108.08	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	805	CLA	CHB-C4A-NA	2.75	128.36	124.40
17	4	314	CLA	C3B-C4B-NB	-2.74	108.08	110.53
17	b	836	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
17	a	808	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
17	b	837	CLA	C3B-C4B-NB	-2.74	108.08	110.53
23	b	850	BCR	C20-C21-C22	-2.74	123.44	127.28
17	a	824	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	b	831	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	f	803	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	b	823	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	b	830	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
17	b	826	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
17	b	813	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
17	l	203	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	a	814	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	b	832	CLA	C3B-C4B-NB	-2.73	108.09	110.53
15	j	101	XAT	C15-C35-C34	-2.73	117.94	123.52
17	a	824	CLA	C3B-C4B-NB	-2.73	108.10	110.53
17	5	308	CLA	C3B-C4B-NB	-2.73	108.10	110.53
15	j	101	XAT	C31-C30-C29	-2.72	123.46	127.28
17	l	309	CLA	C3B-C4B-NB	-2.72	108.10	110.53
17	a	827	CLA	C3B-C4B-NB	-2.72	108.10	110.53
23	b	846	BCR	C7-C8-C9	-2.72	122.21	126.23
17	4	315	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
17	4	316	CLA	CAA-C2A-C3A	-2.72	110.00	116.23
17	b	818	CLA	CMB-C2B-C1B	-2.71	121.28	125.42
17	4	316	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
17	b	810	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
17	b	807	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	b	849	LHG	O8-C23-C24	2.71	120.09	111.83
17	b	825	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	b	833	CLA	C3B-C4B-NB	-2.71	108.11	110.53
15	j	101	XAT	C31-C32-C33	-2.71	118.94	126.36
17	b	831	CLA	CAA-C2A-C3A	-2.70	110.03	116.23
17	a	802	CLA	C1-C2-C3	-2.70	121.77	126.20
17	a	815	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	4	306	XAT	C31-C32-C33	-2.70	118.96	126.36
17	b	815	CLA	C3B-C4B-NB	-2.70	108.12	110.53
23	m	102	BCR	C33-C5-C6	-2.70	121.54	124.48
17	a	841	CLA	C1-C2-C3	-2.70	121.78	126.20
15	4	304	XAT	C39-C29-C28	2.70	122.21	118.09
17	a	814	CLA	O2D-CGD-O1D	-2.70	118.60	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	303	XAT	C15-C14-C13	-2.70	123.50	127.28
20	1	304	A1L1F	C26-C30-C31	-2.70	121.55	124.97
21	b	842	PQN	C2M-C2-C3	-2.70	120.02	124.45
17	5	312	CLA	C3B-C4B-NB	-2.69	108.12	110.53
17	l	203	CLA	CHB-C4A-NA	2.69	128.29	124.40
25	j	105	LMG	O8-C28-C29	2.69	120.04	111.83
17	b	806	CLA	C3B-C4B-NB	-2.69	108.13	110.53
17	b	803	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	4	302	XAT	C27-C28-C29	-2.68	121.37	125.53
17	a	835	CLA	CHB-C4A-NA	2.68	128.27	124.40
17	4	311	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
17	a	812	CLA	C3B-C4B-NB	-2.68	108.14	110.53
17	5	307	CLA	C3B-C4B-NB	-2.68	108.14	110.53
17	a	801	CLA	C3B-C4B-NB	-2.67	108.14	110.53
23	b	845	BCR	C11-C10-C9	-2.66	123.54	127.28
20	1	304	A1L1F	O15-C25-C14	-2.66	109.24	116.88
17	a	821	CLA	CHB-C4A-NA	2.66	128.24	124.40
20	1	304	A1L1F	O13-C45-C47	2.66	119.95	111.83
17	b	838	CLA	C3B-C4B-NB	-2.66	108.16	110.53
17	a	834	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
17	a	810	CLA	C3B-C4B-NB	-2.66	108.16	110.53
23	f	801	BCR	C2-C1-C6	2.66	114.30	110.44
17	a	810	CLA	C1-C2-C3	-2.66	121.85	126.20
17	a	840	CLA	C3B-C4B-NB	-2.65	108.16	110.53
17	a	822	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
15	5	304	XAT	C30-C31-C32	-2.65	115.52	123.20
15	5	301	XAT	C35-C15-C14	-2.65	118.09	123.52
18	5	316	SQD	C44-O6-C1	-2.65	108.11	113.80
22	a	845	LHG	O8-C23-C24	2.65	119.92	111.83
15	5	304	XAT	C31-C30-C29	-2.65	123.56	127.28
17	1	308	CLA	C3B-C4B-NB	-2.65	108.17	110.53
17	a	810	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
15	4	305	XAT	C31-C30-C29	-2.64	123.57	127.28
19	b	851	DGD	C1E-O6E-C5E	2.64	118.88	113.72
17	b	825	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	a	826	CLA	CHB-C4A-NA	2.64	128.21	124.40
23	a	847	BCR	C16-C15-C14	-2.64	118.12	123.52
23	a	849	BCR	C16-C15-C14	-2.64	118.12	123.52
17	5	314	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	b	834	CLA	C3B-C4B-NB	-2.64	108.17	110.53
17	4	318	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
17	4	310	CLA	C3B-C4B-NB	-2.64	108.18	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	316	CLA	CHB-C4A-NA	2.64	128.20	124.40
17	b	826	CLA	C3B-C4B-NB	-2.64	108.18	110.53
17	a	829	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
23	b	846	BCR	C21-C20-C19	-2.63	115.58	123.20
17	l	311	CLA	C3B-C4B-NB	-2.63	108.18	110.53
15	4	306	XAT	C7-C8-C9	-2.63	121.45	125.53
17	b	823	CLA	C3B-C4B-NB	-2.63	108.19	110.53
17	i	102	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
23	m	102	BCR	C15-C16-C17	-2.62	118.15	123.52
23	j	104	BCR	C27-C26-C25	-2.62	119.16	122.70
17	a	842	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
17	a	814	CLA	CHB-C4A-NA	2.62	128.18	124.40
23	j	104	BCR	C33-C5-C6	-2.62	121.63	124.48
23	a	849	BCR	C23-C24-C25	-2.62	120.01	127.00
23	b	847	BCR	C8-C7-C6	-2.61	120.02	127.00
17	a	821	CLA	C3B-C4B-NB	-2.61	108.20	110.53
23	l	201	BCR	C21-C20-C19	-2.61	115.64	123.20
17	l	202	CLA	C3B-C4B-NB	-2.61	108.20	110.53
23	b	848	BCR	C34-C9-C8	2.60	122.07	118.09
25	a	853	LMG	C8-O7-C10	-2.60	111.56	117.80
15	4	303	XAT	C10-C11-C12	-2.60	115.66	123.20
17	b	834	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
17	5	311	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
17	b	806	CLA	CHB-C4A-NA	2.60	128.15	124.40
17	b	802	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
17	a	805	CLA	C3B-C4B-NB	-2.59	108.21	110.53
17	b	811	CLA	CHB-C4A-NA	2.59	128.14	124.40
17	b	821	CLA	C1-C2-C3	-2.59	122.57	126.76
17	l	309	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
23	l	205	BCR	C28-C27-C26	-2.59	109.44	114.06
17	5	311	CLA	C3B-C4B-NB	-2.59	108.22	110.53
23	l	201	BCR	C20-C21-C22	-2.59	123.65	127.28
17	4	311	CLA	CHB-C4A-NA	2.59	128.14	124.40
17	a	832	CLA	CHB-C4A-NA	2.59	128.13	124.40
17	5	306	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
17	4	318	CLA	CHB-C4A-NA	2.59	128.13	124.40
17	b	809	CLA	CHB-C4A-NA	2.58	128.13	124.40
15	4	301	XAT	C27-C28-C29	-2.58	121.52	125.53
15	5	304	XAT	C8-C9-C10	-2.58	114.94	119.01
17	a	838	CLA	C3B-C4B-NB	-2.58	108.22	110.53
17	a	819	CLA	CHB-C4A-NA	2.58	128.13	124.40
17	l	307	CLA	C3B-C4B-NB	-2.58	108.22	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	848	BCR	C24-C23-C22	-2.58	122.42	126.23
19	b	851	DGD	O2G-C1B-O1B	-2.58	117.67	123.70
17	a	854	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
23	b	844	BCR	C24-C23-C22	-2.58	122.42	126.23
17	a	809	CLA	CHB-C4A-NA	2.57	128.12	124.40
17	b	803	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
17	1	306	CLA	CHB-C4A-NA	2.57	128.11	124.40
17	a	833	CLA	CHB-C4A-NA	2.57	128.11	124.40
15	5	304	XAT	C15-C35-C34	-2.57	118.26	123.52
23	b	850	BCR	C28-C27-C26	-2.57	109.47	114.06
17	a	828	CLA	C1-C2-C3	-2.57	121.99	126.20
17	a	807	CLA	CHB-C4A-NA	2.57	128.11	124.40
17	j	103	CLA	CHB-C4A-NA	2.57	128.11	124.40
17	4	312	CLA	CHB-C4A-NA	2.56	128.10	124.40
17	a	804	CLA	C3B-C4B-NB	-2.56	108.24	110.53
17	b	808	CLA	C3B-C4B-NB	-2.56	108.24	110.53
17	1	314	CLA	CHB-C4A-NA	2.56	128.09	124.40
17	b	814	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
23	b	843	BCR	C29-C30-C25	2.56	114.16	110.44
20	1	304	A1L1F	C27-C34-C33	2.56	122.00	118.09
23	a	850	BCR	C10-C11-C12	-2.56	115.79	123.20
15	5	301	XAT	C4-C3-C2	-2.56	106.01	110.79
17	b	807	CLA	C3B-C4B-NB	-2.56	108.25	110.53
17	b	807	CLA	C1-C2-C3	-2.56	122.01	126.20
17	b	801	CLA	CHB-C4A-NA	2.56	128.09	124.40
17	a	832	CLA	C1-C2-C3	-2.56	122.63	126.76
23	b	847	BCR	C38-C26-C25	-2.55	121.70	124.48
17	a	835	CLA	C3B-C4B-NB	-2.55	108.25	110.53
17	b	818	CLA	CHB-C4A-NA	2.55	128.08	124.40
17	5	313	CLA	CHB-C4A-NA	2.55	128.07	124.40
23	b	843	BCR	C21-C20-C19	-2.55	115.83	123.20
17	b	836	CLA	CHB-C4A-NA	2.55	128.07	124.40
17	b	822	CLA	C3B-C4B-NB	-2.55	108.26	110.53
17	1	204	CLA	C3B-C4B-NB	-2.54	108.26	110.53
17	a	804	CLA	CHB-C4A-NA	2.54	128.07	124.40
17	b	836	CLA	C3B-C4B-NB	-2.54	108.26	110.53
15	4	303	XAT	C30-C31-C32	-2.54	115.84	123.20
17	5	308	CLA	CHB-C4A-NA	2.54	128.07	124.40
17	5	312	CLA	CHB-C4A-NA	2.54	128.07	124.40
17	a	806	CLA	CHB-C4A-NA	2.54	128.07	124.40
17	a	801	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
17	b	814	CLA	CHB-C4A-NA	2.54	128.06	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	303	XAT	C35-C15-C14	-2.54	118.33	123.52
17	a	810	CLA	CHB-C4A-NA	2.53	128.06	124.40
17	b	805	CLA	CHB-C4A-NA	2.53	128.06	124.40
23	b	850	BCR	C10-C11-C12	-2.53	115.86	123.20
23	b	852	BCR	C15-C14-C13	-2.53	123.73	127.28
17	a	827	CLA	CHB-C4A-NA	2.53	128.05	124.40
23	l	205	BCR	C15-C16-C17	-2.53	118.34	123.52
23	j	104	BCR	C38-C26-C27	2.53	118.99	113.60
17	b	821	CLA	O2D-CGD-CBD	2.53	115.65	111.23
17	a	830	CLA	C1-C2-C3	-2.53	122.06	126.20
17	1	312	CLA	CHB-C4A-NA	2.53	128.04	124.40
15	5	304	XAT	C39-C29-C28	2.52	121.94	118.09
17	b	821	CLA	C3B-C4B-NB	-2.52	108.28	110.53
23	f	804	BCR	C15-C16-C17	-2.52	118.36	123.52
23	b	843	BCR	C33-C5-C4	2.52	118.97	113.60
17	a	825	CLA	CHB-C4A-NA	2.52	128.04	124.40
17	4	307	CLA	CHB-C4A-NA	2.52	128.04	124.40
17	f	802	CLA	CHB-C4A-NA	2.51	128.03	124.40
17	b	821	CLA	CHB-C4A-NA	2.51	128.03	124.40
17	4	309	CLA	C3B-C4B-NB	-2.51	108.29	110.53
23	b	848	BCR	C20-C21-C22	-2.51	123.76	127.28
15	4	301	XAT	C35-C15-C14	-2.51	118.38	123.52
17	4	315	CLA	CHB-C4A-NA	2.51	128.02	124.40
17	a	806	CLA	C6-C5-C3	-2.51	107.36	113.47
17	a	838	CLA	CHB-C4A-NA	2.51	128.02	124.40
17	b	834	CLA	CHB-C4A-NA	2.51	128.02	124.40
17	b	813	CLA	CHB-C4A-NA	2.51	128.02	124.40
17	1	306	CLA	C3B-C4B-NB	-2.50	108.29	110.53
17	a	804	CLA	O2D-CGD-CBD	2.50	115.61	111.23
17	a	817	CLA	CHB-C4A-NA	2.50	128.01	124.40
17	b	832	CLA	CHB-C4A-NA	2.50	128.01	124.40
20	1	304	A1L1F	C31-C32-C33	-2.50	115.95	123.20
17	a	830	CLA	C3B-C4B-NB	-2.50	108.30	110.53
17	4	308	CLA	CHB-C4A-NA	2.50	128.01	124.40
17	5	306	CLA	CHB-C4A-NA	2.50	128.01	124.40
17	l	204	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	a	848	BCR	C10-C11-C12	-2.50	115.96	123.20
17	f	803	CLA	CHB-C4A-NA	2.50	128.00	124.40
17	a	836	CLA	CHB-C4A-NA	2.50	128.00	124.40
17	a	806	CLA	O1D-CGD-CBD	2.50	129.44	124.52
17	a	815	CLA	CHB-C4A-NA	2.50	128.00	124.40
17	a	826	CLA	C3B-C4B-NB	-2.49	108.30	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	851	DGD	C6D-O5D-C1E	2.49	119.14	113.80
23	j	104	BCR	C15-C16-C17	-2.49	118.43	123.52
23	a	850	BCR	C38-C26-C27	2.48	118.89	113.60
17	a	840	CLA	CHB-C4A-NA	2.48	127.98	124.40
17	l	308	CLA	CHB-C4A-NA	2.48	127.98	124.40
17	a	802	CLA	CHB-C4A-NA	2.48	127.98	124.40
17	b	840	CLA	CHB-C4A-NA	2.48	127.97	124.40
17	a	803	CLA	C3B-C4B-NB	-2.48	108.32	110.53
17	b	837	CLA	CHB-C4A-NA	2.47	127.97	124.40
17	b	812	CLA	CMB-C2B-C3B	2.47	130.10	123.53
17	a	822	CLA	CHB-C4A-NA	2.47	127.97	124.40
17	a	823	CLA	CHB-C4A-NA	2.47	127.97	124.40
17	b	828	CLA	C3B-C4B-NB	-2.47	108.33	110.53
17	l	313	CLA	CAA-C2A-C3A	-2.47	110.57	116.23
17	a	844	CLA	C3B-C4B-NB	-2.47	108.33	110.53
17	l	202	CLA	CHB-C4A-NA	2.47	127.96	124.40
17	a	816	CLA	CHB-C4A-NA	2.47	127.96	124.40
17	4	317	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	l	310	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	f	804	BCR	C28-C27-C26	-2.46	109.66	114.06
17	b	816	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	b	835	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	b	847	BCR	C39-C30-C25	-2.46	106.38	110.24
23	l	201	BCR	C28-C27-C26	-2.46	109.67	114.06
17	a	808	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	b	807	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	a	802	CLA	CMB-C2B-C1B	-2.46	121.67	125.42
17	5	305	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	a	837	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	a	811	CLA	CHB-C4A-NA	2.46	127.95	124.40
17	a	835	CLA	O2D-CGD-CBD	2.45	115.52	111.23
25	j	105	LMG	C8-O7-C10	-2.45	111.92	117.80
23	b	844	BCR	C15-C16-C17	-2.45	118.50	123.52
17	5	310	CLA	CHB-C4A-NA	2.45	127.94	124.40
17	l	307	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	j	104	BCR	C38-C26-C25	-2.45	121.81	124.48
23	a	850	BCR	C8-C7-C6	-2.45	120.46	127.00
17	b	810	CLA	C1-C2-C3	-2.45	122.19	126.20
23	b	848	BCR	C38-C26-C25	-2.44	121.82	124.48
15	5	302	XAT	C31-C30-C29	-2.44	123.85	127.28
17	f	802	CLA	C3B-C4B-NB	-2.44	108.35	110.53
17	a	812	CLA	CHB-C4A-NA	2.44	127.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	809	CLA	C3B-C4B-NB	-2.44	108.35	110.53
17	a	854	CLA	CHB-C4A-NA	2.44	127.92	124.40
16	5	303	A1L1G	C43-C44-C42	-2.44	118.87	122.82
17	5	315	CLA	CHB-C4A-NA	2.44	127.91	124.40
23	b	843	BCR	C15-C16-C17	-2.43	118.54	123.52
17	b	822	CLA	C1-C2-C3	-2.43	122.21	126.20
17	b	839	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	a	848	BCR	C21-C20-C19	-2.43	116.16	123.20
17	a	818	CLA	CHB-C4A-NA	2.43	127.91	124.40
17	b	820	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	b	847	BCR	C21-C20-C19	-2.43	116.16	123.20
17	b	822	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	b	850	BCR	C8-C7-C6	-2.43	120.51	127.00
17	b	808	CLA	CHB-C4A-NA	2.43	127.90	124.40
17	a	839	CLA	CHB-C4A-NA	2.42	127.90	124.40
23	b	846	BCR	C33-C5-C6	-2.42	121.84	124.48
17	b	812	CLA	CAB-C3B-C2B	2.42	129.95	123.53
21	b	842	PQN	C11-C3-C2	-2.41	120.75	124.89
23	a	848	BCR	C15-C16-C17	-2.41	118.58	123.52
21	b	842	PQN	C14-C13-C15	2.41	119.41	115.23
17	4	313	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	5	311	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	4	310	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	b	819	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	b	833	CLA	CHB-C4A-NA	2.41	127.87	124.40
17	b	810	CLA	C3B-C4B-NB	-2.41	108.38	110.53
17	4	314	CLA	CHB-C4A-NA	2.40	127.87	124.40
23	b	845	BCR	C28-C27-C26	-2.40	109.78	114.06
17	i	102	CLA	CHB-C4A-NA	2.40	127.86	124.40
17	1	311	CLA	CHB-C4A-NA	2.39	127.86	124.40
17	a	828	CLA	CHB-C4A-NA	2.39	127.85	124.40
17	b	817	CLA	CHB-C4A-NA	2.39	127.85	124.40
17	b	826	CLA	CHB-C4A-NA	2.39	127.85	124.40
23	a	850	BCR	C16-C15-C14	-2.39	118.63	123.52
17	b	836	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
17	a	833	CLA	C1-C2-C3	-2.39	122.28	126.20
17	j	102	CLA	CHB-C4A-NA	2.39	127.85	124.40
23	a	849	BCR	C21-C20-C19	-2.39	116.28	123.20
23	b	846	BCR	C16-C15-C14	-2.39	118.64	123.52
17	b	823	CLA	CHB-C4A-NA	2.39	127.84	124.40
23	b	844	BCR	C23-C24-C25	-2.38	120.63	127.00
15	5	301	XAT	C30-C31-C32	-2.38	116.29	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	838	CLA	C1-C2-C3	-2.38	122.30	126.20
17	l	313	CLA	CHB-C4A-NA	2.38	127.83	124.40
23	f	801	BCR	C33-C5-C4	2.38	118.67	113.60
17	b	828	CLA	CHB-C4A-NA	2.38	127.83	124.40
17	a	820	CLA	CHB-C4A-NA	2.38	127.83	124.40
17	a	829	CLA	C3B-C4B-NB	-2.38	108.41	110.53
17	b	812	CLA	CHB-C4A-NA	2.38	127.83	124.40
15	5	301	XAT	O24-C25-C38	2.38	117.70	115.05
17	a	842	CLA	CHB-C4A-NA	2.37	127.83	124.40
17	b	840	CLA	C3B-C4B-NB	-2.37	108.41	110.53
17	a	834	CLA	C1-C2-C3	-2.37	122.31	126.20
23	b	843	BCR	C11-C12-C13	-2.37	119.86	126.36
17	b	814	CLA	C1-C2-C3	-2.37	122.32	126.20
23	m	102	BCR	C8-C7-C6	-2.37	120.68	127.00
15	j	101	XAT	C39-C29-C28	2.37	121.70	118.09
17	4	309	CLA	CHB-C4A-NA	2.37	127.81	124.40
15	4	306	XAT	O24-C25-C38	2.36	117.69	115.05
17	a	823	CLA	C3B-C4B-NB	-2.36	108.42	110.53
17	b	810	CLA	CHB-C4A-NA	2.36	127.81	124.40
23	a	847	BCR	C23-C24-C25	-2.36	120.69	127.00
17	b	824	CLA	CHB-C4A-NA	2.36	127.81	124.40
23	l	201	BCR	C15-C16-C17	-2.36	118.69	123.52
17	b	812	CLA	C3B-C4B-NB	-2.36	107.88	110.33
17	l	305	CLA	CHB-C4A-NA	2.36	127.80	124.40
17	a	831	CLA	CHB-C4A-NA	2.35	127.80	124.40
23	b	845	BCR	C34-C9-C10	-2.35	119.00	122.82
17	5	309	CLA	CHB-C4A-NA	2.35	127.80	124.40
17	a	841	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
15	a	852	XAT	C19-C9-C8	2.35	121.68	118.09
23	b	852	BCR	C23-C24-C25	-2.35	120.72	127.00
20	l	304	A1L1F	O7-C54-O55	-2.35	118.45	122.99
23	b	844	BCR	C28-C27-C26	-2.35	109.87	114.06
17	a	834	CLA	CHB-C4A-NA	2.34	127.78	124.40
23	b	845	BCR	C7-C6-C5	-2.34	116.16	121.56
17	a	813	CLA	CHB-C4A-NA	2.34	127.78	124.40
17	b	836	CLA	C1-C2-C3	-2.34	122.36	126.20
17	a	824	CLA	CHB-C4A-NA	2.34	127.78	124.40
23	l	201	BCR	C29-C30-C25	2.34	113.83	110.44
17	b	811	CLA	C3B-C4B-NB	-2.33	108.45	110.53
23	f	804	BCR	C11-C12-C13	-2.33	119.98	126.36
23	b	847	BCR	C34-C9-C8	2.33	121.64	118.09
17	a	810	CLA	O2A-CGA-O1A	-2.33	117.81	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	304	A1L1F	C37-C36-C35	-2.32	118.76	123.52
17	a	844	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	i	101	BCR	C16-C15-C14	-2.32	118.76	123.52
17	5	307	CLA	CHB-C4A-NA	2.32	127.75	124.40
17	1	309	CLA	CHB-C4A-NA	2.32	127.75	124.40
17	b	830	CLA	C1-C2-C3	-2.32	122.39	126.20
23	l	201	BCR	C23-C24-C25	-2.32	120.80	127.00
23	b	845	BCR	C37-C22-C21	-2.32	119.06	122.82
23	m	102	BCR	C24-C23-C22	-2.32	122.80	126.23
16	1	301	A1L1G	C17-C20-C21	2.32	116.85	114.24
17	5	314	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
15	4	302	XAT	C15-C35-C34	-2.32	118.78	123.52
17	b	824	CLA	C1-C2-C3	-2.32	122.40	126.20
17	b	840	CLA	C1-C2-C3	-2.31	122.41	126.20
17	b	819	CLA	C3B-C4B-NB	-2.31	108.47	110.53
23	b	850	BCR	C37-C22-C23	2.31	121.62	118.09
17	b	831	CLA	CHB-C4A-NA	2.31	127.74	124.40
17	4	311	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
23	a	848	BCR	C16-C15-C14	-2.30	118.81	123.52
17	a	816	CLA	C1-C2-C3	-2.30	123.04	126.76
17	4	314	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
17	a	836	CLA	C1-C2-C3	-2.30	123.05	126.76
16	1	301	A1L1G	C14-C29-C30	-2.30	121.56	125.47
23	f	804	BCR	C3-C4-C5	-2.29	109.96	114.06
15	5	304	XAT	O24-C25-C38	2.29	117.61	115.05
15	j	101	XAT	O24-C25-C38	2.29	117.61	115.05
17	a	805	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
23	b	847	BCR	C29-C30-C25	2.29	113.77	110.44
17	a	818	CLA	O2D-CGD-CBD	2.29	115.23	111.23
23	i	101	BCR	C10-C11-C12	-2.29	116.56	123.20
15	5	302	XAT	O4-C5-C18	2.29	117.61	115.05
17	a	826	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
15	5	302	XAT	C15-C35-C34	-2.29	118.84	123.52
18	5	316	SQD	C45-O47-C7	-2.29	112.32	117.80
17	1	306	CLA	C1-C2-C3	-2.29	122.45	126.20
17	b	838	CLA	CHB-C4A-NA	2.29	127.70	124.40
17	a	844	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
17	a	833	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
17	f	803	CLA	C1-C2-C3	-2.28	122.46	126.20
15	4	304	XAT	O24-C25-C38	2.28	117.60	115.05
23	a	849	BCR	C10-C11-C12	-2.28	116.59	123.20
23	b	847	BCR	C33-C5-C4	2.28	118.45	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	804	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
17	b	841	CLA	CHB-C4A-NA	2.27	127.68	124.40
23	l	205	BCR	C38-C26-C27	2.27	118.44	113.60
17	b	809	CLA	O2D-CGD-CBD	2.27	115.20	111.23
17	b	822	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
17	a	844	CLA	C1-C2-C3	-2.27	122.47	126.20
17	b	835	CLA	C1-C2-C3	-2.27	122.48	126.20
15	4	301	XAT	C39-C29-C30	-2.27	119.14	122.82
17	b	817	CLA	C1-C2-C3	-2.27	122.48	126.20
15	4	302	XAT	O4-C5-C18	2.27	117.58	115.05
17	b	815	CLA	C1-C2-C3	-2.27	122.48	126.20
17	a	827	CLA	CAA-C2A-C1A	-2.26	104.55	111.97
15	5	302	XAT	C11-C12-C13	-2.26	120.16	126.36
17	b	837	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
15	4	306	XAT	C15-C35-C34	-2.26	118.89	123.52
15	4	305	XAT	O4-C5-C18	2.26	117.57	115.05
23	f	801	BCR	C35-C13-C12	2.26	121.54	118.09
23	b	848	BCR	C35-C13-C12	2.25	121.53	118.09
17	b	811	CLA	C1-C2-C3	-2.25	122.50	126.20
23	f	801	BCR	C34-C9-C8	2.25	121.53	118.09
17	5	307	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
23	f	801	BCR	C28-C27-C26	-2.25	110.04	114.06
17	b	804	CLA	O1D-CGD-CBD	2.25	128.96	124.52
15	5	304	XAT	O4-C5-C18	2.25	117.56	115.05
17	a	819	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
17	b	818	CLA	CMB-C2B-C3B	2.25	131.84	126.55
17	f	802	CLA	C1-C2-C3	-2.25	122.51	126.20
17	5	311	CLA	C1-C2-C3	-2.25	122.52	126.20
17	a	806	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
17	b	826	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
15	4	306	XAT	O4-C5-C18	2.25	117.56	115.05
17	a	829	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
15	1	303	XAT	C19-C9-C8	2.24	121.52	118.09
23	a	850	BCR	C20-C19-C18	-2.24	120.21	126.36
21	a	843	PQN	C11-C12-C13	-2.24	122.97	126.83
23	b	846	BCR	C34-C9-C8	2.24	121.51	118.09
15	4	303	XAT	O24-C25-C38	2.24	117.55	115.05
23	b	847	BCR	C23-C24-C25	-2.24	121.02	127.00
23	l	205	BCR	C33-C5-C4	2.24	118.37	113.60
23	b	846	BCR	C11-C10-C9	-2.24	124.14	127.28
15	1	303	XAT	C27-C28-C29	-2.23	122.06	125.53
15	5	302	XAT	C30-C31-C32	-2.23	116.73	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	852	XAT	O24-C25-C38	2.23	117.54	115.05
17	b	803	CLA	CHB-C4A-NA	2.23	127.61	124.40
17	a	820	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
17	a	823	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
17	b	818	CLA	C1-C2-C3	-2.22	122.56	126.20
15	a	852	XAT	C40-C33-C32	2.22	121.48	118.09
23	a	848	BCR	C33-C5-C4	2.22	118.33	113.60
15	5	301	XAT	O4-C5-C18	2.22	117.53	115.05
15	1	302	XAT	O24-C25-C38	2.22	117.53	115.05
23	b	844	BCR	C36-C18-C19	2.22	121.47	118.09
17	a	838	CLA	C1-C2-C3	-2.22	122.57	126.20
23	b	850	BCR	C35-C13-C12	2.22	121.47	118.09
17	a	831	CLA	O2D-CGD-CBD	2.21	115.10	111.23
23	f	801	BCR	C15-C14-C13	-2.21	124.17	127.28
17	b	836	CLA	CAC-C3C-C4C	2.21	127.67	124.79
17	1	312	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
17	a	804	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
15	4	302	XAT	O24-C25-C38	2.21	117.52	115.05
15	4	303	XAT	C20-C13-C12	2.21	121.46	118.09
23	b	844	BCR	C37-C22-C23	2.21	121.46	118.09
17	a	811	CLA	C1-C2-C3	-2.21	122.58	126.20
15	4	303	XAT	O4-C5-C18	2.21	117.52	115.05
17	a	840	CLA	C1-C2-C3	-2.21	122.58	126.20
17	a	829	CLA	CHB-C4A-NA	2.21	127.58	124.40
17	b	805	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
17	a	809	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
17	a	820	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
15	4	306	XAT	C39-C29-C30	-2.20	119.25	122.82
15	4	303	XAT	C39-C29-C28	2.20	121.45	118.09
23	b	850	BCR	C33-C5-C4	2.20	118.29	113.60
23	a	849	BCR	C8-C7-C6	-2.20	121.12	127.00
23	l	201	BCR	C39-C30-C25	-2.20	106.79	110.24
17	b	830	CLA	CHB-C4A-NA	2.20	127.57	124.40
17	a	806	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
23	j	104	BCR	C29-C30-C25	2.20	113.63	110.44
21	a	843	PQN	C2M-C2-C3	-2.20	120.84	124.45
23	b	844	BCR	C11-C12-C13	-2.20	120.34	126.36
15	1	302	XAT	O4-C5-C18	2.20	117.50	115.05
17	b	827	CLA	CHB-C4A-NA	2.19	127.56	124.40
15	1	303	XAT	O24-C25-C38	2.19	117.49	115.05
17	a	803	CLA	CMB-C2B-C3B	2.19	131.69	126.55
15	4	301	XAT	O4-C5-C18	2.19	117.49	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	848	BCR	C23-C24-C25	-2.18	121.16	127.00
17	5	311	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
17	a	801	CLA	CHB-C4A-NA	2.18	127.55	124.40
17	b	824	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
15	5	302	XAT	O24-C25-C26	-2.18	57.20	58.93
17	b	828	CLA	C1-C2-C3	-2.18	122.63	126.20
15	4	302	XAT	C8-C9-C10	-2.18	115.58	119.01
23	a	847	BCR	C8-C7-C6	-2.18	121.18	127.00
17	5	312	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
23	f	804	BCR	C21-C20-C19	-2.17	116.90	123.20
17	a	834	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
17	b	815	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
17	b	829	CLA	CHB-C4A-NA	2.17	127.54	124.40
17	a	812	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
17	a	831	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
23	l	201	BCR	C37-C22-C23	2.17	121.40	118.09
17	b	841	CLA	C1-C2-C3	-2.16	122.65	126.20
15	4	304	XAT	C7-C8-C9	-2.16	122.17	125.53
23	j	104	BCR	C21-C20-C19	-2.16	116.93	123.20
17	a	830	CLA	CHB-C4A-NA	2.16	127.52	124.40
17	a	816	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
17	4	312	CLA	O2D-CGD-CBD	2.16	115.01	111.23
15	4	304	XAT	O4-C5-C18	2.16	117.46	115.05
23	b	845	BCR	C1-C6-C7	2.16	121.51	115.65
17	b	831	CLA	CMA-C3A-C2A	-2.16	111.28	116.23
23	b	846	BCR	C23-C24-C25	-2.16	121.23	127.00
17	l	308	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
15	4	305	XAT	O24-C25-C38	2.16	117.46	115.05
17	a	838	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
17	f	802	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
17	5	308	CLA	C1-C2-C3	-2.16	122.66	126.20
17	4	309	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
23	a	848	BCR	C34-C9-C8	2.16	121.38	118.09
17	b	819	CLA	C1-C2-C3	-2.15	122.67	126.20
17	i	102	CLA	C1-C2-C3	-2.15	122.67	126.20
17	b	833	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
23	a	849	BCR	C15-C16-C17	-2.15	119.11	123.52
23	b	846	BCR	C15-C16-C17	-2.15	119.12	123.52
17	a	826	CLA	CMB-C2B-C3B	2.15	131.60	126.55
23	j	104	BCR	C16-C15-C14	-2.15	119.13	123.52
23	l	201	BCR	C3-C4-C5	-2.15	110.23	114.06
17	a	806	CLA	C5-C3-C2	-2.15	116.35	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	102	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
17	a	839	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
17	b	839	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
17	b	827	CLA	C1-C2-C3	-2.14	122.69	126.20
23	m	102	BCR	C15-C14-C13	-2.14	124.28	127.28
17	a	829	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
17	4	309	CLA	O2D-CGD-CBD	2.14	114.97	111.23
17	b	802	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
23	b	852	BCR	C32-C1-C6	-2.14	106.89	110.24
17	a	804	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
17	b	823	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
17	4	308	CLA	O2D-CGD-CBD	2.14	114.96	111.23
23	b	843	BCR	C37-C22-C23	2.13	121.35	118.09
17	a	807	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
17	a	842	CLA	C1-C2-C3	-2.13	122.71	126.20
15	5	304	XAT	C35-C15-C14	-2.13	119.16	123.52
15	1	302	XAT	C10-C11-C12	-2.13	117.03	123.20
17	b	807	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
17	b	830	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
23	b	847	BCR	C2-C1-C6	2.13	113.53	110.44
15	1	302	XAT	C30-C31-C32	-2.12	117.04	123.20
23	a	849	BCR	C37-C22-C23	2.12	121.33	118.09
15	4	304	XAT	C35-C15-C14	-2.12	119.18	123.52
23	b	848	BCR	C23-C24-C25	-2.12	121.34	127.00
18	5	316	SQD	O7-S-C6	2.12	109.92	106.76
17	1	307	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
17	b	820	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
17	b	821	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
17	a	836	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
17	b	801	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
17	b	830	CLA	O2D-CGD-CBD	2.11	114.92	111.23
17	a	803	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
15	5	302	XAT	O24-C25-C38	2.11	117.41	115.05
17	b	811	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
17	4	314	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
17	1	306	CLA	CAC-C3C-C4C	2.11	127.53	124.79
17	b	804	CLA	O2D-CGD-CBD	2.11	114.91	111.23
23	b	848	BCR	C37-C22-C23	2.11	121.31	118.09
17	4	310	CLA	C1-C2-C3	-2.11	123.35	126.76
15	a	852	XAT	C39-C29-C28	2.11	121.31	118.09
17	a	826	CLA	C1-C2-C3	-2.10	122.75	126.20
23	a	847	BCR	C28-C27-C26	-2.10	110.30	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	818	CLA	C1-C2-C3	-2.10	122.75	126.20
17	a	802	CLA	CMB-C2B-C3B	2.10	131.50	126.55
17	4	318	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
23	a	847	BCR	C33-C5-C4	2.10	118.08	113.60
23	b	844	BCR	C33-C5-C4	2.10	118.08	113.60
17	a	827	CLA	C1-C2-C3	-2.10	122.75	126.20
17	b	838	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
17	b	836	CLA	CMB-C2B-C3B	2.10	131.49	126.55
17	a	809	CLA	O2D-CGD-CBD	2.10	114.90	111.23
17	b	813	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
23	b	846	BCR	C35-C13-C12	2.10	121.29	118.09
17	1	310	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
17	b	832	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
17	a	854	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
19	b	851	DGD	O3D-C3D-C4D	-2.10	105.43	110.38
17	b	828	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
17	b	803	CLA	O2D-CGD-CBD	2.10	114.89	111.23
17	a	808	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
23	b	843	BCR	C38-C26-C27	2.09	118.06	113.60
17	b	820	CLA	C1-C2-C3	-2.09	122.77	126.20
17	b	826	CLA	C1-C2-C3	-2.09	122.77	126.20
23	j	104	BCR	C3-C4-C5	-2.09	110.33	114.06
17	a	825	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
17	1	311	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
17	a	829	CLA	CMB-C2B-C3B	2.09	131.46	126.55
17	5	307	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
23	l	201	BCR	C34-C9-C10	-2.09	119.43	122.82
17	b	818	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
17	a	805	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
19	b	851	DGD	O5E-C6E-C5E	-2.09	104.23	111.33
17	b	830	CLA	CHB-C1B-NB	2.09	127.18	124.05
17	b	808	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
15	1	303	XAT	C11-C10-C9	-2.08	124.36	127.28
23	b	845	BCR	C16-C15-C14	-2.08	119.26	123.52
17	b	840	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
17	5	308	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
17	a	831	CLA	C3B-C4B-NB	-2.08	108.67	110.53
15	1	303	XAT	O4-C5-C18	2.08	117.37	115.05
15	5	301	XAT	C39-C29-C28	2.08	121.27	118.09
15	1	303	XAT	C20-C13-C12	2.08	121.27	118.09
17	a	844	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
15	4	301	XAT	C10-C11-C12	-2.08	117.18	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	835	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
15	4	305	XAT	C30-C31-C32	-2.08	117.18	123.20
17	b	817	CLA	O2D-CGD-CBD	2.08	114.86	111.23
15	5	302	XAT	C19-C9-C10	-2.08	119.45	122.82
17	a	818	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
17	a	806	CLA	C6-C7-C8	-2.08	109.07	115.97
17	a	801	CLA	O1D-CGD-CBD	2.07	128.61	124.52
17	a	806	CLA	CAA-C2A-C3A	-2.07	107.39	113.00
17	1	306	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
15	j	101	XAT	O4-C5-C18	2.07	117.36	115.05
17	b	841	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
17	j	102	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
17	1	311	CLA	O2D-CGD-CBD	2.07	114.85	111.23
15	4	305	XAT	C19-C9-C8	2.07	121.25	118.09
17	a	827	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
23	a	849	BCR	C38-C26-C27	2.07	118.01	113.60
23	i	101	BCR	C23-C22-C21	2.07	122.27	119.01
17	b	811	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
17	a	832	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
17	a	822	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
23	a	847	BCR	C20-C19-C18	-2.06	120.71	126.36
17	a	814	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
17	b	808	CLA	O2D-CGD-CBD	2.06	114.83	111.23
23	b	845	BCR	C21-C20-C19	-2.06	117.23	123.20
17	b	805	CLA	C1-C2-C3	-2.06	122.83	126.20
15	1	302	XAT	C39-C29-C28	2.06	121.23	118.09
15	4	305	XAT	C20-C13-C12	2.05	121.23	118.09
17	b	839	CLA	C1-C2-C3	-2.05	122.83	126.20
15	a	852	XAT	O4-C5-C18	2.05	117.34	115.05
17	a	814	CLA	C1-C2-C3	-2.05	122.84	126.20
17	b	830	CLA	C3B-C4B-NB	-2.05	108.70	110.53
23	a	848	BCR	C28-C27-C26	-2.05	110.40	114.06
17	a	823	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
23	f	804	BCR	C8-C7-C6	-2.05	121.53	127.00
17	5	311	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
17	a	839	CLA	CMB-C2B-C1B	-2.05	122.31	125.42
17	a	854	CLA	C1-C2-C3	-2.04	122.85	126.20
17	b	806	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
17	b	837	CLA	O2D-CGD-CBD	2.04	114.80	111.23
17	b	826	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
17	a	809	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
25	j	105	LMG	O7-C10-O9	-2.04	118.94	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	809	CLA	C1-C2-C3	-2.04	122.86	126.20
17	b	815	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
15	4	301	XAT	C24-C23-C22	-2.04	106.98	110.79
17	b	802	CLA	C3B-C4B-NB	-2.04	108.71	110.53
17	1	307	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
17	b	822	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
17	a	830	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
23	b	852	BCR	C38-C26-C27	2.03	117.93	113.60
17	1	311	CLA	C1-C2-C3	-2.03	122.87	126.20
23	a	849	BCR	C35-C13-C12	2.03	121.19	118.09
17	a	844	CLA	CMB-C2B-C3B	2.03	131.33	126.55
16	1	301	A1L1G	C29-C30-C31	2.03	122.15	119.00
17	a	809	CLA	CMB-C2B-C3B	2.03	131.33	126.55
17	b	810	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
23	a	849	BCR	C29-C30-C25	2.03	113.38	110.44
17	b	810	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
17	b	807	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
17	b	804	CLA	CAC-C3C-C4C	2.03	127.42	124.79
23	1	205	BCR	C10-C11-C12	-2.02	117.33	123.20
17	a	842	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
17	1	203	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
17	a	833	CLA	CMB-C2B-C3B	2.02	131.31	126.55
17	a	816	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
17	b	827	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
17	b	835	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
17	b	812	CLA	C1-C2-C3	-2.02	122.89	126.20
17	b	825	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
15	4	302	XAT	C30-C31-C32	-2.02	117.35	123.20
17	a	811	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
17	b	802	CLA	C1-C2-C3	-2.02	122.89	126.20
15	4	305	XAT	C39-C29-C28	2.02	121.17	118.09
17	1	305	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
17	a	831	CLA	CHB-C1B-NB	2.02	127.07	124.05
23	a	850	BCR	C35-C13-C12	2.01	121.17	118.09
17	4	308	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
17	4	314	CLA	CMB-C2B-C3B	2.01	131.29	126.55
17	b	833	CLA	CMB-C2B-C3B	2.01	131.28	126.55
23	b	843	BCR	C16-C15-C14	-2.01	119.40	123.52
15	5	301	XAT	C10-C11-C12	-2.01	117.37	123.20
17	a	833	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
17	a	809	CLA	C1-C2-C3	-2.01	122.90	126.20
23	b	843	BCR	C33-C5-C6	-2.01	122.29	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	847	BCR	C10-C11-C12	-2.01	117.38	123.20
17	b	829	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
23	b	847	BCR	C38-C26-C27	2.01	117.87	113.60
15	4	301	XAT	C28-C29-C30	2.01	122.16	119.01
23	b	846	BCR	C28-C27-C26	-2.01	110.48	114.06
19	4	319	DGD	O2G-C1B-O1B	-2.00	119.02	123.70
17	b	818	CLA	CHB-C1B-NB	2.00	127.05	124.05
17	a	813	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
17	a	803	CLA	CHB-C4A-NA	2.00	127.29	124.40

All (126) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	5	305	CLA	ND
17	5	306	CLA	ND
17	5	307	CLA	ND
17	5	308	CLA	ND
17	5	309	CLA	ND
17	5	310	CLA	ND
17	5	311	CLA	ND
17	5	312	CLA	ND
17	5	313	CLA	ND
17	5	314	CLA	ND
17	5	315	CLA	ND
17	4	307	CLA	ND
17	4	308	CLA	ND
17	4	309	CLA	ND
17	4	310	CLA	ND
17	4	311	CLA	ND
17	4	312	CLA	ND
17	4	313	CLA	ND
17	4	314	CLA	ND
17	4	315	CLA	ND
17	4	316	CLA	ND
17	4	317	CLA	ND
17	4	318	CLA	ND
17	1	305	CLA	ND
17	1	306	CLA	ND
17	1	307	CLA	ND
17	1	308	CLA	ND
17	1	309	CLA	ND
17	1	310	CLA	ND

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Mol	Chain	Res	Type	Atom
17	1	311	CLA	ND
17	1	312	CLA	ND
17	1	313	CLA	ND
17	1	314	CLA	ND
17	a	801	CLA	ND
17	a	802	CLA	ND
17	a	803	CLA	ND
17	a	804	CLA	ND
17	a	805	CLA	ND
17	a	806	CLA	ND
17	a	807	CLA	ND
17	a	808	CLA	ND
17	a	809	CLA	ND
17	a	810	CLA	ND
17	a	811	CLA	ND
17	a	812	CLA	ND
17	a	813	CLA	ND
17	a	814	CLA	ND
17	a	815	CLA	ND
17	a	816	CLA	ND
17	a	817	CLA	ND
17	a	818	CLA	ND
17	a	819	CLA	ND
17	a	820	CLA	ND
17	a	821	CLA	ND
17	a	822	CLA	ND
17	a	823	CLA	ND
17	a	824	CLA	ND
17	a	825	CLA	ND
17	a	826	CLA	ND
17	a	827	CLA	ND
17	a	828	CLA	ND
17	a	829	CLA	ND
17	a	830	CLA	ND
17	a	831	CLA	ND
17	a	832	CLA	ND
17	a	833	CLA	ND
17	a	834	CLA	ND
17	a	835	CLA	ND
17	a	836	CLA	ND
17	a	837	CLA	ND
17	a	838	CLA	ND

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Mol	Chain	Res	Type	Atom
17	a	839	CLA	ND
17	a	840	CLA	ND
17	a	841	CLA	ND
17	a	842	CLA	ND
17	a	844	CLA	ND
17	a	854	CLA	ND
17	b	801	CLA	ND
17	b	802	CLA	ND
17	b	803	CLA	ND
17	b	804	CLA	ND
17	b	805	CLA	ND
17	b	806	CLA	ND
17	b	807	CLA	ND
17	b	808	CLA	ND
17	b	809	CLA	ND
17	b	810	CLA	ND
17	b	811	CLA	ND
17	b	812	CLA	ND
17	b	813	CLA	ND
17	b	814	CLA	ND
17	b	815	CLA	ND
17	b	816	CLA	ND
17	b	817	CLA	ND
17	b	818	CLA	ND
17	b	819	CLA	ND
17	b	820	CLA	ND
17	b	821	CLA	ND
17	b	822	CLA	ND
17	b	823	CLA	ND
17	b	824	CLA	ND
17	b	825	CLA	ND
17	b	826	CLA	ND
17	b	827	CLA	ND
17	b	828	CLA	ND
17	b	829	CLA	ND
17	b	830	CLA	ND
17	b	831	CLA	ND
17	b	832	CLA	ND
17	b	833	CLA	ND
17	b	834	CLA	ND
17	b	835	CLA	ND
17	b	836	CLA	ND

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Mol	Chain	Res	Type	Atom
17	b	837	CLA	ND
17	b	838	CLA	ND
17	b	839	CLA	ND
17	b	840	CLA	ND
17	b	841	CLA	ND
17	f	802	CLA	ND
17	f	803	CLA	ND
17	i	102	CLA	ND
17	j	102	CLA	ND
17	j	103	CLA	ND
17	l	202	CLA	ND
17	l	203	CLA	ND
17	l	204	CLA	ND

All (1419) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	5	302	XAT	O4-C6-C7-C8
15	5	302	XAT	C7-C8-C9-C10
15	5	302	XAT	C7-C8-C9-C19
15	4	301	XAT	C27-C28-C29-C30
15	4	301	XAT	C27-C28-C29-C39
15	4	302	XAT	O4-C6-C7-C8
15	4	302	XAT	C27-C28-C29-C30
15	4	302	XAT	C27-C28-C29-C39
15	4	304	XAT	O4-C6-C7-C8
15	4	304	XAT	C7-C8-C9-C10
15	4	304	XAT	C7-C8-C9-C19
15	4	306	XAT	O24-C26-C27-C28
15	a	852	XAT	C7-C8-C9-C10
15	a	852	XAT	C7-C8-C9-C19
15	a	852	XAT	C11-C12-C13-C14
15	a	852	XAT	C27-C28-C29-C30
15	j	101	XAT	O4-C6-C7-C8
15	j	101	XAT	C7-C8-C9-C10
15	j	101	XAT	O24-C26-C27-C28
16	5	303	A1L1G	C26-C30-C31-C32
16	5	303	A1L1G	C31-C32-C33-C34
16	5	303	A1L1G	C32-C33-C34-C27
16	5	303	A1L1G	C32-C33-C34-C35
16	5	303	A1L1G	C41-C42-C44-C2
16	5	303	A1L1G	C41-C42-C44-C43

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Mol	Chain	Res	Type	Atoms
16	1	301	A1L1G	C45-C2-C44-C42
16	1	301	A1L1G	C45-C2-C44-C43
16	1	301	A1L1G	O13-C26-C30-C29
16	1	301	A1L1G	C27-C34-C35-C36
16	1	301	A1L1G	C33-C34-C35-C36
16	1	301	A1L1G	C35-C36-C37-C38
16	1	301	A1L1G	C38-C39-C40-C41
16	1	301	A1L1G	C39-C40-C41-C42
17	5	308	CLA	CBD-CGD-O2D-CED
17	5	309	CLA	CAD-CBD-CGD-O1D
17	5	309	CLA	CAD-CBD-CGD-O2D
17	5	310	CLA	CBD-CGD-O2D-CED
17	5	314	CLA	C1A-C2A-CAA-CBA
17	5	314	CLA	C3A-C2A-CAA-CBA
17	5	315	CLA	CBD-CGD-O2D-CED
17	5	315	CLA	O1D-CGD-O2D-CED
17	4	307	CLA	C1A-C2A-CAA-CBA
17	4	308	CLA	CHA-CBD-CGD-O1D
17	4	308	CLA	CHA-CBD-CGD-O2D
17	4	310	CLA	CBD-CGD-O2D-CED
17	4	311	CLA	C1A-C2A-CAA-CBA
17	4	312	CLA	CBA-CGA-O2A-C1
17	4	312	CLA	CBD-CGD-O2D-CED
17	4	313	CLA	C1A-C2A-CAA-CBA
17	4	313	CLA	C3A-C2A-CAA-CBA
17	4	316	CLA	CAD-CBD-CGD-O2D
17	4	317	CLA	CBD-CGD-O2D-CED
17	4	318	CLA	CBD-CGD-O2D-CED
17	1	305	CLA	C11-C10-C8-C9
17	1	310	CLA	CBD-CGD-O2D-CED
17	1	313	CLA	CBD-CGD-O2D-CED
17	1	314	CLA	C1A-C2A-CAA-CBA
17	1	314	CLA	C3A-C2A-CAA-CBA
17	a	801	CLA	CBD-CGD-O2D-CED
17	a	804	CLA	CHA-CBD-CGD-O1D
17	a	804	CLA	CHA-CBD-CGD-O2D
17	a	805	CLA	C1A-C2A-CAA-CBA
17	a	805	CLA	C3A-C2A-CAA-CBA
17	a	806	CLA	CAD-CBD-CGD-O2D
17	a	809	CLA	C1A-C2A-CAA-CBA
17	a	809	CLA	C3A-C2A-CAA-CBA
17	a	809	CLA	CHA-CBD-CGD-O1D

