



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 04:14 AM UTC

PDB ID : 6TRC / pdb_00006trc
EMDB ID : EMD-10558
Title : Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6
Authors : Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Mielke, T.; Lisdat, F.; Zouni, A.; Wendler, P.
Deposited on : 2019-12-18
Resolution : 2.98 Å(reported)

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

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A user guide is available at

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

The types of validation reports are described at

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

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

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

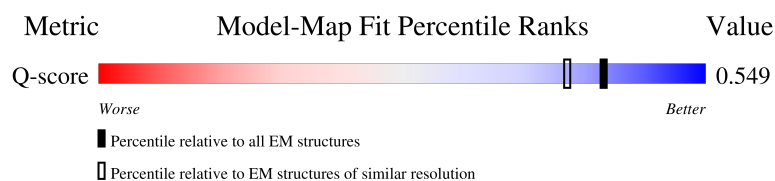
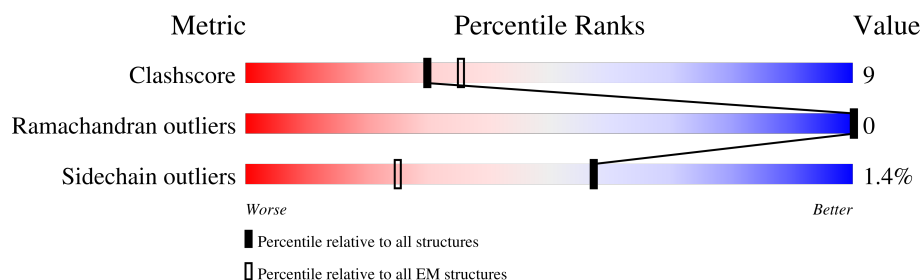
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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	13236 (2.48 - 3.48)

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	1	755	25% 79% 20% .
1	A	755	25% 79% 20% .
1	a	755	24% 79% 19% .
2	2	741	18% 80% 19%

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Mol	Chain	Length	Quality of chain
2	B	741	
2	b	741	
3	3	81	
3	C	81	
3	c	81	
4	4	139	
4	D	139	
4	d	139	
5	5	76	
5	E	76	
5	e	76	
6	6	141	
6	F	141	
6	f	141	
7	7	38	
7	I	38	
7	i	38	
8	8	41	
8	J	41	
8	j	41	
9	9	83	
9	K	83	
9	k	83	
10	0	155	
10	L	155	

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Mol	Chain	Length	Quality of chain
10	l	155	
11	M	31	
11	m	31	
11	y	31	
12	X	36	
12	x	36	
12	z	36	

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
13	CL0	1	801	X	-	-	-
13	CL0	A	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	CLA	0	203	X	-	-	-
14	CLA	0	204	X	-	-	-
14	CLA	0	207	X	-	-	-
14	CLA	0	208	X	-	-	-
14	CLA	0	209	X	-	-	-
14	CLA	1	802	X	-	-	-
14	CLA	1	803	X	-	-	-
14	CLA	1	804	X	-	-	-
14	CLA	1	805	X	-	-	-
14	CLA	1	806	X	-	-	-
14	CLA	1	807	X	-	-	-
14	CLA	1	808	X	-	-	-
14	CLA	1	809	X	-	-	-
14	CLA	1	810	X	-	-	-
14	CLA	1	811	X	-	-	-
14	CLA	1	812	X	-	-	-
14	CLA	1	813	X	-	-	-
14	CLA	1	814	X	-	-	-
14	CLA	1	815	X	-	-	-
14	CLA	1	816	X	-	-	-
14	CLA	1	817	X	-	-	-
14	CLA	1	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	1	819	X	-	-	-
14	CLA	1	820	X	-	-	-
14	CLA	1	821	X	-	-	-
14	CLA	1	822	X	-	-	-
14	CLA	1	823	X	-	-	-
14	CLA	1	824	X	-	-	-
14	CLA	1	825	X	-	-	-
14	CLA	1	826	X	-	-	-
14	CLA	1	827	X	-	-	-
14	CLA	1	828	X	-	-	-
14	CLA	1	829	X	-	-	-
14	CLA	1	830	X	-	-	-
14	CLA	1	831	X	-	-	-
14	CLA	1	832	X	-	-	-
14	CLA	1	833	X	-	-	-
14	CLA	1	834	X	-	-	-
14	CLA	1	835	X	-	-	-
14	CLA	1	836	X	-	-	-
14	CLA	1	837	X	-	-	-
14	CLA	1	838	X	-	-	-
14	CLA	1	839	X	-	-	-
14	CLA	1	840	X	-	-	-
14	CLA	1	841	X	-	-	-
14	CLA	1	842	X	-	-	-
14	CLA	1	843	X	-	-	-
14	CLA	1	844	X	-	-	-
14	CLA	2	3003	X	-	-	-
14	CLA	2	3004	X	-	-	-
14	CLA	2	3005	X	-	-	-
14	CLA	2	3006	X	-	-	-
14	CLA	2	3007	X	-	-	-
14	CLA	2	3008	X	-	-	-
14	CLA	2	3009	X	-	-	-
14	CLA	2	3010	X	-	-	-
14	CLA	2	3011	X	-	-	-
14	CLA	2	3012	X	-	-	-
14	CLA	2	3014	X	-	-	-
14	CLA	2	3015	X	-	-	-
14	CLA	2	3016	X	-	-	-
14	CLA	2	3017	X	-	-	-
14	CLA	2	3019	X	-	-	-
14	CLA	2	3020	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	2	3021	X	-	-	-
14	CLA	2	3022	X	-	-	-
14	CLA	2	3023	X	-	-	-
14	CLA	2	3025	X	-	-	-
14	CLA	2	3026	X	-	-	-
14	CLA	2	3027	X	-	-	-
14	CLA	2	3028	X	-	-	-
14	CLA	2	3029	X	-	-	-
14	CLA	2	3030	X	-	-	-
14	CLA	2	3031	X	-	-	-
14	CLA	2	3032	X	-	-	-
14	CLA	2	3033	X	-	-	-
14	CLA	2	3034	X	-	-	-
14	CLA	2	3035	X	-	-	-
14	CLA	2	3036	X	-	-	-
14	CLA	2	3037	X	-	-	-
14	CLA	2	3038	X	-	-	-
14	CLA	2	3039	X	-	-	-
14	CLA	2	3041	X	-	-	-
14	CLA	2	3042	X	-	-	-
14	CLA	6	201	X	-	-	-
14	CLA	6	203	X	-	-	-
14	CLA	6	204	X	-	-	-
14	CLA	8	101	X	-	-	-
14	CLA	8	102	X	-	-	-
14	CLA	9	101	X	-	-	-
14	CLA	9	103	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	855	X	-	-	-
14	CLA	B	3003	X	-	-	-
14	CLA	B	3004	X	-	-	-
14	CLA	B	3005	X	-	-	-
14	CLA	B	3006	X	-	-	-
14	CLA	B	3007	X	-	-	-
14	CLA	B	3008	X	-	-	-
14	CLA	B	3009	X	-	-	-
14	CLA	B	3010	X	-	-	-
14	CLA	B	3011	X	-	-	-
14	CLA	B	3012	X	-	-	-
14	CLA	B	3014	X	-	-	-
14	CLA	B	3015	X	-	-	-
14	CLA	B	3016	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	3017	X	-	-	-
14	CLA	B	3019	X	-	-	-
14	CLA	B	3020	X	-	-	-
14	CLA	B	3021	X	-	-	-
14	CLA	B	3022	X	-	-	-
14	CLA	B	3023	X	-	-	-
14	CLA	B	3025	X	-	-	-
14	CLA	B	3026	X	-	-	-
14	CLA	B	3027	X	-	-	-
14	CLA	B	3028	X	-	-	-
14	CLA	B	3029	X	-	-	-
14	CLA	B	3030	X	-	-	-
14	CLA	B	3031	X	-	-	-
14	CLA	B	3032	X	-	-	-
14	CLA	B	3033	X	-	-	-
14	CLA	B	3034	X	-	-	-
14	CLA	B	3035	X	-	-	-
14	CLA	B	3036	X	-	-	-
14	CLA	B	3037	X	-	-	-
14	CLA	B	3038	X	-	-	-
14	CLA	B	3039	X	-	-	-
14	CLA	B	3041	X	-	-	-
14	CLA	B	3042	X	-	-	-
14	CLA	F	201	X	-	-	-
14	CLA	F	203	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	203	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	M	1601	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	802	X	-	-	-
14	CLA	a	803	X	-	-	-
14	CLA	a	804	X	-	-	-
14	CLA	a	805	X	-	-	-
14	CLA	a	806	X	-	-	-
14	CLA	a	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	808	X	-	-	-
14	CLA	a	809	X	-	-	-
14	CLA	a	810	X	-	-	-
14	CLA	a	811	X	-	-	-
14	CLA	a	812	X	-	-	-
14	CLA	a	813	X	-	-	-
14	CLA	a	814	X	-	-	-
14	CLA	a	815	X	-	-	-
14	CLA	a	816	X	-	-	-
14	CLA	a	817	X	-	-	-
14	CLA	a	818	X	-	-	-
14	CLA	a	819	X	-	-	-
14	CLA	a	820	X	-	-	-
14	CLA	a	821	X	-	-	-
14	CLA	a	822	X	-	-	-
14	CLA	a	823	X	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	X	-	-	-
14	CLA	a	826	X	-	-	-
14	CLA	a	827	X	-	-	-
14	CLA	a	828	X	-	-	-
14	CLA	a	829	X	-	-	-
14	CLA	a	830	X	-	-	-
14	CLA	a	831	X	-	-	-
14	CLA	a	832	X	-	-	-
14	CLA	a	833	X	-	-	-
14	CLA	a	834	X	-	-	-
14	CLA	a	835	X	-	-	-
14	CLA	a	836	X	-	-	-
14	CLA	a	837	X	-	-	-
14	CLA	a	838	X	-	-	-
14	CLA	a	839	X	-	-	-
14	CLA	a	840	X	-	-	-
14	CLA	a	841	X	-	-	-
14	CLA	a	842	X	-	-	-
14	CLA	a	843	X	-	-	-
14	CLA	b	3003	X	-	-	-
14	CLA	b	3004	X	-	-	-
14	CLA	b	3005	X	-	-	-
14	CLA	b	3006	X	-	-	-
14	CLA	b	3007	X	-	-	-
14	CLA	b	3008	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	3009	X	-	-	-
14	CLA	b	3010	X	-	-	-
14	CLA	b	3011	X	-	-	-
14	CLA	b	3012	X	-	-	-
14	CLA	b	3014	X	-	-	-
14	CLA	b	3015	X	-	-	-
14	CLA	b	3016	X	-	-	-
14	CLA	b	3017	X	-	-	-
14	CLA	b	3019	X	-	-	-
14	CLA	b	3020	X	-	-	-
14	CLA	b	3021	X	-	-	-
14	CLA	b	3022	X	-	-	-
14	CLA	b	3023	X	-	-	-
14	CLA	b	3025	X	-	-	-
14	CLA	b	3026	X	-	-	-
14	CLA	b	3027	X	-	-	-
14	CLA	b	3028	X	-	-	-
14	CLA	b	3029	X	-	-	-
14	CLA	b	3030	X	-	-	-
14	CLA	b	3031	X	-	-	-
14	CLA	b	3032	X	-	-	-
14	CLA	b	3033	X	-	-	-
14	CLA	b	3034	X	-	-	-
14	CLA	b	3035	X	-	-	-
14	CLA	b	3036	X	-	-	-
14	CLA	b	3037	X	-	-	-
14	CLA	b	3038	X	-	-	-
14	CLA	b	3039	X	-	-	-
14	CLA	b	3041	X	-	-	-
14	CLA	b	3042	X	-	-	-
14	CLA	f	201	X	-	-	-
14	CLA	f	203	X	-	-	-
14	CLA	f	204	X	-	-	-
14	CLA	j	1101	X	-	-	-
14	CLA	j	1102	X	-	-	-
14	CLA	j	1103	X	-	-	-
14	CLA	k	101	X	-	-	-
14	CLA	k	102	X	-	-	-
14	CLA	l	203	X	-	-	-
14	CLA	l	206	X	-	-	-
14	CLA	l	207	X	-	-	-
14	CLA	l	208	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	x	1701	X	-	-	-
14	CLA	z	1701	X	-	-	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 75591 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	a	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	1	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	b	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	2	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	4	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	70	Total	C	N	O		0	0
			546	347	94	105			
5	e	70	Total	C	N	O		0	0
			546	347	94	105			
5	5	70	Total	C	N	O		0	0
			546	347	94	105			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	f	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	6	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	i	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	7	38	Total	C	N	O	S	0	0
			303	209	40	49	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			340	232	51	55	2		
8	j	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	k	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	9	79	Total	C	N	O	S	0	0
			571	377	92	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	l	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	0	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4
l	143	LEU	SER	conflict	UNP Q8DGB4
0	143	LEU	SER	conflict	UNP Q8DGB4

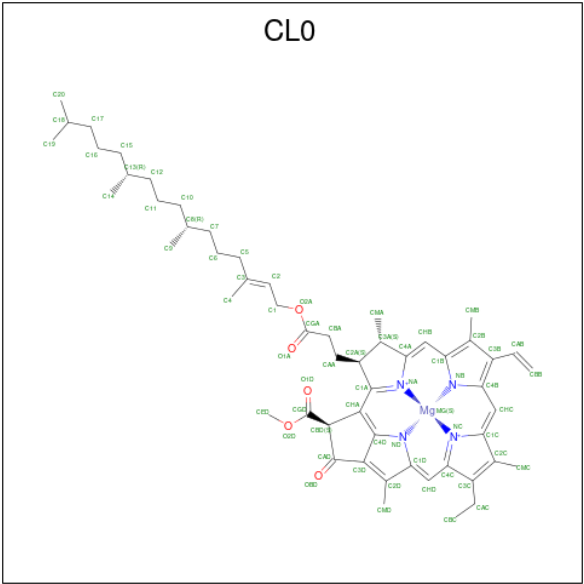
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	m	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	y	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I 4.8K protein.

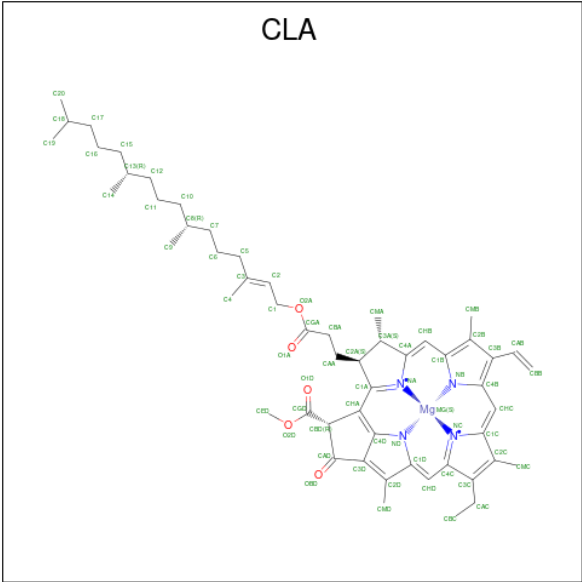
Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	27	Total	C	N	O	0	0
			228	163	33	32		
12	x	27	Total	C	N	O	0	0
			228	163	33	32		
12	z	27	Total	C	N	O	0	0
			228	163	33	32		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 36	C 30	Mg 1	N 4	O 1	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	M	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	k	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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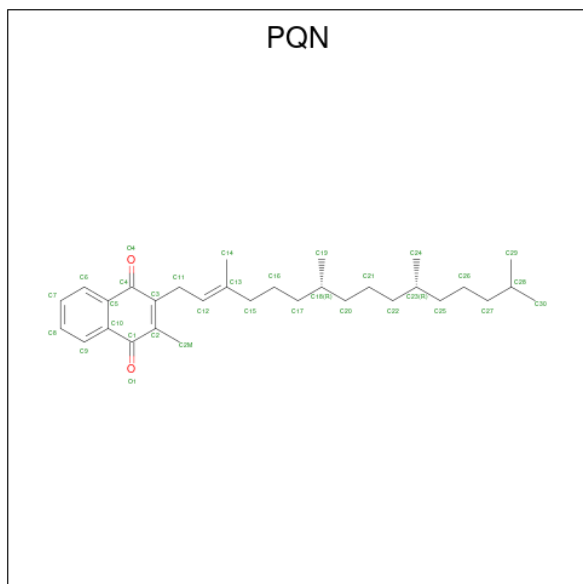
Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	8	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	9	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	0	1	Total 36	C 30	Mg 1	N 4	O 1	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0

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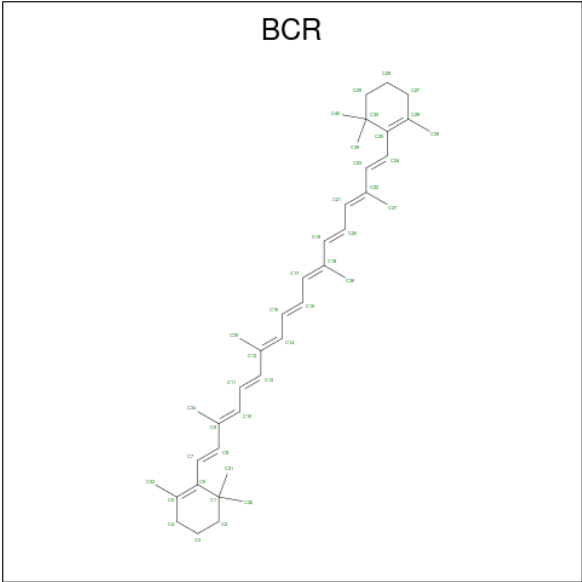
Mol	Chain	Residues	Atoms					AltConf
14	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	
15	1	1	Total	C	O	0
			33	31	2	
15	2	1	Total	C	O	0
			33	31	2	

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			25	25	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 25 25	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 25 25	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0

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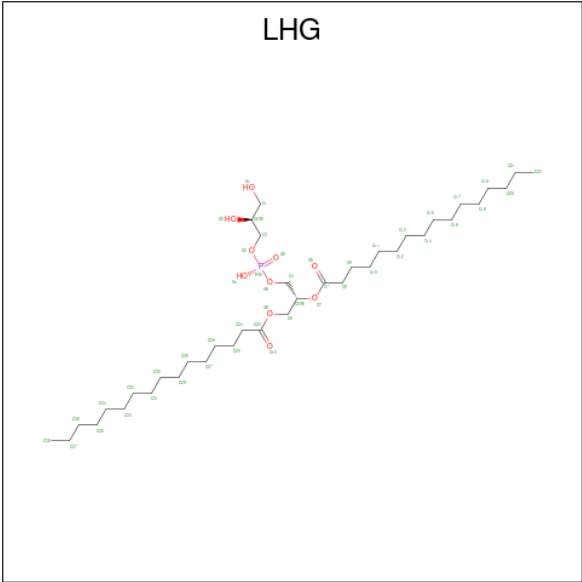
Mol	Chain	Residues	Atoms	AltConf
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	i	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 25 25	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	m	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 25 25	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	7	1	Total C 40 40	0
16	8	1	Total C 40 40	0
16	8	1	Total C 40 40	0
16	9	1	Total C 40 40	0
16	9	1	Total C 25 25	0
16	0	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	y	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



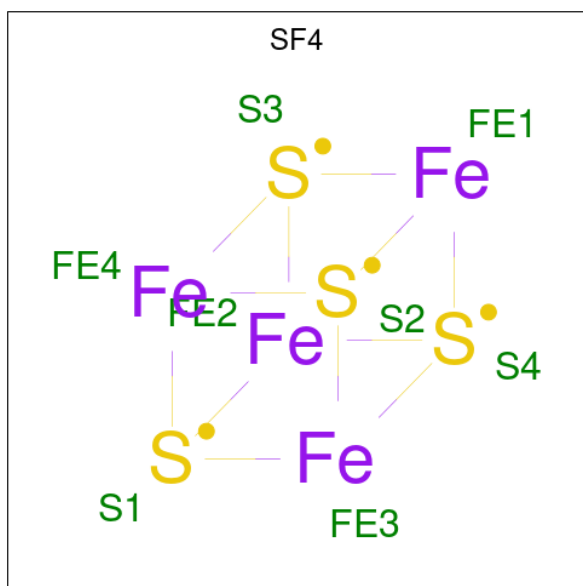
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	B	1	Total	C	O	P	0
			49	38	10	1	
17	L	1	Total	C	O	P	0
			49	38	10	1	
17	L	1	Total	C	O	P	0
			39	28	10	1	
17	a	1	Total	C	O	P	0
			49	38	10	1	
17	a	1	Total	C	O	P	0
			41	30	10	1	
17	b	1	Total	C	O	P	0
			49	38	10	1	
17	l	1	Total	C	O	P	0
			49	38	10	1	
17	l	1	Total	C	O	P	0
			39	28	10	1	
17	1	1	Total	C	O	P	0
			49	38	10	1	
17	1	1	Total	C	O	P	0
			41	30	10	1	
17	2	1	Total	C	O	P	0
			49	38	10	1	
17	0	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
17	0	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

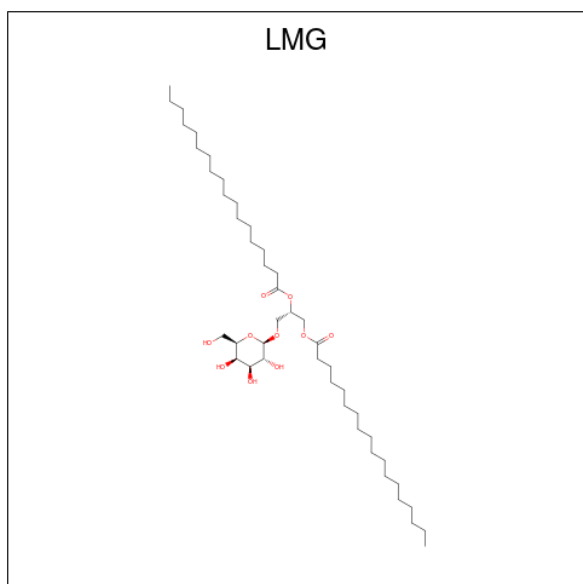


Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	b	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			8	4	4	
18	2	1	Total	Fe	S	0
			8	4	4	
18	3	1	Total	Fe	S	0
			8	4	4	
18	3	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total 1	Ca 1	0
19	L	1	Total 1	Ca 1	0
19	b	1	Total 1	Ca 1	0
19	1	1	Total 1	Ca 1	0
19	2	1	Total 1	Ca 1	0
19	0	1	Total 1	Ca 1	0

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total 55	C 45	O 10	0
20	b	1	Total 55	C 45	O 10	0
20	2	1	Total 55	C 45	O 10	0

- Molecule 21 is water.

Mol	Chain	Residues	Atoms	AltConf
21	A	65	Total O 65 65	0
21	B	77	Total O 77 77	0
21	C	28	Total O 28 28	0
21	D	22	Total O 22 22	0
21	E	7	Total O 7 7	0
21	F	4	Total O 4 4	0
21	I	1	Total O 1 1	0
21	J	1	Total O 1 1	0
21	K	1	Total O 1 1	0
21	L	10	Total O 10 10	0
21	M	1	Total O 1 1	0
21	a	65	Total O 65 65	0
21	b	74	Total O 74 74	0
21	c	28	Total O 28 28	0
21	d	19	Total O 19 19	0
21	e	9	Total O 9 9	0
21	f	5	Total O 5 5	0
21	i	2	Total O 2 2	0
21	j	1	Total O 1 1	0
21	k	1	Total O 1 1	0
21	l	11	Total O 11 11	0
21	m	2	Total O 2 2	0

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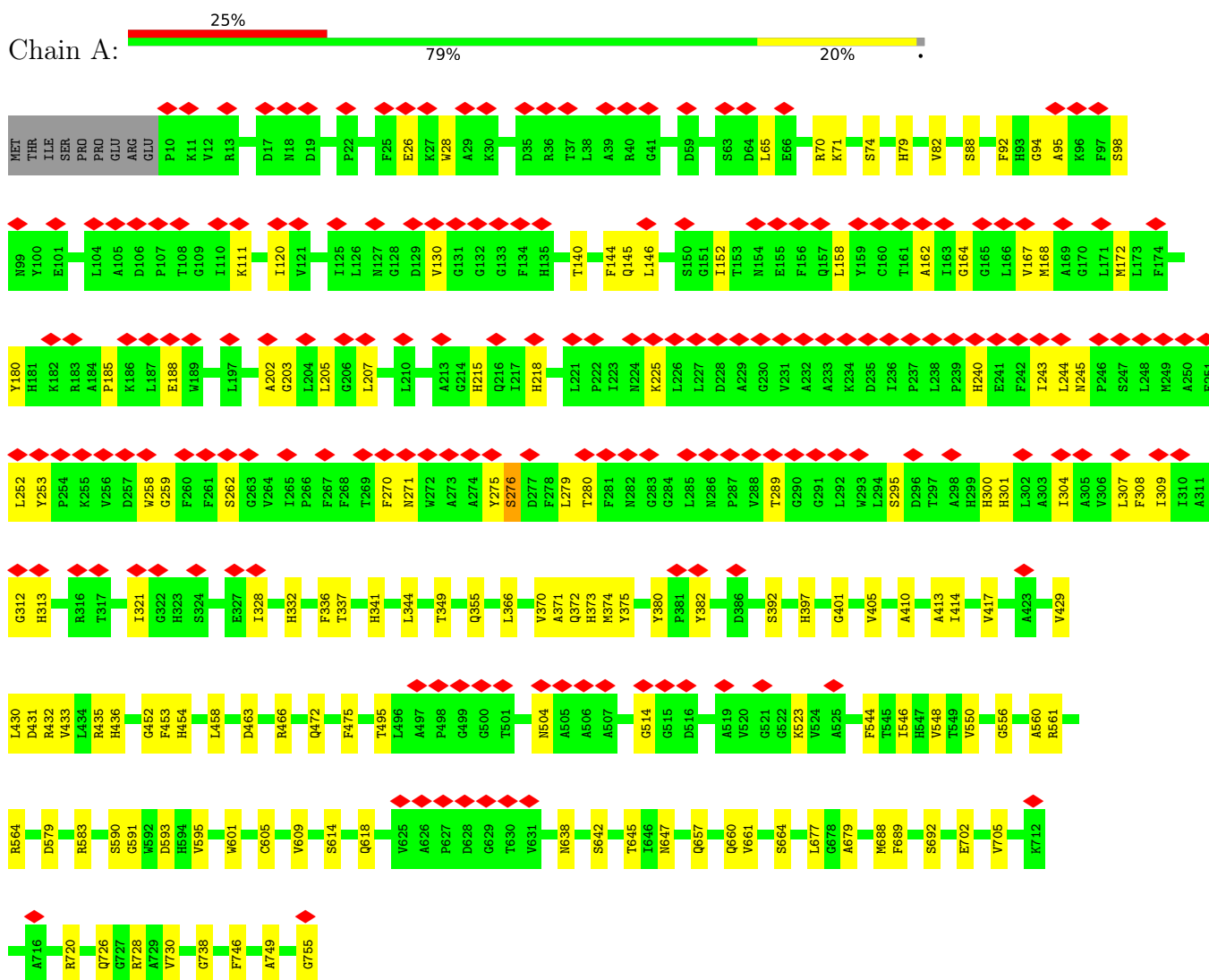
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Mol	Chain	Residues	Atoms		AltConf
21	1	65	Total 65	O 65	0
21	2	75	Total 75	O 75	0
21	3	27	Total 27	O 27	0
21	4	22	Total 22	O 22	0
21	5	8	Total 8	O 8	0
21	6	4	Total 4	O 4	0
21	7	2	Total 2	O 2	0
21	8	1	Total 1	O 1	0
21	9	1	Total 1	O 1	0
21	0	10	Total 10	O 10	0
21	y	2	Total 2	O 2	0

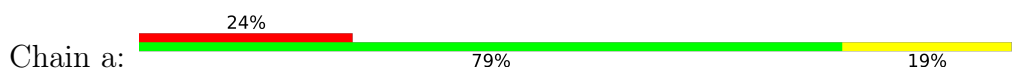
3 Residue-property plots

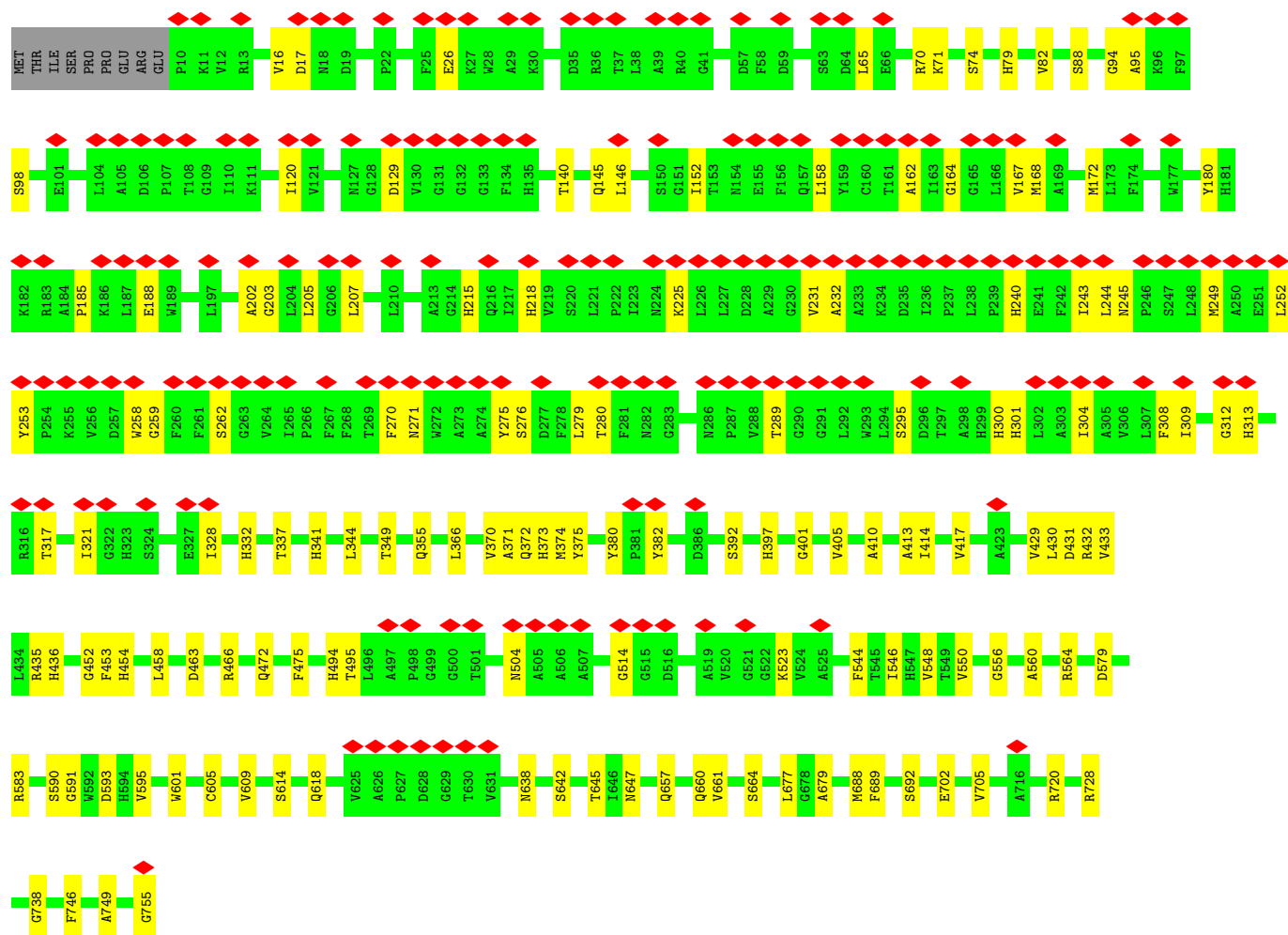
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

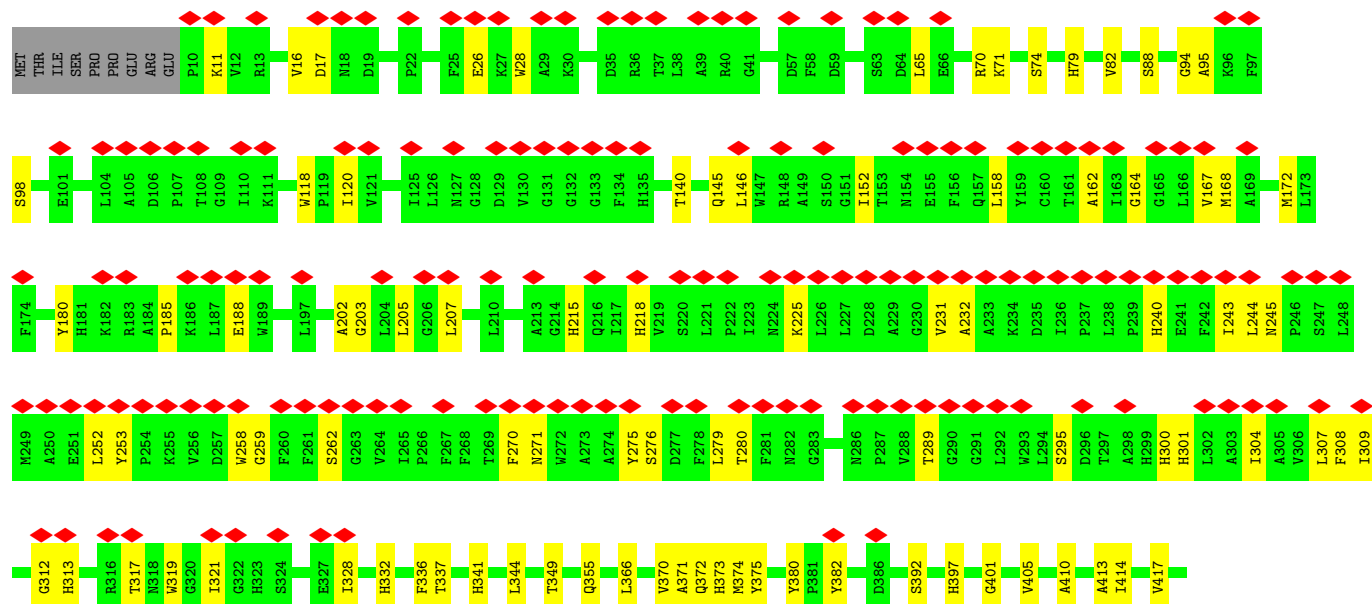
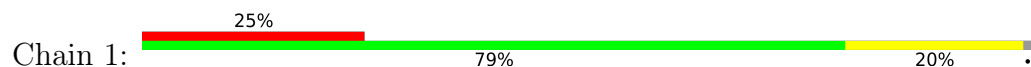


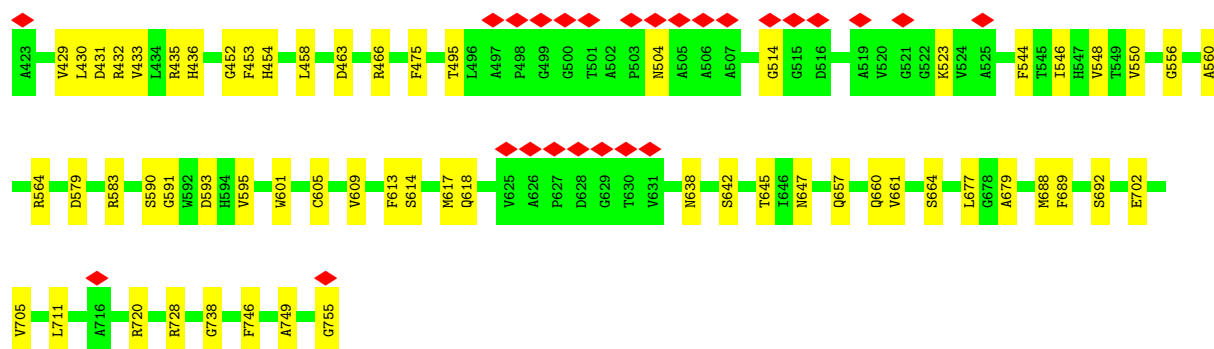
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