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

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Mol	Chain	Res	Type	Atoms
17	b	811	CLA	CAD-CBD-CGD-O2D
17	b	813	CLA	C1A-C2A-CAA-CBA
17	b	813	CLA	C2-C3-C5-C6
17	b	813	CLA	C4-C3-C5-C6
17	b	815	CLA	C1A-C2A-CAA-CBA
17	b	815	CLA	CBD-CGD-O2D-CED
17	b	816	CLA	CHA-CBD-CGD-O1D
17	b	816	CLA	CHA-CBD-CGD-O2D
17	b	818	CLA	C3A-C2A-CAA-CBA
17	b	819	CLA	C1A-C2A-CAA-CBA
17	b	819	CLA	C3A-C2A-CAA-CBA
17	b	820	CLA	C4B-C3B-CAB-CBB
17	b	821	CLA	C1A-C2A-CAA-CBA
17	b	821	CLA	C3A-C2A-CAA-CBA
17	b	822	CLA	CHA-CBD-CGD-O2D
17	b	825	CLA	CHA-CBD-CGD-O1D
17	b	825	CLA	CHA-CBD-CGD-O2D
17	b	829	CLA	C1A-C2A-CAA-CBA
17	b	829	CLA	C3A-C2A-CAA-CBA
17	b	830	CLA	CHA-CBD-CGD-O1D
17	b	830	CLA	CHA-CBD-CGD-O2D
17	b	833	CLA	C1A-C2A-CAA-CBA
17	b	833	CLA	C3A-C2A-CAA-CBA
17	b	834	CLA	C1A-C2A-CAA-CBA
17	b	834	CLA	C3A-C2A-CAA-CBA
17	b	834	CLA	C11-C12-C13-C14
17	b	835	CLA	CHA-CBD-CGD-O1D
17	b	835	CLA	CHA-CBD-CGD-O2D
17	b	835	CLA	CBD-CGD-O2D-CED
17	b	839	CLA	C4B-C3B-CAB-CBB
17	b	840	CLA	C1A-C2A-CAA-CBA
17	b	840	CLA	C3A-C2A-CAA-CBA
17	b	840	CLA	CAD-CBD-CGD-O1D
17	b	840	CLA	CAD-CBD-CGD-O2D
17	b	840	CLA	CBD-CGD-O2D-CED
17	j	102	CLA	C1A-C2A-CAA-CBA
17	j	103	CLA	CAD-CBD-CGD-O1D
17	j	103	CLA	CAD-CBD-CGD-O2D
17	j	103	CLA	CBD-CGD-O2D-CED
17	l	203	CLA	C6-C7-C8-C9
18	5	316	SQD	O49-C7-O47-C45
18	5	316	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
18	5	316	SQD	C5-C6-S-O7
18	5	316	SQD	C5-C6-S-O8
18	5	316	SQD	C5-C6-S-O9
18	1	315	SQD	O5-C5-C6-S
18	1	315	SQD	C5-C6-S-O7
18	1	315	SQD	C5-C6-S-O8
18	1	315	SQD	C5-C6-S-O9
19	4	319	DGD	C2B-C1B-O2G-C2G
19	4	319	DGD	O1B-C1B-O2G-C2G
20	1	304	A1L1F	C29-C14-C25-C24
20	1	304	A1L1F	C32-C33-C34-C35
20	1	304	A1L1F	C38-C39-C40-C41
22	a	845	LHG	O1-C1-C2-C3
22	a	845	LHG	C3-O3-P-O4
22	a	845	LHG	C3-O3-P-O6
22	a	845	LHG	C4-O6-P-O3
22	a	845	LHG	C4-O6-P-O5
22	a	845	LHG	O6-C4-C5-O7
22	a	845	LHG	O7-C5-C6-O8
22	a	846	LHG	O1-C1-C2-C3
22	a	846	LHG	O6-C4-C5-O7
22	b	849	LHG	O1-C1-C2-C3
22	b	849	LHG	C1-C2-C3-O3
22	b	849	LHG	O2-C2-C3-O3
22	b	849	LHG	C3-O3-P-O5
22	b	849	LHG	C3-O3-P-O6
22	b	849	LHG	C4-O6-P-O3
22	b	849	LHG	C4-O6-P-O4
22	b	849	LHG	C4-O6-P-O5
22	m	101	LHG	C1-C2-C3-O3
22	m	101	LHG	C3-O3-P-O4
22	m	101	LHG	O9-C7-O7-C5
22	m	101	LHG	C8-C7-O7-C5
23	a	850	BCR	C23-C24-C25-C26
23	b	843	BCR	C7-C8-C9-C10
23	b	843	BCR	C7-C8-C9-C34
23	b	845	BCR	C1-C6-C7-C8
23	b	845	BCR	C5-C6-C7-C8
23	i	101	BCR	C21-C22-C23-C24
23	i	101	BCR	C37-C22-C23-C24
23	j	104	BCR	C7-C8-C9-C10
23	j	104	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
23	m	102	BCR	C21-C22-C23-C24
23	m	102	BCR	C37-C22-C23-C24
25	a	853	LMG	C11-C10-O7-C8
25	j	105	LMG	O9-C10-O7-C8
25	j	105	LMG	C11-C10-O7-C8
17	5	310	CLA	O1D-CGD-O2D-CED
17	4	310	CLA	O1D-CGD-O2D-CED
17	1	313	CLA	O1D-CGD-O2D-CED
17	a	812	CLA	O1D-CGD-O2D-CED
17	b	803	CLA	O1D-CGD-O2D-CED
17	b	835	CLA	O1D-CGD-O2D-CED
17	5	313	CLA	CBD-CGD-O2D-CED
17	4	307	CLA	CBD-CGD-O2D-CED
17	1	309	CLA	CBD-CGD-O2D-CED
17	a	812	CLA	CBD-CGD-O2D-CED
17	i	102	CLA	CBD-CGD-O2D-CED
17	1	307	CLA	O1A-CGA-O2A-C1
17	a	806	CLA	O1A-CGA-O2A-C1
17	b	815	CLA	O1A-CGA-O2A-C1
22	m	101	LHG	O10-C23-O8-C6
17	4	317	CLA	O1D-CGD-O2D-CED
17	b	804	CLA	O1D-CGD-O2D-CED
17	a	801	CLA	O1D-CGD-O2D-CED
17	1	307	CLA	CBA-CGA-O2A-C1
17	a	806	CLA	CBA-CGA-O2A-C1
17	b	815	CLA	CBA-CGA-O2A-C1
22	m	101	LHG	C24-C23-O8-C6
17	4	311	CLA	O1A-CGA-O2A-C1
17	a	805	CLA	O1A-CGA-O2A-C1
17	a	818	CLA	O1A-CGA-O2A-C1
17	b	822	CLA	O1A-CGA-O2A-C1
17	f	802	CLA	O1A-CGA-O2A-C1
22	b	849	LHG	O10-C23-O8-C6
25	a	853	LMG	O10-C28-O8-C9
17	4	312	CLA	O1A-CGA-O2A-C1
17	b	815	CLA	O1D-CGD-O2D-CED
17	5	308	CLA	O1D-CGD-O2D-CED
17	4	318	CLA	O1D-CGD-O2D-CED
17	1	310	CLA	O1D-CGD-O2D-CED
17	a	811	CLA	O1D-CGD-O2D-CED
17	a	829	CLA	O1D-CGD-O2D-CED
17	b	840	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	j	103	CLA	O1D-CGD-O2D-CED
25	a	853	LMG	O9-C10-O7-C8
17	1	309	CLA	CBA-CGA-O2A-C1
17	1	309	CLA	O1A-CGA-O2A-C1
17	l	204	CLA	O1A-CGA-O2A-C1
17	a	810	CLA	C3-C5-C6-C7
17	b	802	CLA	C3-C5-C6-C7
17	b	805	CLA	C3-C5-C6-C7
17	b	807	CLA	C3-C5-C6-C7
17	b	809	CLA	C3-C5-C6-C7
17	a	805	CLA	CBA-CGA-O2A-C1
17	a	818	CLA	CBA-CGA-O2A-C1
17	a	836	CLA	CBA-CGA-O2A-C1
17	b	822	CLA	CBA-CGA-O2A-C1
17	b	824	CLA	CBA-CGA-O2A-C1
17	f	802	CLA	CBA-CGA-O2A-C1
25	a	853	LMG	C29-C28-O8-C9
20	1	304	A1L1F	C56-C54-O7-C8
20	1	304	A1L1F	O55-C54-O7-C8
17	5	305	CLA	CBD-CGD-O2D-CED
17	5	309	CLA	CBD-CGD-O2D-CED
17	a	804	CLA	CBD-CGD-O2D-CED
17	a	814	CLA	CBD-CGD-O2D-CED
17	b	806	CLA	CBD-CGD-O2D-CED
17	b	820	CLA	CBD-CGD-O2D-CED
17	b	836	CLA	CBD-CGD-O2D-CED
17	4	312	CLA	O1D-CGD-O2D-CED
17	a	825	CLA	C4-C3-C5-C6
17	a	831	CLA	C4-C3-C5-C6
17	a	839	CLA	C4-C3-C5-C6
17	j	102	CLA	C4-C3-C5-C6
17	a	831	CLA	C2-C3-C5-C6
17	a	839	CLA	C2-C3-C5-C6
17	j	102	CLA	C2-C3-C5-C6
17	l	204	CLA	CBA-CGA-O2A-C1
17	5	306	CLA	CBD-CGD-O2D-CED
17	1	309	CLA	O1D-CGD-O2D-CED
17	a	817	CLA	C2A-CAA-CBA-CGA
17	b	810	CLA	C2A-CAA-CBA-CGA
17	1	307	CLA	C3-C5-C6-C7
17	1	310	CLA	C3-C5-C6-C7
17	b	819	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	4	311	CLA	CBA-CGA-O2A-C1
17	1	305	CLA	CBA-CGA-O2A-C1
17	a	807	CLA	CBA-CGA-O2A-C1
17	a	811	CLA	CBA-CGA-O2A-C1
17	b	806	CLA	CBA-CGA-O2A-C1
17	b	811	CLA	CBA-CGA-O2A-C1
17	b	819	CLA	CBA-CGA-O2A-C1
22	b	849	LHG	C24-C23-O8-C6
25	j	105	LMG	C29-C28-O8-C9
25	j	105	LMG	C4-C5-C6-O5
17	5	311	CLA	O1A-CGA-O2A-C1
17	1	305	CLA	O1A-CGA-O2A-C1
17	a	811	CLA	O1A-CGA-O2A-C1
17	a	812	CLA	O1A-CGA-O2A-C1
17	a	820	CLA	O1A-CGA-O2A-C1
17	b	806	CLA	O1A-CGA-O2A-C1
17	b	819	CLA	O1A-CGA-O2A-C1
25	j	105	LMG	O10-C28-O8-C9
17	4	308	CLA	CBD-CGD-O2D-CED
17	a	818	CLA	CBD-CGD-O2D-CED
17	a	837	CLA	CBD-CGD-O2D-CED
25	j	105	LMG	C12-C13-C14-C15
22	a	845	LHG	O2-C2-C3-O3
22	m	101	LHG	O2-C2-C3-O3
17	a	812	CLA	CBA-CGA-O2A-C1
17	b	840	CLA	CBA-CGA-O2A-C1
17	a	836	CLA	O1A-CGA-O2A-C1
17	b	824	CLA	O1A-CGA-O2A-C1
17	b	811	CLA	CBD-CGD-O2D-CED
17	b	840	CLA	O1A-CGA-O2A-C1
17	i	102	CLA	O1D-CGD-O2D-CED
17	5	309	CLA	C3-C5-C6-C7
17	a	807	CLA	C3-C5-C6-C7
17	a	835	CLA	C3-C5-C6-C7
17	a	841	CLA	CBD-CGD-O2D-CED
17	b	824	CLA	CBD-CGD-O2D-CED
17	b	828	CLA	CBD-CGD-O2D-CED
19	b	851	DGD	O6E-C5E-C6E-O5E
17	4	307	CLA	O1D-CGD-O2D-CED
17	5	311	CLA	CBA-CGA-O2A-C1
17	a	820	CLA	CBA-CGA-O2A-C1
17	a	813	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	b	829	CLA	C4-C3-C5-C6
17	a	825	CLA	C2-C3-C5-C6
17	a	807	CLA	O1A-CGA-O2A-C1
17	b	811	CLA	O1A-CGA-O2A-C1
17	a	835	CLA	CBD-CGD-O2D-CED
17	1	312	CLA	C3-C5-C6-C7
19	4	319	DGD	O6E-C1E-O5D-C6D
17	4	309	CLA	CBD-CGD-O2D-CED
17	a	807	CLA	CBD-CGD-O2D-CED
17	a	810	CLA	CBD-CGD-O2D-CED
17	a	834	CLA	CBD-CGD-O2D-CED
17	b	841	CLA	CBD-CGD-O2D-CED
22	a	845	LHG	C23-C24-C25-C26
25	a	853	LMG	O6-C5-C6-O5
25	j	105	LMG	O6-C5-C6-O5
17	5	313	CLA	O1D-CGD-O2D-CED
22	a	845	LHG	C12-C13-C14-C15
16	5	303	A1L1G	C40-C41-C42-C44
22	a	845	LHG	C1-C2-C3-O3
17	5	308	CLA	CBA-CGA-O2A-C1
17	a	809	CLA	CBA-CGA-O2A-C1
17	a	839	CLA	CBA-CGA-O2A-C1
17	a	854	CLA	CBA-CGA-O2A-C1
17	b	821	CLA	CBA-CGA-O2A-C1
17	b	827	CLA	CBA-CGA-O2A-C1
17	b	834	CLA	CBA-CGA-O2A-C1
17	5	311	CLA	CBD-CGD-O2D-CED
25	a	853	LMG	C4-C5-C6-O5
17	a	804	CLA	O1D-CGD-O2D-CED
17	b	806	CLA	O1D-CGD-O2D-CED
22	a	845	LHG	C28-C29-C30-C31
17	a	813	CLA	C2-C3-C5-C6
17	b	823	CLA	CBD-CGD-O2D-CED
17	1	306	CLA	C6-C7-C8-C9
17	1	306	CLA	C11-C12-C13-C14
17	1	310	CLA	C14-C13-C15-C16
17	a	829	CLA	C11-C10-C8-C9
17	b	801	CLA	C11-C10-C8-C9
17	b	801	CLA	C14-C13-C15-C16
17	b	805	CLA	C11-C10-C8-C9
17	b	819	CLA	C11-C10-C8-C9
17	b	825	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	b	830	CLA	C14-C13-C15-C16
17	b	839	CLA	C6-C7-C8-C9
17	f	802	CLA	C11-C12-C13-C14
17	i	102	CLA	C11-C10-C8-C9
17	i	102	CLA	C11-C12-C13-C14
19	4	319	DGD	C2E-C1E-O5D-C6D
22	a	846	LHG	O2-C2-C3-O3
17	b	836	CLA	O1D-CGD-O2D-CED
17	a	809	CLA	O1A-CGA-O2A-C1
17	a	854	CLA	O1A-CGA-O2A-C1
15	a	852	XAT	C11-C12-C13-C20
15	a	852	XAT	C27-C28-C29-C39
15	j	101	XAT	C7-C8-C9-C19
16	1	301	A1L1G	C28-C39-C40-C41
20	1	304	A1L1F	C32-C33-C34-C27
20	1	304	A1L1F	C28-C39-C40-C41
23	b	852	BCR	C7-C8-C9-C34
23	l	205	BCR	C7-C8-C9-C34
23	l	205	BCR	C37-C22-C23-C24
23	m	102	BCR	C7-C8-C9-C34
23	b	852	BCR	C7-C8-C9-C10
23	l	205	BCR	C7-C8-C9-C10
23	l	205	BCR	C21-C22-C23-C24
17	5	310	CLA	C2A-CAA-CBA-CGA
17	4	312	CLA	C2A-CAA-CBA-CGA
17	4	317	CLA	C2A-CAA-CBA-CGA
17	b	805	CLA	C2A-CAA-CBA-CGA
17	b	827	CLA	C2A-CAA-CBA-CGA
25	a	853	LMG	C28-C29-C30-C31
17	5	305	CLA	O1D-CGD-O2D-CED
17	b	821	CLA	O1A-CGA-O2A-C1
17	4	317	CLA	CBA-CGA-O2A-C1
17	b	839	CLA	CBA-CGA-O2A-C1
17	a	810	CLA	C13-C15-C16-C17
17	a	814	CLA	O1D-CGD-O2D-CED
17	b	807	CLA	CBD-CGD-O2D-CED
17	a	807	CLA	C5-C6-C7-C8
17	b	809	CLA	C5-C6-C7-C8
17	i	102	CLA	C8-C10-C11-C12
17	b	824	CLA	C3-C5-C6-C7
17	5	308	CLA	O1A-CGA-O2A-C1
17	b	827	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	4	316	CLA	CBD-CGD-O2D-CED
17	1	310	CLA	C11-C10-C8-C7
17	a	801	CLA	C12-C13-C15-C16
17	a	809	CLA	C12-C13-C15-C16
17	a	828	CLA	C12-C13-C15-C16
17	a	844	CLA	C12-C13-C15-C16
17	b	808	CLA	C12-C13-C15-C16
17	b	834	CLA	C13-C15-C16-C17
19	b	851	DGD	C1A-C2A-C3A-C4A
17	5	309	CLA	O1D-CGD-O2D-CED
17	b	807	CLA	C15-C16-C17-C18
22	b	849	LHG	C7-C8-C9-C10
17	a	839	CLA	O1A-CGA-O2A-C1
17	b	834	CLA	O1A-CGA-O2A-C1
17	b	828	CLA	CBA-CGA-O2A-C1
17	a	834	CLA	C15-C16-C17-C18
17	b	801	CLA	C15-C16-C17-C18
17	a	825	CLA	C2A-CAA-CBA-CGA
17	a	830	CLA	C2A-CAA-CBA-CGA
17	a	842	CLA	C2A-CAA-CBA-CGA
17	b	821	CLA	C2A-CAA-CBA-CGA
17	b	834	CLA	C2A-CAA-CBA-CGA
17	b	839	CLA	C2A-CAA-CBA-CGA
17	4	309	CLA	C10-C11-C12-C13
17	a	802	CLA	C5-C6-C7-C8
17	a	809	CLA	C5-C6-C7-C8
17	a	814	CLA	C13-C15-C16-C17
17	b	833	CLA	C13-C15-C16-C17
17	b	841	CLA	C13-C15-C16-C17
17	i	102	CLA	C10-C11-C12-C13
20	1	304	A1L1F	C45-C47-C48-C49
22	a	846	LHG	C7-C8-C9-C10
25	a	853	LMG	C10-C11-C12-C13
17	a	801	CLA	C3-C5-C6-C7
20	1	304	A1L1F	C49-C50-C51-C52
17	b	820	CLA	O1D-CGD-O2D-CED
17	5	309	CLA	C13-C15-C16-C17
17	1	306	CLA	C5-C6-C7-C8
17	1	306	CLA	C8-C10-C11-C12
17	a	809	CLA	C8-C10-C11-C12
17	a	830	CLA	C13-C15-C16-C17
17	a	831	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	b	809	CLA	C8-C10-C11-C12
17	b	814	CLA	C15-C16-C17-C18
17	b	830	CLA	C8-C10-C11-C12
17	l	203	CLA	C10-C11-C12-C13
17	a	807	CLA	C15-C16-C17-C18
17	a	841	CLA	C5-C6-C7-C8
17	b	815	CLA	C5-C6-C7-C8
17	5	305	CLA	CBA-CGA-O2A-C1
17	5	306	CLA	O1D-CGD-O2D-CED
17	a	837	CLA	O1D-CGD-O2D-CED
17	b	837	CLA	C5-C6-C7-C8
17	b	829	CLA	C2-C3-C5-C6
19	b	851	DGD	C4E-C5E-C6E-O5E
17	l	306	CLA	C15-C16-C17-C18
17	a	841	CLA	C15-C16-C17-C18
17	4	318	CLA	CBA-CGA-O2A-C1
17	a	816	CLA	CBA-CGA-O2A-C1
17	b	802	CLA	CBA-CGA-O2A-C1
17	b	832	CLA	CBA-CGA-O2A-C1
17	b	802	CLA	CBD-CGD-O2D-CED
17	f	802	CLA	CBD-CGD-O2D-CED
17	a	818	CLA	O1D-CGD-O2D-CED
17	b	841	CLA	C10-C11-C12-C13
17	4	314	CLA	C3-C5-C6-C7
17	a	801	CLA	C8-C10-C11-C12
17	b	801	CLA	C2A-CAA-CBA-CGA
17	4	308	CLA	O1D-CGD-O2D-CED
17	a	814	CLA	CBA-CGA-O2A-C1
17	a	838	CLA	CBA-CGA-O2A-C1
17	a	828	CLA	C13-C15-C16-C17
17	a	828	CLA	C15-C16-C17-C18
17	f	802	CLA	C13-C15-C16-C17
21	b	842	PQN	C23-C25-C26-C27
17	a	826	CLA	CBD-CGD-O2D-CED
17	b	837	CLA	C8-C10-C11-C12
17	f	802	CLA	C5-C6-C7-C8
17	a	831	CLA	C15-C16-C17-C18
17	a	839	CLA	C13-C15-C16-C17
17	b	801	CLA	C13-C15-C16-C17
17	b	802	CLA	C8-C10-C11-C12
17	b	828	CLA	C13-C15-C16-C17
17	a	833	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	a	844	CLA	CBA-CGA-O2A-C1
19	4	319	DGD	C3B-C4B-C5B-C6B
17	b	801	CLA	C8-C10-C11-C12
17	l	203	CLA	C8-C10-C11-C12
18	1	315	SQD	C8-C7-O47-C45
17	b	811	CLA	O1D-CGD-O2D-CED
18	1	315	SQD	O49-C7-O47-C45
17	a	824	CLA	CBA-CGA-O2A-C1
18	1	315	SQD	C24-C23-O48-C46
17	a	801	CLA	C16-C17-C18-C20
17	b	811	CLA	C16-C17-C18-C20
17	b	839	CLA	O1A-CGA-O2A-C1
23	a	850	BCR	C37-C22-C23-C24
23	f	801	BCR	C37-C22-C23-C24
23	a	850	BCR	C21-C22-C23-C24
23	f	801	BCR	C21-C22-C23-C24
17	4	318	CLA	O1A-CGA-O2A-C1
17	a	816	CLA	O1A-CGA-O2A-C1
17	b	802	CLA	O1A-CGA-O2A-C1
17	b	828	CLA	O1A-CGA-O2A-C1
17	b	832	CLA	C2A-CAA-CBA-CGA
17	b	830	CLA	C10-C11-C12-C13
17	b	840	CLA	C5-C6-C7-C8
17	a	806	CLA	O2A-C1-C2-C3
16	5	303	A1L1G	C29-C30-C31-C32
17	4	309	CLA	C16-C17-C18-C20
17	b	834	CLA	C16-C17-C18-C19
17	b	841	CLA	C16-C17-C18-C20
17	a	841	CLA	O1D-CGD-O2D-CED
17	b	824	CLA	O1D-CGD-O2D-CED
17	a	814	CLA	O1A-CGA-O2A-C1
17	5	315	CLA	C2C-C3C-CAC-CBC
17	b	825	CLA	C5-C6-C7-C8
17	a	836	CLA	CBD-CGD-O2D-CED
17	a	835	CLA	O1D-CGD-O2D-CED
17	a	818	CLA	C2-C1-O2A-CGA
17	b	811	CLA	C16-C17-C18-C19
17	b	812	CLA	C6-C7-C8-C9
17	b	828	CLA	O1D-CGD-O2D-CED
19	b	851	DGD	C9B-CAB-CBB-CCB
23	m	102	BCR	C14-C15-C16-C17
17	a	834	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	a	854	CLA	C5-C6-C7-C8
17	b	828	CLA	C8-C10-C11-C12
21	a	843	PQN	C25-C26-C27-C28
22	a	845	LHG	C11-C10-C9-C8
17	b	832	CLA	O1A-CGA-O2A-C1
17	b	817	CLA	CBA-CGA-O2A-C1
22	a	845	LHG	O1-C1-C2-O2
22	a	846	LHG	O1-C1-C2-O2
22	b	849	LHG	O1-C1-C2-O2
22	a	845	LHG	C27-C28-C29-C30
17	4	313	CLA	C4B-C3B-CAB-CBB
17	a	801	CLA	C4B-C3B-CAB-CBB
17	a	841	CLA	C4B-C3B-CAB-CBB
17	b	841	CLA	C4B-C3B-CAB-CBB
22	m	101	LHG	C9-C10-C11-C12
17	b	834	CLA	C16-C17-C18-C20
17	f	802	CLA	C16-C17-C18-C19
17	f	802	CLA	C16-C17-C18-C20
17	1	314	CLA	C2A-CAA-CBA-CGA
17	b	829	CLA	C2A-CAA-CBA-CGA
17	a	814	CLA	C10-C11-C12-C13
17	a	827	CLA	C8-C10-C11-C12
17	a	841	CLA	C8-C10-C11-C12
17	b	806	CLA	C15-C16-C17-C18
17	b	836	CLA	C5-C6-C7-C8
17	1	308	CLA	C11-C10-C8-C7
22	a	845	LHG	C13-C14-C15-C16
17	b	809	CLA	C10-C11-C12-C13
17	4	311	CLA	C3A-C2A-CAA-CBA
17	a	807	CLA	C3A-C2A-CAA-CBA
17	a	838	CLA	C3A-C2A-CAA-CBA
17	a	854	CLA	C3A-C2A-CAA-CBA
17	b	810	CLA	C3A-C2A-CAA-CBA
17	b	813	CLA	C3A-C2A-CAA-CBA
17	b	815	CLA	C3A-C2A-CAA-CBA
17	f	803	CLA	C3A-C2A-CAA-CBA
17	b	841	CLA	O1D-CGD-O2D-CED
17	b	812	CLA	C6-C7-C8-C10
17	a	833	CLA	O1A-CGA-O2A-C1
17	a	838	CLA	O1A-CGA-O2A-C1
17	a	844	CLA	O1A-CGA-O2A-C1
22	m	101	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
17	a	814	CLA	C5-C6-C7-C8
17	a	823	CLA	CBA-CGA-O2A-C1
17	b	807	CLA	CBA-CGA-O2A-C1
17	b	836	CLA	CBA-CGA-O2A-C1
18	1	315	SQD	O10-C23-O48-C46
18	1	315	SQD	C11-C10-C9-C8
19	4	319	DGD	C2B-C3B-C4B-C5B
22	m	101	LHG	C14-C15-C16-C17
17	a	807	CLA	O1D-CGD-O2D-CED
17	4	309	CLA	O1D-CGD-O2D-CED
17	a	810	CLA	O1D-CGD-O2D-CED
19	b	851	DGD	C4A-C5A-C6A-C7A
17	b	801	CLA	C16-C17-C18-C20
17	4	312	CLA	C2B-C3B-CAB-CBB
17	4	313	CLA	C2B-C3B-CAB-CBB
17	4	315	CLA	C2B-C3B-CAB-CBB
17	a	808	CLA	C2B-C3B-CAB-CBB
17	a	836	CLA	C2B-C3B-CAB-CBB
17	b	820	CLA	C2B-C3B-CAB-CBB
17	b	839	CLA	C2B-C3B-CAB-CBB
23	a	850	BCR	C23-C24-C25-C30
23	l	205	BCR	C23-C24-C25-C26
23	l	205	BCR	C23-C24-C25-C30
17	j	102	CLA	CBD-CGD-O2D-CED
17	b	825	CLA	CBA-CGA-O2A-C1
17	b	808	CLA	C5-C6-C7-C8
17	b	808	CLA	C3-C5-C6-C7
17	5	306	CLA	C2A-CAA-CBA-CGA
17	a	814	CLA	C2A-CAA-CBA-CGA
19	b	851	DGD	C4B-C5B-C6B-C7B
22	m	101	LHG	C11-C12-C13-C14
17	a	811	CLA	C11-C10-C8-C7
17	1	308	CLA	C4-C3-C5-C6
17	1	310	CLA	C4-C3-C5-C6
19	b	851	DGD	C2B-C3B-C4B-C5B
16	5	303	A1L1G	C39-C40-C41-C42
19	b	851	DGD	C3B-C4B-C5B-C6B
17	a	825	CLA	CBA-CGA-O2A-C1
17	b	826	CLA	C11-C10-C8-C9
19	4	319	DGD	O6D-C1D-O3G-C3G
17	b	817	CLA	O1A-CGA-O2A-C1
17	4	317	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	a	840	CLA	C13-C15-C16-C17
19	b	851	DGD	C2B-C1B-O2G-C2G
22	a	846	LHG	C8-C7-O7-C5
17	a	809	CLA	C13-C15-C16-C17
17	b	839	CLA	C15-C16-C17-C18
17	b	804	CLA	C2C-C3C-CAC-CBC
17	a	810	CLA	C2A-CAA-CBA-CGA
17	b	833	CLA	C2A-CAA-CBA-CGA
17	b	801	CLA	C16-C17-C18-C19
17	4	311	CLA	C4-C3-C5-C6
17	b	835	CLA	C4-C3-C5-C6
17	b	840	CLA	C4-C3-C5-C6
17	1	308	CLA	C2-C3-C5-C6
20	1	304	A1L1F	C47-C48-C49-C50
17	b	830	CLA	C15-C16-C17-C18
17	j	102	CLA	C8-C10-C11-C12
22	a	845	LHG	C26-C27-C28-C29
17	a	823	CLA	O1A-CGA-O2A-C1
17	b	807	CLA	O1A-CGA-O2A-C1
17	4	308	CLA	C3-C5-C6-C7
17	b	805	CLA	C13-C15-C16-C17
17	b	810	CLA	C5-C6-C7-C8
22	b	849	LHG	O6-C4-C5-O7
17	b	833	CLA	C15-C16-C17-C18
17	a	806	CLA	C16-C17-C18-C19
17	b	841	CLA	C16-C17-C18-C19
17	b	836	CLA	O1A-CGA-O2A-C1
18	1	315	SQD	C7-C8-C9-C10
17	4	309	CLA	C13-C15-C16-C17
17	4	309	CLA	C15-C16-C17-C18
19	4	319	DGD	O1G-C1G-C2G-O2G
17	a	806	CLA	C13-C15-C16-C17
17	a	801	CLA	C16-C17-C18-C19
17	a	820	CLA	C16-C17-C18-C20
17	b	825	CLA	O1A-CGA-O2A-C1
17	4	311	CLA	C2-C3-C5-C6
17	b	840	CLA	C2-C3-C5-C6
22	a	846	LHG	O9-C7-O7-C5
17	b	810	CLA	C10-C11-C12-C13
17	a	822	CLA	C2A-CAA-CBA-CGA
17	a	808	CLA	CBD-CGD-O2D-CED
17	5	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	1	305	CLA	C8-C10-C11-C12
17	a	844	CLA	C10-C11-C12-C13
17	b	814	CLA	C3-C5-C6-C7
17	5	306	CLA	C1A-C2A-CAA-CBA
17	4	314	CLA	C1A-C2A-CAA-CBA
17	1	306	CLA	C1A-C2A-CAA-CBA
17	a	807	CLA	C1A-C2A-CAA-CBA
17	a	817	CLA	C1A-C2A-CAA-CBA
17	a	819	CLA	C1A-C2A-CAA-CBA
17	a	825	CLA	C1A-C2A-CAA-CBA
17	b	817	CLA	C1A-C2A-CAA-CBA
17	b	818	CLA	C1A-C2A-CAA-CBA
17	b	838	CLA	C1A-C2A-CAA-CBA
17	f	803	CLA	C1A-C2A-CAA-CBA
17	b	809	CLA	C15-C16-C17-C18
22	a	845	LHG	O6-C4-C5-C6
17	a	839	CLA	C3-C5-C6-C7
17	b	801	CLA	C3-C5-C6-C7
17	a	807	CLA	C12-C13-C15-C16
17	a	810	CLA	C12-C13-C15-C16
17	a	822	CLA	C6-C7-C8-C10
17	a	830	CLA	C12-C13-C15-C16
17	a	841	CLA	C11-C10-C8-C7
17	a	844	CLA	C11-C12-C13-C15
17	b	807	CLA	C11-C10-C8-C7
17	b	807	CLA	C12-C13-C15-C16
17	b	811	CLA	C11-C12-C13-C15
17	b	819	CLA	C6-C7-C8-C10
17	b	823	CLA	C6-C7-C8-C10
17	b	825	CLA	C11-C10-C8-C7
17	b	826	CLA	C6-C7-C8-C10
17	b	828	CLA	C6-C7-C8-C10
17	b	834	CLA	C11-C12-C13-C15
17	b	839	CLA	C6-C7-C8-C10
17	f	802	CLA	C11-C12-C13-C15
17	b	815	CLA	C6-C7-C8-C10
17	b	811	CLA	C2-C3-C5-C6
19	b	851	DGD	CAB-CBB-CCB-CDB
17	5	311	CLA	O1D-CGD-O2D-CED
17	a	812	CLA	C10-C11-C12-C13
17	b	830	CLA	C13-C15-C16-C17
17	b	836	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	b	849	LHG	C8-C7-O7-C5
17	a	806	CLA	C2A-CAA-CBA-CGA
17	4	309	CLA	C11-C12-C13-C14
17	1	308	CLA	C11-C10-C8-C9
17	a	807	CLA	C11-C12-C13-C14
17	a	809	CLA	C14-C13-C15-C16
17	a	814	CLA	C11-C10-C8-C9
17	a	822	CLA	C6-C7-C8-C9
17	a	827	CLA	C11-C10-C8-C9
17	a	842	CLA	C11-C12-C13-C14
17	a	844	CLA	C14-C13-C15-C16
17	b	801	CLA	C11-C12-C13-C14
17	b	803	CLA	C11-C10-C8-C9
17	b	807	CLA	C14-C13-C15-C16
17	b	808	CLA	C11-C10-C8-C9
17	b	823	CLA	C6-C7-C8-C9
17	b	825	CLA	C11-C10-C8-C9
17	b	826	CLA	C6-C7-C8-C9
17	b	837	CLA	C14-C13-C15-C16
19	b	851	DGD	CBB-CCB-CDB-CEB
17	5	315	CLA	C4C-C3C-CAC-CBC
19	b	851	DGD	C6A-C7A-C8A-C9A
19	4	319	DGD	O1G-C1G-C2G-C3G
22	a	845	LHG	C4-C5-C6-O8
22	b	849	LHG	C4-C5-C6-O8
17	b	807	CLA	O1D-CGD-O2D-CED
17	b	823	CLA	O1D-CGD-O2D-CED
17	a	835	CLA	CBA-CGA-O2A-C1
17	a	844	CLA	C16-C17-C18-C19
22	m	101	LHG	C29-C30-C31-C32
17	a	825	CLA	O1A-CGA-O2A-C1
17	4	316	CLA	O1D-CGD-O2D-CED
17	a	829	CLA	C10-C11-C12-C13
17	b	839	CLA	C4-C3-C5-C6
17	a	820	CLA	C8-C10-C11-C12
17	b	840	CLA	C13-C15-C16-C17
17	b	815	CLA	C6-C7-C8-C9
17	b	819	CLA	C11-C12-C13-C14
22	m	101	LHG	C11-C10-C9-C8
15	4	306	XAT	C27-C28-C29-C30
17	1	308	CLA	C13-C15-C16-C17
17	a	854	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	a	843	PQN	C23-C25-C26-C27
17	4	308	CLA	CBA-CGA-O2A-C1
17	a	841	CLA	CBA-CGA-O2A-C1
17	1	310	CLA	C5-C6-C7-C8
17	a	844	CLA	C16-C17-C18-C20
17	b	837	CLA	C2C-C3C-CAC-CBC
17	b	804	CLA	C15-C16-C17-C18
19	b	851	DGD	C2A-C1A-O1G-C1G
17	b	802	CLA	C4-C3-C5-C6
17	b	811	CLA	C4-C3-C5-C6
17	b	803	CLA	C2-C3-C5-C6
20	1	304	A1L1F	C50-C51-C52-C53
22	m	101	LHG	C12-C13-C14-C15
17	b	805	CLA	C16-C17-C18-C20
17	b	828	CLA	C15-C16-C17-C18
25	a	853	LMG	C14-C15-C16-C17
25	j	105	LMG	C13-C14-C15-C16
17	5	310	CLA	CAA-CBA-CGA-O2A
19	b	851	DGD	C3A-C4A-C5A-C6A
17	1	306	CLA	CBA-CGA-O2A-C1
17	1	310	CLA	CBA-CGA-O2A-C1
17	b	829	CLA	CBA-CGA-O2A-C1
17	1	311	CLA	CBD-CGD-O2D-CED
17	4	318	CLA	C3-C5-C6-C7
17	b	802	CLA	O1D-CGD-O2D-CED
17	f	802	CLA	O1D-CGD-O2D-CED
17	a	810	CLA	C5-C6-C7-C8
17	a	829	CLA	C8-C10-C11-C12
17	a	811	CLA	C11-C10-C8-C9
17	a	805	CLA	C6-C7-C8-C9
17	a	824	CLA	O1A-CGA-O2A-C1
17	a	801	CLA	C4-C3-C5-C6
17	a	804	CLA	C2-C3-C5-C6
17	a	831	CLA	CBA-CGA-O2A-C1
17	b	812	CLA	CBA-CGA-O2A-C1
17	4	311	CLA	C11-C10-C8-C9
17	a	810	CLA	C14-C13-C15-C16
17	a	814	CLA	C11-C12-C13-C14
17	a	830	CLA	C14-C13-C15-C16
17	a	835	CLA	C6-C7-C8-C9
17	a	841	CLA	C11-C10-C8-C9
17	a	844	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	a	844	CLA	C11-C12-C13-C14
17	b	803	CLA	C6-C7-C8-C9
17	b	810	CLA	C6-C7-C8-C9
17	b	811	CLA	C11-C12-C13-C14
17	b	819	CLA	C6-C7-C8-C9
17	b	829	CLA	C11-C12-C13-C14
17	b	838	CLA	C14-C13-C15-C16
17	j	102	CLA	C6-C7-C8-C9
17	a	826	CLA	C15-C16-C17-C18
22	m	101	LHG	C2-C3-O3-P
17	5	308	CLA	C4B-C3B-CAB-CBB
17	4	312	CLA	C4B-C3B-CAB-CBB
17	4	315	CLA	C4B-C3B-CAB-CBB
17	1	305	CLA	C4B-C3B-CAB-CBB
17	1	309	CLA	C4B-C3B-CAB-CBB
17	1	313	CLA	C4B-C3B-CAB-CBB
17	1	314	CLA	C4B-C3B-CAB-CBB
17	a	808	CLA	C4B-C3B-CAB-CBB
17	a	825	CLA	C4B-C3B-CAB-CBB
17	a	836	CLA	C4B-C3B-CAB-CBB
17	a	837	CLA	C4B-C3B-CAB-CBB
17	b	818	CLA	C4B-C3B-CAB-CBB
17	b	819	CLA	C4B-C3B-CAB-CBB
17	j	102	CLA	C4B-C3B-CAB-CBB
19	b	851	DGD	CCB-CDB-CEB-CFB
17	a	844	CLA	C15-C16-C17-C18
17	b	807	CLA	C10-C11-C12-C13
17	a	819	CLA	C2A-CAA-CBA-CGA
19	4	319	DGD	C2D-C1D-O3G-C3G
17	1	308	CLA	C15-C16-C17-C18
17	b	833	CLA	C3-C5-C6-C7
17	b	834	CLA	C3-C5-C6-C7
22	b	849	LHG	C9-C10-C11-C12
22	b	849	LHG	O6-C4-C5-C6
17	4	309	CLA	C12-C13-C15-C16
17	4	311	CLA	C11-C10-C8-C7
17	1	308	CLA	C11-C12-C13-C15
17	a	807	CLA	C11-C12-C13-C15
17	a	809	CLA	C6-C7-C8-C10
17	a	812	CLA	C6-C7-C8-C10
17	a	814	CLA	C11-C12-C13-C15
17	a	827	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	a	829	CLA	C6-C7-C8-C10
17	a	835	CLA	C6-C7-C8-C10
17	a	842	CLA	C11-C12-C13-C15
17	a	844	CLA	C11-C10-C8-C7
17	b	801	CLA	C11-C12-C13-C15
17	b	803	CLA	C6-C7-C8-C10
17	b	803	CLA	C11-C10-C8-C7
17	b	803	CLA	C12-C13-C15-C16
17	b	808	CLA	C11-C10-C8-C7
17	b	810	CLA	C6-C7-C8-C10
17	b	837	CLA	C12-C13-C15-C16
17	b	838	CLA	C12-C13-C15-C16
17	b	839	CLA	C12-C13-C15-C16
17	j	102	CLA	C6-C7-C8-C10
17	a	812	CLA	C8-C10-C11-C12
22	a	845	LHG	C7-C8-C9-C10
17	4	312	CLA	C3A-C2A-CAA-CBA
17	a	804	CLA	C4-C3-C5-C6
17	a	820	CLA	C4-C3-C5-C6
17	a	829	CLA	C3A-C2A-CAA-CBA
17	a	840	CLA	C4-C3-C5-C6
17	b	803	CLA	C4-C3-C5-C6
17	j	102	CLA	C3A-C2A-CAA-CBA
17	a	828	CLA	C2-C3-C5-C6
17	a	835	CLA	O1A-CGA-O2A-C1
17	b	801	CLA	C5-C6-C7-C8
25	j	105	LMG	C28-C29-C30-C31
15	5	301	XAT	C7-C8-C9-C19
15	4	306	XAT	C27-C28-C29-C39
17	4	308	CLA	O1A-CGA-O2A-C1
17	a	826	CLA	O1D-CGD-O2D-CED
17	a	809	CLA	C2A-CAA-CBA-CGA
17	b	813	CLA	C5-C6-C7-C8
17	a	836	CLA	O1D-CGD-O2D-CED
18	1	315	SQD	O6-C44-C45-C46
22	a	846	LHG	C4-C5-C6-O8
17	b	836	CLA	C3-C5-C6-C7
17	4	309	CLA	C16-C17-C18-C19
17	a	805	CLA	C6-C7-C8-C10
17	b	819	CLA	C11-C12-C13-C15
17	j	102	CLA	C5-C6-C7-C8
17	a	828	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	b	814	CLA	C4-C3-C5-C6
17	a	801	CLA	C2-C3-C5-C6
17	b	807	CLA	C2-C3-C5-C6
17	a	827	CLA	C3-C5-C6-C7
17	1	310	CLA	C16-C17-C18-C20
19	b	851	DGD	O1B-C1B-O2G-C2G
17	1	309	CLA	C2B-C3B-CAB-CBB
17	a	825	CLA	C2B-C3B-CAB-CBB
17	a	837	CLA	C2B-C3B-CAB-CBB
17	a	841	CLA	C2B-C3B-CAB-CBB
17	b	818	CLA	C2B-C3B-CAB-CBB
17	j	102	CLA	C2B-C3B-CAB-CBB
23	b	844	BCR	C1-C6-C7-C8
23	m	102	BCR	C1-C6-C7-C8
17	b	823	CLA	C10-C11-C12-C13
17	a	830	CLA	C5-C6-C7-C8
22	a	845	LHG	C34-C35-C36-C37
17	a	806	CLA	C16-C17-C18-C20
17	b	807	CLA	C4-C3-C5-C6
17	5	309	CLA	C5-C6-C7-C8
17	a	820	CLA	C2-C3-C5-C6
17	b	814	CLA	C2-C3-C5-C6
17	a	820	CLA	C16-C17-C18-C19
17	a	803	CLA	C15-C16-C17-C18
17	1	308	CLA	C11-C12-C13-C14
17	1	310	CLA	C6-C7-C8-C9
17	1	310	CLA	C11-C10-C8-C9
17	a	807	CLA	C14-C13-C15-C16
17	a	829	CLA	C6-C7-C8-C9
17	b	802	CLA	C11-C10-C8-C9
17	b	825	CLA	C11-C12-C13-C14
17	b	833	CLA	C14-C13-C15-C16
19	b	851	DGD	C7A-C8A-C9A-CAA
17	4	318	CLA	C5-C6-C7-C8
17	a	841	CLA	O1A-CGA-O2A-C1
17	j	103	CLA	C1A-C2A-CAA-CBA
17	b	803	CLA	C13-C15-C16-C17
17	b	806	CLA	C10-C11-C12-C13
17	a	806	CLA	CBD-CGD-O2D-CED
20	1	304	A1L1F	C14-C29-C30-C31
17	b	812	CLA	O1A-CGA-O2A-C1
17	4	314	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	a	846	LHG	O6-C4-C5-C6
22	m	101	LHG	O6-C4-C5-C6
17	a	854	CLA	C8-C10-C11-C12
17	1	306	CLA	C6-C7-C8-C10
17	a	801	CLA	C6-C7-C8-C10
17	a	802	CLA	C6-C7-C8-C10
17	a	814	CLA	C6-C7-C8-C10
17	a	820	CLA	C11-C12-C13-C15
17	a	829	CLA	C11-C10-C8-C7
17	b	814	CLA	C11-C10-C8-C7
17	b	825	CLA	C6-C7-C8-C10
17	b	829	CLA	C12-C13-C15-C16
17	b	830	CLA	C12-C13-C15-C16
17	b	833	CLA	C12-C13-C15-C16
17	i	102	CLA	C11-C10-C8-C7
17	4	311	CLA	C15-C16-C17-C18
17	b	839	CLA	C13-C15-C16-C17
17	b	828	CLA	C16-C17-C18-C20
22	b	849	LHG	O9-C7-O7-C5
17	a	807	CLA	C4-C3-C5-C6
17	b	810	CLA	CAA-CBA-CGA-O2A
17	1	310	CLA	C2-C3-C5-C6
17	a	840	CLA	C2-C3-C5-C6
25	a	853	LMG	C12-C13-C14-C15
17	b	807	CLA	C5-C6-C7-C8
17	b	829	CLA	C5-C6-C7-C8
25	a	853	LMG	C9-C8-O7-C10
17	1	306	CLA	O1A-CGA-O2A-C1
17	a	831	CLA	O1A-CGA-O2A-C1
17	b	829	CLA	O1A-CGA-O2A-C1
19	b	851	DGD	O1A-C1A-O1G-C1G
17	1	310	CLA	O1A-CGA-O2A-C1
17	i	102	CLA	CBA-CGA-O2A-C1
17	a	842	CLA	C8-C10-C11-C12
18	1	315	SQD	C9-C10-C11-C12
17	1	306	CLA	C16-C17-C18-C20
17	1	310	CLA	C16-C17-C18-C19
17	b	805	CLA	C16-C17-C18-C19
17	a	827	CLA	C5-C6-C7-C8
17	b	835	CLA	C2-C3-C5-C6
17	1	306	CLA	C3-C5-C6-C7
17	1	306	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	a	801	CLA	C6-C7-C8-C9
17	a	802	CLA	C6-C7-C8-C9
17	a	820	CLA	C11-C12-C13-C14
17	a	840	CLA	C11-C10-C8-C9
17	b	802	CLA	C6-C7-C8-C9
17	b	802	CLA	C11-C12-C13-C14
17	b	804	CLA	C6-C7-C8-C9
17	b	806	CLA	C6-C7-C8-C9
17	b	814	CLA	C11-C10-C8-C9
17	b	839	CLA	C11-C12-C13-C14
17	b	839	CLA	C14-C13-C15-C16
22	a	845	LHG	C9-C10-C11-C12
17	4	314	CLA	O1A-CGA-O2A-C1
17	a	841	CLA	C13-C15-C16-C17
17	a	808	CLA	O1D-CGD-O2D-CED
17	b	808	CLA	C16-C17-C18-C20
17	b	818	CLA	C10-C11-C12-C13
17	b	810	CLA	C16-C17-C18-C19
17	j	102	CLA	O1D-CGD-O2D-CED
17	5	305	CLA	C4B-C3B-CAB-CBB
17	5	306	CLA	C4B-C3B-CAB-CBB
17	5	310	CLA	C4B-C3B-CAB-CBB
17	4	307	CLA	C4B-C3B-CAB-CBB
17	4	308	CLA	C4B-C3B-CAB-CBB
17	4	316	CLA	C4B-C3B-CAB-CBB
17	4	318	CLA	C4B-C3B-CAB-CBB
17	a	807	CLA	C4B-C3B-CAB-CBB
17	a	813	CLA	C4B-C3B-CAB-CBB
17	a	817	CLA	C4B-C3B-CAB-CBB
17	a	819	CLA	C4B-C3B-CAB-CBB
17	a	824	CLA	C1A-C2A-CAA-CBA
17	a	824	CLA	C4B-C3B-CAB-CBB
17	b	801	CLA	C4B-C3B-CAB-CBB
17	b	809	CLA	C4B-C3B-CAB-CBB
17	b	814	CLA	C1A-C2A-CAA-CBA
17	b	824	CLA	C1A-C2A-CAA-CBA
17	b	829	CLA	C4B-C3B-CAB-CBB
17	b	835	CLA	C4B-C3B-CAB-CBB
17	b	838	CLA	C4B-C3B-CAB-CBB
17	f	803	CLA	C4B-C3B-CAB-CBB
17	i	102	CLA	C4B-C3B-CAB-CBB
17	j	103	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	b	819	CLA	C8-C10-C11-C12
15	5	301	XAT	C7-C8-C9-C10
17	b	802	CLA	C2A-CAA-CBA-CGA
17	b	808	CLA	C2A-CAA-CBA-CGA
17	5	311	CLA	C2-C3-C5-C6
17	5	307	CLA	C11-C10-C8-C7
17	a	842	CLA	C12-C13-C15-C16
17	b	801	CLA	C11-C10-C8-C7
17	b	801	CLA	C12-C13-C15-C16
17	b	806	CLA	C11-C12-C13-C15
17	b	810	CLA	C11-C10-C8-C7
17	b	828	CLA	C11-C10-C8-C7
17	b	830	CLA	C11-C12-C13-C15
21	a	843	PQN	C22-C23-C25-C26
25	a	853	LMG	C31-C32-C33-C34
17	1	307	CLA	C5-C6-C7-C8
17	b	811	CLA	C3A-C2A-CAA-CBA
22	m	101	LHG	O6-C4-C5-O7
18	1	315	SQD	C13-C14-C15-C16
17	a	809	CLA	C6-C7-C8-C9
17	a	814	CLA	C6-C7-C8-C9
17	a	830	CLA	C8-C10-C11-C12
15	4	301	XAT	C29-C30-C31-C32
23	m	102	BCR	C13-C14-C15-C16
17	4	313	CLA	CBA-CGA-O2A-C1
17	a	823	CLA	C1-C2-C3-C4
17	b	832	CLA	C1-C2-C3-C4
17	b	815	CLA	C3-C5-C6-C7
17	i	102	CLA	O1A-CGA-O2A-C1
18	5	316	SQD	O47-C45-C46-O48
18	1	315	SQD	O6-C44-C45-O47
22	a	846	LHG	O7-C5-C6-O8
22	b	849	LHG	O7-C5-C6-O8
17	b	841	CLA	C15-C16-C17-C18
17	a	806	CLA	O1D-CGD-O2D-CED
18	5	316	SQD	C44-C45-C46-O48
17	a	809	CLA	C10-C11-C12-C13
17	1	313	CLA	CAD-CBD-CGD-O2D
17	a	814	CLA	CAD-CBD-CGD-O2D
17	a	839	CLA	CAD-CBD-CGD-O2D
17	a	844	CLA	CAD-CBD-CGD-O2D
17	b	833	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	b	837	CLA	CAD-CBD-CGD-O2D
17	1	311	CLA	CBA-CGA-O2A-C1
17	b	825	CLA	C2A-CAA-CBA-CGA
22	a	846	LHG	C10-C11-C12-C13
15	j	101	XAT	C9-C10-C11-C12
16	1	301	A1L1G	C37-C38-C39-C28
17	5	313	CLA	CHA-CBD-CGD-O1D
17	5	313	CLA	CHA-CBD-CGD-O2D
17	4	315	CLA	CHA-CBD-CGD-O1D
17	4	315	CLA	CHA-CBD-CGD-O2D
17	4	316	CLA	CAD-CBD-CGD-O1D
17	1	313	CLA	CAD-CBD-CGD-O1D
17	a	806	CLA	CAD-CBD-CGD-O1D
17	a	814	CLA	CAD-CBD-CGD-O1D
17	a	828	CLA	CAD-CBD-CGD-O1D
17	a	839	CLA	CAD-CBD-CGD-O1D
17	a	844	CLA	CAD-CBD-CGD-O1D
17	b	822	CLA	CHA-CBD-CGD-O1D
17	b	833	CLA	CAD-CBD-CGD-O1D
17	b	836	CLA	CAD-CBD-CGD-O1D
17	b	837	CLA	CAD-CBD-CGD-O1D
17	f	802	CLA	CAD-CBD-CGD-O1D
17	f	803	CLA	CHA-CBD-CGD-O2D
17	j	102	CLA	CHA-CBD-CGD-O1D
17	j	102	CLA	CHA-CBD-CGD-O2D
22	a	845	LHG	C3-O3-P-O5
22	a	846	LHG	C3-O3-P-O5
22	a	846	LHG	C4-O6-P-O3
22	a	846	LHG	C4-O6-P-O5
22	m	101	LHG	C3-O3-P-O5
22	m	101	LHG	C3-O3-P-O6
22	m	101	LHG	C4-O6-P-O3
22	m	101	LHG	C4-O6-P-O5
17	b	823	CLA	C3-C5-C6-C7
17	1	308	CLA	CBD-CGD-O2D-CED
17	a	841	CLA	C4-C3-C5-C6
17	5	306	CLA	C2B-C3B-CAB-CBB
17	5	310	CLA	C2B-C3B-CAB-CBB
17	4	318	CLA	C2B-C3B-CAB-CBB
17	1	314	CLA	C2B-C3B-CAB-CBB
17	a	819	CLA	C2B-C3B-CAB-CBB
17	b	801	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	b	835	CLA	C2B-C3B-CAB-CBB
17	b	838	CLA	C2B-C3B-CAB-CBB
17	b	841	CLA	C2B-C3B-CAB-CBB
17	i	102	CLA	C2B-C3B-CAB-CBB
23	l	201	BCR	C1-C6-C7-C8
17	a	807	CLA	C2-C3-C5-C6
17	b	839	CLA	C2-C3-C5-C6
17	a	834	CLA	C5-C6-C7-C8
17	b	825	CLA	C8-C10-C11-C12
17	1	308	CLA	C16-C17-C18-C19
17	b	808	CLA	C16-C17-C18-C19
17	a	821	CLA	C2A-CAA-CBA-CGA
17	b	803	CLA	C3-C5-C6-C7
17	b	840	CLA	C2C-C3C-CAC-CBC
22	m	101	LHG	C10-C11-C12-C13
17	a	830	CLA	C16-C17-C18-C19
18	1	315	SQD	C46-C45-O47-C7
17	b	805	CLA	CBA-CGA-O2A-C1
17	1	311	CLA	O1A-CGA-O2A-C1
17	5	309	CLA	C6-C7-C8-C9
17	4	309	CLA	C14-C13-C15-C16
17	a	807	CLA	C6-C7-C8-C9
17	a	812	CLA	C6-C7-C8-C9
17	b	803	CLA	C14-C13-C15-C16
17	b	804	CLA	C11-C12-C13-C14
17	b	807	CLA	C11-C12-C13-C14
17	b	810	CLA	C11-C10-C8-C9
17	b	829	CLA	C14-C13-C15-C16
17	b	802	CLA	C11-C12-C13-C15
17	b	807	CLA	C11-C12-C13-C15
17	a	839	CLA	C15-C16-C17-C18
17	b	805	CLA	O1A-CGA-O2A-C1
22	m	101	LHG	C13-C14-C15-C16
17	b	833	CLA	C2C-C3C-CAC-CBC
17	a	854	CLA	CBD-CGD-O2D-CED
17	b	818	CLA	O1A-CGA-O2A-C1
17	b	828	CLA	C10-C11-C12-C13
17	b	818	CLA	CBA-CGA-O2A-C1
17	1	305	CLA	C2A-CAA-CBA-CGA
17	1	308	CLA	C2A-CAA-CBA-CGA
17	a	802	CLA	C4-C3-C5-C6
17	b	828	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	1	311	CLA	O1D-CGD-O2D-CED
17	a	801	CLA	CAA-CBA-CGA-O2A
22	b	849	LHG	C25-C26-C27-C28
17	b	801	CLA	O1A-CGA-O2A-C1
18	5	316	SQD	C7-C8-C9-C10
17	4	318	CLA	C2A-CAA-CBA-CGA
17	a	813	CLA	C2A-CAA-CBA-CGA
17	b	828	CLA	C2A-CAA-CBA-CGA
16	1	301	A1L1G	C40-C41-C42-C44
17	a	841	CLA	C2-C3-C5-C6
17	b	803	CLA	C16-C17-C18-C20
17	a	801	CLA	C14-C13-C15-C16
17	a	826	CLA	C11-C10-C8-C9
17	a	842	CLA	C14-C13-C15-C16
17	b	828	CLA	C11-C10-C8-C9
21	a	843	PQN	C24-C23-C25-C26
17	1	308	CLA	O1D-CGD-O2D-CED
17	b	801	CLA	CBA-CGA-O2A-C1
17	a	854	CLA	C15-C16-C17-C18
17	a	832	CLA	C4B-C3B-CAB-CBB
17	b	831	CLA	C4B-C3B-CAB-CBB
17	5	307	CLA	C8-C10-C11-C12
17	a	813	CLA	CBA-CGA-O2A-C1
17	a	830	CLA	C15-C16-C17-C18
17	a	813	CLA	O1A-CGA-O2A-C1
17	5	315	CLA	CAA-CBA-CGA-O2A
17	a	802	CLA	C2-C3-C5-C6
17	b	802	CLA	C2-C3-C5-C6
17	a	830	CLA	C16-C17-C18-C20
17	a	826	CLA	C11-C10-C8-C7
17	a	831	CLA	C11-C10-C8-C7
17	b	802	CLA	C12-C13-C15-C16
17	f	802	CLA	C6-C7-C8-C10
17	1	308	CLA	C16-C17-C18-C20
19	b	851	DGD	O2G-C2G-C3G-O3G
17	a	830	CLA	C4-C3-C5-C6
17	b	814	CLA	C3A-C2A-CAA-CBA
17	b	832	CLA	C3A-C2A-CAA-CBA
17	a	854	CLA	O1D-CGD-O2D-CED
17	5	310	CLA	CAA-CBA-CGA-O1A
23	b	845	BCR	C11-C10-C9-C34
23	b	845	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	f	804	BCR	C35-C13-C14-C15
23	l	201	BCR	C11-C10-C9-C34
17	a	812	CLA	C3-C5-C6-C7
17	5	306	CLA	CAA-CBA-CGA-O1A
17	b	840	CLA	C16-C17-C18-C20
17	a	820	CLA	C13-C15-C16-C17
17	5	311	CLA	C4-C3-C5-C6
17	b	814	CLA	C10-C11-C12-C13
17	4	311	CLA	CBD-CGD-O2D-CED
17	5	307	CLA	C11-C10-C8-C9
17	1	310	CLA	C11-C12-C13-C14
17	a	822	CLA	C11-C10-C8-C9
17	a	829	CLA	C11-C12-C13-C14
17	a	831	CLA	C6-C7-C8-C9
17	a	831	CLA	C11-C10-C8-C9
17	a	844	CLA	C6-C7-C8-C9
17	a	854	CLA	C11-C10-C8-C9
17	b	808	CLA	C6-C7-C8-C9
22	a	845	LHG	C25-C26-C27-C28
17	a	839	CLA	C16-C17-C18-C20
17	a	832	CLA	CBD-CGD-O2D-CED
17	b	841	CLA	O1A-CGA-O2A-C1
17	4	315	CLA	CAA-CBA-CGA-O1A
17	4	315	CLA	CAA-CBA-CGA-O2A
17	5	309	CLA	C2A-CAA-CBA-CGA
17	a	803	CLA	C2A-CAA-CBA-CGA
17	b	811	CLA	C2A-CAA-CBA-CGA
17	4	312	CLA	C1A-C2A-CAA-CBA
17	4	317	CLA	C1A-C2A-CAA-CBA
17	b	816	CLA	C1A-C2A-CAA-CBA
17	b	835	CLA	C1A-C2A-CAA-CBA
23	b	845	BCR	C11-C10-C9-C8
23	b	845	BCR	C20-C21-C22-C23
23	f	804	BCR	C12-C13-C14-C15
23	l	201	BCR	C11-C10-C9-C8
17	a	801	CLA	O1A-CGA-O2A-C1
17	5	305	CLA	C2B-C3B-CAB-CBB
17	5	308	CLA	C2B-C3B-CAB-CBB
17	4	307	CLA	C2B-C3B-CAB-CBB
17	4	308	CLA	C2B-C3B-CAB-CBB
17	4	316	CLA	C2B-C3B-CAB-CBB
17	1	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	1	313	CLA	C2B-C3B-CAB-CBB
17	a	801	CLA	C2B-C3B-CAB-CBB
17	a	807	CLA	C2B-C3B-CAB-CBB
17	a	810	CLA	C2B-C3B-CAB-CBB
17	a	813	CLA	C2B-C3B-CAB-CBB
17	a	817	CLA	C2B-C3B-CAB-CBB
17	a	824	CLA	C2B-C3B-CAB-CBB
17	a	832	CLA	C2B-C3B-CAB-CBB
17	b	809	CLA	C2B-C3B-CAB-CBB
17	b	829	CLA	C2B-C3B-CAB-CBB
17	b	831	CLA	C2B-C3B-CAB-CBB
17	f	803	CLA	C2B-C3B-CAB-CBB
17	j	103	CLA	C2B-C3B-CAB-CBB
23	b	844	BCR	C5-C6-C7-C8
23	b	852	BCR	C23-C24-C25-C30
23	l	205	BCR	C1-C6-C7-C8
23	m	102	BCR	C5-C6-C7-C8
17	5	306	CLA	CAA-CBA-CGA-O2A
17	a	801	CLA	CBA-CGA-O2A-C1
17	b	841	CLA	CBA-CGA-O2A-C1
17	b	808	CLA	C4-C3-C5-C6
17	a	832	CLA	O1D-CGD-O2D-CED
17	a	830	CLA	C2-C3-C5-C6
17	5	313	CLA	CAA-CBA-CGA-O1A
17	b	809	CLA	C2A-CAA-CBA-CGA
17	a	817	CLA	CAA-CBA-CGA-O1A
22	a	845	LHG	C14-C15-C16-C17
17	1	305	CLA	C3-C5-C6-C7
17	a	817	CLA	CAA-CBA-CGA-O2A
22	m	101	LHG	C15-C16-C17-C18
22	a	846	LHG	C1-C2-C3-O3
17	1	307	CLA	C6-C7-C8-C9
17	b	818	CLA	CBD-CGD-O2D-CED
17	b	808	CLA	C2-C3-C5-C6
17	b	840	CLA	C4C-C3C-CAC-CBC
17	4	311	CLA	O1D-CGD-O2D-CED
17	b	838	CLA	C11-C12-C13-C14
17	4	311	CLA	C13-C15-C16-C17
25	a	853	LMG	C11-C12-C13-C14
17	5	313	CLA	CAA-CBA-CGA-O2A
17	a	835	CLA	C4-C3-C5-C6
17	a	835	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	4	307	CLA	C2A-CAA-CBA-CGA
18	1	315	SQD	C15-C16-C17-C18
17	5	310	CLA	CBA-CGA-O2A-C1
17	5	314	CLA	C4-C3-C5-C6
17	b	834	CLA	C4-C3-C5-C6
17	a	819	CLA	CAA-CBA-CGA-O2A
17	a	826	CLA	C13-C15-C16-C17
17	4	311	CLA	C4B-C3B-CAB-CBB
17	a	810	CLA	C4B-C3B-CAB-CBB
17	a	842	CLA	O1A-CGA-O2A-C1
17	1	306	CLA	C16-C17-C18-C19
17	a	830	CLA	O1A-CGA-O2A-C1
17	1	314	CLA	CAA-CBA-CGA-O2A
17	a	804	CLA	O1A-CGA-O2A-C1
17	5	307	CLA	C11-C12-C13-C14
17	b	814	CLA	C16-C17-C18-C19
17	b	818	CLA	O1D-CGD-O2D-CED
17	b	802	CLA	C10-C11-C12-C13
17	1	314	CLA	CAA-CBA-CGA-O1A
17	a	813	CLA	C6-C7-C8-C9
17	a	828	CLA	C14-C13-C15-C16
17	a	839	CLA	C6-C7-C8-C9
17	a	840	CLA	C14-C13-C15-C16
17	b	806	CLA	C11-C12-C13-C14
17	b	830	CLA	C11-C12-C13-C14
17	5	307	CLA	C2A-CAA-CBA-CGA
17	a	839	CLA	C2A-CAA-CBA-CGA
17	a	830	CLA	CBA-CGA-O2A-C1
17	a	842	CLA	CBA-CGA-O2A-C1
17	4	307	CLA	C3A-C2A-CAA-CBA
17	1	310	CLA	C3A-C2A-CAA-CBA
17	b	809	CLA	C3A-C2A-CAA-CBA
17	b	814	CLA	C5-C6-C7-C8
19	b	851	DGD	C1B-C2B-C3B-C4B
17	b	814	CLA	C13-C15-C16-C17
17	1	204	CLA	CAA-CBA-CGA-O2A
25	j	105	LMG	C11-C12-C13-C14
15	5	301	XAT	O4-C6-C7-C8
15	5	304	XAT	O24-C26-C27-C28
15	4	301	XAT	O4-C6-C7-C8
15	4	306	XAT	O4-C6-C7-C8
17	b	834	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	a	843	PQN	C18-C20-C21-C22
17	b	811	CLA	C8-C10-C11-C12
17	a	804	CLA	CBA-CGA-O2A-C1
17	4	309	CLA	C3-C5-C6-C7
17	a	804	CLA	C6-C7-C8-C9
22	m	101	LHG	C35-C36-C37-C38
17	4	307	CLA	CAA-CBA-CGA-O2A
17	4	309	CLA	C6-C7-C8-C9
17	4	313	CLA	O1A-CGA-O2A-C1
15	a	852	XAT	C31-C32-C33-C34
17	b	803	CLA	C10-C11-C12-C13
17	4	310	CLA	CAA-CBA-CGA-O2A
17	a	829	CLA	CAA-CBA-CGA-O2A
17	b	803	CLA	CAA-CBA-CGA-O2A
17	b	819	CLA	C2A-CAA-CBA-CGA
17	1	305	CLA	C11-C10-C8-C7
17	a	801	CLA	C11-C10-C8-C7
17	a	835	CLA	C11-C12-C13-C15
17	a	839	CLA	C6-C7-C8-C10
17	a	840	CLA	C12-C13-C15-C16
17	b	838	CLA	C11-C12-C13-C15
17	b	819	CLA	C2B-C3B-CAB-CBB
23	b	848	BCR	C1-C6-C7-C8
23	b	848	BCR	C5-C6-C7-C8
23	b	852	BCR	C23-C24-C25-C26
23	f	804	BCR	C23-C24-C25-C26
23	f	804	BCR	C23-C24-C25-C30
23	j	104	BCR	C1-C6-C7-C8
23	l	201	BCR	C5-C6-C7-C8
23	l	205	BCR	C5-C6-C7-C8
17	5	311	CLA	C2-C1-O2A-CGA
17	a	814	CLA	C2-C1-O2A-CGA
17	a	822	CLA	C2-C1-O2A-CGA
17	b	810	CLA	C2-C1-O2A-CGA
17	b	825	CLA	C10-C11-C12-C13
17	1	306	CLA	CAA-CBA-CGA-O2A
17	1	309	CLA	CAA-CBA-CGA-O2A
17	a	818	CLA	CAA-CBA-CGA-O2A
17	b	838	CLA	CAA-CBA-CGA-O2A
17	a	827	CLA	C10-C11-C12-C13
17	b	801	CLA	CAA-CBA-CGA-O2A
17	4	309	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	b	836	CLA	C4C-C3C-CAC-CBC
17	j	102	CLA	C3-C5-C6-C7
17	b	807	CLA	C16-C17-C18-C19
18	1	315	SQD	O47-C7-C8-C9
18	5	316	SQD	C4-C5-C6-S
17	a	829	CLA	C2A-CAA-CBA-CGA
17	a	801	CLA	C11-C10-C8-C9
17	a	801	CLA	C11-C12-C13-C14
17	b	803	CLA	C5-C6-C7-C8
17	b	807	CLA	CAA-CBA-CGA-O2A
25	j	105	LMG	C7-C8-C9-O8
17	4	317	CLA	C4B-C3B-CAB-CBB
17	a	803	CLA	C1A-C2A-CAA-CBA
17	a	814	CLA	C1A-C2A-CAA-CBA
17	a	840	CLA	C4B-C3B-CAB-CBB
17	b	803	CLA	C4B-C3B-CAB-CBB
17	b	823	CLA	C1A-C2A-CAA-CBA
17	b	826	CLA	C1A-C2A-CAA-CBA
17	4	307	CLA	CAA-CBA-CGA-O1A
23	m	102	BCR	C22-C23-C24-C25
17	a	810	CLA	CAA-CBA-CGA-O2A
23	f	801	BCR	C17-C18-C19-C20
17	b	810	CLA	CAA-CBA-CGA-O1A
17	a	836	CLA	CAA-CBA-CGA-O2A
17	b	818	CLA	CAA-CBA-CGA-O2A
17	a	841	CLA	C2A-CAA-CBA-CGA
17	b	839	CLA	C3-C5-C6-C7
17	b	820	CLA	C6-C7-C8-C9
17	b	809	CLA	CAA-CBA-CGA-O2A
17	b	833	CLA	CAA-CBA-CGA-O2A
22	m	101	LHG	O1-C1-C2-C3
17	a	810	CLA	C2-C1-O2A-CGA
17	1	312	CLA	CAA-CBA-CGA-O2A
17	1	310	CLA	C12-C13-C15-C16
17	a	801	CLA	C11-C12-C13-C15
17	a	834	CLA	C11-C12-C13-C15
17	b	805	CLA	C11-C12-C13-C15
17	b	819	CLA	C11-C10-C8-C7
17	l	203	CLA	C6-C7-C8-C10
17	a	826	CLA	C10-C11-C12-C13
17	b	810	CLA	C16-C17-C18-C20
22	m	101	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
17	a	834	CLA	C10-C11-C12-C13
17	a	814	CLA	C16-C17-C18-C19
22	m	101	LHG	C30-C31-C32-C33
17	a	801	CLA	C5-C6-C7-C8
17	j	102	CLA	CAA-CBA-CGA-O2A
17	b	838	CLA	CAA-CBA-CGA-O1A
17	j	102	CLA	C10-C11-C12-C13
17	1	306	CLA	C3A-C2A-CAA-CBA
17	a	814	CLA	C3A-C2A-CAA-CBA
17	5	309	CLA	C15-C16-C17-C18
17	a	810	CLA	C16-C17-C18-C20
22	a	845	LHG	O8-C23-C24-C25
17	4	311	CLA	C8-C10-C11-C12
17	b	818	CLA	CAA-CBA-CGA-O1A
17	a	818	CLA	CAA-CBA-CGA-O1A
17	b	801	CLA	CAA-CBA-CGA-O1A
17	a	834	CLA	C11-C12-C13-C14
17	f	802	CLA	C6-C7-C8-C9
17	4	310	CLA	CAA-CBA-CGA-O1A
18	1	315	SQD	O49-C7-C8-C9
18	5	316	SQD	O5-C5-C6-S
17	b	825	CLA	C15-C16-C17-C18
23	i	101	BCR	C17-C18-C19-C20
17	b	807	CLA	CAA-CBA-CGA-O1A
18	5	316	SQD	C10-C11-C12-C13
17	b	833	CLA	CAA-CBA-CGA-O1A
17	a	813	CLA	CAA-CBA-CGA-O2A
17	b	809	CLA	CAA-CBA-CGA-O1A
17	5	314	CLA	CAD-CBD-CGD-O2D
17	a	810	CLA	CAD-CBD-CGD-O2D
17	a	816	CLA	CAD-CBD-CGD-O2D
17	a	828	CLA	CAD-CBD-CGD-O2D
17	a	832	CLA	CAD-CBD-CGD-O2D
17	a	854	CLA	CAD-CBD-CGD-O2D
17	b	836	CLA	CAD-CBD-CGD-O2D
17	1	312	CLA	CAA-CBA-CGA-O1A
17	a	836	CLA	CAA-CBA-CGA-O1A
17	b	814	CLA	CBD-CGD-O2D-CED
17	a	816	CLA	C2-C1-O2A-CGA
17	a	839	CLA	C2-C1-O2A-CGA
17	a	826	CLA	C8-C10-C11-C12
17	b	830	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	a	835	CLA	CAA-CBA-CGA-O2A
17	b	804	CLA	CAA-CBA-CGA-O2A
17	a	813	CLA	CBD-CGD-O2D-CED
17	a	840	CLA	C16-C17-C18-C19
17	j	102	CLA	CAA-CBA-CGA-O1A
18	1	315	SQD	C12-C13-C14-C15
17	a	820	CLA	CBD-CGD-O2D-CED
17	a	810	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

158 monomers are involved in 480 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	304	XAT	9	0
17	b	830	CLA	4	0
17	a	804	CLA	4	0
17	4	307	CLA	2	0
17	1	312	CLA	2	0
17	a	824	CLA	1	0
17	4	312	CLA	1	0
17	a	841	CLA	7	0
17	1	311	CLA	2	0
17	b	834	CLA	5	0
17	a	803	CLA	4	0
17	4	311	CLA	6	0
17	a	830	CLA	7	0
15	5	302	XAT	10	0
17	b	813	CLA	4	0
17	b	829	CLA	3	0
17	a	810	CLA	4	0
17	a	813	CLA	1	0
17	a	835	CLA	5	0
16	1	301	A1L1G	1	0
17	4	314	CLA	4	0
23	1	205	BCR	11	0
17	5	315	CLA	2	0
17	a	818	CLA	10	0
17	a	825	CLA	4	0
17	a	838	CLA	1	0
17	b	801	CLA	4	0
25	j	105	LMG	7	0
17	b	802	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	b	818	CLA	7	0
17	b	812	CLA	2	0
17	a	806	CLA	7	0
17	b	827	CLA	4	0
17	4	315	CLA	1	0
15	a	852	XAT	5	0
17	5	307	CLA	7	0
17	a	854	CLA	3	0
17	a	844	CLA	5	0
17	b	831	CLA	5	0
23	i	101	BCR	2	0
19	4	319	DGD	11	0
17	a	833	CLA	2	0
17	b	817	CLA	4	0
17	b	823	CLA	5	0
17	1	310	CLA	1	0
17	j	102	CLA	5	0
21	b	842	PQN	2	0
17	b	804	CLA	4	0
15	5	304	XAT	5	0
15	1	303	XAT	3	0
17	a	802	CLA	5	0
17	b	839	CLA	5	0
17	a	823	CLA	3	0
17	b	811	CLA	6	0
17	a	837	CLA	1	0
17	a	819	CLA	6	0
17	a	842	CLA	5	0
15	4	301	XAT	4	0
17	1	308	CLA	4	0
15	5	301	XAT	5	0
17	b	815	CLA	3	0
17	l	202	CLA	1	0
17	a	839	CLA	6	0
17	b	822	CLA	3	0
17	b	841	CLA	4	0
17	4	310	CLA	3	0
25	a	853	LMG	11	0
17	b	828	CLA	4	0
17	4	317	CLA	1	0
19	b	851	DGD	6	0
23	b	845	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	306	CLA	6	0
23	b	848	BCR	2	0
17	a	815	CLA	1	0
23	j	104	BCR	8	0
23	f	801	BCR	9	0
17	a	834	CLA	7	0
17	a	816	CLA	2	0
15	4	302	XAT	5	0
17	a	822	CLA	5	0
17	b	806	CLA	2	0
23	f	804	BCR	5	0
17	4	313	CLA	1	0
22	a	846	LHG	3	0
17	b	805	CLA	3	0
17	j	103	CLA	2	0
17	b	835	CLA	1	0
15	4	303	XAT	3	0
17	b	807	CLA	7	0
23	b	844	BCR	2	0
17	5	309	CLA	4	0
17	b	814	CLA	7	0
17	b	825	CLA	6	0
17	5	311	CLA	1	0
23	b	843	BCR	3	0
23	b	847	BCR	7	0
17	4	309	CLA	8	0
17	f	802	CLA	1	0
17	a	826	CLA	6	0
17	4	308	CLA	2	0
17	b	809	CLA	4	0
17	b	824	CLA	6	0
17	a	809	CLA	3	0
17	a	807	CLA	4	0
17	5	310	CLA	2	0
17	b	808	CLA	1	0
17	a	814	CLA	3	0
23	a	848	BCR	5	0
23	b	846	BCR	2	0
17	5	312	CLA	3	0
23	a	847	BCR	2	0
17	b	803	CLA	2	0
15	4	306	XAT	4	0

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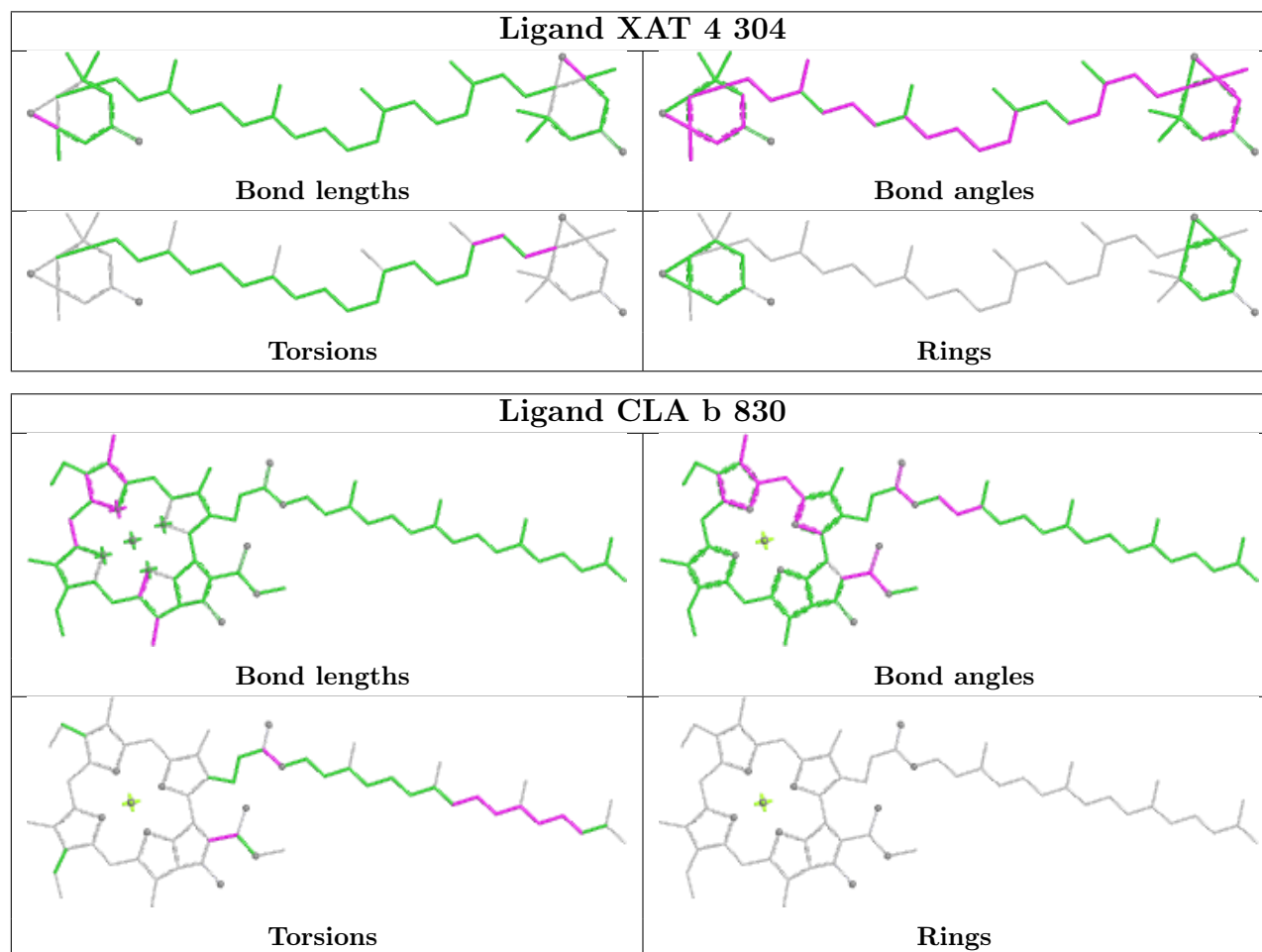
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	j	101	XAT	5	0
22	m	101	LHG	1	0
17	b	837	CLA	6	0
17	a	831	CLA	6	0
23	l	201	BCR	5	0
17	b	821	CLA	2	0
23	b	852	BCR	5	0
17	b	836	CLA	4	0
17	a	828	CLA	5	0
17	b	810	CLA	1	0
18	1	315	SQD	3	0
17	a	829	CLA	6	0
15	1	302	XAT	4	0
18	5	316	SQD	1	0
20	1	304	A1L1F	2	0
23	m	102	BCR	3	0
17	b	833	CLA	3	0
22	a	845	LHG	3	0
23	b	850	BCR	4	0
17	b	832	CLA	2	0
17	b	838	CLA	5	0
17	b	820	CLA	2	0
17	b	840	CLA	3	0
17	a	808	CLA	1	0
23	a	850	BCR	4	0
17	a	832	CLA	2	0
17	a	820	CLA	6	0
17	l	203	CLA	2	0
17	a	840	CLA	6	0
17	a	827	CLA	3	0
17	5	305	CLA	2	0
17	a	805	CLA	3	0
17	5	314	CLA	1	0
17	4	318	CLA	5	0
17	5	308	CLA	2	0
16	5	303	A1L1G	1	0
17	b	826	CLA	3	0
17	b	819	CLA	3	0
17	4	316	CLA	1	0
17	i	102	CLA	4	0
17	a	801	CLA	6	0
24	c	102	SF4	3	0

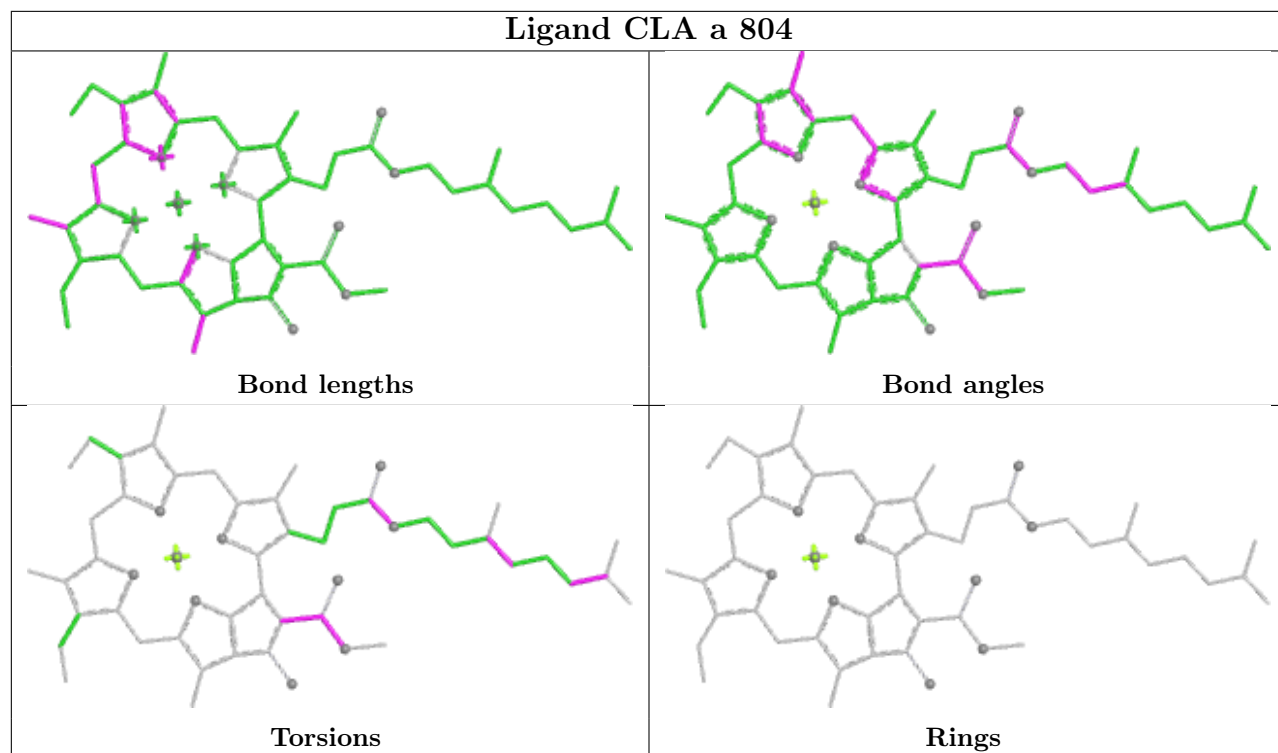
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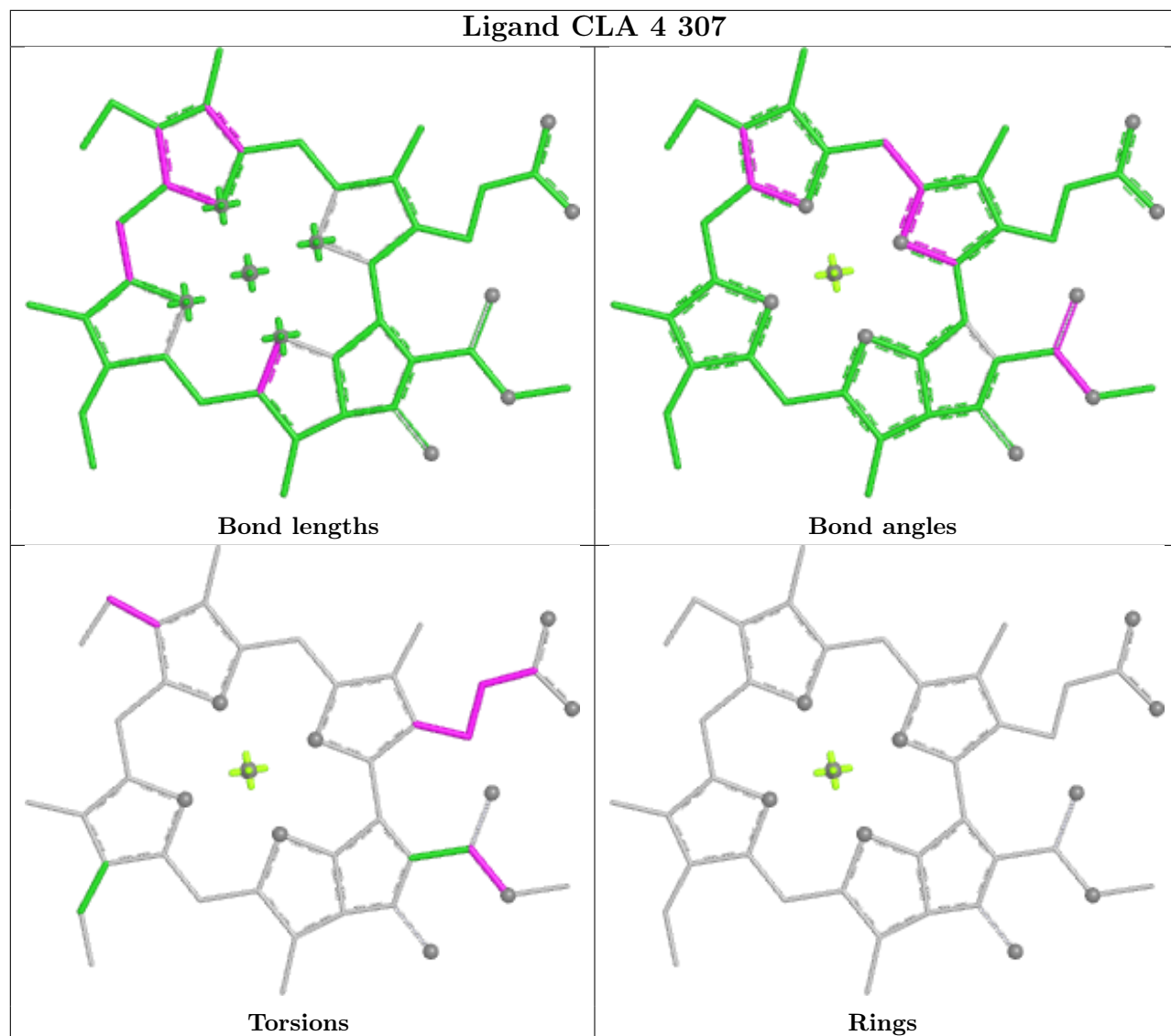
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	a	843	PQN	3	0
23	a	849	BCR	2	0

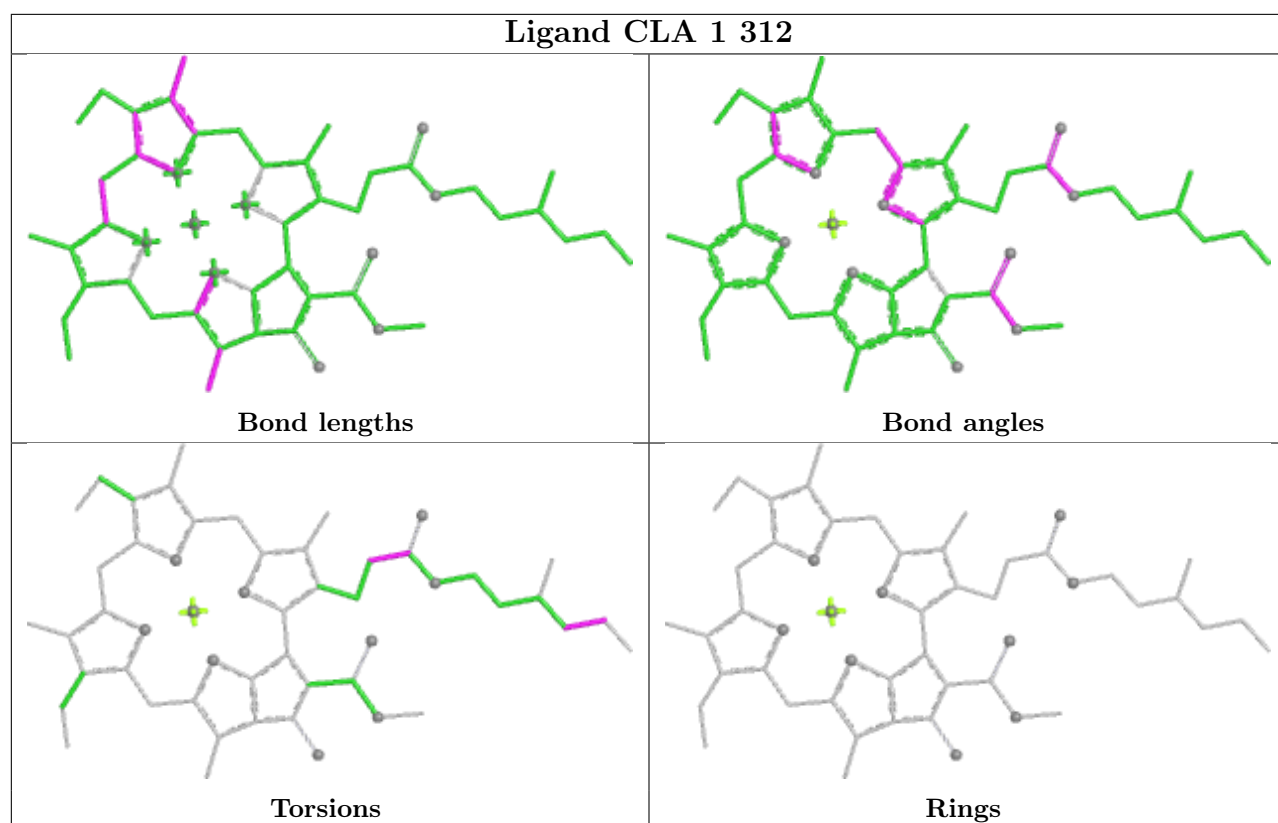
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



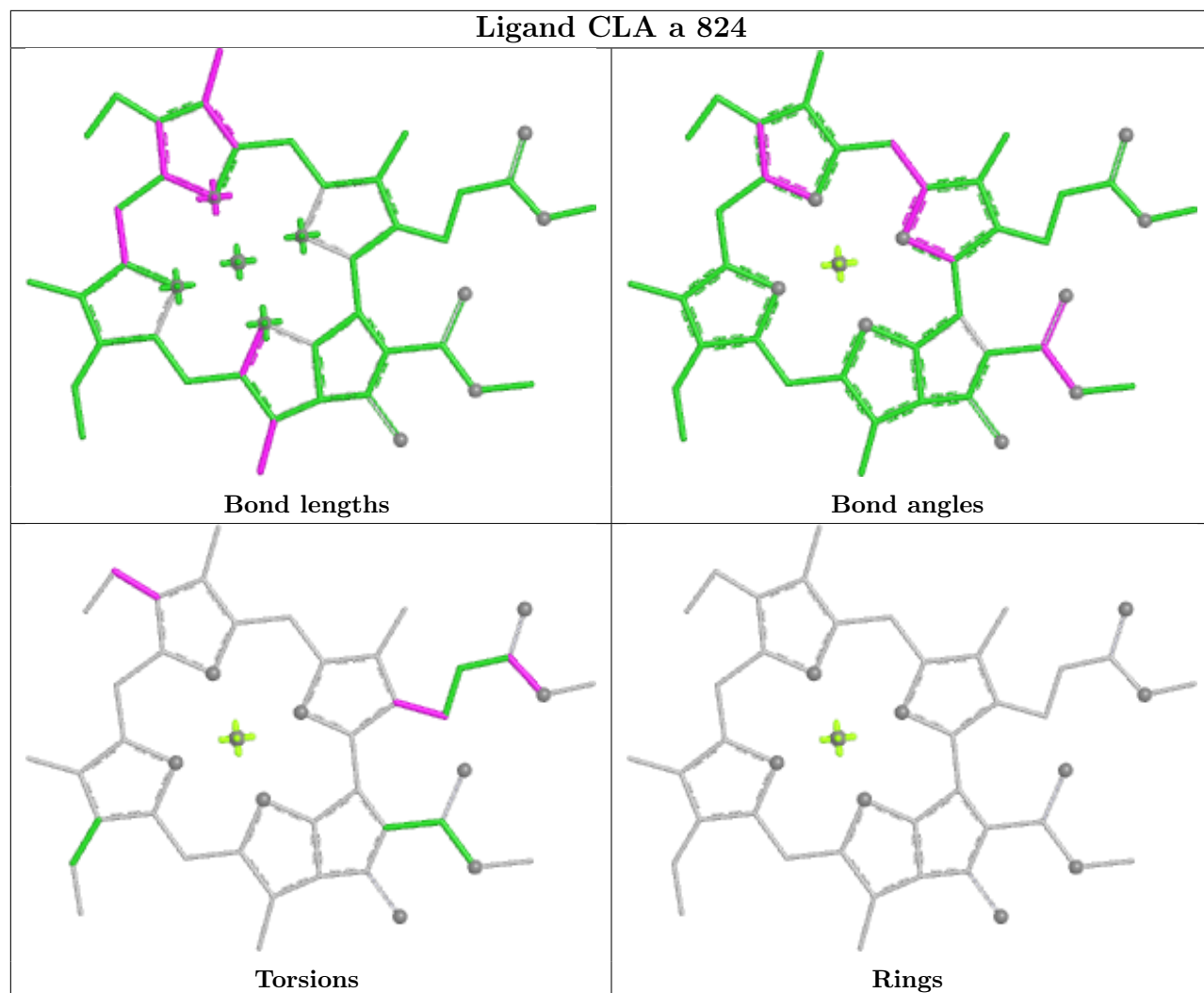


Ligand CLA 4 307

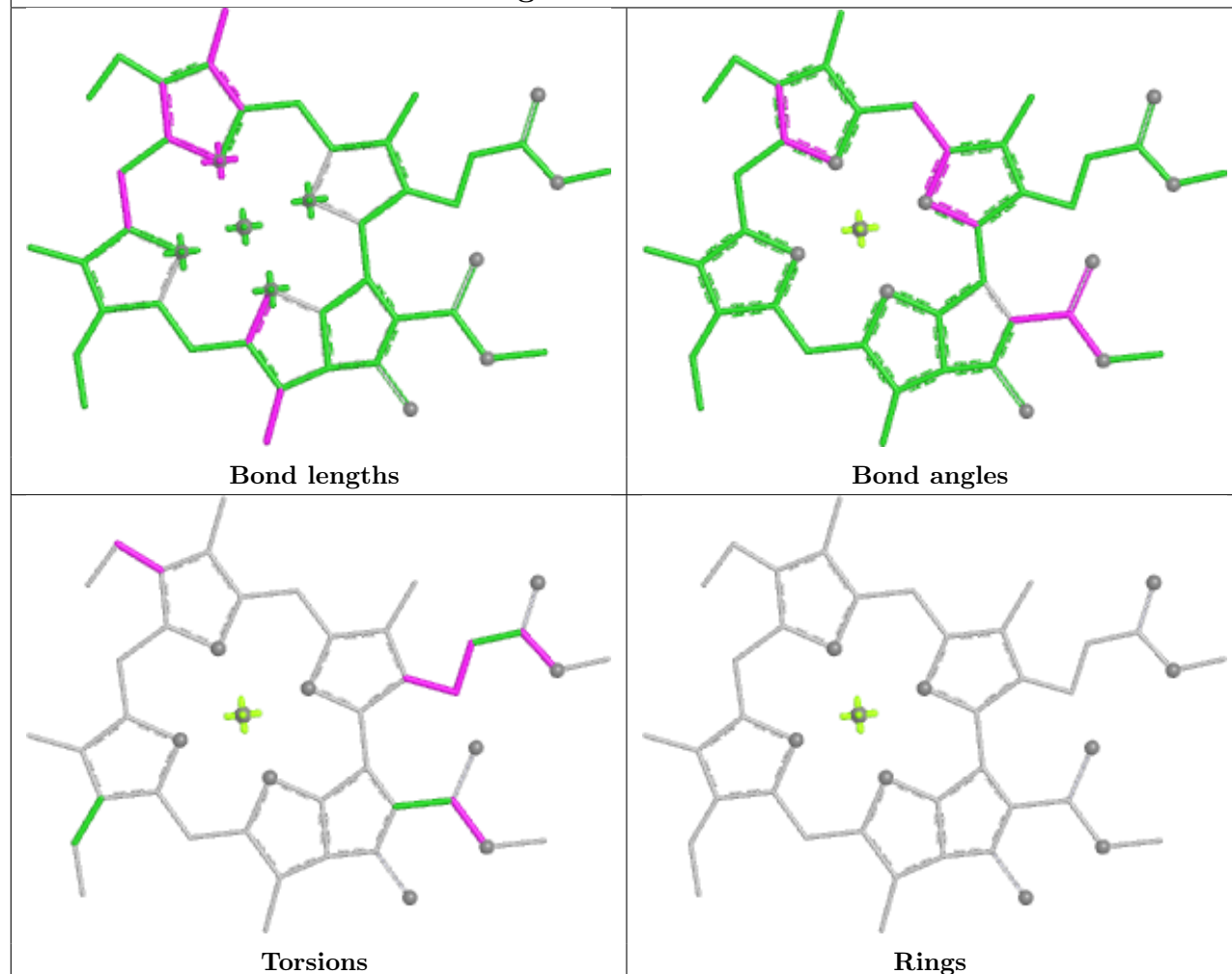




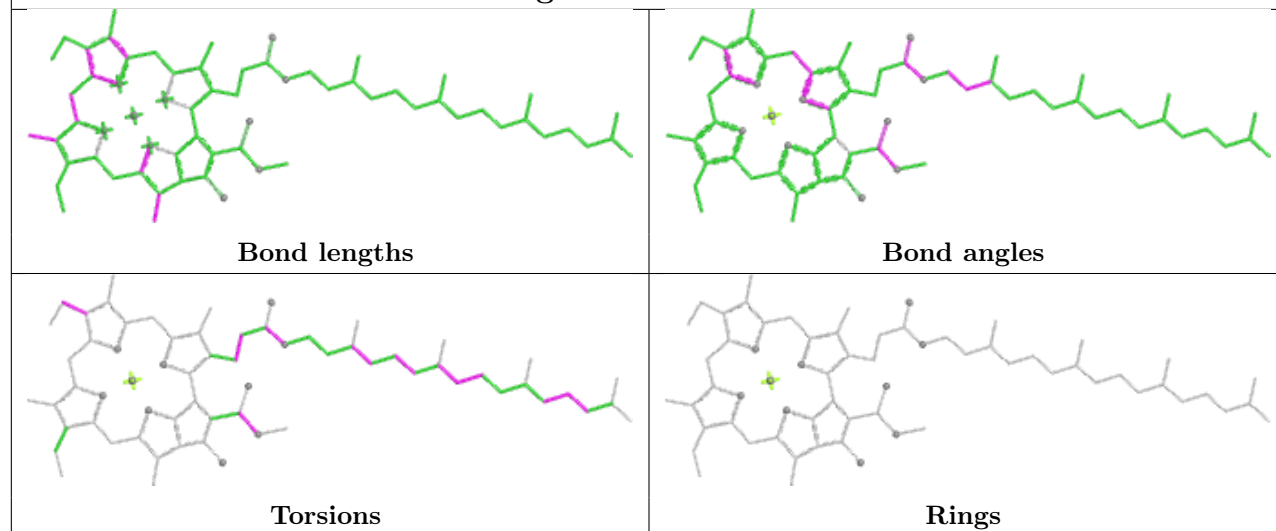
Ligand CLA a 824

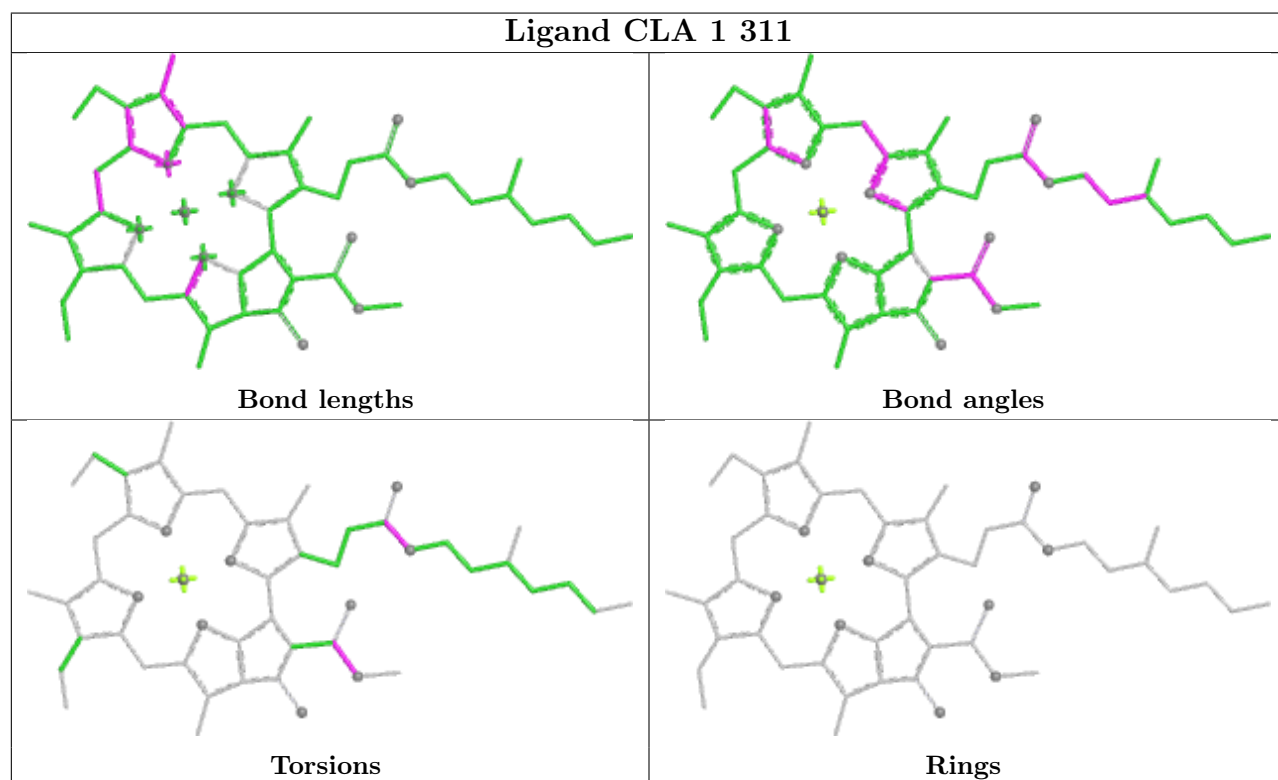
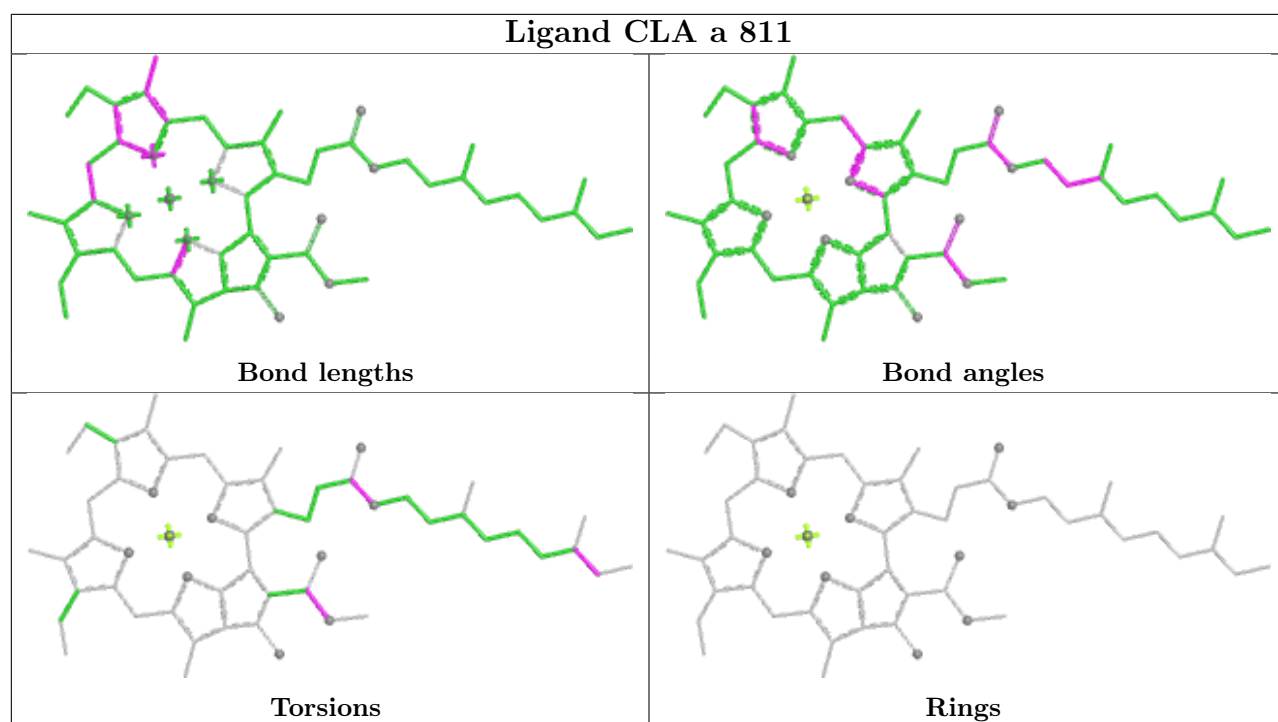


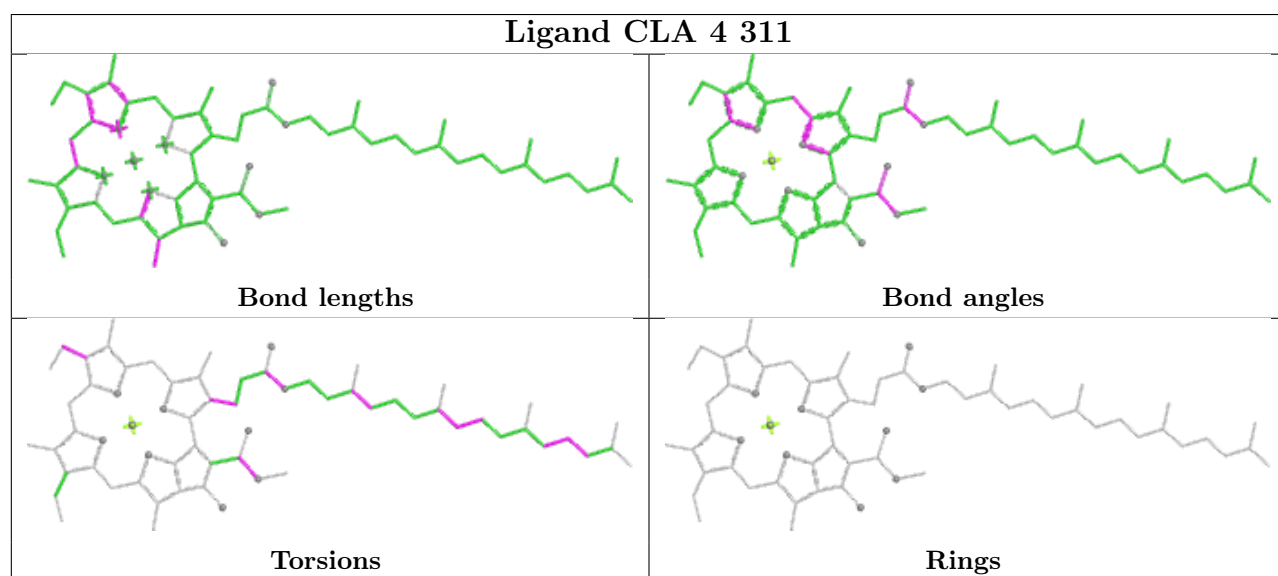
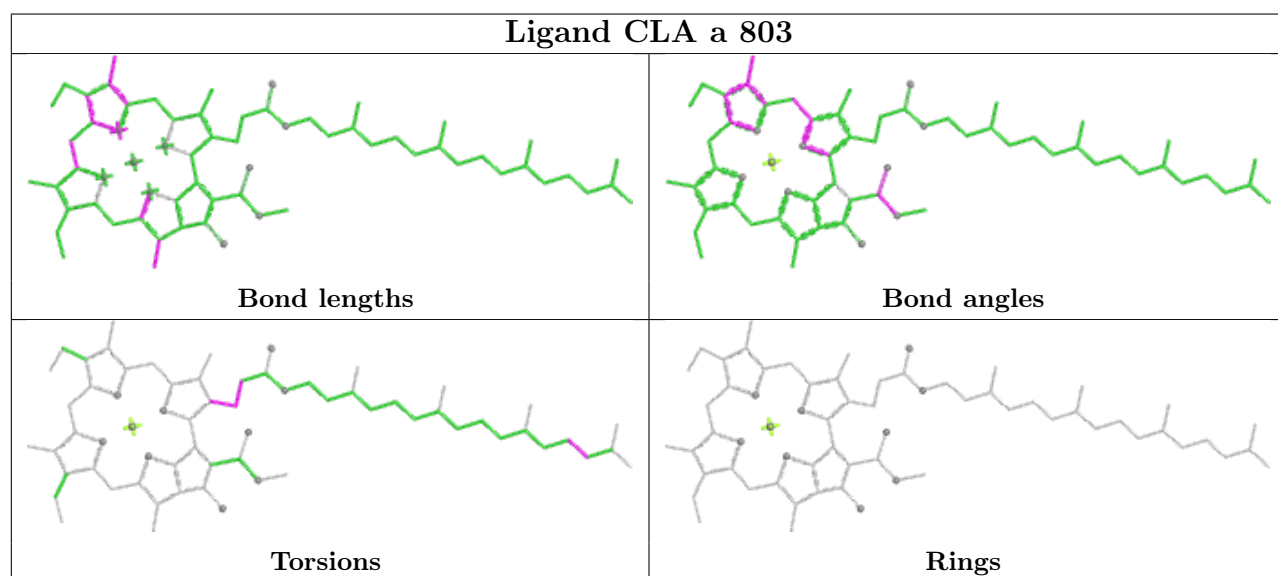
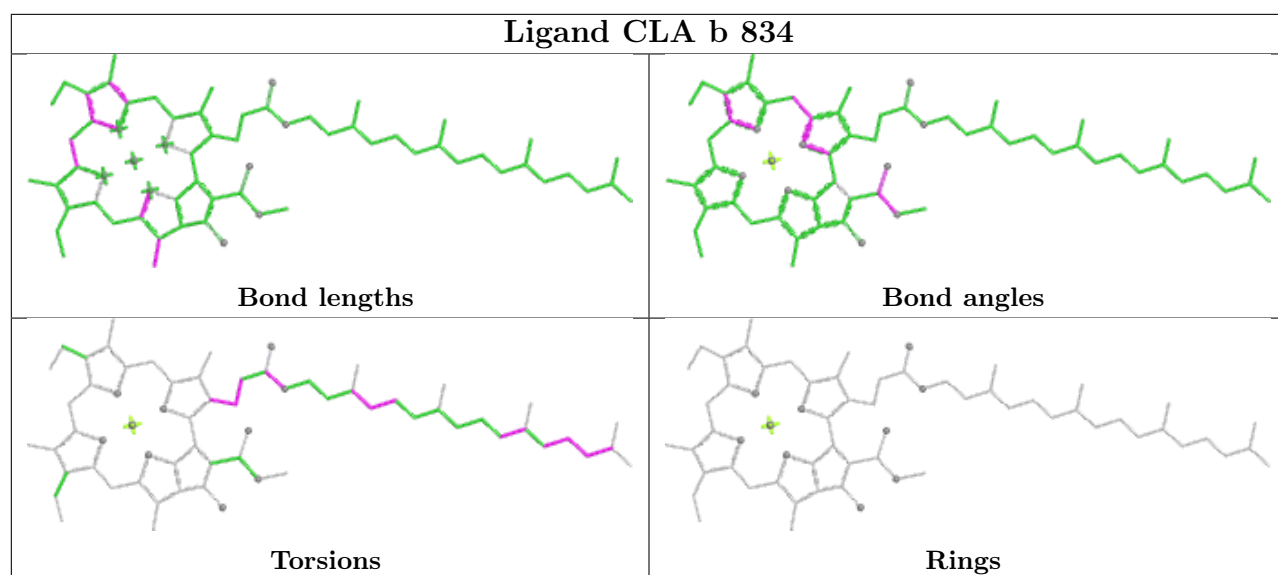
Ligand CLA 4 312

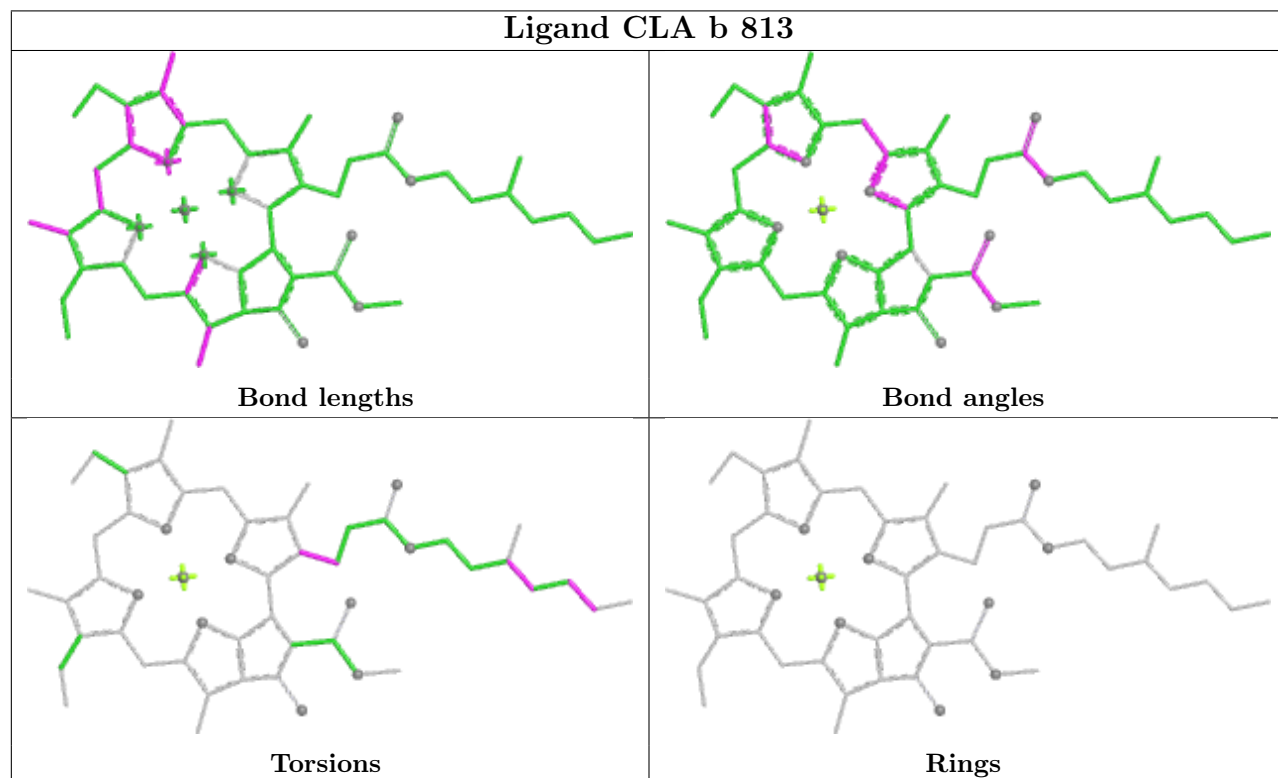
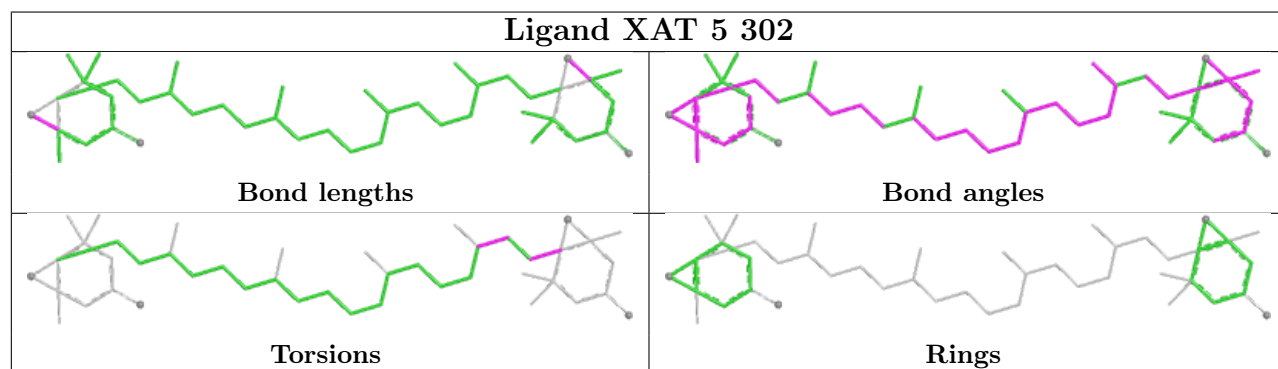
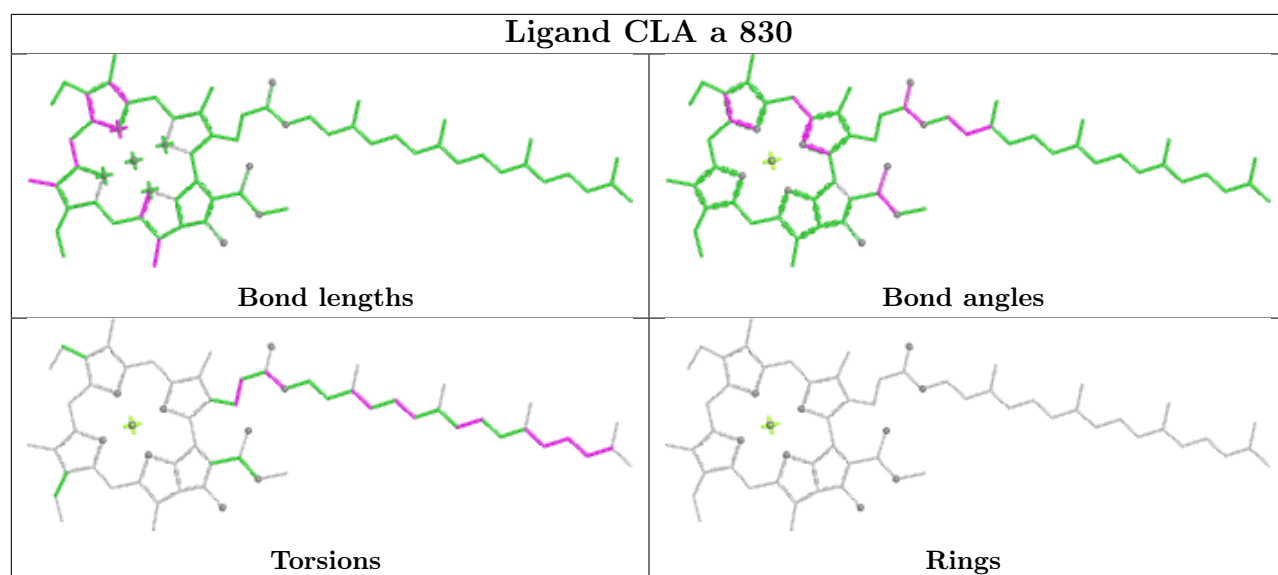


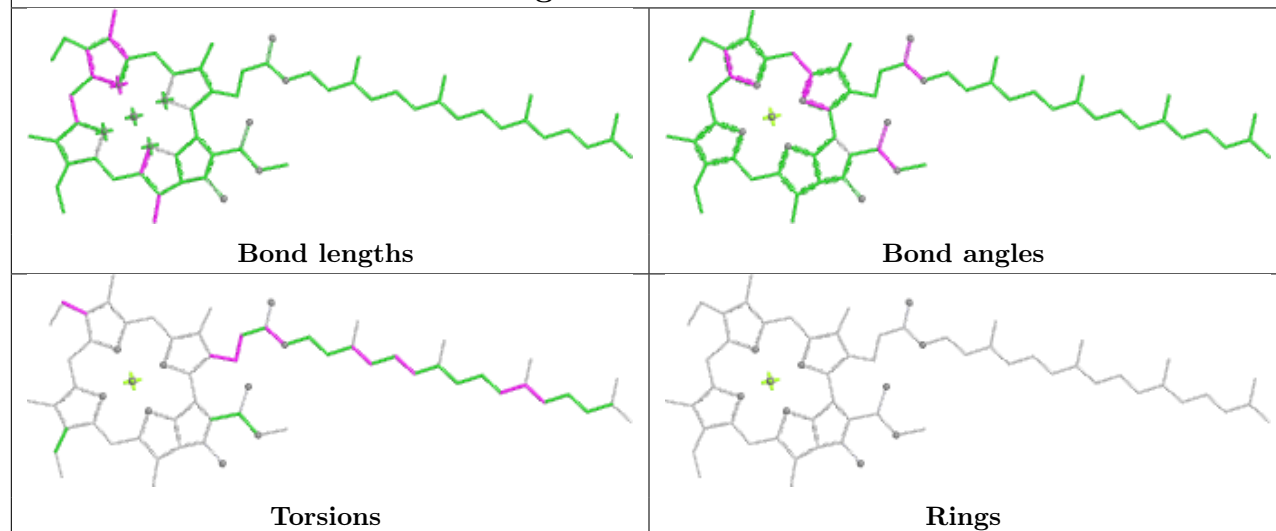
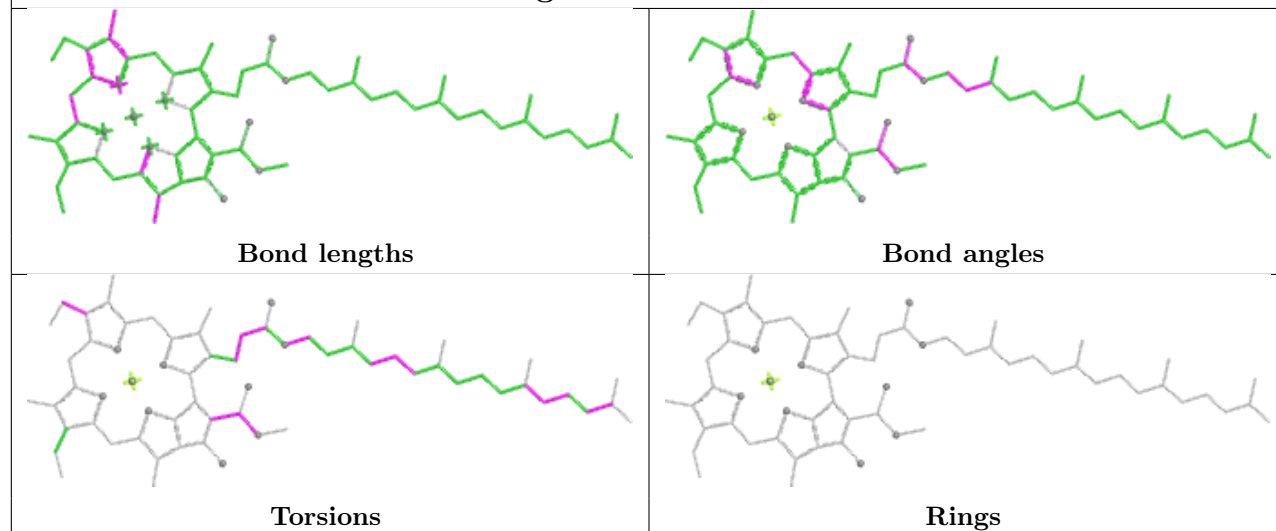
Ligand CLA a 841

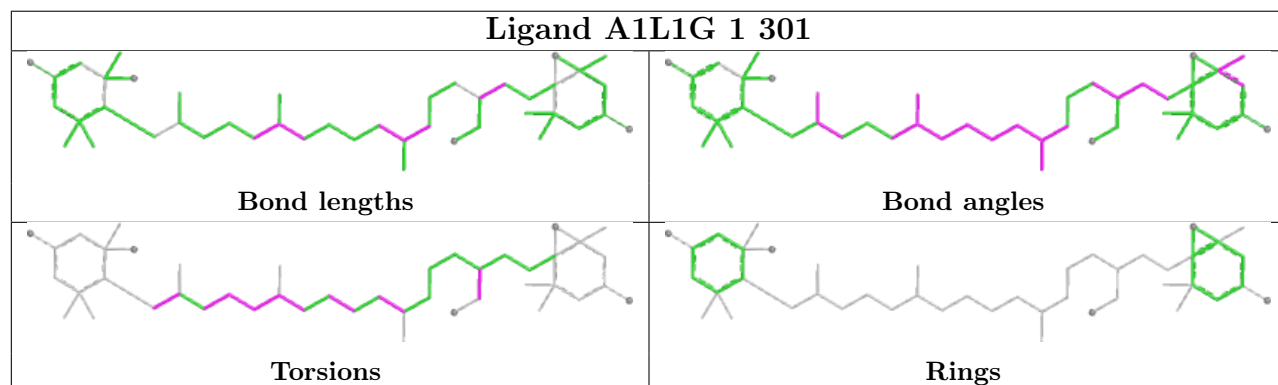
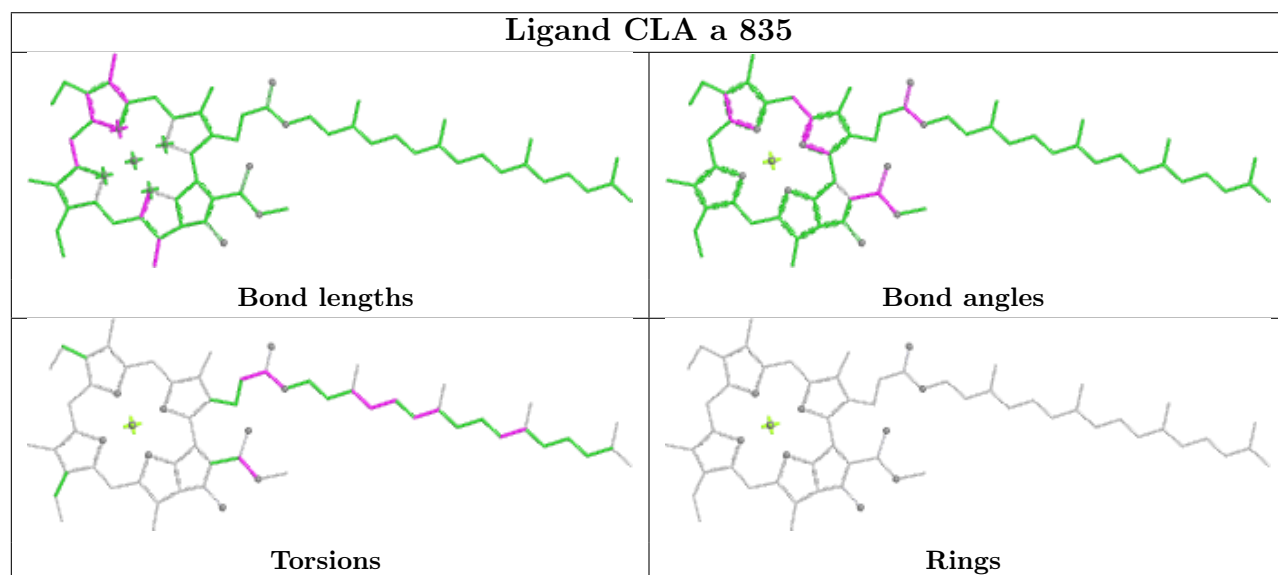
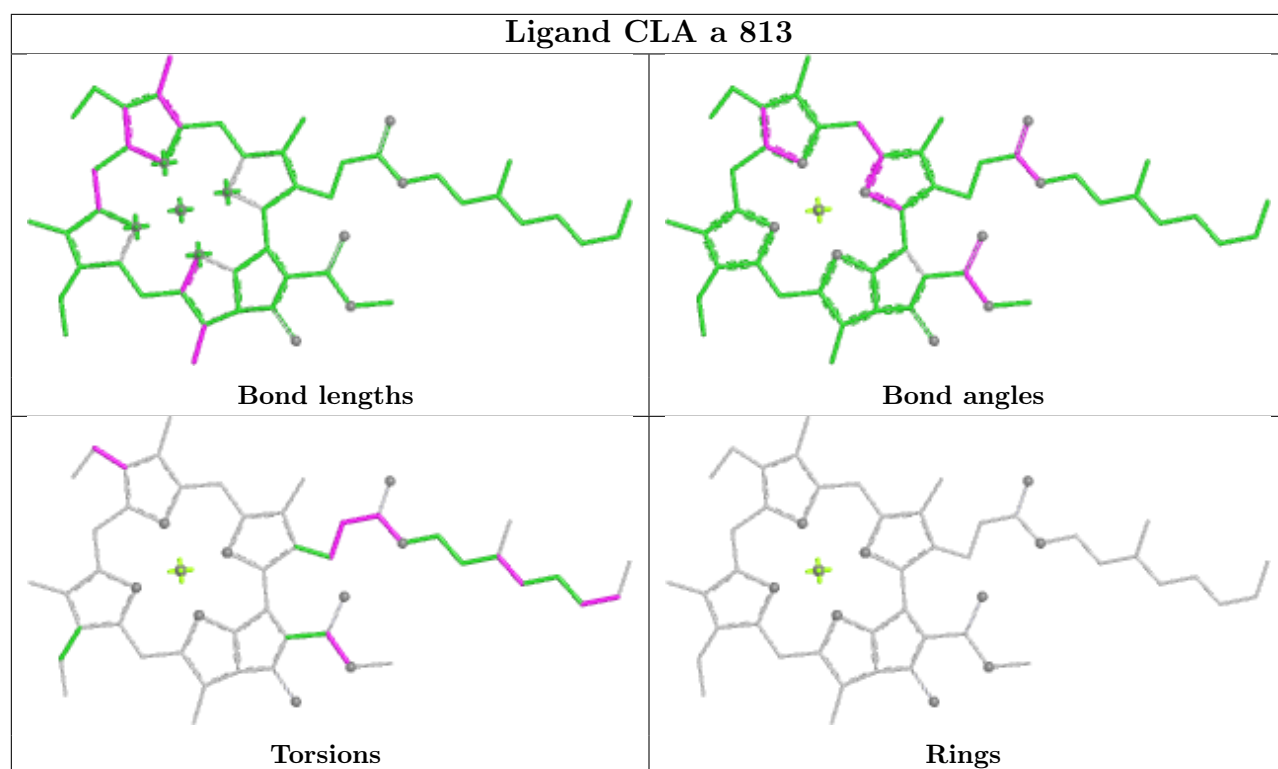


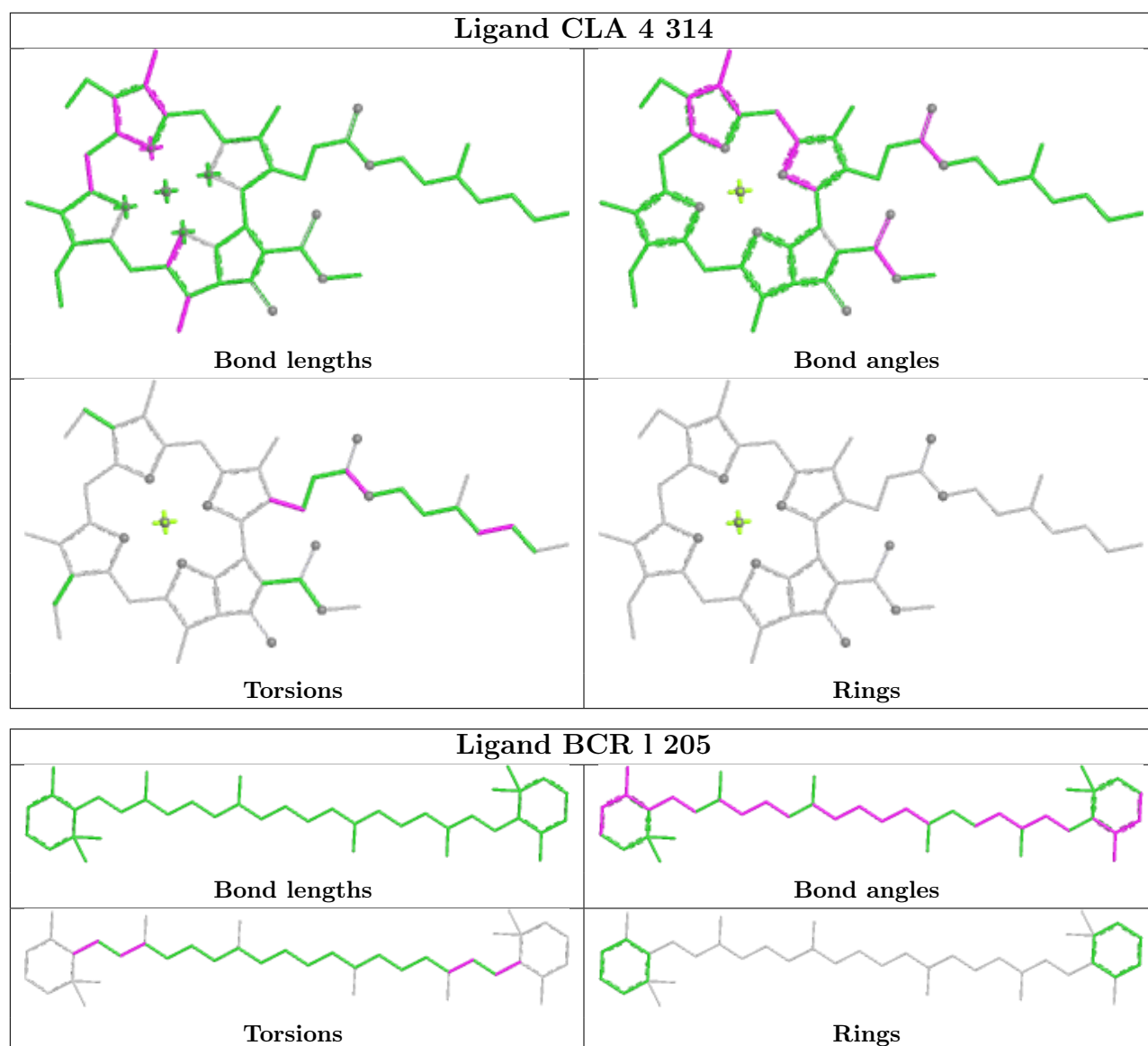




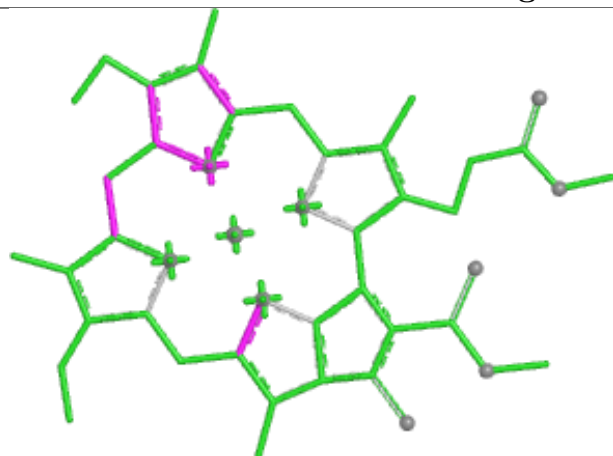


Ligand CLA b 829**Ligand CLA a 810**

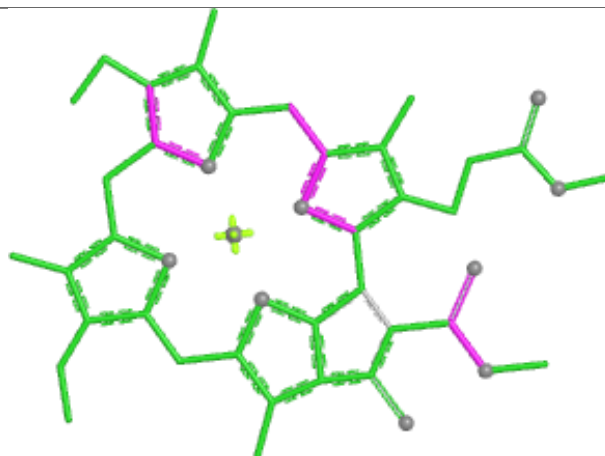




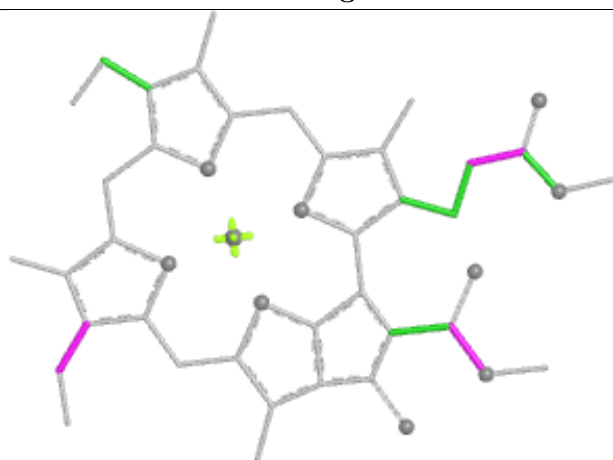
Ligand CLA 5 315



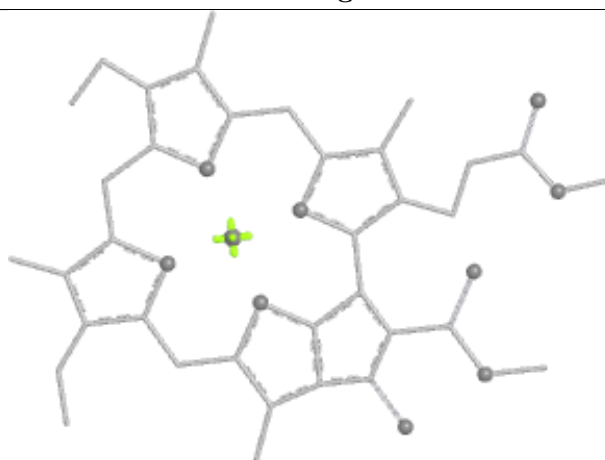
Bond lengths



Bond angles

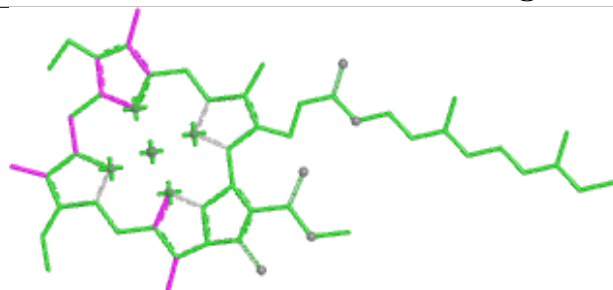


Torsions

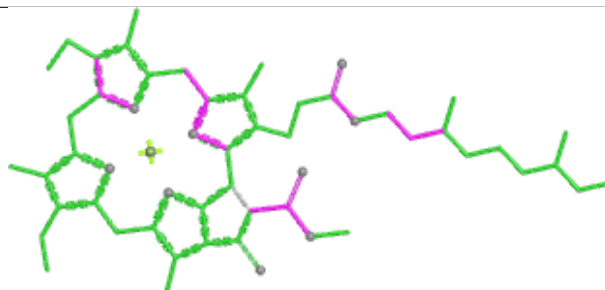


Rings

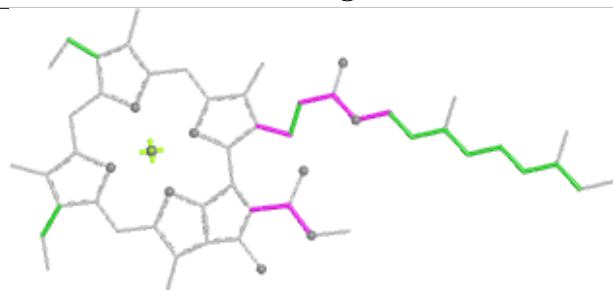
Ligand CLA a 818



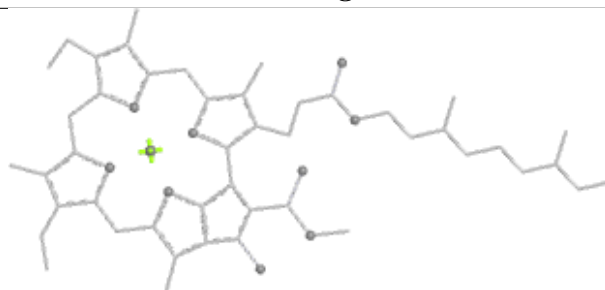
Bond lengths



Bond angles

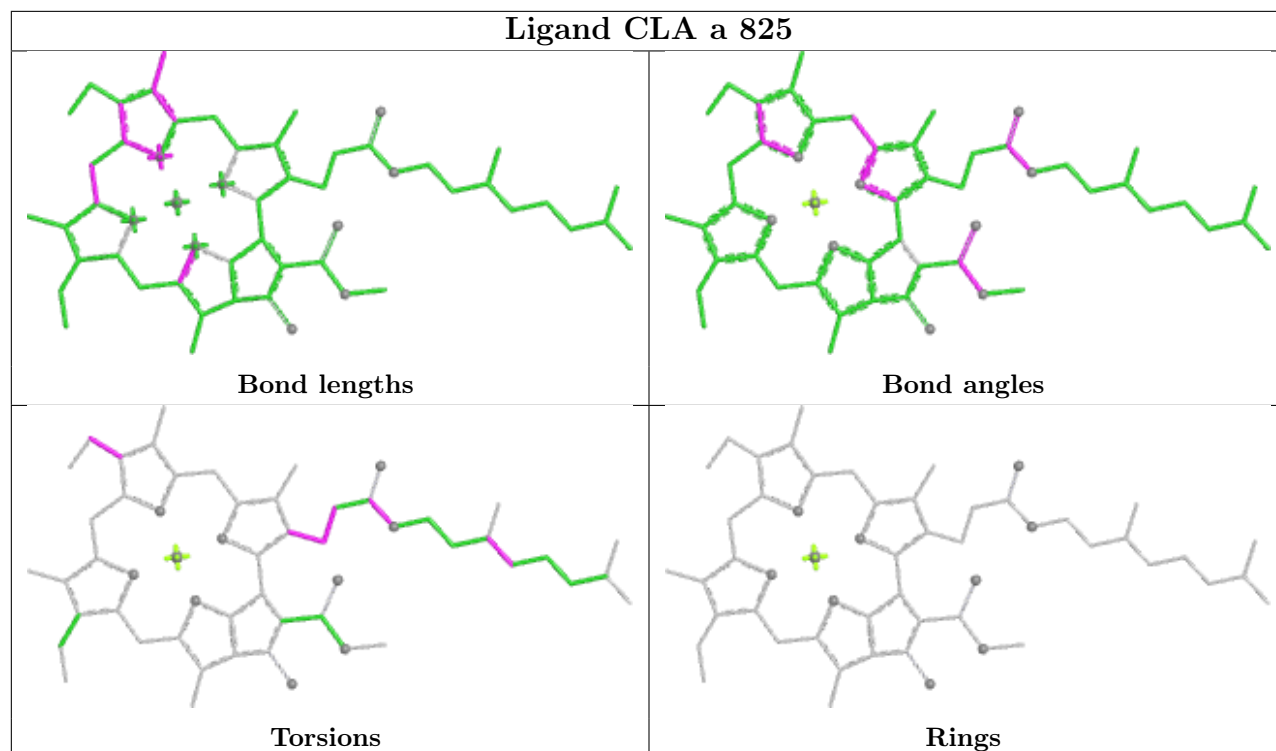


Torsions

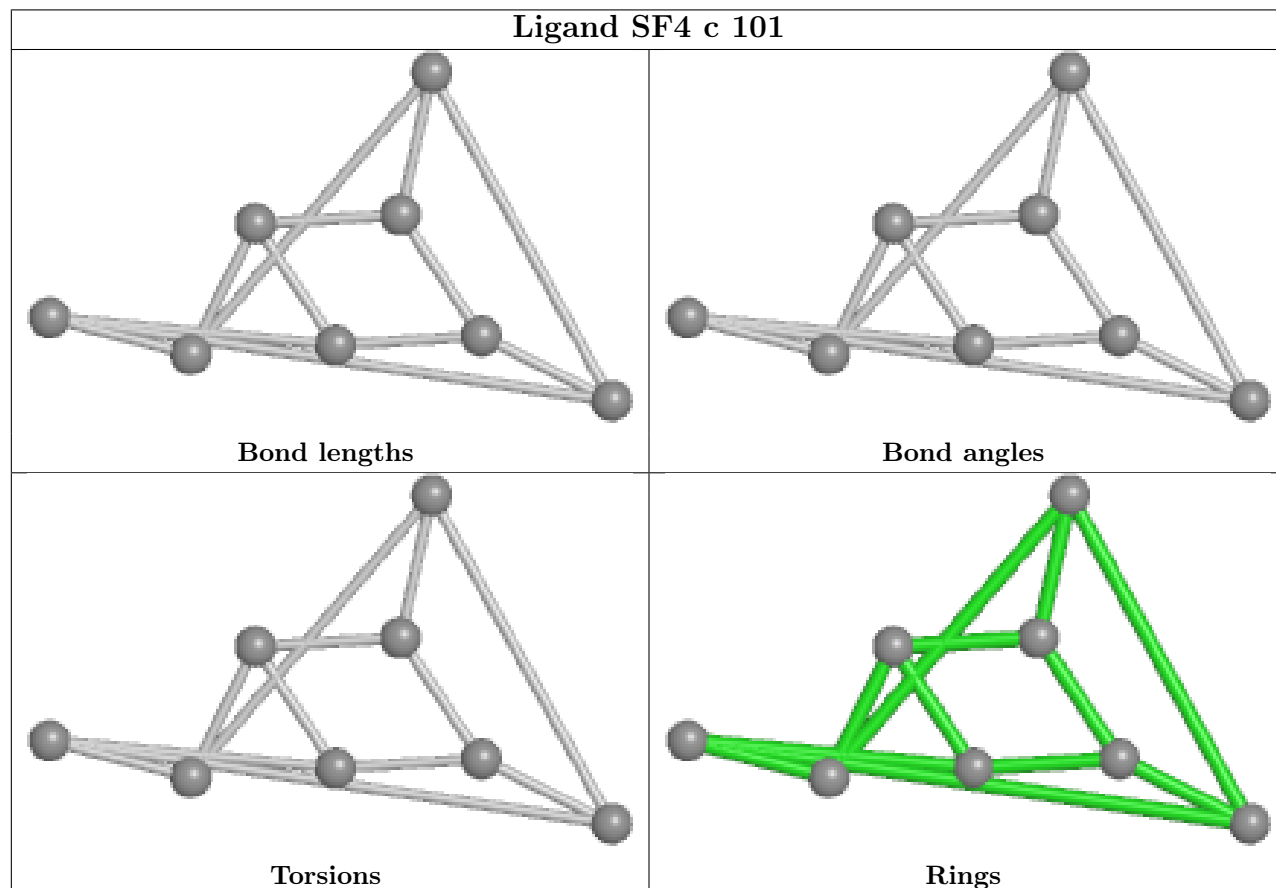


Rings

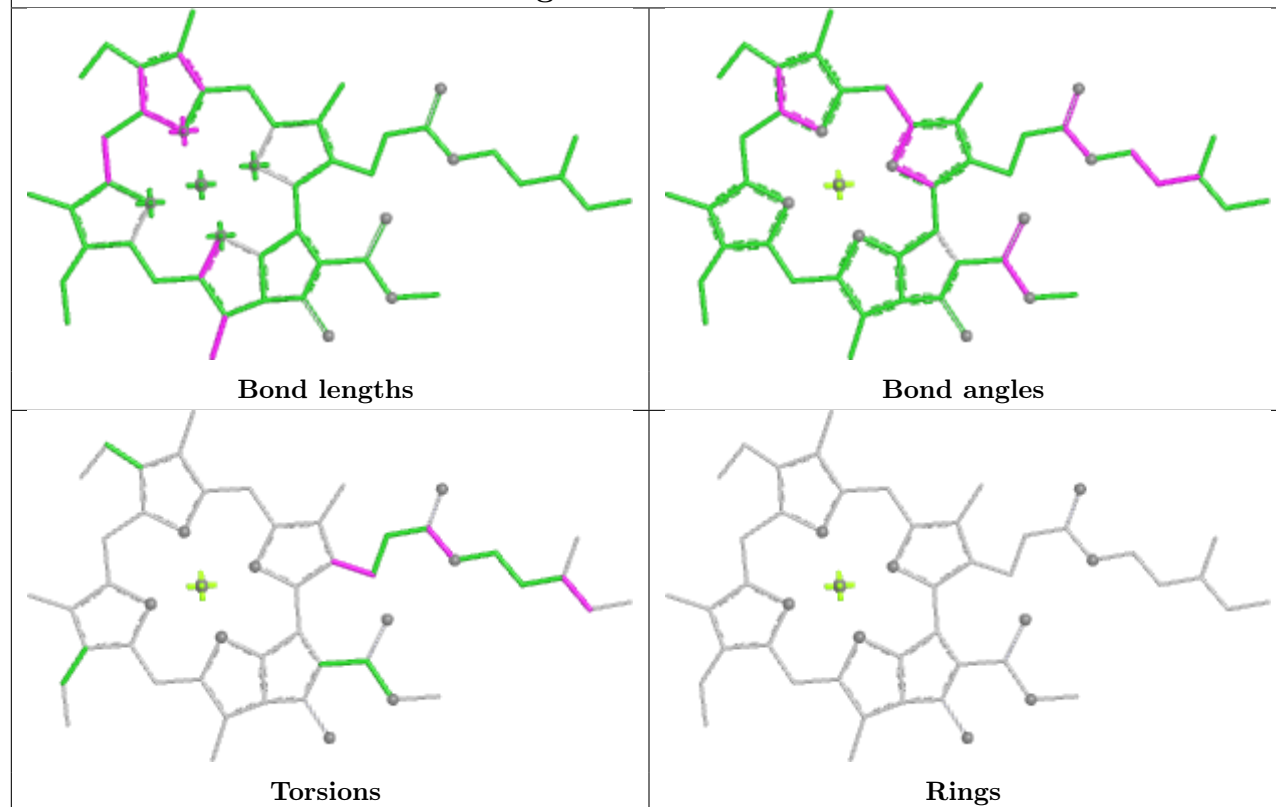
Ligand CLA a 825



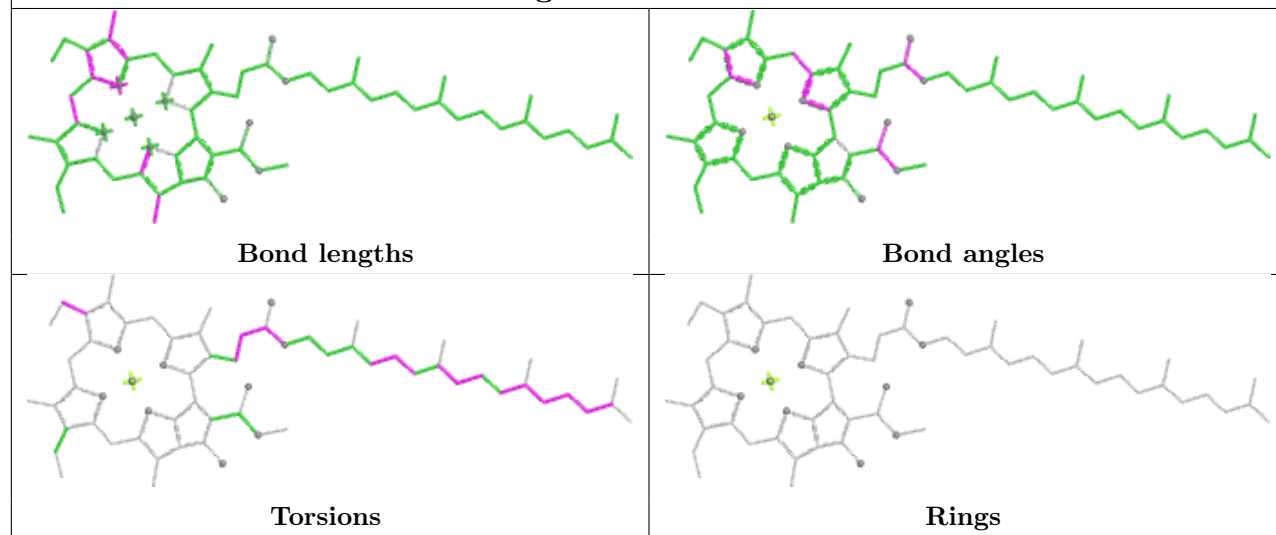
Ligand SF4 c 101

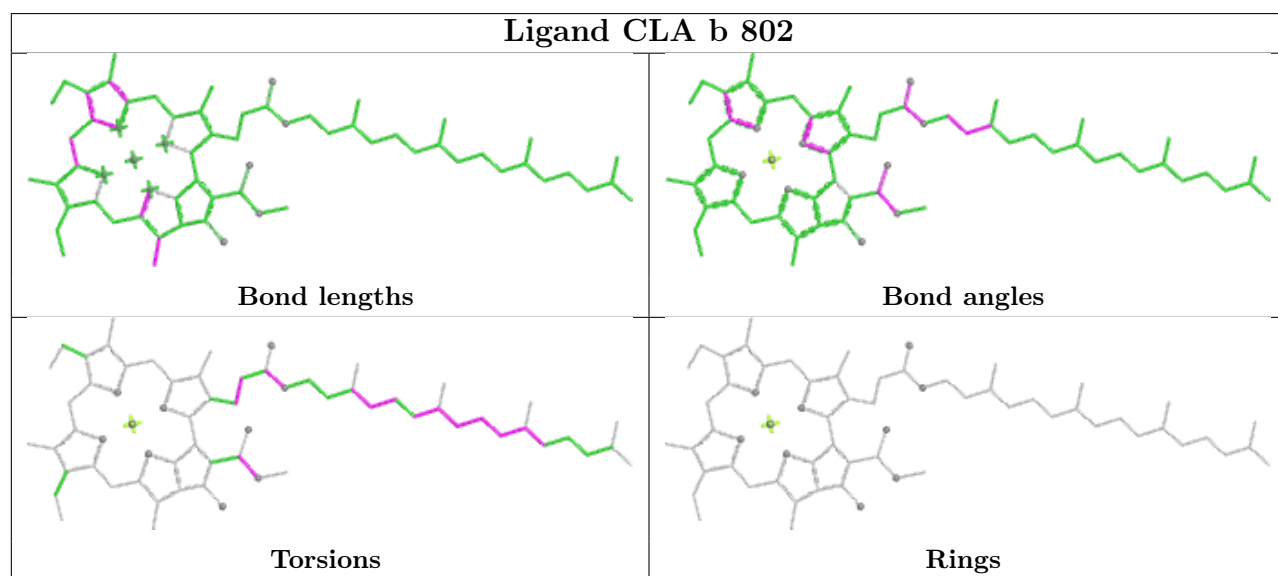
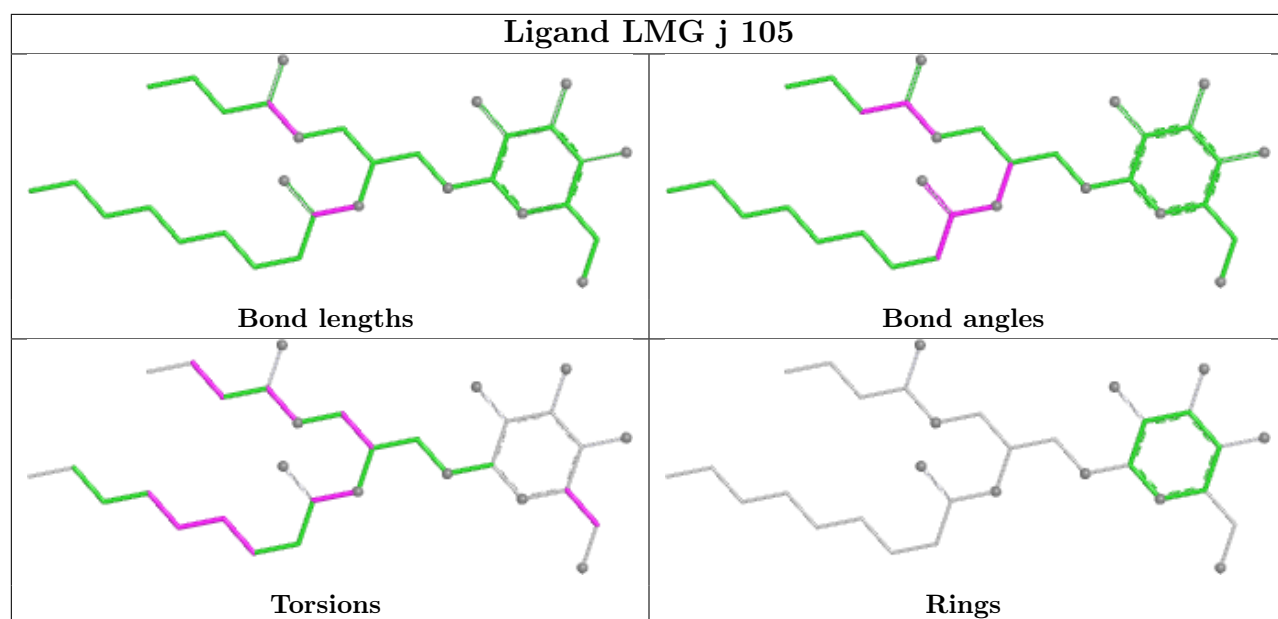


Ligand CLA a 838

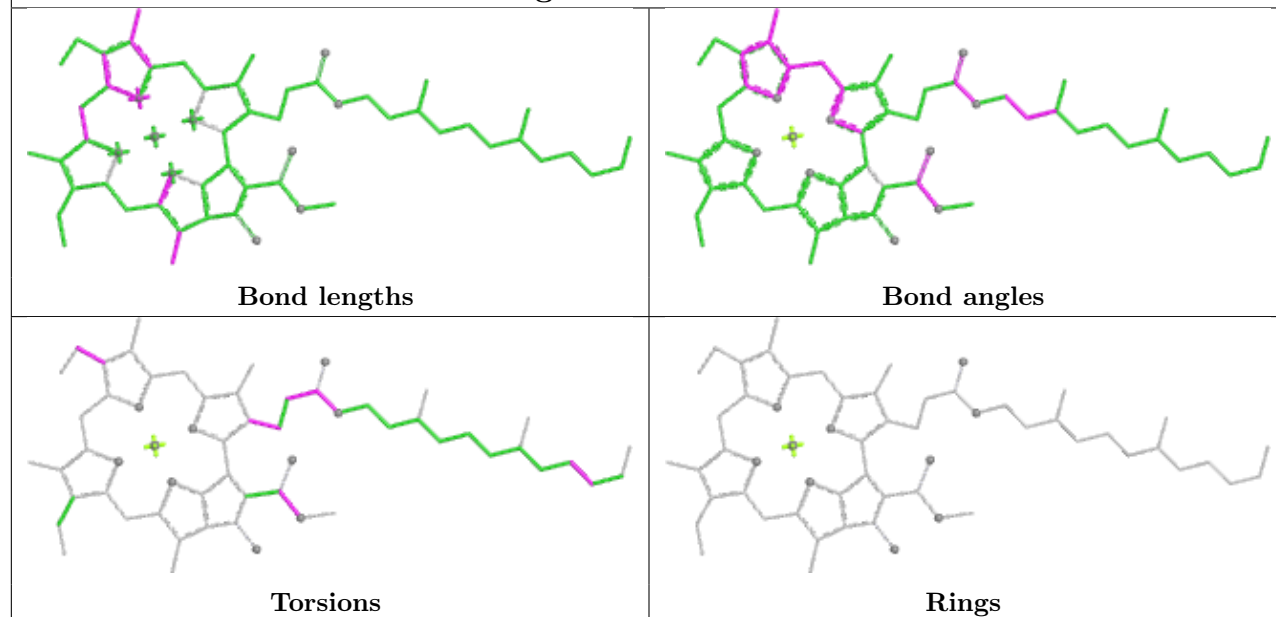


Ligand CLA b 801

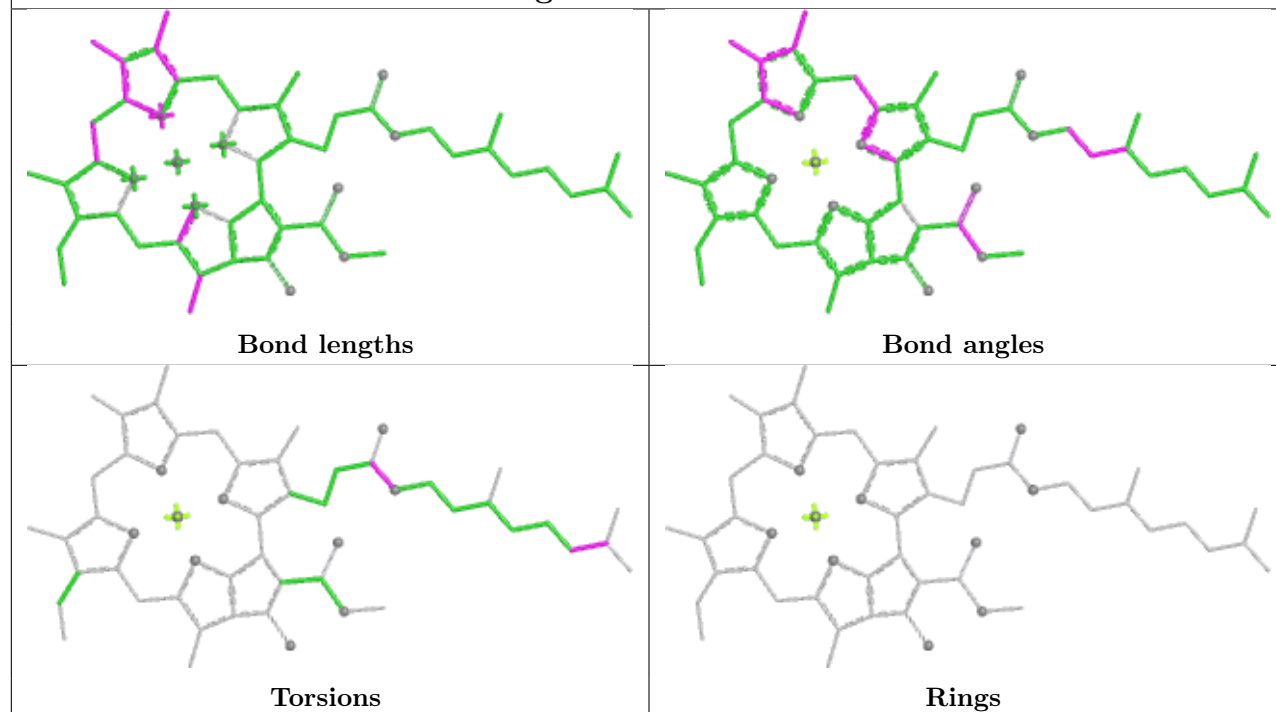


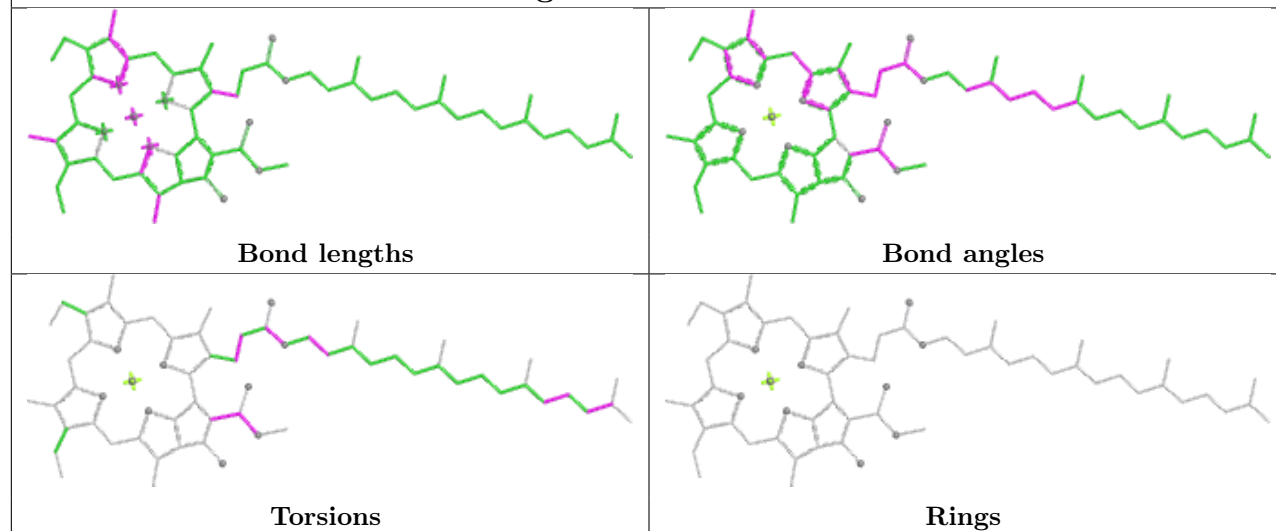
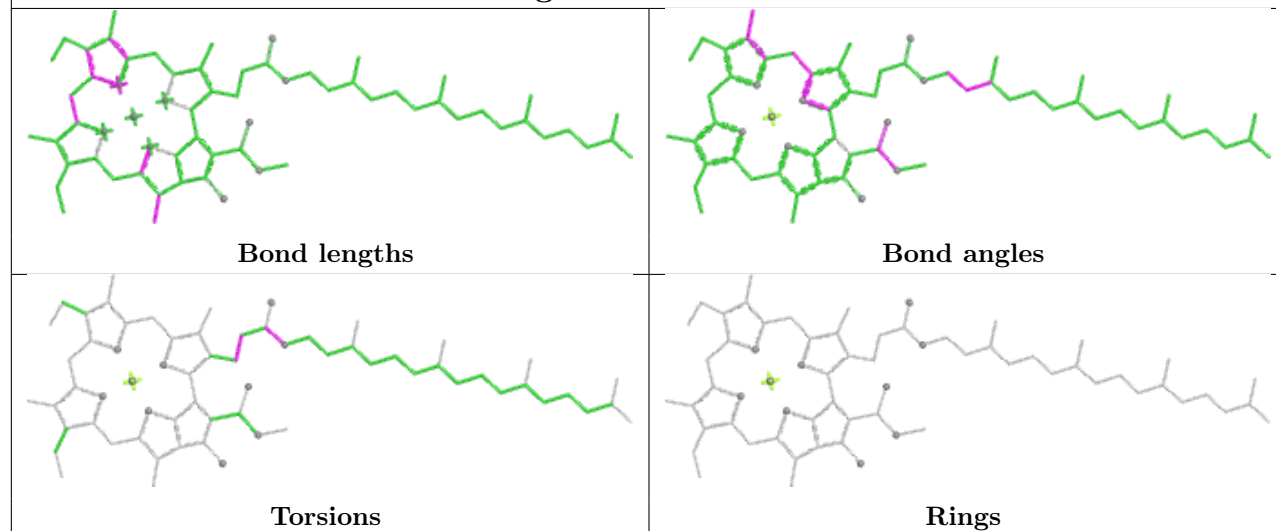


Ligand CLA b 818

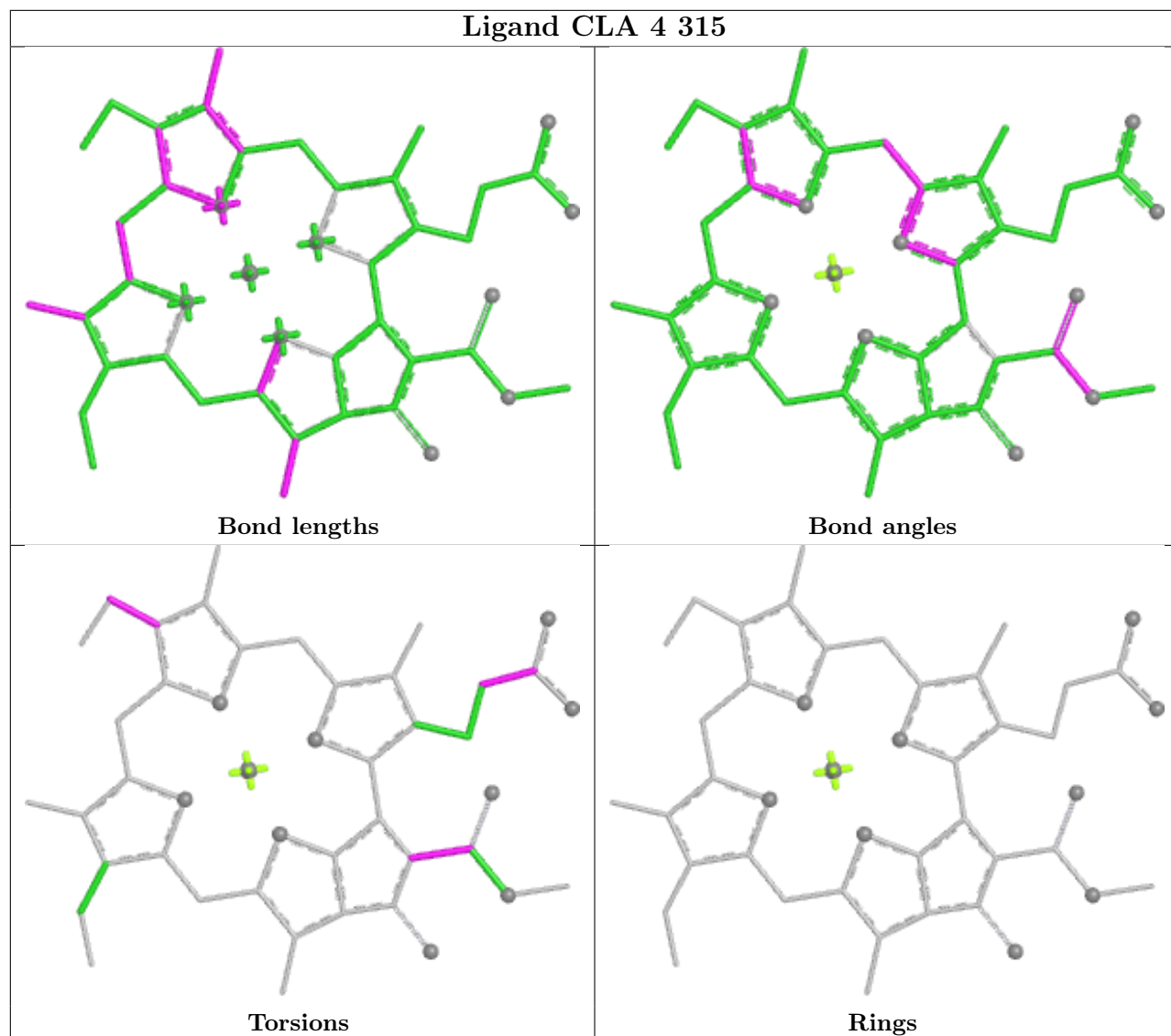


Ligand CLA b 812

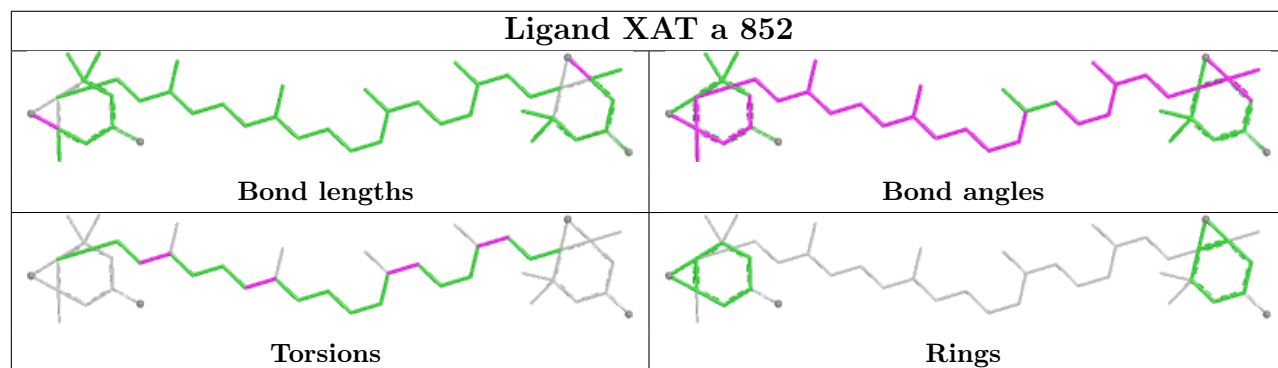


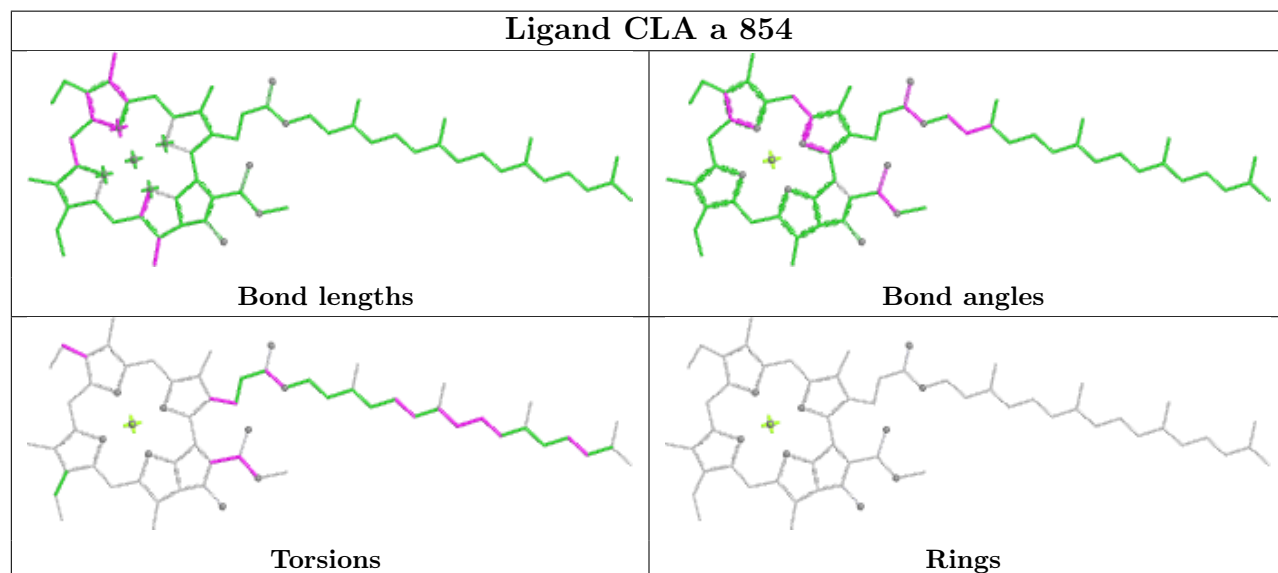
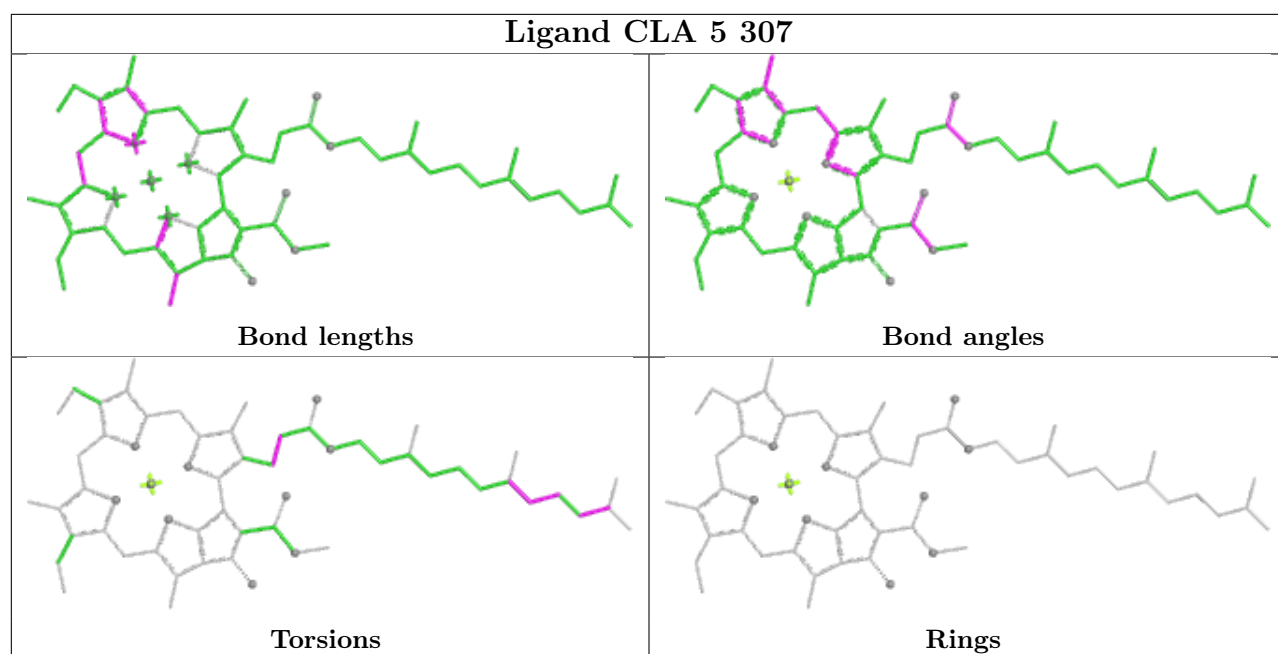
Ligand CLA a 806**Ligand CLA b 827**