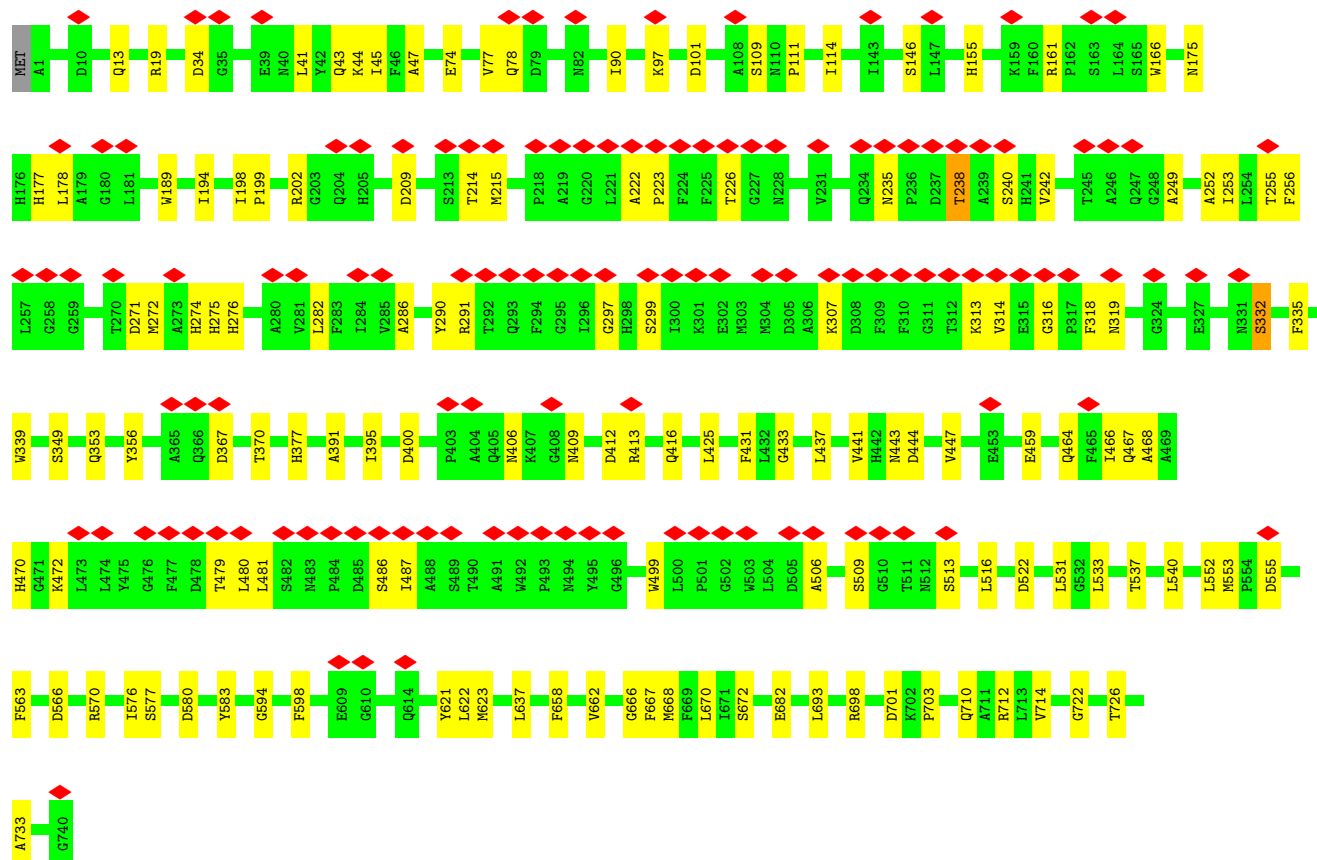
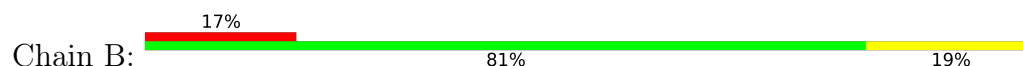


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

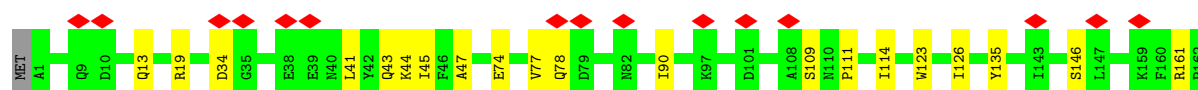
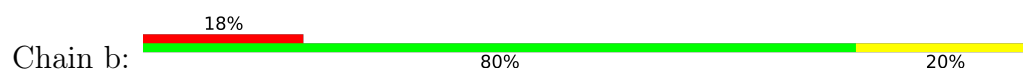


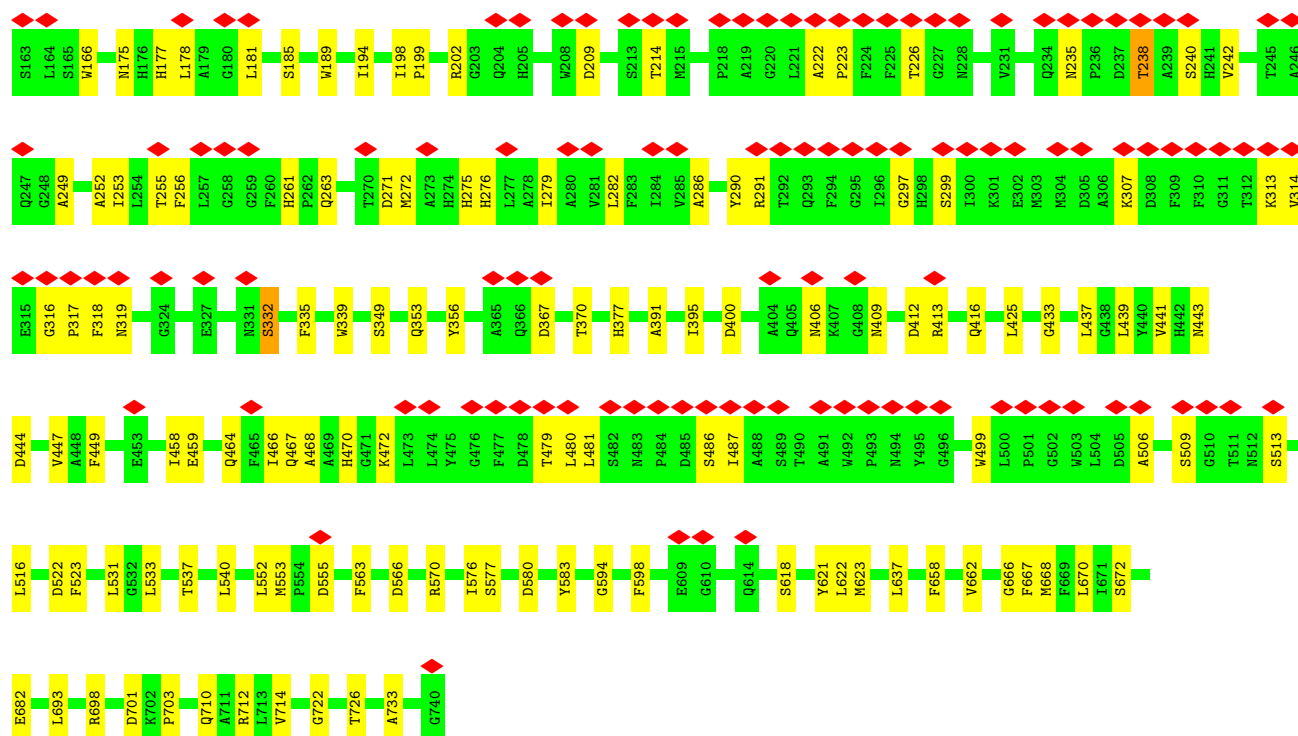


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

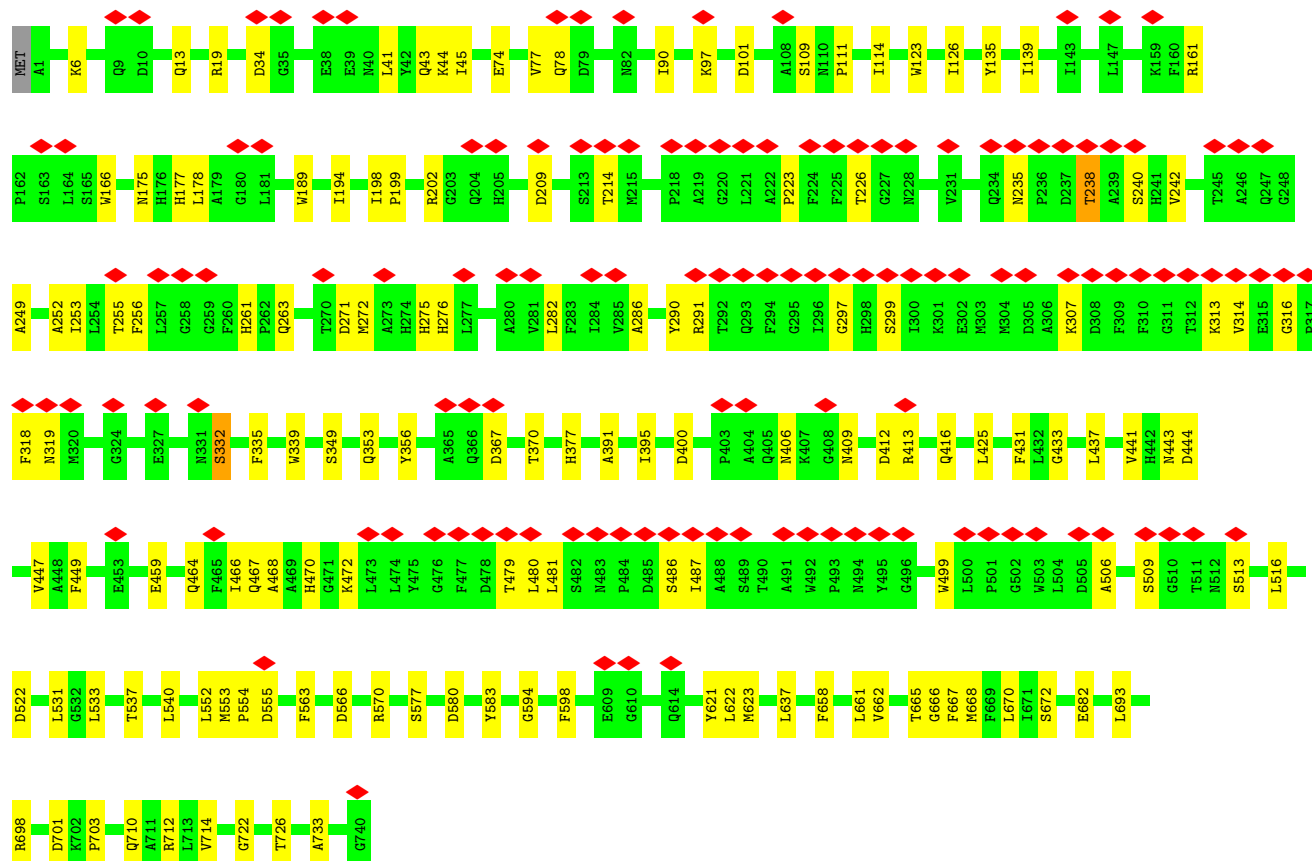
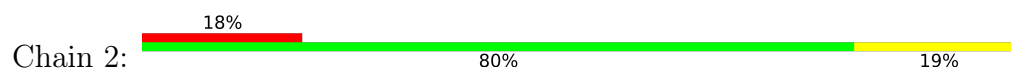


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



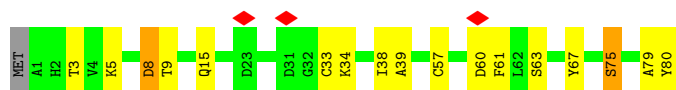


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



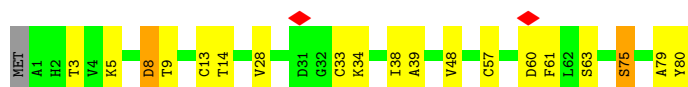
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  78% 19% ..



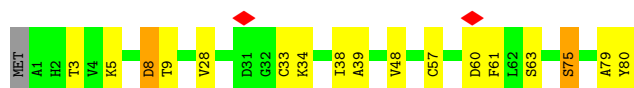
- Molecule 3: Photosystem I iron-sulfur center

Chain c:  75% 21% ..



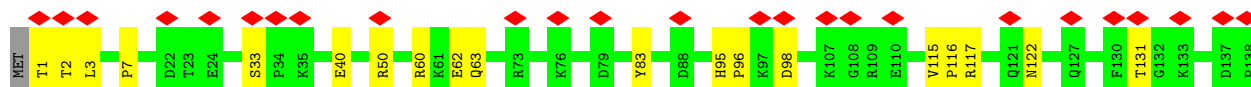
- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  78% 19% ..



- Molecule 4: Photosystem I reaction center subunit II

Chain D:  18% 86% 14% .



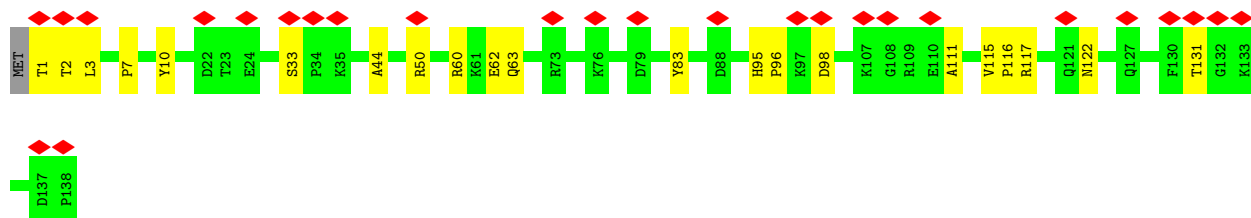
- Molecule 4: Photosystem I reaction center subunit II

Chain d:  18% 86% 13% .

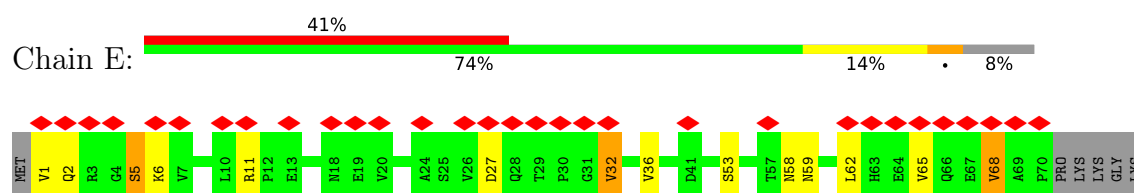


- Molecule 4: Photosystem I reaction center subunit II

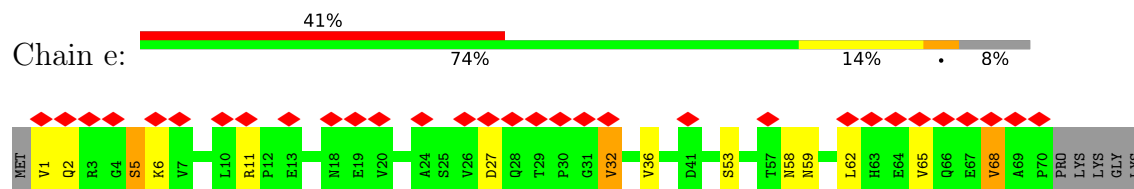
Chain 4:  19% 84% 15% .



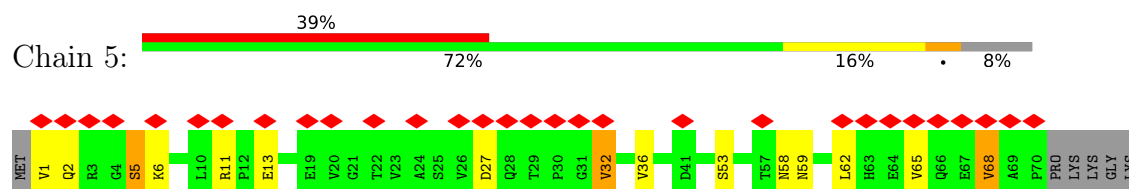
- Molecule 5: Photosystem I reaction center subunit IV



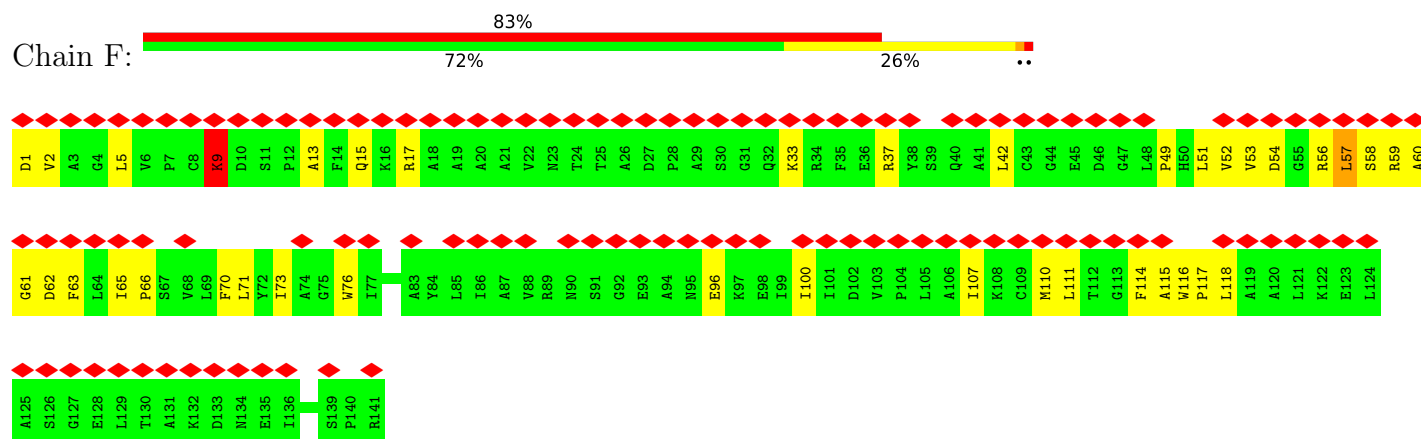
- Molecule 5: Photosystem I reaction center subunit IV



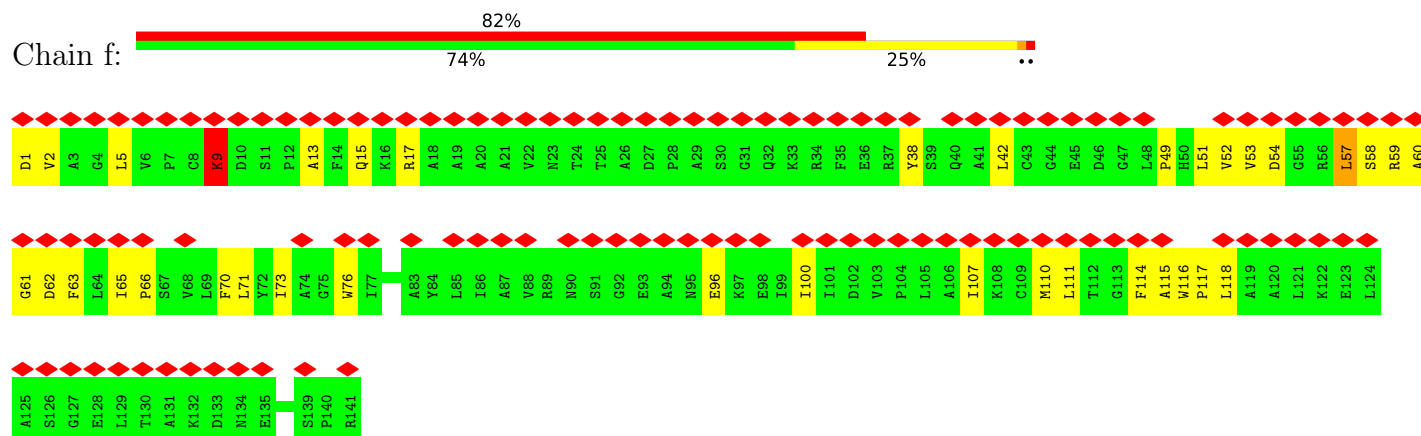
- Molecule 5: Photosystem I reaction center subunit IV



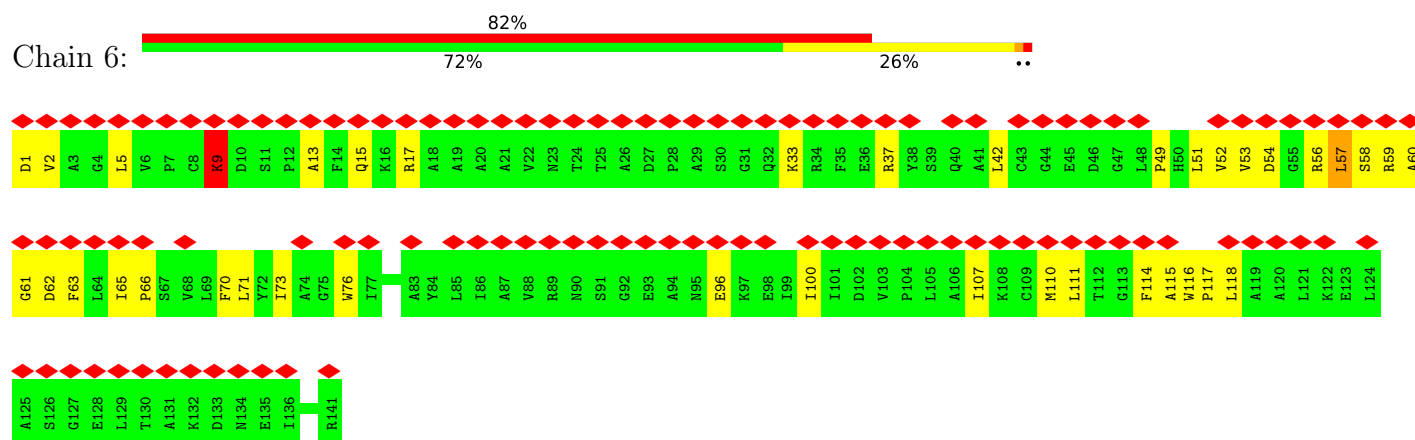
- Molecule 6: Photosystem I reaction center subunit III



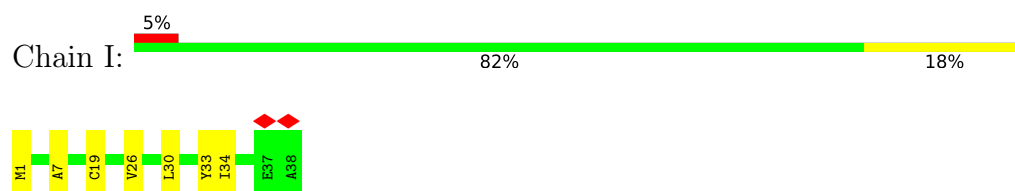
- Molecule 6: Photosystem I reaction center subunit III



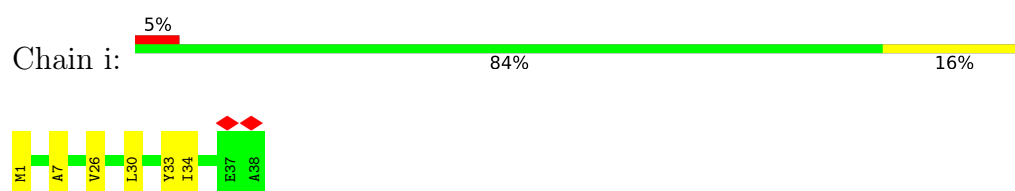
- Molecule 6: Photosystem I reaction center subunit III



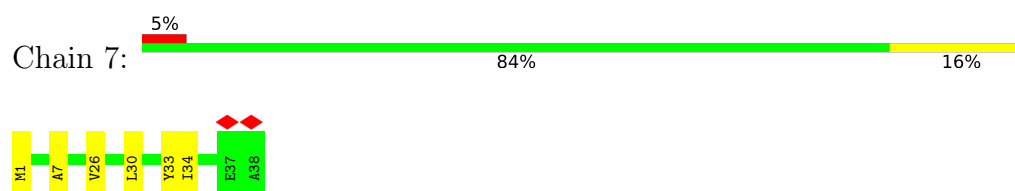
- Molecule 7: Photosystem I reaction center subunit VIII



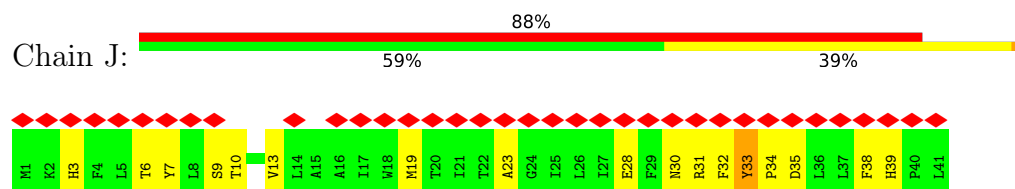
- Molecule 7: Photosystem I reaction center subunit VIII



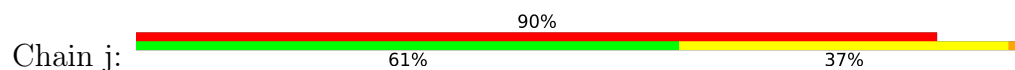
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX

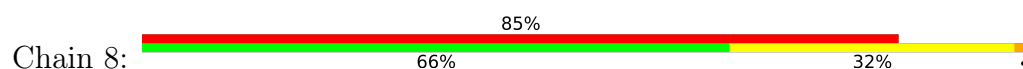


- Molecule 8: Photosystem I reaction center subunit IX

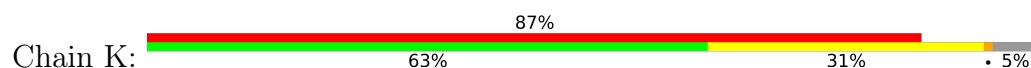




• Molecule 8: Photosystem I reaction center subunit IX



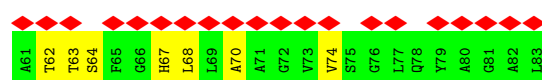
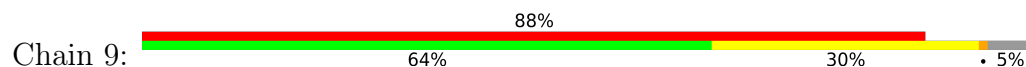
• Molecule 9: Photosystem I reaction center subunit PsaK



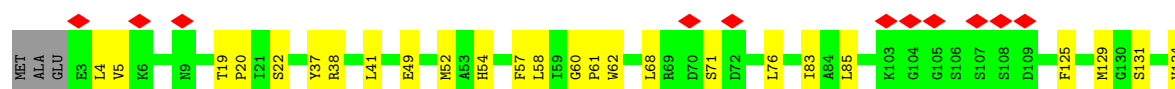
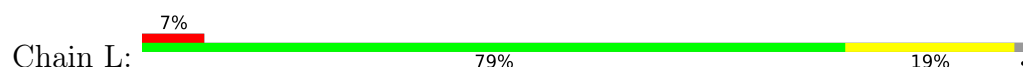
• Molecule 9: Photosystem I reaction center subunit PsaK



• Molecule 9: Photosystem I reaction center subunit PsaK

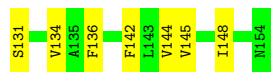
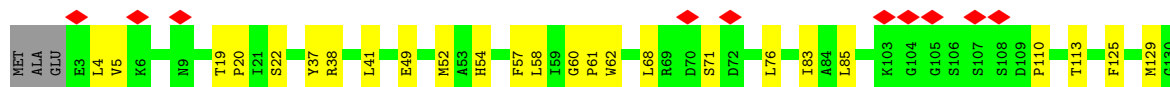
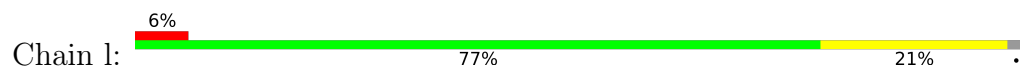


• Molecule 10: Photosystem I reaction center subunit XI

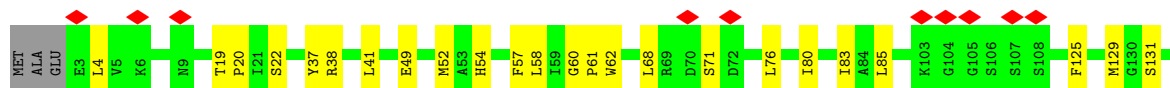




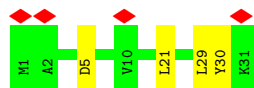
- Molecule 10: Photosystem I reaction center subunit XI



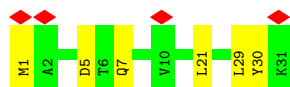
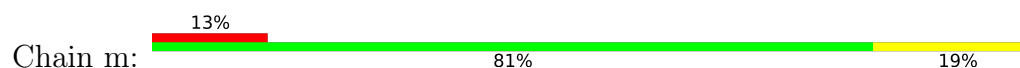
- Molecule 10: Photosystem I reaction center subunit XI



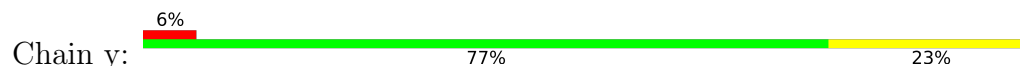
- Molecule 11: Photosystem I reaction center subunit XII



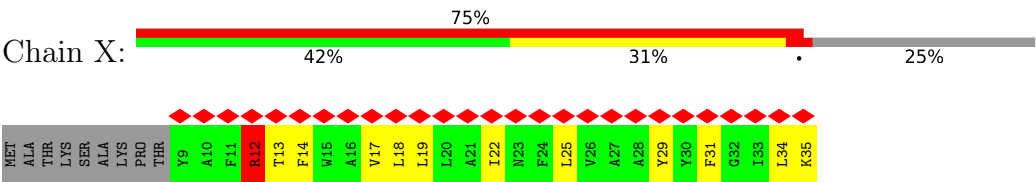
- Molecule 11: Photosystem I reaction center subunit XII



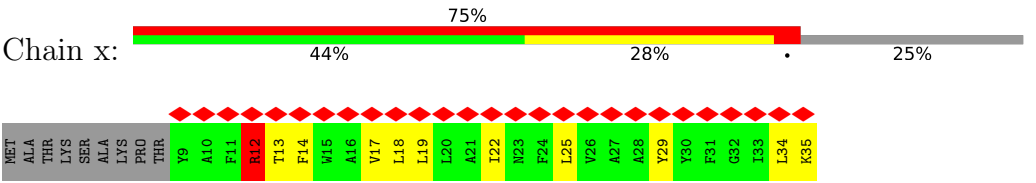
- Molecule 11: Photosystem I reaction center subunit XII



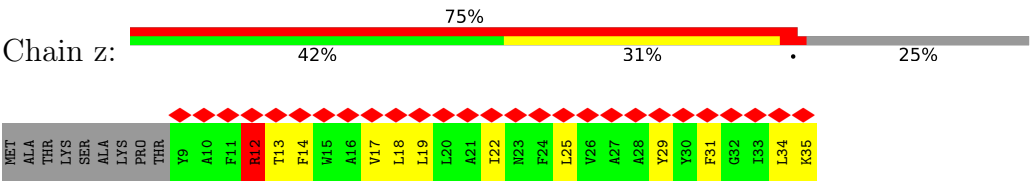
- Molecule 12: Photosystem I 4.8K protein



• Molecule 12: Photosystem I 4.8K protein



• Molecule 12: Photosystem I 4.8K protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	351.68002, 351.68002, 351.68002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.628, 0.628, 0.628	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, LMG, CLA, BCR, LHG, PQN, FME, CL0, SF4

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	1	0.37	0/6027	0.45	0/8220
1	A	0.37	0/6027	0.45	0/8220
1	a	0.37	0/6027	0.45	0/8220
2	2	0.38	0/6112	0.45	0/8350
2	B	0.38	0/6112	0.45	0/8350
2	b	0.38	0/6112	0.45	0/8350
3	3	0.42	0/608	0.52	0/824
3	C	0.42	0/608	0.53	0/824
3	c	0.42	0/608	0.52	0/824
4	4	0.36	0/1101	0.44	0/1492
4	D	0.36	0/1101	0.44	0/1492
4	d	0.36	0/1101	0.44	0/1492
5	5	0.27	0/559	0.39	0/762
5	E	0.27	0/559	0.39	0/762
5	e	0.27	0/559	0.39	0/762
6	6	0.25	0/1087	0.53	1/1476 (0.1%)
6	F	0.25	0/1087	0.53	1/1476 (0.1%)
6	f	0.25	0/1087	0.53	1/1476 (0.1%)
7	7	0.39	0/304	0.42	0/415
7	I	0.39	0/304	0.42	0/415
7	i	0.39	0/304	0.42	0/415
8	8	0.30	0/342	0.49	0/467
8	J	0.30	0/342	0.49	0/467
8	j	0.30	0/342	0.49	0/467
9	9	0.22	0/585	0.56	0/800
9	K	0.23	0/585	0.56	0/800
9	k	0.22	0/585	0.56	0/800
10	0	0.41	0/1153	0.43	0/1565
10	L	0.41	0/1153	0.43	0/1565
10	l	0.41	0/1153	0.43	0/1565
11	M	0.35	0/244	0.41	0/332
11	m	0.35	0/244	0.41	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	y	0.35	0/244	0.41	0/332
12	X	0.29	0/236	0.82	1/321 (0.3%)
12	x	0.28	0/236	0.82	1/321 (0.3%)
12	z	0.29	0/236	0.82	1/321 (0.3%)
All	All	0.36	0/55074	0.46	6/75072 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	B	0	1
2	b	0	1
6	6	0	1
6	F	0	1
6	f	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	9	LYS	CD-CE-NZ	5.22	128.60	111.90
6	f	9	LYS	CD-CE-NZ	5.21	128.58	111.90
6	6	9	LYS	CD-CE-NZ	5.20	128.55	111.90
12	x	12	ARG	CA-CB-CG	5.20	124.50	114.10
12	z	12	ARG	CA-CB-CG	5.20	124.50	114.10
12	X	12	ARG	CA-CB-CG	5.17	124.45	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	479	THR	Peptide
6	6	57	LEU	Peptide
2	B	479	THR	Peptide
6	F	57	LEU	Peptide
2	b	479	THR	Peptide
6	f	57	LEU	Peptide

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	1	5826	0	5692	119	0
1	A	5826	0	5692	122	0
1	a	5826	0	5692	117	0
2	2	5894	0	5653	113	0
2	B	5894	0	5653	110	0
2	b	5894	0	5653	123	0
3	3	598	0	580	17	0
3	C	598	0	580	17	0
3	c	598	0	580	18	0
4	4	1075	0	1077	18	0
4	D	1075	0	1077	16	0
4	d	1075	0	1077	16	0
5	5	546	0	535	11	0
5	E	546	0	535	10	0
5	e	546	0	535	9	0
6	6	1065	0	1077	31	0
6	F	1065	0	1077	32	0
6	f	1065	0	1077	28	0
7	7	303	0	305	4	0
7	I	303	0	305	5	0
7	i	303	0	305	4	0
8	8	340	0	346	11	0
8	J	340	0	346	16	0
8	j	340	0	346	16	0
9	9	571	0	593	23	0
9	K	571	0	593	25	0
9	k	571	0	593	23	0
10	0	1124	0	1127	22	0
10	L	1124	0	1127	22	0
10	l	1124	0	1127	23	0
11	M	241	0	264	6	0
11	m	241	0	264	7	0
11	y	241	0	264	11	0
12	X	228	0	234	18	0
12	x	228	0	234	14	0
12	z	228	0	234	15	0
13	1	65	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	65	0	72	1	0
13	a	65	0	72	1	0
14	0	296	0	312	6	0
14	1	2674	0	2849	55	0
14	2	2446	0	2562	73	0
14	6	153	0	127	6	0
14	8	82	0	58	0	0
14	9	104	0	88	0	0
14	A	2710	0	2873	53	0
14	B	2446	0	2562	71	0
14	F	153	0	127	7	0
14	J	82	0	58	0	0
14	K	104	0	88	2	0
14	L	260	0	288	7	0
14	M	36	0	24	0	0
14	X	45	0	33	0	0
14	a	2609	0	2777	54	0
14	b	2446	0	2562	69	0
14	f	153	0	127	7	0
14	j	147	0	130	4	0
14	k	104	0	88	0	0
14	l	260	0	288	5	0
14	x	45	0	33	0	0
14	z	45	0	33	2	0
15	1	33	0	46	1	0
15	2	33	0	46	0	0
15	A	33	0	46	1	0
15	B	33	0	46	0	0
15	a	33	0	46	3	0
15	b	33	0	46	0	0
16	0	120	0	168	1	0
16	1	225	0	313	11	0
16	2	280	0	392	11	0
16	6	80	0	112	0	0
16	7	40	0	56	0	0
16	8	80	0	112	6	0
16	9	65	0	89	3	0
16	A	265	0	369	13	0
16	B	320	0	448	10	0
16	F	80	0	112	0	0
16	I	80	0	112	1	0
16	J	80	0	112	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	25	0	33	2	0
16	L	40	0	56	0	0
16	M	40	0	56	1	0
16	a	265	0	369	12	0
16	b	240	0	336	8	0
16	f	80	0	112	0	0
16	i	40	0	56	0	0
16	j	120	0	168	13	0
16	k	25	0	33	2	0
16	l	120	0	168	1	0
16	m	40	0	56	1	0
16	y	40	0	56	4	0
17	0	88	0	125	1	0
17	1	90	0	129	2	0
17	2	49	0	74	3	0
17	A	90	0	129	2	0
17	B	49	0	74	5	0
17	L	88	0	125	2	0
17	a	90	0	129	2	0
17	b	49	0	74	3	0
17	l	88	0	125	2	0
18	2	8	0	0	0	0
18	3	16	0	0	0	0
18	B	8	0	0	0	0
18	C	16	0	0	0	0
18	b	8	0	0	0	0
18	c	16	0	0	0	0
19	0	1	0	0	0	0
19	2	1	0	0	0	0
19	B	1	0	0	0	0
19	L	1	0	0	0	0
19	b	1	0	0	0	0
19	l	1	0	0	0	0
20	2	55	0	86	1	0
20	B	55	0	86	0	0
20	b	55	0	86	0	0
21	0	10	0	0	0	0
21	1	65	0	0	12	0
21	2	75	0	0	11	0
21	3	27	0	0	4	0
21	4	22	0	0	2	0
21	5	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	6	4	0	0	0	0
21	7	2	0	0	0	0
21	8	1	0	0	0	0
21	9	1	0	0	0	0
21	A	65	0	0	14	0
21	B	77	0	0	11	0
21	C	28	0	0	4	0
21	D	22	0	0	2	0
21	E	7	0	0	0	0
21	F	4	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	10	0	0	0	0
21	M	1	0	0	0	0
21	a	65	0	0	14	0
21	b	74	0	0	9	0
21	c	28	0	0	4	0
21	d	19	0	0	1	0
21	e	9	0	0	0	0
21	f	5	0	0	0	0
21	i	2	0	0	0	0
21	j	1	0	0	0	0
21	k	1	0	0	0	0
21	l	11	0	0	0	0
21	m	2	0	0	0	0
21	y	2	0	0	0	0
All	All	75591	0	76164	1368	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 9.