Ligand CLA 4 315

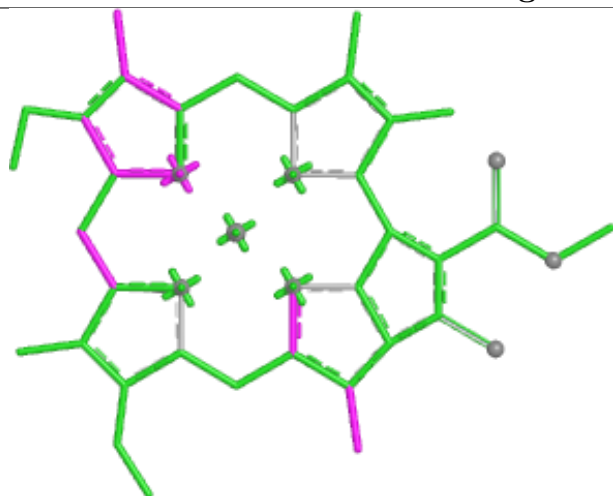


Ligand XAT a 852

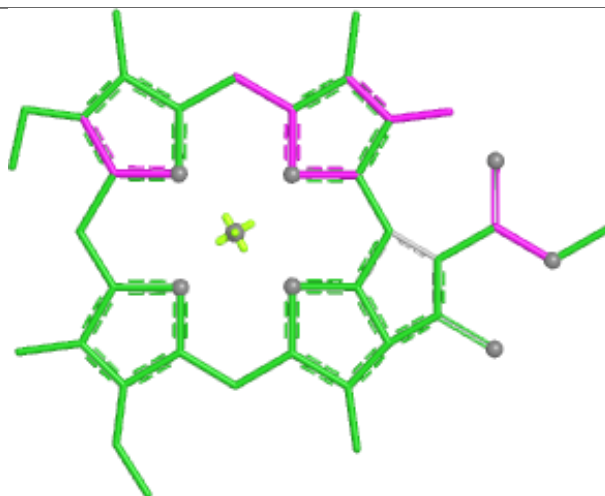




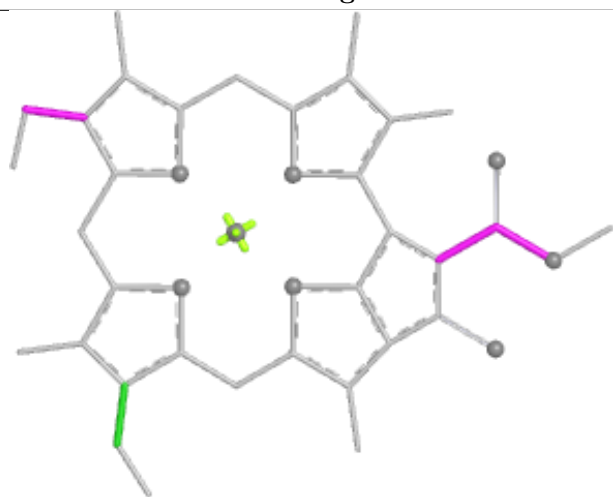
Ligand CLA 1 313



Bond lengths



Bond angles

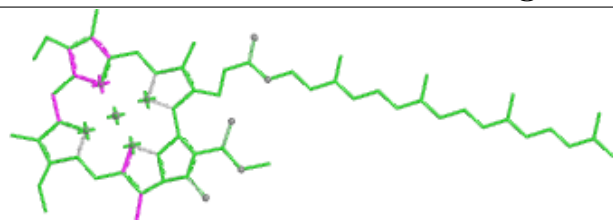


Torsions

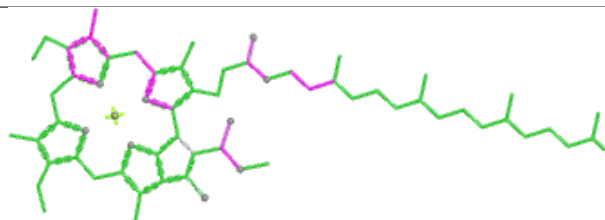


Rings

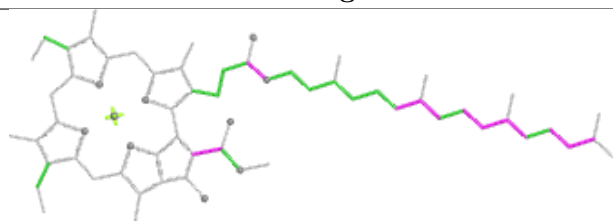
Ligand CLA a 844



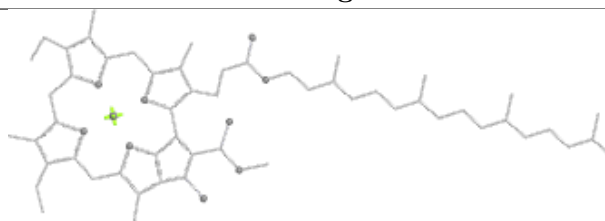
Bond lengths



Bond angles

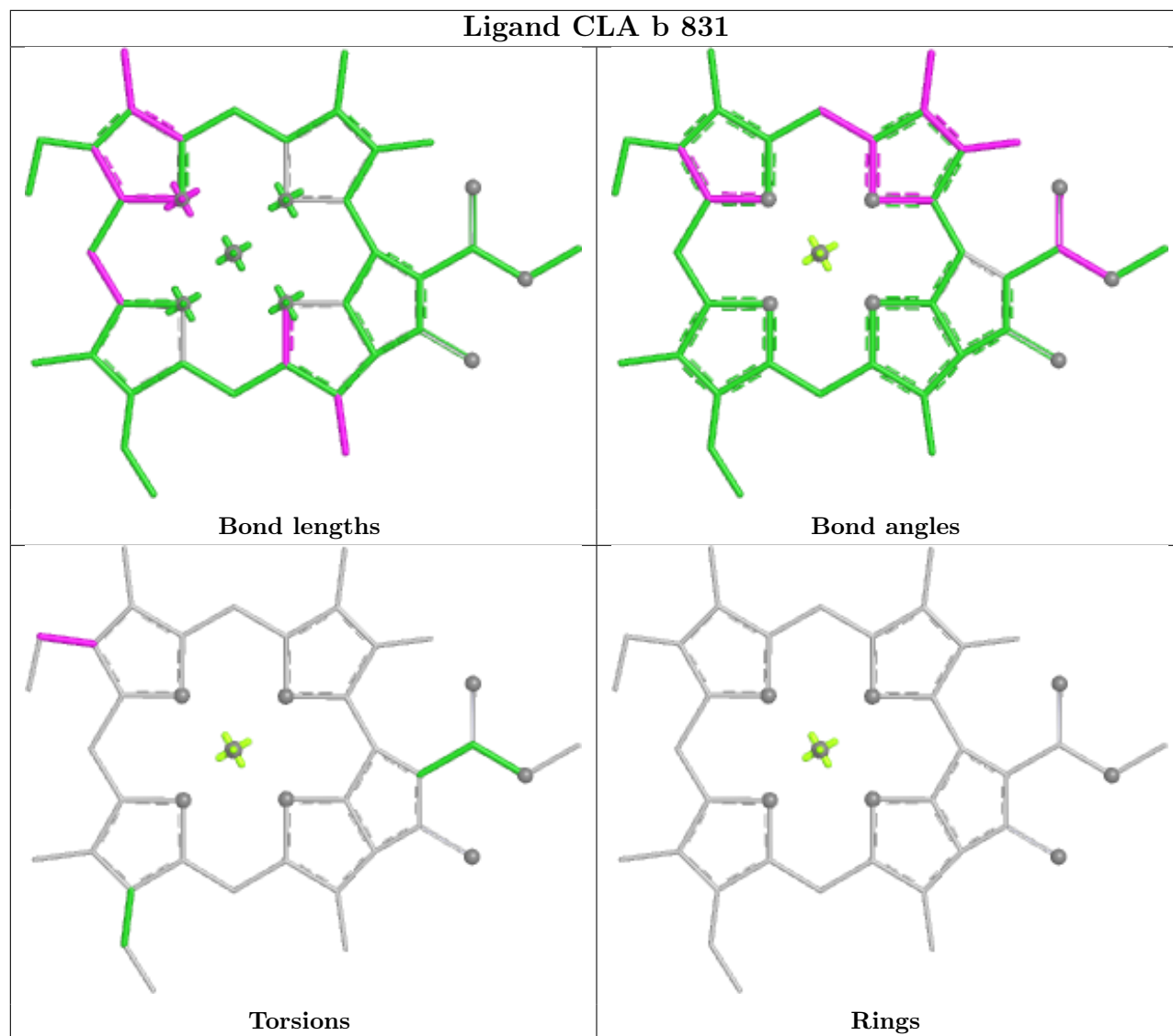


Torsions

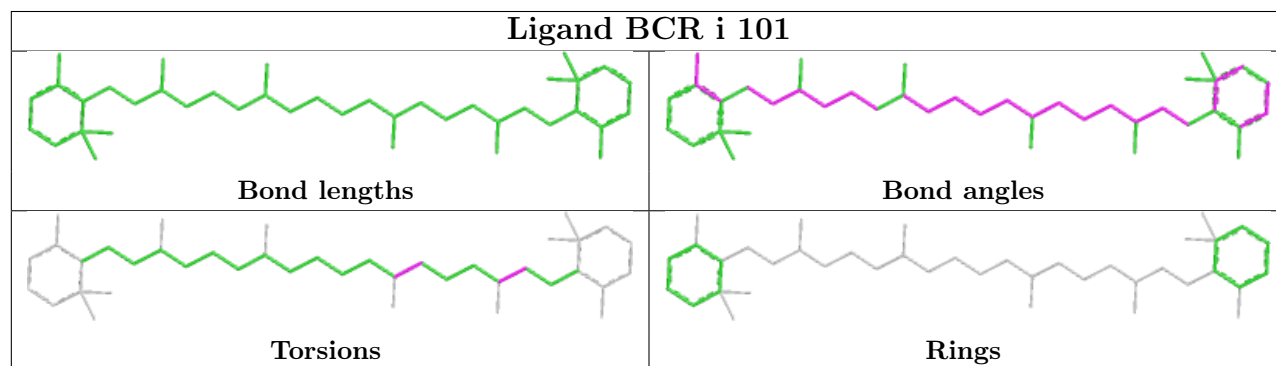


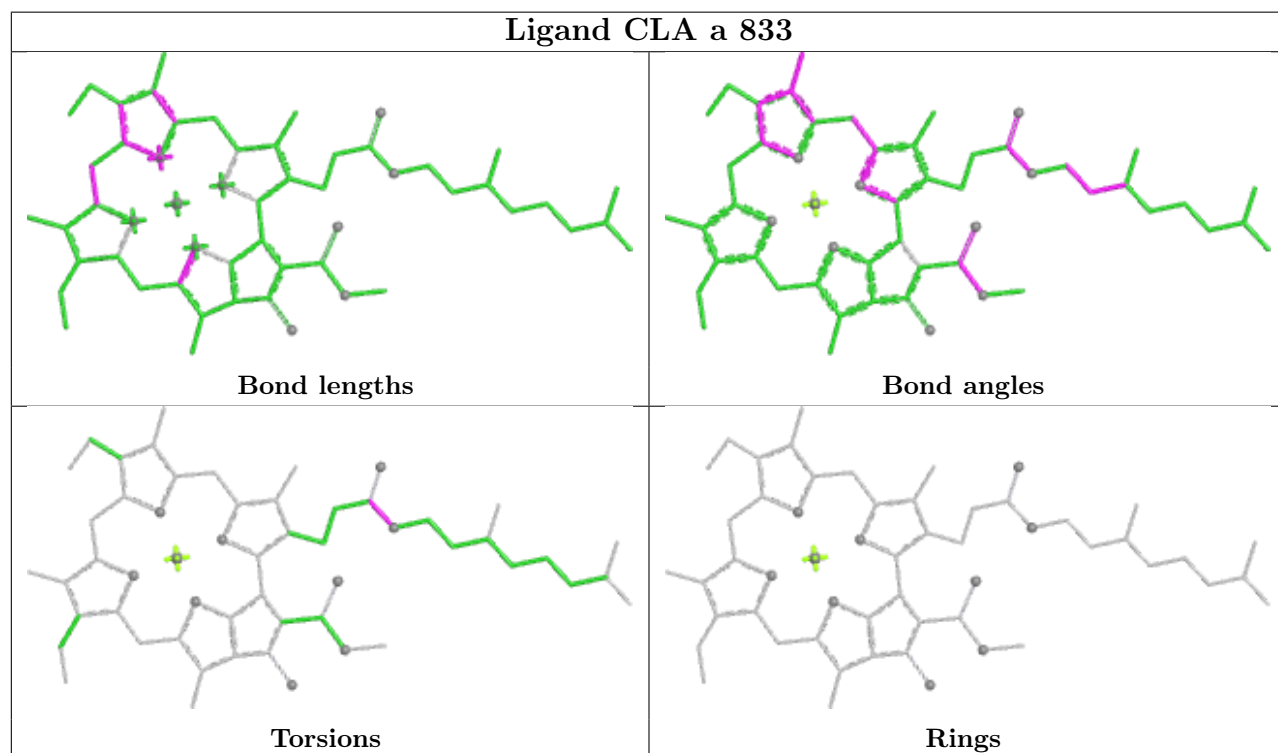
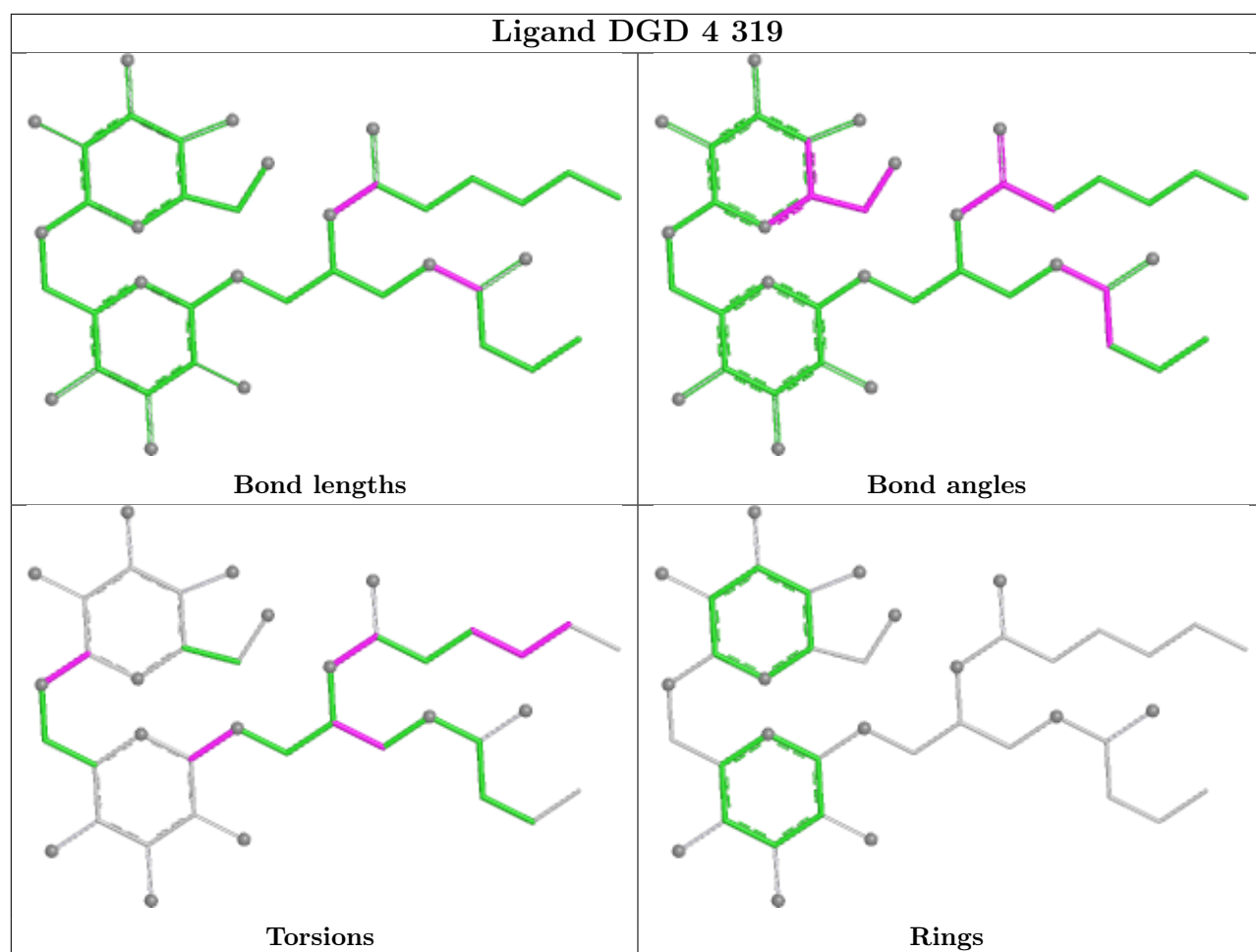
Rings

Ligand CLA b 831

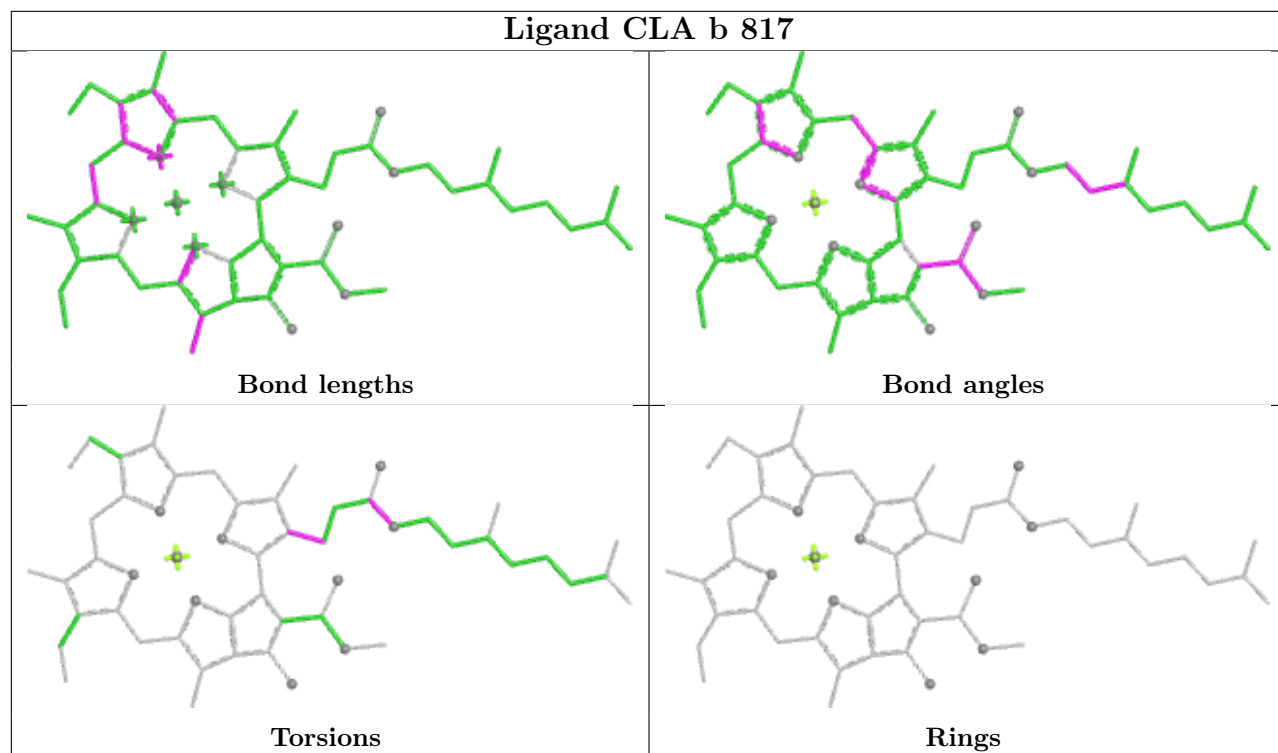


Ligand BCR i 101

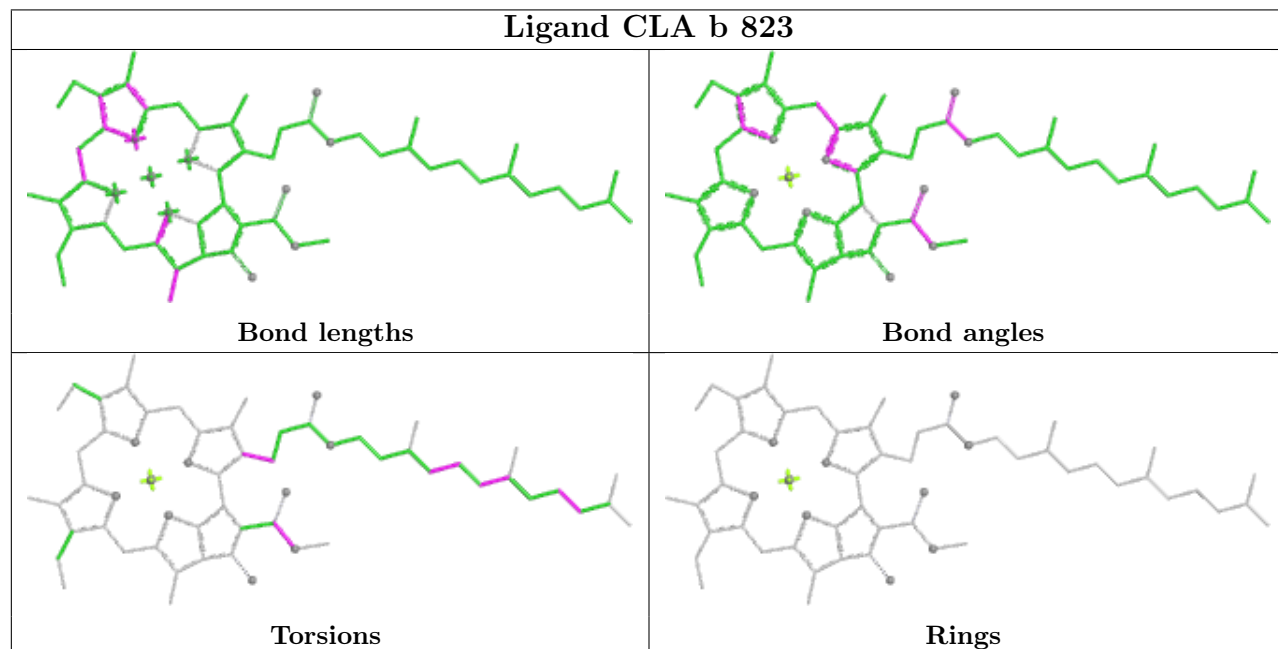


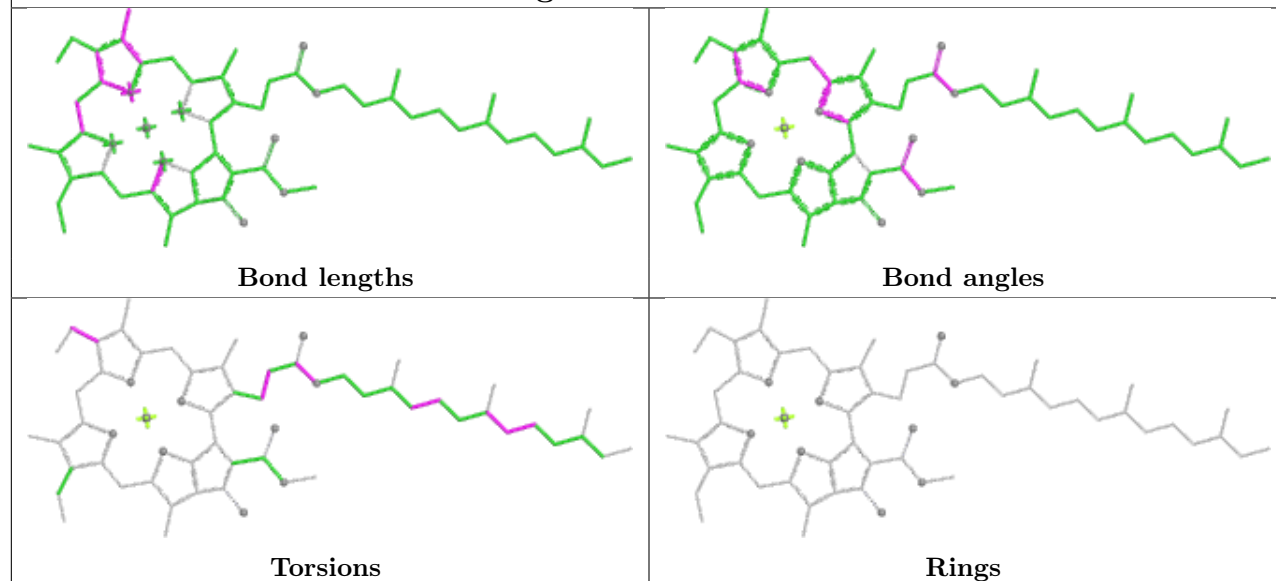
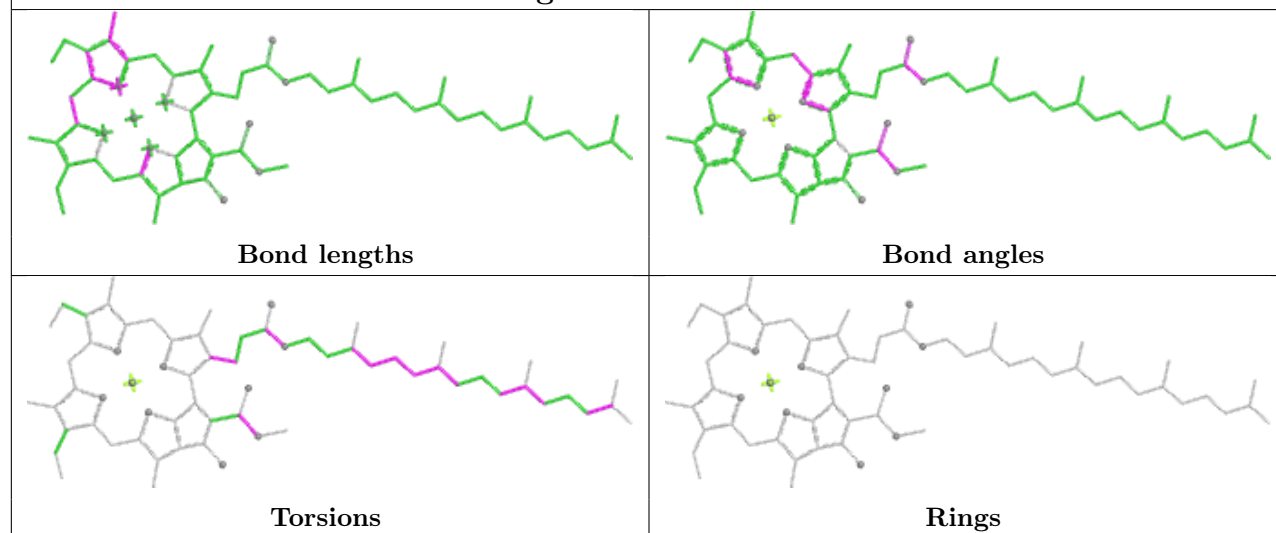


Ligand CLA b 817

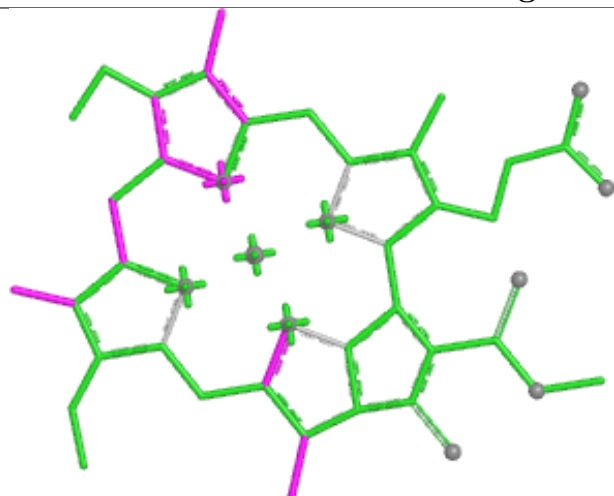


Ligand CLA b 823

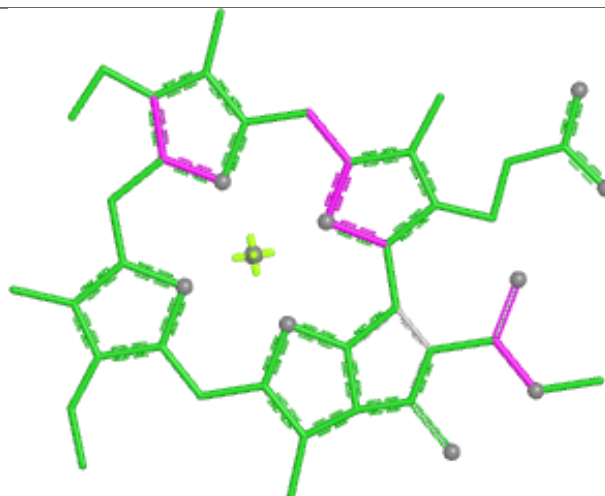


Ligand CLA 1 305**Ligand CLA 1 310**

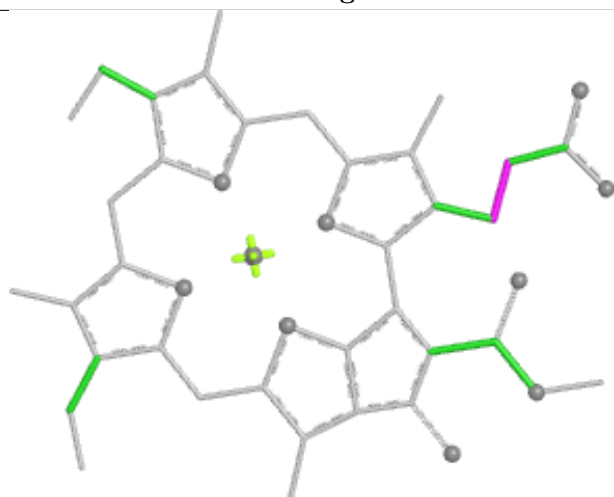
Ligand CLA a 821



Bond lengths



Bond angles

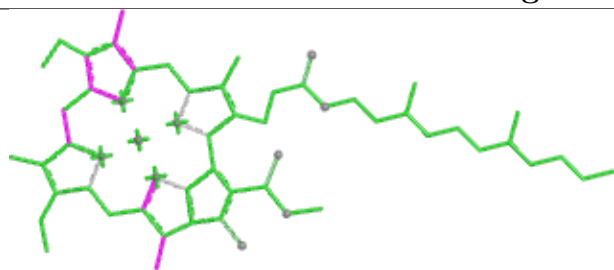


Torsions

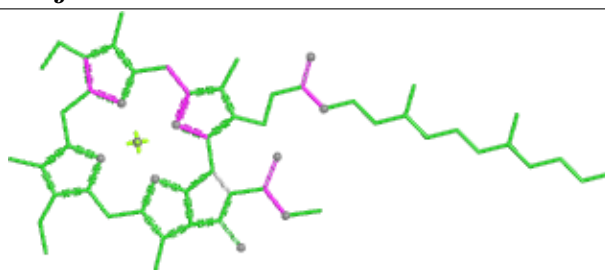


Rings

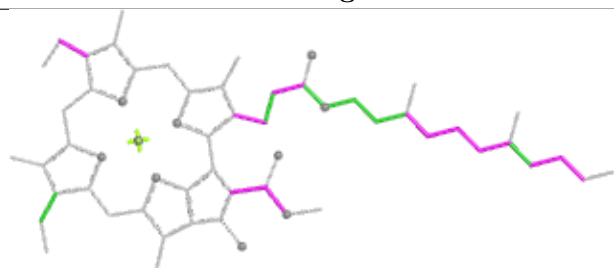
Ligand CLA j 102



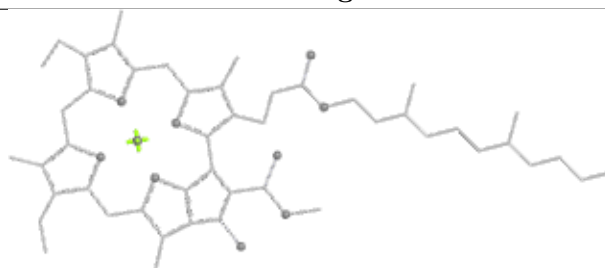
Bond lengths



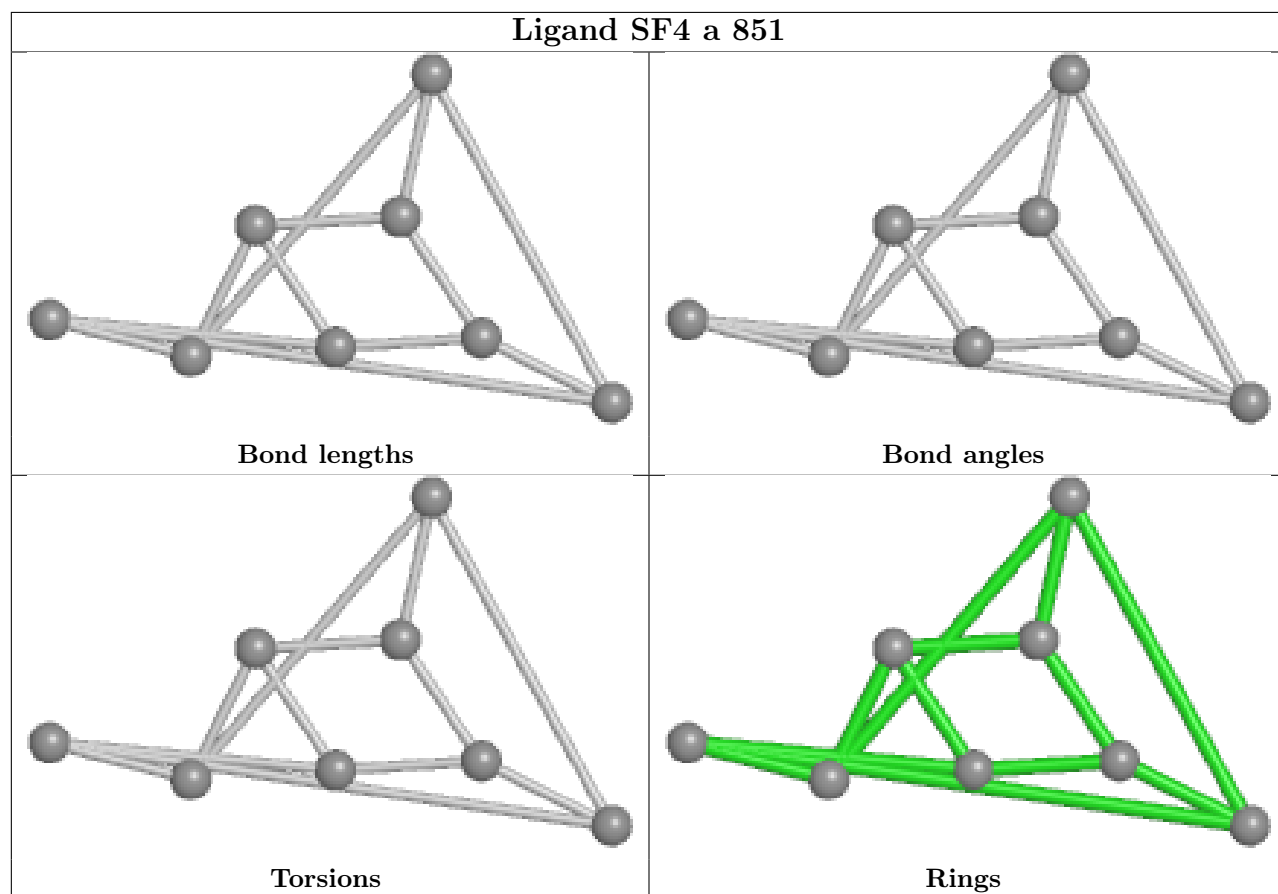
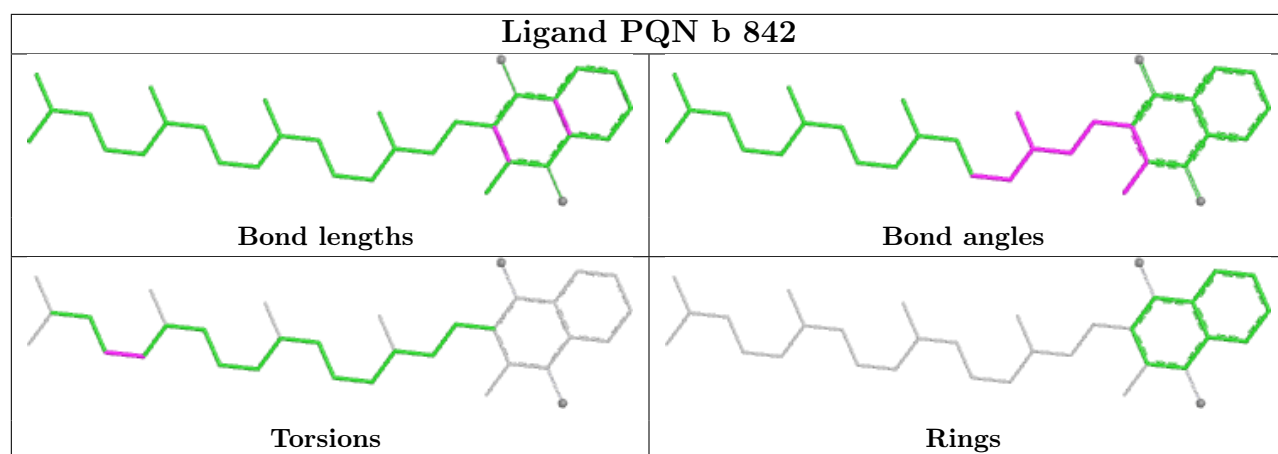
Bond angles

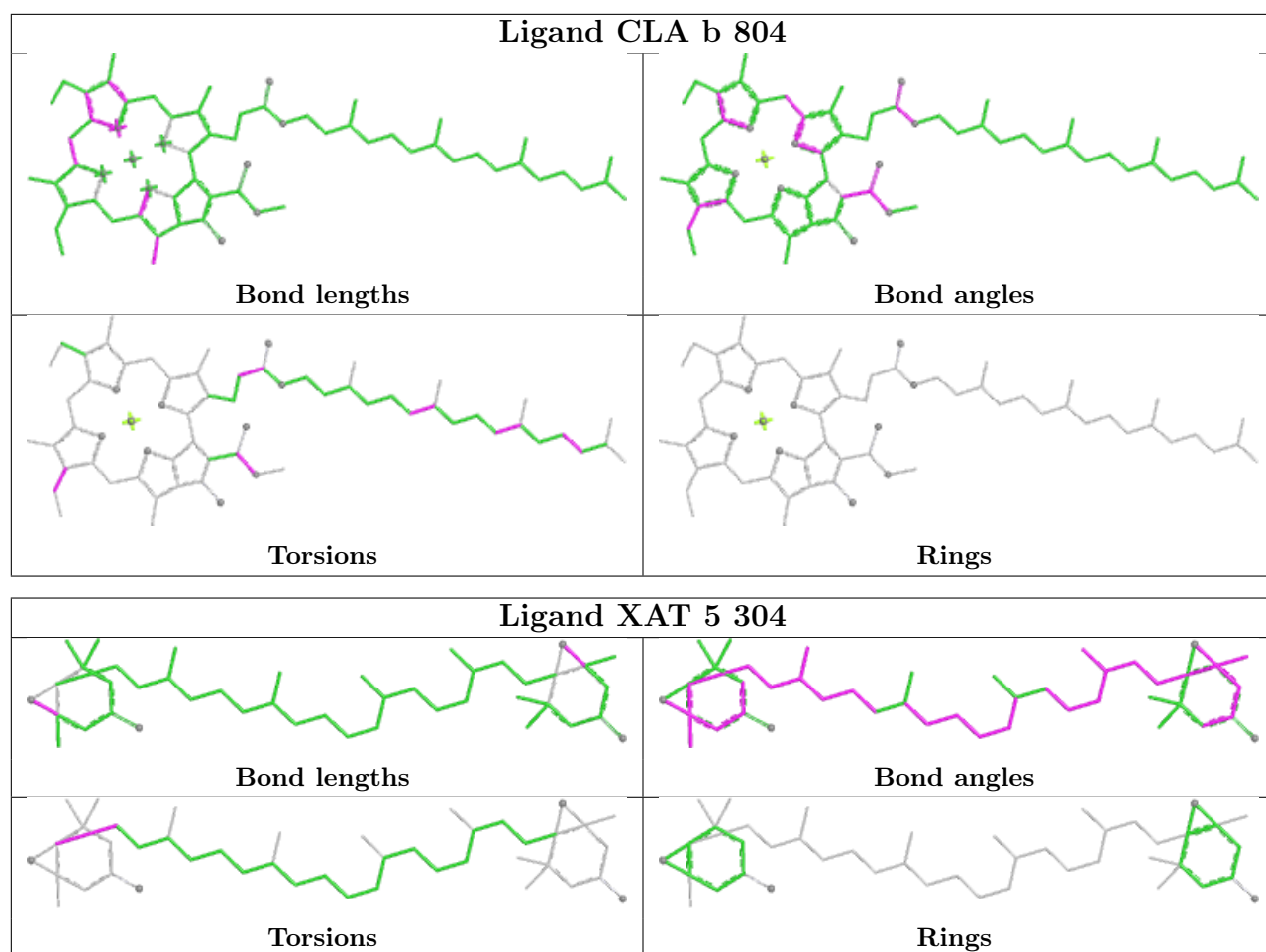


Torsions

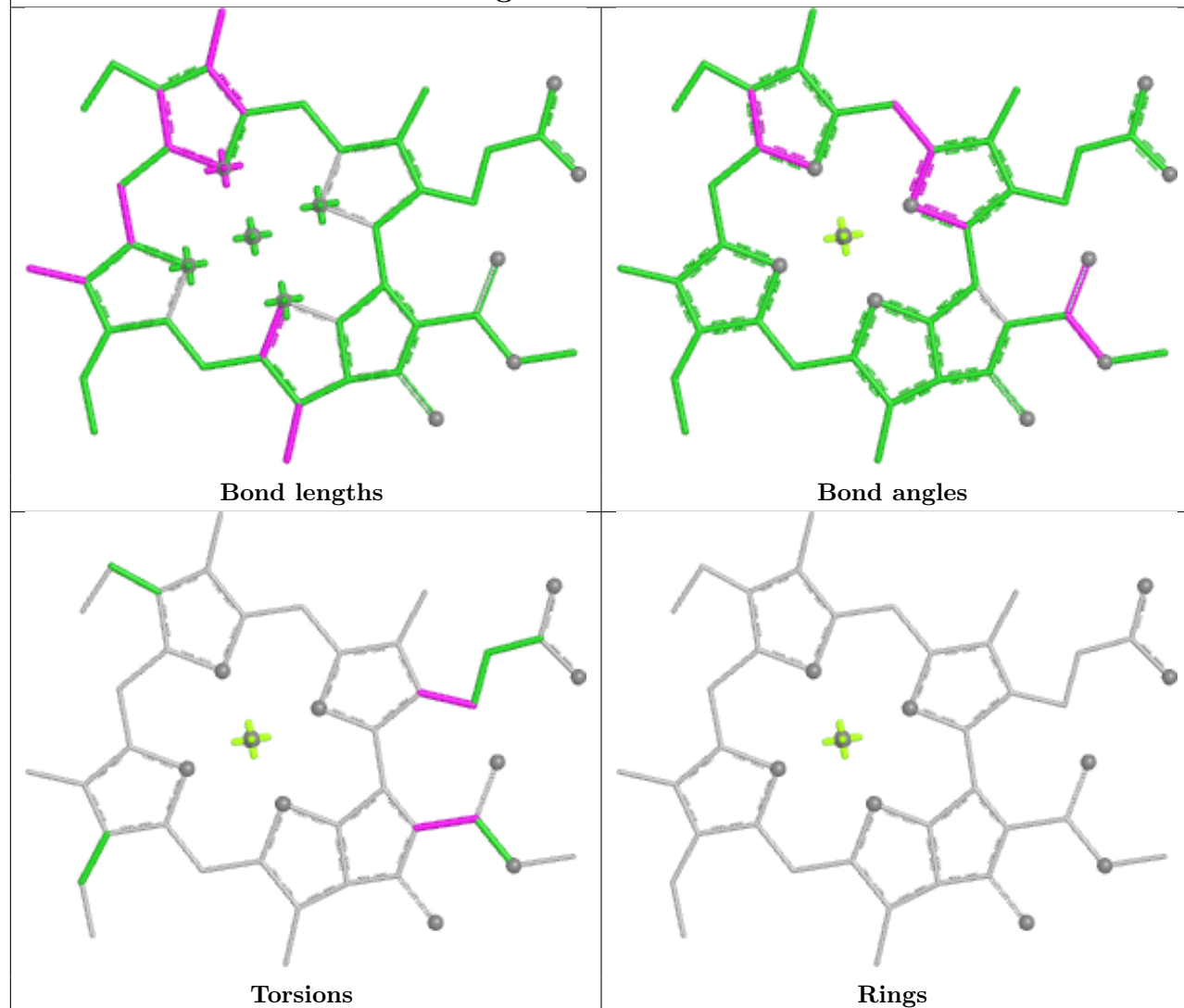


Rings

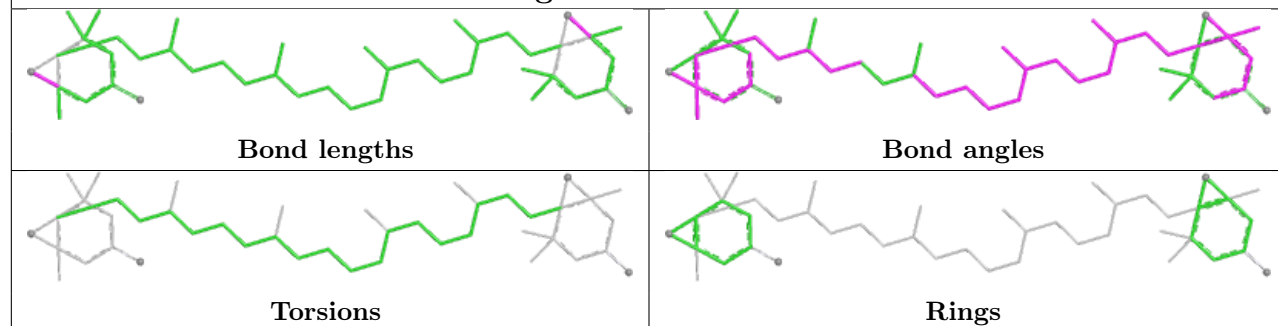


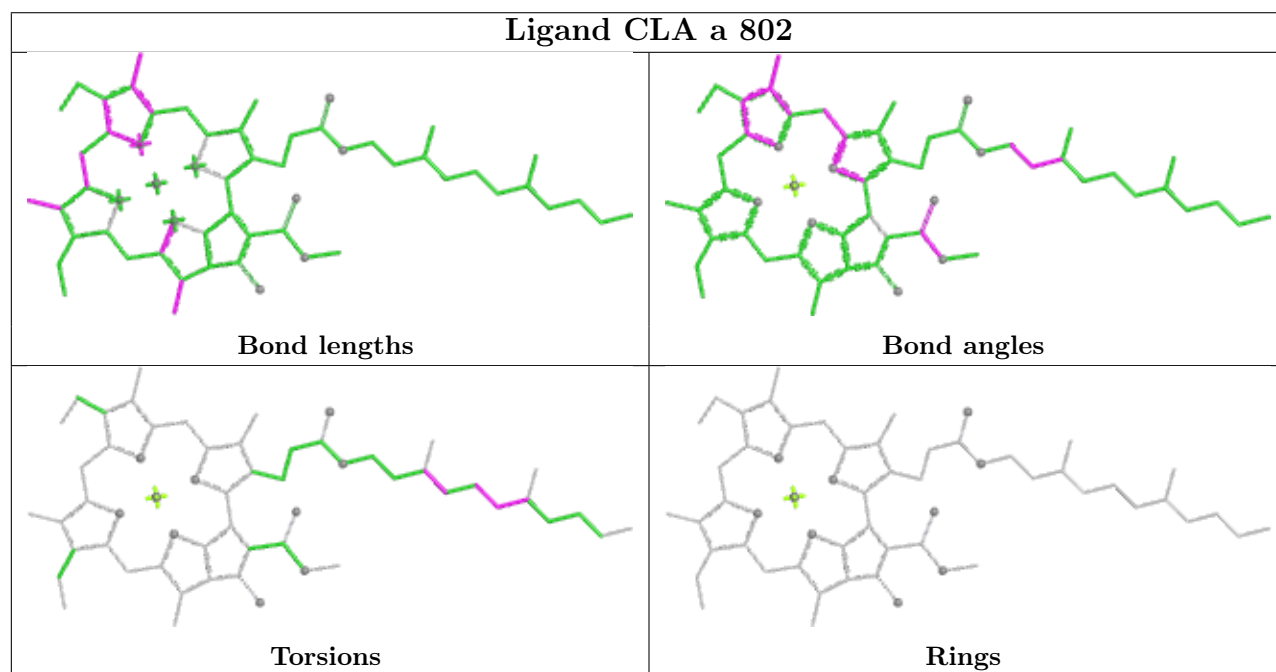
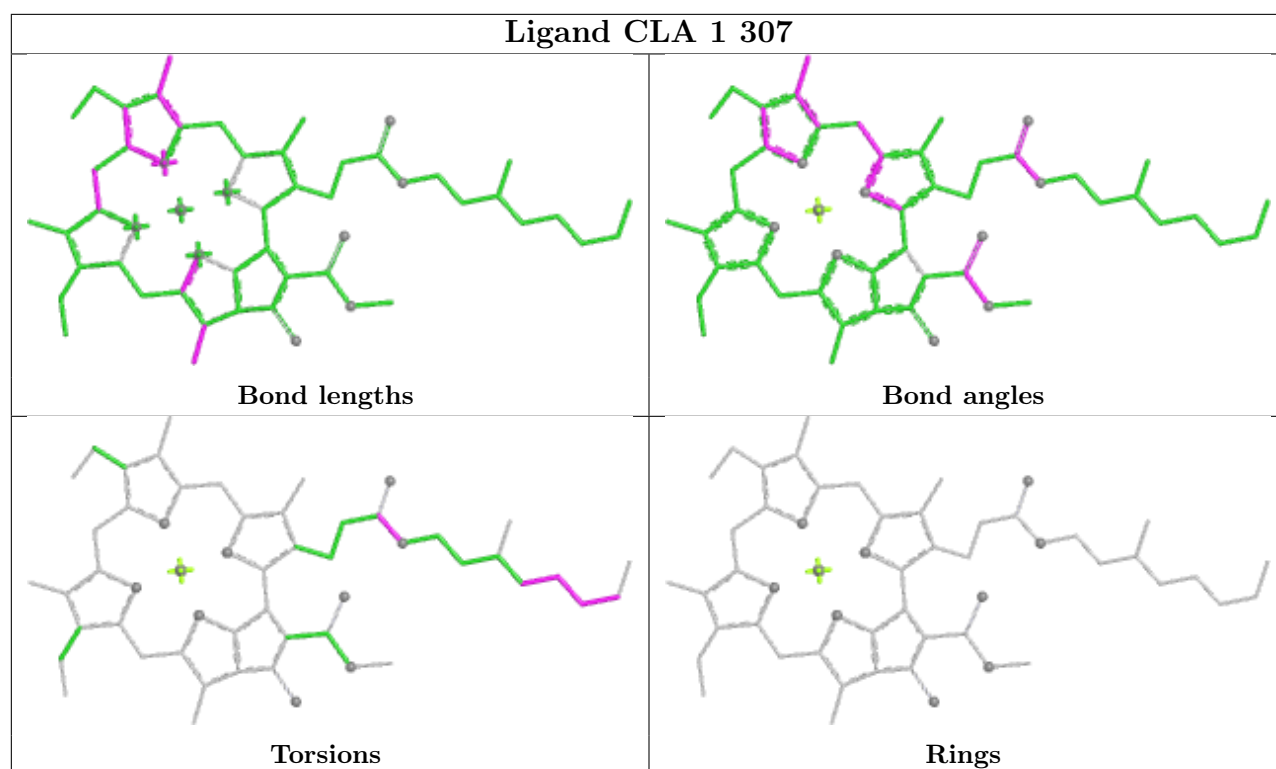


Ligand CLA b 816

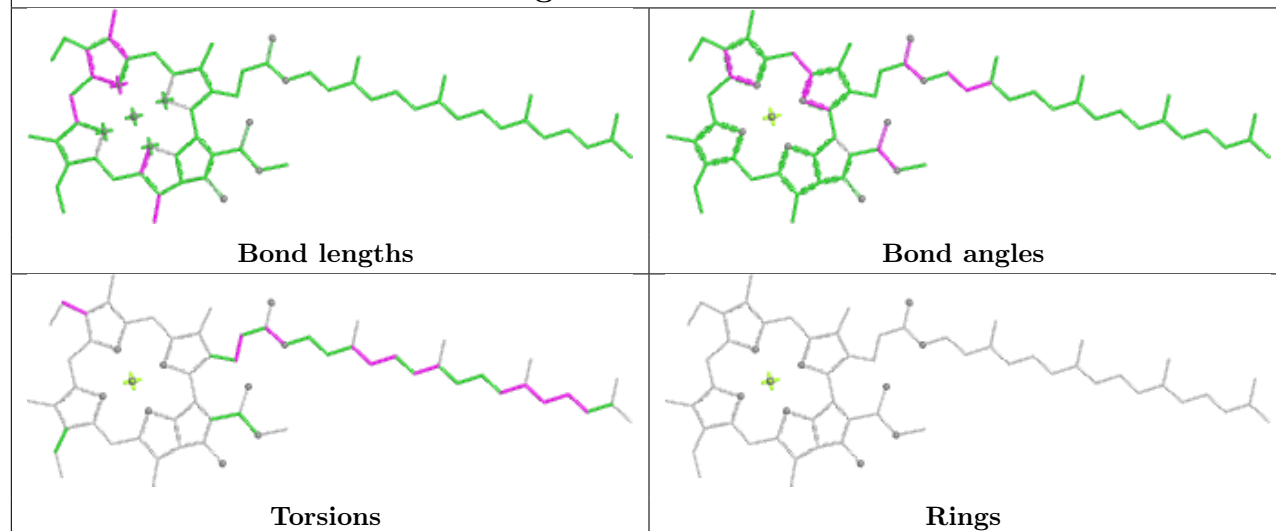


Ligand XAT 1 303

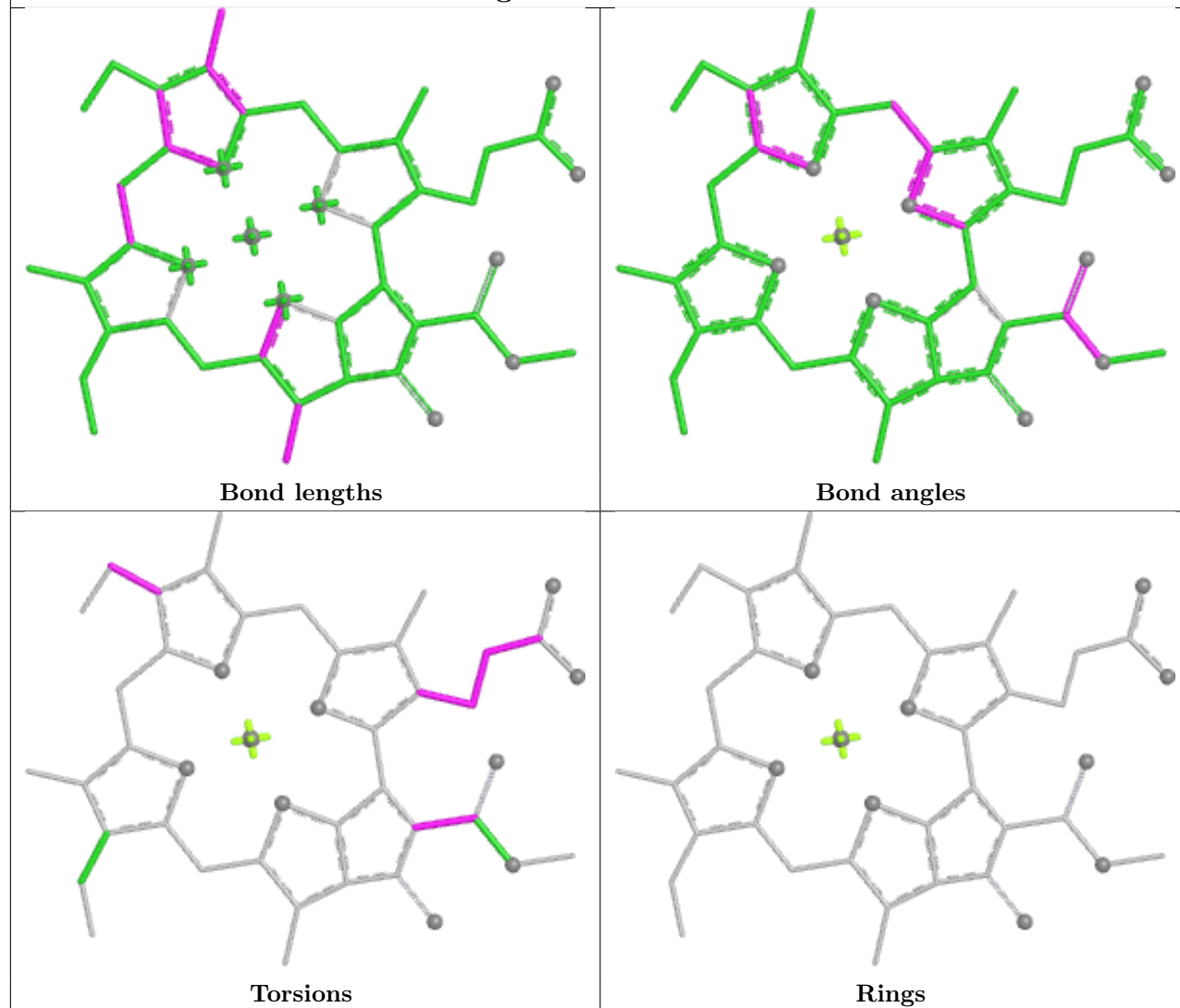




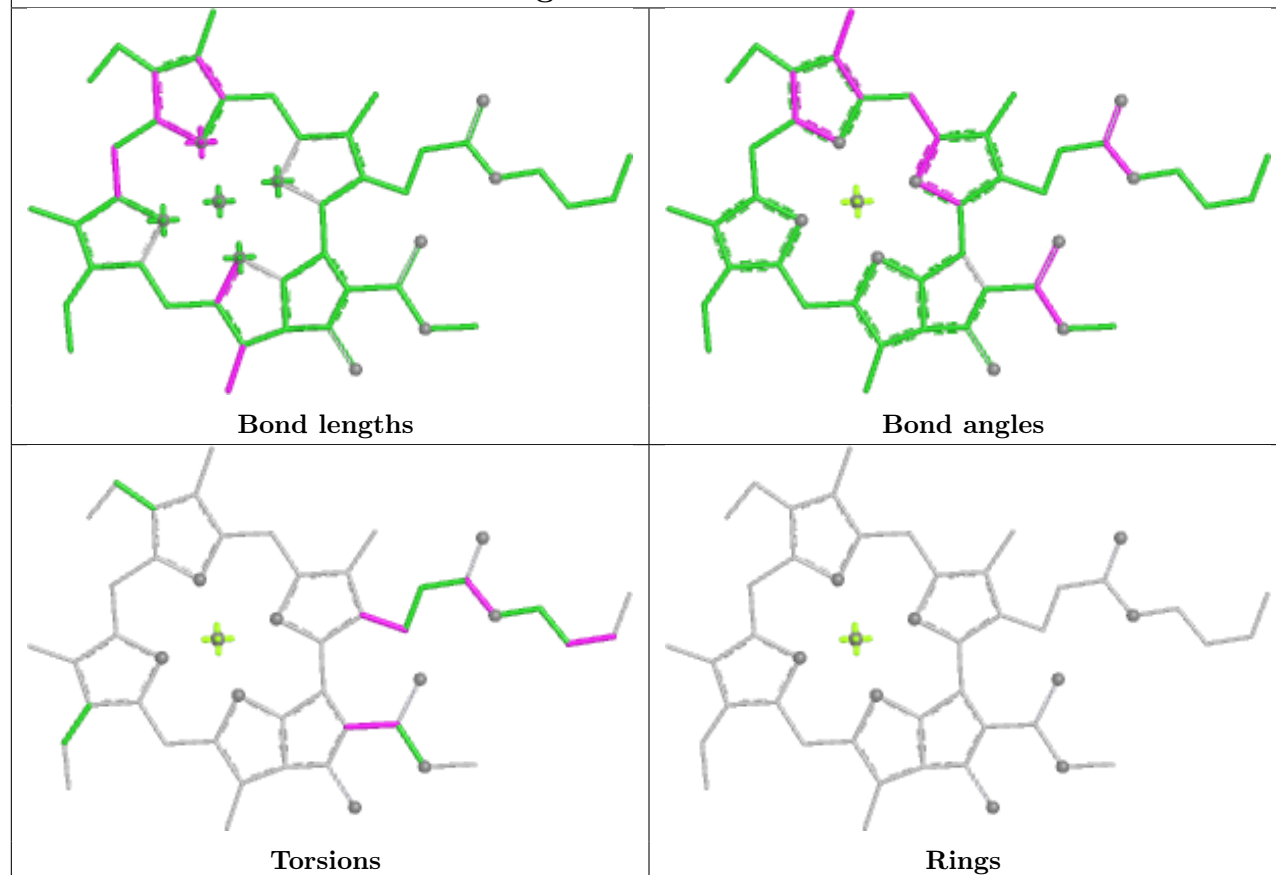
Ligand CLA b 839



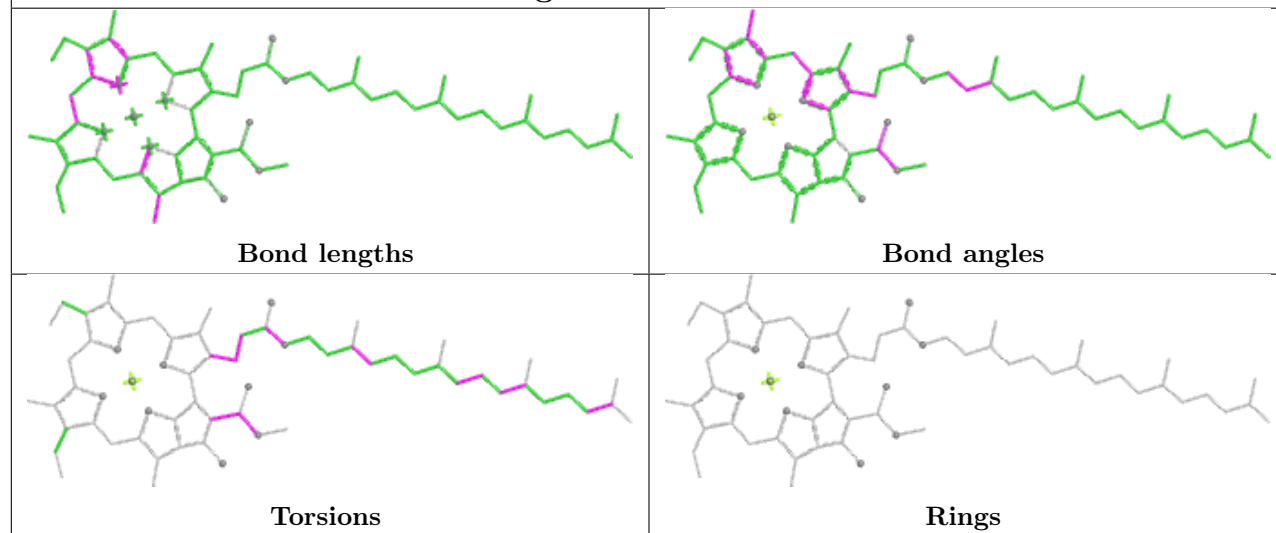
Ligand CLA a 817



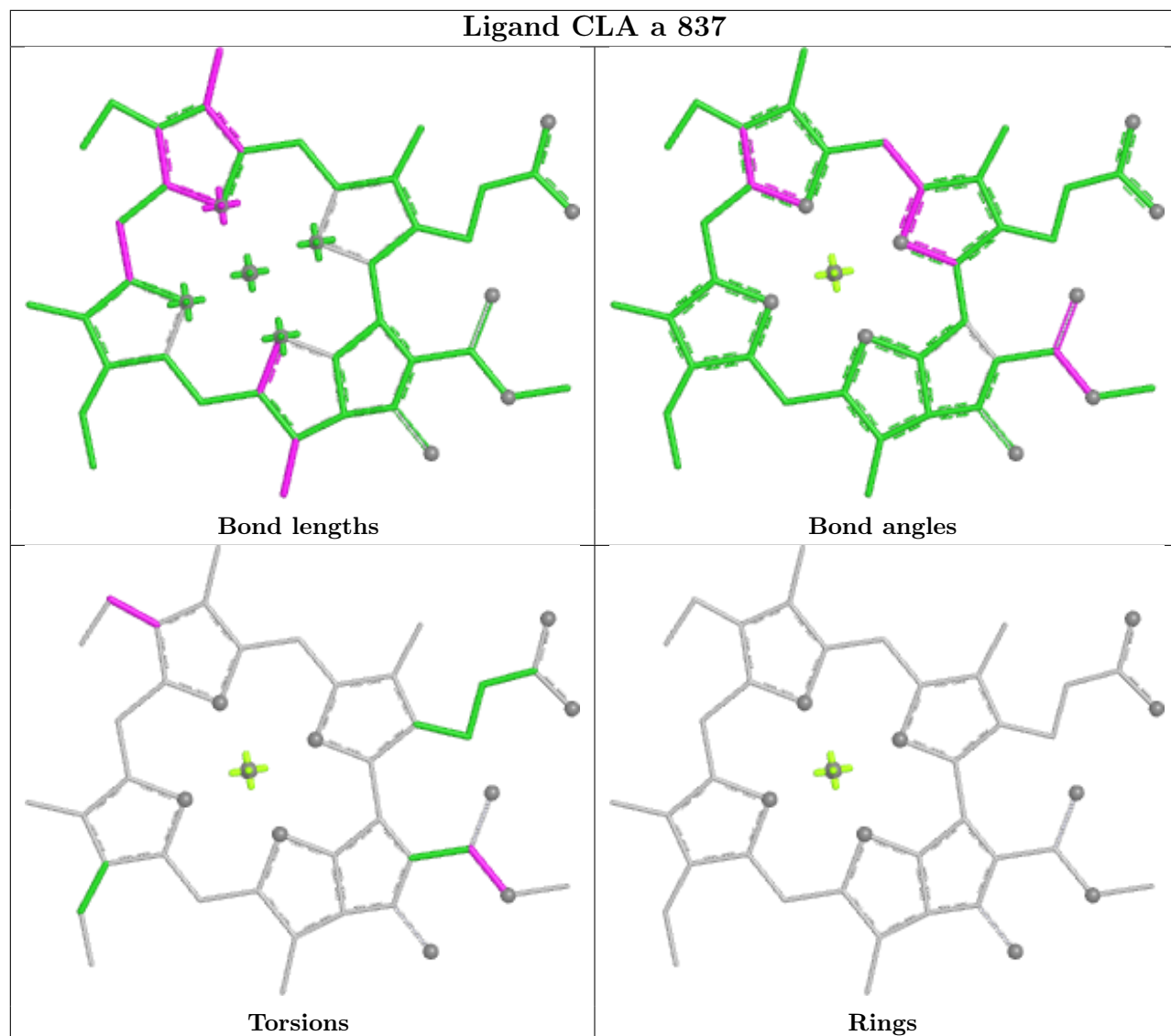
Ligand CLA a 823

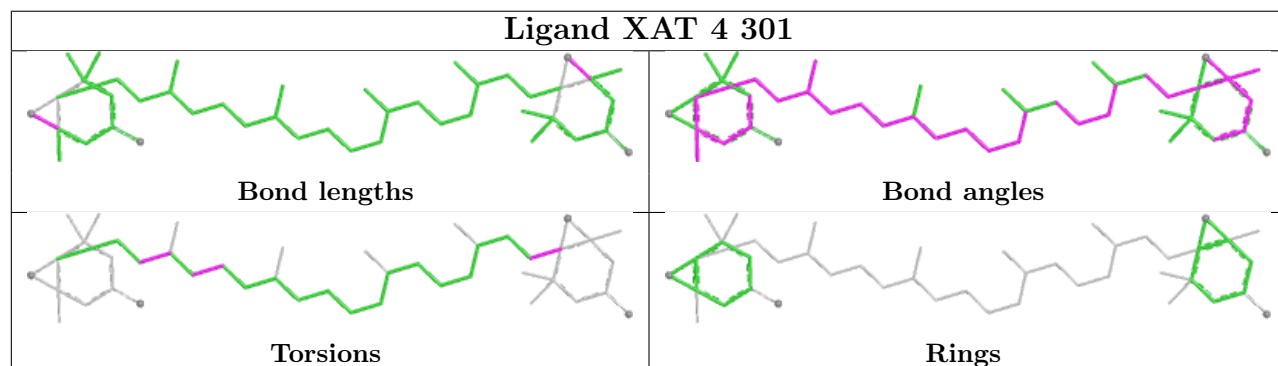
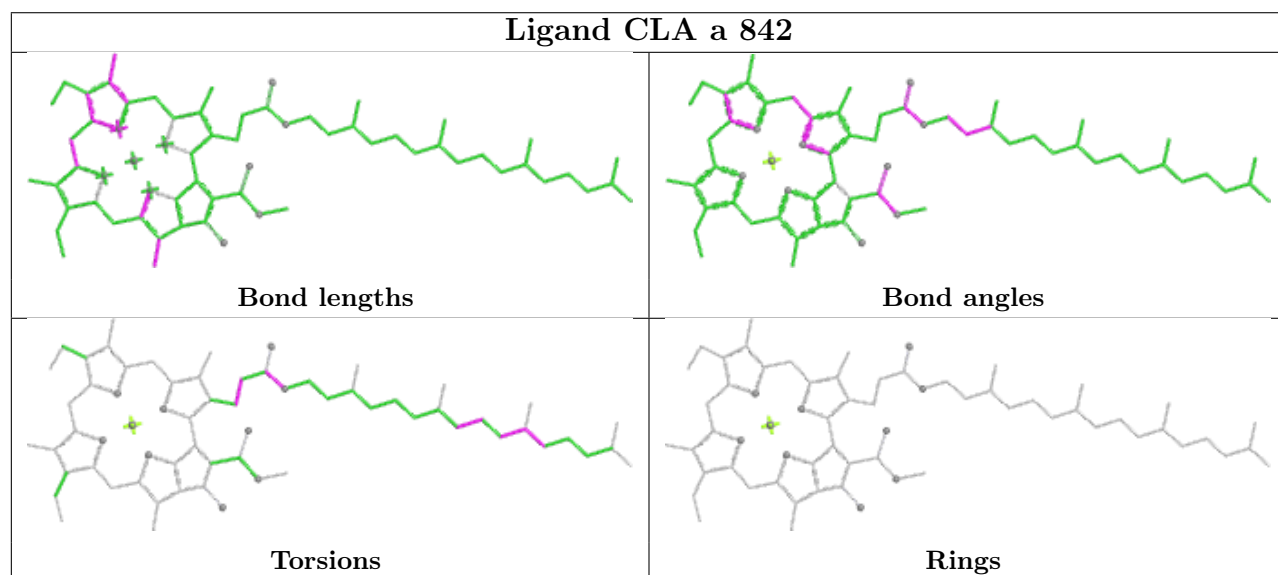
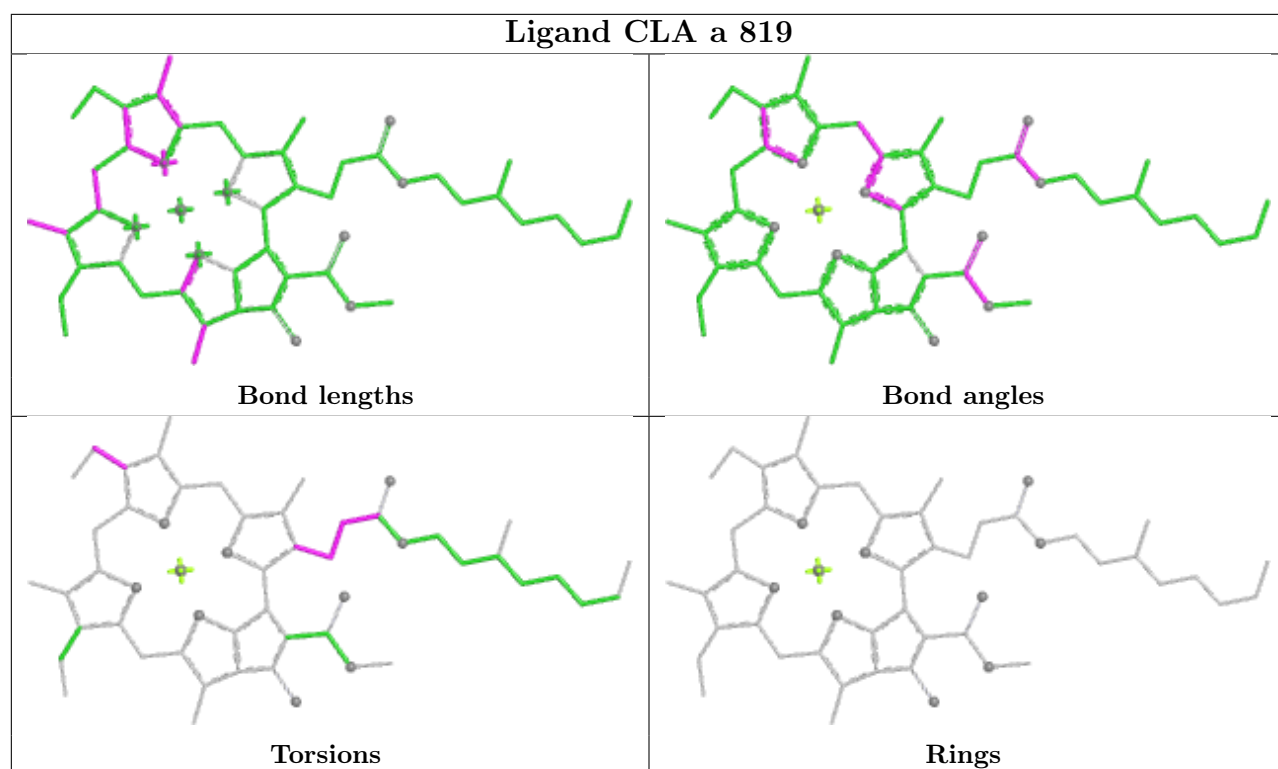