All (1368) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:33:SER:OG	4:4:50:ARG:O	1.83	0.96
4:D:33:SER:OG	4:D:50:ARG:O	1.83	0.96
4:d:33:SER:OG	4:d:50:ARG:O	1.83	0.95
1:1:657:GLN:O	21:1:901:HOH:O	1.88	0.92
1:A:657:GLN:O	21:A:901:HOH:O	1.88	0.92
1:a:657:GLN:O	21:a:901:HOH:O	1.88	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:9:LYS:O	6:6:15:GLN:NE2	2.05	0.89
6:f:9:LYS:O	6:f:15:GLN:NE2	2.05	0.89
6:F:9:LYS:O	6:F:15:GLN:NE2	2.05	0.89
7:I:33:TYR:OH	11:M:30:TYR:OH	1.90	0.87
1:A:259:GLY:N	1:A:262:SER:OG	2.09	0.86
1:1:259:GLY:N	1:1:262:SER:OG	2.09	0.86
2:b:406:ASN:ND2	21:b:3105:HOH:O	2.08	0.86
1:A:657:GLN:OE1	21:A:902:HOH:O	1.94	0.86
2:B:555:ASP:OD1	21:B:3101:HOH:O	1.94	0.85
2:2:406:ASN:ND2	21:2:3105:HOH:O	2.08	0.85
2:b:555:ASP:OD1	21:b:3101:HOH:O	1.92	0.85
4:4:60:ARG:NH2	4:4:62:GLU:OE1	2.10	0.85
2:B:406:ASN:ND2	21:B:3106:HOH:O	2.09	0.85
2:2:555:ASP:OD1	21:2:3101:HOH:O	1.94	0.85
2:2:74:GLU:OE1	11:y:1:MET:N	2.10	0.85
1:a:259:GLY:N	1:a:262:SER:OG	2.09	0.85
4:d:95:HIS:O	21:d:201:HOH:O	1.94	0.84
2:2:577:SER:OG	2:2:580:ASP:OD2	1.95	0.84
4:D:60:ARG:NH2	4:D:62:GLU:OE1	2.10	0.84
4:d:60:ARG:NH2	4:d:62:GLU:OE1	2.10	0.84
1:1:657:GLN:OE1	21:1:902:HOH:O	1.94	0.84
4:D:95:HIS:O	21:D:201:HOH:O	1.94	0.84
1:a:657:GLN:OE1	21:a:902:HOH:O	1.94	0.84
17:2:3051:LHG:O5	12:z:12:ARG:NH2	2.11	0.84
1:A:688:MET:O	1:A:692:SER:OG	1.96	0.83
2:b:577:SER:OG	2:b:580:ASP:OD2	1.95	0.83
2:2:367:ASP:OD2	2:2:370:THR:OG1	1.96	0.83
1:a:688:MET:O	1:a:692:SER:OG	1.97	0.83
2:B:367:ASP:OD2	2:B:370:THR:OG1	1.96	0.83
4:4:95:HIS:O	21:4:201:HOH:O	1.95	0.82
2:B:577:SER:OG	2:B:580:ASP:OD2	1.95	0.82
1:1:688:MET:O	1:1:692:SER:OG	1.96	0.82
2:b:367:ASP:OD2	2:b:370:THR:OG1	1.96	0.82
1:1:94:GLY:O	1:1:98:SER:OG	1.99	0.81
1:A:94:GLY:O	1:A:98:SER:OG	1.99	0.81
1:a:94:GLY:O	1:a:98:SER:OG	1.99	0.80
1:A:523:LYS:NZ	1:A:755:GLY:O	2.14	0.80
1:a:523:LYS:NZ	1:a:755:GLY:O	2.14	0.80
14:2:3034:CLA:O1A	8:8:30:ASN:ND2	2.14	0.80
14:B:3034:CLA:O1A	8:J:30:ASN:ND2	2.14	0.79
3:C:80:TYR:O	21:C:201:HOH:O	1.99	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:523:LYS:NZ	1:1:755:GLY:O	2.14	0.79
3:c:80:TYR:O	21:c:201:HOH:O	2.01	0.78
3:c:57:CYS:O	21:c:202:HOH:O	2.02	0.78
3:3:80:TYR:O	21:3:201:HOH:O	2.00	0.77
14:B:3033:CLA:HBC2	14:B:3033:CLA:HHD	1.66	0.77
14:2:3033:CLA:HHD	14:2:3033:CLA:HBC2	1.66	0.77
3:C:60:ASP:OD2	5:E:11:ARG:NH1	2.18	0.77
14:b:3033:CLA:HBC2	14:b:3033:CLA:HHD	1.67	0.77
1:a:120:ILE:O	21:a:903:HOH:O	2.03	0.76
3:3:57:CYS:O	21:3:202:HOH:O	2.02	0.76
1:A:702:GLU:OE1	21:A:903:HOH:O	2.04	0.76
17:B:3051:LHG:O5	12:X:12:ARG:NH2	2.19	0.76
1:1:702:GLU:OE1	21:1:903:HOH:O	2.03	0.76
3:C:57:CYS:O	21:C:202:HOH:O	2.02	0.76
2:B:400:ASP:OD2	21:B:3102:HOH:O	2.04	0.75
2:2:522:ASP:OD1	21:2:3102:HOH:O	2.03	0.75
1:a:579:ASP:O	21:a:904:HOH:O	2.04	0.75
3:3:60:ASP:OD2	5:5:11:ARG:NH1	2.19	0.75
2:B:522:ASP:OD1	21:B:3103:HOH:O	2.05	0.75
1:a:702:GLU:OE1	21:a:905:HOH:O	2.04	0.74
17:a:852:LHG:O5	21:a:906:HOH:O	2.05	0.74
14:b:3005:CLA:HBC3	14:b:3005:CLA:HHD	1.69	0.74
14:2:3005:CLA:HBC3	14:2:3005:CLA:HHD	1.69	0.74
2:b:413:ARG:NE	14:b:3031:CLA:OBD	2.21	0.74
1:a:647:ASN:OD1	21:a:907:HOH:O	2.05	0.74
2:b:291:ARG:NH2	2:b:297:GLY:O	2.21	0.74
17:A:853:LHG:O5	21:A:904:HOH:O	2.05	0.73
2:b:682:GLU:OE2	21:b:3104:HOH:O	2.07	0.73
2:B:291:ARG:NH2	2:B:297:GLY:O	2.21	0.73
2:2:413:ARG:NE	14:2:3031:CLA:OBD	2.21	0.73
1:A:647:ASN:OD1	21:A:905:HOH:O	2.05	0.73
2:b:522:ASP:OD1	21:b:3102:HOH:O	2.05	0.73
1:1:120:ILE:O	21:1:904:HOH:O	2.05	0.73
2:b:400:ASP:OD2	21:b:3103:HOH:O	2.06	0.73
6:6:61:GLY:O	8:8:39:HIS:N	2.20	0.73
1:A:720:ARG:O	21:A:906:HOH:O	2.06	0.73
2:B:413:ARG:NE	14:B:3031:CLA:OBD	2.21	0.73
1:1:720:ARG:O	21:1:905:HOH:O	2.06	0.73
12:z:34:LEU:HG	12:z:35:LYS:H	1.54	0.73
14:B:3005:CLA:HBC3	14:B:3005:CLA:HHD	1.69	0.73
2:2:291:ARG:NH2	2:2:297:GLY:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:GLN:OE1	21:B:3104:HOH:O	2.07	0.72
2:2:400:ASP:OD2	21:2:3103:HOH:O	2.06	0.72
2:B:682:GLU:OE2	21:B:3105:HOH:O	2.08	0.72
12:x:34:LEU:HG	12:x:35:LYS:H	1.54	0.71
2:2:566:ASP:OD2	2:2:570:ARG:NH2	2.24	0.71
2:b:566:ASP:OD2	2:b:570:ARG:NH2	2.24	0.71
17:1:852:LHG:O5	21:1:906:HOH:O	2.08	0.71
1:A:120:ILE:O	21:A:907:HOH:O	2.08	0.71
12:X:34:LEU:HG	12:X:35:LYS:H	1.54	0.71
2:2:682:GLU:OE2	21:2:3104:HOH:O	2.07	0.71
2:B:566:ASP:OD2	2:B:570:ARG:NH2	2.24	0.71
2:B:316:GLY:O	2:B:319:ASN:N	2.24	0.70
1:a:494:HIS:O	21:a:908:HOH:O	2.09	0.70
2:2:316:GLY:O	2:2:319:ASN:N	2.24	0.70
2:b:316:GLY:O	2:b:319:ASN:N	2.24	0.70
1:A:472:GLN:OE1	21:A:908:HOH:O	2.08	0.70
7:i:33:TYR:OH	11:m:30:TYR:OH	1.98	0.69
9:9:43:LEU:HG	9:9:47:LEU:HD13	1.75	0.69
14:1:802:CLA:O1A	2:2:531:LEU:HD11	1.92	0.69
1:a:720:ARG:O	21:a:909:HOH:O	2.10	0.69
2:2:13:GLN:OE1	21:2:3106:HOH:O	2.10	0.69
9:K:43:LEU:HG	9:K:47:LEU:HD13	1.75	0.69
2:B:698:ARG:NH1	21:B:3112:HOH:O	2.26	0.68
2:2:698:ARG:NH1	21:2:3110:HOH:O	2.25	0.68
14:B:3038:CLA:H141	12:X:19:LEU:HD13	1.76	0.68
2:B:459:GLU:OE1	2:B:464:GLN:NE2	2.27	0.68
2:b:13:GLN:OE1	21:b:3106:HOH:O	2.11	0.68
1:1:689:PHE:O	21:1:907:HOH:O	2.10	0.68
2:B:540:LEU:O	21:B:3107:HOH:O	2.11	0.67
16:I:102:BCR:H403	16:I:102:BCR:H23C	1.77	0.67
1:A:243:ILE:HB	14:A:817:CLA:HBC2	1.77	0.67
14:A:802:CLA:O1A	2:B:531:LEU:HD11	1.93	0.67
16:0:210:BCR:H403	16:0:210:BCR:H23C	1.77	0.67
1:a:259:GLY:N	1:a:262:SER:HG	1.91	0.67
1:1:243:ILE:HB	14:1:817:CLA:HBC2	1.77	0.67
3:3:48:VAL:O	21:3:203:HOH:O	2.12	0.67
14:B:3003:CLA:H201	16:J:103:BCR:H362	1.76	0.67
1:a:243:ILE:HB	14:a:816:CLA:HBC2	1.77	0.67
10:l:38:ARG:NH2	10:l:49:GLU:OE1	2.28	0.67
9:k:43:LEU:HG	9:k:47:LEU:HD13	1.75	0.66
2:2:459:GLU:OE1	2:2:464:GLN:NE2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:NH2	2:B:701:ASP:OD2	2.29	0.66
14:a:802:CLA:O1A	2:b:531:LEU:HD11	1.95	0.66
2:b:698:ARG:NH1	21:b:3111:HOH:O	2.29	0.66
10:0:38:ARG:NH2	10:0:49:GLU:OE1	2.28	0.66
2:b:449:PHE:O	21:b:3107:HOH:O	2.14	0.66
16:l:209:BCR:H403	16:l:209:BCR:H23C	1.77	0.66
1:1:647:ASN:OD1	21:1:908:HOH:O	2.13	0.66
1:1:660:GLN:O	1:1:664:SER:OG	2.12	0.66
2:2:19:ARG:NH2	2:2:701:ASP:OD2	2.29	0.66
1:A:270:PHE:CD2	9:K:74:VAL:HG21	2.30	0.66
2:B:43:GLN:OE1	2:B:161:ARG:NH2	2.29	0.66
3:c:48:VAL:O	21:c:203:HOH:O	2.13	0.66
2:b:43:GLN:OE1	2:b:161:ARG:NH2	2.29	0.66
3:C:8:ASP:OD1	4:D:116:PRO:HA	1.96	0.65
1:A:660:GLN:O	1:A:664:SER:OG	2.12	0.65
2:b:413:ARG:NH2	14:b:3031:CLA:OBD	2.29	0.65
14:b:3034:CLA:O1A	8:j:30:ASN:ND2	2.29	0.65
2:2:43:GLN:OE1	2:2:161:ARG:NH2	2.29	0.65
2:2:413:ARG:NH2	14:2:3031:CLA:OBD	2.29	0.65
10:L:38:ARG:NH2	10:L:49:GLU:OE1	2.28	0.65
1:1:579:ASP:O	21:1:909:HOH:O	2.14	0.65
2:b:19:ARG:NH2	2:b:701:ASP:OD2	2.29	0.65
2:b:459:GLU:OE1	2:b:464:GLN:NE2	2.27	0.65
14:b:3039:CLA:HMA3	14:b:3040:CLA:HED2	1.79	0.65
1:a:660:GLN:O	1:a:664:SER:OG	2.13	0.65
3:c:60:ASP:OD2	5:e:11:ARG:NH1	2.29	0.65
1:A:593:ASP:OD2	1:A:728:ARG:NH1	2.30	0.65
14:2:3039:CLA:HMA3	14:2:3040:CLA:HED2	1.79	0.65
1:1:593:ASP:OD2	1:1:728:ARG:NH1	2.30	0.64
1:A:689:PHE:O	21:A:909:HOH:O	2.15	0.64
2:B:413:ARG:NH2	14:B:3031:CLA:OBD	2.29	0.64
1:a:593:ASP:OD2	1:a:728:ARG:NH1	2.30	0.64
2:b:458:ILE:HD13	16:j:1106:BCR:H342	1.77	0.64
1:a:454:HIS:O	1:a:458:LEU:HG	1.98	0.64
14:b:3038:CLA:H141	12:x:19:LEU:HD13	1.80	0.64
5:5:2:GLN:O	5:5:5:SER:OG	2.16	0.64
14:B:3039:CLA:HMA3	14:B:3040:CLA:HED2	1.79	0.64
1:1:454:HIS:O	1:1:458:LEU:HG	1.98	0.64
8:8:28:GLU:OE2	8:8:31:ARG:NH2	2.31	0.63
1:A:454:HIS:O	1:A:458:LEU:HG	1.98	0.63
14:A:833:CLA:OBD	10:L:19:THR:HG21	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:33:TYR:OH	11:y:30:TYR:OH	1.86	0.63
2:b:583:TYR:OH	2:b:670:LEU:CD2	2.47	0.62
2:2:583:TYR:OH	2:2:670:LEU:CD2	2.47	0.62
8:J:28:GLU:OE2	8:J:31:ARG:NH2	2.31	0.62
5:e:2:GLN:O	5:e:5:SER:OG	2.16	0.62
12:z:12:ARG:HD3	12:z:12:ARG:N	2.15	0.62
5:E:2:GLN:O	5:E:5:SER:OG	2.16	0.62
8:j:28:GLU:OE2	8:j:31:ARG:NH2	2.31	0.62
12:X:12:ARG:HD3	12:X:12:ARG:N	2.15	0.62
2:B:583:TYR:OH	2:B:670:LEU:CD2	2.47	0.62
3:3:8:ASP:OD1	4:4:116:PRO:HA	2.00	0.62
8:j:7:TYR:HE1	14:j:1101:CLA:HBC2	1.63	0.62
16:B:3053:BCR:H401	8:J:33:TYR:CD2	2.35	0.62
14:1:833:CLA:OBD	10:0:19:THR:HG21	2.01	0.61
2:B:271:ASP:OD1	14:B:3018:CLA:HMB1	2.00	0.61
6:F:51:LEU:HD22	6:F:62:ASP:HB2	1.83	0.61
2:b:540:LEU:O	21:b:3108:HOH:O	2.16	0.61
6:f:51:LEU:HD22	6:f:62:ASP:HB2	1.83	0.61
12:x:12:ARG:HD3	12:x:12:ARG:N	2.15	0.61
6:6:51:LEU:HD22	6:6:62:ASP:HB2	1.83	0.61
8:j:33:TYR:CD2	16:j:1106:BCR:H401	2.35	0.61
16:2:3052:BCR:H401	8:8:33:TYR:CD2	2.35	0.61
17:b:3051:LHG:O5	12:x:12:ARG:NH2	2.33	0.60
8:j:7:TYR:HE1	14:j:1101:CLA:CBC	2.14	0.60
2:2:540:LEU:O	21:2:3107:HOH:O	2.16	0.60
3:c:8:ASP:OD1	4:d:116:PRO:HA	2.01	0.60
2:2:175:ASN:ND2	2:2:290:TYR:O	2.34	0.60
3:c:33:CYS:SG	3:c:34:LYS:N	2.75	0.60
1:a:590:SER:OG	1:a:593:ASP:OD1	2.20	0.60
1:A:590:SER:OG	1:A:593:ASP:OD1	2.20	0.60
6:F:96:GLU:OE1	6:F:100:ILE:HD12	2.02	0.60
1:a:661:VAL:HG21	1:a:746:PHE:HA	1.84	0.60
2:2:506:ALA:O	2:2:509:SER:OG	2.16	0.60
14:a:832:CLA:OBD	10:l:19:THR:HG21	2.01	0.60
6:6:96:GLU:OE1	6:6:100:ILE:HD12	2.02	0.60
1:A:661:VAL:HG21	1:A:746:PHE:HA	1.84	0.59
2:B:175:ASN:ND2	2:B:290:TYR:O	2.34	0.59
2:b:175:ASN:ND2	2:b:290:TYR:O	2.34	0.59
6:f:96:GLU:OE1	6:f:100:ILE:HD12	2.02	0.59
3:C:33:CYS:SG	3:C:34:LYS:N	2.75	0.59
6:F:61:GLY:O	8:J:39:HIS:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:95:ALA:HB2	1:a:158:LEU:HB2	1.85	0.59
14:b:3028:CLA:HBC2	14:b:3028:CLA:HHD	1.84	0.59
1:A:215:HIS:ND1	14:A:815:CLA:NB	2.51	0.59
6:F:52:VAL:HB	6:F:59:ARG:HG2	1.85	0.59
1:1:215:HIS:ND1	14:1:815:CLA:NB	2.51	0.59
1:1:661:VAL:HG21	1:1:746:PHE:HA	1.84	0.59
2:b:506:ALA:O	2:b:509:SER:OG	2.17	0.58
1:1:371:ALA:HB2	1:1:397:HIS:HB2	1.85	0.58
14:f:204:CLA:HHC	14:f:204:CLA:HBB1	1.86	0.58
4:D:63:GLN:NE2	21:D:203:HOH:O	2.32	0.58
14:2:3028:CLA:HBC2	14:2:3028:CLA:HHD	1.84	0.58
3:3:33:CYS:SG	3:3:34:LYS:N	2.75	0.58
14:B:3028:CLA:HBC2	14:B:3028:CLA:HHD	1.84	0.58
1:a:638:ASN:O	1:a:642:SER:OG	2.17	0.58
6:f:52:VAL:HB	6:f:59:ARG:HG2	1.84	0.58
2:2:235:ASN:O	2:2:252:ALA:N	2.33	0.58
1:A:328:ILE:O	1:A:332:HIS:ND1	2.36	0.58
9:K:70:ALA:O	9:K:74:VAL:HG22	2.03	0.58
1:a:215:HIS:ND1	14:a:814:CLA:NB	2.51	0.58
1:A:313:HIS:NE2	14:A:821:CLA:NC	2.51	0.58
4:D:117:ARG:NH2	4:D:122:ASN:OD1	2.36	0.58
9:9:70:ALA:O	9:9:74:VAL:HG22	2.03	0.58
8:8:32:PHE:C	8:8:33:TYR:HD1	2.12	0.58
9:k:70:ALA:O	9:k:74:VAL:HG22	2.03	0.58
14:B:3031:CLA:C10	12:X:12:ARG:HB3	2.34	0.58
8:J:32:PHE:C	8:J:33:TYR:HD1	2.12	0.58
1:1:95:ALA:HB2	1:1:158:LEU:HB2	1.85	0.58
14:F:204:CLA:HHC	14:F:204:CLA:HBB1	1.86	0.57
6:6:52:VAL:HB	6:6:59:ARG:HG2	1.85	0.57
1:A:372:GLN:HA	1:A:375:TYR:HE1	1.70	0.57
10:L:125:PHE:O	10:L:129:MET:HG2	2.04	0.57
8:j:32:PHE:C	8:j:33:TYR:HD1	2.12	0.57
1:1:372:GLN:HA	1:1:375:TYR:HE1	1.70	0.57
1:A:145:GLN:N	1:A:145:GLN:OE1	2.37	0.57
1:a:371:ALA:HB2	1:a:397:HIS:HB2	1.85	0.57
3:c:60:ASP:N	3:c:60:ASP:OD1	2.37	0.57
1:1:661:VAL:HG22	1:1:749:ALA:HB3	1.86	0.57
1:A:638:ASN:O	1:A:642:SER:OG	2.17	0.57
2:B:307:LYS:HE3	2:B:313:LYS:HG2	1.86	0.57
1:a:661:VAL:HG22	1:a:749:ALA:HB3	1.86	0.57
1:a:689:PHE:O	21:a:910:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:203:GLY:HA2	1:1:207:LEU:HD13	1.87	0.57
10:0:125:PHE:O	10:0:129:MET:HG2	2.04	0.57
1:A:371:ALA:HB2	1:A:397:HIS:HB2	1.85	0.57
1:a:313:HIS:NE2	14:a:820:CLA:NC	2.51	0.57
1:A:203:GLY:HA2	1:A:207:LEU:HD13	1.87	0.57
1:a:328:ILE:O	1:a:332:HIS:ND1	2.36	0.57
1:1:313:HIS:NE2	14:1:821:CLA:NC	2.51	0.57
2:2:307:LYS:HE3	2:2:313:LYS:HG2	1.86	0.57
14:2:3039:CLA:HBC1	6:6:53:VAL:HG11	1.87	0.57
14:6:204:CLA:HHC	14:6:204:CLA:HBB1	1.86	0.57
1:1:590:SER:OG	1:1:593:ASP:OD1	2.20	0.57
1:a:372:GLN:HA	1:a:375:TYR:HE1	1.70	0.57
2:b:255:THR:HG22	2:b:256:PHE:H	1.70	0.57
1:1:328:ILE:O	1:1:332:HIS:ND1	2.36	0.57
1:A:95:ALA:HB2	1:A:158:LEU:HB2	1.85	0.57
14:2:3003:CLA:H201	16:8:103:BCR:H362	1.86	0.57
3:C:60:ASP:OD1	3:C:60:ASP:N	2.37	0.56
1:a:145:GLN:OE1	1:a:145:GLN:N	2.37	0.56
2:b:339:TRP:CH2	16:b:3047:BCR:H372	2.40	0.56
1:1:145:GLN:OE1	1:1:145:GLN:N	2.37	0.56
2:2:255:THR:HG22	2:2:256:PHE:H	1.70	0.56
2:B:339:TRP:CH2	16:B:3047:BCR:H372	2.40	0.56
1:a:203:GLY:HA2	1:a:207:LEU:HD13	1.87	0.56
2:b:552:LEU:O	2:b:570:ARG:NH1	2.38	0.56
2:B:255:THR:HG22	2:B:256:PHE:H	1.70	0.56
2:b:307:LYS:HE3	2:b:313:LYS:HG2	1.86	0.56
1:A:564:ARG:O	4:D:60:ARG:NH1	2.39	0.56
4:d:117:ARG:NH2	4:d:122:ASN:OD1	2.36	0.56
14:2:3038:CLA:H141	12:z:19:LEU:HD13	1.88	0.56
4:4:117:ARG:NH2	4:4:122:ASN:OD1	2.36	0.56
10:l:125:PHE:O	10:l:129:MET:HG2	2.04	0.56
1:1:429:VAL:HG23	14:1:825:CLA:HBC2	1.88	0.56
2:B:552:LEU:O	2:B:570:ARG:NH1	2.39	0.56
2:2:135:TYR:OH	11:y:10:VAL:HG23	2.06	0.56
12:z:25:LEU:HD11	12:z:34:LEU:CD2	2.36	0.56
14:2:3037:CLA:HHC	14:2:3037:CLA:HBB1	1.88	0.56
1:a:374:MET:HE1	14:a:829:CLA:O1D	2.06	0.56
1:1:374:MET:HE1	14:1:830:CLA:O1D	2.06	0.56
14:B:3037:CLA:HHC	14:B:3037:CLA:HBB1	1.88	0.55
1:1:579:ASP:OD2	1:1:583:ARG:NH1	2.37	0.55
2:2:339:TRP:CH2	16:2:3047:BCR:H372	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:VAL:HG22	1:A:749:ALA:HB3	1.86	0.55
12:X:25:LEU:HD11	12:X:34:LEU:CD2	2.36	0.55
2:b:235:ASN:O	2:b:252:ALA:N	2.33	0.55
12:x:25:LEU:HD11	12:x:34:LEU:CD2	2.36	0.55
12:x:34:LEU:HG	12:x:35:LYS:N	2.22	0.55
14:0:207:CLA:HHC	14:0:207:CLA:HBB1	1.89	0.55
14:b:3039:CLA:HBC1	6:f:53:VAL:HG11	1.88	0.55
14:f:203:CLA:C2C	8:j:19:MET:HE1	2.36	0.55
9:K:27:ILE:HG12	9:K:62:THR:CG2	2.37	0.55
1:a:429:VAL:HG23	14:a:824:CLA:HBC2	1.88	0.55
2:b:439:LEU:HD11	16:j:1106:BCR:H311	1.89	0.55
2:2:722:GLY:O	2:2:726:THR:HG22	2.07	0.55
2:2:552:LEU:O	2:2:570:ARG:NH1	2.38	0.55
1:A:374:MET:HE1	14:A:830:CLA:O1D	2.06	0.55
3:3:60:ASP:N	3:3:60:ASP:OD1	2.37	0.55
14:b:3037:CLA:HHC	14:b:3037:CLA:HBB1	1.88	0.55
1:a:410:ALA:O	1:a:414:ILE:HG13	2.08	0.54
1:a:579:ASP:OD2	1:a:583:ARG:NH1	2.37	0.54
9:k:27:ILE:HG12	9:k:62:THR:CG2	2.37	0.54
14:l:206:CLA:HHC	14:l:206:CLA:HBB1	1.89	0.54
2:2:449:PHE:O	21:2:3109:HOH:O	2.18	0.54
1:A:579:ASP:OD2	1:A:583:ARG:NH1	2.37	0.54
1:1:466:ARG:NE	21:1:915:HOH:O	2.40	0.54
4:4:63:GLN:NE2	21:4:204:HOH:O	2.37	0.54
1:A:429:VAL:HG23	14:A:825:CLA:HBC2	1.88	0.54
2:B:722:GLY:O	2:B:726:THR:HG22	2.07	0.54
14:L:203:CLA:HHC	14:L:203:CLA:HBB1	1.89	0.54
1:a:564:ARG:O	4:d:60:ARG:NH1	2.40	0.54
14:1:818:CLA:HBC1	14:1:819:CLA:H122	1.90	0.54
1:a:472:GLN:OE1	21:a:911:HOH:O	2.18	0.54
3:3:9:THR:O	3:3:63:SER:OG	2.20	0.54
2:b:722:GLY:O	2:b:726:THR:HG22	2.07	0.54
9:9:27:ILE:HG12	9:9:62:THR:CG2	2.37	0.54
2:b:194:ILE:HD12	2:b:253:ILE:HB	1.90	0.54
9:9:27:ILE:HG23	9:9:54:PHE:CE2	2.43	0.54
4:d:95:HIS:HB3	4:d:96:PRO:HD3	1.90	0.54
1:1:244:LEU:O	1:1:245:ASN:OD1	2.26	0.54
1:1:564:ARG:O	4:4:60:ARG:NH1	2.40	0.54
2:2:467:GLN:NE2	2:2:516:LEU:O	2.39	0.54
8:8:3:HIS:HA	8:8:6:THR:HG22	1.90	0.54
6:F:76:TRP:HZ3	6:F:114:PHE:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:828:CLA:O1D	14:a:829:CLA:HMA1	2.08	0.54
2:2:194:ILE:HD12	2:2:253:ILE:HB	1.90	0.54
1:A:413:ALA:O	1:A:417:VAL:HG23	2.08	0.53
1:1:259:GLY:N	1:1:262:SER:HG	2.04	0.53
2:B:194:ILE:HD12	2:B:253:ILE:HB	1.90	0.53
1:a:413:ALA:O	1:a:417:VAL:HG23	2.08	0.53
4:4:95:HIS:HB3	4:4:96:PRO:HD3	1.90	0.53
1:A:240:HIS:HB2	14:A:817:CLA:HBC3	1.90	0.53
1:A:458:LEU:HD22	1:A:475:PHE:CE2	2.44	0.53
14:a:817:CLA:HBC1	14:a:818:CLA:H122	1.90	0.53
10:0:38:ARG:HB3	10:0:41:LEU:HD13	1.90	0.53
6:F:1:ASP:OD1	6:F:2:VAL:N	2.41	0.53
1:a:240:HIS:HB2	14:a:816:CLA:HBC3	1.91	0.53
14:b:3033:CLA:HHC	14:b:3033:CLA:HBB1	1.91	0.53
8:j:3:HIS:HA	8:j:6:THR:HG22	1.89	0.53
1:1:413:ALA:O	1:1:417:VAL:HG23	2.08	0.53
1:A:410:ALA:O	1:A:414:ILE:HG13	2.08	0.53
1:A:466:ARG:NE	21:A:915:HOH:O	2.41	0.53
1:a:244:LEU:O	1:a:245:ASN:OD1	2.26	0.53
1:a:458:LEU:HD22	1:a:475:PHE:CE2	2.44	0.53
9:k:27:ILE:HG23	9:k:54:PHE:CE2	2.43	0.53
14:2:3033:CLA:HHC	14:2:3033:CLA:HBB1	1.91	0.53
2:B:274:HIS:HB3	14:B:3018:CLA:HMB2	1.90	0.53
9:K:27:ILE:HG23	9:K:54:PHE:CE2	2.43	0.53
10:L:38:ARG:HB3	10:L:41:LEU:HD13	1.90	0.53
1:1:410:ALA:O	1:1:414:ILE:HG13	2.08	0.53
10:0:4:LEU:HD23	10:0:20:PRO:HG3	1.91	0.53
1:A:259:GLY:N	1:A:262:SER:HG	2.05	0.53
1:a:466:ARG:NE	21:a:920:HOH:O	2.42	0.53
1:A:244:LEU:O	1:A:245:ASN:OD1	2.26	0.53
14:A:829:CLA:O1D	14:A:830:CLA:HMA1	2.08	0.53
14:B:3033:CLA:HHC	14:B:3033:CLA:HBB1	1.91	0.53
8:J:3:HIS:HA	8:J:6:THR:HG22	1.90	0.53
3:c:9:THR:O	3:c:63:SER:OG	2.19	0.53
4:d:1:THR:O	4:d:2:THR:OG1	2.22	0.53
7:i:7:ALA:N	11:m:5:ASP:OD1	2.41	0.53
1:a:79:HIS:CE1	14:a:805:CLA:HMA3	2.45	0.52
6:f:1:ASP:OD1	6:f:2:VAL:N	2.41	0.52
6:6:76:TRP:HZ3	6:6:114:PHE:HA	1.73	0.52
1:A:79:HIS:CE1	14:A:806:CLA:HMA3	2.45	0.52
2:b:214:THR:O	14:b:3016:CLA:HED3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:240:HIS:HB2	14:1:817:CLA:HBC3	1.90	0.52
14:B:3039:CLA:HBC1	6:F:53:VAL:HG11	1.90	0.52
12:z:34:LEU:HG	12:z:35:LYS:N	2.22	0.52
10:l:38:ARG:HB3	10:l:41:LEU:HD13	1.90	0.52
2:B:214:THR:O	14:B:3016:CLA:HED3	2.09	0.52
14:B:3017:CLA:CBC	14:B:3017:CLA:HHD	2.40	0.52
1:1:458:LEU:HD22	1:1:475:PHE:CE2	2.44	0.52
6:6:57:LEU:HD23	6:6:60:ALA:HB2	1.92	0.52
6:F:57:LEU:HD23	6:F:60:ALA:HB2	1.92	0.52
6:f:76:TRP:HZ3	6:f:114:PHE:HA	1.73	0.52
6:6:1:ASP:OD1	6:6:2:VAL:N	2.41	0.52
4:D:95:HIS:HB3	4:D:96:PRO:HD3	1.90	0.52
1:1:79:HIS:CE1	14:1:806:CLA:HMA3	2.45	0.52
14:A:818:CLA:HBC1	14:A:819:CLA:H122	1.90	0.52
14:a:803:CLA:HHC	14:a:803:CLA:HBB1	1.92	0.52
14:1:829:CLA:O1D	14:1:830:CLA:HMA1	2.08	0.52
21:B:3101:HOH:O	3:C:67:TYR:OH	2.16	0.52
3:C:8:ASP:CG	4:D:116:PRO:HA	2.35	0.52
10:L:4:LEU:HD23	10:L:20:PRO:HG3	1.91	0.52
14:b:3017:CLA:CBC	14:b:3017:CLA:HHD	2.40	0.52
14:1:803:CLA:HHC	14:1:803:CLA:HBB1	1.92	0.52
10:l:4:LEU:HD23	10:l:20:PRO:HG3	1.91	0.52
2:2:44:LYS:NZ	11:y:29:LEU:O	2.43	0.52
1:a:355:GLN:NE2	21:a:917:HOH:O	2.38	0.51
2:2:214:THR:O	14:2:3016:CLA:HED3	2.09	0.51
9:k:27:ILE:HG23	9:k:54:PHE:CD2	2.45	0.51
10:l:145:VAL:O	10:l:148:ILE:HG12	2.11	0.51
14:2:3017:CLA:CBC	14:2:3017:CLA:HHD	2.40	0.51
10:0:58:LEU:HD21	10:0:85:LEU:HD23	1.93	0.51
6:F:1:ASP:N	6:F:5:LEU:O	2.44	0.51
6:f:57:LEU:HD23	6:f:60:ALA:HB2	1.92	0.51
10:l:58:LEU:HD21	10:l:85:LEU:HD23	1.93	0.51
9:K:63:THR:O	9:K:67:HIS:ND1	2.38	0.51
1:1:661:VAL:HG23	21:1:901:HOH:O	2.10	0.51
1:A:355:GLN:NE2	21:A:913:HOH:O	2.36	0.51
1:a:172:MET:HE1	14:a:813:CLA:H92	1.93	0.51
10:0:68:LEU:O	10:0:71:SER:OG	2.24	0.51
12:X:34:LEU:HG	12:X:35:LYS:N	2.22	0.51
2:b:202:ARG:HG2	2:b:249:ALA:HB1	1.93	0.51
1:1:638:ASN:O	1:1:642:SER:OG	2.17	0.51
9:9:27:ILE:HG23	9:9:54:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:661:VAL:HG23	21:a:901:HOH:O	2.10	0.51
1:1:79:HIS:O	1:1:82:VAL:HG22	2.11	0.51
3:3:75:SER:O	21:3:203:HOH:O	2.19	0.51
10:0:145:VAL:O	10:0:148:ILE:HG12	2.11	0.51
1:A:205:LEU:HB3	1:A:308:PHE:CD2	2.46	0.51
14:A:841:CLA:O2D	14:A:841:CLA:H2A	2.10	0.51
1:1:172:MET:HE1	14:1:814:CLA:H92	1.93	0.51
1:1:205:LEU:HB3	1:1:308:PHE:CD2	2.46	0.51
6:f:1:ASP:N	6:f:5:LEU:O	2.44	0.51
6:f:61:GLY:O	8:j:39:HIS:N	2.41	0.51
2:2:413:ARG:CZ	14:2:3031:CLA:OBD	2.59	0.51
2:2:666:GLY:O	2:2:670:LEU:HG	2.11	0.51
1:A:79:HIS:O	1:A:82:VAL:HG22	2.11	0.51
2:B:202:ARG:HG2	2:B:249:ALA:HB1	1.93	0.51
14:a:840:CLA:H2A	14:a:840:CLA:O2D	2.10	0.51
2:b:666:GLY:O	2:b:670:LEU:HG	2.11	0.51
6:f:59:ARG:NE	6:f:62:ASP:OD2	2.42	0.51
14:A:803:CLA:HHC	14:A:803:CLA:HBB1	1.92	0.50
1:A:172:MET:HE1	14:A:814:CLA:H92	1.92	0.50
2:B:666:GLY:O	2:B:670:LEU:HG	2.11	0.50
14:1:841:CLA:H2A	14:1:841:CLA:O2D	2.10	0.50
2:2:583:TYR:OH	2:2:670:LEU:HD22	2.12	0.50
6:6:1:ASP:N	6:6:5:LEU:O	2.44	0.50
1:A:432:ARG:NE	14:A:832:CLA:OBD	2.43	0.50
1:A:661:VAL:HG23	21:A:901:HOH:O	2.11	0.50
2:b:291:ARG:NH1	2:b:299:SER:OG	2.43	0.50
3:3:60:ASP:HB3	5:5:58:ASN:ND2	2.25	0.50
9:K:27:ILE:HG23	9:K:54:PHE:CD2	2.45	0.50
10:L:58:LEU:HD21	10:L:85:LEU:HD23	1.93	0.50
2:B:431:PHE:CZ	16:B:3053:BCR:H332	2.47	0.50
2:2:291:ARG:NH1	2:2:299:SER:OG	2.43	0.50
1:A:74:SER:OG	1:A:180:TYR:HB2	2.12	0.50
1:A:579:ASP:O	21:A:910:HOH:O	2.19	0.50
2:B:255:THR:HG22	2:B:256:PHE:N	2.27	0.50
10:L:145:VAL:O	10:L:148:ILE:HG12	2.11	0.50
2:B:44:LYS:NZ	11:M:29:LEU:O	2.45	0.50
1:A:705:VAL:HG22	14:F:201:CLA:HBC2	1.94	0.50
1:a:705:VAL:HG22	14:f:201:CLA:HBC2	1.94	0.50
1:1:218:HIS:NE2	14:1:816:CLA:NA	2.60	0.50
1:1:270:PHE:CD2	9:9:74:VAL:HG21	2.47	0.50
14:2:3040:CLA:HBC2	14:z:1701:CLA:HBC3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:z:22:ILE:O	12:z:25:LEU:HB3	2.12	0.50
1:A:207:LEU:HD12	1:A:309:ILE:HD11	1.93	0.50
2:B:339:TRP:HH2	16:B:3047:BCR:H372	1.76	0.50
2:B:413:ARG:CZ	14:B:3031:CLA:OBD	2.59	0.50
3:C:9:THR:O	3:C:63:SER:OG	2.20	0.50
2:b:467:GLN:NE2	2:b:516:LEU:O	2.39	0.50
2:2:202:ARG:HG2	2:2:249:ALA:HB1	1.93	0.50
2:2:339:TRP:HH2	16:2:3047:BCR:H372	1.76	0.50
2:2:513:SER:HA	2:2:516:LEU:HD21	1.94	0.50
1:a:207:LEU:HD12	1:a:309:ILE:HD11	1.93	0.49
1:A:313:HIS:CD2	14:A:821:CLA:ND	2.81	0.49
2:B:658:PHE:O	2:B:662:VAL:HG23	2.12	0.49
6:F:116:TRP:N	6:F:117:PRO:CD	2.76	0.49
10:L:68:LEU:O	10:L:71:SER:OG	2.24	0.49
2:b:255:THR:HG22	2:b:256:PHE:N	2.27	0.49
2:b:413:ARG:CZ	14:b:3031:CLA:OBD	2.59	0.49
6:f:116:TRP:N	6:f:117:PRO:CD	2.75	0.49
2:2:255:THR:HG22	2:2:256:PHE:N	2.27	0.49
2:2:658:PHE:O	2:2:662:VAL:HG23	2.12	0.49
1:A:583:ARG:NH2	4:D:62:GLU:OE2	2.41	0.49
2:B:467:GLN:NE2	2:B:516:LEU:O	2.39	0.49
2:b:658:PHE:O	2:b:662:VAL:HG23	2.12	0.49
1:1:207:LEU:HD12	1:1:309:ILE:HD11	1.93	0.49
1:A:313:HIS:NE2	14:A:821:CLA:ND	2.61	0.49
16:A:851:BCR:H24C	14:B:3034:CLA:CMC	2.42	0.49
2:B:291:ARG:NH1	2:B:299:SER:OG	2.43	0.49
15:1:845:PQN:H241	15:1:845:PQN:H271	1.95	0.49
14:2:3031:CLA:C10	12:z:12:ARG:HB3	2.42	0.49
6:6:59:ARG:NE	6:6:62:ASP:OD2	2.42	0.49
6:6:116:TRP:N	6:6:117:PRO:CD	2.76	0.49
2:B:513:SER:HA	2:B:516:LEU:HD21	1.94	0.49
1:a:205:LEU:HB3	1:a:308:PHE:CD2	2.46	0.49
1:a:677:LEU:HD11	2:b:623:MET:HB2	1.93	0.49
14:b:3042:CLA:HHC	14:b:3042:CLA:HBB1	1.95	0.49
1:1:432:ARG:NE	14:1:832:CLA:OBD	2.43	0.49
12:z:13:THR:O	12:z:17:VAL:HG12	2.13	0.49
1:A:28:TRP:O	8:J:7:TYR:HD1	1.96	0.49
1:a:270:PHE:CD2	9:k:74:VAL:HG21	2.47	0.49
2:b:272:MET:O	2:b:275:HIS:HB3	2.13	0.49
4:d:7:PRO:O	4:d:50:ARG:NE	2.34	0.49
12:x:22:ILE:O	12:x:25:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:677:LEU:HD11	2:2:623:MET:HB2	1.94	0.49
2:2:6:LYS:NZ	11:y:30:TYR:O	2.38	0.49
1:a:79:HIS:O	1:a:82:VAL:HG22	2.11	0.49
1:a:218:HIS:NE2	14:a:815:CLA:NA	2.60	0.49
2:b:339:TRP:HH2	16:b:3047:BCR:H372	1.76	0.49
1:A:218:HIS:NE2	14:A:816:CLA:NA	2.60	0.49
14:2:3042:CLA:HHC	14:2:3042:CLA:HBB1	1.95	0.49
6:6:59:ARG:O	6:6:59:ARG:HG3	2.13	0.49
14:A:816:CLA:HBC3	16:A:846:BCR:H312	1.95	0.49
14:B:3012:CLA:O1D	14:B:3012:CLA:H2A	2.13	0.49
4:D:7:PRO:O	4:D:50:ARG:NE	2.34	0.49
12:x:13:THR:O	12:x:17:VAL:HG12	2.13	0.49
15:A:845:PQN:H271	15:A:845:PQN:H241	1.95	0.49
12:X:13:THR:O	12:X:17:VAL:HG12	2.13	0.49
1:1:355:GLN:NE2	21:1:914:HOH:O	2.37	0.49
14:1:816:CLA:HBC3	16:9:102:BCR:H312	1.95	0.49
9:9:63:THR:O	9:9:67:HIS:ND1	2.38	0.49
1:A:349:THR:O	1:A:349:THR:HG22	2.13	0.48
2:B:189:TRP:HD1	2:B:276:HIS:CD2	2.31	0.48
6:F:59:ARG:O	6:F:59:ARG:HG3	2.13	0.48
1:a:74:SER:OG	1:a:180:TYR:HB2	2.12	0.48
1:a:313:HIS:CD2	14:a:820:CLA:ND	2.81	0.48
2:b:189:TRP:HD1	2:b:276:HIS:CD2	2.31	0.48
14:b:3003:CLA:H201	16:j:1104:BCR:H362	1.95	0.48
10:l:68:LEU:O	10:l:71:SER:OG	2.24	0.48
1:1:202:ALA:HB2	1:1:312:GLY:HA3	1.95	0.48
14:1:825:CLA:H2A	14:1:825:CLA:HED3	1.95	0.48
1:A:677:LEU:HD11	2:B:623:MET:HB2	1.93	0.48
2:B:235:ASN:O	2:B:252:ALA:N	2.33	0.48
6:F:56:ARG:HB2	12:X:31:PHE:CZ	2.48	0.48
1:a:202:ALA:HB2	1:a:312:GLY:HA3	1.95	0.48
1:a:313:HIS:NE2	14:a:820:CLA:ND	2.61	0.48
1:a:349:THR:O	1:a:349:THR:HG22	2.13	0.48
14:a:815:CLA:HBC3	16:a:845:BCR:H312	1.95	0.48
1:1:74:SER:OG	1:1:180:TYR:HB2	2.12	0.48
2:B:583:TYR:OH	2:B:670:LEU:HD22	2.12	0.48
2:b:580:ASP:OD1	2:b:712:ARG:CZ	2.61	0.48
10:l:83:ILE:HA	10:l:129:MET:HE1	1.94	0.48
1:1:313:HIS:CD2	14:1:821:CLA:ND	2.81	0.48
3:C:15:GLN:O	21:C:203:HOH:O	2.20	0.48
12:X:22:ILE:O	12:X:25:LEU:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:513:SER:HA	2:b:516:LEU:HD21	1.94	0.48
1:1:705:VAL:HG22	14:6:201:CLA:HBC2	1.94	0.48
2:2:189:TRP:HD1	2:2:276:HIS:CD2	2.31	0.48
2:2:272:MET:O	2:2:275:HIS:HB3	2.13	0.48
2:2:319:ASN:HB3	17:2:3051:LHG:H112	1.96	0.48
14:A:825:CLA:HED3	14:A:825:CLA:H2A	1.95	0.48
6:F:53:VAL:HG13	6:F:63:PHE:CD2	2.49	0.48
1:1:313:HIS:NE2	14:1:821:CLA:ND	2.61	0.48
14:A:806:CLA:O1D	14:A:806:CLA:H2A	2.14	0.48
2:B:580:ASP:OD1	2:B:712:ARG:CZ	2.61	0.48
14:B:3042:CLA:HHC	14:B:3042:CLA:HBB1	1.95	0.48
14:a:824:CLA:HED3	14:a:824:CLA:H2A	1.95	0.48
15:a:844:PQN:H241	15:a:844:PQN:H271	1.95	0.48
2:b:583:TYR:OH	2:b:670:LEU:HD22	2.12	0.48
2:2:580:ASP:OD1	2:2:712:ARG:CZ	2.61	0.48
3:3:8:ASP:CG	4:4:116:PRO:HA	2.38	0.48
1:A:28:TRP:HB3	8:J:7:TYR:CD1	2.49	0.48
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.95	0.48
1:A:463:ASP:OD1	1:A:645:THR:HB	2.14	0.48
2:B:272:MET:O	2:B:275:HIS:HB3	2.13	0.48
14:b:3012:CLA:H2A	14:b:3012:CLA:O1D	2.13	0.48
3:c:3:THR:HG22	3:c:5:LYS:HD3	1.96	0.48
6:f:59:ARG:HG3	6:f:59:ARG:O	2.13	0.48
10:0:83:ILE:HA	10:0:129:MET:HE1	1.94	0.48
2:B:443:ASN:O	2:B:447:VAL:HG12	2.14	0.48
6:F:107:ILE:O	6:F:111:LEU:HG	2.14	0.48
10:L:83:ILE:HA	10:L:129:MET:HE1	1.94	0.48
1:a:544:PHE:O	1:a:548:VAL:HG23	2.14	0.48
14:1:806:CLA:O1D	14:1:806:CLA:H2A	2.14	0.48
1:A:544:PHE:O	1:A:548:VAL:HG23	2.14	0.48
14:a:805:CLA:O1D	14:a:805:CLA:H2A	2.14	0.48
2:b:710:GLN:O	2:b:714:VAL:HG23	2.14	0.48
6:f:65:ILE:HB	6:f:66:PRO:HD3	1.96	0.48
14:b:3005:CLA:HHD	14:b:3005:CLA:CBC	2.42	0.48
9:k:63:THR:O	9:k:67:HIS:ND1	2.38	0.48
1:1:349:THR:HG22	1:1:349:THR:O	2.13	0.48
1:1:463:ASP:OD1	1:1:645:THR:HB	2.14	0.48
1:A:70:ARG:NE	1:A:185:PRO:O	2.43	0.47
1:A:207:LEU:HB3	16:A:848:BCR:H352	1.96	0.47
9:K:67:HIS:CE1	16:K:103:BCR:H12C	2.49	0.47
1:a:463:ASP:OD1	1:a:645:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:480:LEU:HD11	14:b:3036:CLA:HMC1	1.96	0.47
1:1:544:PHE:O	1:1:548:VAL:HG23	2.14	0.47
16:1:850:BCR:H24C	14:2:3034:CLA:CMC	2.44	0.47
2:2:443:ASN:O	2:2:447:VAL:HG12	2.14	0.47
14:2:3012:CLA:O1D	14:2:3012:CLA:H2A	2.13	0.47
6:6:53:VAL:HG13	6:6:63:PHE:CD2	2.49	0.47
2:B:319:ASN:HB3	17:B:3051:LHG:H112	1.96	0.47
10:L:54:HIS:HA	10:L:57:PHE:CE1	2.49	0.47
6:6:65:ILE:HB	6:6:66:PRO:HD3	1.96	0.47
6:6:107:ILE:O	6:6:111:LEU:HG	2.14	0.47
2:B:710:GLN:O	2:B:714:VAL:HG23	2.14	0.47
6:f:107:ILE:O	6:f:111:LEU:HG	2.14	0.47
2:2:339:TRP:HE1	14:2:3025:CLA:C2B	2.28	0.47
6:f:53:VAL:HG13	6:f:63:PHE:CD2	2.49	0.47
14:1:807:CLA:HMA2	14:1:807:CLA:H2	1.97	0.47
9:K:16:GLY:HA2	14:K:101:CLA:OBD	2.14	0.47
2:b:319:ASN:HB3	17:b:3051:LHG:H112	1.96	0.47
2:b:339:TRP:HE1	14:b:3025:CLA:C2B	2.28	0.47
1:1:207:LEU:HB3	16:1:847:BCR:H352	1.96	0.47
2:2:710:GLN:O	2:2:714:VAL:HG23	2.14	0.47
6:6:54:ASP:OD1	6:6:54:ASP:N	2.48	0.47
14:B:3018:CLA:C4C	14:B:3018:CLA:H91	2.45	0.47
14:B:3028:CLA:HHC	14:B:3028:CLA:HBB1	1.97	0.47
6:F:54:ASP:N	6:F:54:ASP:OD1	2.48	0.47
9:k:67:HIS:CE1	16:k:103:BCR:H12C	2.49	0.47
9:9:67:HIS:CE1	16:9:104:BCR:H12C	2.49	0.47
12:z:14:PHE:O	12:z:17:VAL:HG12	2.15	0.47
14:A:807:CLA:H2	14:A:807:CLA:HMA2	1.96	0.47
16:A:851:BCR:H362	14:B:3003:CLA:H42	1.97	0.47
2:B:339:TRP:HE1	14:B:3025:CLA:C2B	2.28	0.47
1:a:70:ARG:NE	1:a:185:PRO:O	2.44	0.47
1:a:432:ARG:NE	14:a:831:CLA:OBD	2.43	0.47
13:a:801:CL0:H13	14:b:3003:CLA:OBD	2.14	0.47
15:a:844:PQN:C30	8:j:15:ALA:HB1	2.44	0.47
2:b:439:LEU:HD11	16:j:1106:BCR:C31	2.44	0.47
2:b:443:ASN:O	2:b:447:VAL:HG12	2.14	0.47
10:0:54:HIS:HA	10:0:57:PHE:CE1	2.49	0.47
3:c:75:SER:O	21:c:203:HOH:O	2.20	0.47
8:j:7:TYR:CE1	14:j:1101:CLA:HBC2	2.47	0.47
6:6:5:LEU:HB3	6:6:42:LEU:HD23	1.97	0.47
16:8:103:BCR:HC8	16:8:103:BCR:H311	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.96	0.47
3:c:8:ASP:CG	4:d:116:PRO:HA	2.40	0.47
10:l:54:HIS:HA	10:l:57:PHE:CE1	2.49	0.47
1:1:70:ARG:NE	1:1:185:PRO:O	2.43	0.47
2:2:667:PHE:CB	14:2:3005:CLA:HMC2	2.45	0.47
14:2:3005:CLA:HHD	14:2:3005:CLA:CBC	2.42	0.47
1:A:366:LEU:HD13	14:A:828:CLA:H41	1.97	0.47
1:a:372:GLN:HG2	14:a:826:CLA:HED1	1.97	0.47
1:a:583:ARG:NH2	4:d:62:GLU:OE2	2.42	0.47
5:e:62:LEU:HA	5:e:65:VAL:HG22	1.97	0.47
6:f:5:LEU:HB3	6:f:42:LEU:HD23	1.97	0.47
12:x:14:PHE:O	12:x:17:VAL:HG12	2.15	0.47
5:5:36:VAL:O	5:5:59:ASN:HA	2.15	0.47
2:B:409:ASN:O	2:B:413:ARG:HG3	2.15	0.46
5:E:36:VAL:O	5:E:59:ASN:HA	2.15	0.46
2:b:177:HIS:O	2:b:178:LEU:C	2.58	0.46
6:f:70:PHE:O	6:f:71:LEU:C	2.57	0.46
1:1:140:THR:HG22	1:1:140:THR:O	2.15	0.46
2:2:409:ASN:O	2:2:413:ARG:HG3	2.15	0.46
2:B:480:LEU:HD11	14:B:3036:CLA:HMC1	1.96	0.46
14:L:201:CLA:HHC	14:L:201:CLA:HBB1	1.98	0.46
16:a:850:BCR:H24C	14:b:3034:CLA:CMC	2.44	0.46
9:9:43:LEU:HD22	9:9:55:GLY:HA2	1.98	0.46
14:B:3009:CLA:H92	14:B:3009:CLA:HMC1	1.97	0.46
4:D:1:THR:O	4:D:2:THR:OG1	2.22	0.46
1:a:65:LEU:HD11	14:a:825:CLA:H201	1.97	0.46
1:a:207:LEU:HB3	16:a:847:BCR:H352	1.97	0.46
2:b:409:ASN:O	2:b:413:ARG:HG3	2.15	0.46
14:b:3009:CLA:H92	14:b:3009:CLA:HMC1	1.97	0.46
14:b:3031:CLA:C10	12:x:12:ARG:HB3	2.45	0.46
14:l:203:CLA:HHC	14:l:203:CLA:HBB1	1.98	0.46
1:1:65:LEU:HD11	14:1:826:CLA:H201	1.97	0.46
1:1:372:GLN:HG2	14:1:827:CLA:HED1	1.97	0.46
14:b:3028:CLA:HHC	14:b:3028:CLA:HBB1	1.97	0.46
14:1:820:CLA:H92	14:1:830:CLA:H91	1.98	0.46
14:1:838:CLA:HBC2	14:1:838:CLA:HHD	1.98	0.46
14:A:838:CLA:HBC2	14:A:838:CLA:HHD	1.98	0.46
2:B:209:ASP:O	2:B:209:ASP:OD2	2.33	0.46
6:F:5:LEU:HB3	6:F:42:LEU:HD23	1.97	0.46
9:K:20:ILE:HA	14:K:101:CLA:O1A	2.15	0.46
9:K:45:ILE:HG22	9:K:46:ALA:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:366:LEU:HD13	14:a:827:CLA:H41	1.98	0.46
1:a:504:ASN:OD1	9:k:5:THR:N	2.48	0.46
14:a:806:CLA:HMA2	14:a:806:CLA:H2	1.97	0.46
14:a:819:CLA:H92	14:a:829:CLA:H91	1.98	0.46
13:1:801:CL0:H13	14:2:3003:CLA:OBD	2.15	0.46
1:A:140:THR:HG22	1:A:140:THR:O	2.15	0.46
1:A:300:HIS:HB2	14:A:819:CLA:C1B	2.46	0.46
1:A:372:GLN:HG2	14:A:827:CLA:HED1	1.97	0.46
6:f:13:ALA:O	6:f:17:ARG:HG2	2.16	0.46
5:5:1:VAL:HB	5:5:62:LEU:HD21	1.98	0.46
1:A:225:LYS:HG2	1:A:252:LEU:HD13	1.98	0.46
2:B:667:PHE:HB2	14:B:3005:CLA:HMC2	1.98	0.46
14:B:3010:CLA:HHC	14:B:3010:CLA:HBB1	1.98	0.46
3:C:3:THR:HG22	3:C:5:LYS:HD3	1.96	0.46
2:b:523:PHE:CZ	16:j:1106:BCR:H322	2.50	0.46
3:c:60:ASP:CG	3:c:61:PHE:H	2.24	0.46
2:2:332:SER:OG	2:2:335:PHE:HB2	2.16	0.46
2:2:480:LEU:HD11	14:2:3036:CLA:HMC1	1.96	0.46
10:0:62:TRP:HH2	10:0:85:LEU:HD22	1.81	0.46
4:D:2:THR:O	4:D:3:LEU:C	2.59	0.46
16:J:103:BCR:HC8	16:J:103:BCR:H311	1.97	0.46
12:X:14:PHE:O	12:X:17:VAL:HG12	2.15	0.46
16:a:848:BCR:C23	16:a:848:BCR:H403	2.46	0.46
2:b:332:SER:OG	2:b:335:PHE:HB2	2.16	0.46
2:b:667:PHE:HB2	14:b:3005:CLA:HMC2	1.98	0.46
14:1:843:CLA:HHC	14:1:843:CLA:HBB1	1.98	0.46
2:2:209:ASP:O	2:2:209:ASP:OD2	2.33	0.46
14:2:3018:CLA:H91	14:2:3018:CLA:C4C	2.45	0.46
3:3:3:THR:HG22	3:3:5:LYS:HD3	1.96	0.46
6:6:13:ALA:O	6:6:17:ARG:HG2	2.16	0.46
1:A:65:LEU:HD11	14:A:826:CLA:H201	1.97	0.46
2:B:332:SER:OG	2:B:335:PHE:HB2	2.16	0.46
16:B:3045:BCR:H23C	16:B:3045:BCR:H382	1.98	0.46
14:b:3010:CLA:HHC	14:b:3010:CLA:HBB1	1.98	0.46
1:1:300:HIS:HB2	14:1:819:CLA:C1B	2.45	0.46
2:2:242:VAL:HG23	2:2:242:VAL:O	2.16	0.46
14:2:3033:CLA:O1D	14:2:3033:CLA:H2A	2.16	0.46
2:B:667:PHE:CB	14:B:3005:CLA:HMC2	2.45	0.46
1:a:225:LYS:HG2	1:a:252:LEU:HD13	1.98	0.46
14:b:3018:CLA:C4C	14:b:3018:CLA:H91	2.45	0.46
9:k:43:LEU:HD22	9:k:55:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:366:LEU:HD13	14:1:828:CLA:H41	1.97	0.46
16:2:3045:BCR:H382	16:2:3045:BCR:H23C	1.98	0.46
2:B:506:ALA:O	2:B:509:SER:OG	2.17	0.45
6:F:59:ARG:NE	6:F:62:ASP:OD2	2.42	0.45
14:a:802:CLA:H91	16:a:850:BCR:H20C	1.98	0.45
2:b:667:PHE:CB	14:b:3005:CLA:HMC2	2.45	0.45
4:d:2:THR:O	4:d:3:LEU:C	2.59	0.45
5:e:1:VAL:HB	5:e:62:LEU:HD21	1.98	0.45
9:k:64:SER:O	9:k:68:LEU:HD13	2.17	0.45
14:2:3028:CLA:HHC	14:2:3028:CLA:HBB1	1.97	0.45
5:5:62:LEU:HA	5:5:65:VAL:HG22	1.97	0.45
14:B:3033:CLA:O1D	14:B:3033:CLA:H2A	2.16	0.45
5:E:62:LEU:HA	5:E:65:VAL:HG22	1.97	0.45
14:F:203:CLA:C2C	8:J:19:MET:HE1	2.46	0.45
1:a:140:THR:HG22	1:a:140:THR:O	2.15	0.45
2:b:209:ASP:O	2:b:209:ASP:OD2	2.34	0.45
2:b:391:ALA:O	2:b:395:ILE:HG13	2.16	0.45
5:e:36:VAL:O	5:e:59:ASN:HA	2.15	0.45
3:3:60:ASP:CG	3:3:61:PHE:H	2.24	0.45
9:9:45:ILE:HG22	9:9:46:ALA:N	2.31	0.45
2:B:391:ALA:O	2:B:395:ILE:HG13	2.16	0.45
9:K:43:LEU:HD22	9:K:55:GLY:HA2	1.97	0.45
9:K:64:SER:O	9:K:68:LEU:HD13	2.16	0.45