Ligand CLA b 811

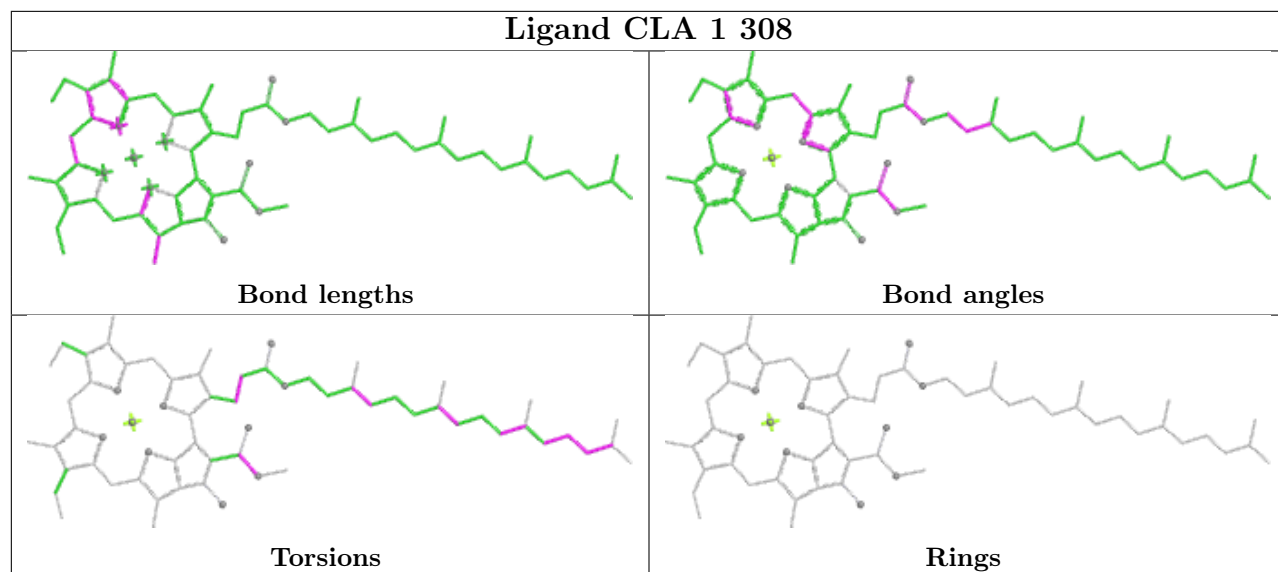


Ligand CLA a 837

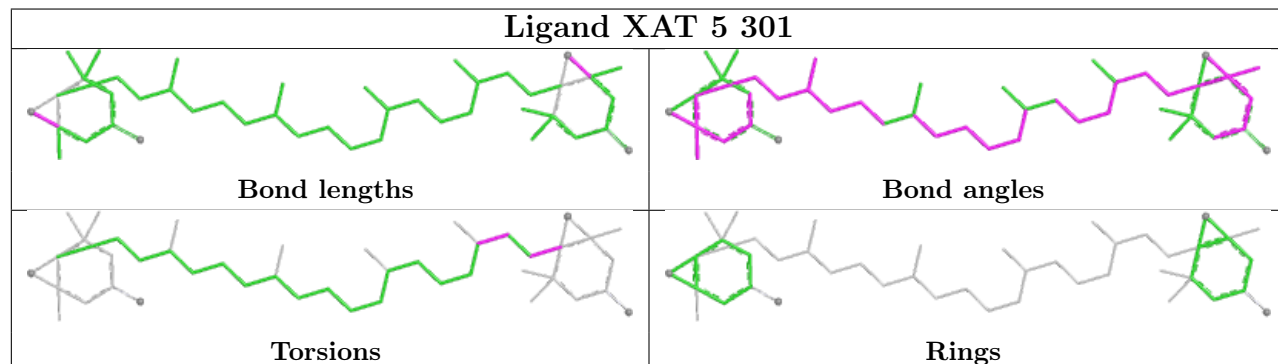




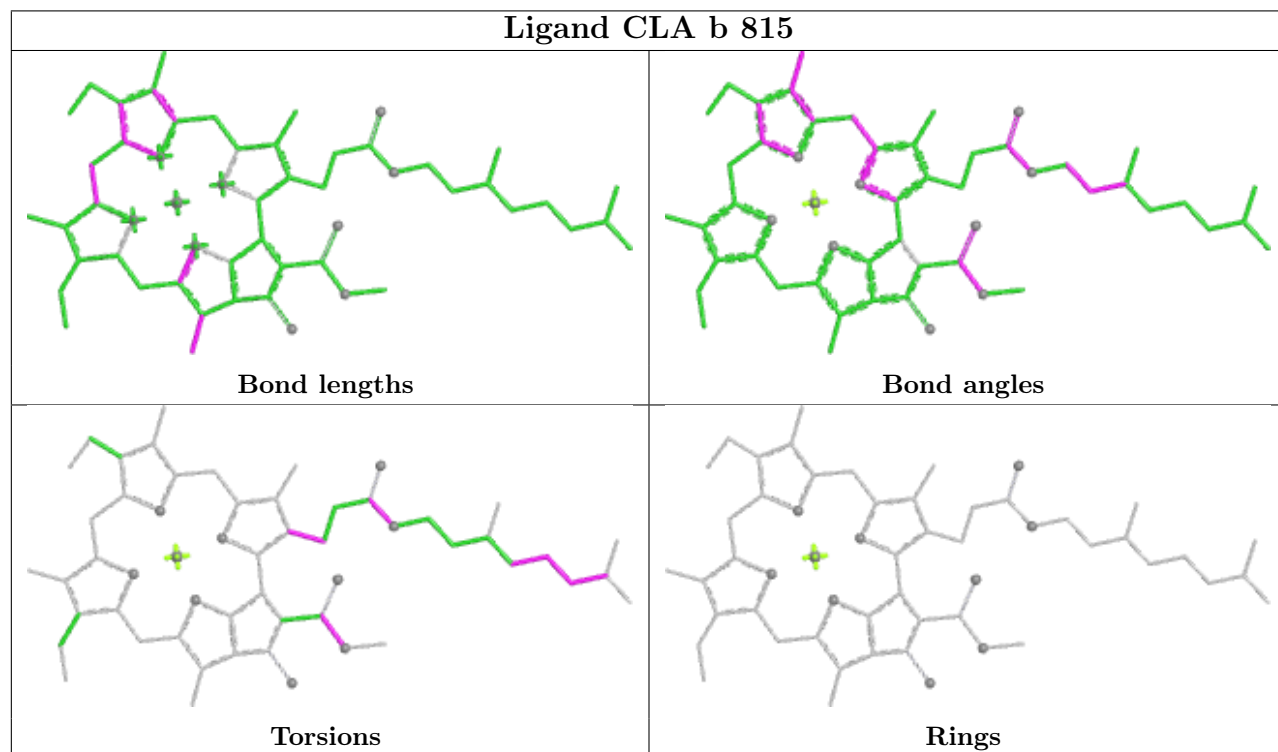
Ligand CLA 1 308



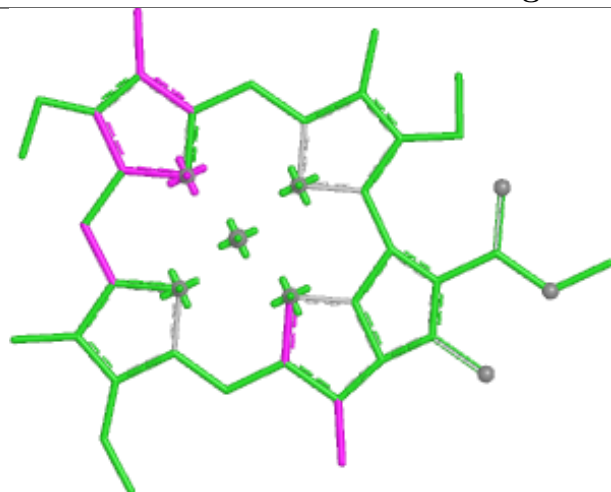
Ligand XAT 5 301



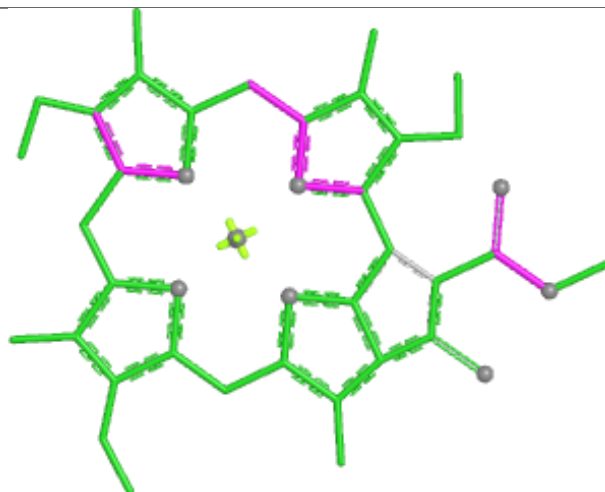
Ligand CLA b 815



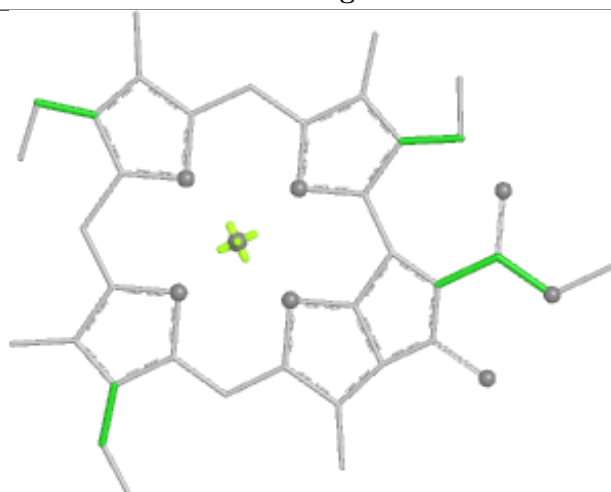
Ligand CLA 1 202



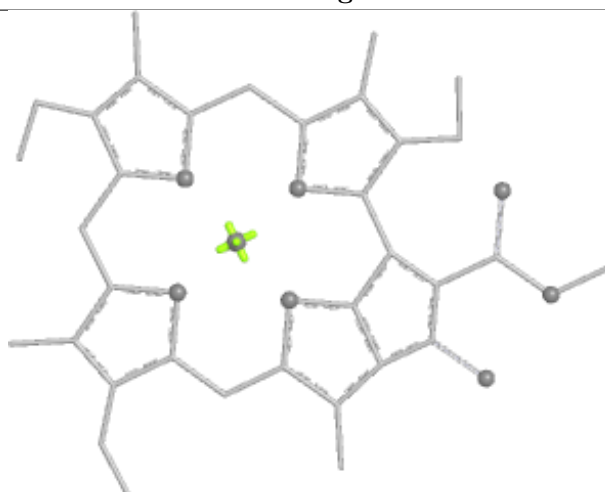
Bond lengths



Bond angles

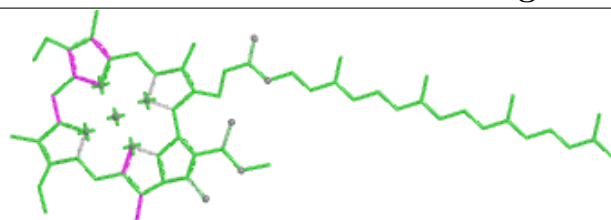


Torsions

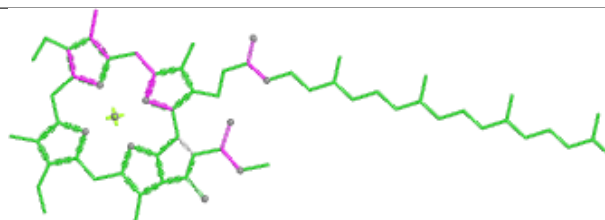


Rings

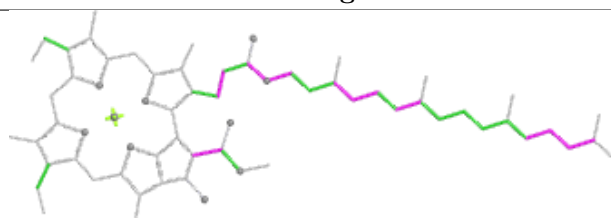
Ligand CLA a 839



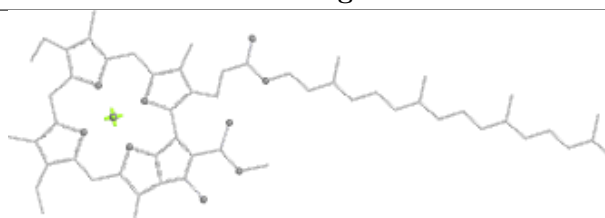
Bond lengths



Bond angles

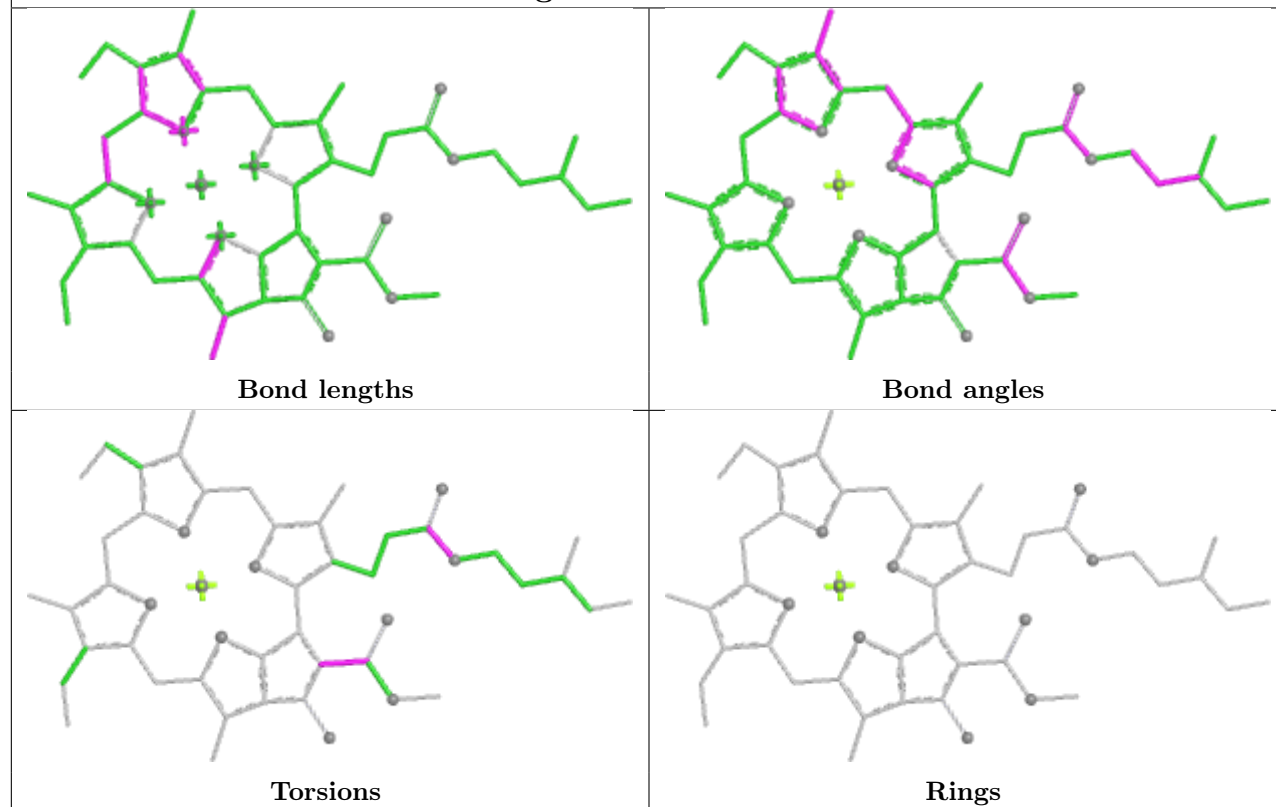


Torsions

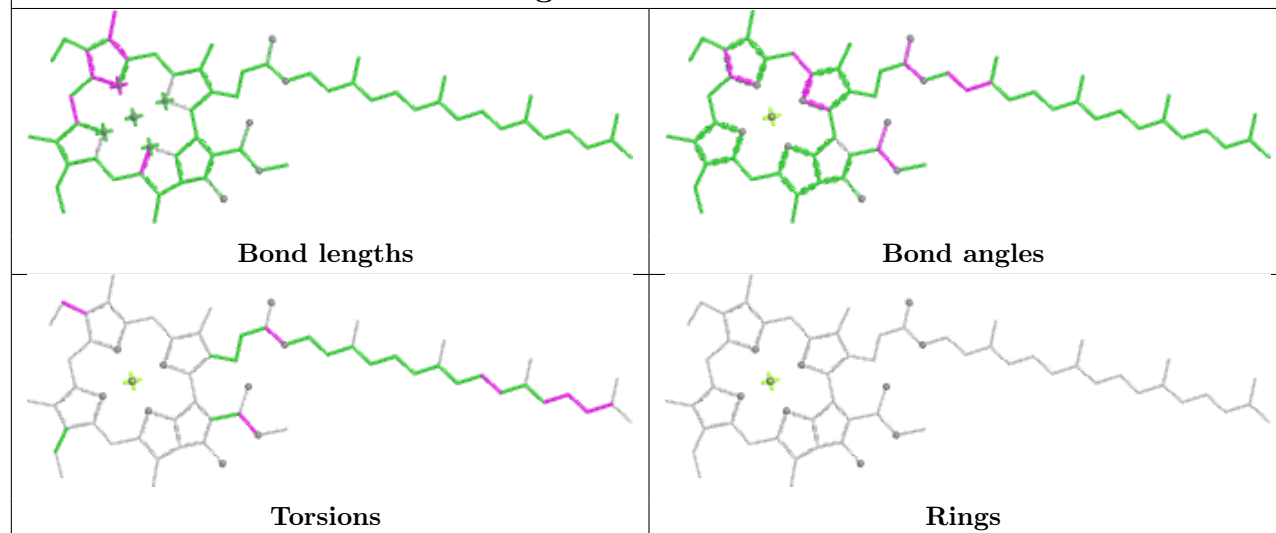


Rings

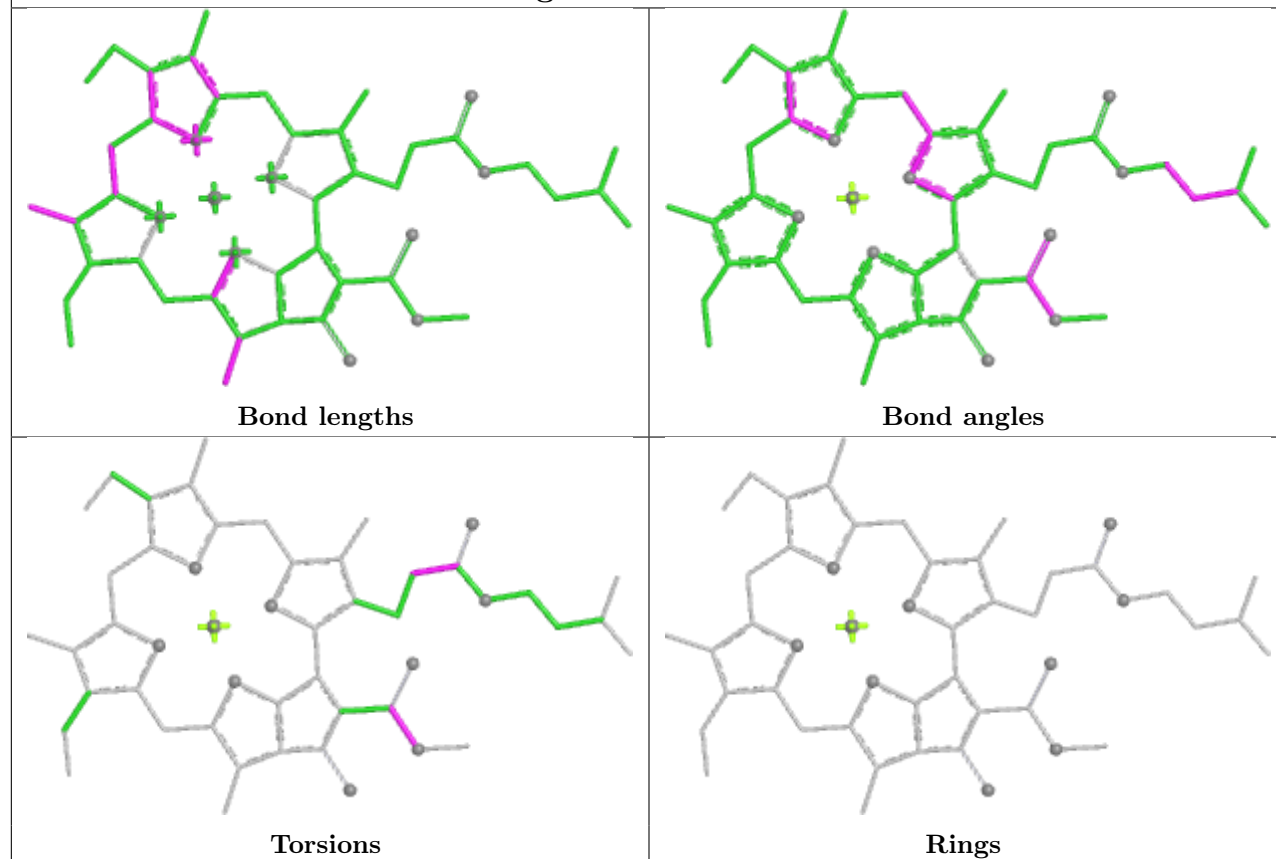
Ligand CLA b 822



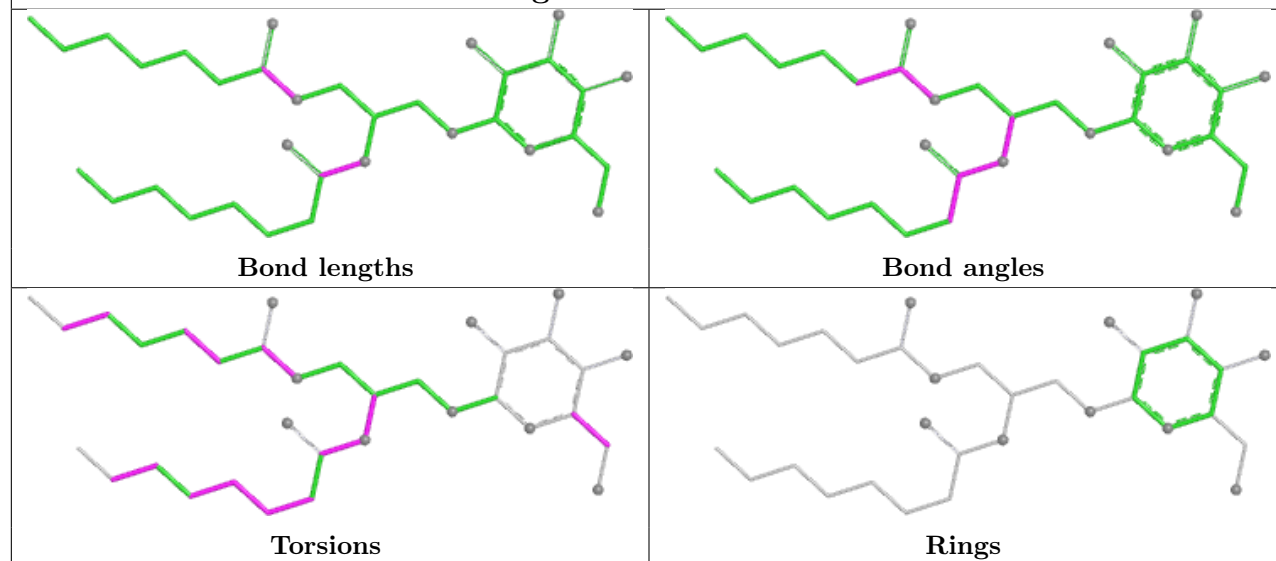
Ligand CLA b 841



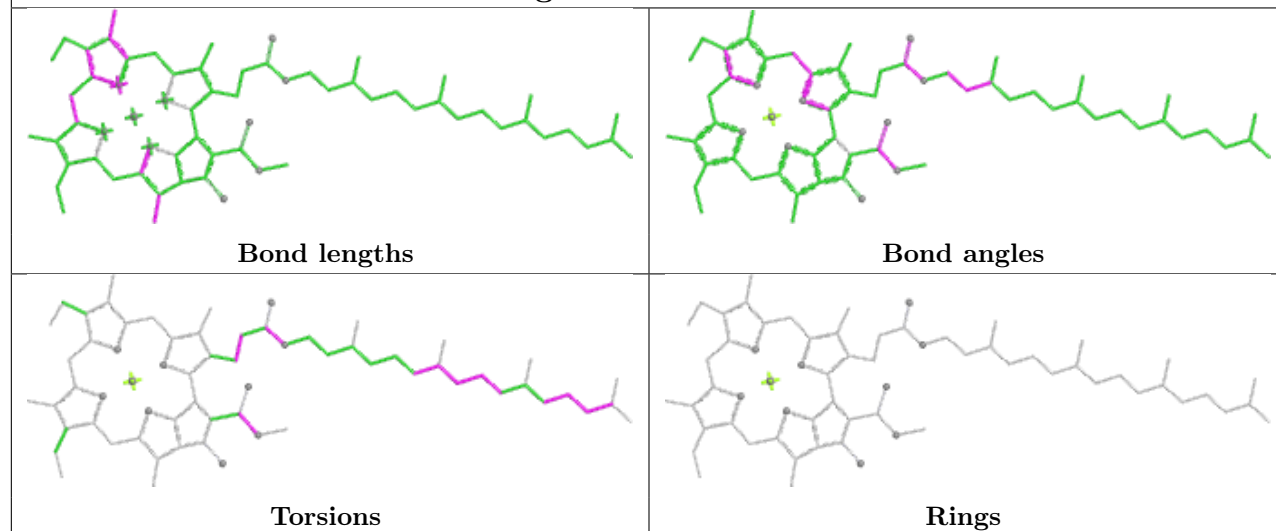
Ligand CLA 4 310



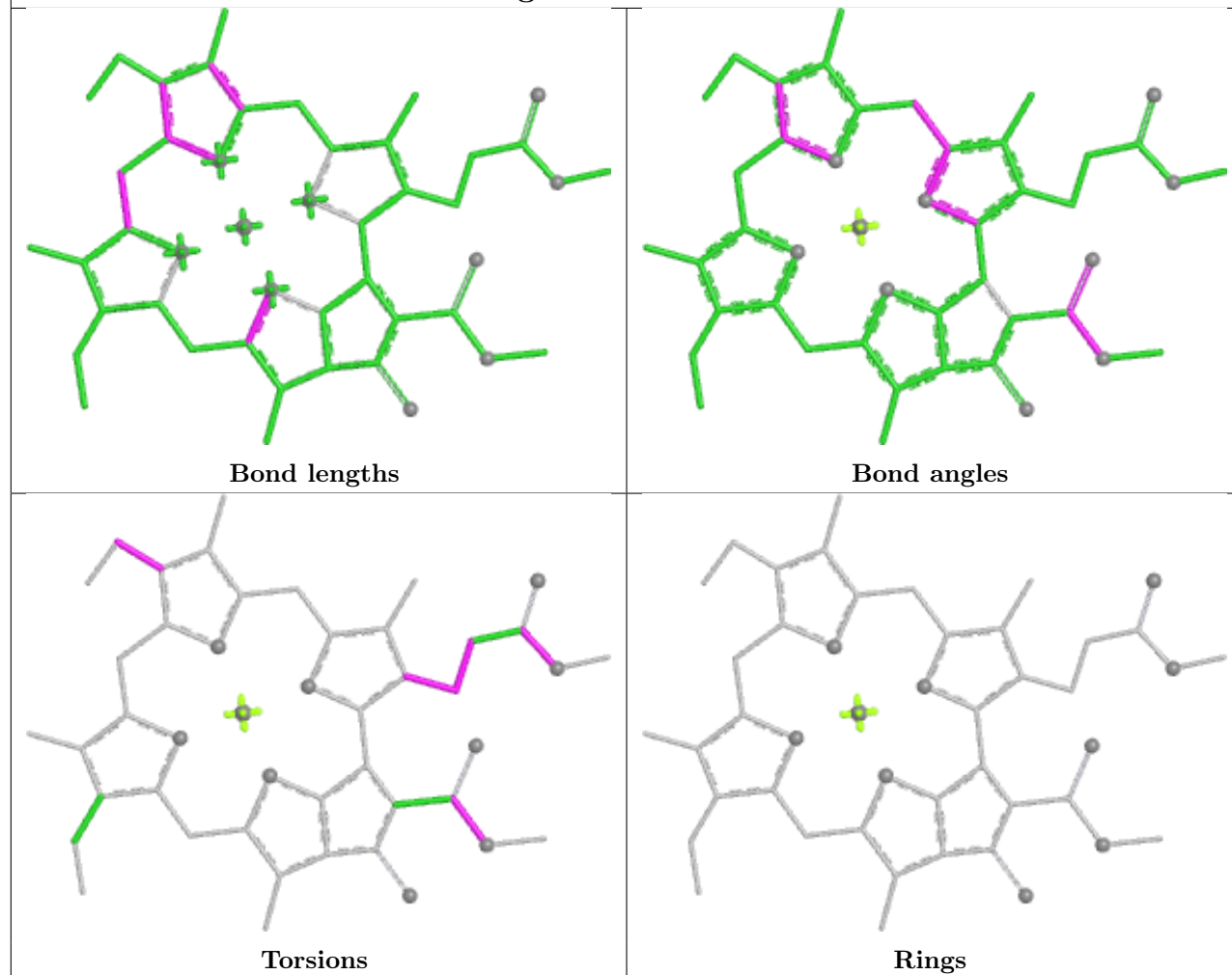
Ligand LMG a 853

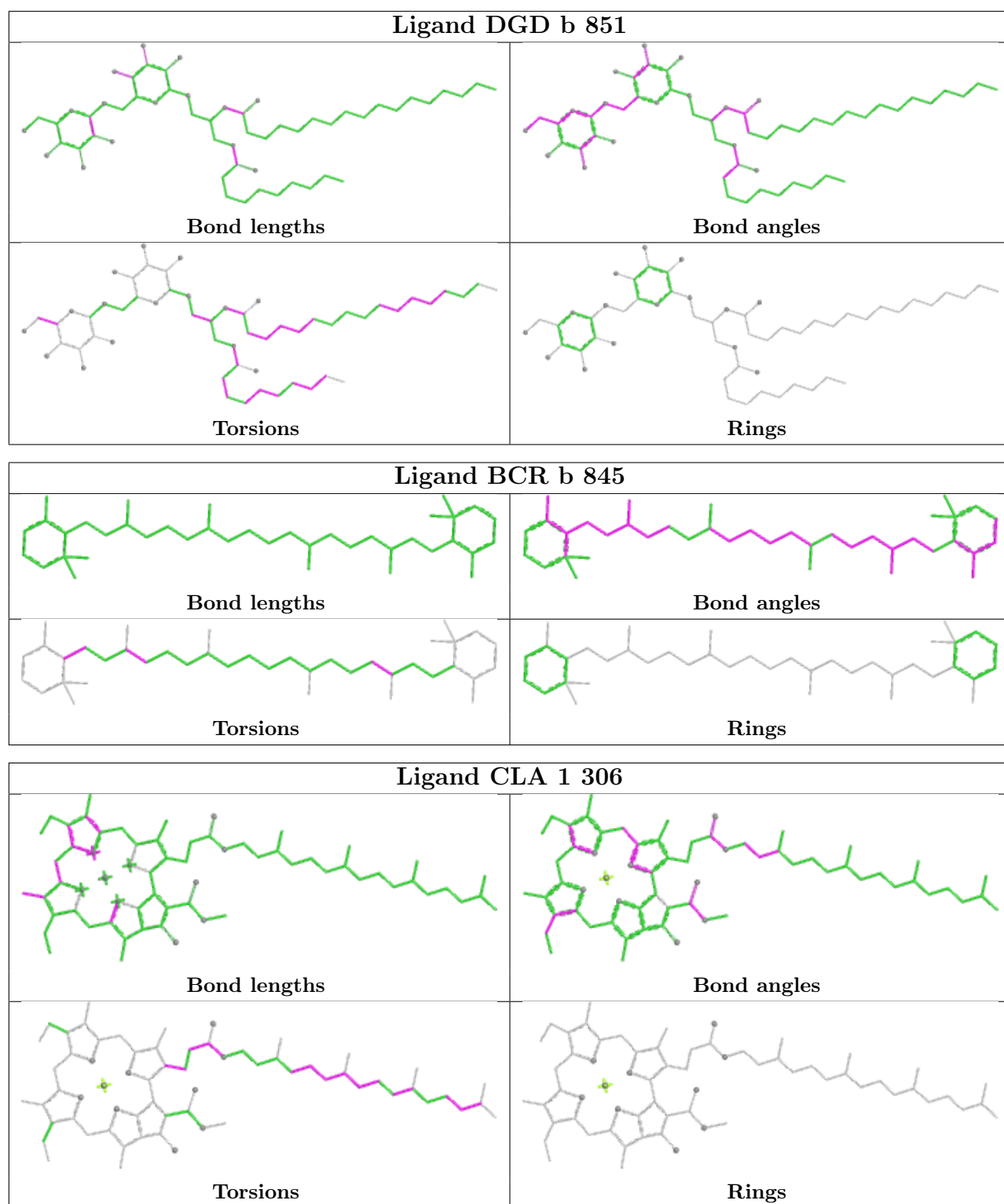


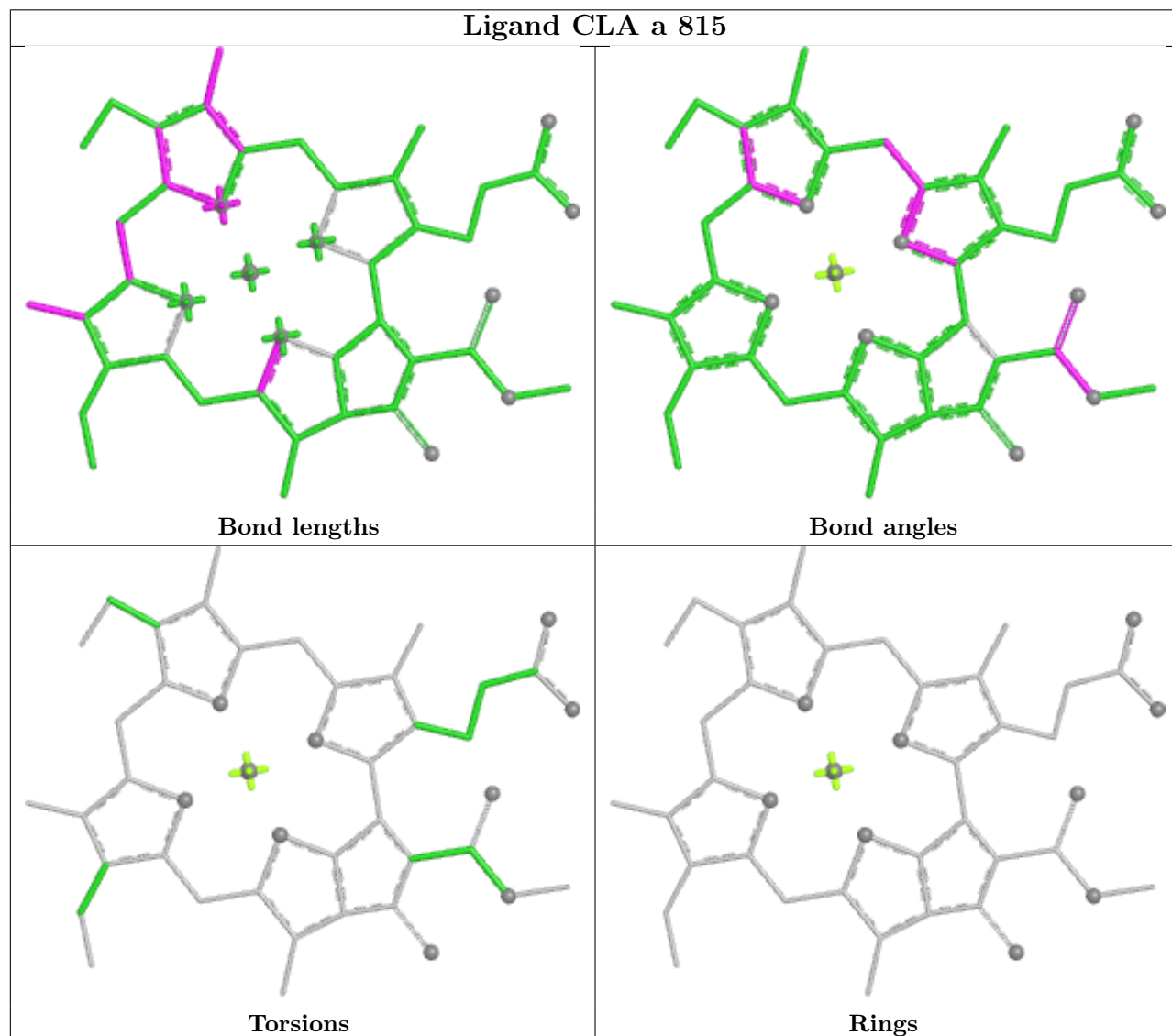
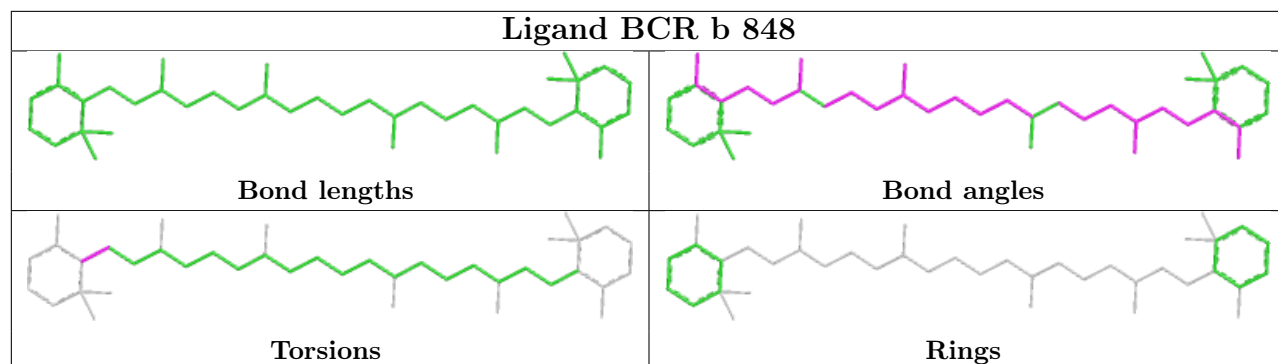
Ligand CLA b 828

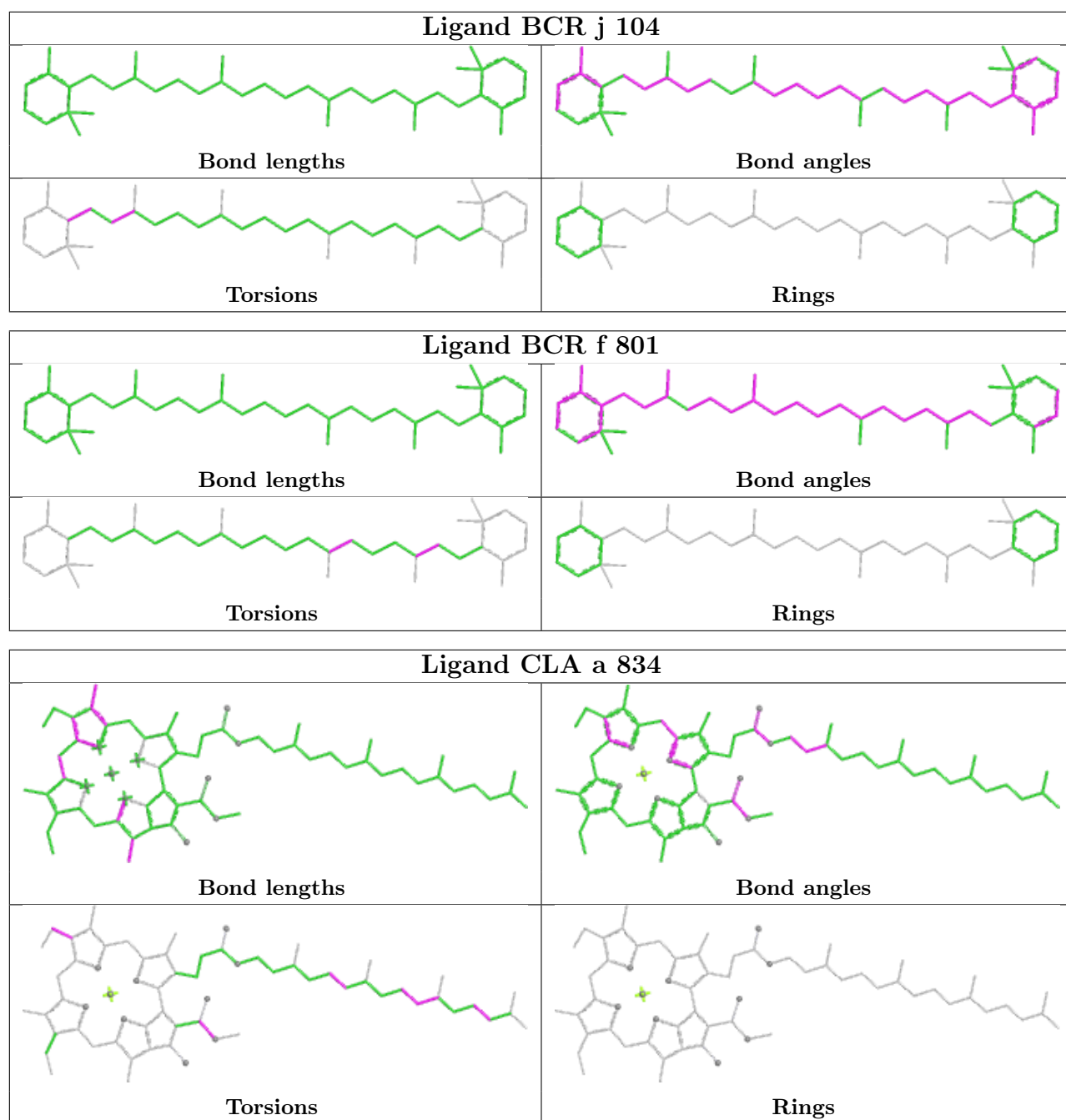


Ligand CLA 4 317

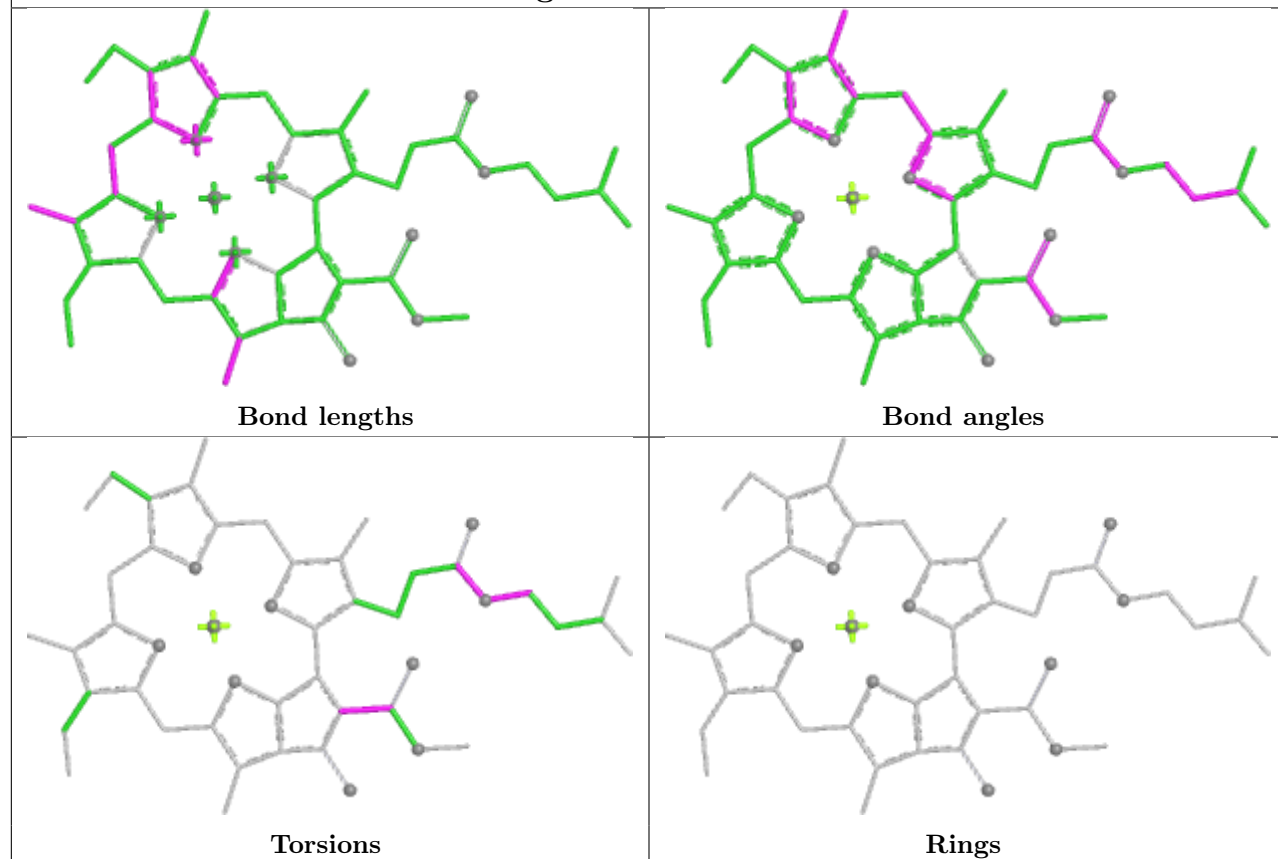




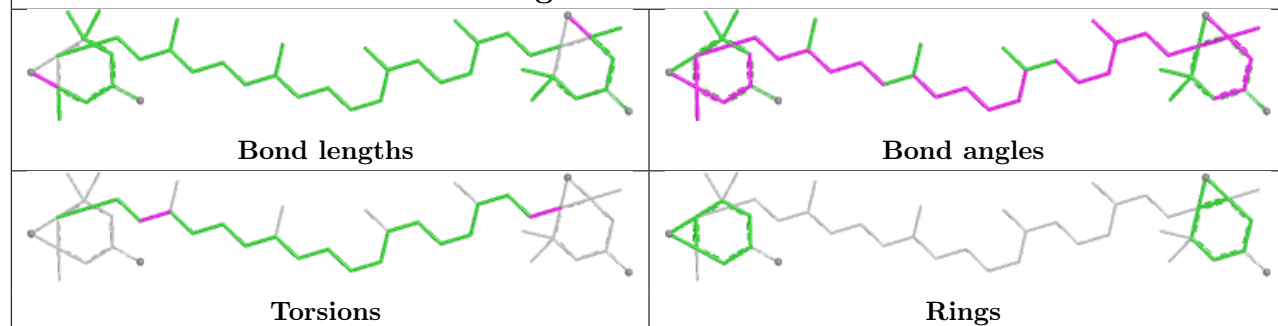


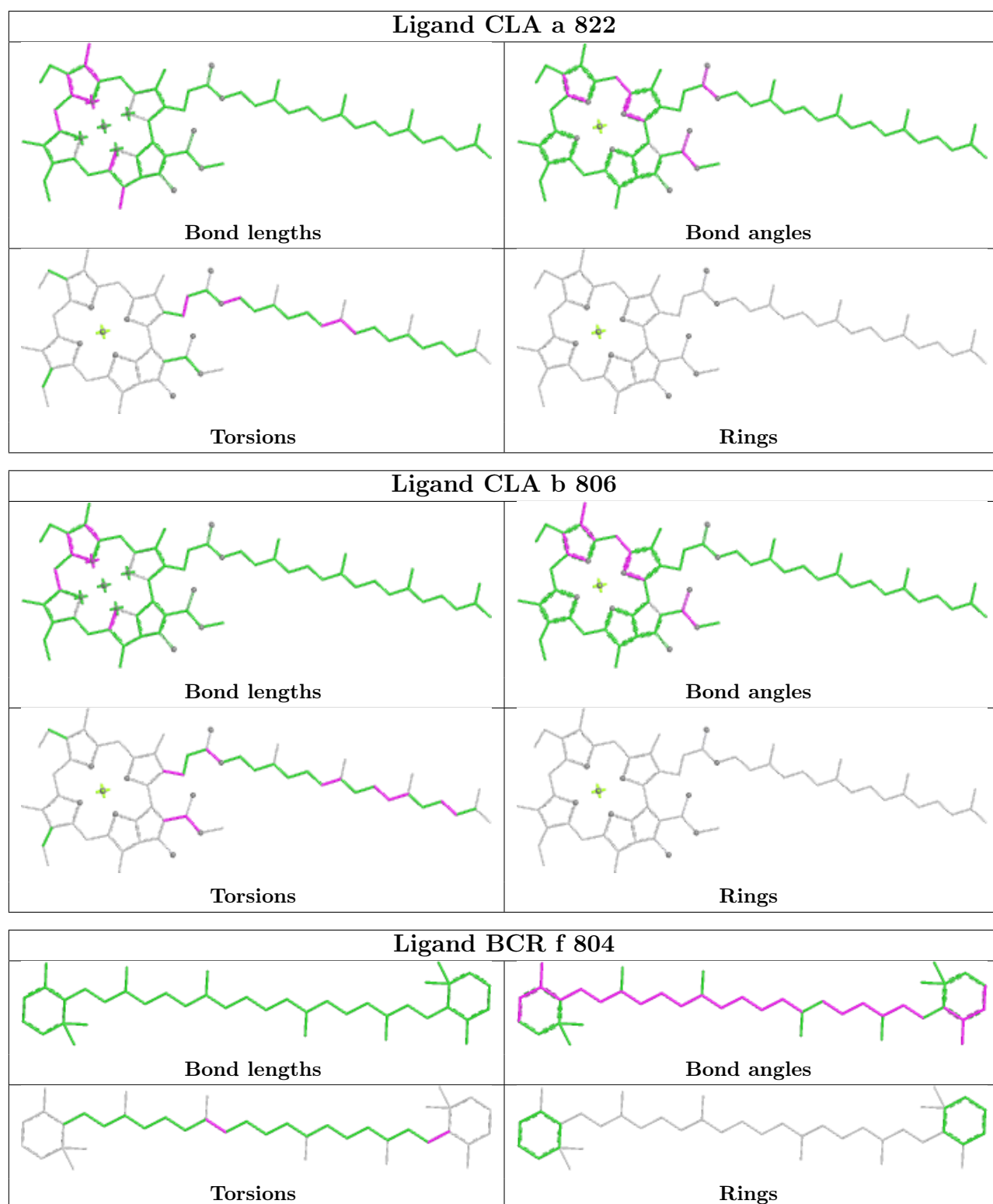


Ligand CLA a 816

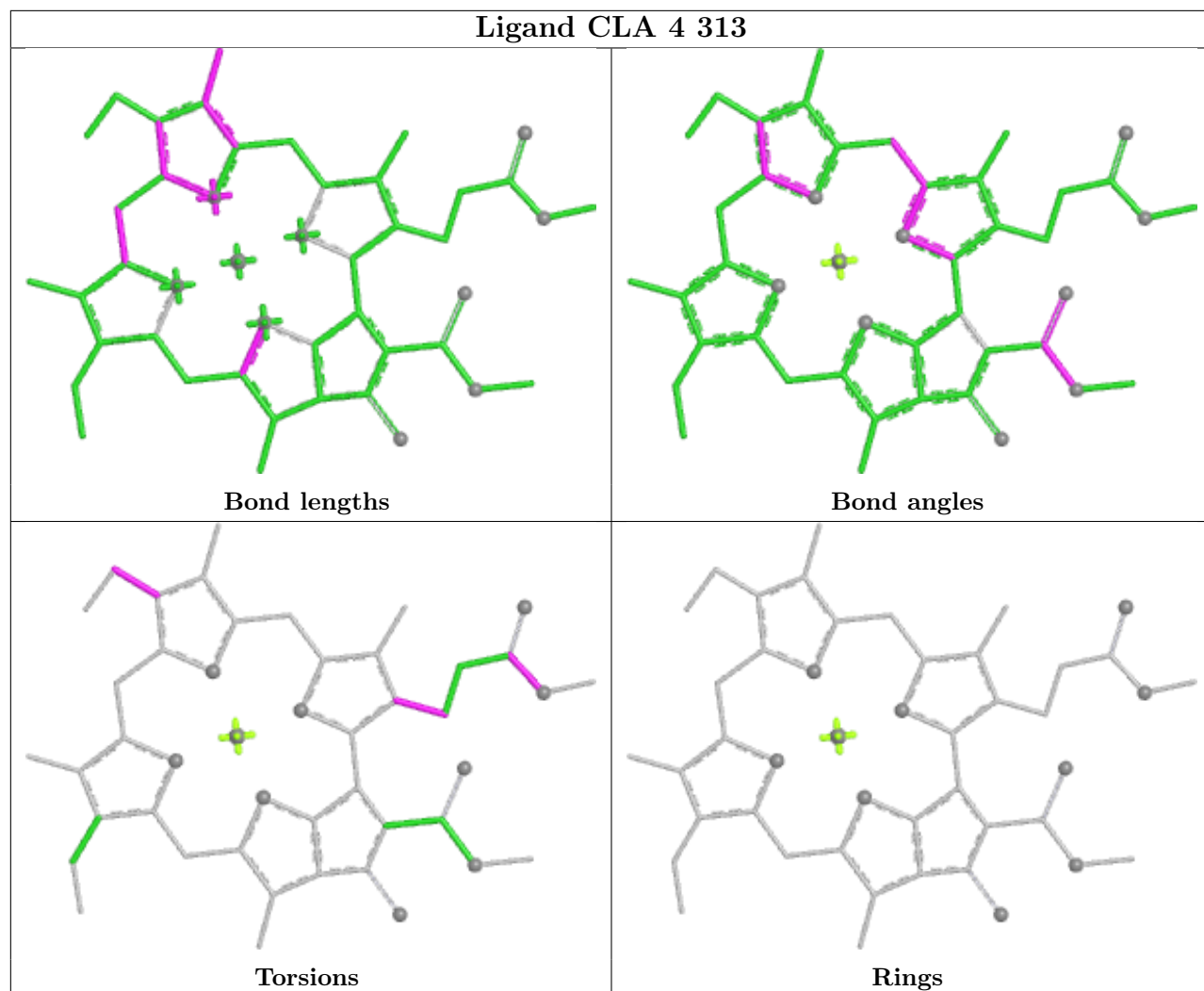


Ligand XAT 4 302

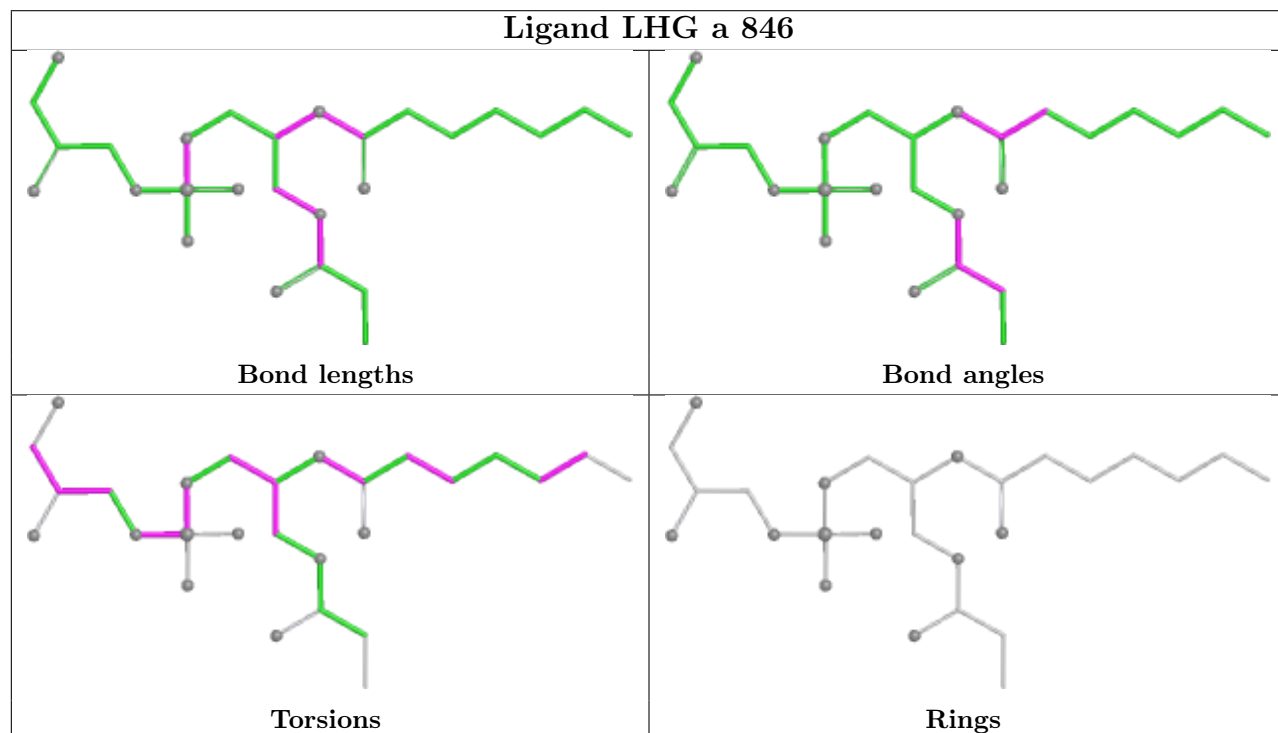


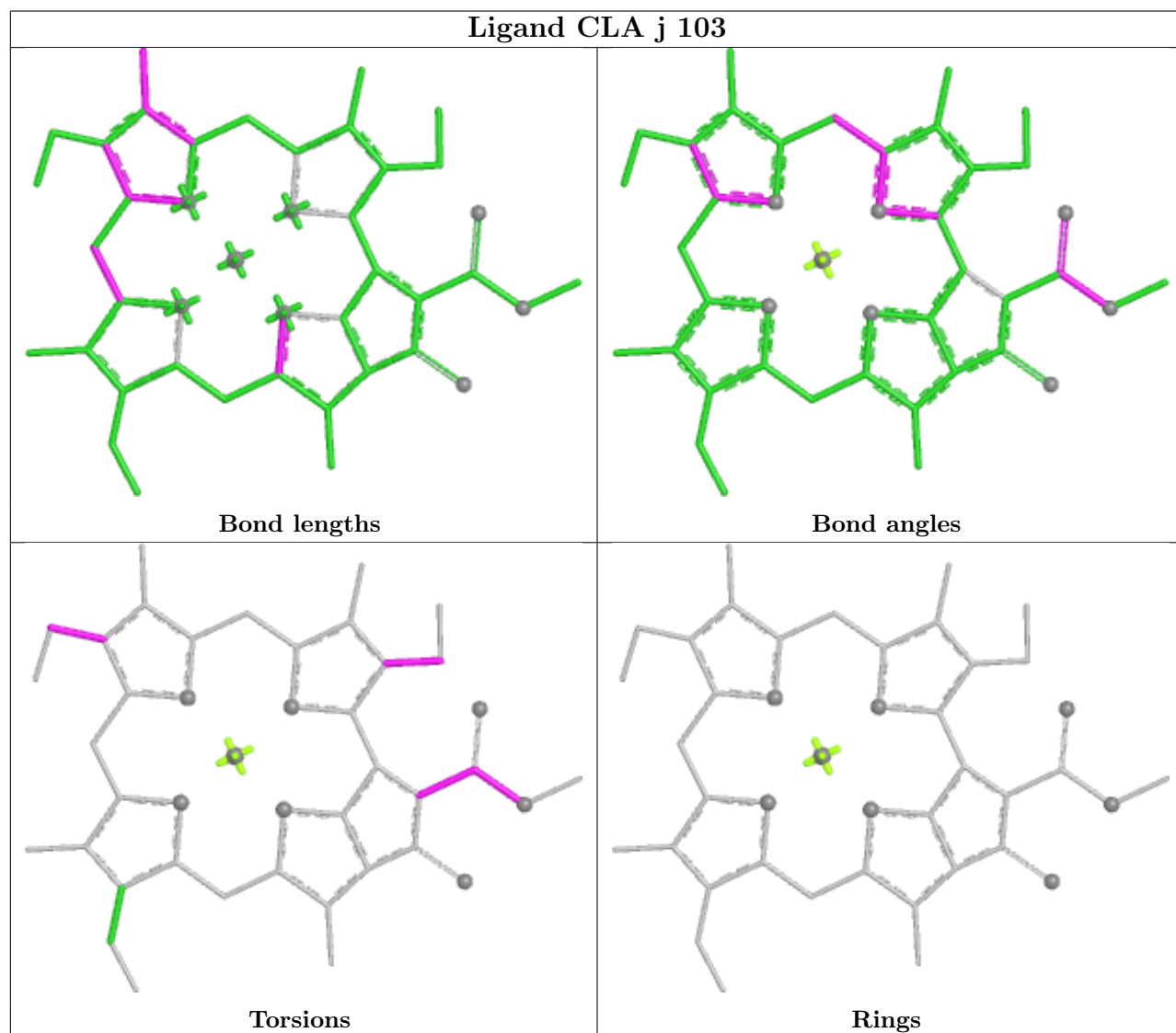
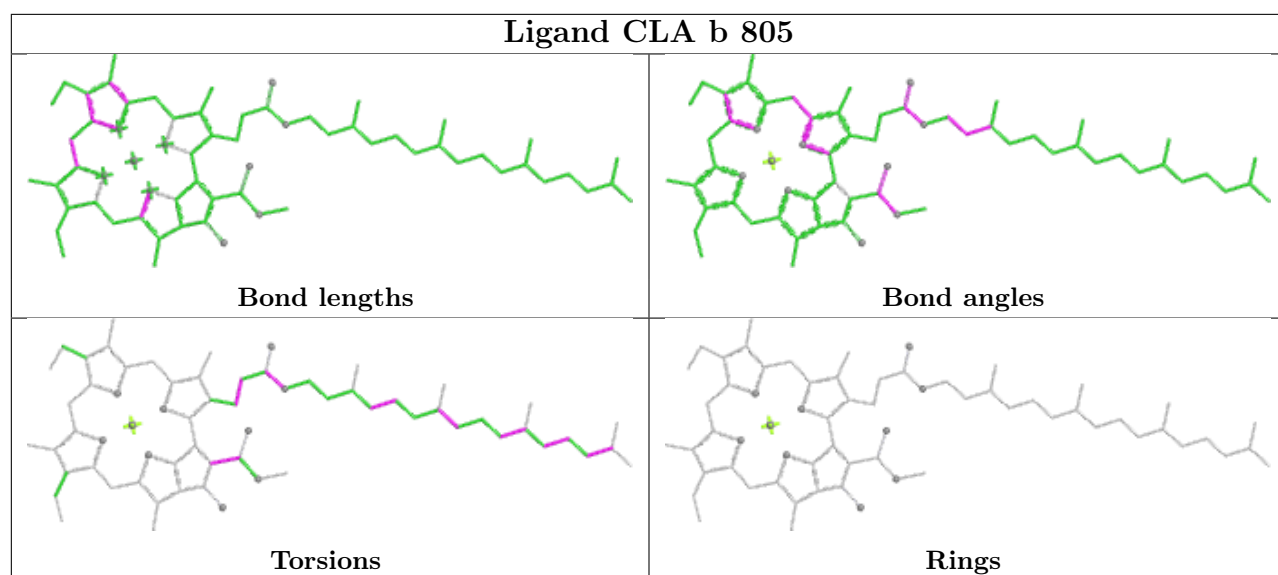


Ligand CLA 4 313

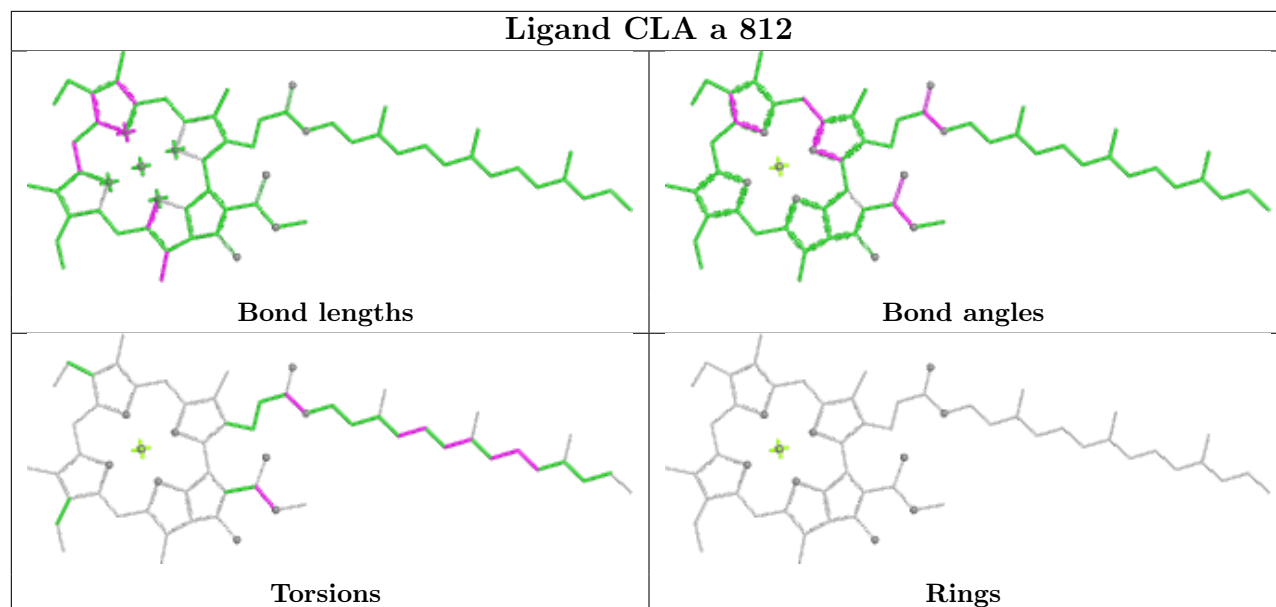


Ligand LHG a 846

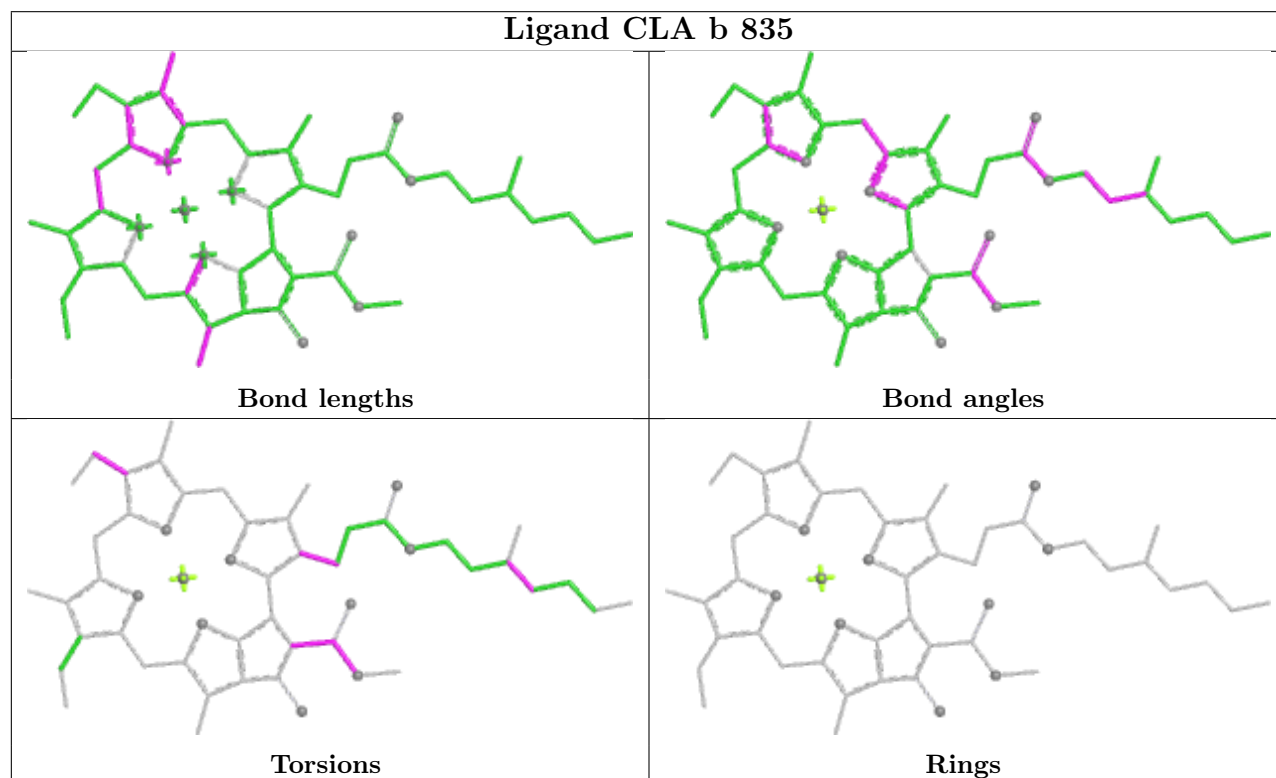




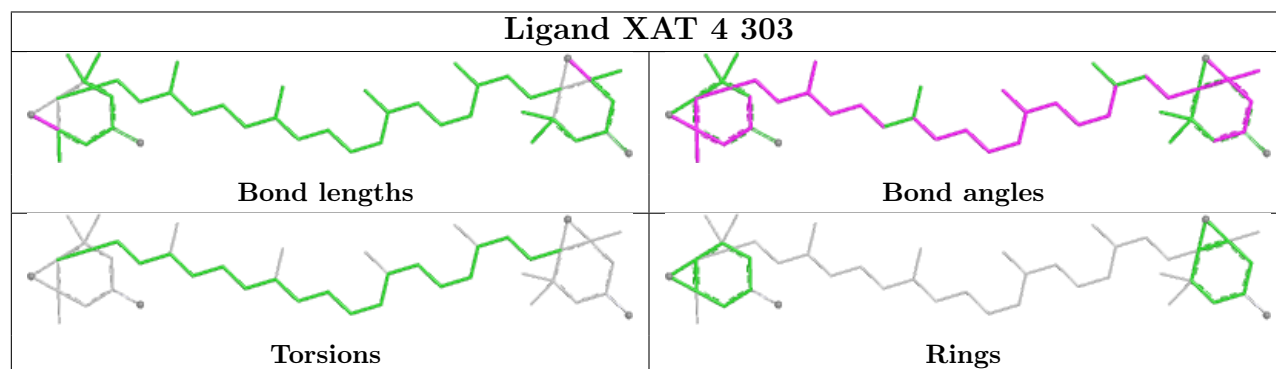
Ligand CLA a 812

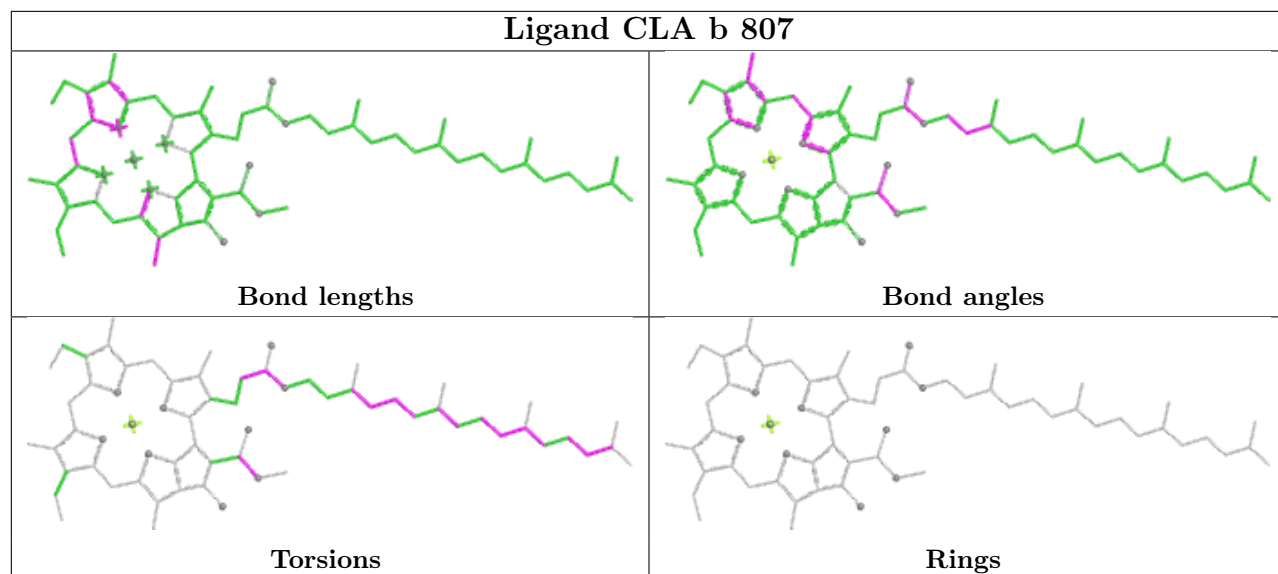
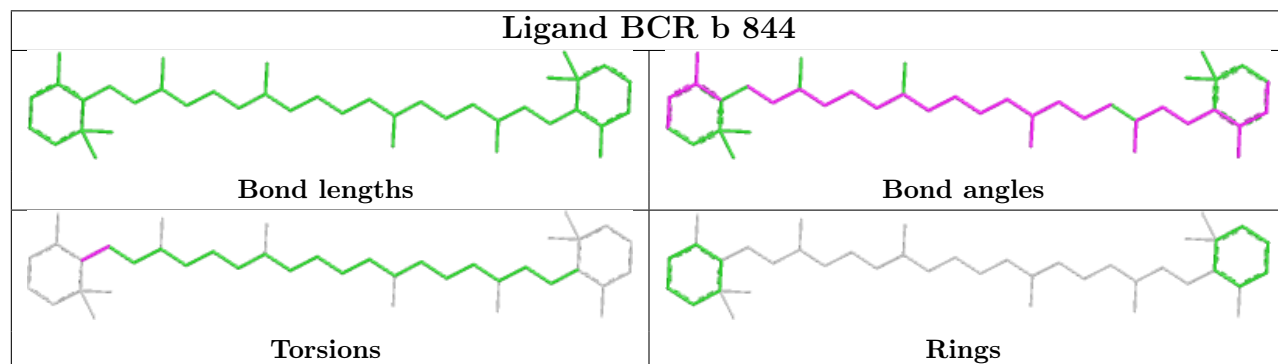
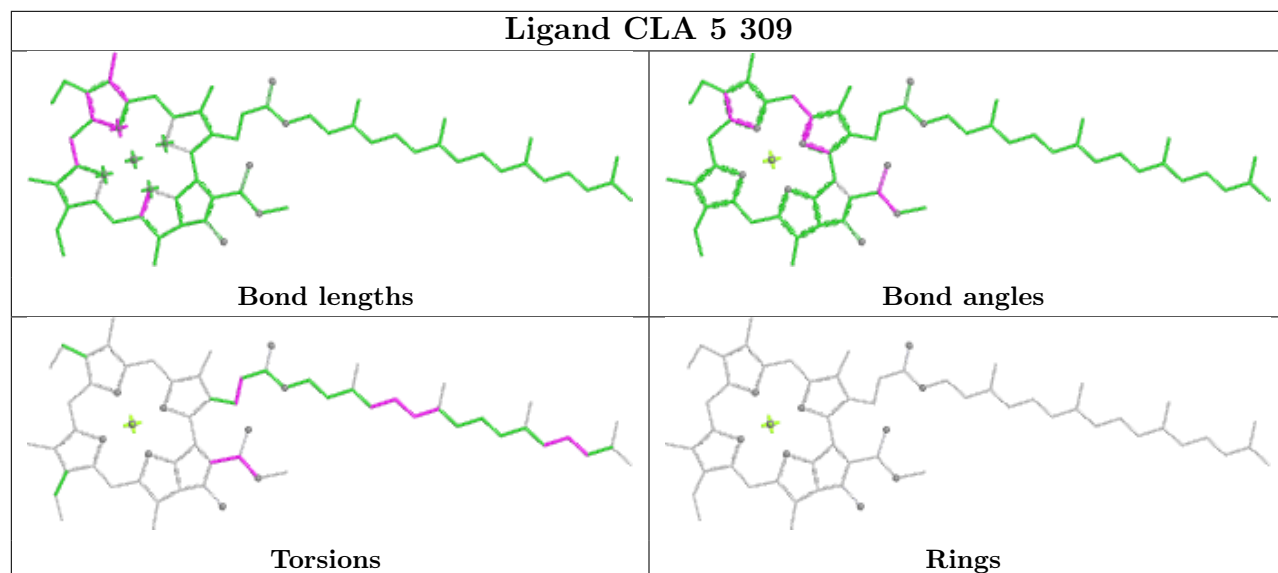


Ligand CLA b 835

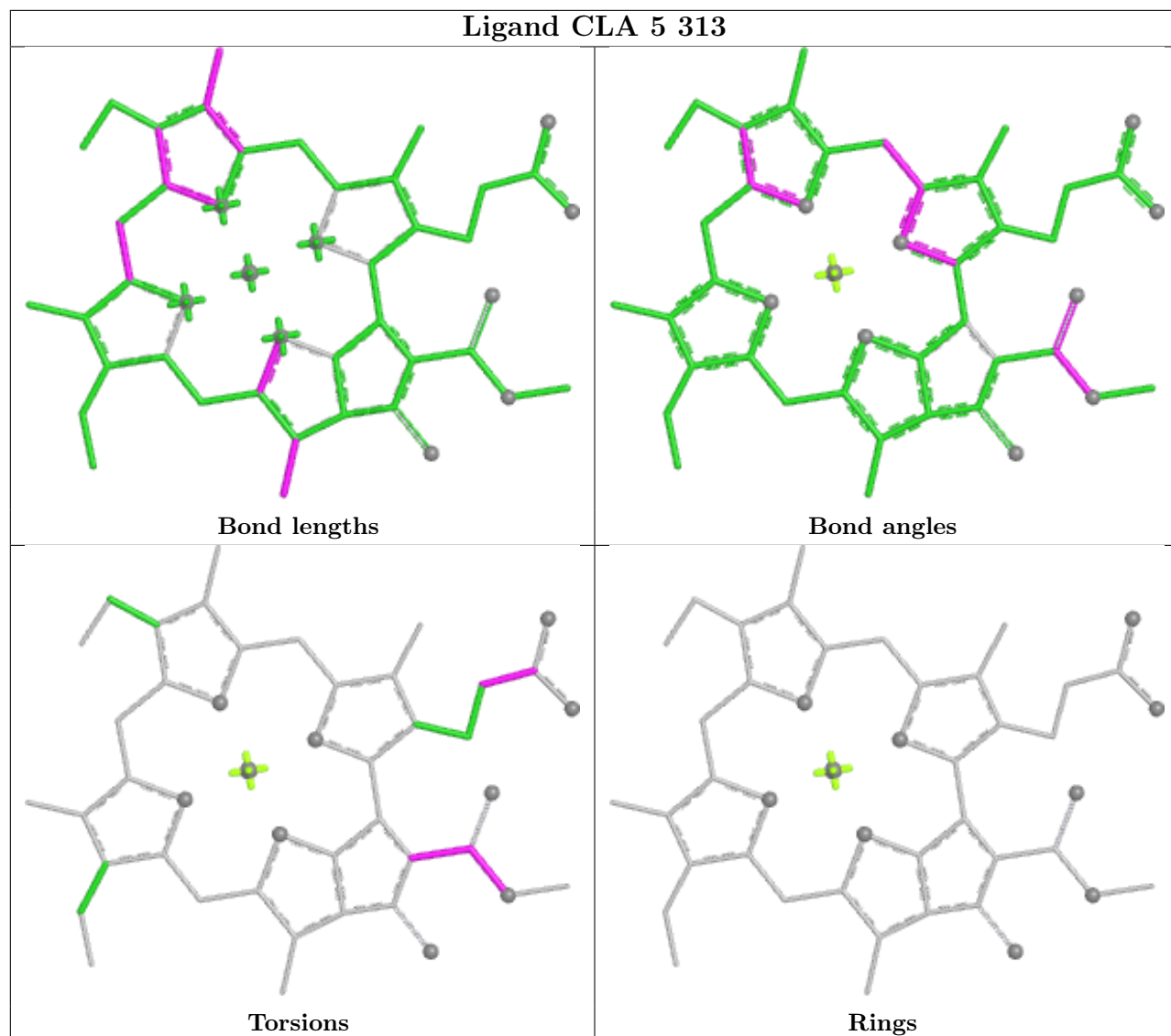


Ligand XAT 4 303

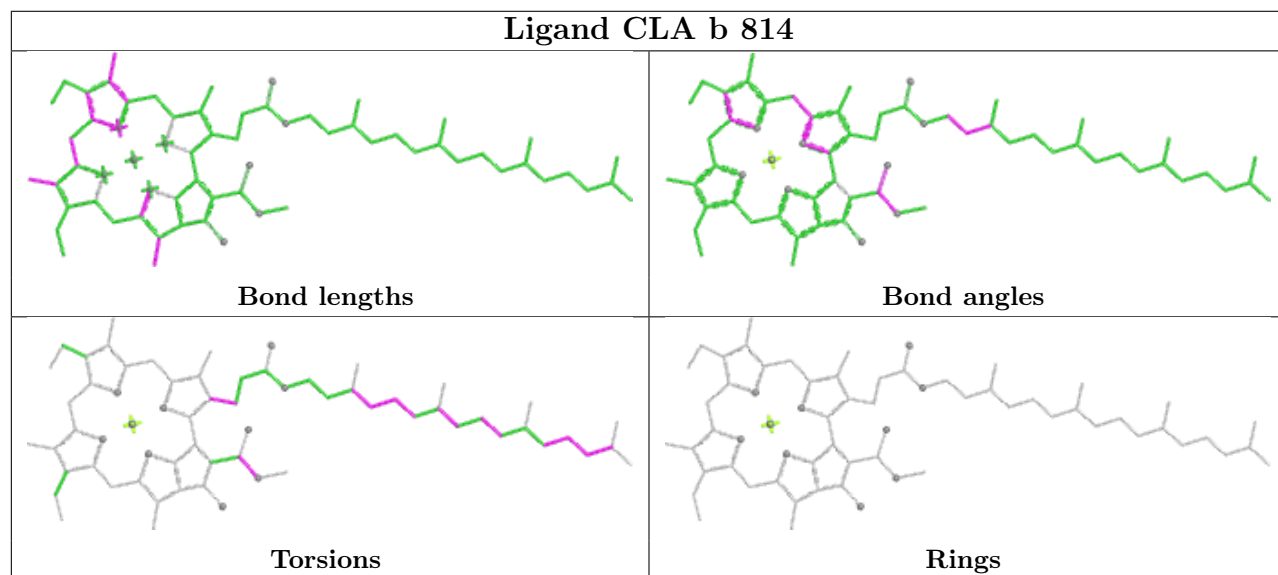


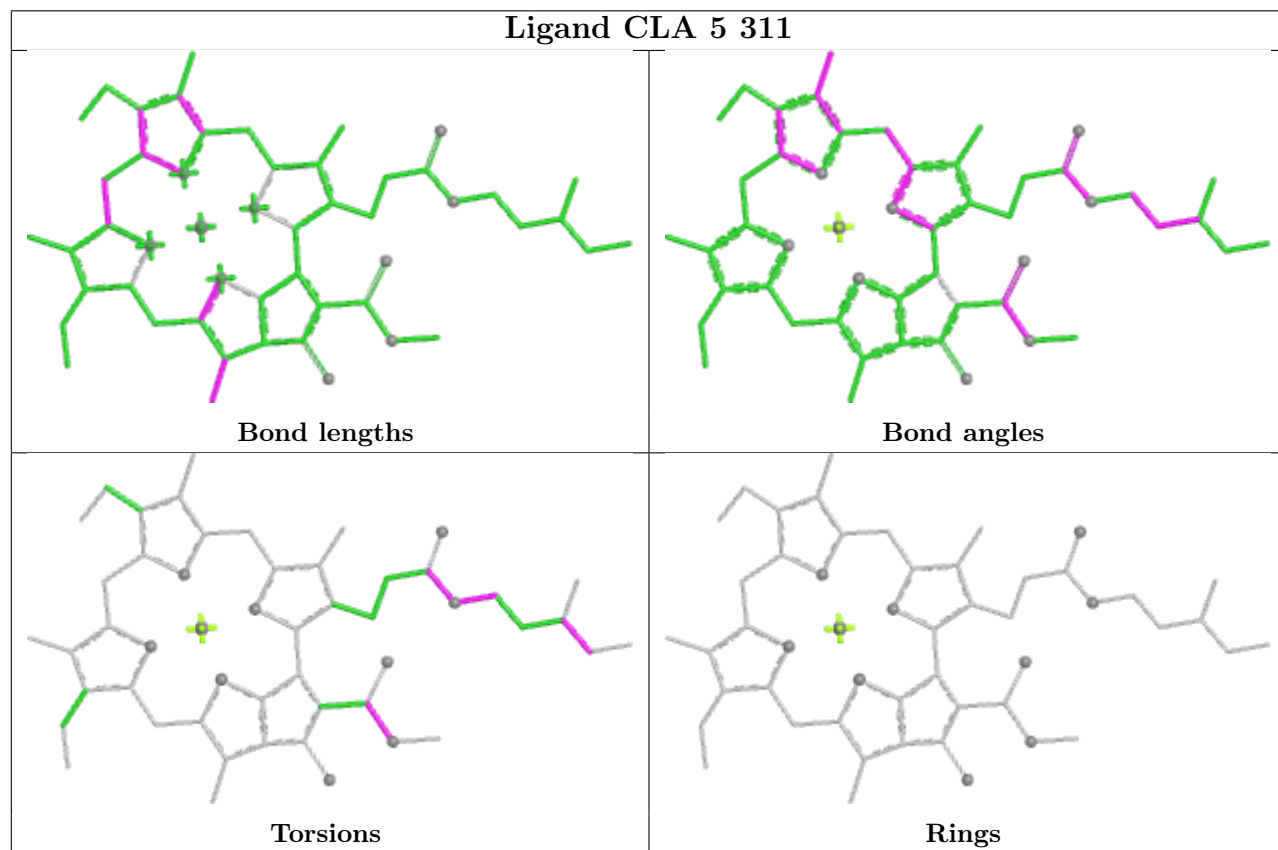
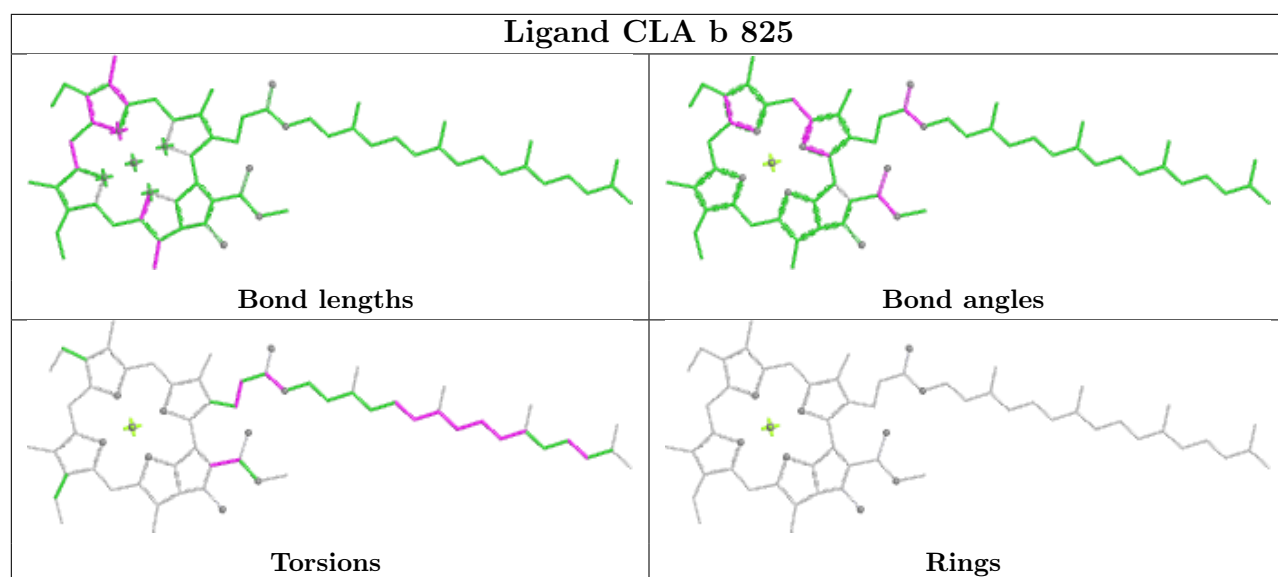
Ligand CLA b 807**Ligand BCR b 844****Ligand CLA 5 309**

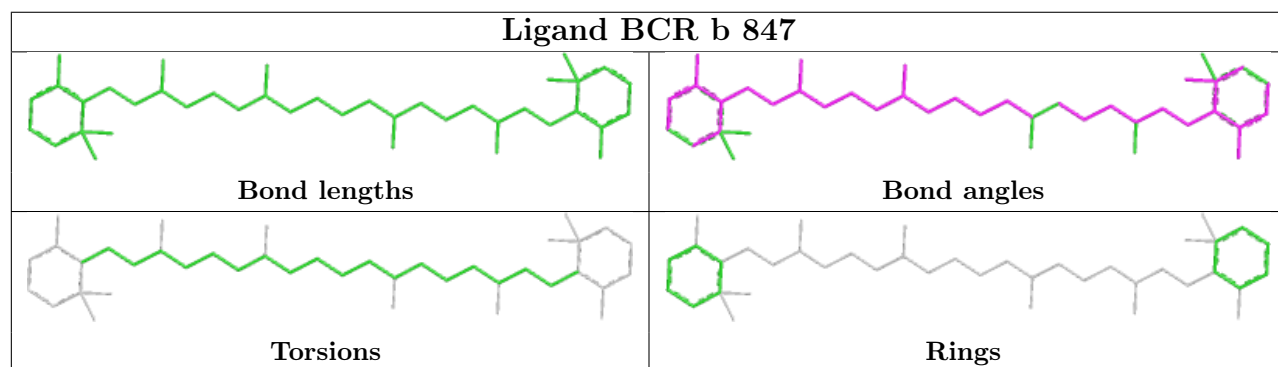
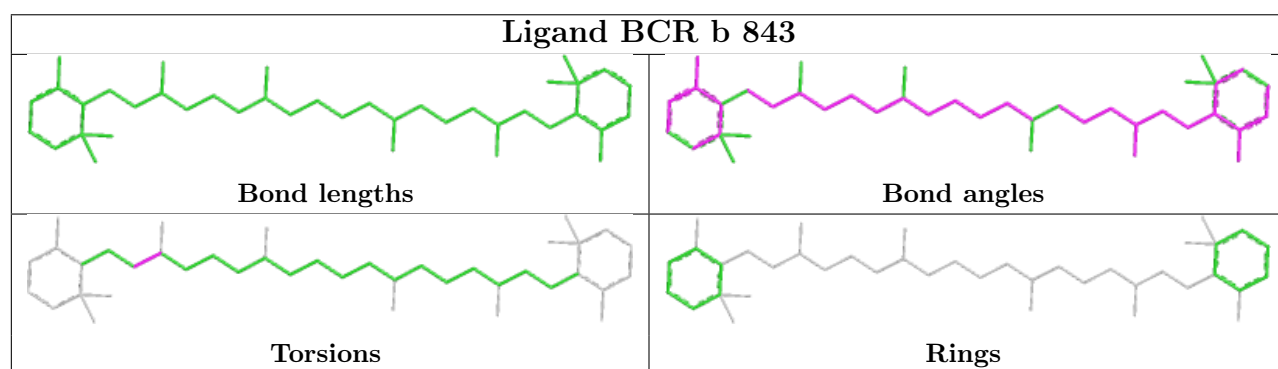
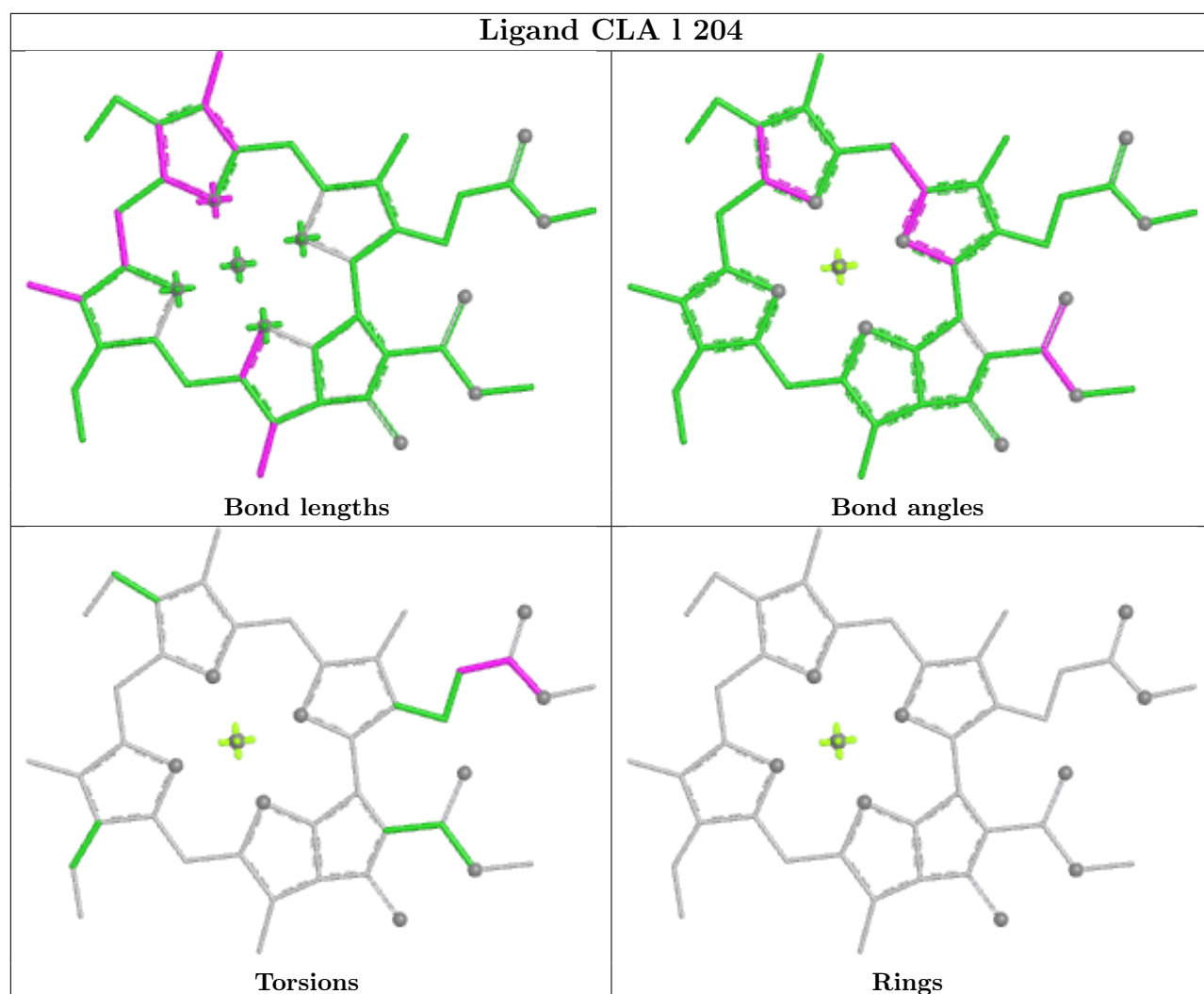
Ligand CLA 5 313

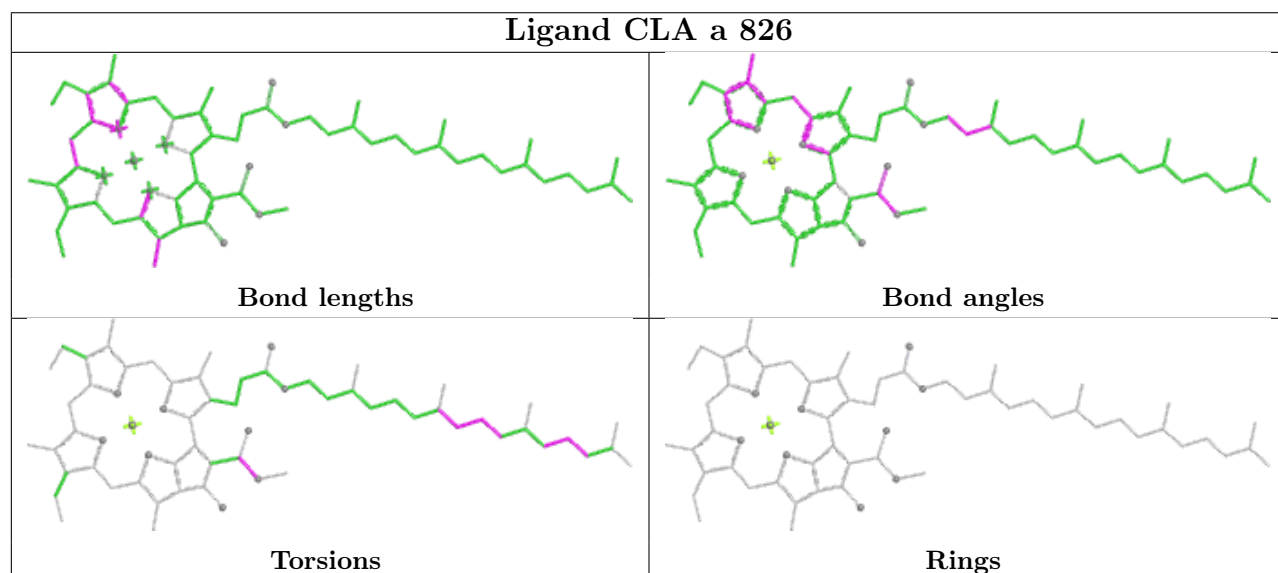
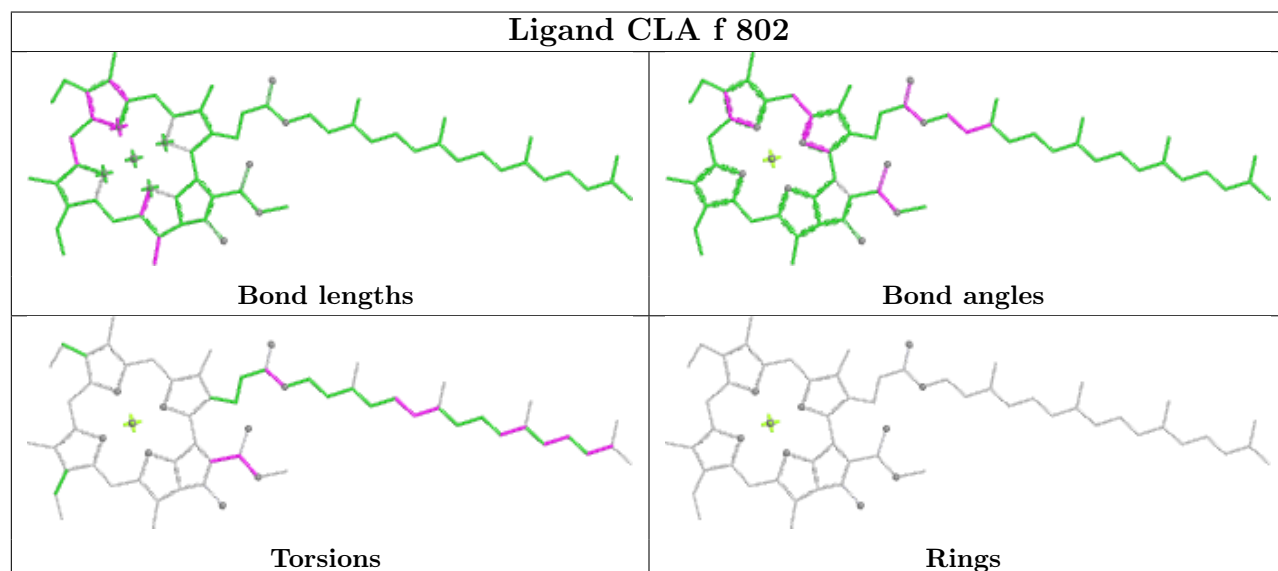
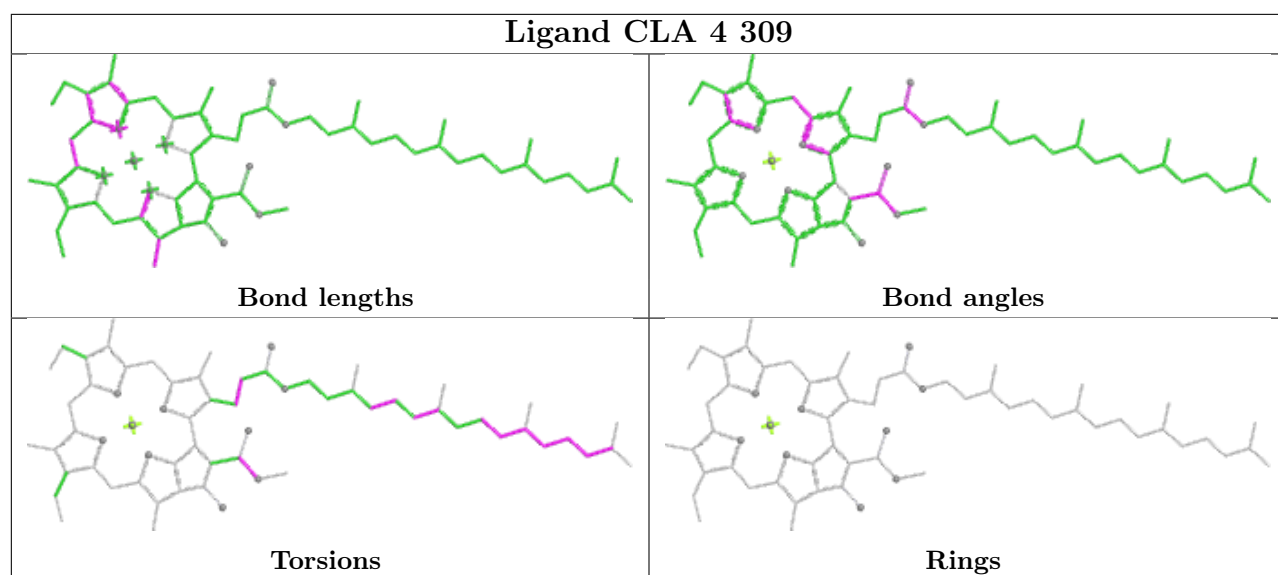


Ligand CLA b 814

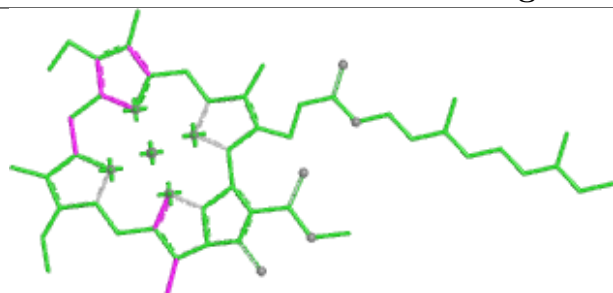




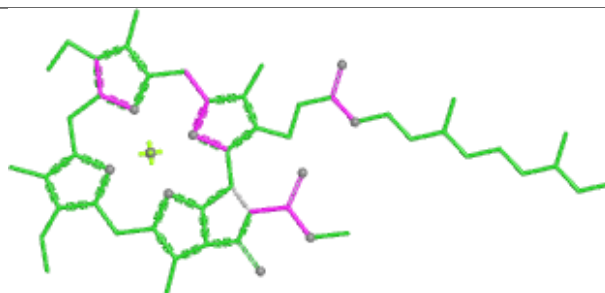




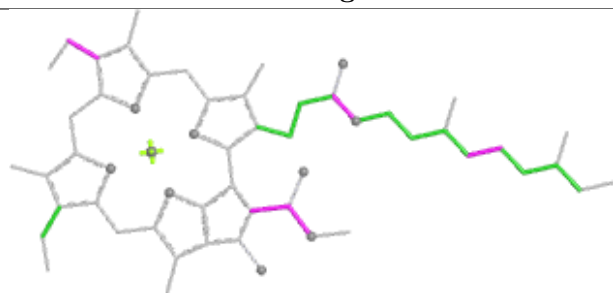
Ligand CLA 4 308



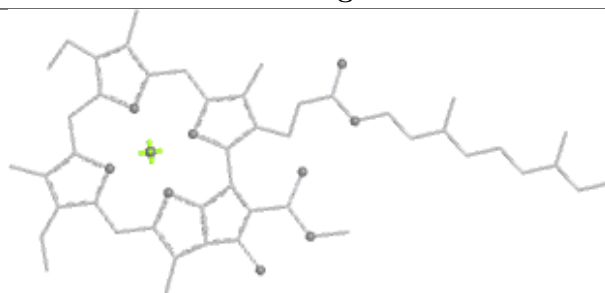
Bond lengths



Bond angles

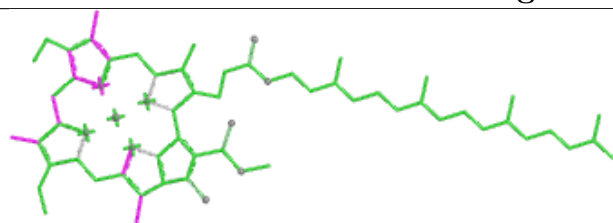


Torsions

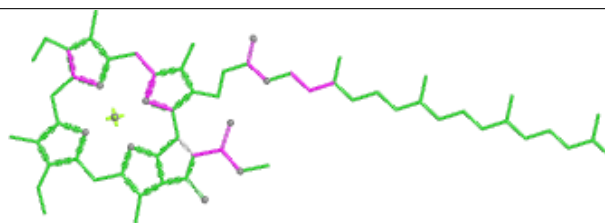


Rings

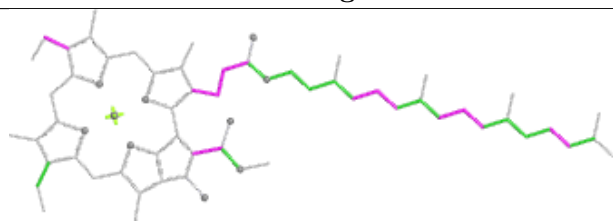
Ligand CLA b 809



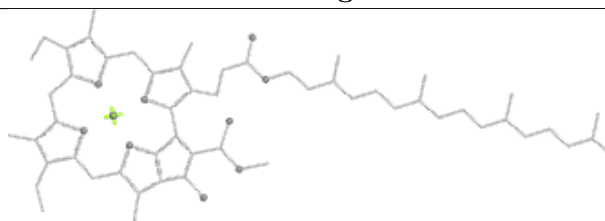
Bond lengths



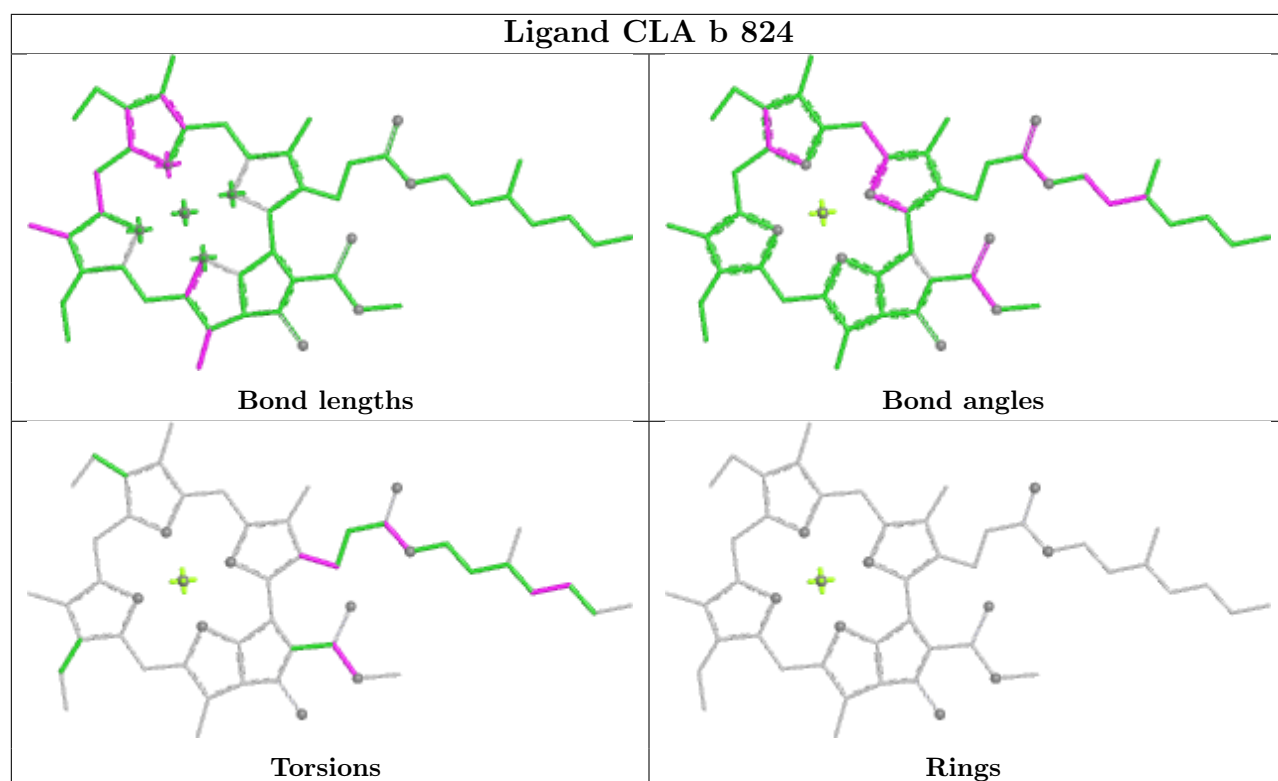
Bond angles



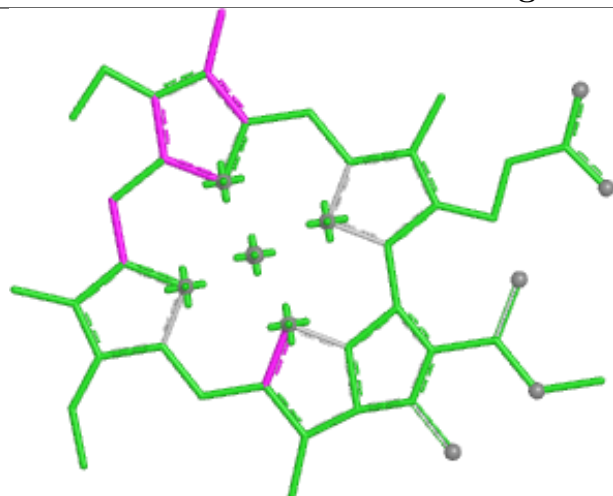
Torsions



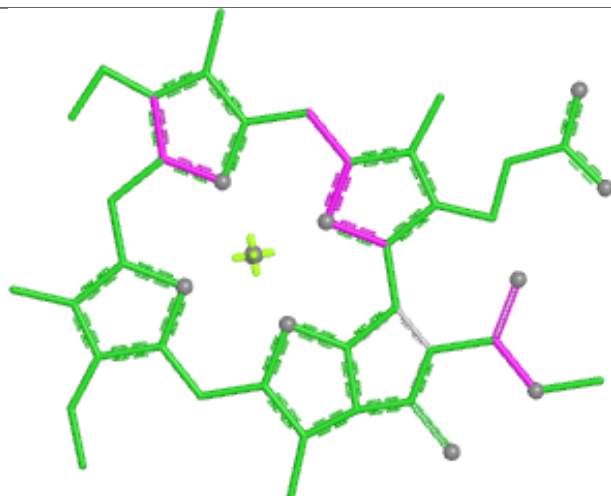
Rings



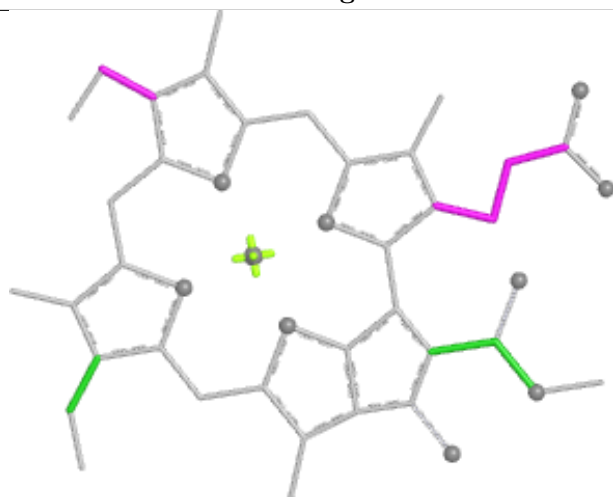
Ligand CLA 1 314



Bond lengths



Bond angles

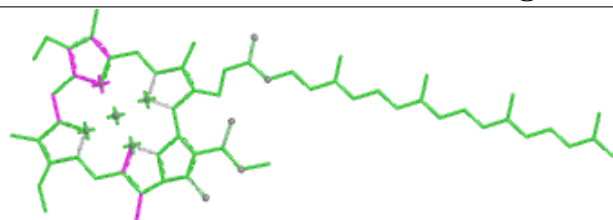


Torsions

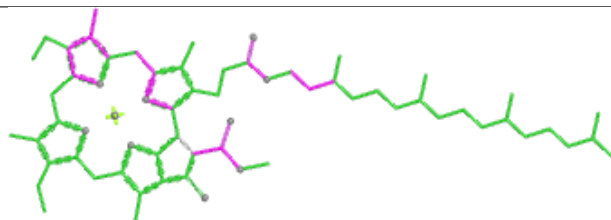


Rings

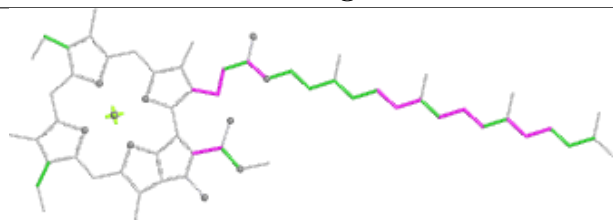
Ligand CLA a 809



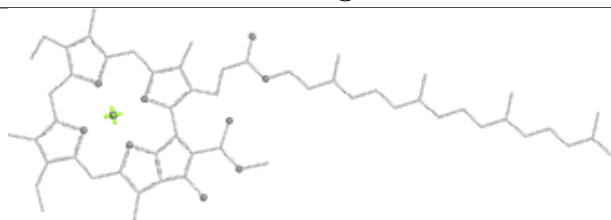
Bond lengths



Bond angles

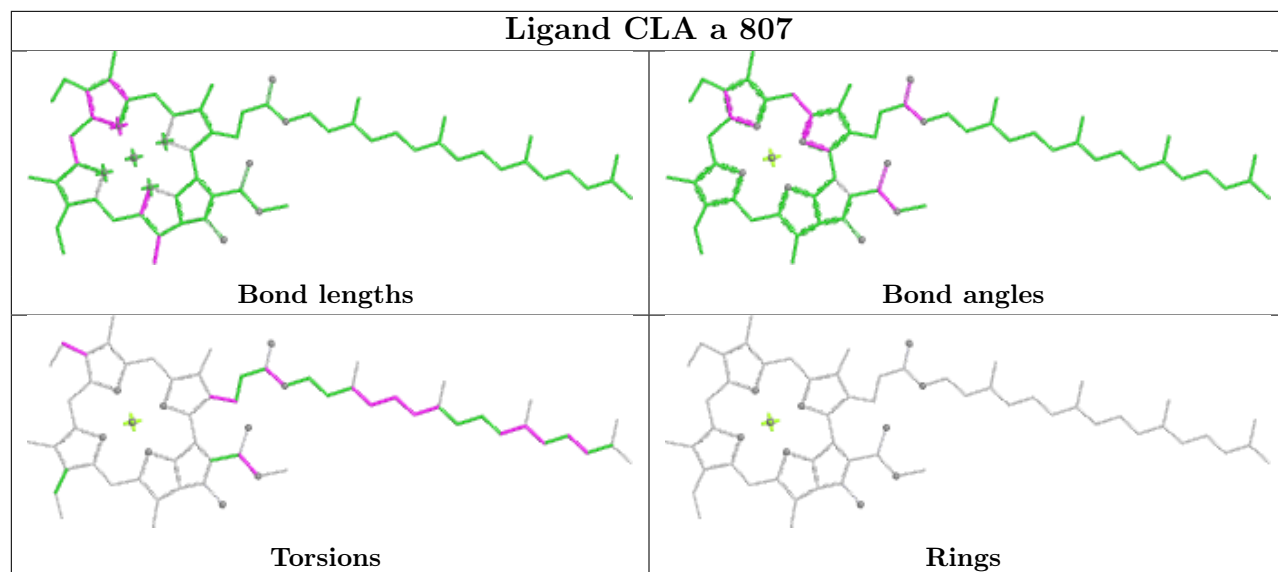


Torsions

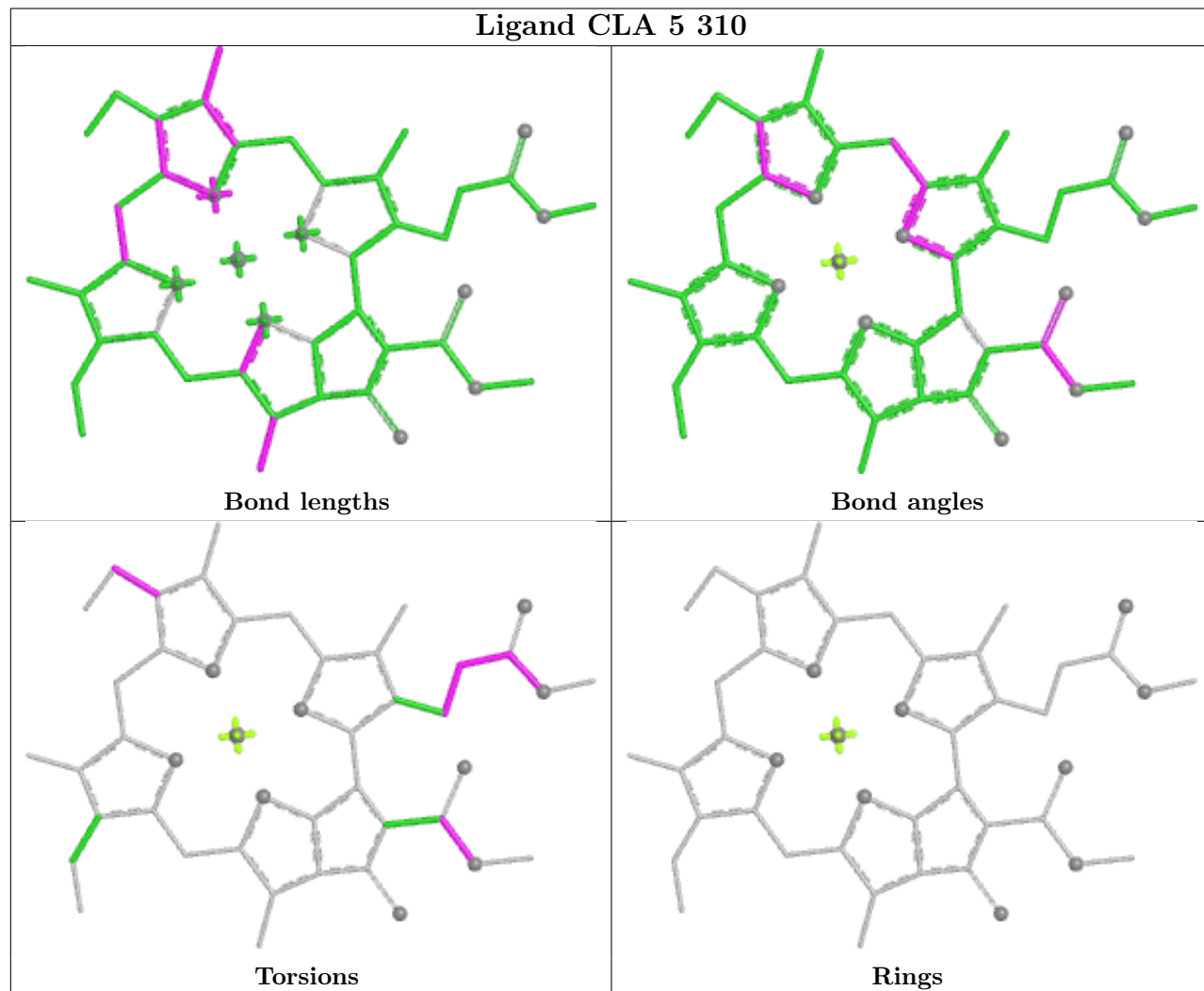


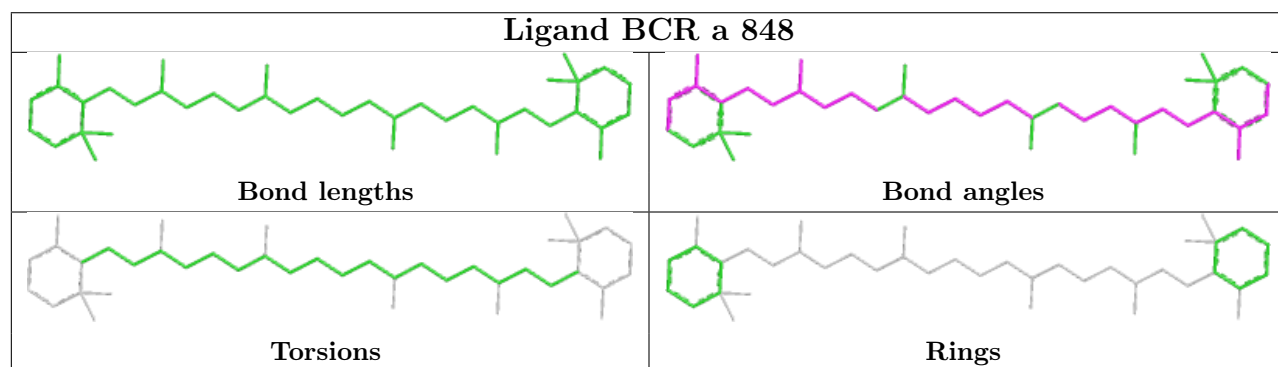
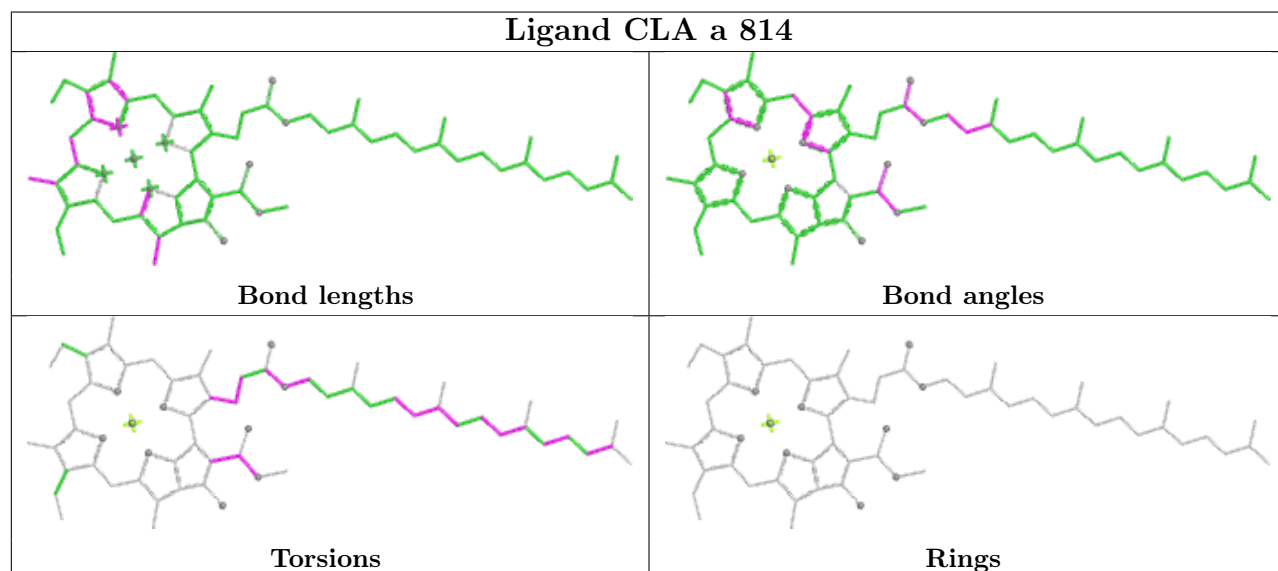
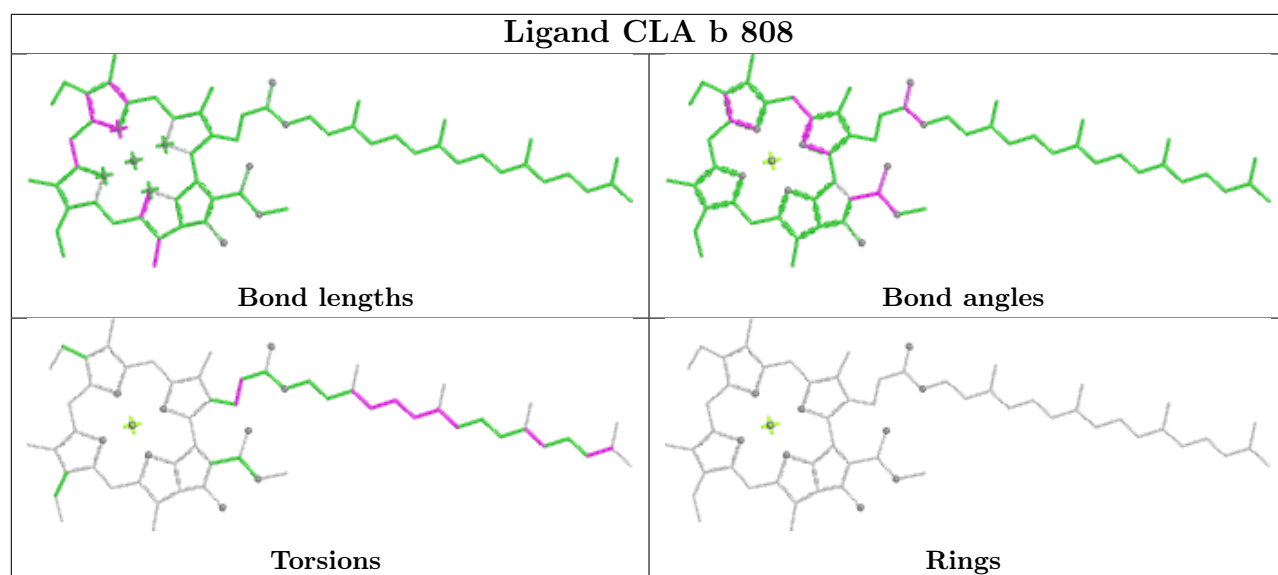
Rings

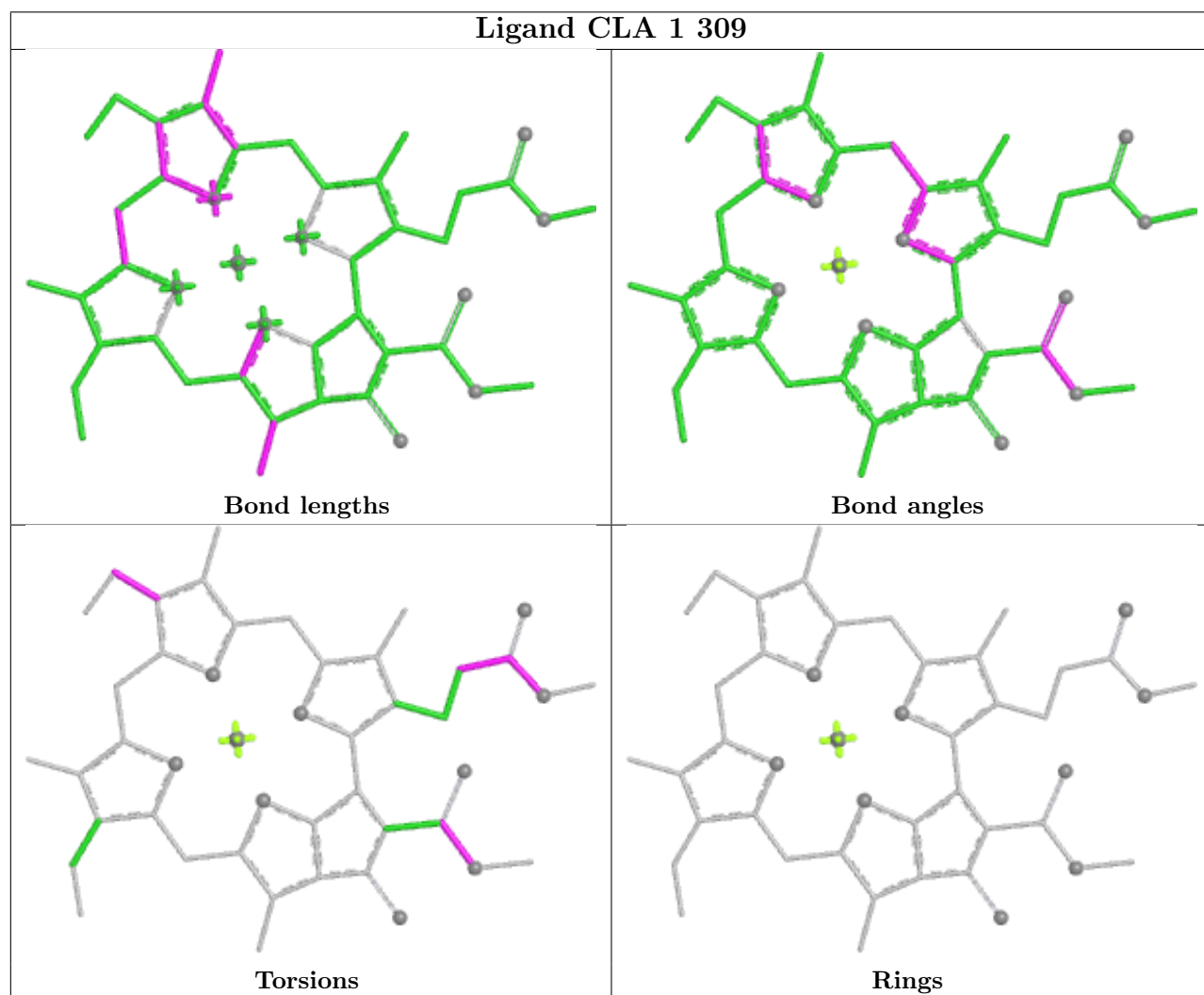
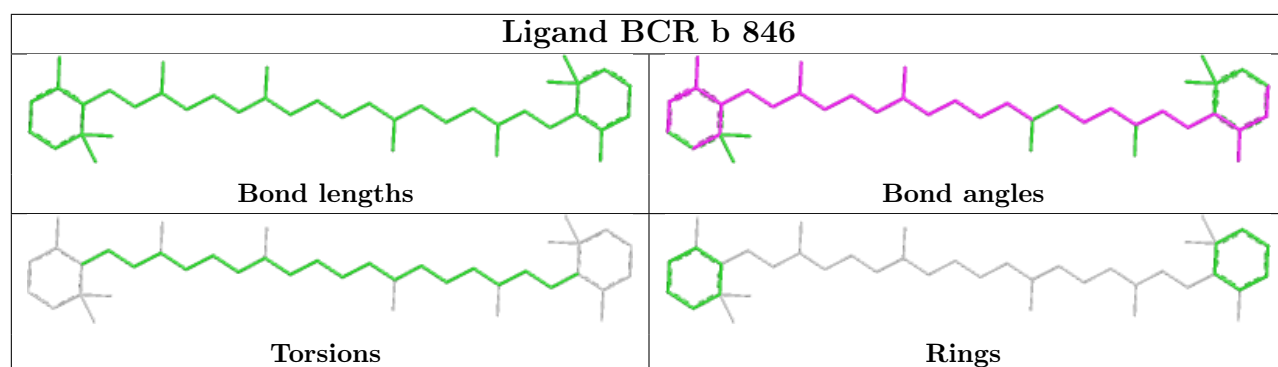
Ligand CLA a 807



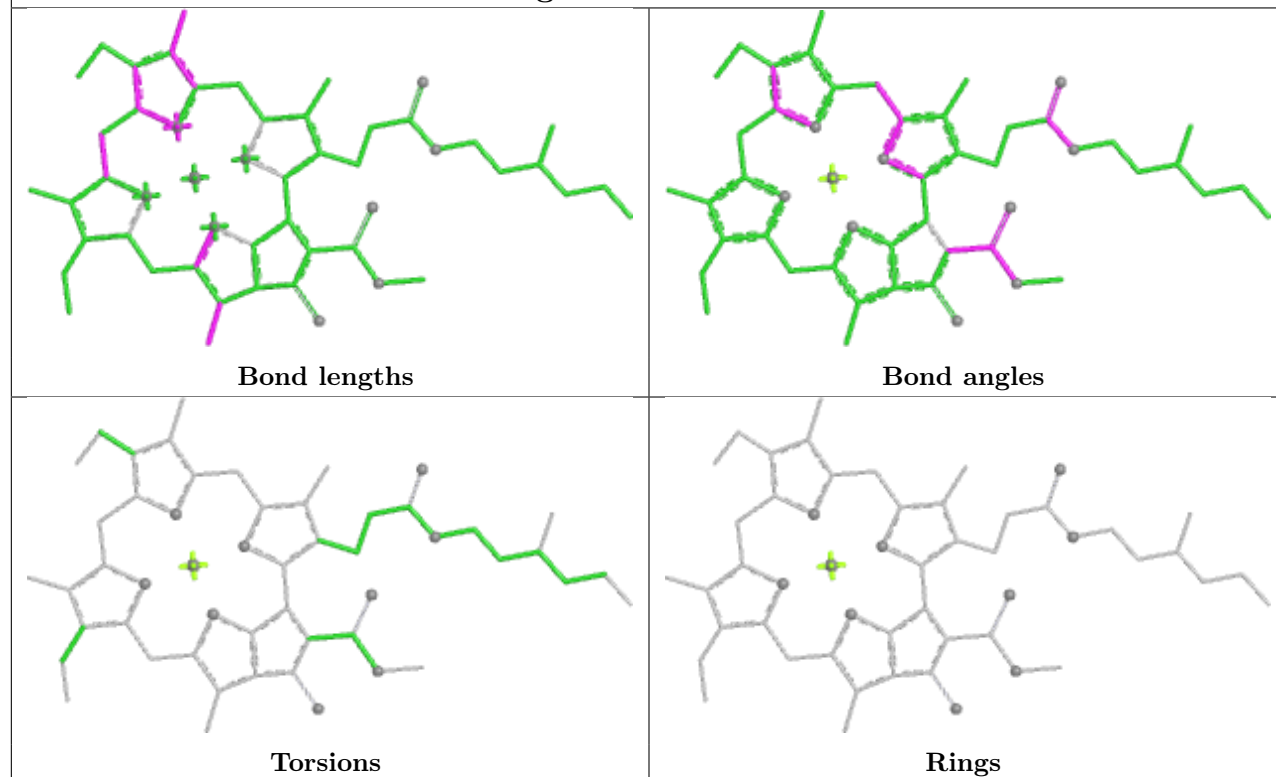
Ligand CLA 5 310



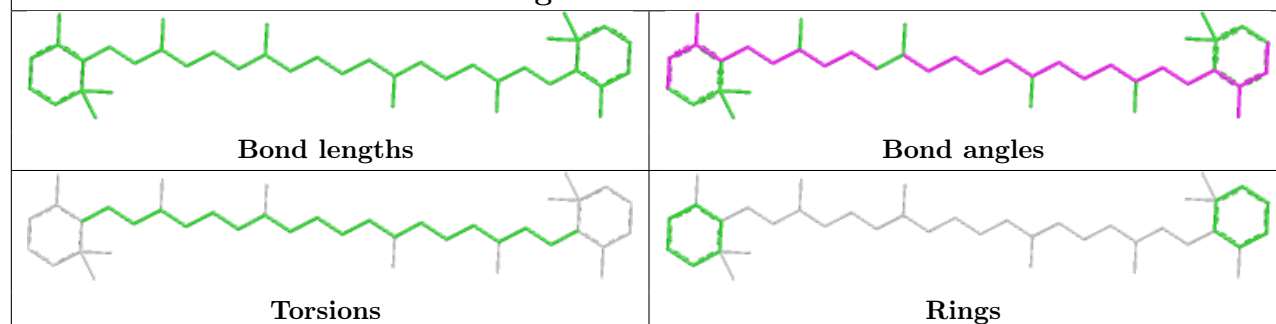




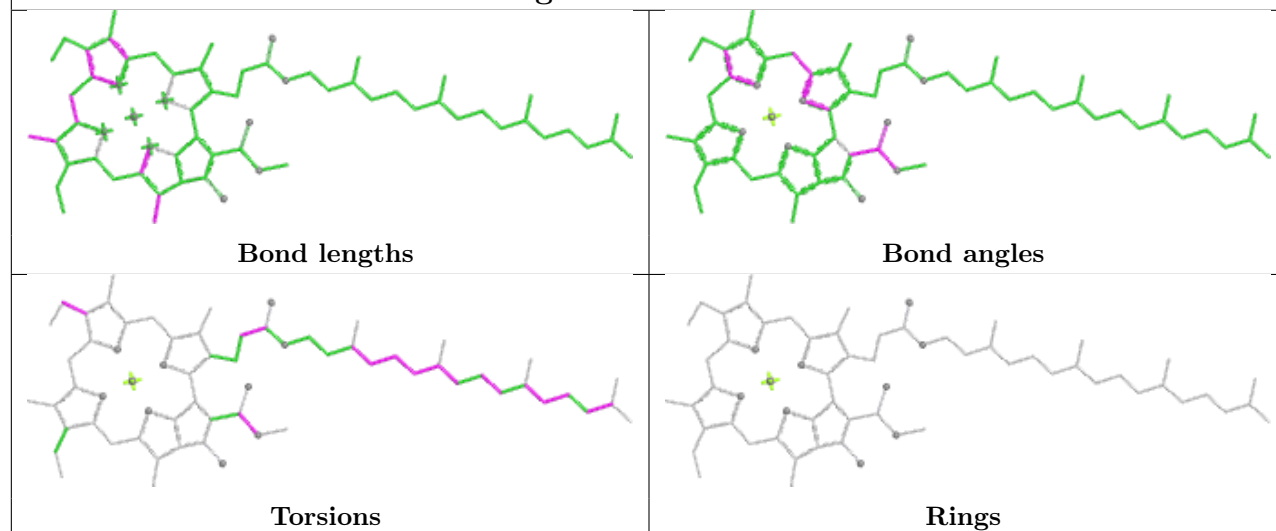
Ligand CLA 5 312

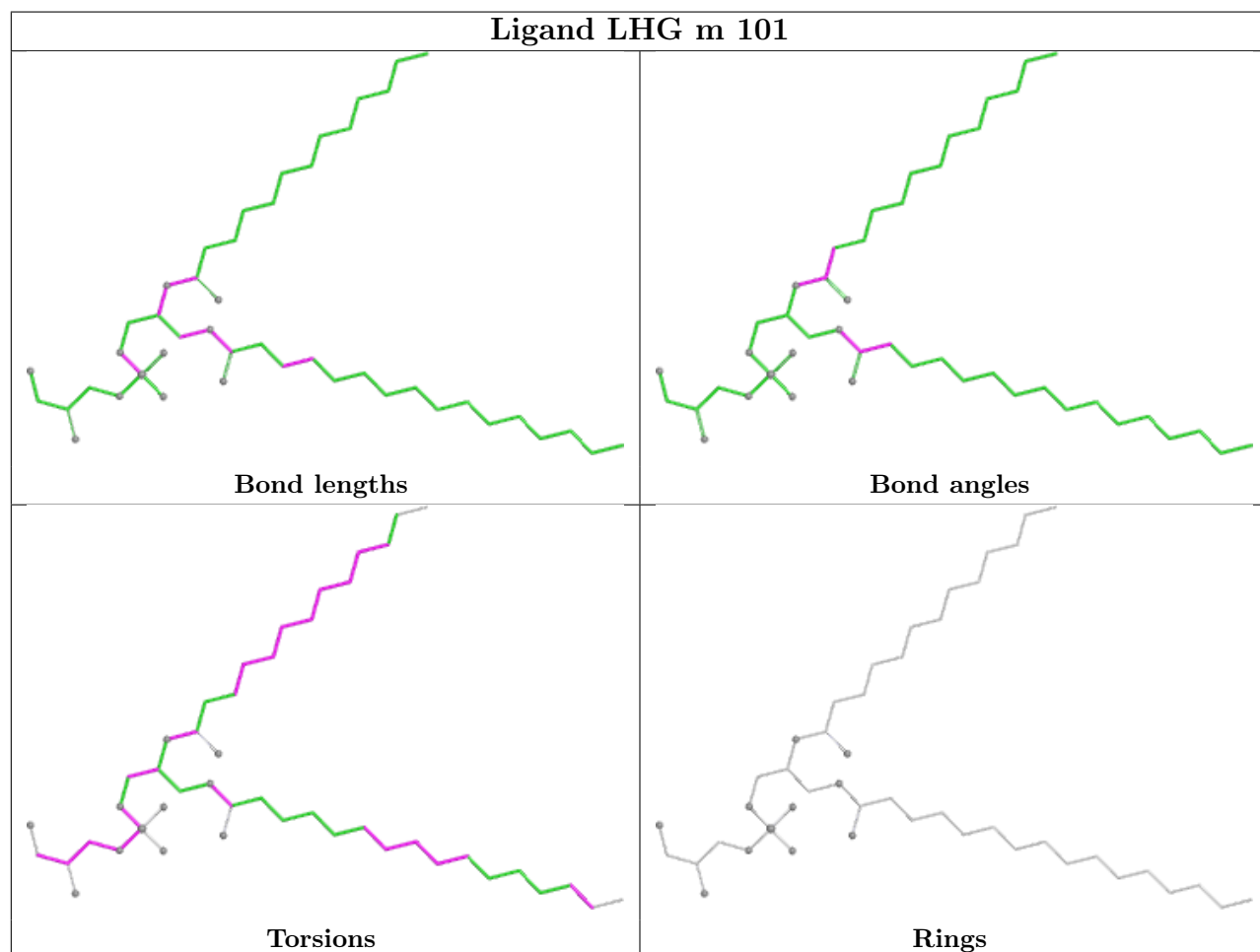
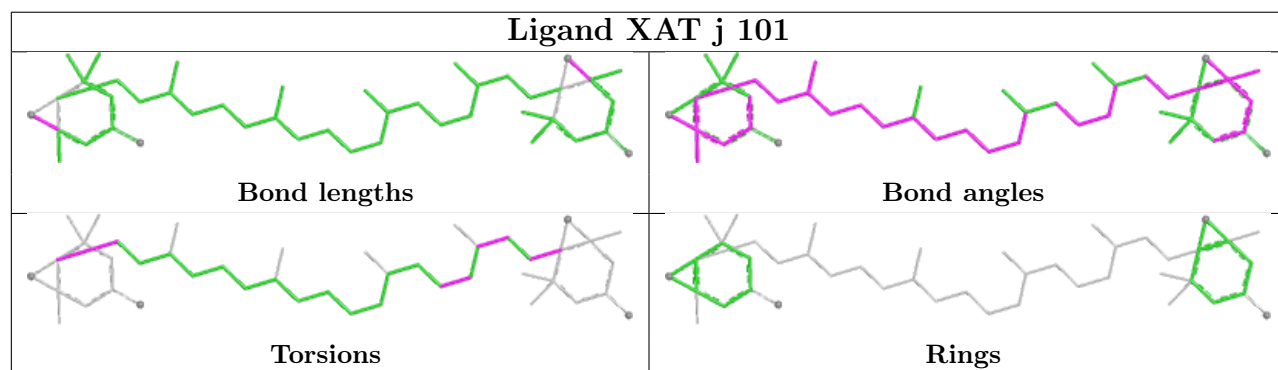
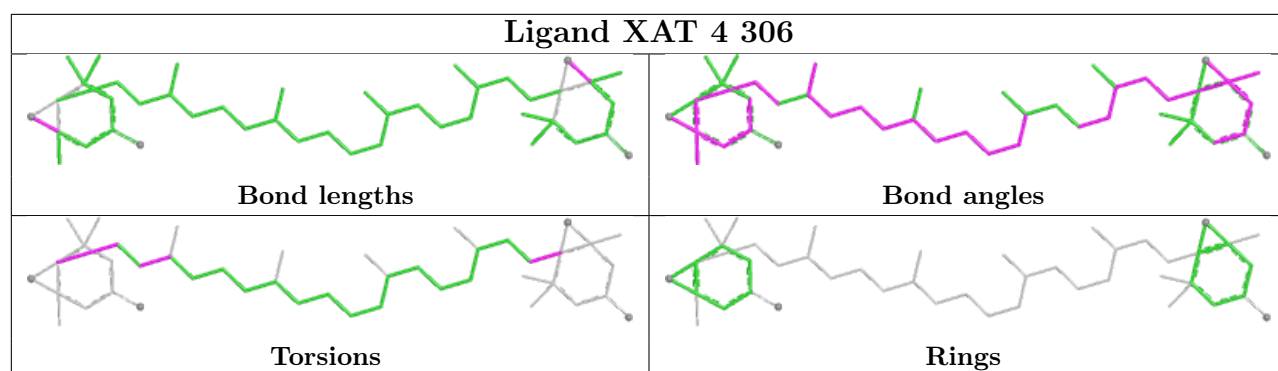