2:b:468:ALA:HA	2:b:472:LYS:O	2.16	0.45
14:l:207:CLA:HBC2	14:l:207:CLA:HHD	1.99	0.45
1:1:140:THR:HG21	1:1:392:SER:OG	2.16	0.45
3:C:60:ASP:CG	3:C:61:PHE:H	2.24	0.45
14:a:842:CLA:HHC	14:a:842:CLA:HBB1	1.98	0.45
6:f:54:ASP:N	6:f:54:ASP:OD1	2.48	0.45
16:j:1104:BCR:HC8	16:j:1104:BCR:H311	1.97	0.45
1:1:225:LYS:HG2	1:1:252:LEU:HD13	1.98	0.45
2:2:468:ALA:HA	2:2:472:LYS:O	2.16	0.45
6:6:62:ASP:HA	8:8:38:PHE:HB2	1.98	0.45
14:0:208:CLA:HBC2	14:0:208:CLA:HHD	1.99	0.45
14:A:844:CLA:CGA	14:A:855:CLA:C2A	2.94	0.45
2:B:198:ILE:N	2:B:199:PRO:HD2	2.32	0.45
5:E:1:VAL:HB	5:E:62:LEU:HD21	1.98	0.45
10:L:62:TRP:HH2	10:L:85:LEU:HD22	1.81	0.45
12:X:25:LEU:HD11	12:X:34:LEU:HD23	1.98	0.45
14:a:837:CLA:HBC2	14:a:837:CLA:HHD	1.98	0.45
9:k:31:ARG:N	9:k:54:PHE:HZ	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:55:GLY:N	9:k:58:GLU:OE1	2.49	0.45
2:2:271:ASP:OD1	14:2:3018:CLA:HMB3	2.16	0.45
2:2:391:ALA:O	2:2:395:ILE:HG13	2.16	0.45
4:4:2:THR:O	4:4:3:LEU:C	2.59	0.45
6:6:70:PHE:O	6:6:71:LEU:C	2.57	0.45
16:A:849:BCR:C23	16:A:849:BCR:H403	2.46	0.45
3:C:60:ASP:HB3	5:E:58:ASN:ND2	2.32	0.45
9:K:31:ARG:N	9:K:54:PHE:HZ	2.15	0.45
1:a:300:HIS:HB2	14:a:818:CLA:C1B	2.46	0.45
2:2:444:ASP:OD1	2:2:621:TYR:HB2	2.17	0.45
9:9:31:ARG:N	9:9:54:PHE:HZ	2.15	0.45
6:F:70:PHE:O	6:F:71:LEU:C	2.57	0.45
16:a:850:BCR:H362	14:b:3003:CLA:H42	1.99	0.45
2:b:47:ALA:HB3	11:m:29:LEU:HD21	1.98	0.45
10:l:62:TRP:HH2	10:l:85:LEU:HD22	1.81	0.45
1:1:556:GLY:O	1:1:560:ALA:HB2	2.17	0.45
14:A:843:CLA:HHC	14:A:843:CLA:HBB1	1.98	0.45
2:B:256:PHE:HE2	2:B:499:TRP:HE3	1.65	0.45
14:B:3006:CLA:O1A	11:M:30:TYR:HB2	2.16	0.45
6:F:62:ASP:HA	8:J:38:PHE:HB2	1.98	0.45
9:K:55:GLY:N	9:K:58:GLU:OE1	2.49	0.45
1:a:556:GLY:O	1:a:560:ALA:HB2	2.17	0.45
2:2:223:PRO:HA	2:2:226:THR:HB	1.99	0.45
14:A:820:CLA:H92	14:A:830:CLA:H91	1.98	0.45
9:k:45:ILE:HG22	9:k:46:ALA:N	2.31	0.45
16:1:850:BCR:H362	14:2:3003:CLA:H42	1.98	0.45
2:2:667:PHE:HB2	14:2:3005:CLA:HMC2	1.98	0.45
2:2:726:THR:HG23	14:2:3004:CLA:O1D	2.17	0.45
14:2:3009:CLA:H92	14:2:3009:CLA:HMC1	1.97	0.45
1:A:94:GLY:C	1:A:98:SER:HG	2.09	0.45
2:B:242:VAL:HG23	2:B:242:VAL:O	2.16	0.45
6:F:13:ALA:O	6:F:17:ARG:HG2	2.16	0.45
2:b:271:ASP:OD1	14:b:3018:CLA:HMB3	2.16	0.45
14:b:3019:CLA:H42	14:b:3019:CLA:O1A	2.17	0.45
12:x:25:LEU:HD11	12:x:34:LEU:HD23	1.98	0.45
14:2:3016:CLA:H3A	16:2:3046:BCR:H311	1.99	0.45
3:3:8:ASP:OD1	4:4:115:VAL:O	2.35	0.45
14:0:204:CLA:HHC	14:0:204:CLA:HBB1	1.98	0.45
1:A:95:ALA:HB2	1:A:158:LEU:CB	2.46	0.44
2:B:223:PRO:HA	2:B:226:THR:HB	1.99	0.44
1:a:466:ARG:HG2	1:a:466:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:439:LEU:CD1	16:j:1106:BCR:C31	2.94	0.44
2:b:444:ASP:OD1	2:b:621:TYR:HB2	2.17	0.44
2:b:458:ILE:CD1	16:j:1106:BCR:H342	2.46	0.44
1:1:88:SER:HB2	1:1:162:ALA:O	2.18	0.44
1:1:372:GLN:NE2	1:1:375:TYR:OH	2.50	0.44
1:1:583:ARG:NH2	4:4:62:GLU:OE2	2.41	0.44
14:1:821:CLA:HBA2	14:1:821:CLA:H3A	1.87	0.44
16:1:848:BCR:C23	16:1:848:BCR:H403	2.46	0.44
14:2:3010:CLA:HHC	14:2:3010:CLA:HBB1	1.98	0.44
14:2:3019:CLA:H42	14:2:3019:CLA:O1A	2.17	0.44
6:6:73:ILE:O	6:6:76:TRP:HB3	2.18	0.44
1:A:140:THR:HG21	1:A:392:SER:OG	2.16	0.44
14:A:832:CLA:O1D	10:L:5:VAL:HG11	2.17	0.44
2:B:146:SER:OG	11:M:21:LEU:HD12	2.17	0.44
2:B:177:HIS:O	2:B:178:LEU:C	2.58	0.44
2:B:413:ARG:HH21	14:B:3031:CLA:CAD	2.30	0.44
16:B:3053:BCR:H401	8:J:33:TYR:HD2	1.82	0.44
2:b:146:SER:OG	11:m:21:LEU:HD12	2.17	0.44
2:b:412:ASP:O	2:b:416:GLN:HG2	2.18	0.44
2:b:726:THR:HG23	14:b:3004:CLA:O1D	2.17	0.44
1:1:95:ALA:HB2	1:1:158:LEU:CB	2.46	0.44
2:2:177:HIS:O	2:2:178:LEU:C	2.58	0.44
2:2:198:ILE:N	2:2:199:PRO:HD2	2.32	0.44
1:a:140:THR:HG21	1:a:392:SER:OG	2.17	0.44
1:1:253:TYR:HB2	1:1:258:TRP:HE1	1.83	0.44
2:2:554:PRO:HB2	5:5:13:GLU:OE1	2.18	0.44
17:2:3051:LHG:P	12:z:12:ARG:NH2	2.90	0.44
1:A:372:GLN:NE2	1:A:375:TYR:OH	2.50	0.44
13:A:801:CL0:H13	14:B:3003:CLA:OBD	2.17	0.44
2:B:155:HIS:O	21:B:3108:HOH:O	2.21	0.44
2:B:444:ASP:OD1	2:B:621:TYR:HB2	2.17	0.44
2:B:637:LEU:HD13	2:B:733:ALA:HB3	1.99	0.44
2:B:726:THR:HG23	14:B:3004:CLA:O1D	2.17	0.44
14:L:204:CLA:HHD	14:L:204:CLA:HBC2	1.99	0.44
1:a:372:GLN:NE2	1:a:375:TYR:OH	2.50	0.44
14:a:802:CLA:H142	16:a:850:BCR:H402	2.00	0.44
14:b:3033:CLA:H2A	14:b:3033:CLA:O1D	2.16	0.44
10:l:58:LEU:O	10:l:62:TRP:HZ3	2.00	0.44
1:1:271:ASN:CG	1:1:271:ASN:O	2.61	0.44
2:2:114:ILE:O	14:2:3010:CLA:HMD1	2.18	0.44
2:2:487:ILE:H	2:2:487:ILE:HD12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:3050:LMG:O5	21:2:3108:HOH:O	2.18	0.44
14:A:802:CLA:H91	16:A:851:BCR:H20C	1.99	0.44
14:A:802:CLA:H142	16:A:851:BCR:H402	1.99	0.44
2:B:353:GLN:HA	2:B:356:TYR:HE1	1.82	0.44
14:B:3016:CLA:H3A	16:B:3046:BCR:H311	1.99	0.44
2:b:114:ILE:O	14:b:3010:CLA:HMD1	2.18	0.44
2:b:135:TYR:OH	11:m:7:GLN:O	2.33	0.44
2:b:481:LEU:HD13	14:b:3035:CLA:HMD2	1.99	0.44
2:b:487:ILE:HD12	2:b:487:ILE:H	1.83	0.44
16:b:3045:BCR:H382	16:b:3045:BCR:H23C	1.98	0.44
3:c:38:ILE:HG12	3:c:39:ALA:H	1.83	0.44
3:c:60:ASP:HB3	5:e:58:ASN:ND2	2.32	0.44
6:f:38:TYR:CE1	8:j:37:LEU:HB3	2.52	0.44
16:2:3048:BCR:H24C	16:2:3048:BCR:H371	1.87	0.44
14:6:204:CLA:HHC	14:6:204:CLA:CBB	2.48	0.44
1:A:271:ASN:CG	1:A:271:ASN:O	2.61	0.44
2:B:412:ASP:O	2:B:416:GLN:HG2	2.18	0.44
14:B:3005:CLA:HHD	14:B:3005:CLA:CBC	2.42	0.44
17:B:3051:LHG:P	12:X:12:ARG:HH21	2.40	0.44
1:a:88:SER:HB2	1:a:162:ALA:O	2.17	0.44
2:b:413:ARG:HE	14:b:3031:CLA:CAD	2.25	0.44
2:2:166:TRP:CZ2	14:2:3012:CLA:HBB	2.52	0.44
4:4:1:THR:OG1	4:4:2:THR:N	2.47	0.44
9:9:23:ASN:HD21	9:9:67:HIS:CE1	2.36	0.44
9:9:64:SER:O	9:9:68:LEU:HD13	2.16	0.44
10:0:76:LEU:HD23	10:0:136:PHE:CZ	2.53	0.44
16:y:101:BCR:H23C	16:y:101:BCR:H382	2.00	0.44
1:A:466:ARG:HH11	1:A:466:ARG:HG2	1.82	0.44
2:B:314:VAL:HG13	2:B:316:GLY:H	1.83	0.44
17:B:3051:LHG:P	12:X:12:ARG:NH2	2.90	0.44
14:a:808:CLA:H93	16:j:1104:BCR:H403	1.99	0.44
2:b:198:ILE:N	2:b:199:PRO:HD2	2.32	0.44
2:b:242:VAL:O	2:b:242:VAL:HG23	2.16	0.44
2:b:353:GLN:HA	2:b:356:TYR:HE1	1.82	0.44
2:b:413:ARG:HH21	14:b:3031:CLA:CAD	2.29	0.44
9:k:23:ASN:HD21	9:k:67:HIS:CE1	2.36	0.44
14:1:802:CLA:H91	16:1:850:BCR:H20C	1.99	0.44
2:2:412:ASP:O	2:2:416:GLN:HG2	2.18	0.44
1:A:88:SER:HB2	1:A:162:ALA:O	2.17	0.44
1:A:556:GLY:O	1:A:560:ALA:HB2	2.17	0.44
14:A:824:CLA:H2A	14:A:824:CLA:O2D	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:95:ALA:HB2	1:a:158:LEU:CB	2.47	0.44
1:a:271:ASN:O	1:a:271:ASN:CG	2.61	0.44
2:b:166:TRP:CZ2	14:b:3012:CLA:HBB	2.52	0.44
2:b:668:MET:O	2:b:672:SER:OG	2.35	0.44
5:e:6:LYS:HB2	5:e:68:VAL:HG23	2.00	0.44
2:2:353:GLN:HA	2:2:356:TYR:HE1	1.82	0.44
2:2:413:ARG:HE	14:2:3031:CLA:CAD	2.25	0.44
2:B:468:ALA:HA	2:B:472:LYS:O	2.16	0.44
2:B:481:LEU:HD13	14:B:3035:CLA:HMD2	1.99	0.44
14:B:3040:CLA:HBB1	14:B:3040:CLA:HHC	2.00	0.44
6:F:100:ILE:HG12	8:J:10:THR:HG22	1.99	0.44
6:f:76:TRP:CZ2	6:f:110:MET:O	2.71	0.44
10:l:76:LEU:HD23	10:l:136:PHE:CZ	2.53	0.44
10:l:142:PHE:CD1	14:l:208:CLA:H43	2.53	0.44
1:1:336:PHE:O	1:1:432:ARG:NH2	2.49	0.44
1:A:253:TYR:HB2	1:A:258:TRP:HE1	1.83	0.43
1:A:300:HIS:HB2	14:A:819:CLA:CHB	2.48	0.43
2:B:166:TRP:CZ2	14:B:3012:CLA:HBB	2.52	0.43
14:F:204:CLA:HHC	14:F:204:CLA:CBB	2.48	0.43
9:K:23:ASN:HD21	9:K:67:HIS:CE1	2.36	0.43
10:L:58:LEU:O	10:L:62:TRP:HZ3	2.00	0.43
10:L:76:LEU:HD23	10:L:136:PHE:CZ	2.53	0.43
2:b:256:PHE:HE2	2:b:499:TRP:HE3	1.65	0.43
1:1:466:ARG:HG2	1:1:466:ARG:HH11	1.82	0.43
2:2:594:GLY:O	2:2:598:PHE:CD1	2.71	0.43
3:3:38:ILE:HG12	3:3:39:ALA:H	1.82	0.43
10:0:58:LEU:O	10:0:62:TRP:HZ3	2.00	0.43
10:0:142:PHE:CD1	14:0:209:CLA:H43	2.53	0.43
2:B:594:GLY:O	2:B:598:PHE:CD1	2.71	0.43
17:L:207:LHG:H341	16:y:101:BCR:HC21	2.01	0.43
1:a:300:HIS:HB2	14:a:818:CLA:CHB	2.48	0.43
14:a:823:CLA:H2A	14:a:823:CLA:O2D	2.18	0.43
14:b:3016:CLA:H3A	16:b:3046:BCR:H311	1.99	0.43
1:1:11:LYS:HZ1	9:9:39:LYS:HE2	1.83	0.43
14:1:807:CLA:C4	17:1:852:LHG:H261	2.48	0.43
2:2:256:PHE:HE2	2:2:499:TRP:HE3	1.65	0.43
2:2:282:LEU:HD23	14:2:3020:CLA:HMC1	2.00	0.43
2:2:622:LEU:HD12	14:2:3003:CLA:H11	2.01	0.43
5:5:6:LYS:HB2	5:5:68:VAL:HG23	2.00	0.43
12:z:25:LEU:HD11	12:z:34:LEU:HD23	1.98	0.43
1:A:564:ARG:HD3	3:C:79:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:ILE:O	6:F:76:TRP:HB3	2.18	0.43
1:a:146:LEU:HD13	1:a:380:TYR:HE2	1.83	0.43
3:c:8:ASP:OD1	4:d:115:VAL:O	2.36	0.43
16:m:101:BCR:H382	16:m:101:BCR:H23C	2.00	0.43
1:1:146:LEU:HD13	1:1:380:TYR:HE2	1.84	0.43
14:2:3038:CLA:H91	14:2:3038:CLA:H13	2.01	0.43
7:7:30:LEU:O	7:7:34:ILE:HG12	2.18	0.43
12:z:22:ILE:HA	12:z:25:LEU:CB	2.49	0.43
2:B:282:LEU:HD23	14:B:3020:CLA:HMC1	2.00	0.43
14:B:3018:CLA:H41	14:B:3018:CLA:H62	1.82	0.43
14:B:3038:CLA:H13	14:B:3038:CLA:H91	2.01	0.43
7:I:7:ALA:N	11:M:5:ASP:OD1	2.51	0.43
7:I:30:LEU:O	7:I:34:ILE:HG12	2.18	0.43
14:b:3026:CLA:H91	16:b:3048:BCR:H342	2.00	0.43
1:1:28:TRP:HB3	8:8:7:TYR:CD1	2.54	0.43
14:1:802:CLA:H142	16:1:850:BCR:H402	1.99	0.43
2:2:90:ILE:HB	2:2:111:PRO:HB2	2.01	0.43
14:2:3006:CLA:H141	16:y:101:BCR:H14C	2.01	0.43
14:2:3040:CLA:HHC	14:2:3040:CLA:HBB1	2.00	0.43
1:A:146:LEU:HD13	1:A:380:TYR:HE2	1.84	0.43
1:A:605:CYS:O	1:A:609:VAL:HG23	2.18	0.43
1:A:720:ARG:NH1	21:A:911:HOH:O	2.29	0.43
14:A:807:CLA:C4	17:A:853:LHG:H261	2.48	0.43
2:B:533:LEU:O	2:B:537:THR:HG22	2.18	0.43
1:a:253:TYR:HB2	1:a:258:TRP:HE1	1.83	0.43
14:b:3038:CLA:H13	14:b:3038:CLA:H91	2.00	0.43
14:b:3040:CLA:HHC	14:b:3040:CLA:HBB1	2.00	0.43
12:x:22:ILE:HA	12:x:25:LEU:CB	2.49	0.43
2:2:637:LEU:HD13	2:2:733:ALA:HB3	1.99	0.43
6:6:57:LEU:O	6:6:58:SER:HB3	2.19	0.43
14:6:203:CLA:C2C	8:8:19:MET:HE1	2.48	0.43
9:9:55:GLY:N	9:9:58:GLU:OE1	2.49	0.43
2:B:622:LEU:HD12	14:B:3003:CLA:H11	2.01	0.43
14:B:3019:CLA:O1A	14:B:3019:CLA:H42	2.18	0.43
16:M:1602:BCR:H382	16:M:1602:BCR:H23C	2.00	0.43
2:b:223:PRO:HA	2:b:226:THR:HB	1.99	0.43
2:b:318:PHE:CD2	14:b:3024:CLA:HMA3	2.54	0.43
1:1:605:CYS:O	1:1:609:VAL:HG23	2.18	0.43
2:2:314:VAL:HG13	2:2:316:GLY:H	1.83	0.43
16:A:851:BCR:H362	14:B:3003:CLA:C4	2.47	0.43
2:B:97:LYS:NZ	2:B:101:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:142:PHE:CD1	14:L:205:CLA:H43	2.53	0.43
12:X:22:ILE:HA	12:X:25:LEU:CB	2.49	0.43
1:a:430:LEU:O	1:a:433:VAL:HG12	2.19	0.43
1:a:433:VAL:HA	1:a:436:HIS:CE1	2.54	0.43
1:a:605:CYS:O	1:a:609:VAL:HG23	2.18	0.43
2:b:594:GLY:O	2:b:598:PHE:CD1	2.71	0.43
6:f:73:ILE:O	6:f:76:TRP:HB3	2.18	0.43
2:2:703:PRO:HB3	14:2:3041:CLA:C1C	2.49	0.43
14:2:3006:CLA:O2A	11:y:26:SER:HB3	2.19	0.43
1:A:301:HIS:HA	1:A:304:ILE:HG12	2.01	0.43
14:A:809:CLA:HAB	14:A:829:CLA:H142	2.01	0.43
3:C:38:ILE:HG12	3:C:39:ALA:H	1.83	0.43
1:a:146:LEU:CD1	1:a:380:TYR:HE2	2.32	0.43
14:a:806:CLA:C4	17:a:852:LHG:H261	2.48	0.43
14:a:808:CLA:HAB	14:a:828:CLA:H142	2.01	0.43
2:b:637:LEU:HD13	2:b:733:ALA:HB3	1.99	0.43
7:i:30:LEU:O	7:i:34:ILE:HG12	2.18	0.43
9:k:23:ASN:ND2	9:k:67:HIS:CE1	2.87	0.43
10:l:110:PRO:O	10:l:113:THR:OG1	2.33	0.43
1:1:430:LEU:O	1:1:433:VAL:HG12	2.19	0.43
4:4:3:LEU:HD11	4:4:83:TYR:CD1	2.54	0.43
2:B:487:ILE:HD12	2:B:487:ILE:H	1.83	0.43
5:E:6:LYS:HB2	5:E:68:VAL:HG23	2.00	0.43
1:a:370:VAL:O	1:a:371:ALA:C	2.62	0.43
14:a:820:CLA:HBA2	14:a:820:CLA:H3A	1.87	0.43
14:a:842:CLA:CGA	14:a:842:CLA:H43	2.49	0.43
2:b:470:HIS:HE1	14:b:3035:CLA:NA	2.17	0.43
14:f:201:CLA:H101	8:j:14:LEU:HD11	1.99	0.43
1:1:301:HIS:HA	1:1:304:ILE:HG12	2.01	0.43
2:2:74:GLU:CD	11:y:1:MET:N	2.76	0.43
2:2:470:HIS:HE1	14:2:3035:CLA:NA	2.17	0.43
14:2:3026:CLA:H91	16:2:3048:BCR:H342	2.01	0.43
1:A:146:LEU:CD1	1:A:380:TYR:HE2	2.32	0.43
1:A:430:LEU:O	1:A:433:VAL:HG12	2.19	0.43
2:B:413:ARG:HE	14:B:3031:CLA:CAD	2.25	0.43
2:B:668:MET:O	2:B:672:SER:OG	2.35	0.43
6:F:76:TRP:CZ2	6:F:110:MET:O	2.71	0.43
1:a:275:TYR:O	1:a:279:LEU:HB2	2.19	0.43
15:a:844:PQN:H301	8:j:15:ALA:HB1	2.00	0.43
2:b:314:VAL:HG13	2:b:316:GLY:H	1.83	0.43
2:b:533:LEU:O	2:b:537:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:76:TRP:HE1	14:f:203:CLA:CAD	2.32	0.43
1:1:300:HIS:HB2	14:1:819:CLA:CHB	2.48	0.43
1:1:601:TRP:CH2	14:1:803:CLA:CBB	3.02	0.43
14:1:843:CLA:H43	14:1:843:CLA:CGA	2.49	0.43
2:2:481:LEU:HD13	14:2:3035:CLA:HMD2	1.99	0.43
14:2:3006:CLA:O1A	11:y:26:SER:O	2.36	0.43
6:6:76:TRP:CZ2	6:6:110:MET:O	2.71	0.43
6:6:115:ALA:HB1	6:6:118:LEU:HD23	2.01	0.43
1:A:504:ASN:OD1	9:K:5:THR:N	2.52	0.42
14:A:843:CLA:CGA	14:A:843:CLA:H43	2.49	0.42
2:B:470:HIS:HE1	14:B:3035:CLA:NA	2.17	0.42
4:D:3:LEU:HD11	4:D:83:TYR:CD1	2.54	0.42
1:a:301:HIS:HA	1:a:304:ILE:HG12	2.01	0.42
2:b:377:HIS:CE1	14:b:3028:CLA:ND	2.87	0.42
14:f:204:CLA:HHC	14:f:204:CLA:CBB	2.48	0.42
7:i:26:VAL:HG13	17:0:202:LHG:H152	2.01	0.42
1:1:504:ASN:OD1	9:9:5:THR:N	2.52	0.42
14:1:839:CLA:O1D	14:1:839:CLA:H2A	2.19	0.42
2:2:74:GLU:HA	2:2:77:VAL:HG22	2.01	0.42
4:4:7:PRO:O	4:4:50:ARG:NE	2.34	0.42
2:B:114:ILE:O	14:B:3010:CLA:HMD1	2.18	0.42
14:B:3026:CLA:H91	16:B:3048:BCR:H342	2.00	0.42
10:L:131:SER:O	10:L:134:VAL:HG12	2.19	0.42
17:L:208:LHG:H152	7:7:26:VAL:HG13	2.01	0.42
14:a:838:CLA:O1D	14:a:838:CLA:H2A	2.19	0.42
2:b:622:LEU:HD12	14:b:3003:CLA:H11	2.01	0.42
2:2:431:PHE:CZ	16:2:3052:BCR:H332	2.54	0.42
14:2:3018:CLA:H41	14:2:3018:CLA:H62	1.82	0.42
14:2:3019:CLA:H62	14:2:3019:CLA:H41	1.90	0.42
9:9:20:ILE:HG13	9:9:21:LEU:N	2.34	0.42
1:A:152:ILE:HG21	1:A:158:LEU:HD21	2.02	0.42
14:A:839:CLA:O1D	14:A:839:CLA:H2A	2.19	0.42
16:A:851:BCR:C8	16:A:851:BCR:H321	2.50	0.42
2:B:90:ILE:HB	2:B:111:PRO:HB2	2.01	0.42
1:a:366:LEU:O	1:a:370:VAL:HG23	2.20	0.42
2:b:74:GLU:OE1	11:m:1:MET:N	2.52	0.42
2:b:282:LEU:HD23	14:b:3020:CLA:HMC1	2.00	0.42
1:1:275:TYR:O	1:1:279:LEU:HB2	2.19	0.42
1:1:433:VAL:HA	1:1:436:HIS:CE1	2.54	0.42
14:1:824:CLA:O2D	14:1:824:CLA:H2A	2.18	0.42
2:2:533:LEU:O	2:2:537:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:7:ALA:N	11:y:5:ASP:OD1	2.52	0.42
14:A:807:CLA:H193	14:A:807:CLA:H151	2.02	0.42
16:A:849:BCR:H24C	16:A:849:BCR:H371	1.88	0.42
14:B:3034:CLA:O1D	8:J:35:ASP:HA	2.19	0.42
9:K:34:ILE:H	9:K:34:ILE:HD12	1.85	0.42
9:k:18:VAL:HG11	9:k:74:VAL:HG12	2.01	0.42
9:k:30:GLY:C	9:k:54:PHE:HZ	2.28	0.42
1:1:146:LEU:CD1	1:1:380:TYR:HE2	2.32	0.42
1:A:370:VAL:O	1:A:371:ALA:C	2.62	0.42
1:A:679:ALA:HB1	1:A:738:GLY:O	2.19	0.42
2:B:215:MET:HE1	9:k:82:ALA:HB2	2.02	0.42
1:a:679:ALA:HB1	1:a:738:GLY:O	2.20	0.42
2:b:90:ILE:HB	2:b:111:PRO:HB2	2.01	0.42
2:b:693:LEU:HD23	10:l:37:TYR:CE2	2.55	0.42
3:c:13:CYS:O	3:c:14:THR:OG1	2.26	0.42
9:k:20:ILE:HG13	9:k:21:LEU:N	2.34	0.42
10:l:60:GLY:N	10:l:61:PRO:CD	2.83	0.42
1:1:71:LYS:HE3	14:1:812:CLA:OBD	2.20	0.42
1:1:152:ILE:HG21	1:1:158:LEU:HD21	2.01	0.42
14:1:809:CLA:HAB	14:1:829:CLA:H142	2.01	0.42
2:2:318:PHE:CD2	14:2:3024:CLA:HMA3	2.54	0.42
3:3:28:VAL:HG21	4:4:111:ALA:HB2	2.01	0.42
9:9:23:ASN:ND2	9:9:67:HIS:CE1	2.87	0.42
10:0:60:GLY:N	10:0:61:PRO:CD	2.83	0.42
10:0:144:VAL:O	10:0:148:ILE:HG23	2.19	0.42
1:A:276:SER:O	1:A:276:SER:OG	2.36	0.42
1:A:373:HIS:CD2	14:A:828:CLA:NC	2.88	0.42
16:A:851:BCR:H24C	14:B:3034:CLA:HMC3	2.02	0.42
2:B:318:PHE:CD2	14:B:3024:CLA:HMA3	2.54	0.42
2:B:377:HIS:CE1	14:B:3028:CLA:ND	2.87	0.42
1:a:26:GLU:C	1:a:26:GLU:OE1	2.63	0.42
1:a:71:LYS:HE3	14:a:811:CLA:OBD	2.20	0.42
1:a:152:ILE:HG21	1:a:158:LEU:HD21	2.01	0.42
1:a:601:TRP:CH2	14:a:803:CLA:CBB	3.02	0.42
2:b:307:LYS:HE3	2:b:313:LYS:CG	2.49	0.42
1:1:366:LEU:O	1:1:370:VAL:HG23	2.20	0.42
2:2:693:LEU:HD23	10:0:37:TYR:CE2	2.55	0.42
14:2:3022:CLA:O2D	14:2:3022:CLA:H2A	2.20	0.42
10:0:131:SER:O	10:0:134:VAL:HG12	2.19	0.42
1:A:26:GLU:C	1:A:26:GLU:OE1	2.63	0.42
1:A:601:TRP:CH2	14:A:803:CLA:CBB	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:PRO:HB3	14:B:3041:CLA:C1C	2.49	0.42
6:F:57:LEU:O	6:F:58:SER:HB3	2.19	0.42
6:F:76:TRP:HE1	14:F:203:CLA:CAD	2.32	0.42
10:L:60:GLY:N	10:L:61:PRO:CD	2.83	0.42
2:b:74:GLU:HA	2:b:77:VAL:HG22	2.01	0.42
14:b:3022:CLA:H2A	14:b:3022:CLA:O2D	2.20	0.42
4:d:3:LEU:HD11	4:d:83:TYR:CD1	2.54	0.42
14:l:807:CLA:H151	14:l:807:CLA:H193	2.02	0.42
4:4:10:TYR:OH	4:4:44:ALA:O	2.25	0.42
6:6:76:TRP:HE1	14:6:203:CLA:CAD	2.32	0.42
9:9:18:VAL:HG11	9:9:74:VAL:HG12	2.01	0.42
1:A:275:TYR:O	1:A:279:LEU:HB2	2.19	0.42
7:l:26:VAL:HG13	17:l:202:LHG:H152	2.01	0.42
9:K:30:GLY:C	9:K:54:PHE:HZ	2.28	0.42
10:L:144:VAL:O	10:L:148:ILE:HG23	2.19	0.42
1:a:289:THR:HA	1:a:382:TYR:CE1	2.55	0.42
2:b:74:GLU:O	2:b:78:GLN:HG2	2.20	0.42
3:c:28:VAL:HG21	4:d:111:ALA:HB2	2.02	0.42
2:2:553:MET:HE1	2:2:563:PHE:CE2	2.55	0.42
9:9:34:ILE:HD12	9:9:34:ILE:H	1.85	0.42
1:A:432:ARG:O	1:A:436:HIS:ND1	2.53	0.42
9:K:18:VAL:HG11	9:K:74:VAL:HG12	2.01	0.42
2:b:703:PRO:HB3	14:b:3041:CLA:C1C	2.49	0.42
16:b:3047:BCR:H24C	16:b:3047:BCR:H371	1.81	0.42
9:k:34:ILE:H	9:k:34:ILE:HD12	1.85	0.42
2:2:377:HIS:CE1	14:2:3028:CLA:ND	2.87	0.42
10:0:57:PHE:CD1	14:0:209:CLA:HBC2	2.55	0.42
2:B:74:GLU:HA	2:B:77:VAL:HG22	2.01	0.42
3:C:75:SER:O	21:C:204:HOH:O	2.22	0.42
5:E:27:ASP:OD2	5:E:32:VAL:HG21	2.20	0.42
9:K:23:ASN:ND2	9:K:67:HIS:CE1	2.87	0.42
9:K:30:GLY:O	9:K:37:ARG:NH2	2.47	0.42
10:L:57:PHE:CD1	14:L:205:CLA:HBC2	2.55	0.42
1:a:168:MET:HE1	14:a:805:CLA:H201	2.02	0.42
1:a:337:THR:O	1:a:337:THR:CG2	2.68	0.42
14:a:806:CLA:H151	14:a:806:CLA:H193	2.02	0.42
14:a:841:CLA:HHC	14:a:841:CLA:HBB1	2.02	0.42
10:l:144:VAL:O	10:l:148:ILE:HG23	2.19	0.42
1:1:231:VAL:HG12	1:1:232:ALA:N	2.35	0.42
1:1:289:THR:HA	1:1:382:TYR:CE1	2.55	0.42
1:1:679:ALA:HB1	1:1:738:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:805:CLA:HBC3	14:1:805:CLA:HHD	2.02	0.42
14:1:809:CLA:HBA2	14:1:809:CLA:H3A	1.92	0.42
14:2:3017:CLA:H2A	14:2:3017:CLA:O2D	2.20	0.42
1:A:321:ILE:HD11	14:A:821:CLA:H2A	2.02	0.41
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.54	0.41
14:A:809:CLA:H93	16:J:103:BCR:H403	2.01	0.41
2:B:553:MET:HE1	2:B:563:PHE:CE2	2.55	0.41
14:B:3026:CLA:C10	16:B:3048:BCR:H333	2.50	0.41
6:F:115:ALA:HB1	6:F:118:LEU:HD23	2.01	0.41
14:F:203:CLA:HBC2	8:J:19:MET:HE3	2.01	0.41
14:a:831:CLA:O1D	10:l:5:VAL:HG11	2.20	0.41
16:a:850:BCR:H362	14:b:3003:CLA:C4	2.50	0.41
14:b:3012:CLA:H203	14:b:3015:CLA:H91	2.02	0.41
14:b:3039:CLA:HBC2	16:j:1106:BCR:HC7	2.01	0.41
1:1:321:ILE:HD11	14:1:821:CLA:H2A	2.02	0.41
14:1:810:CLA:H143	16:8:104:BCR:H383	2.01	0.41
16:1:850:BCR:C8	16:1:850:BCR:H321	2.50	0.41
2:2:261:HIS:HD2	2:2:263:GLN:H	1.68	0.41
2:2:413:ARG:HH21	14:2:3031:CLA:CAD	2.30	0.41
14:2:3026:CLA:C10	16:2:3048:BCR:H333	2.50	0.41
14:2:3036:CLA:HHC	14:2:3036:CLA:HBB1	2.02	0.41
1:A:280:THR:HG23	1:A:295:SER:OG	2.20	0.41
1:A:366:LEU:O	1:A:370:VAL:HG23	2.20	0.41
1:A:372:GLN:HA	1:A:375:TYR:CE1	2.54	0.41
14:a:804:CLA:HBC3	14:a:804:CLA:HHD	2.02	0.41
14:b:3003:CLA:H61	14:b:3003:CLA:H41	1.93	0.41
14:b:3017:CLA:O2D	14:b:3017:CLA:H2A	2.20	0.41
6:f:57:LEU:O	6:f:58:SER:HB3	2.19	0.41
10:l:131:SER:O	10:l:134:VAL:HG12	2.19	0.41
1:1:337:THR:O	1:1:337:THR:CG2	2.68	0.41
2:2:286:ALA:HB2	14:2:3020:CLA:HBC2	2.03	0.41
2:2:470:HIS:CE1	14:2:3035:CLA:NA	2.89	0.41
6:6:42:LEU:O	6:6:49:PRO:HA	2.21	0.41
2:B:319:ASN:O	17:B:3051:LHG:HC91	2.21	0.41
2:B:470:HIS:CE1	14:B:3035:CLA:NA	2.89	0.41
1:a:564:ARG:HD3	3:c:79:ALA:HB3	2.02	0.41
2:b:123:TRP:HA	2:b:126:ILE:HG12	2.03	0.41
2:b:238:THR:HG22	2:b:240:SER:H	1.86	0.41
14:b:3026:CLA:H102	16:b:3048:BCR:H333	2.02	0.41
1:1:280:THR:HG23	1:1:295:SER:OG	2.21	0.41
1:1:452:GLY:O	1:1:453:PHE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:27:ILE:HG12	9:9:62:THR:HB	2.02	0.41
1:A:431:ASP:O	1:A:435:ARG:HG3	2.21	0.41
14:A:842:CLA:C19	8:J:23:ALA:HB2	2.51	0.41
2:B:238:THR:HG22	2:B:240:SER:H	1.86	0.41
14:B:3012:CLA:H203	14:B:3015:CLA:H91	2.02	0.41
10:L:52:MET:HA	10:L:131:SER:HB2	2.01	0.41
10:L:57:PHE:CD2	10:L:57:PHE:C	2.98	0.41
14:L:205:CLA:H92	14:L:205:CLA:H62	1.93	0.41
1:a:341:HIS:HB3	1:a:344:LEU:HD12	2.02	0.41
2:b:487:ILE:HG22	14:b:3036:CLA:HMD1	2.03	0.41
9:k:67:HIS:CE1	16:k:103:BCR:C12	3.04	0.41
10:l:52:MET:HA	10:l:131:SER:HB2	2.01	0.41
1:1:373:HIS:CD2	14:1:828:CLA:NC	2.88	0.41
1:1:564:ARG:HD3	3:3:79:ALA:HB3	2.03	0.41
2:2:668:MET:O	2:2:672:SER:OG	2.35	0.41
9:9:30:GLY:C	9:9:54:PHE:HZ	2.28	0.41
1:A:337:THR:O	1:A:337:THR:CG2	2.68	0.41
1:A:401:GLY:O	1:A:405:VAL:HG23	2.21	0.41
1:A:495:THR:HG21	1:A:514:GLY:HA3	2.02	0.41
14:A:817:CLA:HED2	14:A:817:CLA:HBD	1.92	0.41
2:B:286:ALA:HB2	14:B:3020:CLA:HBC2	2.03	0.41
1:a:401:GLY:O	1:a:405:VAL:HG23	2.21	0.41
16:a:848:BCR:H24C	16:a:848:BCR:H371	1.88	0.41
14:b:3010:CLA:CGA	14:b:3010:CLA:C1A	2.99	0.41
6:f:115:ALA:HB1	6:f:118:LEU:HD23	2.01	0.41
14:j:1101:CLA:H202	14:j:1101:CLA:H161	1.92	0.41
10:l:57:PHE:CD2	10:l:57:PHE:C	2.98	0.41
10:l:57:PHE:CD1	14:l:208:CLA:HBC2	2.55	0.41
14:1:842:CLA:HHC	14:1:842:CLA:HBB1	2.02	0.41
16:1:850:BCR:H362	14:2:3003:CLA:C4	2.51	0.41
2:2:466:ILE:O	2:2:470:HIS:HD2	2.04	0.41
2:2:487:ILE:HG22	14:2:3036:CLA:HMD1	2.03	0.41
2:2:661:LEU:O	2:2:665:THR:OG1	2.35	0.41
6:6:33:LYS:HE3	6:6:37:ARG:NH1	2.36	0.41
1:A:71:LYS:HE3	14:A:812:CLA:OBD	2.20	0.41
14:A:815:CLA:CHC	16:A:847:BCR:H352	2.50	0.41
2:B:47:ALA:HB3	11:M:29:LEU:HD21	2.02	0.41
14:B:3022:CLA:H2A	14:B:3022:CLA:O2D	2.20	0.41
1:a:431:ASP:O	1:a:435:ARG:HG3	2.21	0.41
1:a:466:ARG:HG2	1:a:466:ARG:NH1	2.36	0.41
2:b:553:MET:HE1	2:b:563:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:164:GLY:O	1:1:167:VAL:HG22	2.20	0.41
1:1:546:ILE:O	1:1:550:VAL:HG23	2.21	0.41
14:1:815:CLA:CHC	16:1:846:BCR:H352	2.50	0.41
2:2:74:GLU:O	2:2:78:GLN:HG2	2.20	0.41
14:2:3010:CLA:CGA	14:2:3010:CLA:C1A	2.99	0.41
14:2:3012:CLA:H203	14:2:3015:CLA:H91	2.02	0.41
12:z:29:TYR:CE1	12:z:34:LEU:HD23	2.56	0.41
1:A:289:THR:HA	1:A:382:TYR:CE1	2.55	0.41
1:A:452:GLY:O	1:A:453:PHE:C	2.64	0.41
14:A:820:CLA:HBA2	14:A:820:CLA:H3A	1.96	0.41
14:B:3003:CLA:H61	14:B:3003:CLA:H41	1.93	0.41
9:K:20:ILE:HG13	9:K:21:LEU:N	2.34	0.41
1:a:546:ILE:O	1:a:550:VAL:HG23	2.21	0.41
2:b:41:LEU:O	2:b:45:ILE:HG13	2.20	0.41
2:b:286:ALA:HB2	14:b:3020:CLA:HBC2	2.03	0.41
4:d:1:THR:OG1	4:d:2:THR:N	2.47	0.41
8:j:33:TYR:HD2	16:j:1106:BCR:H401	1.81	0.41
16:1:850:BCR:H24C	14:2:3034:CLA:HMC1	2.03	0.41
2:2:97:LYS:NZ	2:2:101:ASP:OD1	2.51	0.41
14:2:3009:CLA:H203	14:2:3028:CLA:H191	2.03	0.41
1:A:168:MET:HE1	14:A:806:CLA:H201	2.02	0.41
14:A:817:CLA:H61	14:A:817:CLA:H41	1.87	0.41
2:B:437:LEU:O	2:B:441:VAL:HG23	2.21	0.41
6:F:51:LEU:HD22	6:F:62:ASP:CB	2.50	0.41
2:b:433:GLY:HA2	2:b:531:LEU:HD22	2.03	0.41
14:b:3026:CLA:C10	16:b:3048:BCR:H333	2.50	0.41
12:x:22:ILE:HA	12:x:25:LEU:HB2	2.03	0.41
2:2:256:PHE:CD2	2:2:256:PHE:O	2.74	0.41
2:2:425:LEU:HG	14:2:3040:CLA:CBB	2.51	0.41
14:2:3026:CLA:H102	16:2:3048:BCR:H333	2.02	0.41
14:2:3034:CLA:H2A	14:2:3034:CLA:HED2	2.03	0.41
1:A:546:ILE:O	1:A:550:VAL:HG23	2.21	0.41
2:B:307:LYS:HE3	2:B:313:LYS:CG	2.50	0.41
2:B:433:GLY:HA2	2:B:531:LEU:HD22	2.03	0.41
2:B:553:MET:HE2	2:B:566:ASP:HB2	2.03	0.41
2:B:693:LEU:HD23	10:L:37:TYR:CE2	2.55	0.41
14:B:3017:CLA:O2D	14:B:3017:CLA:H2A	2.20	0.41
14:B:3036:CLA:HHC	14:B:3036:CLA:HBB1	2.02	0.41
14:B:3036:CLA:HMD3	21:B:3147:HOH:O	2.21	0.41
3:C:8:ASP:OD1	4:D:115:VAL:O	2.38	0.41
6:F:42:LEU:O	6:F:49:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:118:LEU:CD2	14:F:204:CLA:HBB2	2.51	0.41
8:J:32:PHE:C	8:J:34:PRO:HD3	2.46	0.41
12:X:29:TYR:CE1	12:X:34:LEU:HD23	2.56	0.41
1:a:164:GLY:O	1:a:167:VAL:HG22	2.20	0.41
1:a:231:VAL:HG12	1:a:232:ALA:N	2.35	0.41
1:a:280:THR:HG23	1:a:295:SER:OG	2.21	0.41
1:a:373:HIS:CD2	14:a:827:CLA:NC	2.88	0.41
1:a:432:ARG:O	1:a:436:HIS:ND1	2.53	0.41
1:a:495:THR:HG21	1:a:514:GLY:HA3	2.02	0.41
2:b:181:LEU:O	2:b:185:SER:HB2	2.21	0.41
2:b:437:LEU:O	2:b:441:VAL:HG23	2.21	0.41
2:b:523:PHE:HZ	16:j:1106:BCR:C32	2.34	0.41
14:b:3018:CLA:HBA1	14:b:3018:CLA:H3A	1.92	0.41
5:e:27:ASP:OD2	5:e:32:VAL:HG21	2.20	0.41
6:f:118:LEU:CD2	14:f:204:CLA:HBB2	2.51	0.41
9:k:27:ILE:HG12	9:k:62:THR:HB	2.03	0.41
12:x:29:TYR:CE1	12:x:34:LEU:HD23	2.56	0.41
1:1:26:GLU:OE1	1:1:26:GLU:C	2.63	0.41
1:1:307:LEU:HD21	14:1:818:CLA:H141	2.03	0.41
1:1:401:GLY:O	1:1:405:VAL:HG23	2.21	0.41
1:1:614:SER:O	1:1:618:GLN:HG3	2.21	0.41
1:1:711:LEU:HD21	14:2:3032:CLA:H3A	2.03	0.41
16:1:847:BCR:H311	16:1:847:BCR:H342	2.03	0.41
2:2:41:LEU:O	2:2:45:ILE:HG13	2.21	0.41
2:2:135:TYR:OH	11:y:10:VAL:CG2	2.68	0.41
2:2:139:ILE:HD12	11:y:14:ILE:HD12	2.03	0.41
2:2:437:LEU:O	2:2:441:VAL:HG23	2.21	0.41
2:2:553:MET:HE2	2:2:566:ASP:HB2	2.03	0.41
16:2:3052:BCR:H401	8:8:33:TYR:HD2	1.82	0.41
10:0:52:MET:HA	10:0:131:SER:HB2	2.01	0.41
1:A:164:GLY:O	1:A:167:VAL:HG22	2.20	0.41
1:A:614:SER:O	1:A:618:GLN:HG3	2.21	0.41
16:A:848:BCR:H311	16:A:848:BCR:H342	2.03	0.41
5:E:36:VAL:CG2	5:E:62:LEU:HD12	2.52	0.41
9:K:67:HIS:CE1	16:K:103:BCR:C12	3.04	0.41
1:a:317:THR:HG21	14:a:812:CLA:CMA	2.51	0.41
1:a:614:SER:O	1:a:618:GLN:HG3	2.21	0.41
14:a:832:CLA:H142	14:a:832:CLA:H112	1.95	0.41
16:a:850:BCR:C8	16:a:850:BCR:H321	2.50	0.41
2:b:466:ILE:O	2:b:470:HIS:HD2	2.04	0.41
1:1:16:VAL:HG12	1:1:17:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:168:MET:HE1	14:1:806:CLA:H201	2.03	0.41
14:2:3006:CLA:H142	16:y:101:BCR:H12C	2.03	0.41
1:A:336:PHE:O	1:A:432:ARG:NH2	2.49	0.40
1:A:591:GLY:O	1:A:595:VAL:HG23	2.21	0.40
2:B:41:LEU:O	2:B:45:ILE:HG13	2.21	0.40
2:B:425:LEU:HG	14:B:3040:CLA:CBB	2.51	0.40
2:B:576:ILE:HG12	2:B:576:ILE:O	2.22	0.40
14:B:3038:CLA:C14	12:X:19:LEU:HD13	2.47	0.40
6:F:33:LYS:HE3	6:F:37:ARG:NH1	2.36	0.40
9:K:27:ILE:HG12	9:K:62:THR:HB	2.03	0.40
14:a:814:CLA:CHC	16:a:846:BCR:H352	2.50	0.40
16:a:849:BCR:H20C	16:a:849:BCR:H361	1.97	0.40
14:b:3036:CLA:HHC	14:b:3036:CLA:HBB1	2.02	0.40
6:f:42:LEU:O	6:f:49:PRO:HA	2.21	0.40
1:1:495:THR:HG21	1:1:514:GLY:HA3	2.02	0.40
1:1:591:GLY:O	1:1:595:VAL:HG23	2.21	0.40
14:1:809:CLA:H93	16:8:103:BCR:H403	2.04	0.40
2:2:123:TRP:HA	2:2:126:ILE:HG12	2.03	0.40
8:8:32:PHE:C	8:8:34:PRO:HD3	2.46	0.40
10:0:80:ILE:HG22	14:0:204:CLA:H41	2.04	0.40
1:A:111:LYS:O	1:A:130:VAL:HB	2.22	0.40
14:B:3006:CLA:C1	17:l:201:LHG:H282	2.51	0.40
14:B:3010:CLA:CGA	14:B:3010:CLA:C1A	2.99	0.40
14:B:3033:CLA:HHD	14:B:3033:CLA:CBC	2.45	0.40
16:B:3047:BCR:H20C	16:B:3047:BCR:H361	1.97	0.40
7:I:19:CYS:HB3	14:L:201:CLA:CBB	2.50	0.40
1:a:16:VAL:HG12	1:a:17:ASP:N	2.36	0.40
1:a:591:GLY:O	1:a:595:VAL:HG23	2.21	0.40
2:b:261:HIS:HD2	2:b:263:GLN:H	1.68	0.40
2:b:425:LEU:HG	14:b:3040:CLA:CBB	2.51	0.40
2:b:576:ILE:HG12	2:b:576:ILE:O	2.22	0.40
1:1:319:TRP:O	1:1:321:ILE:N	2.52	0.40
6:6:56:ARG:HB2	12:z:31:PHE:CZ	2.56	0.40
10:0:57:PHE:CD2	10:0:57:PHE:C	2.98	0.40
14:z:1701:CLA:HBC2	14:z:1701:CLA:HHD	2.04	0.40
1:A:341:HIS:HB3	1:A:344:LEU:HD12	2.02	0.40
1:A:561:ARG:NE	4:D:40:GLU:OE2	2.52	0.40
14:A:810:CLA:H93	14:A:810:CLA:H111	1.97	0.40
2:B:222:ALA:HB3	2:B:223:PRO:HD3	2.04	0.40
5:E:36:VAL:CG2	5:E:62:LEU:CD1	3.00	0.40
12:X:22:ILE:HA	12:X:25:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:256:PHE:CD2	2:b:256:PHE:O	2.74	0.40
2:b:470:HIS:CE1	14:b:3035:CLA:NA	2.89	0.40
2:b:487:ILE:HG22	14:b:3036:CLA:CMD	2.52	0.40
14:b:3014:CLA:H141	14:b:3014:CLA:H162	1.97	0.40
5:e:36:VAL:CG2	5:e:62:LEU:CD1	2.99	0.40
1:1:317:THR:HG21	14:1:813:CLA:CMA	2.51	0.40
1:1:466:ARG:HG2	1:1:466:ARG:NH1	2.36	0.40
14:1:839:CLA:HMB3	14:1:839:CLA:HBB1	2.04	0.40
4:4:1:THR:O	4:4:2:THR:OG1	2.22	0.40
5:5:27:ASP:OD2	5:5:32:VAL:HG21	2.20	0.40
6:6:118:LEU:CD2	14:6:204:CLA:HBB2	2.51	0.40
1:A:92:PHE:HB2	1:A:162:ALA:HB1	2.04	0.40
1:A:144:PHE:N	1:A:144:PHE:CD1	2.90	0.40
1:A:307:LEU:HD21	14:A:818:CLA:H141	2.03	0.40
2:B:74:GLU:O	2:B:78:GLN:HG2	2.20	0.40
14:B:3015:CLA:H93	14:B:3015:CLA:H111	1.99	0.40
14:B:3034:CLA:HBB1	14:B:3034:CLA:HMB3	2.03	0.40
1:a:215:HIS:HB2	14:a:814:CLA:CHC	2.52	0.40
14:a:806:CLA:HBB1	14:a:806:CLA:HMB3	2.03	0.40
2:b:44:LYS:NZ	11:m:29:LEU:O	2.55	0.40
2:b:276:HIS:HA	2:b:279:ILE:HG12	2.03	0.40
2:b:316:GLY:O	2:b:317:PRO:C	2.65	0.40
2:b:553:MET:HE2	2:b:566:ASP:HB2	2.03	0.40
14:b:3025:CLA:H141	14:b:3025:CLA:H162	1.92	0.40
14:b:3028:CLA:HBA2	14:b:3028:CLA:H3A	1.86	0.40
14:b:3040:CLA:HHC	14:b:3040:CLA:CBB	2.52	0.40
8:j:32:PHE:C	8:j:34:PRO:HD3	2.46	0.40
1:1:118:TRP:HB3	16:8:104:BCR:H323	2.03	0.40
14:1:829:CLA:H93	16:8:103:BCR:H361	2.02	0.40
2:2:238:THR:HG22	2:2:240:SER:H	1.86	0.40
2:2:433:GLY:HA2	2:2:531:LEU:HD22	2.03	0.40
14:2:3036:CLA:HMD3	21:2:3147:HOH:O	2.21	0.40
5:5:36:VAL:CG2	5:5:62:LEU:CD1	2.99	0.40
5:5:36:VAL:CG2	5:5:62:LEU:HD12	2.51	0.40
6:6:51:LEU:HD22	6:6:62:ASP:CB	2.49	0.40
9:9:67:HIS:CE1	16:9:104:BCR:C12	3.04	0.40
1:A:726:GLN:O	1:A:730:VAL:HG23	2.22	0.40
2:B:316:GLY:O	2:B:319:ASN:CA	2.70	0.40
2:B:466:ILE:O	2:B:470:HIS:HD2	2.03	0.40
1:a:129:ASP:OD2	1:a:129:ASP:N	2.55	0.40
1:a:249:MET:HG2	14:a:815:CLA:HED1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:321:ILE:HG13	14:a:820:CLA:HED2	2.03	0.40
1:a:452:GLY:O	1:a:453:PHE:C	2.64	0.40
2:b:222:ALA:HB3	2:b:223:PRO:HD3	2.04	0.40
2:b:319:ASN:O	17:b:3051:LHG:HC91	2.21	0.40
2:b:618:SER:HA	2:b:621:TYR:CE1	2.57	0.40
1:1:321:ILE:HG13	14:1:821:CLA:HED2	2.03	0.40
1:1:341:HIS:HB3	1:1:344:LEU:HD12	2.02	0.40
1:1:431:ASP:O	1:1:435:ARG:HG3	2.21	0.40
1:1:613:PHE:O	1:1:617:MET:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	744/755 (98%)	688 (92%)	56 (8%)	0	100	100
1	A	744/755 (98%)	688 (92%)	56 (8%)	0	100	100
1	a	744/755 (98%)	688 (92%)	56 (8%)	0	100	100
2	2	738/741 (100%)	685 (93%)	53 (7%)	0	100	100
2	B	738/741 (100%)	685 (93%)	53 (7%)	0	100	100
2	b	738/741 (100%)	685 (93%)	53 (7%)	0	100	100
3	3	78/81 (96%)	66 (85%)	12 (15%)	0	100	100
3	C	78/81 (96%)	66 (85%)	12 (15%)	0	100	100
3	c	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
4	4	136/139 (98%)	119 (88%)	17 (12%)	0	100	100
4	D	136/139 (98%)	119 (88%)	17 (12%)	0	100	100
4	d	136/139 (98%)	119 (88%)	17 (12%)	0	100	100
5	5	68/76 (90%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	68/76 (90%)	67 (98%)	1 (2%)	0	100	100
5	e	68/76 (90%)	67 (98%)	1 (2%)	0	100	100
6	6	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
6	F	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
6	f	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
7	7	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	8	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	j	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	9	77/83 (93%)	73 (95%)	4 (5%)	0	100	100
9	K	77/83 (93%)	73 (95%)	4 (5%)	0	100	100
9	k	77/83 (93%)	73 (95%)	4 (5%)	0	100	100
10	0	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	L	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	l	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	y	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	X	25/36 (69%)	25 (100%)	0	0	100	100
12	x	25/36 (69%)	25 (100%)	0	0	100	100
12	z	25/36 (69%)	25 (100%)	0	0	100	100
All	All	6777/6951 (98%)	6241 (92%)	536 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	1	594/603 (98%)	592 (100%)	2 (0%)	86	91
1	A	594/603 (98%)	592 (100%)	2 (0%)	86	91
1	a	594/603 (98%)	592 (100%)	2 (0%)	86	91
2	2	597/598 (100%)	591 (99%)	6 (1%)	68	83
2	B	597/598 (100%)	591 (99%)	6 (1%)	68	83
2	b	597/598 (100%)	591 (99%)	6 (1%)	68	83
3	3	67/68 (98%)	65 (97%)	2 (3%)	36	67
3	C	67/68 (98%)	65 (97%)	2 (3%)	36	67
3	c	67/68 (98%)	65 (97%)	2 (3%)	36	67
4	4	115/116 (99%)	113 (98%)	2 (2%)	53	77
4	D	115/116 (99%)	113 (98%)	2 (2%)	53	77
4	d	115/116 (99%)	113 (98%)	2 (2%)	53	77
5	5	60/65 (92%)	56 (93%)	4 (7%)	15	44
5	E	60/65 (92%)	56 (93%)	4 (7%)	15	44
5	e	60/65 (92%)	56 (93%)	4 (7%)	15	44
6	6	109/109 (100%)	108 (99%)	1 (1%)	70	85
6	F	109/109 (100%)	108 (99%)	1 (1%)	70	85
6	f	109/109 (100%)	108 (99%)	1 (1%)	70	85
7	7	31/31 (100%)	31 (100%)	0	100	100
7	I	31/31 (100%)	31 (100%)	0	100	100
7	i	31/31 (100%)	31 (100%)	0	100	100
8	8	35/35 (100%)	32 (91%)	3 (9%)	10	34
8	J	35/35 (100%)	32 (91%)	3 (9%)	10	34
8	j	35/35 (100%)	32 (91%)	3 (9%)	10	34
9	9	58/61 (95%)	55 (95%)	3 (5%)	21	53
9	K	58/61 (95%)	55 (95%)	3 (5%)	21	53
9	k	58/61 (95%)	55 (95%)	3 (5%)	21	53
10	0	117/120 (98%)	116 (99%)	1 (1%)	70	85
10	L	117/120 (98%)	116 (99%)	1 (1%)	70	85
10	l	117/120 (98%)	116 (99%)	1 (1%)	70	85
11	M	26/26 (100%)	26 (100%)	0	100	100
11	m	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	y	26/26 (100%)	26 (100%)	0	100	100
12	X	21/28 (75%)	19 (90%)	2 (10%)	8	29
12	x	21/28 (75%)	19 (90%)	2 (10%)	8	29
12	z	21/28 (75%)	19 (90%)	2 (10%)	8	29
All	All	5490/5580 (98%)	5412 (99%)	78 (1%)	57	80