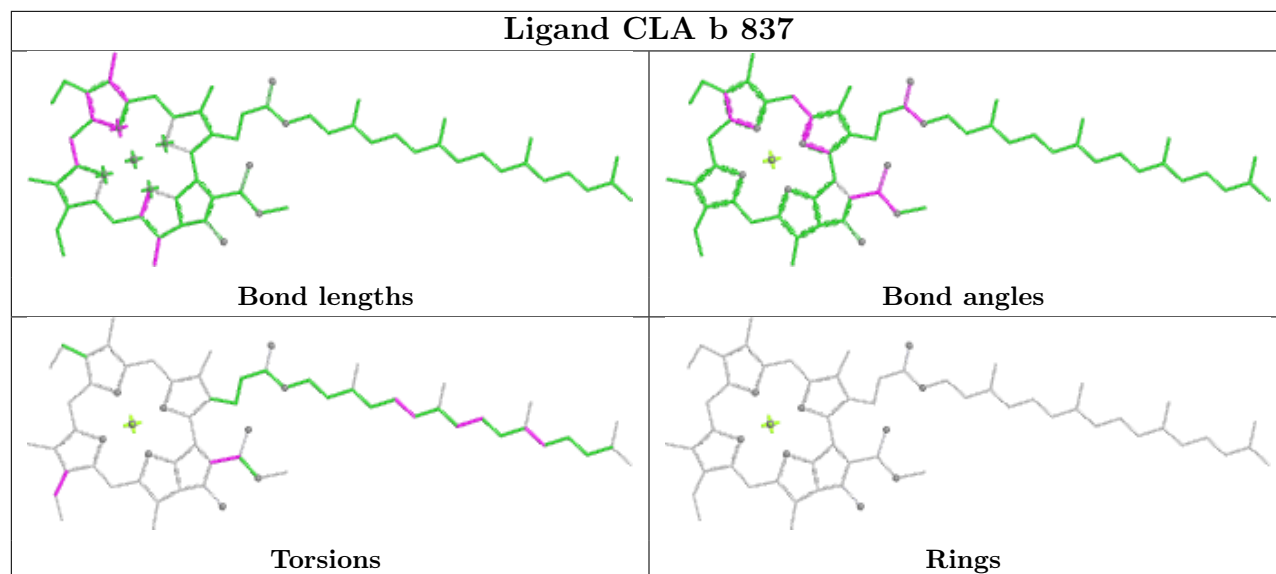
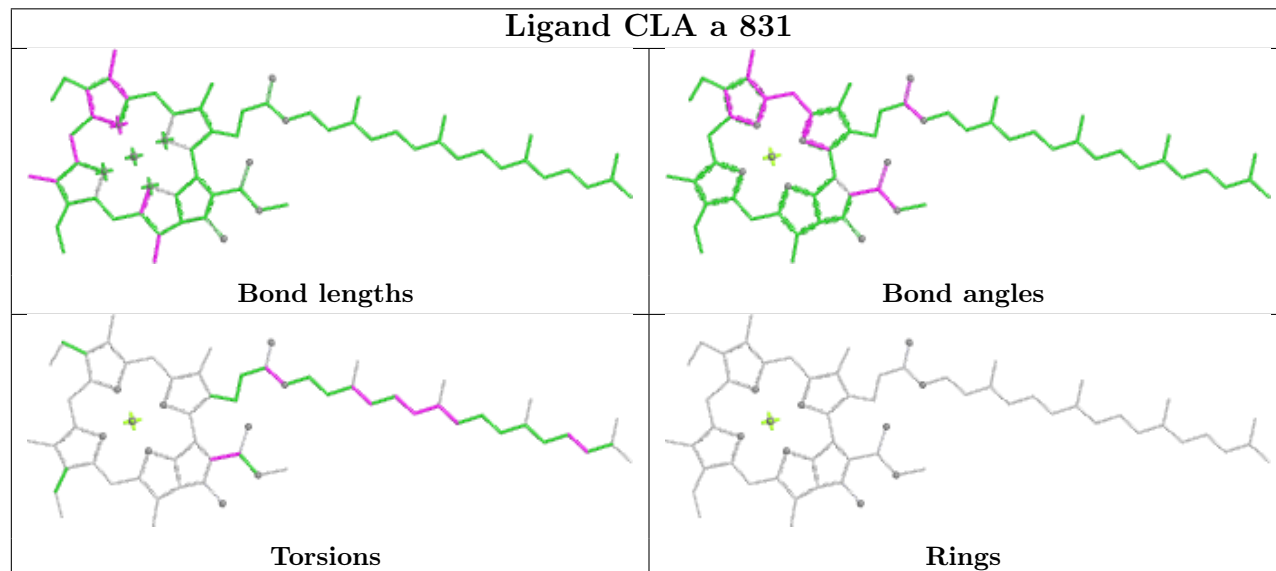
Ligand BCR a 847

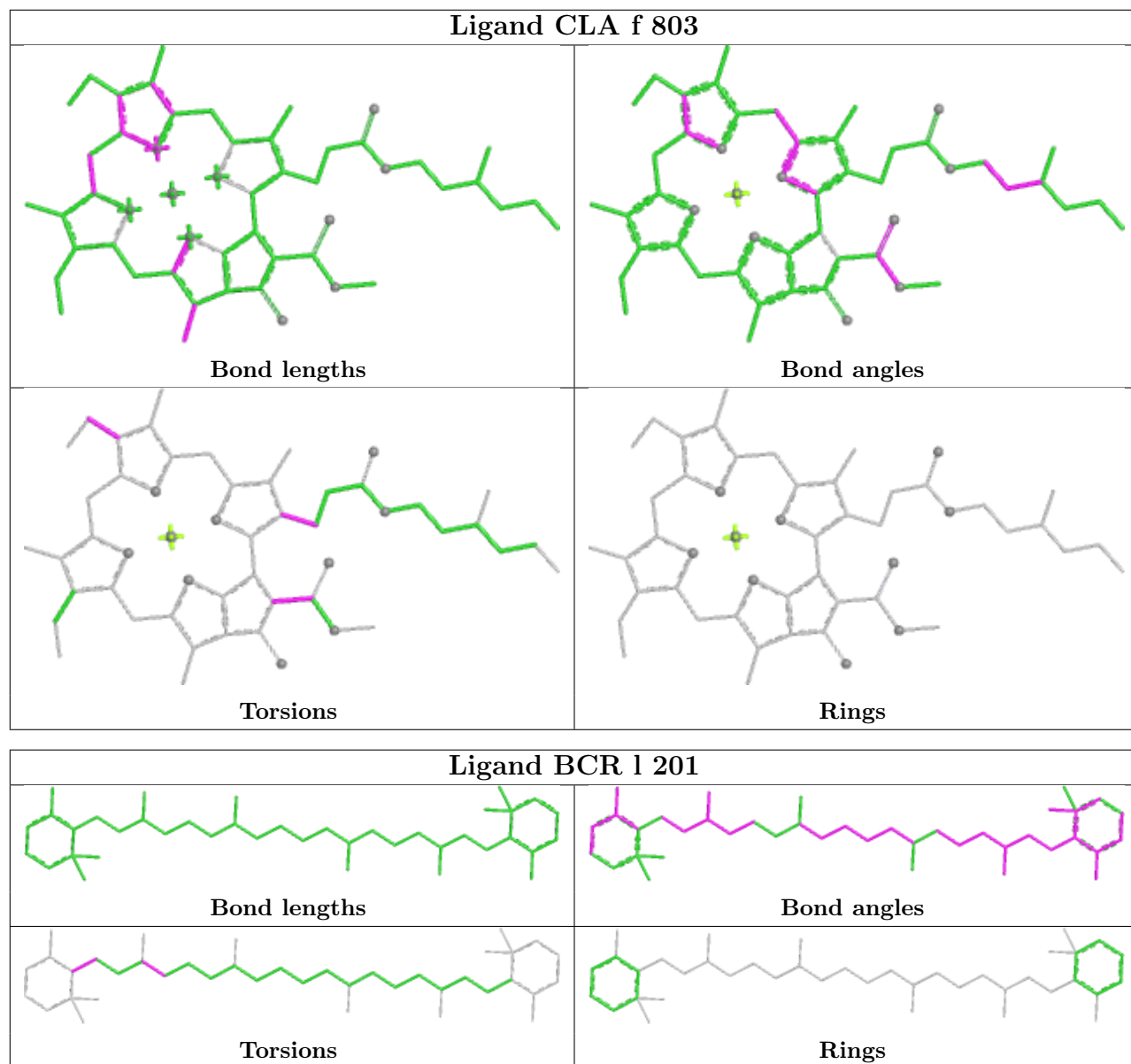


Ligand CLA b 803

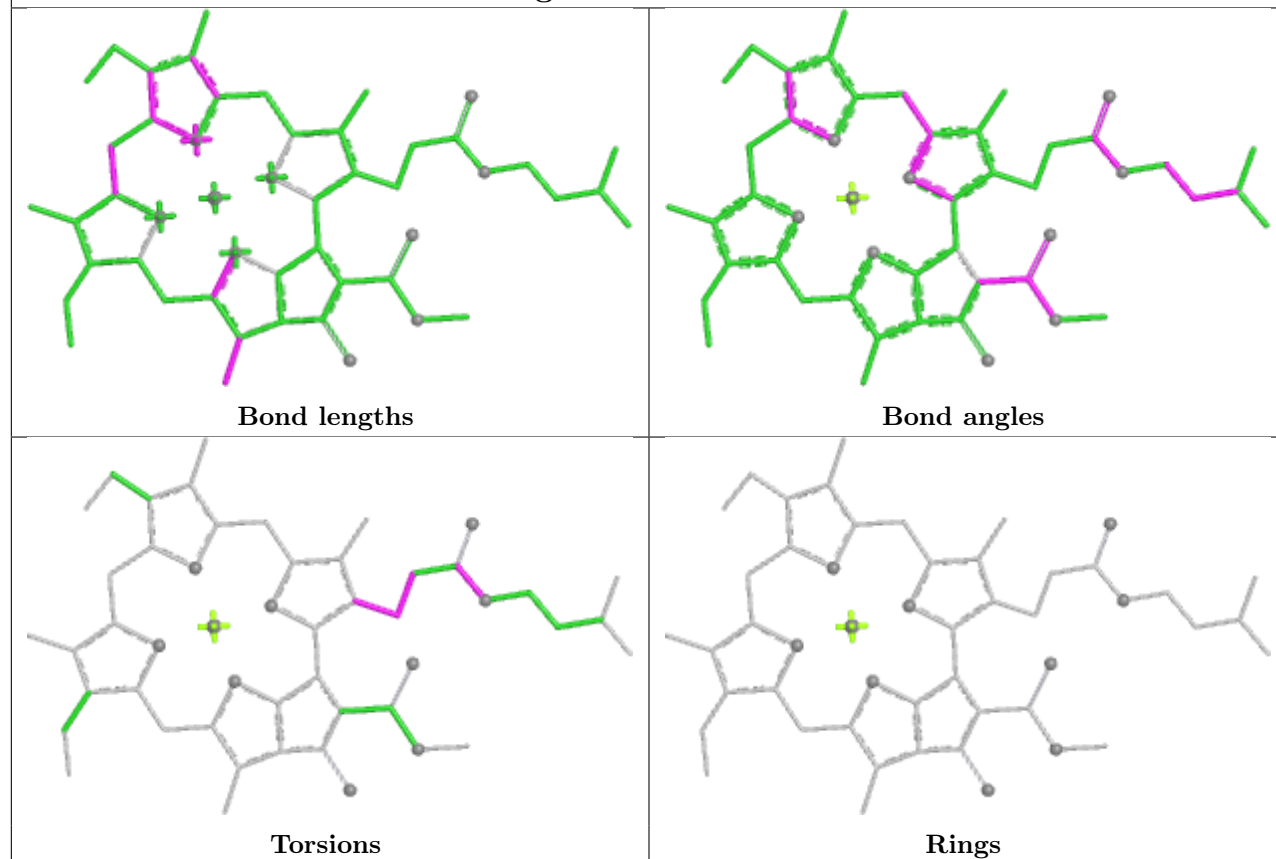




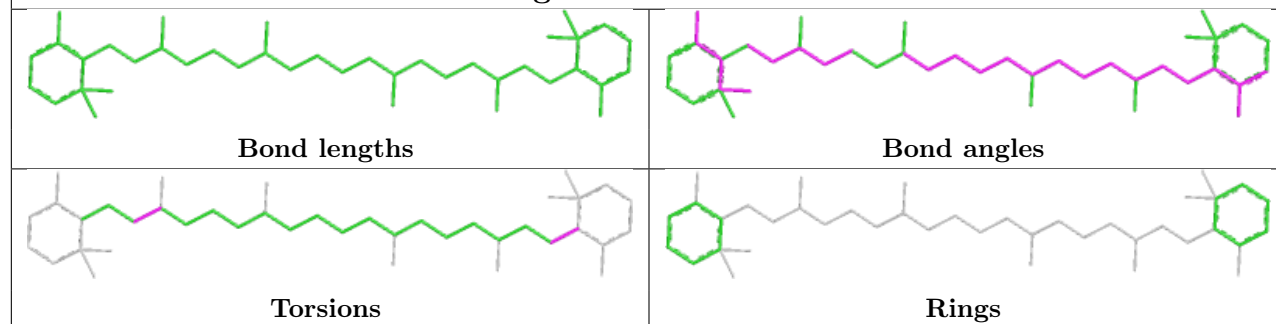
Ligand CLA b 837**Ligand CLA a 831**

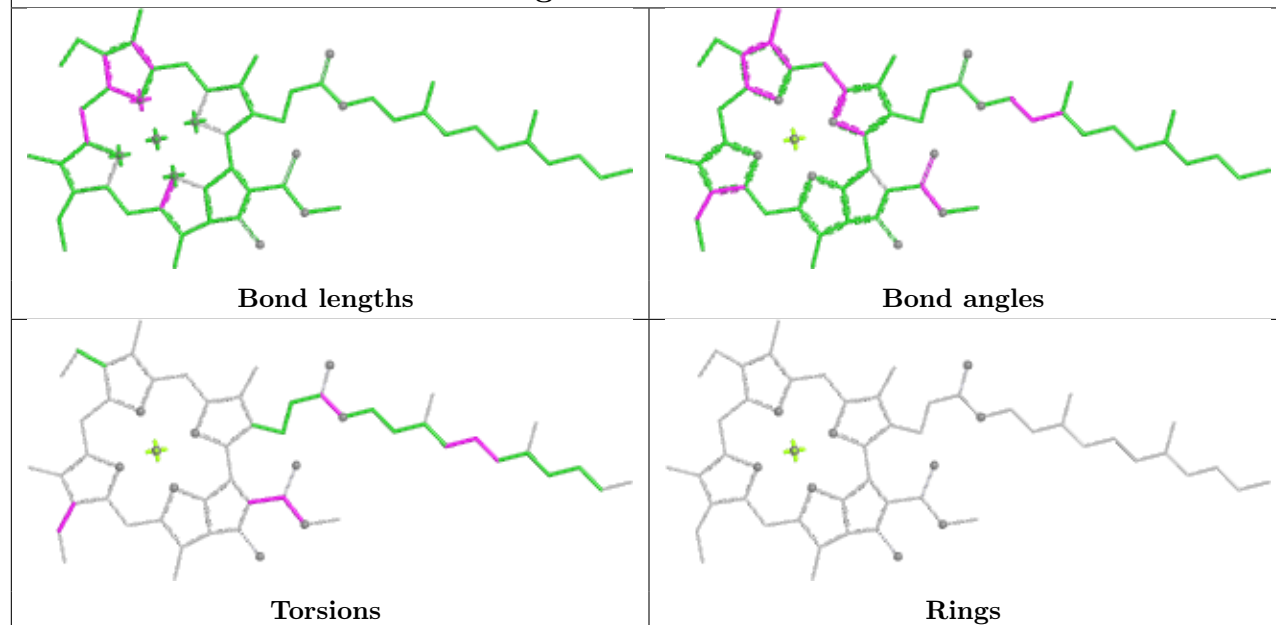
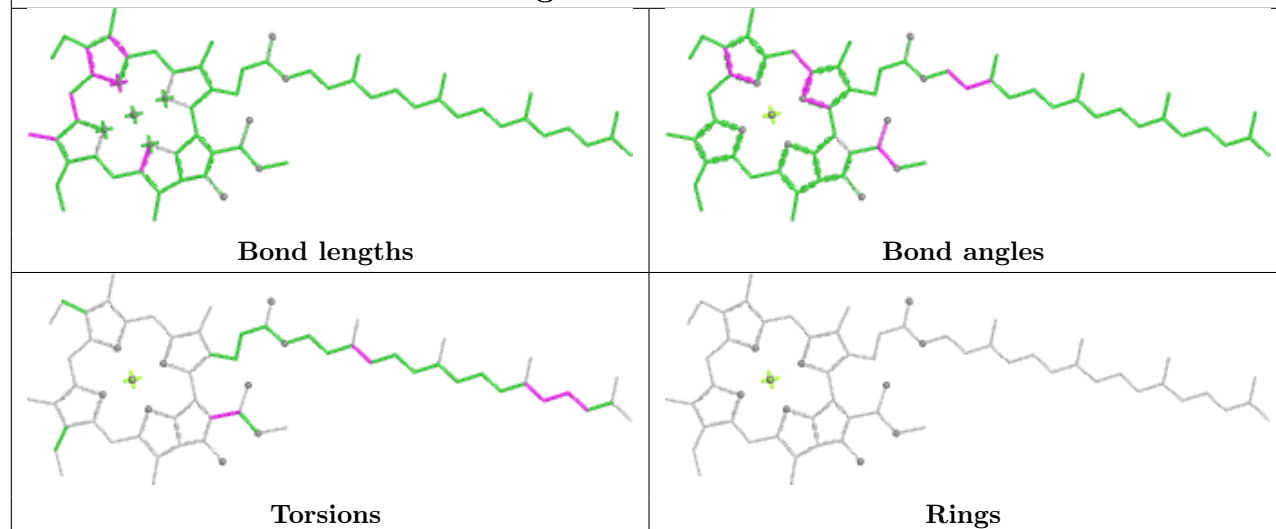


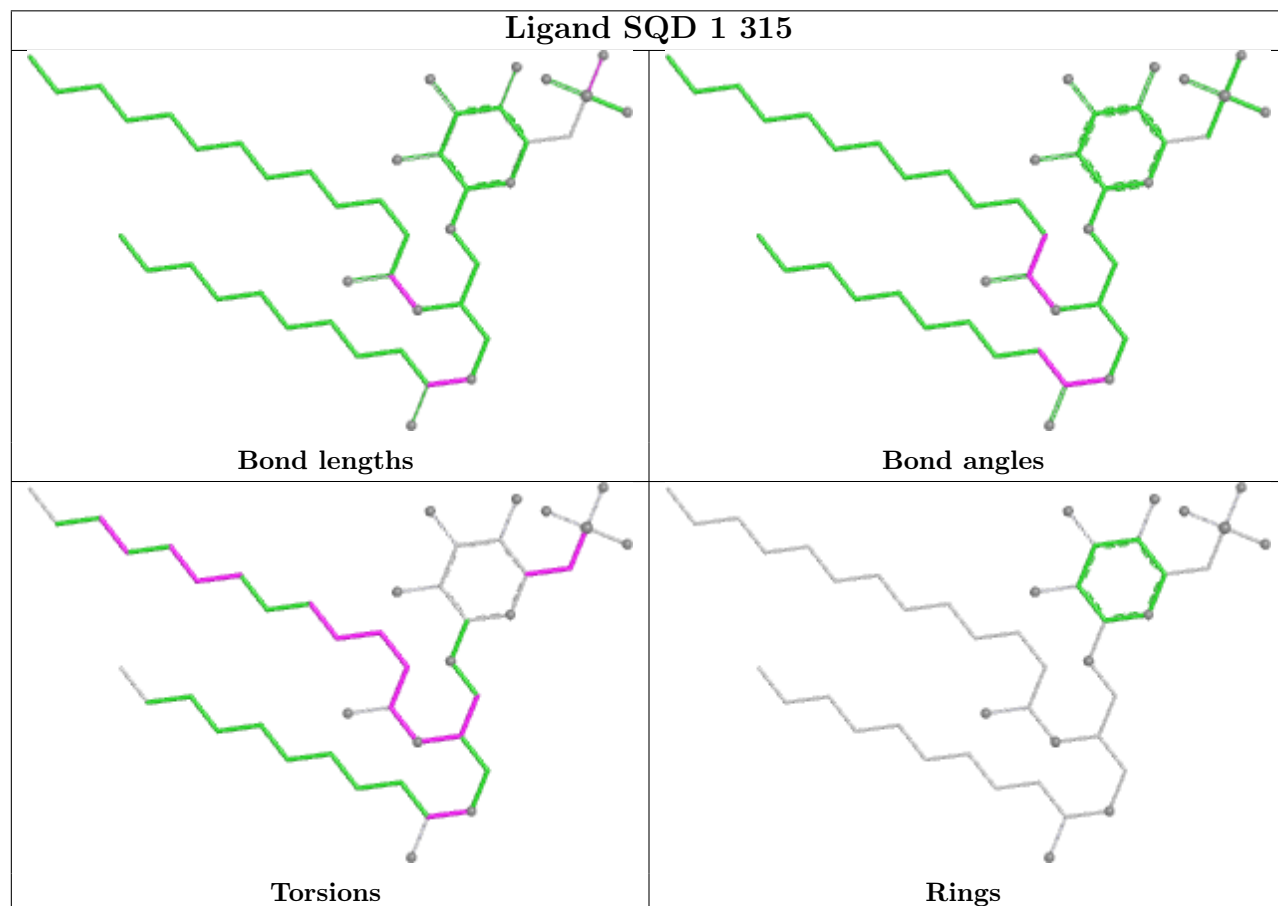
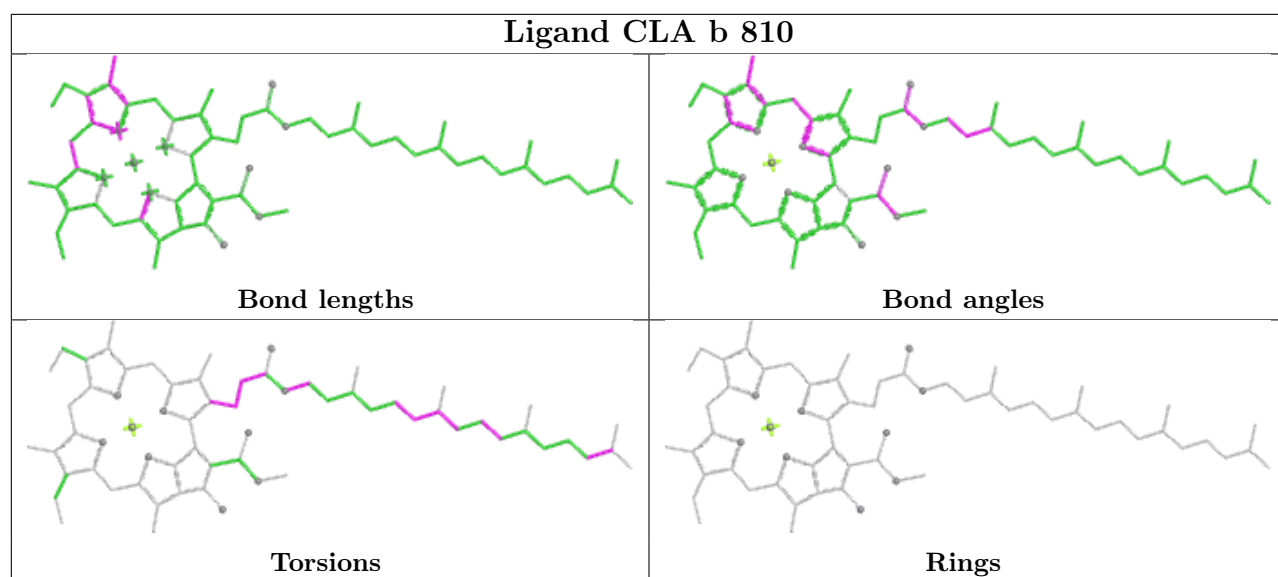
Ligand CLA b 821

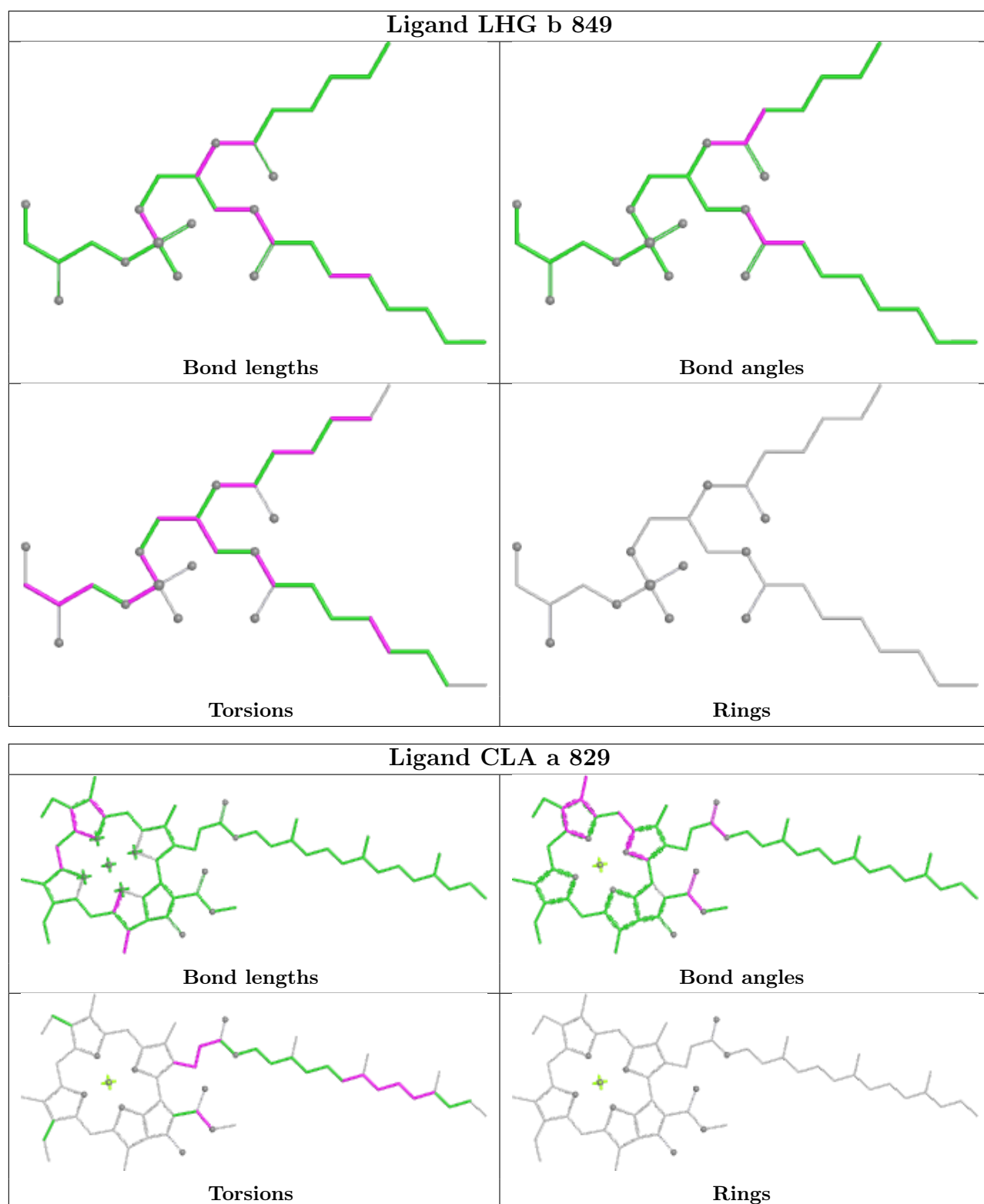


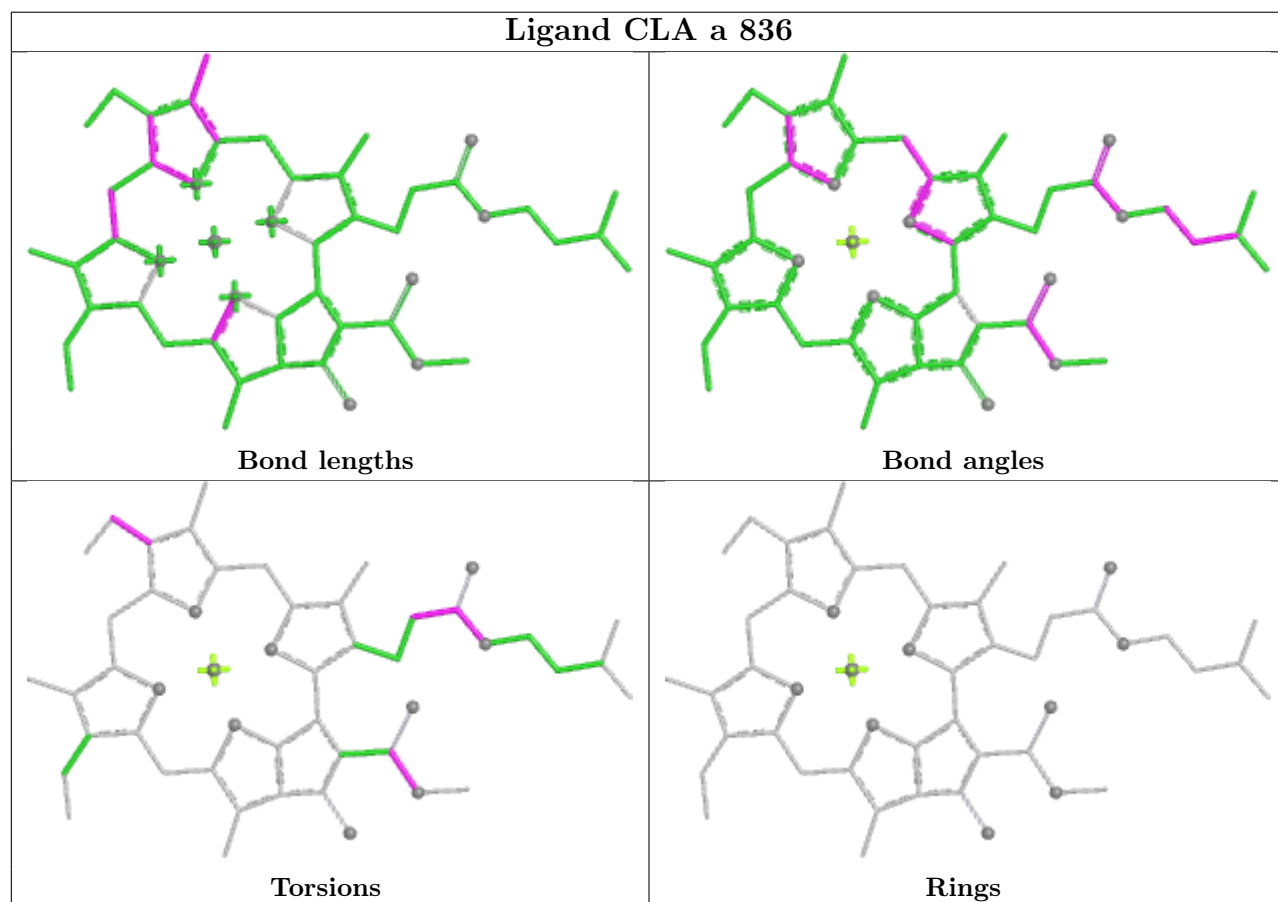
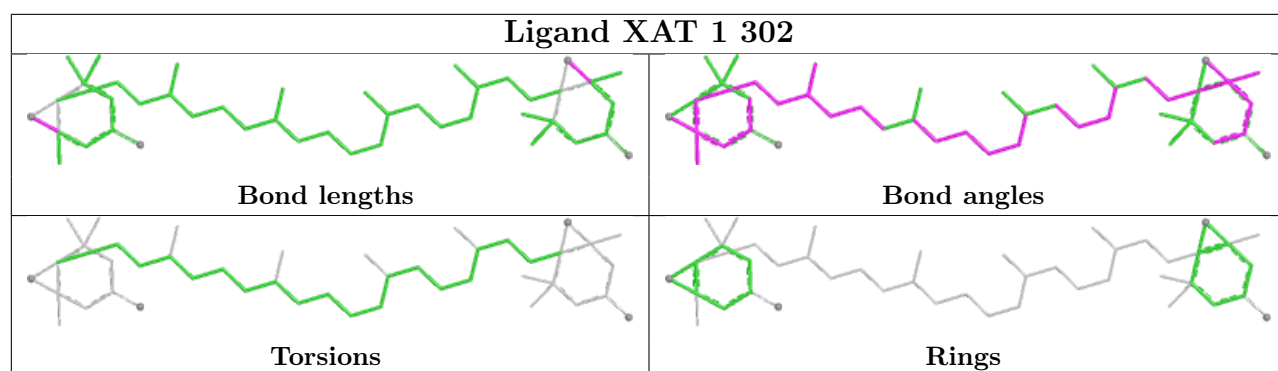
Ligand BCR b 852



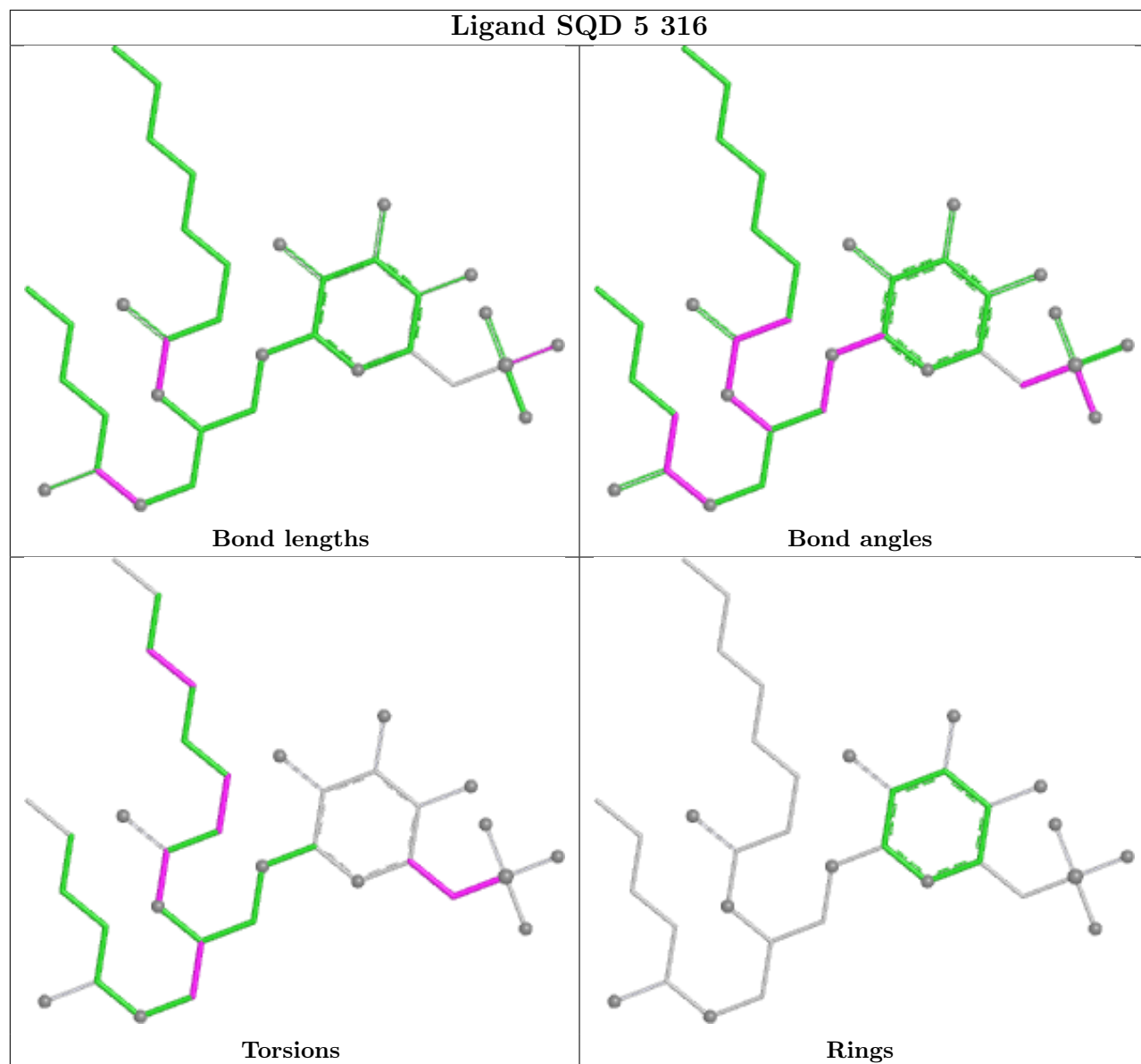
Ligand CLA b 836**Ligand CLA a 828**

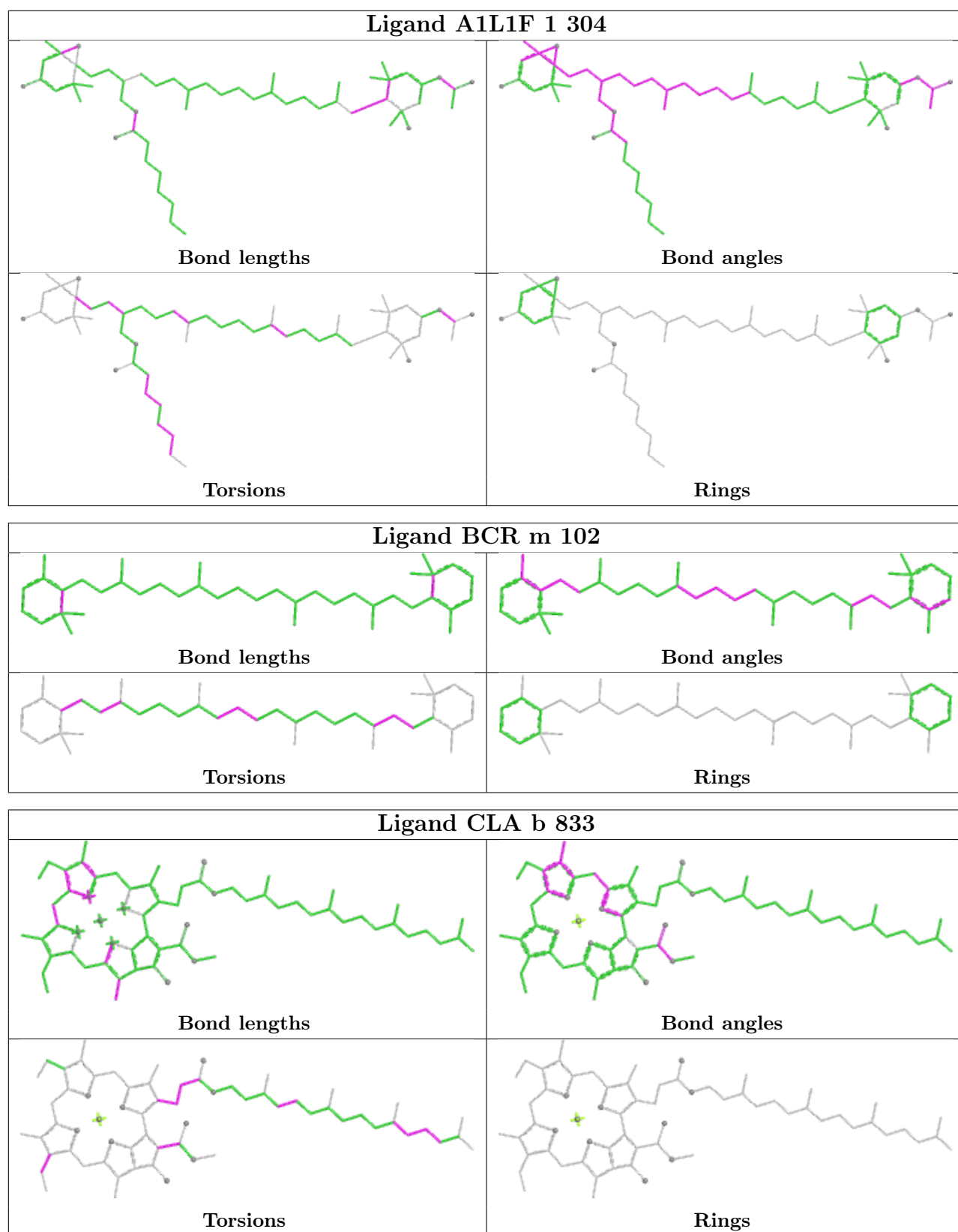


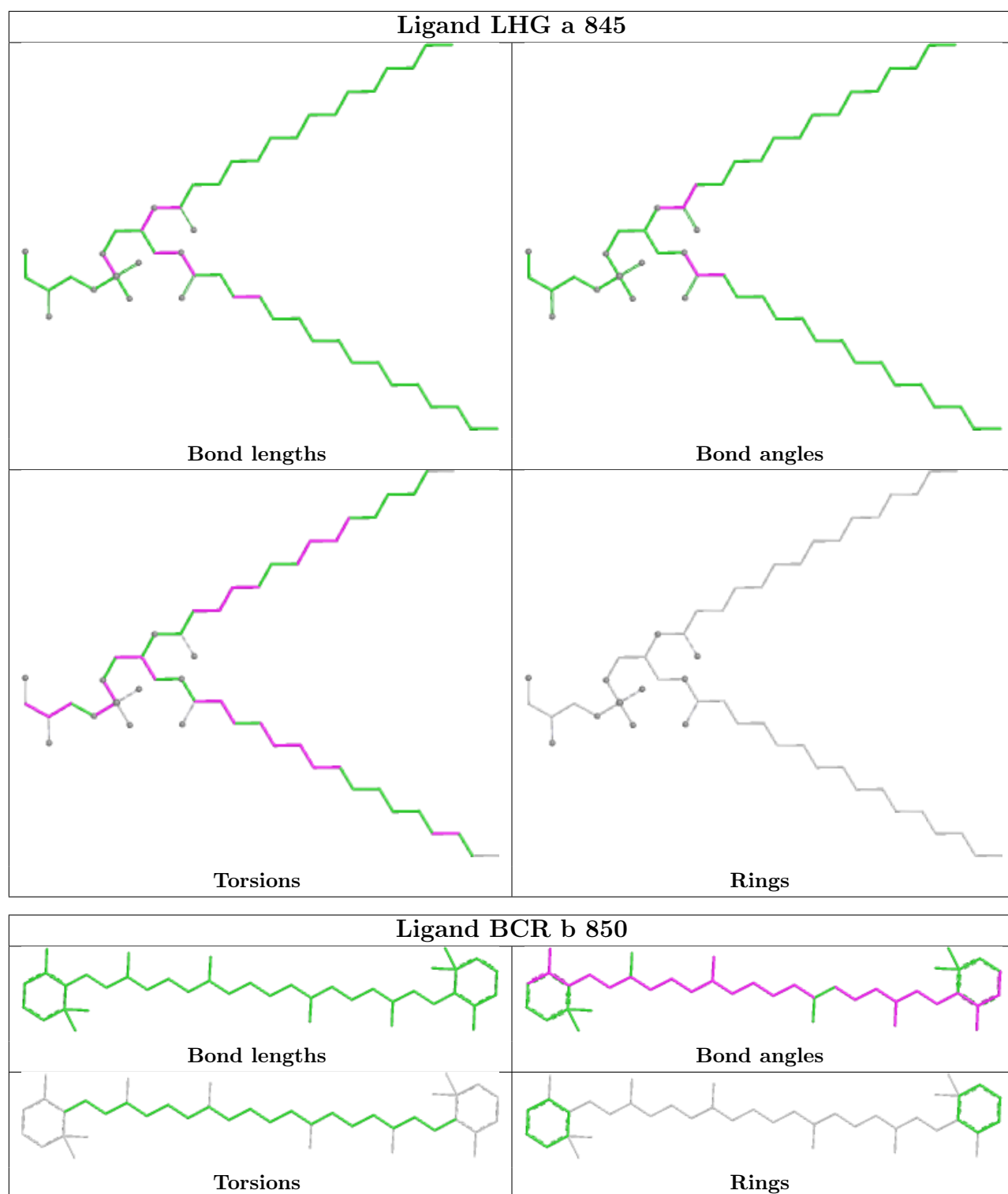




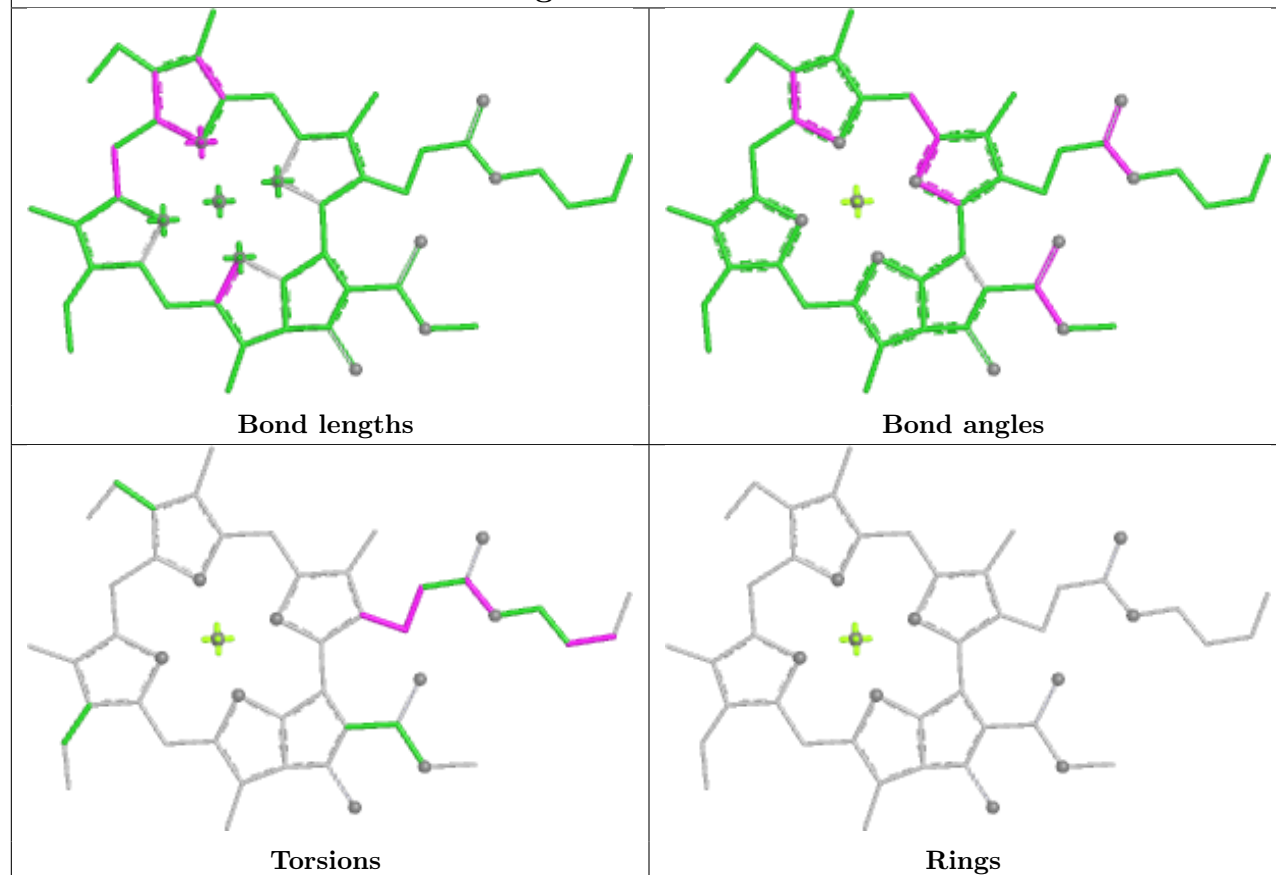
Ligand SQD 5 316



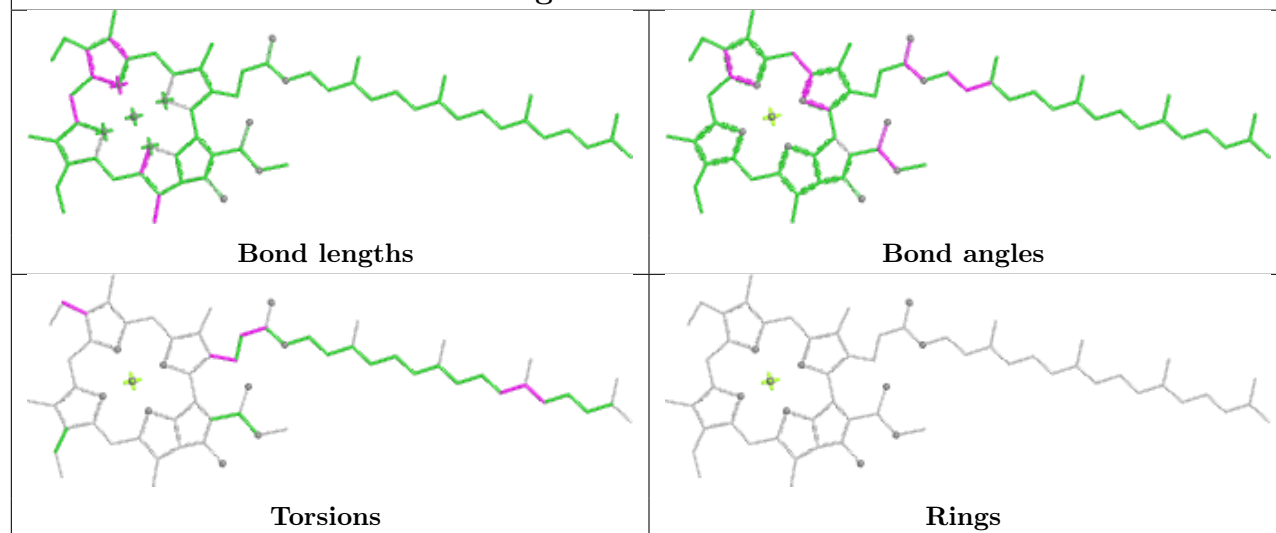




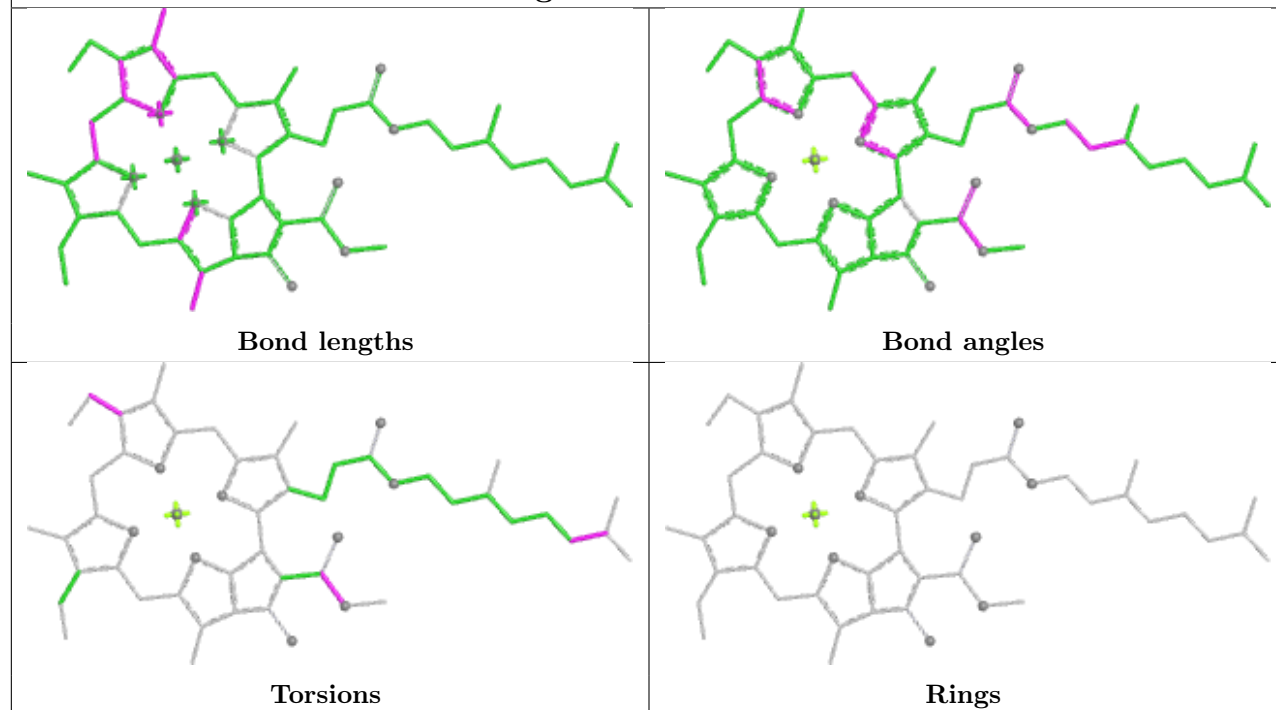
Ligand CLA b 832



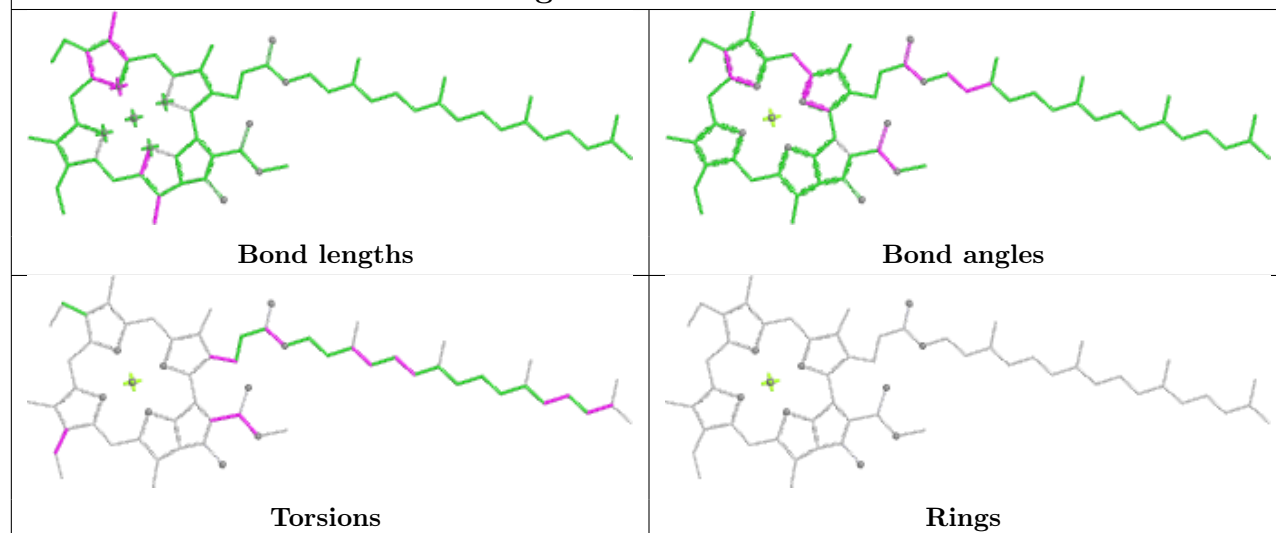
Ligand CLA b 838



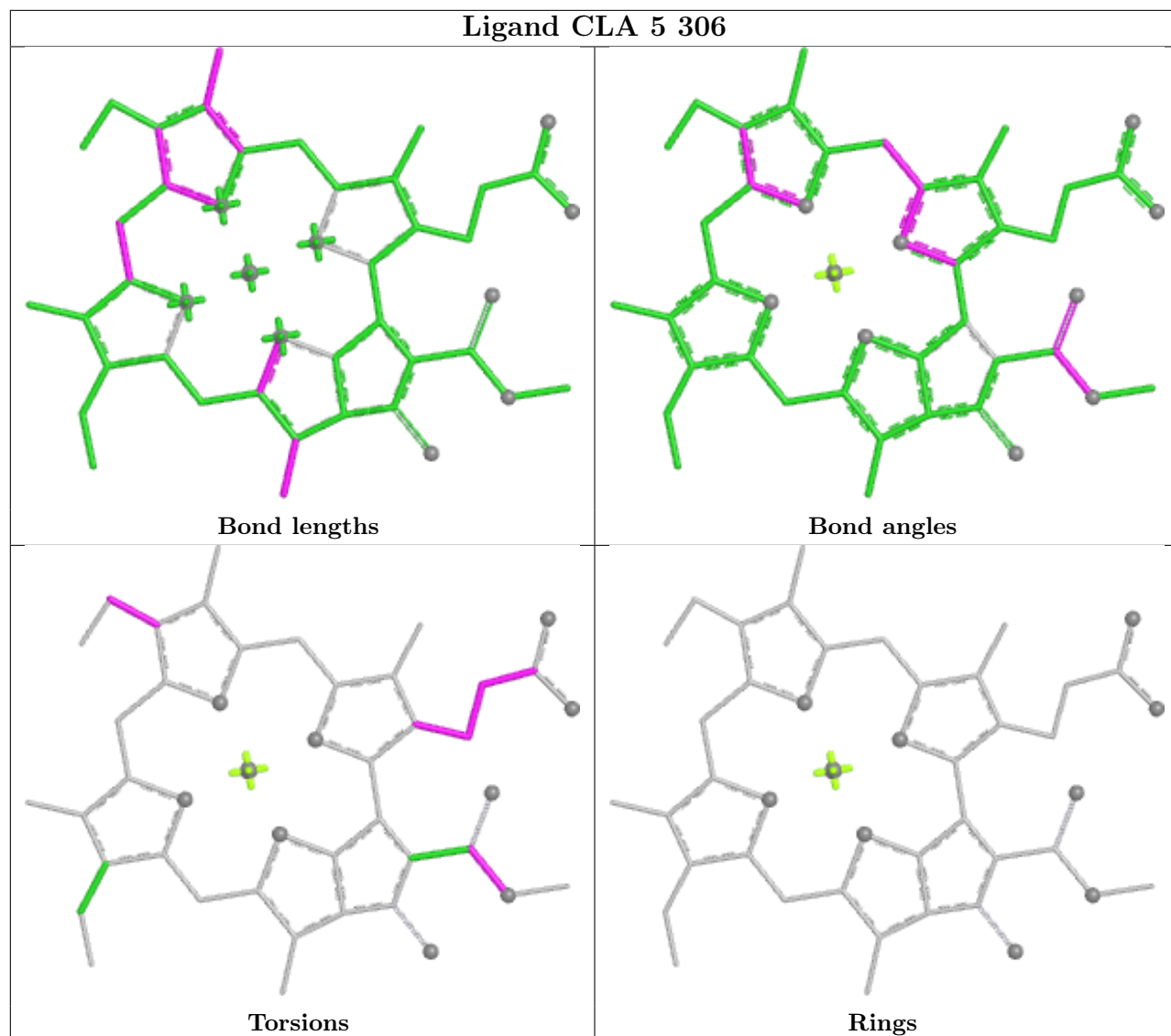
Ligand CLA b 820



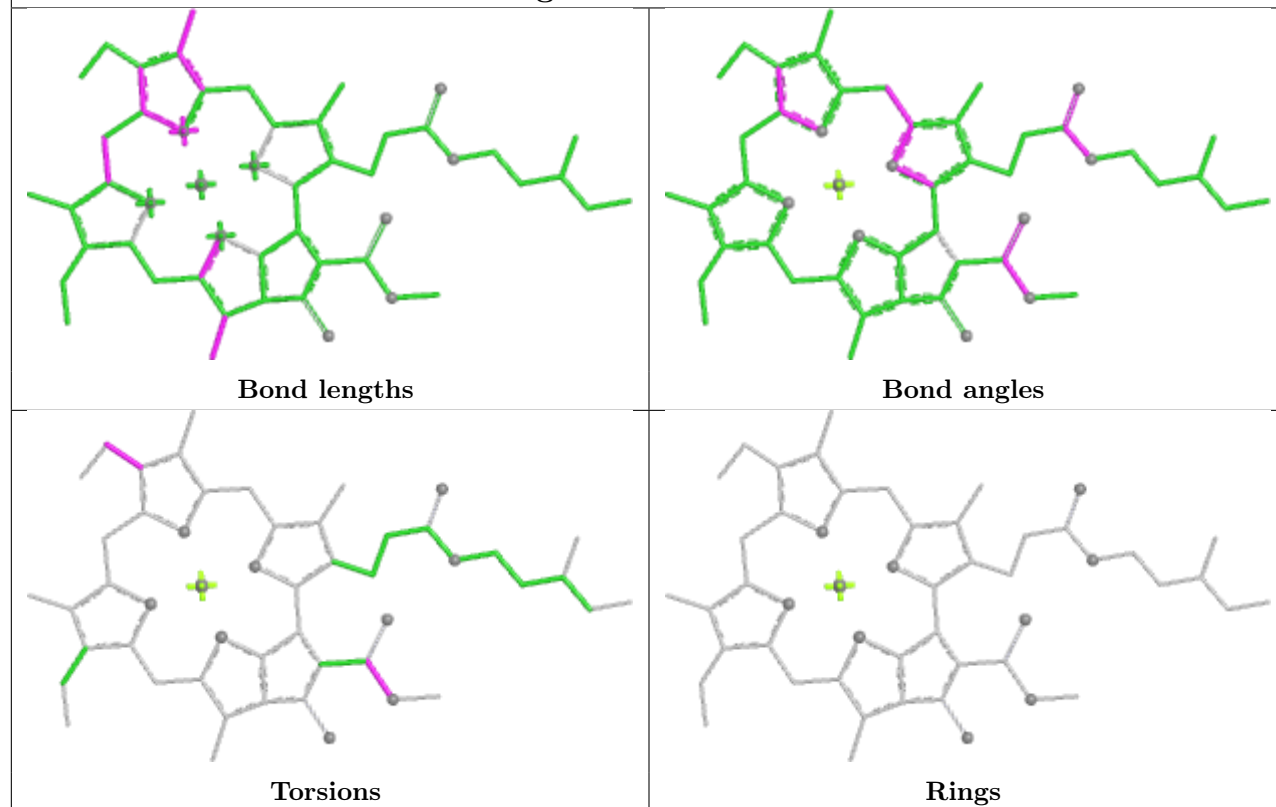
Ligand CLA b 840



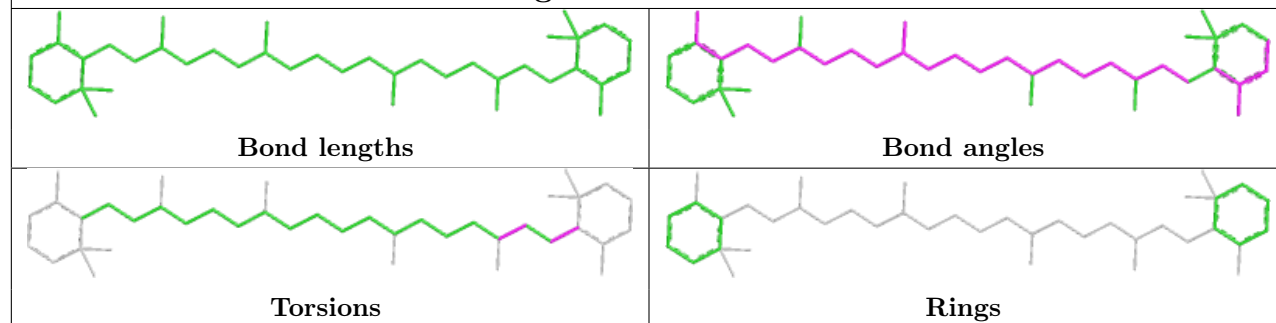
Ligand CLA 5 306



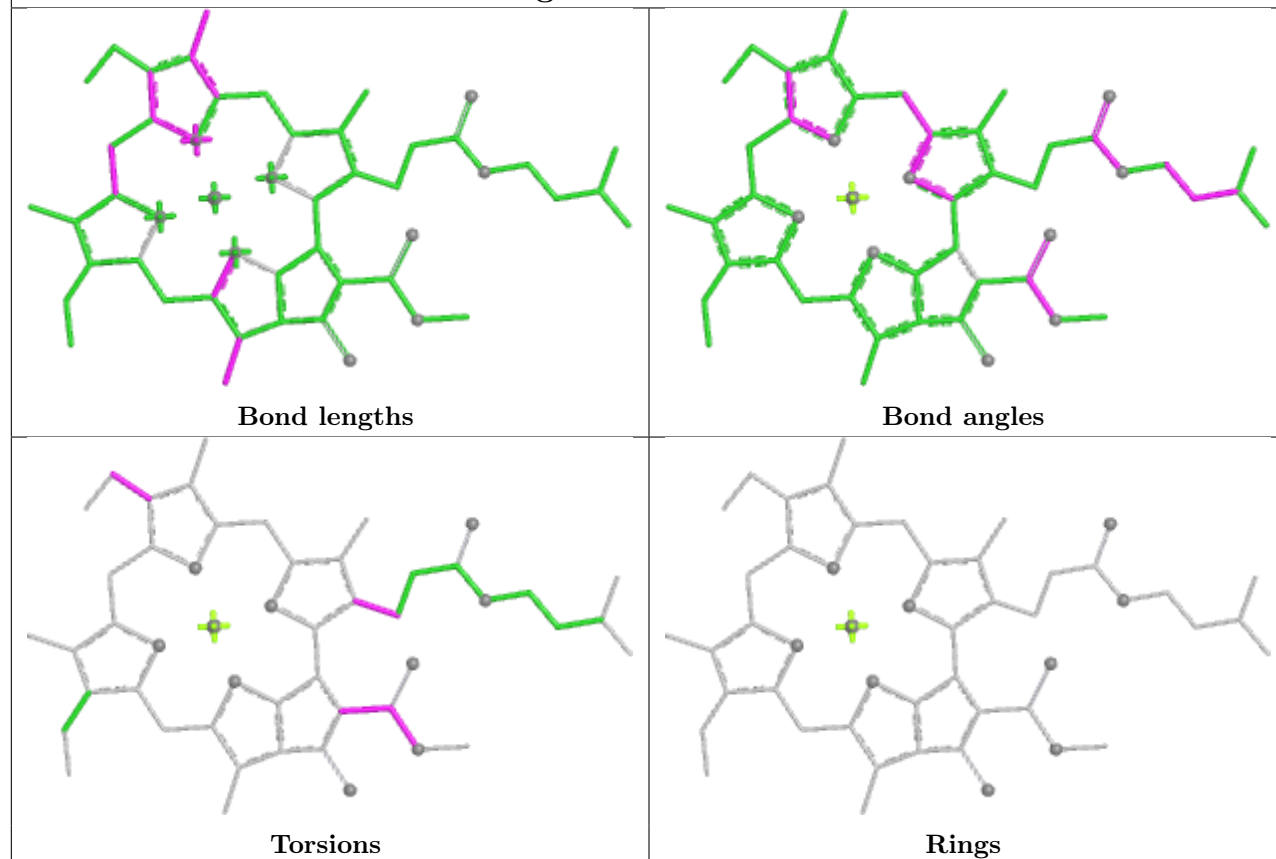
Ligand CLA a 808



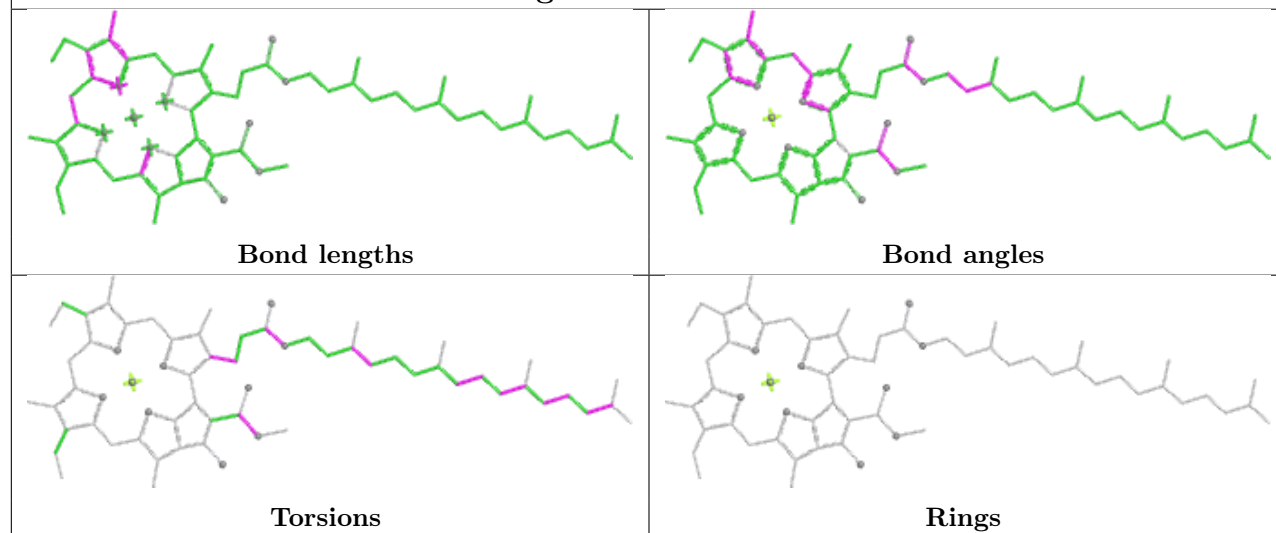
Ligand BCR a 850

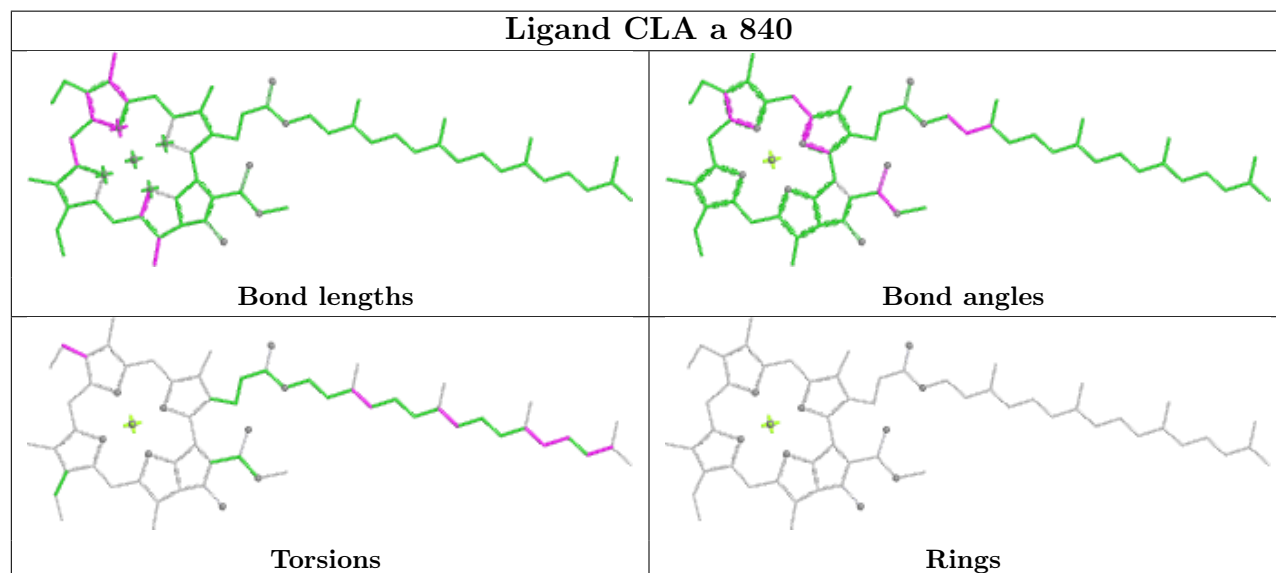
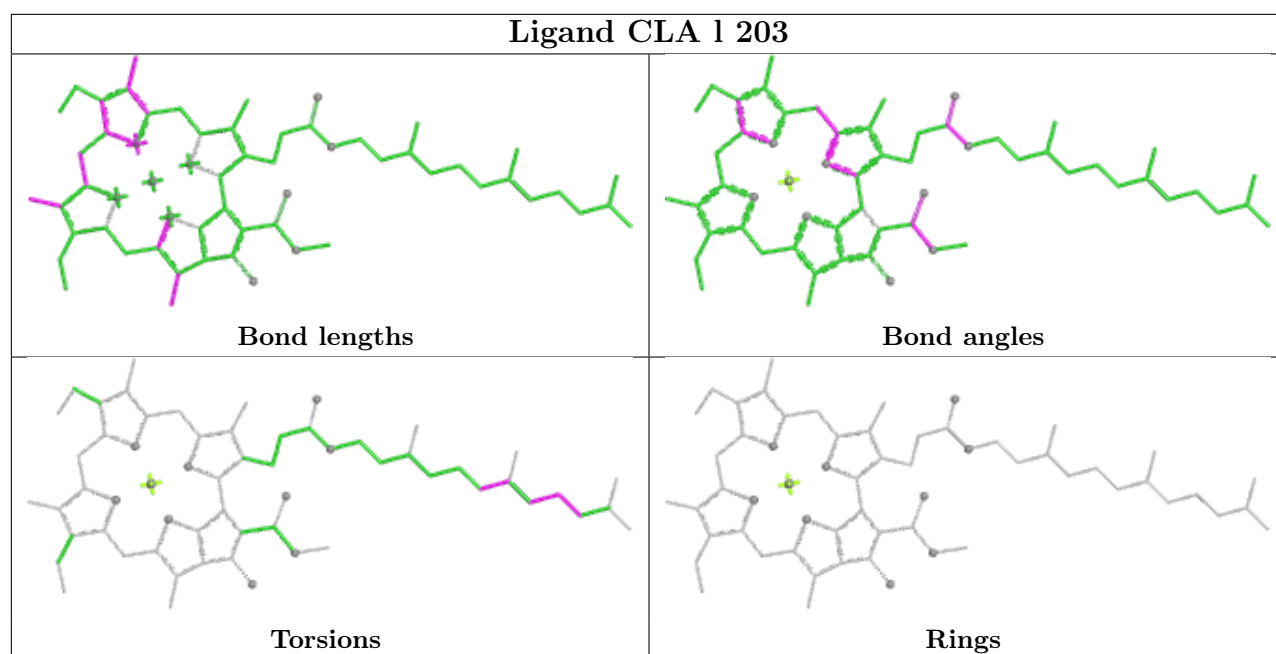