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	GLU
1	A	276	SER
2	B	34	ASP
2	B	109	SER
2	B	238	THR
2	B	332	SER
2	B	349	SER
2	B	486	SER
3	C	8	ASP
3	C	75	SER
4	D	98	ASP
4	D	131	THR
5	E	5	SER
5	E	32	VAL
5	E	53	SER
5	E	68	VAL
6	F	9	LYS
8	J	9	SER
8	J	13	VAL
8	J	33	TYR
9	K	14	SER
9	K	47	LEU
9	K	50	LEU
10	L	22	SER
12	X	12	ARG
12	X	18	LEU
1	a	188	GLU
1	a	276	SER
2	b	34	ASP
2	b	109	SER
2	b	238	THR
2	b	332	SER

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Mol	Chain	Res	Type
2	b	349	SER
2	b	486	SER
3	c	8	ASP
3	c	75	SER
4	d	98	ASP
4	d	131	THR
5	e	5	SER
5	e	32	VAL
5	e	53	SER
5	e	68	VAL
6	f	9	LYS
8	j	9	SER
8	j	13	VAL
8	j	33	TYR
9	k	14	SER
9	k	47	LEU
9	k	50	LEU
10	l	22	SER
12	x	12	ARG
12	x	18	LEU
1	1	188	GLU
1	1	276	SER
2	2	34	ASP
2	2	109	SER
2	2	238	THR
2	2	332	SER
2	2	349	SER
2	2	486	SER
3	3	8	ASP
3	3	75	SER
4	4	98	ASP
4	4	131	THR
5	5	5	SER
5	5	32	VAL
5	5	53	SER
5	5	68	VAL
6	6	9	LYS
8	8	9	SER
8	8	13	VAL
8	8	33	TYR
9	9	14	SER
9	9	47	LEU

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Mol	Chain	Res	Type
9	9	50	LEU
10	0	22	SER
12	z	12	ARG
12	z	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	127	ASN
1	A	191	GLN
1	A	198	ASN
1	A	199	HIS
1	A	286	ASN
1	A	301	HIS
1	A	353	HIS
1	A	372	GLN
1	A	397	HIS
1	A	411	HIS
1	A	618	GLN
1	A	641	GLN
1	A	718	GLN
2	B	157	GLN
2	B	177	HIS
2	B	210	ASN
2	B	261	HIS
2	B	405	GLN
2	B	406	ASN
2	B	416	GLN
2	B	470	HIS
2	B	639	ASN
3	C	15	GLN
4	D	71	GLN
9	K	23	ASN
10	L	9	ASN
10	L	16	HIS
10	L	75	ASN
12	X	23	ASN
1	a	43	GLN
1	a	93	HIS
1	a	127	ASN
1	a	191	GLN

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Mol	Chain	Res	Type
1	a	198	ASN
1	a	199	HIS
1	a	286	ASN
1	a	301	HIS
1	a	353	HIS
1	a	372	GLN
1	a	397	HIS
1	a	411	HIS
1	a	618	GLN
1	a	641	GLN
1	a	718	GLN
2	b	261	HIS
2	b	405	GLN
2	b	406	ASN
2	b	416	GLN
2	b	435	HIS
2	b	470	HIS
2	b	639	ASN
4	d	63	GLN
4	d	71	GLN
6	f	40	GLN
9	k	23	ASN
10	l	9	ASN
10	l	16	HIS
10	l	75	ASN
1	1	93	HIS
1	1	127	ASN
1	1	198	ASN
1	1	199	HIS
1	1	286	ASN
1	1	301	HIS
1	1	353	HIS
1	1	372	GLN
1	1	397	HIS
1	1	411	HIS
1	1	618	GLN
1	1	641	GLN
1	1	718	GLN
2	2	157	GLN
2	2	177	HIS
2	2	261	HIS
2	2	405	GLN

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Mol	Chain	Res	Type
2	2	406	ASN
2	2	416	GLN
2	2	470	HIS
2	2	639	ASN
4	4	71	GLN
4	4	121	GLN
9	9	23	ASN
10	0	9	ASN
10	0	16	HIS
10	0	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
7	FME	I	1	7	8,9,10	1.04	1 (12%)	8,9,11	1.22	1 (12%)
8	FME	8	1	8	8,9,10	0.98	0	8,9,11	0.97	0
8	FME	j	1	8	8,9,10	0.98	0	8,9,11	0.97	0
8	FME	J	1	8	8,9,10	0.98	0	8,9,11	0.97	0
7	FME	i	1	7	8,9,10	1.04	0	8,9,11	1.23	1 (12%)
7	FME	7	1	7	8,9,10	1.04	1 (12%)	8,9,11	1.23	1 (12%)

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
7	FME	I	1	7	-	3/7/9/11	-
8	FME	8	1	8	-	1/7/9/11	-
8	FME	j	1	8	-	1/7/9/11	-
8	FME	J	1	8	-	1/7/9/11	-
7	FME	i	1	7	-	3/7/9/11	-
7	FME	7	1	7	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	1	FME	CA-N	-2.03	1.43	1.46
7	I	1	FME	CA-N	-2.01	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	1	FME	C-CA-N	2.63	114.58	109.50
7	7	1	FME	C-CA-N	2.63	114.57	109.50
7	I	1	FME	C-CA-N	2.62	114.56	109.50

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	1	FME	C-CA-CB-CG
7	i	1	FME	C-CA-CB-CG
7	7	1	FME	C-CA-CB-CG
7	I	1	FME	N-CA-CB-CG
7	i	1	FME	N-CA-CB-CG
7	7	1	FME	N-CA-CB-CG
8	J	1	FME	CB-CG-SD-CE
8	j	1	FME	CB-CG-SD-CE
8	8	1	FME	CB-CG-SD-CE
7	I	1	FME	CB-CG-SD-CE
7	i	1	FME	CB-CG-SD-CE
7	7	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 6 are monoatomic - leaving 396 for Mogul analysis.

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	$\# Z > 2$
14	CLA	1	802	-	69,73,73	1.16	11 (15%)	82,113,113	1.48	10 (12%)
14	CLA	b	3009	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	7 (8%)
14	CLA	a	838	-	69,73,73	1.17	8 (11%)	82,113,113	1.36	6 (7%)
14	CLA	B	3009	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	7 (8%)
14	CLA	1	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	7 (8%)
14	CLA	2	3014	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	B	3016	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	a	823	-	69,73,73	1.17	9 (13%)	82,113,113	1.34	4 (4%)
16	BCR	0	210	-	41,41,41	1.24	5 (12%)	56,56,56	1.33	6 (10%)
14	CLA	a	826	21	69,73,73	1.16	10 (14%)	82,113,113	1.40	9 (10%)
14	CLA	b	3023	21	59,63,73	1.26	8 (13%)	70,101,113	1.38	6 (8%)
14	CLA	a	815	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	5 (6%)
14	CLA	A	827	21	69,73,73	1.15	9 (13%)	82,113,113	1.40	10 (12%)
14	CLA	L	204	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	8 (9%)
14	CLA	A	831	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	5 (6%)
14	CLA	1	811	-	53,57,73	1.31	9 (16%)	61,93,113	1.36	5 (8%)
14	CLA	b	3030	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
14	CLA	A	817	21	69,73,73	1.18	8 (11%)	82,113,113	1.38	8 (9%)
14	CLA	A	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	7 (8%)
16	BCR	9	102	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	10 (17%)
14	CLA	A	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
16	BCR	F	205	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	813	-	49,53,73	1.38	9 (18%)	58,89,113	1.49	4 (6%)
14	CLA	f	203	21	49,53,73	1.38	9 (18%)	58,89,113	1.47	6 (10%)
14	CLA	8	102	-	41,45,73	1.48	8 (19%)	50,78,113	1.39	4 (8%)
14	CLA	a	817	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
17	LHG	2	3051	-	48,48,48	0.69	2 (4%)	51,54,54	1.20	5 (9%)
20	LMG	b	3050	-	55,55,55	0.91	4 (7%)	63,63,63	1.35	9 (14%)
14	CLA	a	809	1	69,73,73	1.17	9 (13%)	82,113,113	1.34	8 (9%)
14	CLA	f	201	21	62,66,73	1.23	9 (14%)	73,104,113	1.37	6 (8%)
14	CLA	1	839	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
14	CLA	1	817	21	69,73,73	1.17	9 (13%)	82,113,113	1.38	8 (9%)
16	BCR	6	205	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	b	3036	21	54,58,73	1.36	8 (14%)	64,95,113	1.41	7 (10%)
16	BCR	A	850	-	41,41,41	1.36	4 (9%)	56,56,56	1.32	7 (12%)
16	BCR	j	1106	-	41,41,41	1.29	2 (4%)	56,56,56	1.44	11 (19%)
14	CLA	2	3003	21	69,73,73	1.16	10 (14%)	82,113,113	1.50	10 (12%)
14	CLA	A	813	-	49,53,73	1.37	9 (18%)	58,89,113	1.48	4 (6%)
16	BCR	A	848	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	7 (12%)
14	CLA	l	203	2	69,73,73	1.17	9 (13%)	82,113,113	1.37	9 (10%)
16	BCR	b	3045	-	41,41,41	1.19	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	2	3013	-	49,53,73	1.35	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	2	3005	-	69,73,73	1.15	6 (8%)	82,113,113	1.47	7 (8%)
14	CLA	A	837	1	49,53,73	1.39	8 (16%)	58,89,113	1.37	6 (10%)
14	CLA	B	3018	-	69,73,73	1.17	7 (10%)	82,113,113	1.33	8 (9%)
14	CLA	2	3019	-	69,73,73	1.15	8 (11%)	82,113,113	1.38	8 (9%)
14	CLA	b	3017	-	69,73,73	1.15	8 (11%)	82,113,113	1.52	10 (12%)
14	CLA	2	3025	2	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
16	BCR	b	3044	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
14	CLA	2	3004	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	5 (6%)
18	SF4	B	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	1	821	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	7 (8%)
14	CLA	B	3042	-	69,73,73	1.18	8 (11%)	82,113,113	1.39	7 (8%)
14	CLA	2	3041	21	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
16	BCR	b	3047	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	7 (12%)
17	LHG	a	853	14	40,40,48	0.79	2 (5%)	43,46,54	1.19	3 (6%)
14	CLA	2	3024	-	49,53,73	1.38	9 (18%)	58,89,113	1.48	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	3008	-	69,73,73	1.18	8 (11%)	82,113,113	1.34	6 (7%)
14	CLA	x	1701	-	49,53,73	1.41	7 (14%)	58,89,113	1.41	4 (6%)
16	BCR	1	847	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	7 (12%)
14	CLA	a	808	1	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)
14	CLA	F	204	-	54,58,73	1.33	7 (12%)	64,95,113	1.45	7 (10%)
14	CLA	A	821	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	7 (8%)
16	BCR	k	103	-	25,25,41	1.11	1 (4%)	33,33,56	1.25	3 (9%)
16	BCR	L	206	-	41,41,41	1.19	4 (9%)	56,56,56	1.20	4 (7%)
16	BCR	0	205	-	41,41,41	1.45	5 (12%)	56,56,56	1.31	6 (10%)
14	CLA	b	3004	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	5 (6%)
14	CLA	b	3006	-	69,73,73	1.17	9 (13%)	82,113,113	1.38	7 (8%)
16	BCR	l	209	-	41,41,41	1.23	5 (12%)	56,56,56	1.33	6 (10%)
14	CLA	b	3031	-	59,63,73	1.27	9 (15%)	70,101,113	1.36	8 (11%)
14	CLA	a	835	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	5 (6%)
16	BCR	6	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	7 (12%)
15	PQN	a	844	-	34,34,34	0.44	0	43,45,45	0.50	1 (2%)
14	CLA	a	833	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	9 (10%)
16	BCR	1	851	-	25,25,41	1.16	1 (4%)	33,33,56	1.29	4 (12%)
14	CLA	2	3036	21	54,58,73	1.36	8 (14%)	64,95,113	1.41	8 (12%)
14	CLA	b	3012	-	69,73,73	1.16	7 (10%)	82,113,113	1.43	8 (9%)
15	PQN	1	845	-	34,34,34	0.44	0	43,45,45	0.49	1 (2%)
14	CLA	1	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	4 (4%)
14	CLA	1	840	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
14	CLA	A	823	-	49,53,73	1.37	8 (16%)	58,89,113	1.46	6 (10%)
14	CLA	2	3038	-	64,68,73	1.22	9 (14%)	76,107,113	1.35	5 (6%)
14	CLA	1	803	21	69,73,73	1.21	9 (13%)	82,113,113	1.22	3 (3%)
14	CLA	A	808	-	55,59,73	1.29	8 (14%)	64,96,113	1.41	6 (9%)
14	CLA	2	3033	-	69,73,73	1.16	9 (13%)	82,113,113	1.43	8 (9%)
14	CLA	B	3028	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	8 (9%)
14	CLA	A	815	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
14	CLA	A	834	-	69,73,73	1.16	10 (14%)	82,113,113	1.41	9 (10%)
14	CLA	b	3021	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	5 (6%)
13	CL0	a	801	-	58,73,73	2.17	13 (22%)	60,113,113	1.78	14 (23%)
14	CLA	A	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	4 (4%)
14	CLA	1	826	21	69,73,73	1.17	9 (13%)	82,113,113	1.39	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	815	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
14	CLA	b	3025	2	69,73,73	1.18	9 (13%)	82,113,113	1.24	5 (6%)
14	CLA	2	3029	-	69,73,73	1.18	8 (11%)	82,113,113	1.19	5 (6%)
16	BCR	A	847	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	5 (8%)
14	CLA	A	803	21	69,73,73	1.22	8 (11%)	82,113,113	1.23	3 (3%)
14	CLA	2	3020	21	69,73,73	1.17	8 (11%)	82,113,113	1.31	5 (6%)
14	CLA	2	3040	-	51,55,73	1.34	8 (15%)	60,91,113	1.33	5 (8%)
14	CLA	L	201	2	69,73,73	1.16	10 (14%)	82,113,113	1.38	9 (10%)
14	CLA	1	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.47	7 (8%)
14	CLA	2	3039	-	69,73,73	1.17	10 (14%)	82,113,113	1.45	9 (10%)
14	CLA	l	206	10	69,73,73	1.18	9 (13%)	82,113,113	1.35	9 (10%)
17	LHG	L	207	-	48,48,48	0.70	1 (2%)	51,54,54	1.32	5 (9%)
14	CLA	B	3035	-	69,73,73	1.16	7 (10%)	82,113,113	1.34	5 (6%)
14	CLA	A	838	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	9 (10%)
14	CLA	1	809	1	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)
14	CLA	b	3040	-	51,55,73	1.35	8 (15%)	60,91,113	1.33	5 (8%)
14	CLA	1	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
16	BCR	b	3046	-	41,41,41	1.28	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	a	842	21	69,73,73	1.19	10 (14%)	82,113,113	1.37	6 (7%)
14	CLA	b	3027	-	69,73,73	1.19	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	A	812	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
14	CLA	A	833	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
14	CLA	1	831	-	69,73,73	1.19	8 (11%)	82,113,113	1.34	6 (7%)
14	CLA	8	101	-	49,53,73	1.39	9 (18%)	58,89,113	1.44	5 (8%)
16	BCR	B	3044	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
14	CLA	L	203	10	69,73,73	1.19	9 (13%)	82,113,113	1.35	9 (10%)
14	CLA	6	203	21	49,53,73	1.38	9 (18%)	58,89,113	1.46	6 (10%)
14	CLA	j	1102	-	49,53,73	1.39	6 (12%)	58,89,113	1.45	5 (8%)
14	CLA	2	3006	-	69,73,73	1.17	9 (13%)	82,113,113	1.39	7 (8%)
18	SF4	c	102	3	0,12,12	-	-	-	-	-
14	CLA	1	812	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
14	CLA	A	816	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	5 (6%)
14	CLA	a	837	-	69,73,73	1.18	9 (13%)	82,113,113	1.44	9 (10%)
17	LHG	B	3051	-	48,48,48	0.69	2 (4%)	51,54,54	1.21	5 (9%)
14	CLA	b	3033	-	69,73,73	1.16	9 (13%)	82,113,113	1.44	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	B	3053	-	41,41,41	1.29	2 (4%)	56,56,56	1.44	11 (19%)
14	CLA	A	842	-	69,73,73	1.18	9 (13%)	82,113,113	1.32	9 (10%)
14	CLA	X	1701	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
17	LHG	1	853	14	40,40,48	0.79	2 (5%)	43,46,54	1.19	3 (6%)
16	BCR	9	104	-	25,25,41	1.10	1 (4%)	33,33,56	1.25	2 (6%)
16	BCR	A	851	-	41,41,41	1.34	4 (9%)	56,56,56	1.32	6 (10%)
16	BCR	B	3045	-	41,41,41	1.18	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	a	807	-	55,59,73	1.30	8 (14%)	64,96,113	1.41	6 (9%)
15	PQN	A	845	-	34,34,34	0.44	0	43,45,45	0.49	1 (2%)
16	BCR	j	1105	-	41,41,41	1.22	3 (7%)	56,56,56	1.30	8 (14%)
14	CLA	2	3035	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	5 (6%)
14	CLA	A	840	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	6 (7%)
16	BCR	a	849	-	41,41,41	1.36	4 (9%)	56,56,56	1.32	7 (12%)
14	CLA	l	208	21	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
14	CLA	B	3004	-	69,73,73	1.16	7 (10%)	82,113,113	1.34	5 (6%)
14	CLA	2	3034	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	K	103	-	25,25,41	1.11	1 (4%)	33,33,56	1.25	2 (6%)
16	BCR	8	103	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	5 (8%)
14	CLA	a	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.39	5 (6%)
16	BCR	j	1104	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	5 (8%)
14	CLA	1	843	21	69,73,73	1.18	10 (14%)	82,113,113	1.37	6 (7%)
14	CLA	2	3022	-	49,53,73	1.37	7 (14%)	58,89,113	1.53	6 (10%)
16	BCR	2	3045	-	41,41,41	1.19	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	1	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	4 (4%)
14	CLA	a	839	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
14	CLA	B	3030	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
14	CLA	A	820	-	69,73,73	1.18	9 (13%)	82,113,113	1.41	9 (10%)
17	LHG	b	3051	-	48,48,48	0.68	2 (4%)	51,54,54	1.20	5 (9%)
14	CLA	1	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	5 (6%)
14	CLA	B	3014	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	a	841	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	8 (9%)
16	BCR	J	103	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	5 (8%)
14	CLA	9	101	-	50,54,73	1.37	9 (18%)	59,90,113	1.39	4 (6%)
14	CLA	1	825	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	813	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	4 (4%)
14	CLA	a	822	-	49,53,73	1.37	9 (18%)	58,89,113	1.48	6 (10%)
14	CLA	j	1103	-	41,45,73	1.48	10 (24%)	50,78,113	1.40	5 (10%)
14	CLA	B	3015	-	69,73,73	1.16	7 (10%)	82,113,113	1.31	9 (10%)
14	CLA	a	820	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	7 (8%)
13	CL0	1	801	-	58,73,73	2.18	13 (22%)	60,113,113	1.79	14 (23%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	F	203	21	49,53,73	1.39	9 (18%)	58,89,113	1.46	6 (10%)
14	CLA	L	205	21	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
16	BCR	I	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.27	4 (7%)
16	BCR	a	847	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	7 (12%)
14	CLA	b	3024	-	49,53,73	1.38	9 (18%)	58,89,113	1.48	6 (10%)
16	BCR	a	850	-	41,41,41	1.34	4 (9%)	56,56,56	1.33	6 (10%)
14	CLA	2	3037	21	49,53,73	1.40	6 (12%)	58,89,113	1.43	5 (8%)
14	CLA	B	3021	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	6 (7%)
16	BCR	y	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.24	5 (8%)
14	CLA	b	3003	21	69,73,73	1.16	10 (14%)	82,113,113	1.51	10 (12%)
14	CLA	a	827	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
14	CLA	A	822	21	69,73,73	1.16	9 (13%)	82,113,113	1.35	7 (8%)
16	BCR	l	210	-	41,41,41	1.19	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	1	838	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	9 (10%)
14	CLA	b	3038	-	64,68,73	1.22	9 (14%)	76,107,113	1.34	5 (6%)
14	CLA	0	209	21	69,73,73	1.16	8 (11%)	82,113,113	1.34	8 (9%)
15	PQN	b	3043	-	34,34,34	0.46	0	43,45,45	0.48	0
14	CLA	z	1701	-	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	B	3008	-	69,73,73	1.17	8 (11%)	82,113,113	1.35	6 (7%)
16	BCR	B	3046	-	41,41,41	1.28	3 (7%)	56,56,56	1.22	5 (8%)
16	BCR	m	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.24	5 (8%)
14	CLA	B	3027	-	69,73,73	1.19	9 (13%)	82,113,113	1.31	6 (7%)
16	BCR	I	102	-	41,41,41	1.23	5 (12%)	56,56,56	1.33	6 (10%)
14	CLA	2	3011	2	69,73,73	1.18	8 (11%)	82,113,113	1.45	9 (10%)
17	LHG	A	853	-	48,48,48	0.81	2 (4%)	51,54,54	1.25	4 (7%)
14	CLA	b	3029	-	69,73,73	1.18	9 (13%)	82,113,113	1.20	5 (6%)
14	CLA	b	3022	-	49,53,73	1.38	7 (14%)	58,89,113	1.55	6 (10%)
14	CLA	b	3026	21	69,73,73	1.18	9 (13%)	82,113,113	1.53	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	f	205	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	8 (14%)
17	LHG	0	201	-	48,48,48	0.70	1 (2%)	51,54,54	1.32	5 (9%)
17	LHG	l	202	-	38,38,48	0.78	0	41,44,54	1.30	4 (9%)
14	CLA	j	1101	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	7 (8%)
14	CLA	a	824	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
14	CLA	1	834	-	69,73,73	1.16	10 (14%)	82,113,113	1.41	9 (10%)
14	CLA	A	843	21	69,73,73	1.19	10 (14%)	82,113,113	1.37	6 (7%)
14	CLA	b	3032	-	53,57,73	1.30	9 (16%)	61,93,113	1.44	7 (11%)
14	CLA	a	810	-	53,57,73	1.31	8 (15%)	61,93,113	1.37	5 (8%)
14	CLA	2	3009	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	7 (8%)
14	CLA	b	3028	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	8 (9%)
14	CLA	2	3016	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	A	832	-	64,68,73	1.22	10 (15%)	76,107,113	1.35	5 (6%)
14	CLA	1	819	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	4 (4%)
14	CLA	9	103	21	62,66,73	1.24	8 (12%)	73,104,113	1.32	6 (8%)
14	CLA	B	3011	2	69,73,73	1.17	8 (11%)	82,113,113	1.44	9 (10%)
14	CLA	b	3005	-	69,73,73	1.16	6 (8%)	82,113,113	1.47	7 (8%)
16	BCR	b	3048	-	41,41,41	1.32	4 (9%)	56,56,56	1.25	6 (10%)
14	CLA	A	829	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
14	CLA	A	805	-	63,67,73	1.21	10 (15%)	74,105,113	1.41	7 (9%)
14	CLA	2	3023	21	59,63,73	1.27	8 (13%)	70,101,113	1.37	6 (8%)
16	BCR	B	3048	-	41,41,41	1.32	4 (9%)	56,56,56	1.25	6 (10%)
14	CLA	A	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	5 (6%)
14	CLA	1	823	-	49,53,73	1.37	8 (16%)	58,89,113	1.47	6 (10%)
16	BCR	l	204	-	41,41,41	1.44	5 (12%)	56,56,56	1.31	7 (12%)
14	CLA	a	840	-	69,73,73	1.15	8 (11%)	82,113,113	1.39	6 (7%)
13	CL0	A	801	-	58,73,73	2.17	13 (22%)	60,113,113	1.79	14 (23%)
14	CLA	1	820	-	69,73,73	1.18	9 (13%)	82,113,113	1.41	9 (10%)
18	SF4	3	101	3	0,12,12	-	-	-	-	-
18	SF4	c	101	3	0,12,12	-	-	-	-	-
14	CLA	A	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
14	CLA	a	805	-	69,73,73	1.17	8 (11%)	82,113,113	1.48	7 (8%)
14	CLA	A	819	-	69,73,73	1.15	8 (11%)	82,113,113	1.31	4 (4%)
14	CLA	b	3039	-	69,73,73	1.17	10 (14%)	82,113,113	1.45	9 (10%)
14	CLA	b	3014	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	842	-	69,73,73	1.18	9 (13%)	82,113,113	1.31	9 (10%)
14	CLA	a	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	1	850	-	41,41,41	1.34	4 (9%)	56,56,56	1.32	6 (10%)
14	CLA	2	3042	-	69,73,73	1.18	8 (11%)	82,113,113	1.39	7 (8%)
14	CLA	1	824	-	69,73,73	1.18	9 (13%)	82,113,113	1.34	5 (6%)
16	BCR	J	104	-	41,41,41	1.22	3 (7%)	56,56,56	1.30	8 (14%)
14	CLA	1	827	21	69,73,73	1.15	10 (14%)	82,113,113	1.39	10 (12%)
16	BCR	M	1602	-	41,41,41	1.24	4 (9%)	56,56,56	1.24	5 (8%)
14	CLA	a	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	7 (8%)
14	CLA	1	841	-	69,73,73	1.16	8 (11%)	82,113,113	1.39	6 (7%)
14	CLA	2	3015	-	69,73,73	1.16	7 (10%)	82,113,113	1.32	9 (10%)
14	CLA	a	816	21	69,73,73	1.17	8 (11%)	82,113,113	1.37	8 (9%)
14	CLA	A	855	-	39,44,73	1.49	8 (20%)	47,76,113	1.46	4 (8%)
14	CLA	b	3034	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	8 (9%)
14	CLA	F	201	21	62,66,73	1.23	9 (14%)	73,104,113	1.37	6 (8%)
14	CLA	B	3040	-	51,55,73	1.34	8 (15%)	60,91,113	1.33	5 (8%)
14	CLA	b	3015	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	10 (12%)
16	BCR	A	846	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	10 (17%)
17	LHG	a	852	-	48,48,48	0.81	2 (4%)	51,54,54	1.25	4 (7%)
14	CLA	B	3003	21	69,73,73	1.16	10 (14%)	82,113,113	1.50	10 (12%)
14	CLA	B	3037	21	49,53,73	1.40	6 (12%)	58,89,113	1.43	5 (8%)
14	CLA	2	3007	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	8 (9%)
14	CLA	K	102	21	62,66,73	1.24	7 (11%)	73,104,113	1.32	6 (8%)
14	CLA	b	3016	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	0	203	-	39,44,73	1.50	9 (23%)	47,76,113	1.45	4 (8%)
14	CLA	b	3019	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	8 (9%)
14	CLA	1	835	-	69,73,73	1.15	7 (10%)	82,113,113	1.40	5 (6%)
14	CLA	B	3019	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	8 (9%)
14	CLA	k	102	21	62,66,73	1.24	7 (11%)	73,104,113	1.32	6 (8%)
16	BCR	A	852	-	25,25,41	1.16	1 (4%)	33,33,56	1.29	4 (12%)
14	CLA	b	3007	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
16	BCR	1	846	-	41,41,41	1.17	3 (7%)	56,56,56	1.29	6 (10%)
16	BCR	1	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.19	5 (8%)
14	CLA	B	3005	-	69,73,73	1.15	6 (8%)	82,113,113	1.47	8 (9%)
14	CLA	B	3023	21	59,63,73	1.26	8 (13%)	70,101,113	1.37	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3036	21	54,58,73	1.37	8 (14%)	64,95,113	1.41	8 (12%)
14	CLA	A	809	1	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
14	CLA	B	3026	21	69,73,73	1.19	9 (13%)	82,113,113	1.52	14 (17%)
14	CLA	a	843	17	49,53,73	1.36	9 (18%)	58,89,113	1.52	6 (10%)
14	CLA	2	3017	-	69,73,73	1.15	8 (11%)	82,113,113	1.51	10 (12%)
14	CLA	A	826	21	69,73,73	1.17	8 (11%)	82,113,113	1.40	10 (12%)
14	CLA	f	204	-	54,58,73	1.32	7 (12%)	64,95,113	1.45	7 (10%)
14	CLA	1	808	-	55,59,73	1.29	8 (14%)	64,96,113	1.40	6 (9%)
14	CLA	a	818	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	4 (4%)
14	CLA	b	3037	21	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
17	LHG	0	202	-	38,38,48	0.78	0	41,44,54	1.30	4 (9%)
14	CLA	B	3013	-	49,53,73	1.35	9 (18%)	58,89,113	1.44	5 (8%)
14	CLA	A	830	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	b	3049	-	41,41,41	1.40	4 (9%)	56,56,56	1.29	7 (12%)
14	CLA	1	805	-	63,67,73	1.21	10 (15%)	74,105,113	1.41	7 (9%)
17	LHG	A	854	14	40,40,48	0.80	2 (5%)	43,46,54	1.19	3 (6%)
20	LMG	B	3050	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	9 (14%)
14	CLA	a	831	-	64,68,73	1.22	10 (15%)	76,107,113	1.35	5 (6%)
14	CLA	2	3028	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	8 (9%)
14	CLA	A	806	-	69,73,73	1.16	7 (10%)	82,113,113	1.48	7 (8%)
14	CLA	l	207	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	8 (9%)
14	CLA	A	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.34	5 (6%)
14	CLA	6	201	21	62,66,73	1.23	9 (14%)	73,104,113	1.37	6 (8%)
14	CLA	M	1601	-	39,44,73	1.50	8 (20%)	47,76,113	1.45	4 (8%)
14	CLA	K	101	-	50,54,73	1.38	9 (18%)	59,90,113	1.39	4 (6%)
14	CLA	a	830	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	6 (7%)
14	CLA	a	821	21	69,73,73	1.16	9 (13%)	82,113,113	1.36	7 (8%)
14	CLA	B	3017	-	69,73,73	1.15	8 (11%)	82,113,113	1.51	10 (12%)
14	CLA	B	3041	21	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
14	CLA	A	841	-	69,73,73	1.15	8 (11%)	82,113,113	1.39	6 (7%)
14	CLA	b	3035	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	5 (6%)
18	SF4	3	102	3	0,12,12	-	-	-	-	-
14	CLA	a	825	21	69,73,73	1.17	9 (13%)	82,113,113	1.39	10 (12%)
14	CLA	A	807	-	69,73,73	1.18	9 (13%)	82,113,113	1.35	7 (8%)
18	SF4	2	3001	2,1	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3024	-	49,53,73	1.38	9 (18%)	58,89,113	1.47	6 (10%)
16	BCR	A	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.19	5 (8%)
16	BCR	2	3047	-	41,41,41	1.22	3 (7%)	56,56,56	1.25	8 (14%)
14	CLA	a	804	-	63,67,73	1.21	9 (14%)	74,105,113	1.41	7 (9%)
20	LMG	2	3050	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	9 (14%)
14	CLA	A	839	-	69,73,73	1.16	7 (10%)	82,113,113	1.35	7 (8%)
14	CLA	b	3018	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	8 (9%)
14	CLA	J	101	-	49,53,73	1.38	8 (16%)	58,89,113	1.45	5 (8%)
14	CLA	B	3033	-	69,73,73	1.16	9 (13%)	82,113,113	1.44	8 (9%)
14	CLA	a	811	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	5 (6%)
14	CLA	B	3034	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	a	851	-	25,25,41	1.15	1 (4%)	33,33,56	1.29	4 (12%)
14	CLA	B	3006	-	69,73,73	1.18	9 (13%)	82,113,113	1.38	7 (8%)
14	CLA	B	3031	-	59,63,73	1.27	9 (15%)	70,101,113	1.36	8 (11%)
15	PQN	B	3043	-	34,34,34	0.46	0	43,45,45	0.48	0
14	CLA	1	816	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	5 (6%)
14	CLA	A	835	-	69,73,73	1.15	7 (10%)	82,113,113	1.39	5 (6%)
14	CLA	1	844	17	49,53,73	1.37	9 (18%)	58,89,113	1.52	6 (10%)
16	BCR	7	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.27	5 (8%)
14	CLA	a	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
14	CLA	A	810	1	69,73,73	1.17	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	a	845	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	11 (19%)
16	BCR	2	3044	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	4 (7%)
16	BCR	B	3047	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	7 (12%)
14	CLA	a	836	1	49,53,73	1.39	9 (18%)	58,89,113	1.38	6 (10%)
14	CLA	B	3029	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	5 (6%)
14	CLA	B	3022	-	49,53,73	1.37	7 (14%)	58,89,113	1.53	6 (10%)
14	CLA	B	3038	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	5 (6%)
14	CLA	B	3012	-	69,73,73	1.17	7 (10%)	82,113,113	1.43	8 (9%)
14	CLA	A	811	-	53,57,73	1.31	8 (15%)	61,93,113	1.37	5 (8%)
14	CLA	1	810	1	69,73,73	1.17	9 (13%)	82,113,113	1.33	8 (9%)
14	CLA	2	3010	-	69,73,73	1.16	8 (11%)	82,113,113	1.52	11 (13%)
14	CLA	2	3008	-	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
16	BCR	a	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.19	5 (8%)
14	CLA	a	819	-	69,73,73	1.18	9 (13%)	82,113,113	1.42	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	l	201	-	48,48,48	0.70	1 (2%)	51,54,54	1.32	5 (9%)
14	CLA	b	3010	-	69,73,73	1.17	8 (11%)	82,113,113	1.51	11 (13%)
14	CLA	B	3032	-	53,57,73	1.31	9 (16%)	61,93,113	1.44	7 (11%)
14	CLA	B	3010	-	69,73,73	1.16	8 (11%)	82,113,113	1.51	11 (13%)
14	CLA	b	3020	21	69,73,73	1.17	9 (13%)	82,113,113	1.31	5 (6%)
14	CLA	2	3032	-	53,57,73	1.30	9 (16%)	61,93,113	1.45	7 (11%)
14	CLA	a	814	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
14	CLA	b	3013	-	49,53,73	1.35	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	k	101	-	50,54,73	1.37	9 (18%)	59,90,113	1.39	5 (8%)
14	CLA	B	3020	21	69,73,73	1.17	9 (13%)	82,113,113	1.31	5 (6%)
14	CLA	2	3027	-	69,73,73	1.19	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	2	3021	-	69,73,73	1.16	8 (11%)	82,113,113	1.20	5 (6%)
14	CLA	b	3011	2	69,73,73	1.17	8 (11%)	82,113,113	1.44	9 (10%)
14	CLA	B	3025	2	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
14	CLA	2	3031	-	59,63,73	1.27	9 (15%)	70,101,113	1.37	7 (10%)
15	PQN	2	3043	-	34,34,34	0.46	0	43,45,45	0.48	0
14	CLA	2	3026	21	69,73,73	1.18	9 (13%)	82,113,113	1.52	14 (17%)
14	CLA	A	818	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
16	BCR	8	104	-	41,41,41	1.23	3 (7%)	56,56,56	1.29	7 (12%)
14	CLA	A	844	17	49,53,73	1.36	9 (18%)	58,89,113	1.53	6 (10%)
14	CLA	0	208	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	8 (9%)
14	CLA	1	830	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
14	CLA	2	3018	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	8 (9%)
18	SF4	b	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	a	802	-	69,73,73	1.16	11 (15%)	82,113,113	1.48	10 (12%)
14	CLA	2	3012	-	69,73,73	1.16	7 (10%)	82,113,113	1.42	7 (8%)
14	CLA	0	204	2	69,73,73	1.16	9 (13%)	82,113,113	1.37	9 (10%)
14	CLA	b	3041	21	69,73,73	1.15	8 (11%)	82,113,113	1.35	6 (7%)
14	CLA	a	803	21	69,73,73	1.22	8 (11%)	82,113,113	1.23	3 (3%)
14	CLA	1	818	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	b	3042	-	69,73,73	1.17	7 (10%)	82,113,113	1.39	7 (8%)
16	BCR	f	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	7 (12%)
16	BCR	2	3048	-	41,41,41	1.32	4 (9%)	56,56,56	1.25	6 (10%)
16	BCR	B	3052	-	41,41,41	1.44	5 (12%)	56,56,56	1.31	6 (10%)
14	CLA	J	102	-	41,45,73	1.48	9 (21%)	50,78,113	1.39	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	2	3052	-	41,41,41	1.29	2 (4%)	56,56,56	1.44	11 (19%)
14	CLA	1	837	1	49,53,73	1.39	9 (18%)	58,89,113	1.39	6 (10%)
14	CLA	B	3039	-	69,73,73	1.17	10 (14%)	82,113,113	1.45	9 (10%)
14	CLA	2	3030	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	7 (8%)
14	CLA	B	3007	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	8 (9%)
16	BCR	B	3049	-	41,41,41	1.39	4 (9%)	56,56,56	1.30	7 (12%)
14	CLA	1	829	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	6 (7%)
16	BCR	2	3049	-	41,41,41	1.40	4 (9%)	56,56,56	1.30	7 (12%)
14	CLA	6	204	-	54,58,73	1.33	6 (11%)	64,95,113	1.45	7 (10%)
17	LHG	1	852	-	48,48,48	0.81	2 (4%)	51,54,54	1.25	4 (7%)
14	CLA	a	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.35	7 (8%)
14	CLA	a	812	-	49,53,73	1.38	9 (18%)	58,89,113	1.49	5 (8%)
14	CLA	A	802	-	69,73,73	1.15	11 (15%)	82,113,113	1.48	10 (12%)
16	BCR	i	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.27	5 (8%)
14	CLA	1	807	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	7 (8%)
16	BCR	0	211	-	41,41,41	1.18	3 (7%)	56,56,56	1.21	4 (7%)
16	BCR	2	3046	-	41,41,41	1.29	3 (7%)	56,56,56	1.22	5 (8%)
16	BCR	1	849	-	41,41,41	1.36	4 (9%)	56,56,56	1.33	7 (12%)
14	CLA	1	822	21	69,73,73	1.16	9 (13%)	82,113,113	1.36	7 (8%)
14	CLA	0	207	10	69,73,73	1.19	9 (13%)	82,113,113	1.35	9 (10%)
16	BCR	F	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	7 (12%)
16	BCR	a	846	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	6 (10%)
17	LHG	L	208	-	38,38,48	0.78	0	41,44,54	1.30	4 (9%)
14	CLA	1	832	-	64,68,73	1.22	10 (15%)	76,107,113	1.35	5 (6%)