Ligand CLA a 832

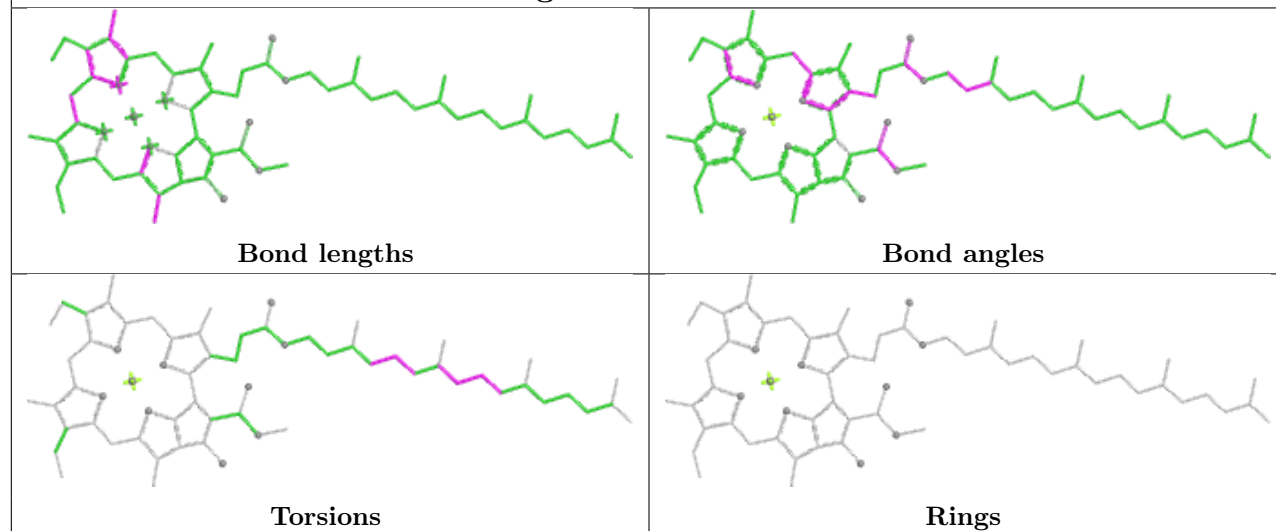


Ligand CLA a 820

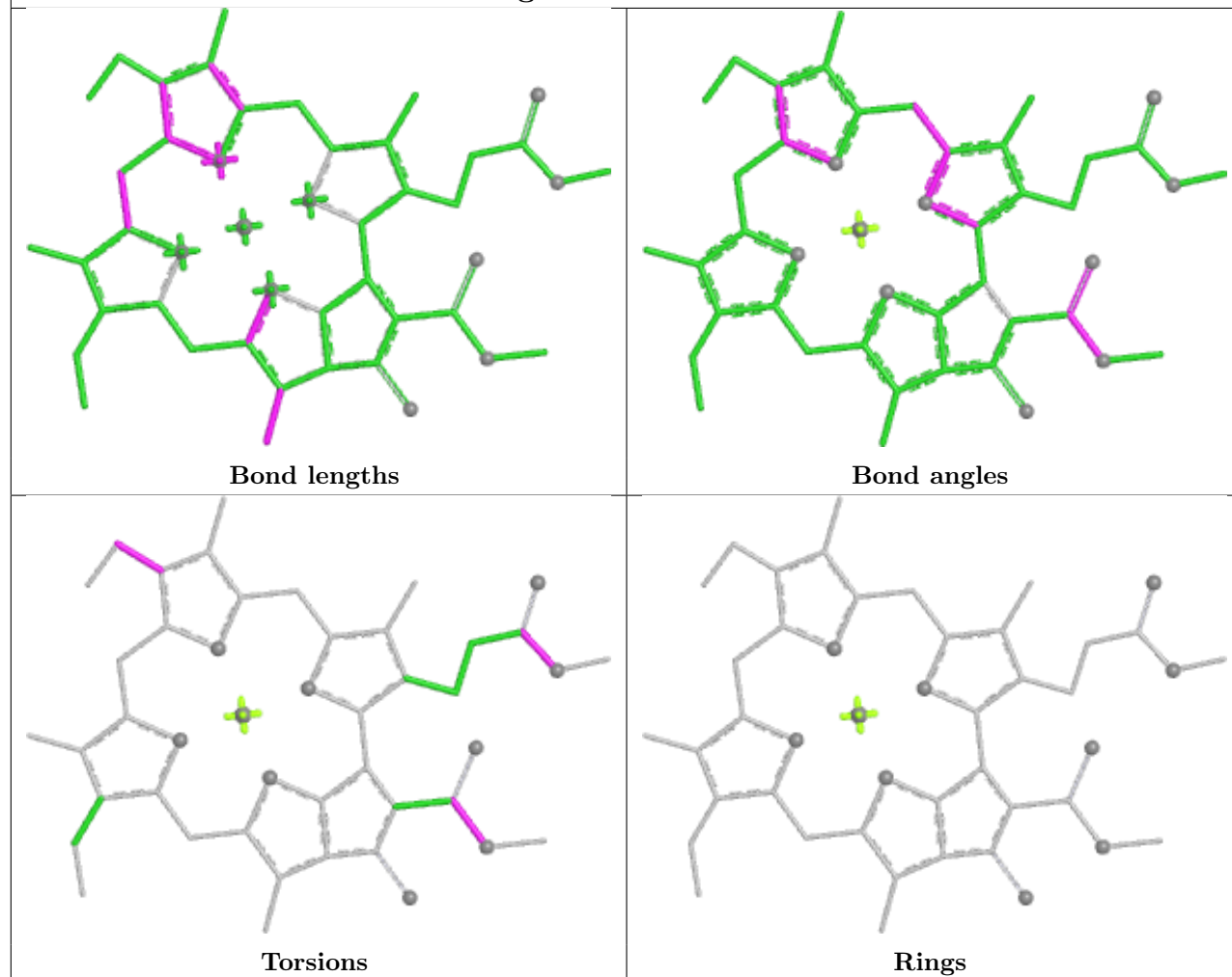




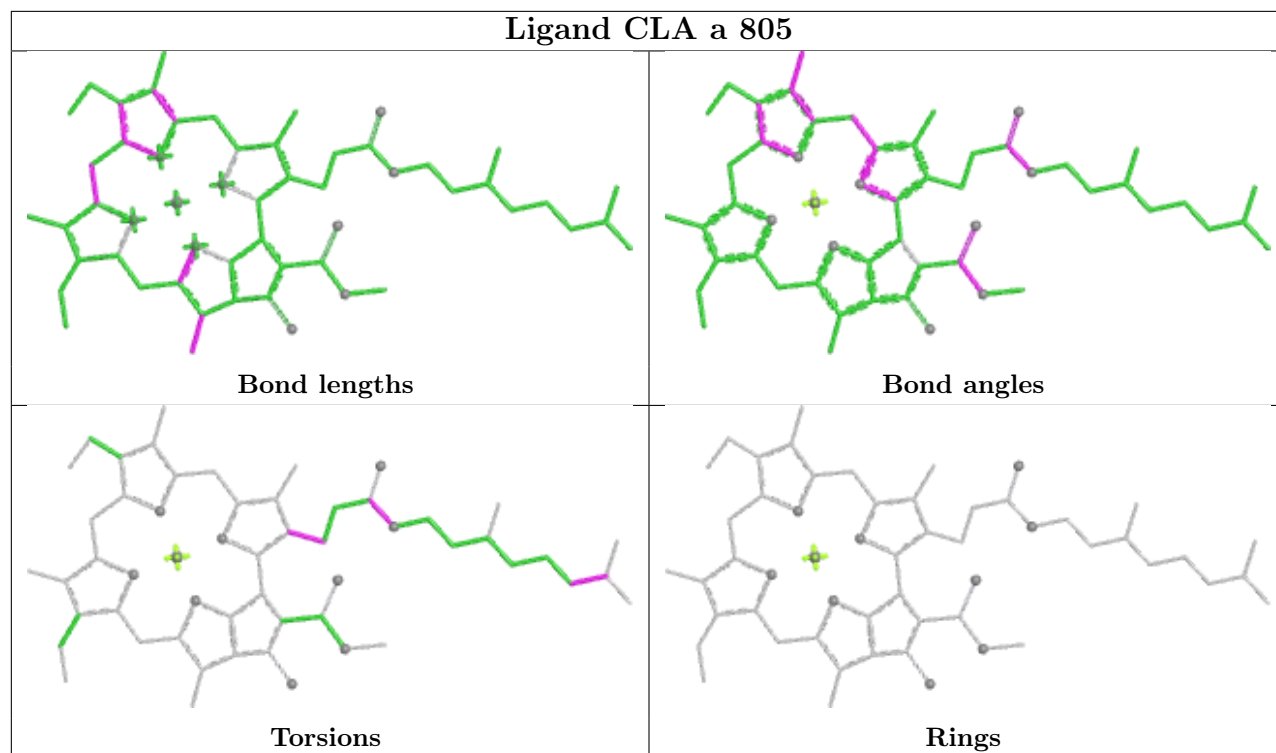
Ligand CLA a 827



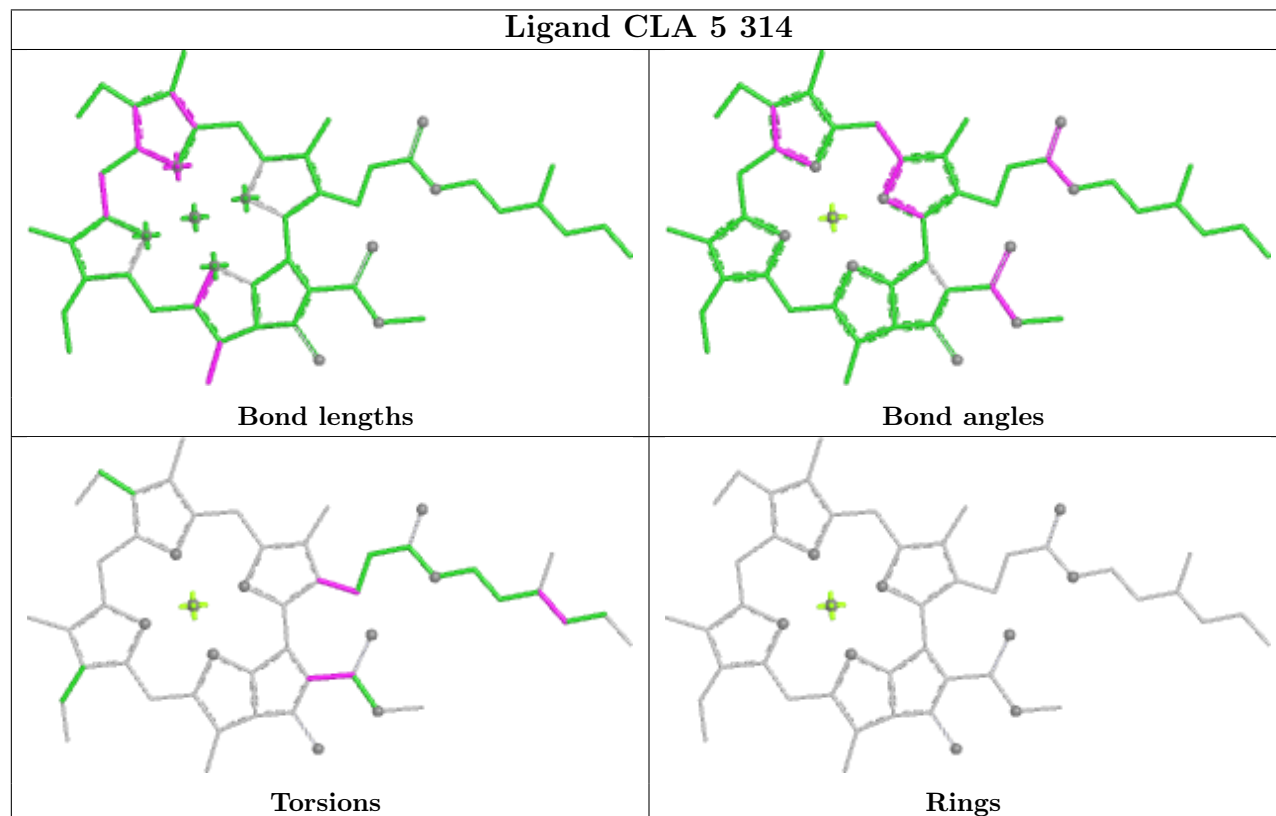
Ligand CLA 5 305



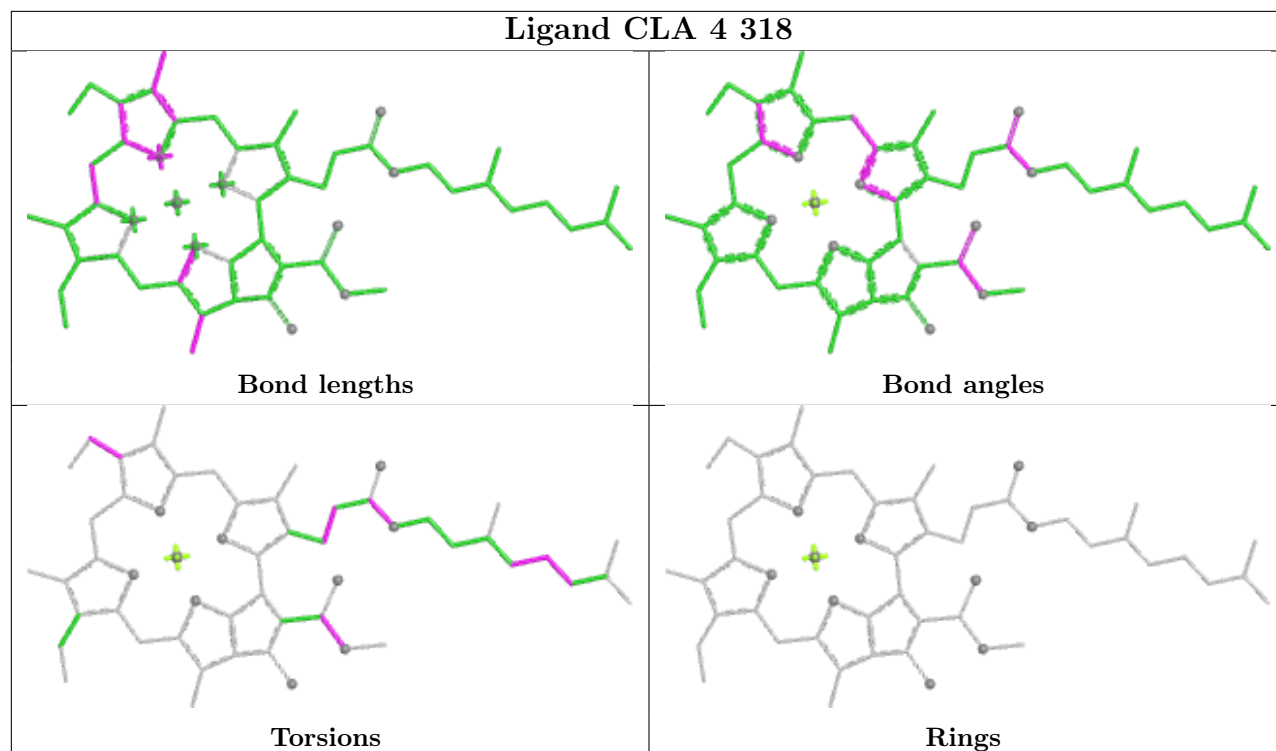
Ligand CLA a 805



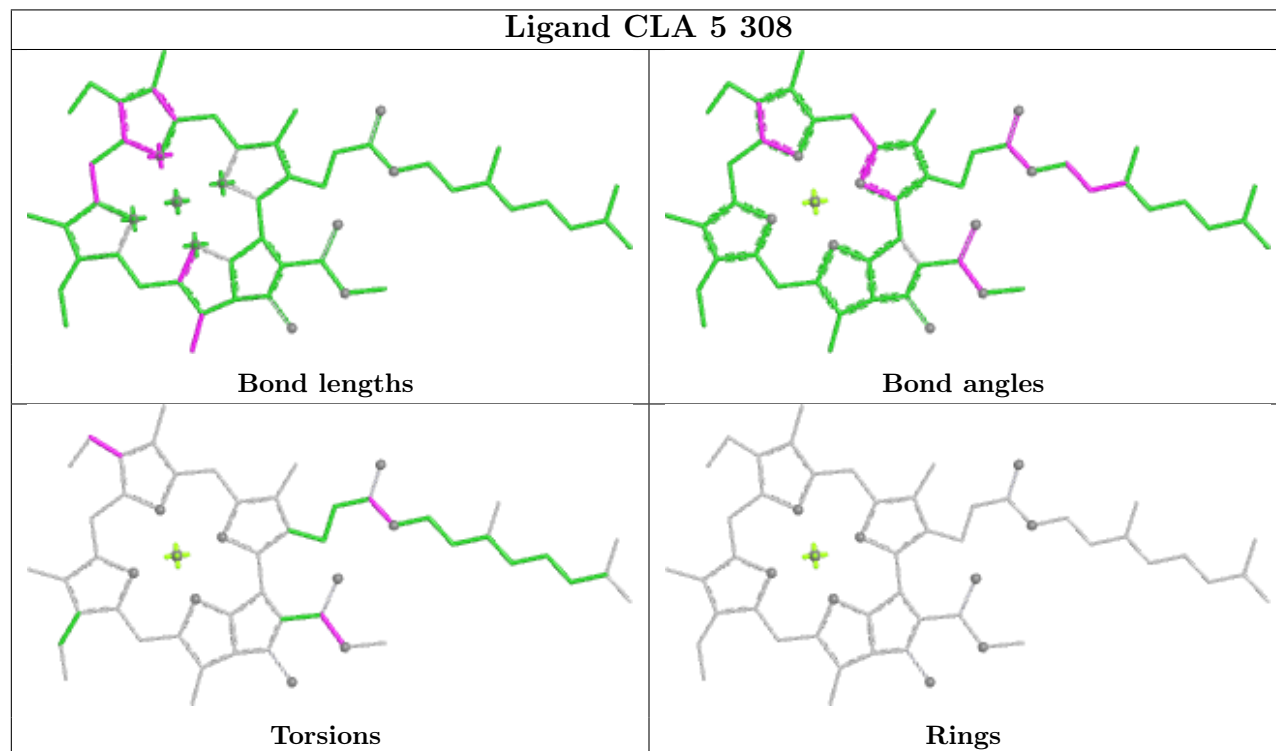
Ligand CLA 5 314

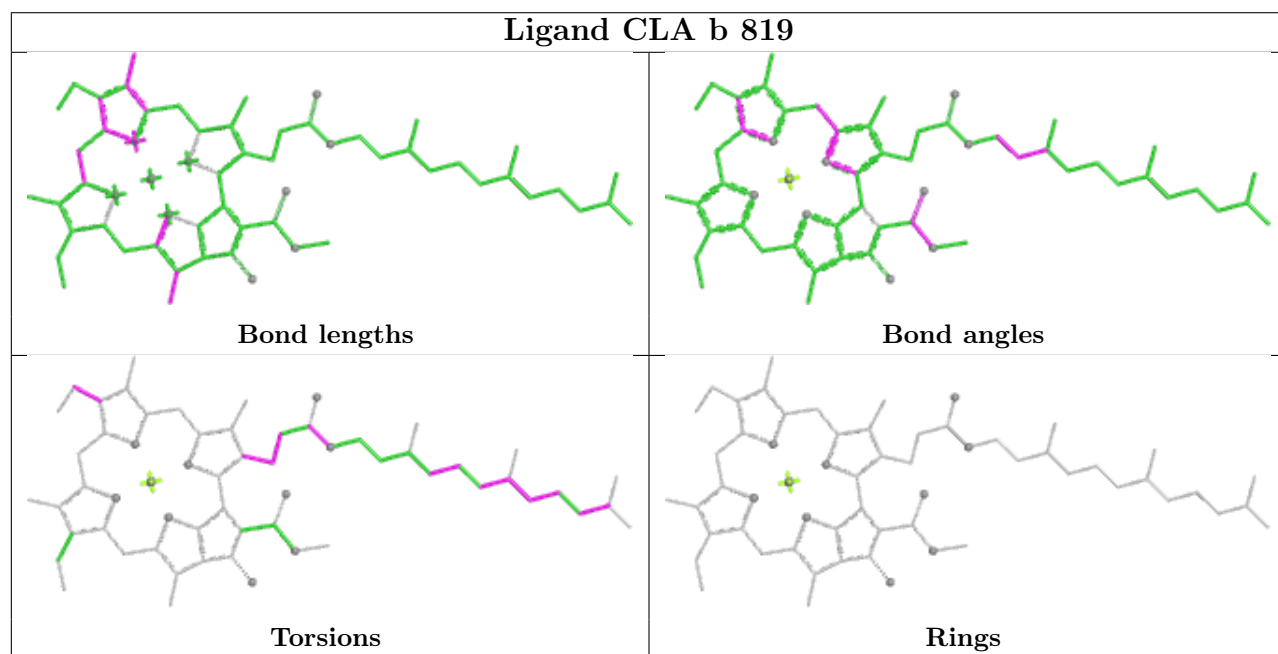
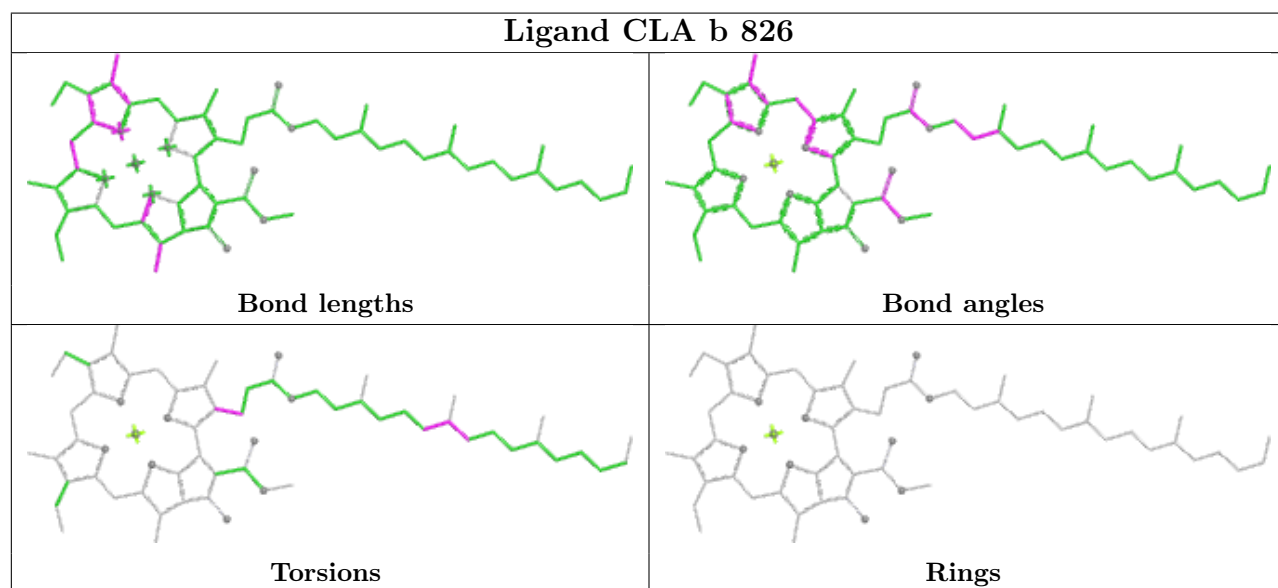
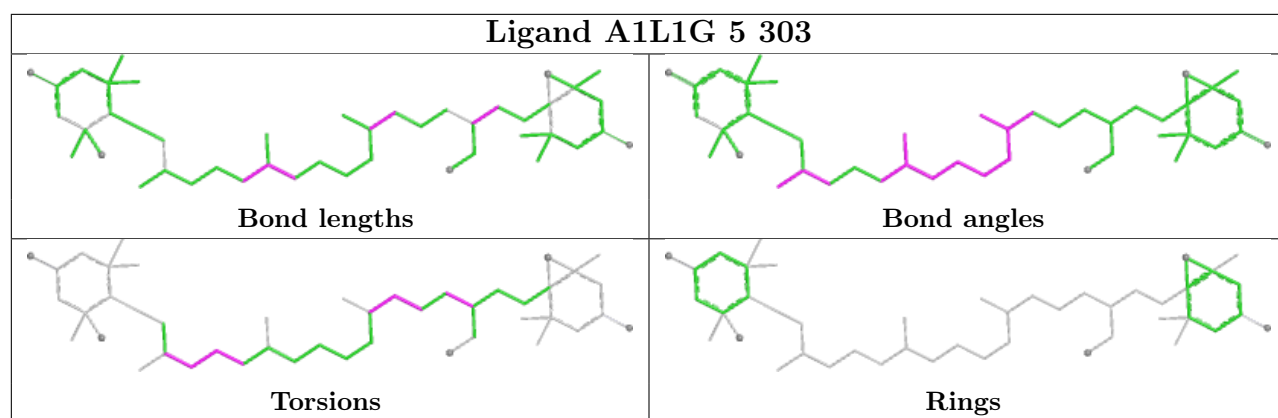


Ligand CLA 4 318

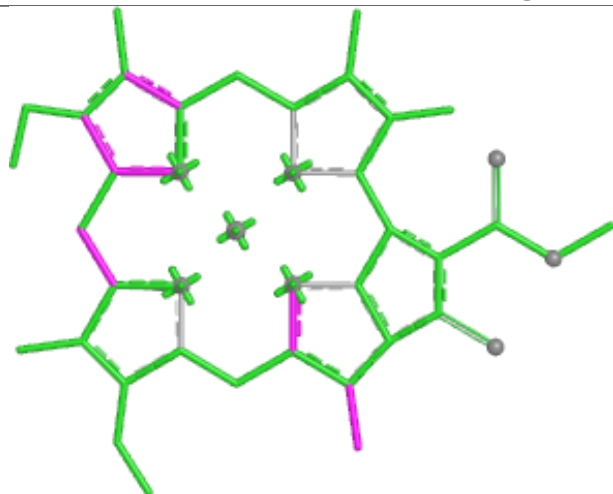


Ligand CLA 5 308

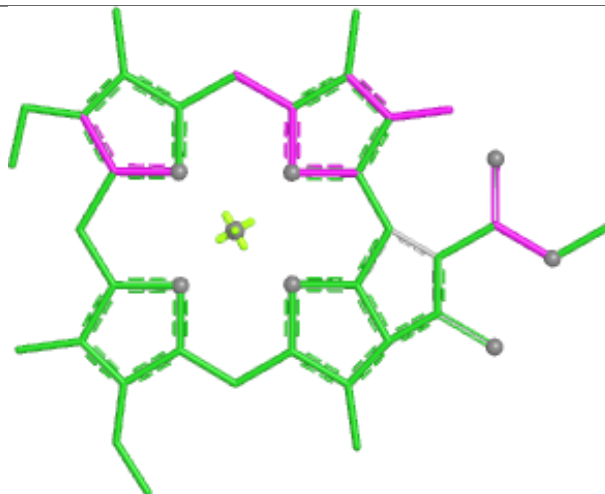




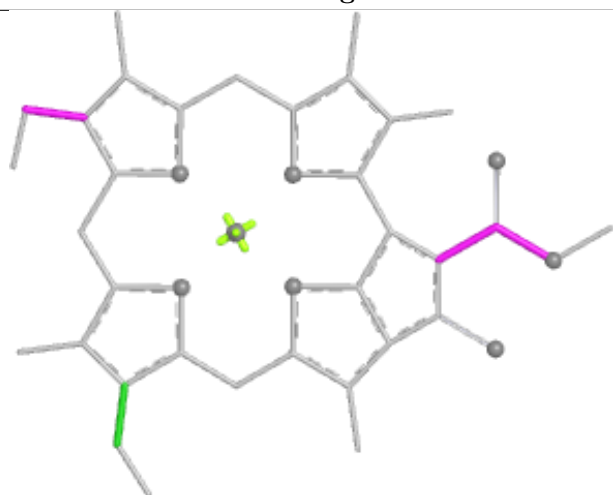
Ligand CLA 4 316



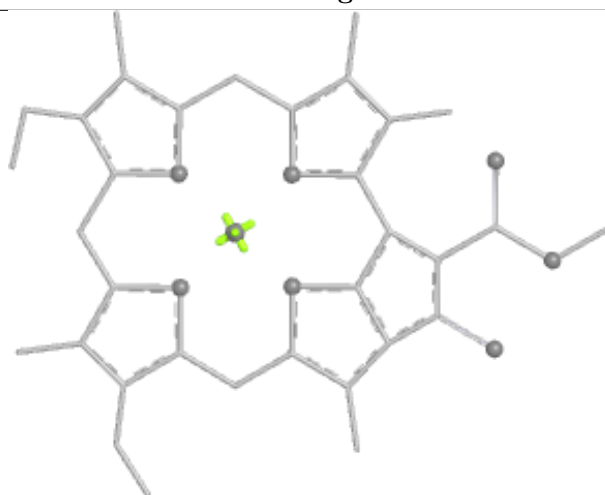
Bond lengths



Bond angles

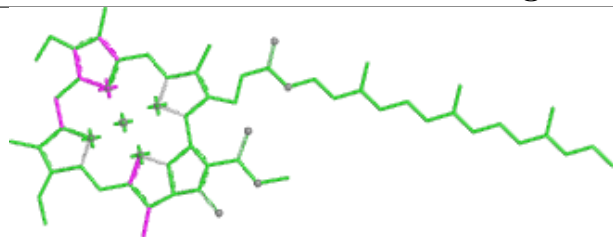


Torsions

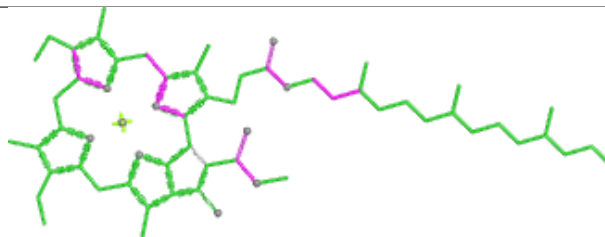


Rings

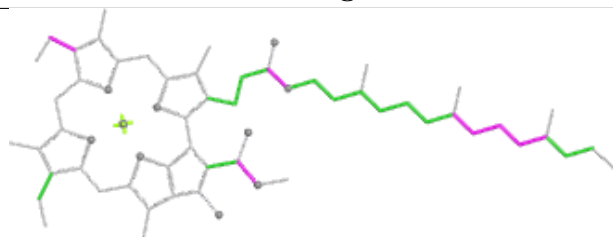
Ligand CLA i 102



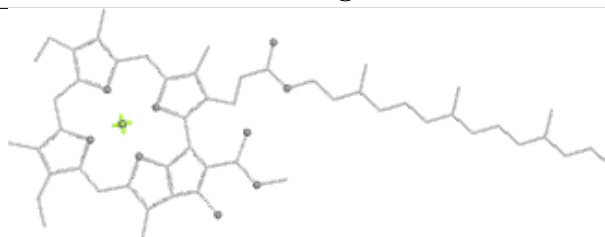
Bond lengths



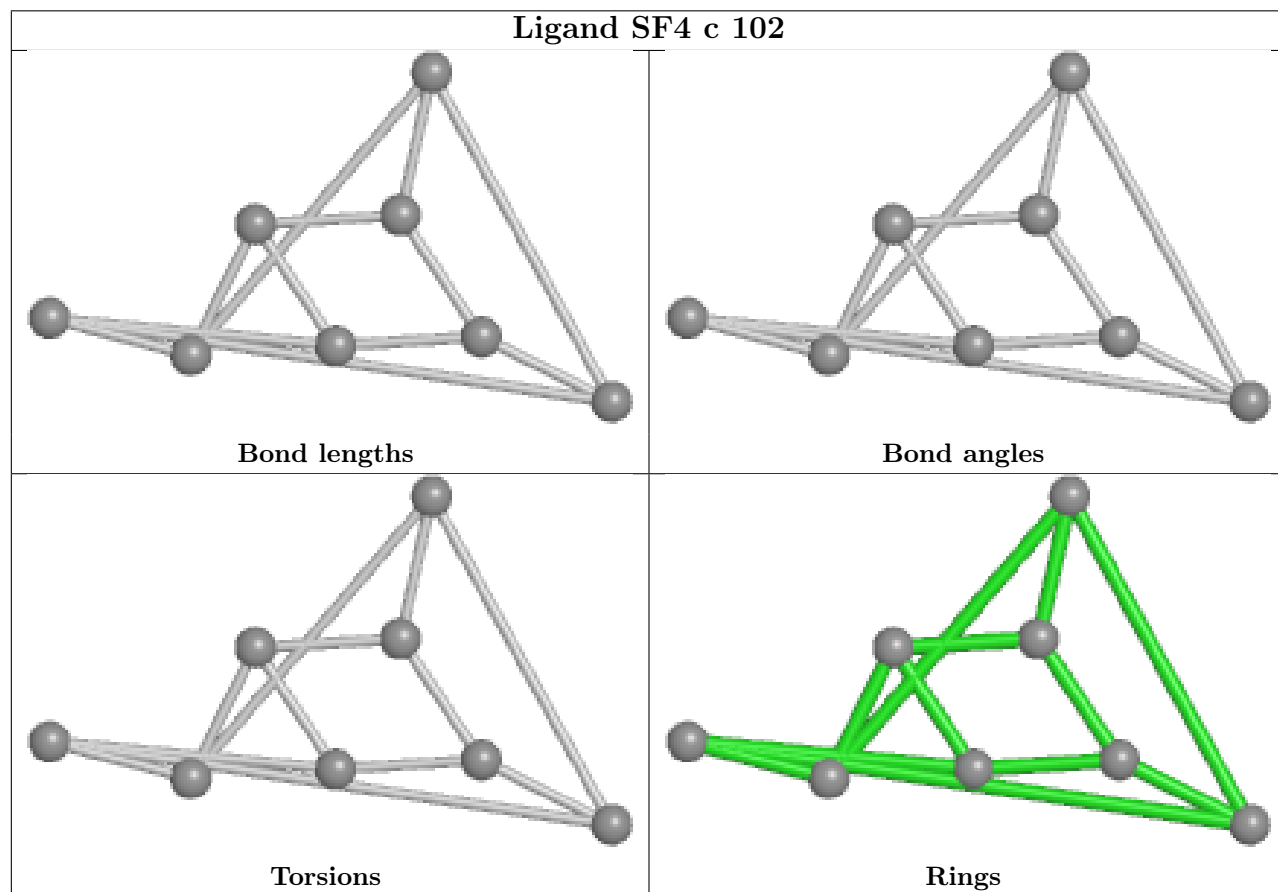
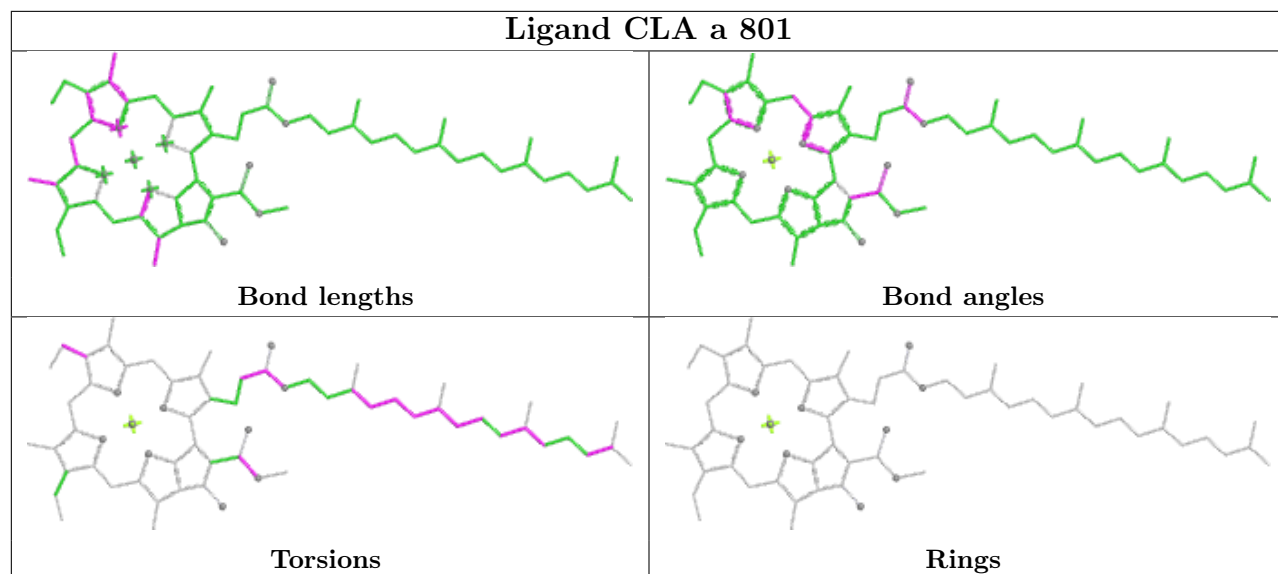
Bond angles

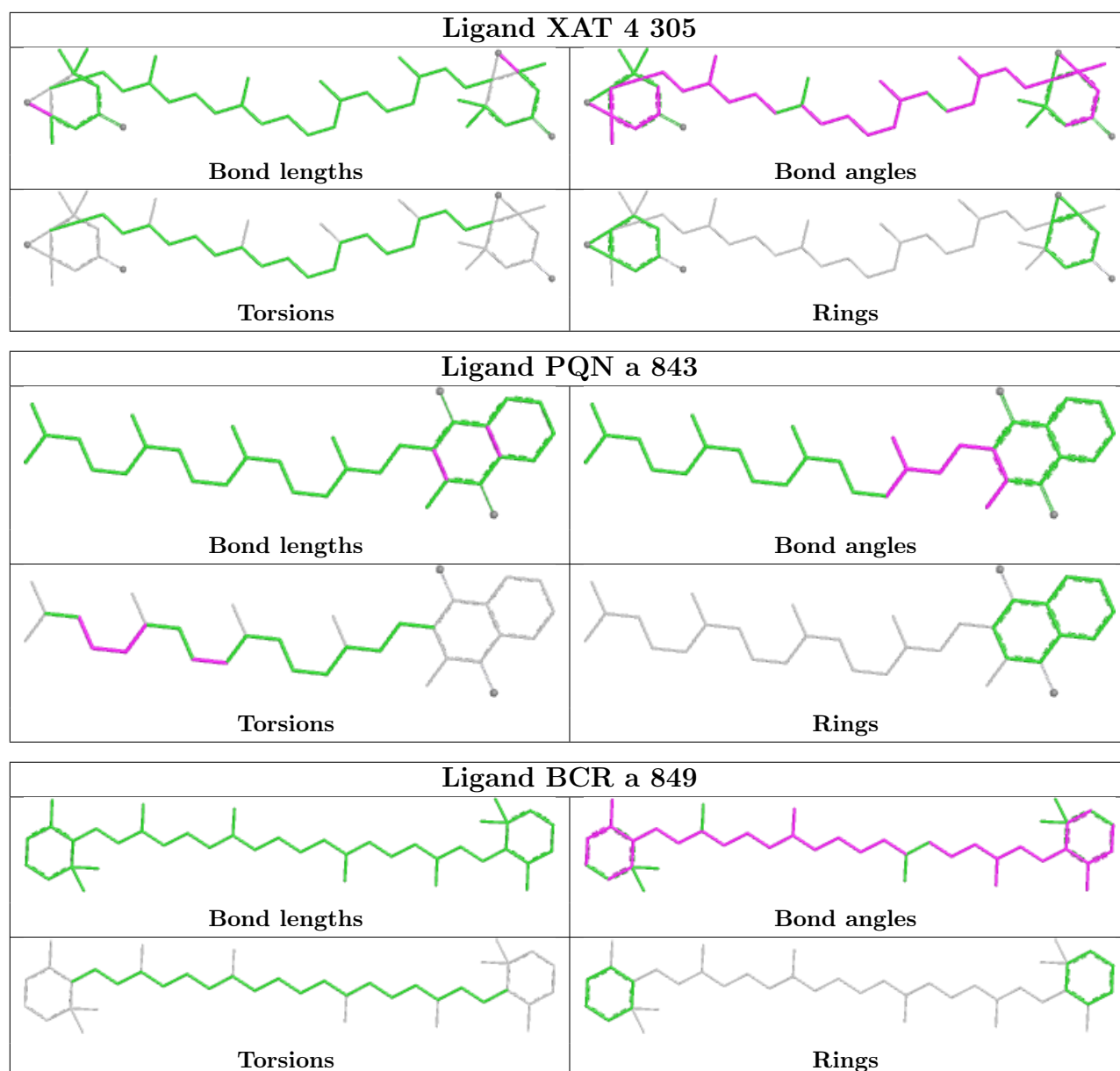


Torsions



Rings





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.

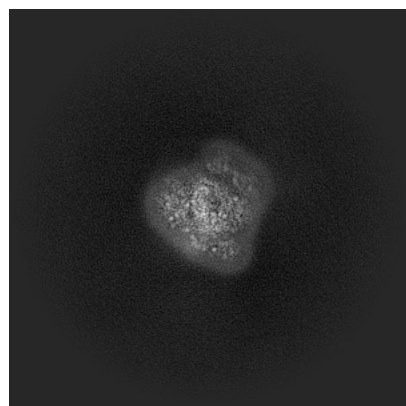
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60291. These allow visual inspection of the internal detail of the map and identification of artifacts.

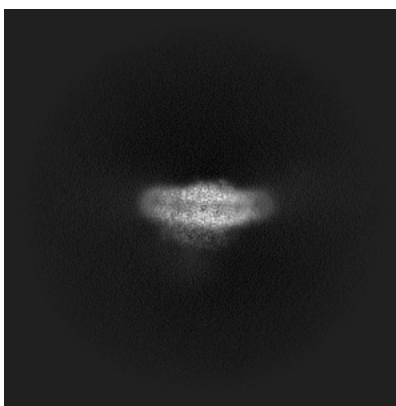
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

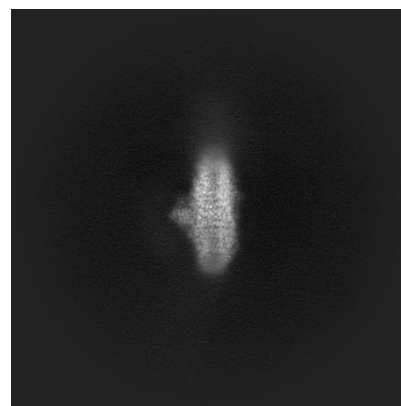
6.1.1 Primary map



X

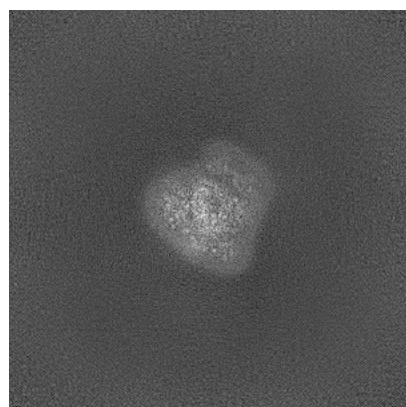


Y

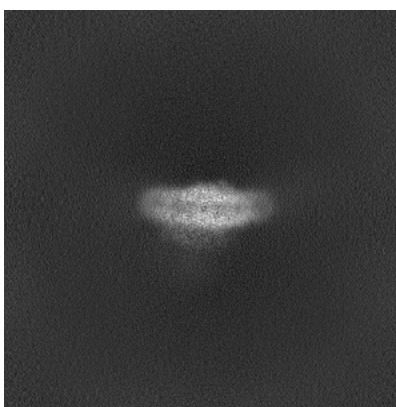


Z

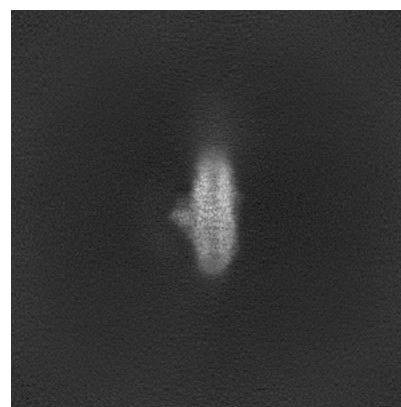
6.1.2 Raw map



X



Y

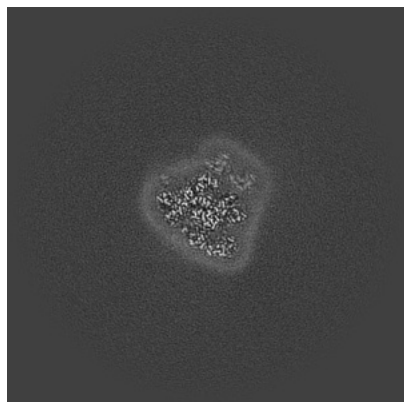


Z

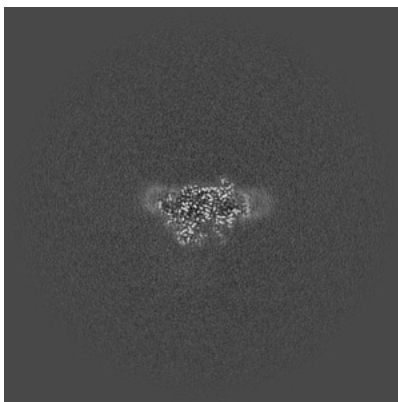
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

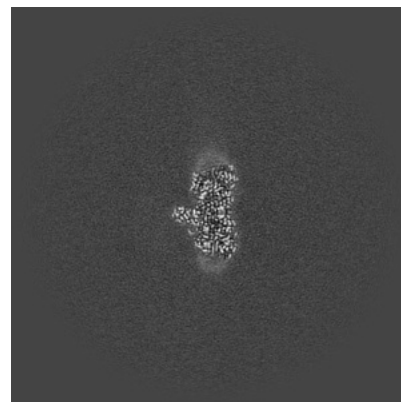
6.2.1 Primary map



X Index: 256

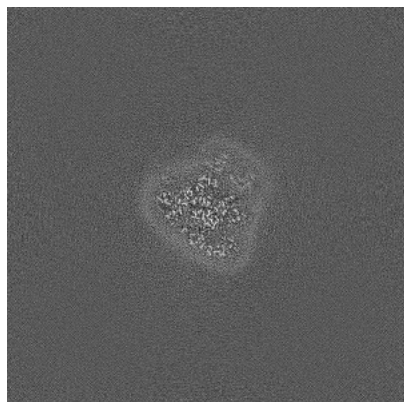


Y Index: 256

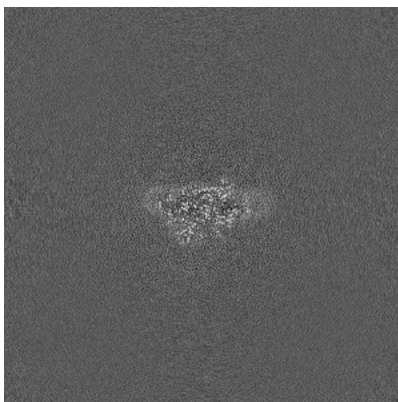


Z Index: 256

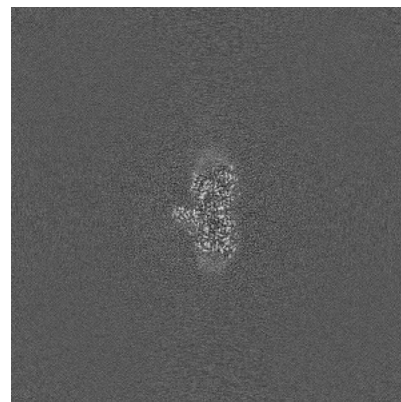
6.2.2 Raw map



X Index: 256



Y Index: 256

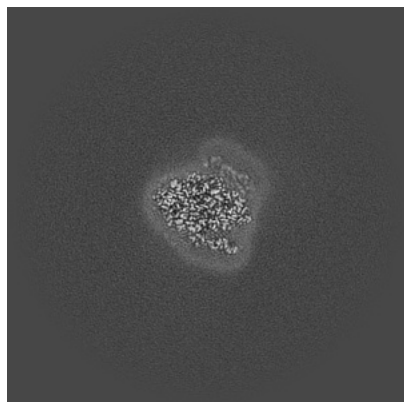


Z Index: 256

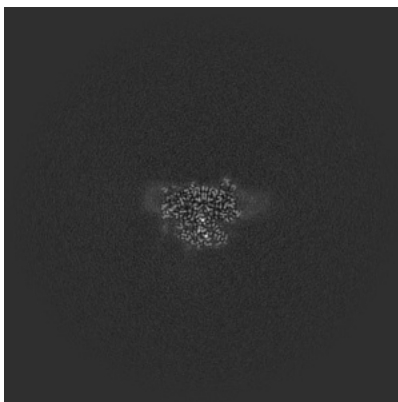
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

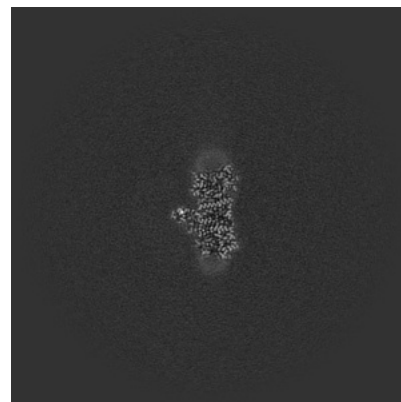
6.3.1 Primary map



X Index: 269

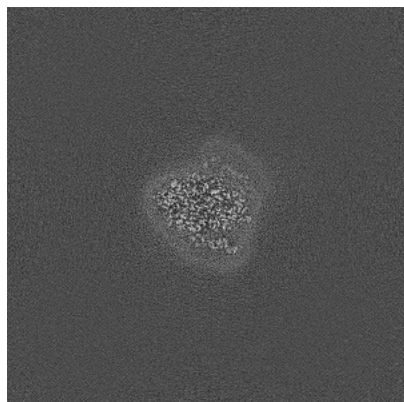


Y Index: 249

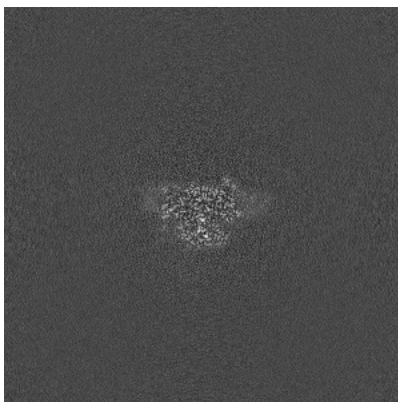


Z Index: 259

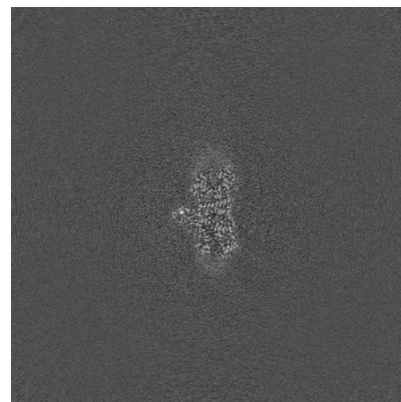
6.3.2 Raw map



X Index: 269



Y Index: 249

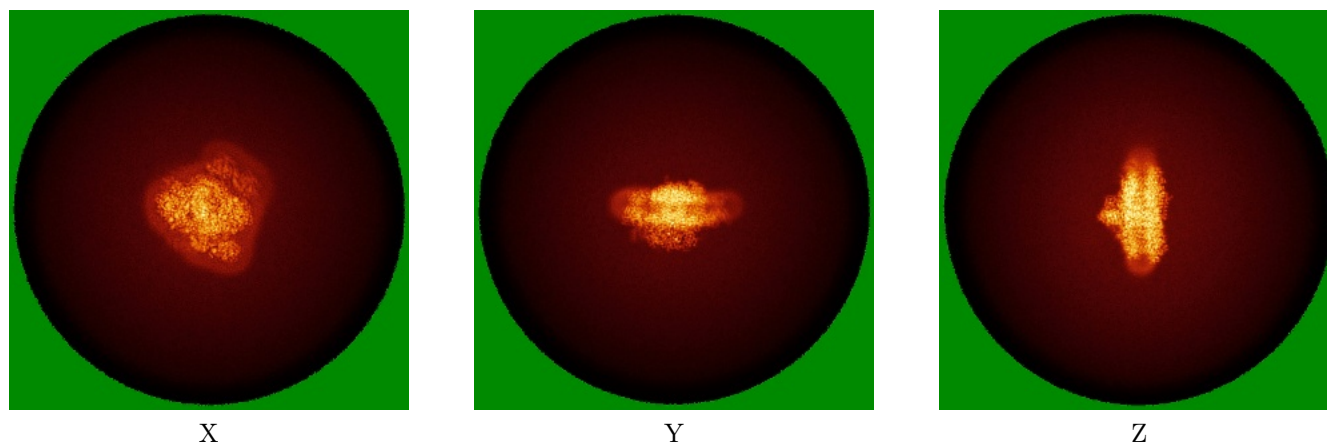


Z Index: 258

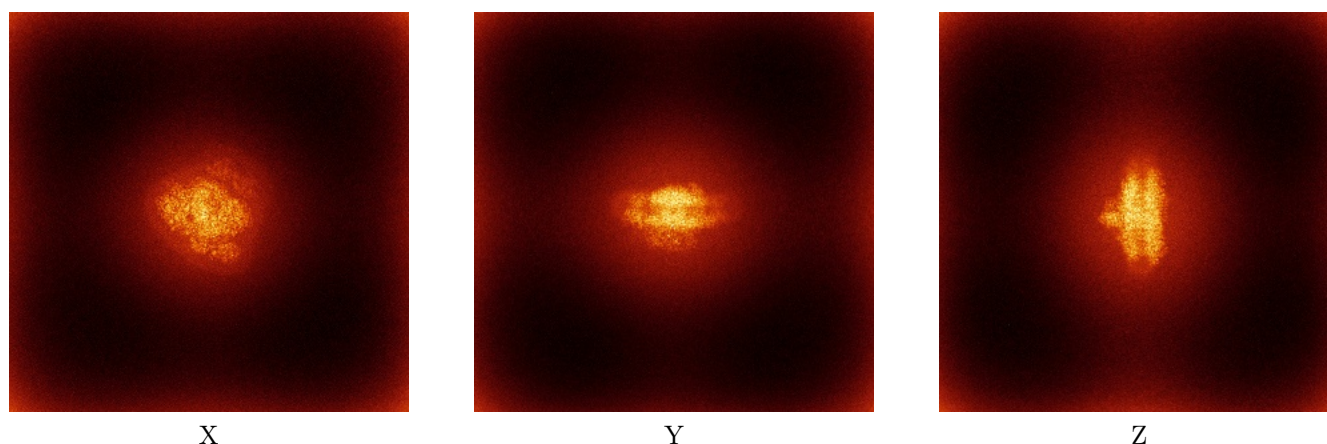
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

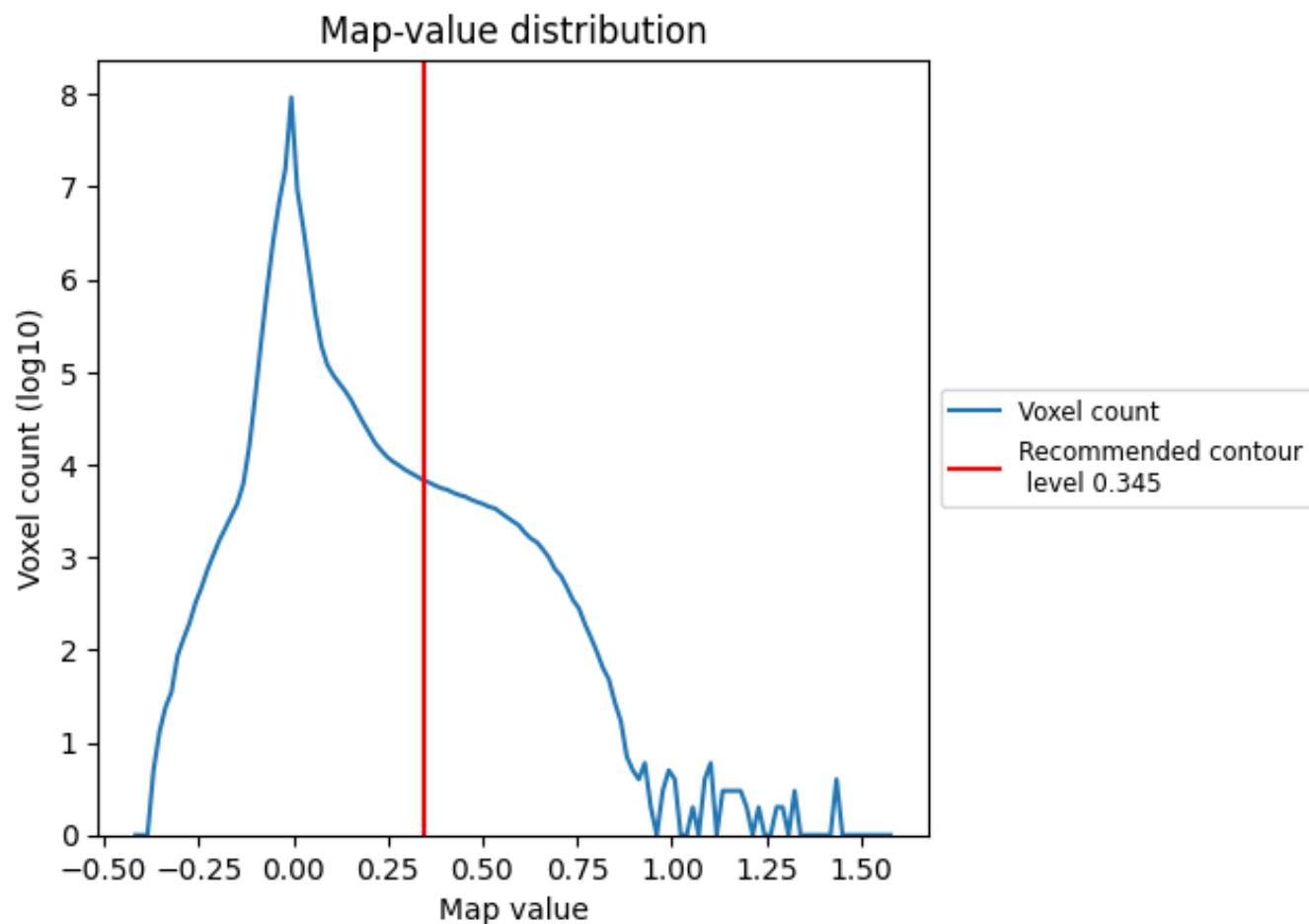
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

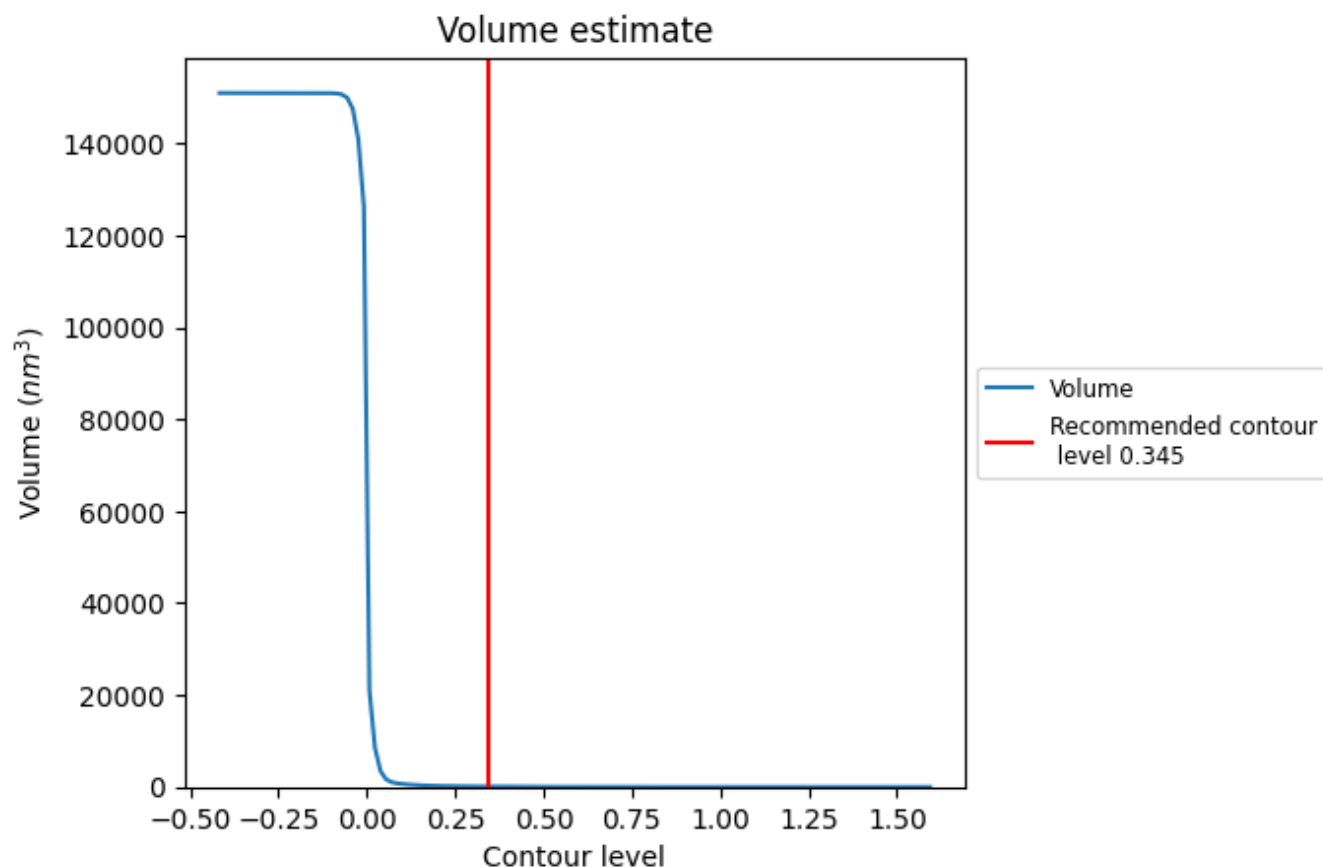
This section contains the results of statistical analysis of the map.

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.

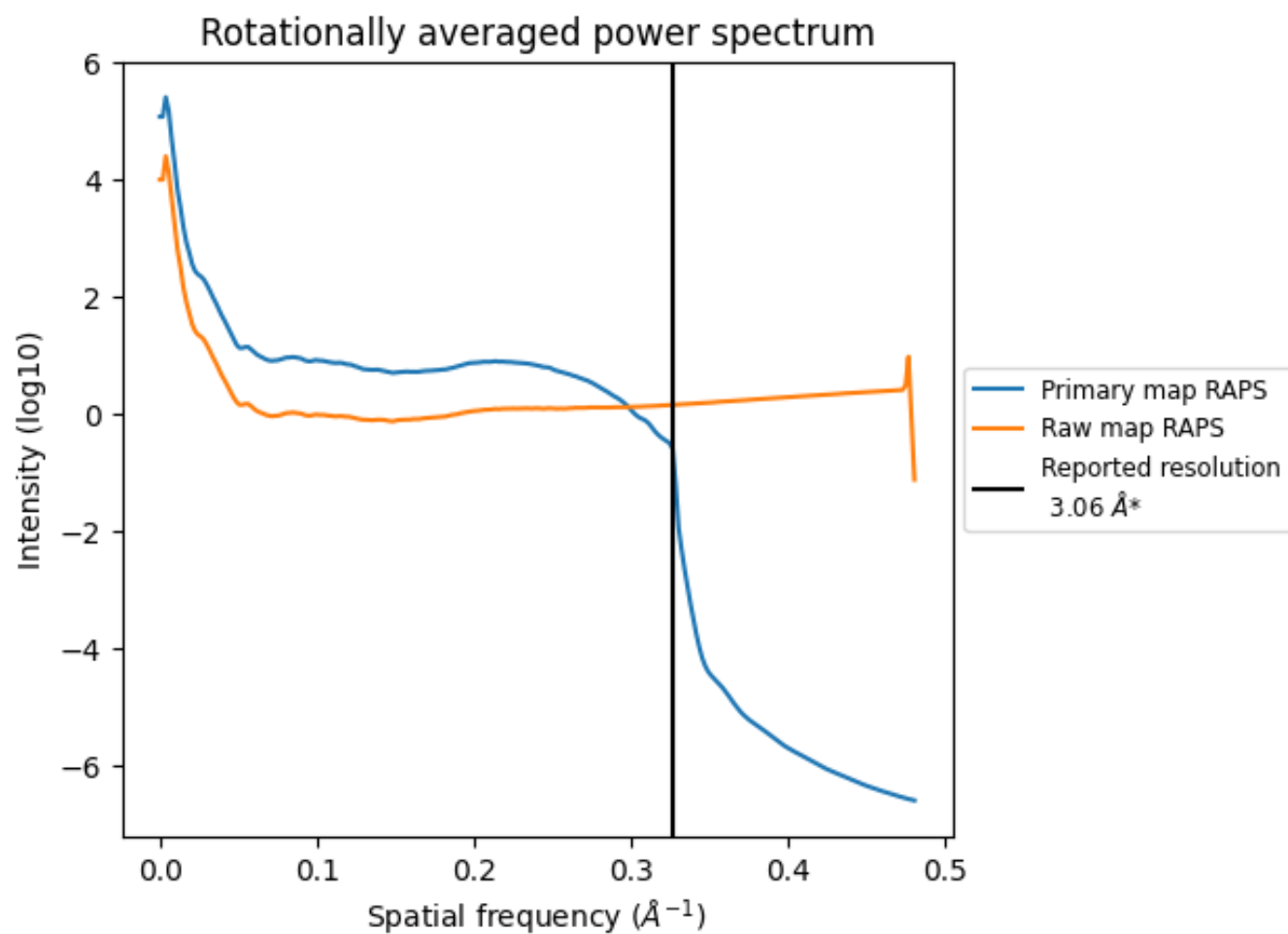
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

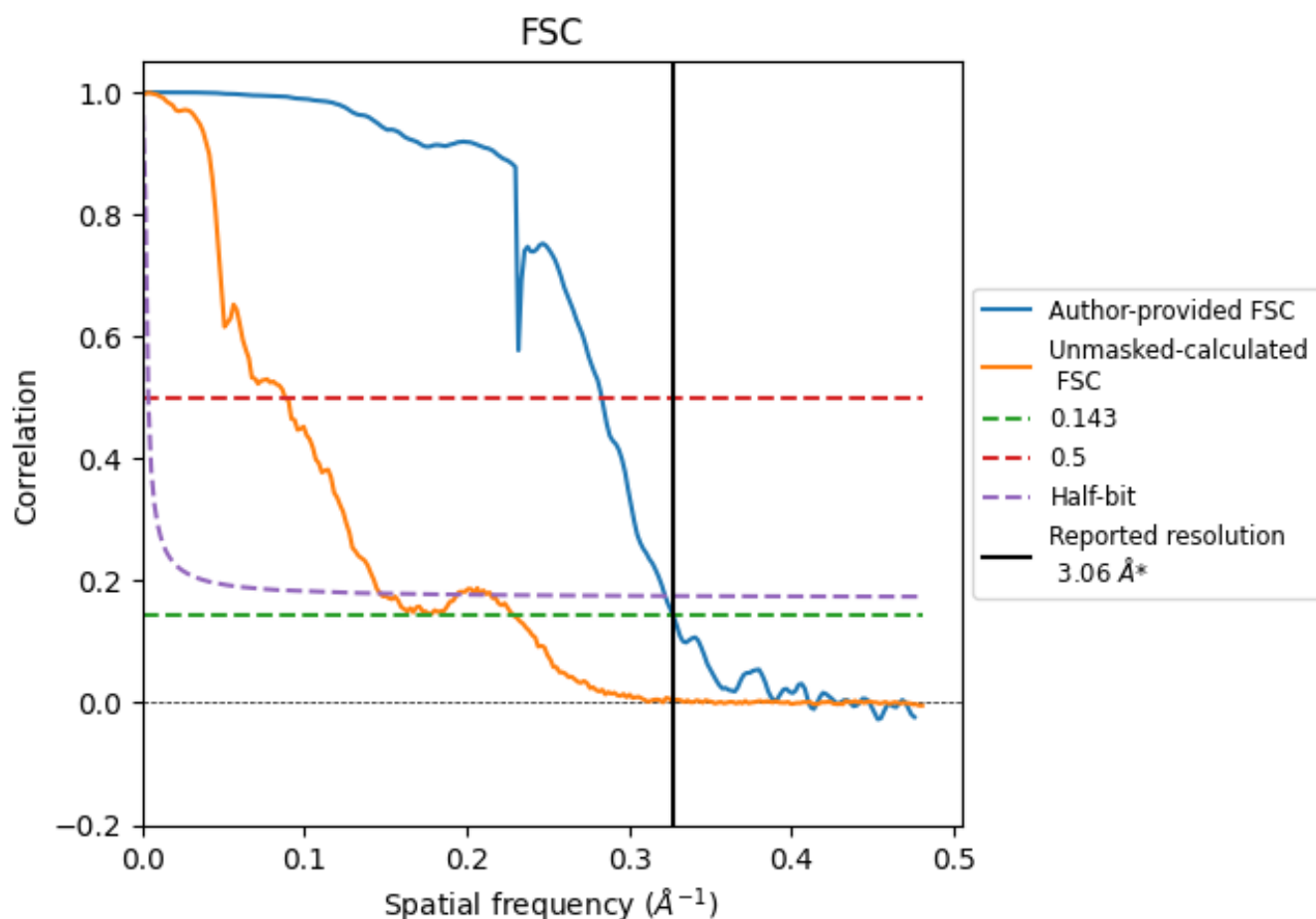


*Reported resolution corresponds to spatial frequency of 0.327 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.327 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

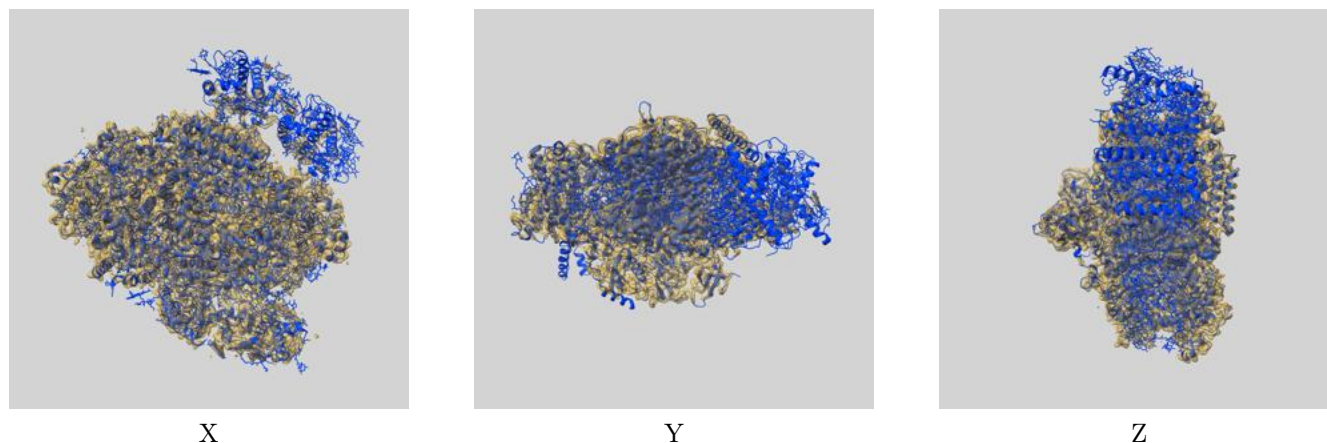
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.53	3.10
Unmasked-calculated*	4.37	11.36	6.82

*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 4.37 differs from the reported value 3.06 by more than 10 %

9 Map-model fit [i](#)

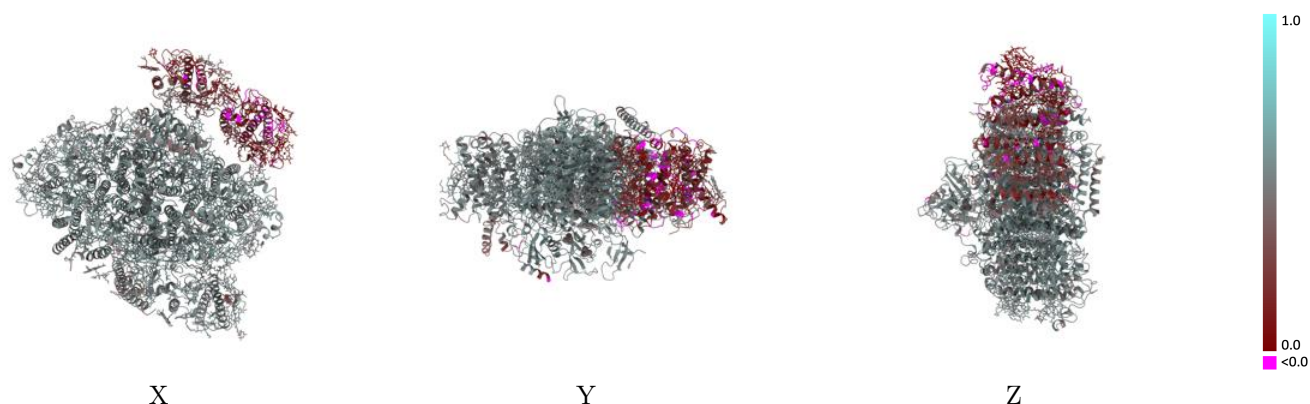
This section contains information regarding the fit between EMDB map EMD-60291 and PDB model 8ZOF. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



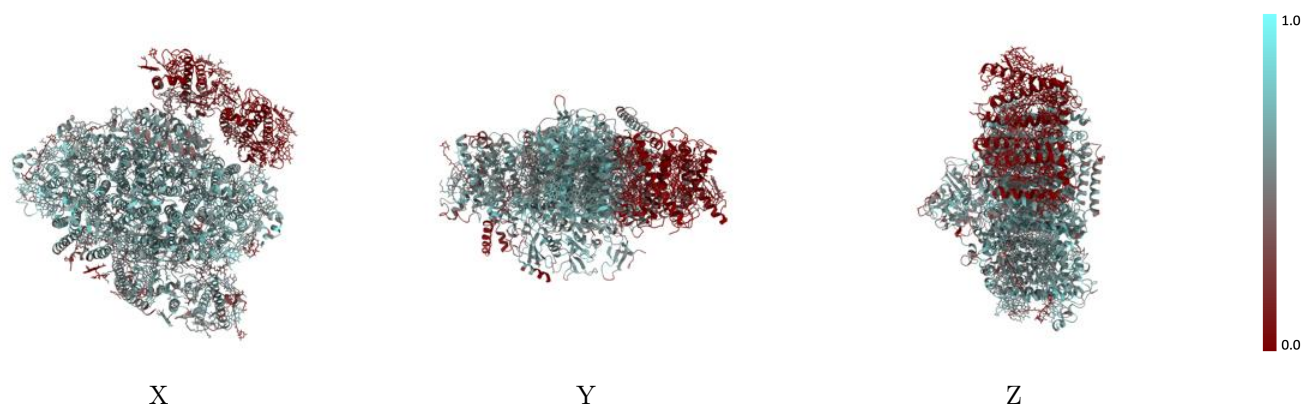
The images above show the 3D surface view of the map at the recommended contour level 0.345 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



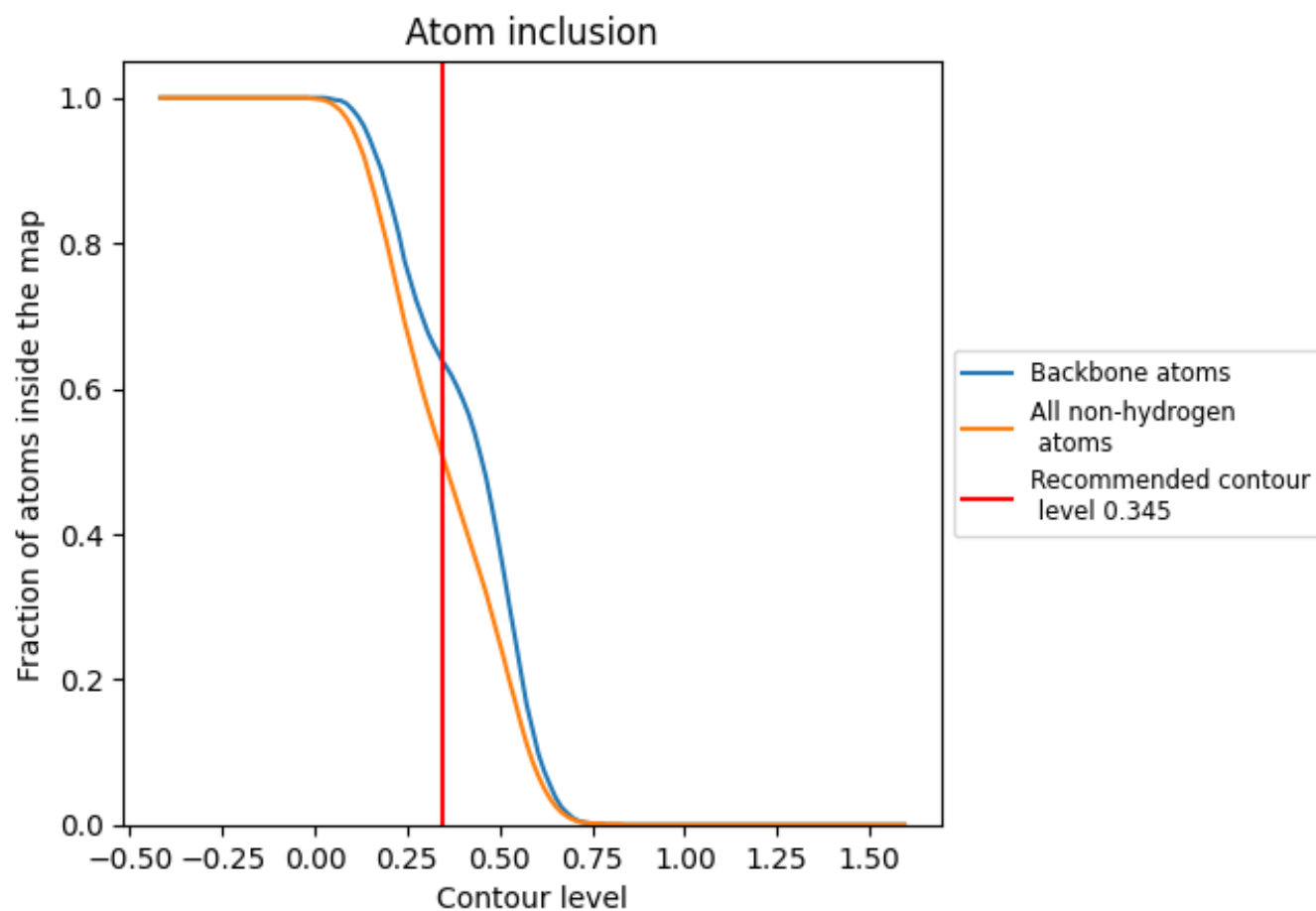
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.345).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 51% 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 (0.345) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5080	0.4790
1	0.5060	0.5080
4	0.0350	0.1180
5	0.0900	0.2380
a	0.6210	0.5430
b	0.6110	0.5390
c	0.6540	0.5300
d	0.5410	0.5250
e	0.5380	0.5150
f	0.5300	0.4960
g	0.2360	0.3820
i	0.3780	0.4890
j	0.5110	0.5320
l	0.5020	0.4900
m	0.4330	0.4670

1.0

0.0

<0.0