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
14	CLA	1	802	-	1/1/15/20	15/39/115/115	-
14	CLA	b	3009	-	1/1/15/20	8/39/115/115	-
14	CLA	a	838	-	1/1/15/20	14/39/115/115	-
14	CLA	B	3009	-	1/1/15/20	8/39/115/115	-
14	CLA	1	804	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	3014	-	1/1/15/20	14/39/115/115	-
14	CLA	B	3016	-	1/1/15/20	11/39/115/115	-
14	CLA	a	823	-	1/1/15/20	18/39/115/115	-
16	BCR	0	210	-	-	9/29/63/63	0/2/2/2
14	CLA	a	826	21	1/1/15/20	13/39/115/115	-
14	CLA	b	3023	21	1/1/13/20	9/27/103/115	-
14	CLA	a	815	-	1/1/15/20	18/39/115/115	-
14	CLA	A	827	21	1/1/15/20	13/39/115/115	-
14	CLA	L	204	-	1/1/15/20	10/39/115/115	-
14	CLA	A	831	-	1/1/15/20	8/39/115/115	-
14	CLA	1	811	-	1/1/11/20	6/20/96/115	-
14	CLA	b	3030	-	1/1/15/20	7/39/115/115	-
14	CLA	A	817	21	1/1/15/20	17/39/115/115	-
14	CLA	A	804	-	1/1/15/20	14/39/115/115	-
16	BCR	9	102	-	-	5/29/63/63	0/2/2/2
14	CLA	A	828	-	1/1/15/20	5/39/115/115	-
16	BCR	F	205	-	-	8/29/63/63	0/2/2/2
14	CLA	1	813	-	1/1/11/20	6/15/91/115	-
14	CLA	f	203	21	1/1/11/20	5/15/91/115	-
14	CLA	8	102	-	1/1/8/20	0/4/76/115	-
14	CLA	a	817	-	1/1/15/20	13/39/115/115	-
17	LHG	2	3051	-	-	24/53/53/53	-
20	LMG	b	3050	-	-	21/50/70/70	0/1/1/1
14	CLA	a	809	1	1/1/15/20	14/39/115/115	-
14	CLA	f	201	21	1/1/13/20	5/31/107/115	-
14	CLA	1	839	-	1/1/15/20	14/39/115/115	-
14	CLA	1	817	21	1/1/15/20	17/39/115/115	-
16	BCR	6	205	-	-	8/29/63/63	0/2/2/2
14	CLA	b	3036	21	1/1/12/20	9/21/97/115	-
16	BCR	A	850	-	-	4/29/63/63	0/2/2/2
16	BCR	j	1106	-	-	16/29/63/63	0/2/2/2
14	CLA	2	3003	21	1/1/15/20	17/39/115/115	-
14	CLA	A	813	-	1/1/11/20	6/15/91/115	-
16	BCR	A	848	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	l	203	2	1/1/15/20	8/39/115/115	-
16	BCR	b	3045	-	-	8/29/63/63	0/2/2/2
14	CLA	2	3013	-	-	4/15/91/115	-
14	CLA	2	3005	-	1/1/15/20	12/39/115/115	-
14	CLA	A	837	1	1/1/11/20	2/15/91/115	-
14	CLA	2	3019	-	1/1/15/20	14/39/115/115	-
14	CLA	B	3018	-	-	16/39/115/115	-
14	CLA	b	3017	-	1/1/15/20	13/39/115/115	-
14	CLA	2	3025	2	1/1/15/20	13/39/115/115	-
16	BCR	b	3044	-	-	7/29/63/63	0/2/2/2
14	CLA	2	3004	-	1/1/15/20	13/39/115/115	-
18	SF4	B	3001	2,1	-	-	0/6/5/5
14	CLA	1	821	-	1/1/15/20	18/39/115/115	-
14	CLA	B	3042	-	1/1/15/20	14/39/115/115	-
14	CLA	2	3041	21	1/1/15/20	7/39/115/115	-
16	BCR	b	3047	-	-	13/29/63/63	0/2/2/2
17	LHG	a	853	14	-	21/45/45/53	-
14	CLA	2	3024	-	-	5/15/91/115	-
14	CLA	b	3008	-	1/1/15/20	12/39/115/115	-
14	CLA	x	1701	-	1/1/11/20	4/15/91/115	-
16	BCR	1	847	-	-	17/29/63/63	0/2/2/2
14	CLA	a	808	1	1/1/15/20	16/39/115/115	-
14	CLA	F	204	-	1/1/12/20	7/21/97/115	-
14	CLA	A	821	-	1/1/15/20	18/39/115/115	-
16	BCR	k	103	-	-	2/18/35/63	0/1/1/2
16	BCR	L	206	-	-	6/29/63/63	0/2/2/2
16	BCR	0	205	-	-	13/29/63/63	0/2/2/2
14	CLA	b	3004	-	1/1/15/20	13/39/115/115	-
14	CLA	b	3006	-	1/1/15/20	17/39/115/115	-
16	BCR	l	209	-	-	9/29/63/63	0/2/2/2
14	CLA	b	3031	-	1/1/13/20	11/27/103/115	-
14	CLA	a	835	-	1/1/15/20	14/39/115/115	-
16	BCR	6	202	-	-	11/29/63/63	0/2/2/2
15	PQN	a	844	-	-	2/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	833	-	1/1/15/20	13/39/115/115	-
16	BCR	1	851	-	-	15/18/35/63	0/1/1/2
14	CLA	2	3036	21	1/1/12/20	9/21/97/115	-
14	CLA	b	3012	-	1/1/15/20	15/39/115/115	-
15	PQN	1	845	-	-	2/23/43/43	0/2/2/2
14	CLA	1	814	-	1/1/15/20	13/39/115/115	-
14	CLA	1	840	-	1/1/15/20	12/39/115/115	-
14	CLA	A	823	-	1/1/11/20	3/15/91/115	-
14	CLA	2	3038	-	1/1/14/20	12/33/109/115	-
14	CLA	1	803	21	1/1/15/20	7/39/115/115	-
14	CLA	A	808	-	1/1/12/20	2/23/99/115	-
14	CLA	2	3033	-	1/1/15/20	13/39/115/115	-
14	CLA	B	3028	-	1/1/15/20	19/39/115/115	-
14	CLA	A	815	-	1/1/15/20	15/39/115/115	-
14	CLA	A	834	-	1/1/15/20	13/39/115/115	-
14	CLA	b	3021	-	1/1/15/20	10/39/115/115	-
13	CL0	a	801	-	3/3/20/25	9/37/135/135	-
14	CLA	A	814	-	1/1/15/20	13/39/115/115	-
14	CLA	1	826	21	1/1/15/20	15/39/115/115	-
14	CLA	1	815	-	1/1/15/20	15/39/115/115	-
14	CLA	b	3025	2	1/1/15/20	13/39/115/115	-
14	CLA	2	3029	-	1/1/15/20	6/39/115/115	-
16	BCR	A	847	-	-	17/29/63/63	0/2/2/2
14	CLA	A	803	21	1/1/15/20	7/39/115/115	-
14	CLA	2	3020	21	1/1/15/20	14/39/115/115	-
14	CLA	2	3040	-	-	2/18/94/115	-
14	CLA	L	201	2	1/1/15/20	8/39/115/115	-
14	CLA	1	806	-	1/1/15/20	21/39/115/115	-
14	CLA	2	3039	-	1/1/15/20	14/39/115/115	-
14	CLA	l	206	10	1/1/15/20	15/39/115/115	-
17	LHG	L	207	-	-	24/53/53/53	-
14	CLA	B	3035	-	1/1/15/20	13/39/115/115	-
14	CLA	A	838	-	1/1/15/20	16/39/115/115	-
14	CLA	1	809	1	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	3040	-	-	2/18/94/115	-
14	CLA	1	828	-	1/1/15/20	5/39/115/115	-
16	BCR	b	3046	-	-	11/29/63/63	0/2/2/2
14	CLA	a	842	21	1/1/15/20	14/39/115/115	-
14	CLA	b	3027	-	1/1/15/20	11/39/115/115	-
14	CLA	A	812	-	1/1/15/20	10/39/115/115	-
14	CLA	A	833	-	1/1/15/20	14/39/115/115	-
14	CLA	1	831	-	1/1/15/20	8/39/115/115	-
14	CLA	8	101	-	1/1/11/20	4/15/91/115	-
16	BCR	B	3044	-	-	7/29/63/63	0/2/2/2
14	CLA	L	203	10	1/1/15/20	15/39/115/115	-
14	CLA	6	203	21	1/1/11/20	5/15/91/115	-
14	CLA	j	1102	-	1/1/11/20	4/15/91/115	-
14	CLA	2	3006	-	1/1/15/20	17/39/115/115	-
18	SF4	c	102	3	-	-	0/6/5/5
14	CLA	1	812	-	1/1/15/20	11/39/115/115	-
14	CLA	A	816	-	1/1/15/20	18/39/115/115	-
14	CLA	a	837	-	1/1/15/20	16/39/115/115	-
17	LHG	B	3051	-	-	24/53/53/53	-
14	CLA	b	3033	-	1/1/15/20	13/39/115/115	-
16	BCR	B	3053	-	-	16/29/63/63	0/2/2/2
14	CLA	A	842	-	1/1/15/20	7/39/115/115	-
14	CLA	X	1701	-	1/1/11/20	4/15/91/115	-
18	SF4	C	102	3	-	-	0/6/5/5
17	LHG	1	853	14	-	21/45/45/53	-
16	BCR	9	104	-	-	2/18/35/63	0/1/1/2
16	BCR	A	851	-	-	21/29/63/63	0/2/2/2
16	BCR	B	3045	-	-	8/29/63/63	0/2/2/2
14	CLA	a	807	-	1/1/12/20	2/23/99/115	-
15	PQN	A	845	-	-	2/23/43/43	0/2/2/2
16	BCR	j	1105	-	-	14/29/63/63	0/2/2/2
14	CLA	2	3035	-	1/1/15/20	13/39/115/115	-
14	CLA	A	840	-	1/1/15/20	12/39/115/115	-
16	BCR	a	849	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	l	208	21	1/1/15/20	12/39/115/115	-
14	CLA	B	3004	-	1/1/15/20	13/39/115/115	-
14	CLA	2	3034	-	1/1/15/20	13/39/115/115	-
16	BCR	K	103	-	-	2/18/35/63	0/1/1/2
16	BCR	8	103	-	-	9/29/63/63	0/2/2/2
14	CLA	a	834	-	1/1/15/20	11/39/115/115	-
16	BCR	j	1104	-	-	9/29/63/63	0/2/2/2
14	CLA	1	843	21	1/1/15/20	14/39/115/115	-
14	CLA	2	3022	-	1/1/11/20	4/15/91/115	-
16	BCR	2	3045	-	-	8/29/63/63	0/2/2/2
14	CLA	1	833	-	1/1/15/20	14/39/115/115	-
14	CLA	a	839	-	1/1/15/20	12/39/115/115	-
14	CLA	B	3030	-	1/1/15/20	7/39/115/115	-
14	CLA	A	820	-	1/1/15/20	9/39/115/115	-
17	LHG	b	3051	-	-	24/53/53/53	-
14	CLA	1	836	-	1/1/15/20	14/39/115/115	-
14	CLA	B	3014	-	1/1/15/20	14/39/115/115	-
14	CLA	a	841	-	1/1/15/20	7/39/115/115	-
16	BCR	J	103	-	-	9/29/63/63	0/2/2/2
14	CLA	9	101	-	1/1/11/20	9/17/93/115	-
14	CLA	1	825	-	1/1/15/20	15/39/115/115	-
14	CLA	a	813	-	1/1/15/20	13/39/115/115	-
14	CLA	a	822	-	1/1/11/20	3/15/91/115	-
14	CLA	j	1103	-	1/1/8/20	0/4/76/115	-
14	CLA	B	3015	-	1/1/15/20	16/39/115/115	-
14	CLA	a	820	-	1/1/15/20	18/39/115/115	-
13	CL0	1	801	-	3/3/20/25	9/37/135/135	-
18	SF4	C	101	3	-	-	0/6/5/5
14	CLA	F	203	21	1/1/11/20	5/15/91/115	-
14	CLA	L	205	21	1/1/15/20	12/39/115/115	-
16	BCR	I	101	-	-	7/29/63/63	0/2/2/2
16	BCR	a	847	-	-	17/29/63/63	0/2/2/2
14	CLA	b	3024	-	-	5/15/91/115	-
16	BCR	a	850	-	-	21/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	3037	21	1/1/11/20	6/15/91/115	-
14	CLA	B	3021	-	1/1/15/20	10/39/115/115	-
16	BCR	y	101	-	-	13/29/63/63	0/2/2/2
14	CLA	b	3003	21	1/1/15/20	17/39/115/115	-
14	CLA	a	827	-	1/1/15/20	5/39/115/115	-
14	CLA	A	822	21	1/1/15/20	9/39/115/115	-
16	BCR	l	210	-	-	6/29/63/63	0/2/2/2
14	CLA	1	838	-	1/1/15/20	16/39/115/115	-
14	CLA	b	3038	-	1/1/14/20	12/33/109/115	-
14	CLA	0	209	21	1/1/15/20	12/39/115/115	-
15	PQN	b	3043	-	-	4/23/43/43	0/2/2/2
14	CLA	z	1701	-	1/1/11/20	4/15/91/115	-
14	CLA	B	3008	-	1/1/15/20	12/39/115/115	-
16	BCR	B	3046	-	-	11/29/63/63	0/2/2/2
16	BCR	m	101	-	-	13/29/63/63	0/2/2/2
14	CLA	B	3027	-	1/1/15/20	11/39/115/115	-
16	BCR	I	102	-	-	9/29/63/63	0/2/2/2
14	CLA	2	3011	2	1/1/15/20	9/39/115/115	-
17	LHG	A	853	-	-	19/53/53/53	-
14	CLA	b	3029	-	1/1/15/20	6/39/115/115	-
14	CLA	b	3022	-	1/1/11/20	4/15/91/115	-
14	CLA	b	3026	21	1/1/15/20	12/39/115/115	-
16	BCR	f	205	-	-	8/29/63/63	0/2/2/2
17	LHG	0	201	-	-	24/53/53/53	-
17	LHG	l	202	-	-	29/43/43/53	-
14	CLA	j	1101	-	1/1/15/20	14/39/115/115	-
14	CLA	a	824	-	1/1/15/20	15/39/115/115	-
14	CLA	1	834	-	1/1/15/20	13/39/115/115	-
14	CLA	A	843	21	1/1/15/20	14/39/115/115	-
14	CLA	b	3032	-	1/1/11/20	9/20/96/115	-
14	CLA	a	810	-	1/1/11/20	6/20/96/115	-
14	CLA	2	3009	-	1/1/15/20	8/39/115/115	-
14	CLA	b	3028	-	1/1/15/20	19/39/115/115	-
14	CLA	2	3016	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	832	-	1/1/14/20	8/33/109/115	-
14	CLA	1	819	-	1/1/15/20	16/39/115/115	-
14	CLA	9	103	21	1/1/13/20	9/31/107/115	-
14	CLA	B	3011	2	1/1/15/20	9/39/115/115	-
14	CLA	b	3005	-	1/1/15/20	12/39/115/115	-
16	BCR	b	3048	-	-	10/29/63/63	0/2/2/2
14	CLA	A	829	-	1/1/15/20	12/39/115/115	-
14	CLA	A	805	-	1/1/13/20	11/32/108/115	-
14	CLA	2	3023	21	1/1/13/20	9/27/103/115	-
16	BCR	B	3048	-	-	10/29/63/63	0/2/2/2
14	CLA	A	836	-	1/1/15/20	14/39/115/115	-
14	CLA	1	823	-	1/1/11/20	3/15/91/115	-
16	BCR	l	204	-	-	13/29/63/63	0/2/2/2
14	CLA	a	840	-	1/1/15/20	10/39/115/115	-
13	CL0	A	801	-	3/3/20/25	9/37/135/135	-
14	CLA	1	820	-	1/1/15/20	9/39/115/115	-
18	SF4	3	101	3	-	-	0/6/5/5
18	SF4	c	101	3	-	-	0/6/5/5
14	CLA	A	825	-	1/1/15/20	15/39/115/115	-
14	CLA	a	805	-	1/1/15/20	21/39/115/115	-
14	CLA	A	819	-	1/1/15/20	16/39/115/115	-
14	CLA	b	3039	-	1/1/15/20	14/39/115/115	-
14	CLA	b	3014	-	1/1/15/20	14/39/115/115	-
14	CLA	1	842	-	1/1/15/20	7/39/115/115	-
14	CLA	a	829	-	1/1/15/20	15/39/115/115	-
16	BCR	1	850	-	-	21/29/63/63	0/2/2/2
14	CLA	2	3042	-	1/1/15/20	13/39/115/115	-
14	CLA	1	824	-	1/1/15/20	18/39/115/115	-
16	BCR	J	104	-	-	14/29/63/63	0/2/2/2
14	CLA	1	827	21	1/1/15/20	13/39/115/115	-
16	BCR	M	1602	-	-	13/29/63/63	0/2/2/2
14	CLA	a	828	-	1/1/15/20	12/39/115/115	-
14	CLA	1	841	-	1/1/15/20	10/39/115/115	-
14	CLA	2	3015	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	816	21	1/1/15/20	17/39/115/115	-
14	CLA	A	855	-	1/1/7/20	1/4/72/115	-
14	CLA	b	3034	-	1/1/15/20	13/39/115/115	-
14	CLA	F	201	21	1/1/13/20	5/31/107/115	-
14	CLA	B	3040	-	-	2/18/94/115	-
14	CLA	b	3015	-	1/1/15/20	16/39/115/115	-
16	BCR	A	846	-	-	5/29/63/63	0/2/2/2
17	LHG	a	852	-	-	19/53/53/53	-
14	CLA	B	3003	21	1/1/15/20	17/39/115/115	-
14	CLA	B	3037	21	1/1/11/20	6/15/91/115	-
14	CLA	2	3007	-	1/1/15/20	12/39/115/115	-
14	CLA	K	102	21	1/1/13/20	9/31/107/115	-
14	CLA	b	3016	-	1/1/15/20	11/39/115/115	-
14	CLA	0	203	-	1/1/7/20	1/4/72/115	-
14	CLA	b	3019	-	1/1/15/20	14/39/115/115	-
14	CLA	1	835	-	1/1/15/20	11/39/115/115	-
14	CLA	B	3019	-	1/1/15/20	14/39/115/115	-
14	CLA	k	102	21	1/1/13/20	9/31/107/115	-
16	BCR	A	852	-	-	15/18/35/63	0/1/1/2
14	CLA	b	3007	-	1/1/15/20	12/39/115/115	-
16	BCR	1	846	-	-	17/29/63/63	0/2/2/2
16	BCR	1	848	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3005	-	1/1/15/20	12/39/115/115	-
14	CLA	B	3023	21	1/1/13/20	9/27/103/115	-
14	CLA	B	3036	21	1/1/12/20	9/21/97/115	-
14	CLA	A	809	1	1/1/15/20	16/39/115/115	-
14	CLA	B	3026	21	1/1/15/20	12/39/115/115	-
14	CLA	a	843	17	1/1/11/20	4/15/91/115	-
14	CLA	2	3017	-	1/1/15/20	13/39/115/115	-
14	CLA	A	826	21	1/1/15/20	15/39/115/115	-
14	CLA	f	204	-	1/1/12/20	7/21/97/115	-
14	CLA	1	808	-	1/1/12/20	2/23/99/115	-
14	CLA	a	818	-	1/1/15/20	16/39/115/115	-
14	CLA	b	3037	21	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	0	202	-	-	29/43/43/53	-
14	CLA	B	3013	-	-	3/15/91/115	-
14	CLA	A	830	-	1/1/15/20	15/39/115/115	-
16	BCR	b	3049	-	-	2/29/63/63	0/2/2/2
14	CLA	1	805	-	1/1/13/20	11/32/108/115	-
17	LHG	A	854	14	-	21/45/45/53	-
20	LMG	B	3050	-	-	21/50/70/70	0/1/1/1
14	CLA	a	831	-	1/1/14/20	8/33/109/115	-
14	CLA	2	3028	-	1/1/15/20	19/39/115/115	-
14	CLA	A	806	-	1/1/15/20	21/39/115/115	-
14	CLA	l	207	-	1/1/15/20	10/39/115/115	-
14	CLA	A	824	-	1/1/15/20	18/39/115/115	-
14	CLA	6	201	21	1/1/13/20	4/31/107/115	-
14	CLA	M	1601	-	1/1/7/20	1/4/72/115	-
14	CLA	K	101	-	1/1/11/20	9/17/93/115	-
14	CLA	a	830	-	1/1/15/20	8/39/115/115	-
14	CLA	a	821	21	1/1/15/20	9/39/115/115	-
14	CLA	B	3017	-	1/1/15/20	13/39/115/115	-
14	CLA	B	3041	21	1/1/15/20	7/39/115/115	-
14	CLA	A	841	-	1/1/15/20	10/39/115/115	-
14	CLA	b	3035	-	1/1/15/20	13/39/115/115	-
18	SF4	3	102	3	-	-	0/6/5/5
14	CLA	a	825	21	1/1/15/20	15/39/115/115	-
14	CLA	A	807	-	1/1/15/20	15/39/115/115	-
18	SF4	2	3001	2,1	-	-	0/6/5/5
14	CLA	B	3024	-	-	5/15/91/115	-
16	BCR	A	849	-	-	7/29/63/63	0/2/2/2
16	BCR	2	3047	-	-	13/29/63/63	0/2/2/2
14	CLA	a	804	-	1/1/13/20	11/32/108/115	-
20	LMG	2	3050	-	-	21/50/70/70	0/1/1/1
14	CLA	A	839	-	1/1/15/20	14/39/115/115	-
14	CLA	b	3018	-	-	16/39/115/115	-
14	CLA	J	101	-	1/1/11/20	4/15/91/115	-
14	CLA	B	3033	-	1/1/15/20	13/39/115/115	-
14	CLA	a	811	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3034	-	1/1/15/20	13/39/115/115	-
16	BCR	a	851	-	-	15/18/35/63	0/1/1/2
14	CLA	B	3006	-	1/1/15/20	17/39/115/115	-
14	CLA	B	3031	-	1/1/13/20	11/27/103/115	-
15	PQN	B	3043	-	-	4/23/43/43	0/2/2/2
14	CLA	1	816	-	1/1/15/20	18/39/115/115	-
14	CLA	A	835	-	1/1/15/20	11/39/115/115	-
14	CLA	1	844	17	1/1/11/20	4/15/91/115	-
16	BCR	7	101	-	-	7/29/63/63	0/2/2/2
14	CLA	a	832	-	1/1/15/20	14/39/115/115	-
14	CLA	A	810	1	1/1/15/20	14/39/115/115	-
16	BCR	a	845	-	-	5/29/63/63	0/2/2/2
16	BCR	2	3044	-	-	7/29/63/63	0/2/2/2
16	BCR	B	3047	-	-	13/29/63/63	0/2/2/2
14	CLA	a	836	1	1/1/11/20	2/15/91/115	-
14	CLA	B	3029	-	1/1/15/20	6/39/115/115	-
14	CLA	B	3022	-	1/1/11/20	4/15/91/115	-
14	CLA	B	3038	-	1/1/14/20	12/33/109/115	-
14	CLA	B	3012	-	1/1/15/20	15/39/115/115	-
14	CLA	A	811	-	1/1/11/20	6/20/96/115	-
14	CLA	1	810	1	1/1/15/20	14/39/115/115	-
14	CLA	2	3010	-	1/1/15/20	9/39/115/115	-
14	CLA	2	3008	-	1/1/15/20	12/39/115/115	-
16	BCR	a	848	-	-	7/29/63/63	0/2/2/2
14	CLA	a	819	-	1/1/15/20	9/39/115/115	-
17	LHG	l	201	-	-	24/53/53/53	-
14	CLA	b	3010	-	1/1/15/20	9/39/115/115	-
14	CLA	B	3032	-	1/1/11/20	9/20/96/115	-
14	CLA	B	3010	-	1/1/15/20	9/39/115/115	-
14	CLA	b	3020	21	1/1/15/20	14/39/115/115	-
14	CLA	2	3032	-	1/1/11/20	9/20/96/115	-
14	CLA	a	814	-	1/1/15/20	15/39/115/115	-
14	CLA	b	3013	-	-	4/15/91/115	-
14	CLA	k	101	-	1/1/11/20	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3020	21	1/1/15/20	14/39/115/115	-
14	CLA	2	3027	-	1/1/15/20	11/39/115/115	-
14	CLA	2	3021	-	1/1/15/20	10/39/115/115	-
14	CLA	b	3011	2	1/1/15/20	9/39/115/115	-
14	CLA	B	3025	2	1/1/15/20	13/39/115/115	-
14	CLA	2	3031	-	1/1/13/20	11/27/103/115	-
15	PQN	2	3043	-	-	4/23/43/43	0/2/2/2
14	CLA	2	3026	21	1/1/15/20	12/39/115/115	-
14	CLA	A	818	-	1/1/15/20	13/39/115/115	-
16	BCR	8	104	-	-	14/29/63/63	0/2/2/2
14	CLA	A	844	17	1/1/11/20	4/15/91/115	-
14	CLA	0	208	-	1/1/15/20	10/39/115/115	-
14	CLA	1	830	-	1/1/15/20	15/39/115/115	-
14	CLA	2	3018	-	-	16/39/115/115	-
18	SF4	b	3001	2,1	-	-	0/6/5/5
14	CLA	a	802	-	1/1/15/20	15/39/115/115	-
14	CLA	2	3012	-	1/1/15/20	15/39/115/115	-
14	CLA	0	204	2	1/1/15/20	8/39/115/115	-
14	CLA	b	3041	21	1/1/15/20	7/39/115/115	-
14	CLA	a	803	21	1/1/15/20	7/39/115/115	-
14	CLA	1	818	-	1/1/15/20	13/39/115/115	-
14	CLA	b	3042	-	1/1/15/20	13/39/115/115	-
16	BCR	f	202	-	-	11/29/63/63	0/2/2/2
16	BCR	2	3048	-	-	10/29/63/63	0/2/2/2
16	BCR	B	3052	-	-	13/29/63/63	0/2/2/2
14	CLA	J	102	-	1/1/8/20	0/4/76/115	-
16	BCR	2	3052	-	-	16/29/63/63	0/2/2/2
14	CLA	1	837	1	1/1/11/20	2/15/91/115	-
14	CLA	B	3039	-	1/1/15/20	14/39/115/115	-
14	CLA	2	3030	-	1/1/15/20	7/39/115/115	-
14	CLA	B	3007	-	1/1/15/20	12/39/115/115	-
16	BCR	B	3049	-	-	2/29/63/63	0/2/2/2
14	CLA	1	829	-	1/1/15/20	12/39/115/115	-
16	BCR	2	3049	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	6	204	-	1/1/12/20	7/21/97/115	-
17	LHG	1	852	-	-	19/53/53/53	-
14	CLA	a	806	-	1/1/15/20	15/39/115/115	-
14	CLA	a	812	-	1/1/11/20	6/15/91/115	-
14	CLA	A	802	-	1/1/15/20	16/39/115/115	-
16	BCR	i	101	-	-	7/29/63/63	0/2/2/2
14	CLA	1	807	-	1/1/15/20	15/39/115/115	-
16	BCR	0	211	-	-	6/29/63/63	0/2/2/2
16	BCR	2	3046	-	-	11/29/63/63	0/2/2/2
16	BCR	1	849	-	-	4/29/63/63	0/2/2/2
14	CLA	1	822	21	1/1/15/20	9/39/115/115	-
14	CLA	0	207	10	1/1/15/20	15/39/115/115	-
16	BCR	F	202	-	-	11/29/63/63	0/2/2/2
16	BCR	a	846	-	-	17/29/63/63	0/2/2/2
17	LHG	L	208	-	-	29/43/43/53	-
14	CLA	1	832	-	1/1/14/20	8/33/109/115	-

All (2709) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	C1B-C2B	8.71	1.49	1.39
13	1	801	CL0	C1B-C2B	8.68	1.49	1.39
13	a	801	CL0	C1B-C2B	8.64	1.49	1.39
13	1	801	CL0	C3B-C4B	6.92	1.48	1.41
13	a	801	CL0	C3B-C4B	6.89	1.48	1.41
13	A	801	CL0	C3B-C4B	6.76	1.48	1.41
13	1	801	CL0	C1D-C2D	6.64	1.47	1.39
13	A	801	CL0	C1D-C2D	6.63	1.47	1.39
13	a	801	CL0	C1D-C2D	6.60	1.47	1.39
16	B	3052	BCR	C1-C6	-4.56	1.47	1.53
16	0	205	BCR	C1-C6	-4.56	1.47	1.53
16	l	204	BCR	C1-C6	-4.55	1.48	1.53
16	A	850	BCR	C30-C25	-4.54	1.48	1.53
16	1	849	BCR	C30-C25	-4.54	1.48	1.53
16	B	3053	BCR	C1-C6	-4.53	1.48	1.53
16	j	1106	BCR	C1-C6	-4.52	1.48	1.53
16	a	849	BCR	C30-C25	-4.48	1.48	1.53
16	2	3052	BCR	C1-C6	-4.46	1.48	1.53
16	2	3048	BCR	C1-C6	-4.34	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	3048	BCR	C1-C6	-4.34	1.48	1.53
16	b	3048	BCR	C1-C6	-4.31	1.48	1.53
16	b	3049	BCR	C30-C25	-4.30	1.48	1.53
16	B	3049	BCR	C30-C25	-4.30	1.48	1.53
16	2	3049	BCR	C30-C25	-4.26	1.48	1.53
16	a	847	BCR	C30-C25	-4.25	1.48	1.53
16	2	3047	BCR	C30-C25	-4.24	1.48	1.53
16	1	847	BCR	C30-C25	-4.24	1.48	1.53
16	A	848	BCR	C30-C25	-4.22	1.48	1.53
16	a	850	BCR	C1-C6	-4.22	1.48	1.53
13	a	801	CL0	C3D-C4D	4.22	1.47	1.41
16	1	850	BCR	C1-C6	-4.20	1.48	1.53
13	A	801	CL0	C3D-C4D	4.20	1.47	1.41
13	1	801	CL0	C3D-C4D	4.20	1.47	1.41
16	A	851	BCR	C1-C6	-4.19	1.48	1.53
16	b	3048	BCR	C30-C25	-4.18	1.48	1.53
16	b	3047	BCR	C30-C25	-4.17	1.48	1.53
16	B	3048	BCR	C30-C25	-4.16	1.48	1.53
16	2	3048	BCR	C30-C25	-4.15	1.48	1.53
16	B	3047	BCR	C30-C25	-4.15	1.48	1.53
16	8	104	BCR	C1-C6	-4.15	1.48	1.53
16	B	3046	BCR	C1-C6	-4.15	1.48	1.53
16	2	3046	BCR	C1-C6	-4.13	1.48	1.53
16	0	205	BCR	C30-C25	-4.11	1.48	1.53
16	b	3046	BCR	C1-C6	-4.10	1.48	1.53
16	j	1105	BCR	C1-C6	-4.07	1.48	1.53
16	J	104	BCR	C1-C6	-4.05	1.48	1.53
16	b	3044	BCR	C1-C6	-4.05	1.48	1.53
16	9	102	BCR	C1-C6	-4.04	1.48	1.53
16	B	3052	BCR	C30-C25	-4.04	1.48	1.53
16	l	204	BCR	C30-C25	-4.04	1.48	1.53
16	B	3044	BCR	C1-C6	-4.02	1.48	1.53
16	A	846	BCR	C1-C6	-4.02	1.48	1.53
16	y	101	BCR	C1-C6	-4.01	1.48	1.53
16	a	850	BCR	C30-C25	-3.98	1.48	1.53
16	7	101	BCR	C1-C6	-3.98	1.48	1.53
16	B	3046	BCR	C30-C25	-3.97	1.48	1.53
16	I	101	BCR	C1-C6	-3.97	1.48	1.53
16	2	3046	BCR	C30-C25	-3.97	1.48	1.53
16	M	1602	BCR	C1-C6	-3.96	1.48	1.53
16	m	101	BCR	C1-C6	-3.96	1.48	1.53
16	2	3044	BCR	C1-C6	-3.96	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	3046	BCR	C30-C25	-3.95	1.48	1.53
16	a	845	BCR	C1-C6	-3.94	1.48	1.53
16	2	3052	BCR	C30-C25	-3.94	1.48	1.53
16	A	851	BCR	C30-C25	-3.93	1.48	1.53
16	i	101	BCR	C1-C6	-3.92	1.48	1.53
16	1	850	BCR	C30-C25	-3.92	1.48	1.53
16	B	3053	BCR	C30-C25	-3.88	1.48	1.53
16	j	1106	BCR	C30-C25	-3.88	1.48	1.53
16	a	848	BCR	C1-C6	-3.88	1.48	1.53
16	2	3049	BCR	C1-C6	-3.87	1.48	1.53
16	1	848	BCR	C1-C6	-3.87	1.48	1.53
16	A	849	BCR	C1-C6	-3.85	1.48	1.53
16	f	202	BCR	C30-C25	-3.84	1.48	1.53
16	b	3049	BCR	C1-C6	-3.84	1.48	1.53
16	6	202	BCR	C30-C25	-3.83	1.48	1.53
16	B	3049	BCR	C1-C6	-3.80	1.48	1.53
16	A	852	BCR	C1-C6	-3.76	1.49	1.53
16	F	202	BCR	C30-C25	-3.75	1.49	1.53
16	f	205	BCR	C30-C25	-3.75	1.49	1.53
16	1	851	BCR	C1-C6	-3.74	1.49	1.53
16	A	850	BCR	C1-C6	-3.72	1.49	1.53
14	j	1102	CLA	C1D-ND	3.69	1.42	1.37
16	l	210	BCR	C1-C6	-3.69	1.49	1.53
16	1	849	BCR	C1-C6	-3.69	1.49	1.53
16	M	1602	BCR	C30-C25	-3.69	1.49	1.53
16	i	101	BCR	C30-C25	-3.68	1.49	1.53
16	L	206	BCR	C1-C6	-3.68	1.49	1.53
16	a	851	BCR	C1-C6	-3.68	1.49	1.53
16	0	211	BCR	C1-C6	-3.68	1.49	1.53
16	F	205	BCR	C30-C25	-3.68	1.49	1.53
16	a	849	BCR	C1-C6	-3.68	1.49	1.53
16	6	205	BCR	C30-C25	-3.67	1.49	1.53
16	m	101	BCR	C30-C25	-3.67	1.49	1.53
16	8	103	BCR	C1-C6	-3.66	1.49	1.53
16	f	205	BCR	C1-C6	-3.65	1.49	1.53
14	8	101	CLA	C1D-ND	3.65	1.42	1.37
16	A	847	BCR	C30-C25	-3.64	1.49	1.53
16	y	101	BCR	C30-C25	-3.63	1.49	1.53
14	J	101	CLA	C1D-ND	3.63	1.42	1.37
16	a	846	BCR	C30-C25	-3.63	1.49	1.53
16	F	205	BCR	C1-C6	-3.62	1.49	1.53
16	I	101	BCR	C30-C25	-3.62	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	7	101	BCR	C30-C25	-3.62	1.49	1.53
16	j	1104	BCR	C1-C6	-3.61	1.49	1.53
16	2	3045	BCR	C1-C6	-3.60	1.49	1.53
16	A	848	BCR	C1-C6	-3.60	1.49	1.53
16	b	3045	BCR	C1-C6	-3.60	1.49	1.53
16	J	103	BCR	C1-C6	-3.57	1.49	1.53
16	6	205	BCR	C1-C6	-3.57	1.49	1.53
16	A	847	BCR	C1-C6	-3.57	1.49	1.53
16	1	847	BCR	C1-C6	-3.57	1.49	1.53
16	a	847	BCR	C1-C6	-3.57	1.49	1.53
14	1	816	CLA	C1D-ND	3.56	1.42	1.37
14	6	204	CLA	C1D-ND	3.56	1.42	1.37
16	B	3045	BCR	C1-C6	-3.56	1.49	1.53
16	1	846	BCR	C30-C25	-3.56	1.49	1.53
14	a	814	CLA	C1D-ND	3.55	1.42	1.37
16	B	3047	BCR	C1-C6	-3.55	1.49	1.53
16	a	846	BCR	C1-C6	-3.55	1.49	1.53
16	2	3047	BCR	C1-C6	-3.55	1.49	1.53
14	1	824	CLA	C1D-ND	3.55	1.42	1.37
16	b	3047	BCR	C1-C6	-3.54	1.49	1.53
16	1	846	BCR	C1-C6	-3.54	1.49	1.53
14	F	204	CLA	C1D-ND	3.53	1.42	1.37
14	a	815	CLA	C1D-ND	3.52	1.42	1.37
14	A	816	CLA	C1D-ND	3.52	1.42	1.37
14	9	103	CLA	C1D-ND	3.52	1.42	1.37
14	j	1103	CLA	C1D-ND	3.52	1.42	1.37
14	b	3022	CLA	C1D-ND	3.52	1.42	1.37
14	A	824	CLA	C1D-ND	3.51	1.42	1.37
14	8	102	CLA	C1D-ND	3.50	1.42	1.37
14	2	3023	CLA	C1D-ND	3.50	1.42	1.37
14	J	102	CLA	C1D-ND	3.50	1.42	1.37
14	a	823	CLA	C1D-ND	3.50	1.42	1.37
14	2	3037	CLA	C4B-NB	3.49	1.42	1.37
14	x	1701	CLA	C1D-ND	3.48	1.42	1.37
14	B	3037	CLA	C4B-NB	3.48	1.42	1.37
14	A	815	CLA	C1D-ND	3.48	1.42	1.37
14	B	3022	CLA	C1D-ND	3.47	1.42	1.37
14	b	3037	CLA	C4B-NB	3.47	1.42	1.37
14	A	821	CLA	C1D-ND	3.47	1.42	1.37
14	2	3022	CLA	C1D-ND	3.47	1.42	1.37
14	A	817	CLA	C1D-ND	3.47	1.42	1.37
16	8	104	BCR	C30-C25	-3.47	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	0	210	BCR	C1-C6	-3.46	1.49	1.53
14	z	1701	CLA	C1D-ND	3.46	1.42	1.37
16	A	846	BCR	C30-C25	-3.46	1.49	1.53
14	k	102	CLA	C1D-ND	3.45	1.42	1.37
16	I	102	BCR	C1-C6	-3.45	1.49	1.53
14	X	1701	CLA	C1D-ND	3.45	1.42	1.37
14	1	815	CLA	C1D-ND	3.45	1.42	1.37
16	l	209	BCR	C1-C6	-3.45	1.49	1.53
16	9	102	BCR	C30-C25	-3.44	1.49	1.53
14	1	821	CLA	C1D-ND	3.44	1.42	1.37
14	K	102	CLA	C1D-ND	3.44	1.42	1.37
14	f	204	CLA	C1D-ND	3.44	1.42	1.37
14	1	817	CLA	C1D-ND	3.43	1.42	1.37
14	B	3037	CLA	C1D-ND	3.42	1.42	1.37
14	a	816	CLA	C1D-ND	3.41	1.42	1.37
16	j	1105	BCR	C30-C25	-3.41	1.49	1.53
14	a	820	CLA	C1D-ND	3.40	1.42	1.37
14	b	3023	CLA	C1D-ND	3.40	1.42	1.37
14	B	3023	CLA	C1D-ND	3.39	1.42	1.37
16	J	104	BCR	C30-C25	-3.39	1.49	1.53
16	a	845	BCR	C30-C25	-3.39	1.49	1.53
14	b	3037	CLA	C1D-ND	3.37	1.42	1.37
14	k	101	CLA	C1D-ND	3.37	1.42	1.37
14	B	3036	CLA	C1D-ND	3.37	1.42	1.37
14	9	101	CLA	C1D-ND	3.36	1.42	1.37
14	b	3036	CLA	C1D-ND	3.36	1.42	1.37
14	1	820	CLA	C1D-ND	3.35	1.42	1.37
14	a	810	CLA	C1D-ND	3.35	1.42	1.37
14	2	3036	CLA	C1D-ND	3.35	1.42	1.37
14	2	3037	CLA	C1D-ND	3.35	1.42	1.37
14	K	101	CLA	C1D-ND	3.34	1.42	1.37
14	B	3021	CLA	C1D-ND	3.34	1.42	1.37
14	0	203	CLA	C1D-ND	3.34	1.42	1.37
14	b	3021	CLA	C1D-ND	3.34	1.42	1.37
16	2	3045	BCR	C30-C25	-3.33	1.49	1.53
14	2	3021	CLA	C1D-ND	3.33	1.42	1.37
14	M	1601	CLA	C1D-ND	3.33	1.42	1.37
14	A	820	CLA	C1D-ND	3.33	1.42	1.37
14	a	807	CLA	C1D-ND	3.33	1.42	1.37
14	A	811	CLA	C1D-ND	3.32	1.42	1.37
14	2	3040	CLA	C1D-ND	3.32	1.42	1.37
14	1	808	CLA	C1D-ND	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	810	CLA	C1D-ND	3.31	1.42	1.37
16	b	3045	BCR	C30-C25	-3.31	1.49	1.53
14	a	836	CLA	C1D-ND	3.31	1.42	1.37
14	B	3025	CLA	C1D-ND	3.31	1.42	1.37
14	a	819	CLA	C1D-ND	3.30	1.42	1.37
14	z	1701	CLA	C4B-NB	3.30	1.42	1.37
14	A	808	CLA	C1D-ND	3.29	1.42	1.37
14	1	811	CLA	C1D-ND	3.29	1.42	1.37
14	B	3040	CLA	C1D-ND	3.29	1.42	1.37
14	b	3035	CLA	C1D-ND	3.29	1.42	1.37
16	2	3044	BCR	C30-C25	-3.29	1.49	1.53
16	B	3044	BCR	C30-C25	-3.29	1.49	1.53
14	b	3040	CLA	C1D-ND	3.29	1.42	1.37
14	b	3027	CLA	C1D-ND	3.28	1.42	1.37
14	A	855	CLA	C1D-ND	3.28	1.42	1.37
14	1	837	CLA	C1D-ND	3.28	1.42	1.37
14	B	3035	CLA	C1D-ND	3.28	1.42	1.37
14	F	204	CLA	C4B-NB	3.28	1.42	1.37
14	2	3025	CLA	C1D-ND	3.28	1.42	1.37
14	a	809	CLA	C1D-ND	3.28	1.42	1.37
14	b	3024	CLA	C1D-ND	3.28	1.42	1.37
14	6	204	CLA	C4B-NB	3.27	1.42	1.37
14	A	810	CLA	C1D-ND	3.27	1.42	1.37
14	a	835	CLA	C1D-ND	3.27	1.42	1.37
14	X	1701	CLA	C4B-NB	3.27	1.42	1.37
14	b	3025	CLA	C1D-ND	3.27	1.42	1.37
14	2	3027	CLA	C1D-ND	3.27	1.42	1.37
14	f	204	CLA	C4B-NB	3.27	1.42	1.37
17	1	852	LHG	O7-C5	-3.26	1.38	1.46
14	x	1701	CLA	C4B-NB	3.26	1.42	1.37
14	b	3031	CLA	C1D-ND	3.26	1.42	1.37
14	B	3024	CLA	C1D-ND	3.26	1.42	1.37
14	A	837	CLA	C1D-ND	3.26	1.42	1.37
14	1	819	CLA	C1D-ND	3.26	1.42	1.37
16	B	3045	BCR	C30-C25	-3.25	1.49	1.53
14	B	3018	CLA	C1D-ND	3.25	1.42	1.37
14	2	3020	CLA	C1D-ND	3.25	1.42	1.37
17	a	852	LHG	O7-C5	-3.25	1.39	1.46
14	B	3020	CLA	C1D-ND	3.25	1.42	1.37
17	A	853	LHG	O7-C5	-3.25	1.39	1.46
14	B	3027	CLA	C1D-ND	3.25	1.42	1.37
14	B	3031	CLA	C1D-ND	3.25	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	3031	CLA	C1D-ND	3.25	1.42	1.37
14	2	3014	CLA	C1D-ND	3.24	1.42	1.37
14	b	3039	CLA	C1D-ND	3.24	1.42	1.37
16	b	3044	BCR	C30-C25	-3.24	1.49	1.53
14	b	3020	CLA	C1D-ND	3.24	1.42	1.37
14	A	836	CLA	C1D-ND	3.23	1.42	1.37
14	A	814	CLA	C1D-ND	3.23	1.42	1.37
14	a	818	CLA	C1D-ND	3.23	1.42	1.37
14	2	3024	CLA	C1D-ND	3.23	1.42	1.37
14	1	844	CLA	C1D-ND	3.23	1.42	1.37
14	1	804	CLA	C1D-ND	3.23	1.42	1.37
14	B	3039	CLA	C1D-ND	3.23	1.42	1.37
14	a	838	CLA	C1D-ND	3.22	1.42	1.37
14	b	3018	CLA	C1D-ND	3.22	1.42	1.37
16	k	103	BCR	C1-C6	-3.22	1.49	1.53
14	2	3035	CLA	C1D-ND	3.21	1.42	1.37
14	1	837	CLA	C4B-NB	3.21	1.42	1.37
14	A	831	CLA	CMB-C2B	-3.20	1.44	1.50
14	a	843	CLA	C1D-ND	3.20	1.42	1.37
14	A	839	CLA	C1D-ND	3.20	1.42	1.37
16	K	103	BCR	C1-C6	-3.20	1.49	1.53
14	a	822	CLA	C1D-ND	3.20	1.42	1.37
14	2	3039	CLA	C1D-ND	3.20	1.42	1.37
14	A	812	CLA	C1D-ND	3.19	1.42	1.37
14	A	819	CLA	C1D-ND	3.19	1.42	1.37
14	1	836	CLA	C1D-ND	3.18	1.42	1.37
14	1	831	CLA	CMB-C2B	-3.18	1.44	1.50
14	A	823	CLA	C1D-ND	3.18	1.42	1.37
14	a	812	CLA	C1D-ND	3.18	1.42	1.37
14	B	3016	CLA	C1D-ND	3.17	1.42	1.37
14	a	830	CLA	CMB-C2B	-3.17	1.44	1.50
16	9	104	BCR	C1-C6	-3.17	1.49	1.53
14	A	804	CLA	C1D-ND	3.17	1.42	1.37
14	a	836	CLA	C4B-NB	3.17	1.42	1.37
14	A	844	CLA	C1D-ND	3.17	1.42	1.37
14	F	203	CLA	C1D-ND	3.17	1.42	1.37
14	a	824	CLA	C1D-ND	3.17	1.42	1.37
14	1	825	CLA	C1D-ND	3.17	1.42	1.37
14	1	839	CLA	C1D-ND	3.17	1.42	1.37
14	A	837	CLA	C4B-NB	3.17	1.42	1.37
14	b	3014	CLA	C1D-ND	3.17	1.42	1.37
14	B	3014	CLA	C1D-ND	3.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	813	CLA	C1D-ND	3.16	1.42	1.37
14	1	812	CLA	C1D-ND	3.16	1.42	1.37
14	1	814	CLA	C1D-ND	3.16	1.42	1.37
14	B	3012	CLA	C1D-ND	3.16	1.42	1.37
14	1	823	CLA	C1D-ND	3.16	1.42	1.37
14	b	3013	CLA	C1D-ND	3.15	1.42	1.37
14	a	811	CLA	C1D-ND	3.15	1.42	1.37
14	2	3018	CLA	C1D-ND	3.15	1.42	1.37
14	B	3013	CLA	C1D-ND	3.15	1.42	1.37
14	B	3018	CLA	C4B-NB	3.15	1.42	1.37
14	j	1103	CLA	C4B-NB	3.14	1.42	1.37
14	1	813	CLA	C1D-ND	3.14	1.42	1.37
14	2	3018	CLA	C4B-NB	3.14	1.42	1.37
14	K	101	CLA	C4B-NB	3.14	1.42	1.37
14	L	203	CLA	C4B-NB	3.14	1.42	1.37
14	b	3016	CLA	C1D-ND	3.14	1.42	1.37
14	B	3006	CLA	C1D-ND	3.13	1.42	1.37
14	1	818	CLA	C1D-ND	3.13	1.42	1.37
14	j	1101	CLA	C1D-ND	3.13	1.42	1.37
13	1	801	CL0	CMD-C2D	-3.13	1.45	1.51
14	b	3012	CLA	C1D-ND	3.13	1.42	1.37
14	b	3015	CLA	C1D-ND	3.13	1.42	1.37
14	0	207	CLA	C4B-NB	3.12	1.42	1.37
14	A	818	CLA	C1D-ND	3.12	1.42	1.37
14	f	203	CLA	C1D-ND	3.12	1.42	1.37
14	2	3032	CLA	C1D-ND	3.12	1.42	1.37
14	a	827	CLA	C1D-ND	3.11	1.42	1.37
14	2	3013	CLA	C1D-ND	3.11	1.42	1.37
14	2	3012	CLA	C1D-ND	3.11	1.41	1.37
14	2	3016	CLA	C1D-ND	3.11	1.41	1.37
14	6	203	CLA	C1D-ND	3.11	1.41	1.37
14	b	3006	CLA	C1D-ND	3.11	1.41	1.37
14	8	102	CLA	C4B-NB	3.11	1.41	1.37
14	A	842	CLA	C1D-ND	3.11	1.41	1.37
16	J	103	BCR	C30-C25	-3.10	1.49	1.53
14	A	813	CLA	C1D-ND	3.10	1.41	1.37
14	0	203	CLA	C4B-NB	3.10	1.41	1.37
14	b	3036	CLA	C4B-NB	3.10	1.41	1.37
14	b	3038	CLA	C1D-ND	3.10	1.41	1.37
14	b	3018	CLA	C4B-NB	3.10	1.41	1.37
14	B	3032	CLA	C1D-ND	3.10	1.41	1.37
13	a	801	CL0	CMD-C2D	-3.09	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	837	CLA	C1D-ND	3.09	1.41	1.37
14	B	3036	CLA	C4B-NB	3.09	1.41	1.37
14	l	206	CLA	C4B-NB	3.09	1.41	1.37
14	b	3040	CLA	C4B-NB	3.09	1.41	1.37
14	A	825	CLA	C1D-ND	3.09	1.41	1.37
14	2	3015	CLA	C1D-ND	3.09	1.41	1.37
14	2	3033	CLA	C4B-NB	3.09	1.41	1.37
14	B	3009	CLA	C1D-ND	3.09	1.41	1.37
13	A	801	CL0	CMD-C2D	-3.08	1.45	1.51
14	L	201	CLA	C1D-ND	3.08	1.41	1.37
14	A	838	CLA	C1D-ND	3.08	1.41	1.37
16	A	849	BCR	C30-C25	-3.08	1.49	1.53
14	b	3032	CLA	C1D-ND	3.08	1.41	1.37
13	A	801	CL0	CMB-C2B	-3.08	1.45	1.51
14	a	808	CLA	C1D-ND	3.08	1.41	1.37
14	1	826	CLA	C1D-ND	3.08	1.41	1.37
14	2	3009	CLA	C1D-ND	3.08	1.41	1.37
14	B	3033	CLA	C4B-NB	3.07	1.41	1.37
14	a	817	CLA	C1D-ND	3.07	1.41	1.37
14	b	3009	CLA	C1D-ND	3.07	1.41	1.37
14	6	201	CLA	C4B-NB	3.07	1.41	1.37
16	8	103	BCR	C30-C25	-3.07	1.49	1.53
14	A	829	CLA	C1D-ND	3.07	1.41	1.37
13	1	801	CL0	CMB-C2B	-3.07	1.45	1.51
14	J	102	CLA	C4B-NB	3.07	1.41	1.37
14	M	1601	CLA	C4B-NB	3.07	1.41	1.37
14	b	3033	CLA	C4B-NB	3.07	1.41	1.37
14	k	101	CLA	C4B-NB	3.07	1.41	1.37
14	2	3036	CLA	C4B-NB	3.07	1.41	1.37
14	2	3026	CLA	C1D-ND	3.07	1.41	1.37
14	a	825	CLA	C1D-ND	3.06	1.41	1.37
13	a	801	CL0	CMB-C2B	-3.06	1.45	1.51
14	B	3015	CLA	C1D-ND	3.06	1.41	1.37
14	l	203	CLA	C1D-ND	3.06	1.41	1.37
14	9	101	CLA	C4B-NB	3.06	1.41	1.37
14	1	805	CLA	C1D-ND	3.06	1.41	1.37
14	A	828	CLA	C1D-ND	3.06	1.41	1.37
14	2	3006	CLA	C1D-ND	3.06	1.41	1.37
14	1	829	CLA	C1D-ND	3.05	1.41	1.37
14	A	855	CLA	C4B-NB	3.05	1.41	1.37
14	A	826	CLA	C1D-ND	3.05	1.41	1.37
16	6	202	BCR	C1-C6	-3.05	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	K	102	CLA	C4B-NB	3.05	1.41	1.37
14	A	805	CLA	C1D-ND	3.05	1.41	1.37
14	2	3021	CLA	C4B-NB	3.05	1.41	1.37
16	l	209	BCR	C30-C25	-3.05	1.49	1.53
14	B	3020	CLA	C4B-NB	3.05	1.41	1.37
16	0	210	BCR	C30-C25	-3.04	1.49	1.53
14	a	828	CLA	C1D-ND	3.04	1.41	1.37
14	F	201	CLA	C4B-NB	3.04	1.41	1.37
14	2	3038	CLA	C1D-ND	3.04	1.41	1.37
14	F	201	CLA	C1D-ND	3.03	1.41	1.37
14	B	3026	CLA	C1D-ND	3.03	1.41	1.37
14	a	821	CLA	C1D-ND	3.03	1.41	1.37
14	A	822	CLA	C1D-ND	3.03	1.41	1.37
16	a	848	BCR	C30-C25	-3.03	1.49	1.53
14	b	3026	CLA	C1D-ND	3.03	1.41	1.37
14	B	3007	CLA	C1D-ND	3.03	1.41	1.37
14	B	3038	CLA	C1D-ND	3.03	1.41	1.37
14	f	201	CLA	C4B-NB	3.02	1.41	1.37
14	1	828	CLA	C1D-ND	3.02	1.41	1.37
14	f	201	CLA	C1D-ND	3.02	1.41	1.37
14	0	207	CLA	C1D-ND	3.02	1.41	1.37
16	j	1104	BCR	C30-C25	-3.02	1.49	1.53
14	1	842	CLA	C1D-ND	3.02	1.41	1.37
14	1	838	CLA	C1D-ND	3.02	1.41	1.37
14	a	804	CLA	C1D-ND	3.02	1.41	1.37
14	A	817	CLA	C4B-NB	3.01	1.41	1.37
16	F	202	BCR	C1-C6	-3.01	1.49	1.53
14	a	841	CLA	C1D-ND	3.01	1.41	1.37
14	2	3040	CLA	C4B-NB	3.01	1.41	1.37
14	B	3040	CLA	C4B-NB	3.01	1.41	1.37
14	1	835	CLA	C1D-ND	3.01	1.41	1.37
14	k	102	CLA	C4B-NB	3.00	1.41	1.37
14	0	204	CLA	C1D-ND	3.00	1.41	1.37
14	b	3007	CLA	C1D-ND	3.00	1.41	1.37
14	2	3023	CLA	C4B-NB	3.00	1.41	1.37
14	A	815	CLA	C4B-NB	3.00	1.41	1.37
14	1	809	CLA	C1D-ND	3.00	1.41	1.37
14	1	841	CLA	C1D-ND	3.00	1.41	1.37
16	1	848	BCR	C30-C25	-2.99	1.49	1.53
14	a	816	CLA	C4B-NB	2.99	1.41	1.37
14	a	840	CLA	C1D-ND	2.99	1.41	1.37
14	1	817	CLA	C4B-NB	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	834	CLA	C1D-ND	2.99	1.41	1.37
14	b	3028	CLA	C4B-NB	2.99	1.41	1.37
14	A	809	CLA	C1D-ND	2.99	1.41	1.37
14	l	206	CLA	C1D-ND	2.99	1.41	1.37
14	B	3021	CLA	C4B-NB	2.98	1.41	1.37
14	a	815	CLA	C4B-NB	2.98	1.41	1.37
16	f	202	BCR	C1-C6	-2.98	1.50	1.53
14	2	3034	CLA	C1D-ND	2.98	1.41	1.37
14	2	3020	CLA	C4B-NB	2.98	1.41	1.37
14	6	201	CLA	C1D-ND	2.98	1.41	1.37
14	L	203	CLA	C1D-ND	2.98	1.41	1.37
14	B	3028	CLA	C4B-NB	2.97	1.41	1.37
14	a	839	CLA	C1D-ND	2.97	1.41	1.37
14	2	3007	CLA	C1D-ND	2.97	1.41	1.37
14	b	3020	CLA	C4B-NB	2.97	1.41	1.37
14	b	3021	CLA	C4B-NB	2.97	1.41	1.37
16	I	102	BCR	C30-C25	-2.97	1.50	1.53
14	1	842	CLA	C4B-NB	2.97	1.41	1.37
14	1	822	CLA	C1D-ND	2.97	1.41	1.37
14	1	840	CLA	C1D-ND	2.97	1.41	1.37
14	2	3028	CLA	C4B-NB	2.97	1.41	1.37
14	A	816	CLA	C4B-NB	2.96	1.41	1.37
14	b	3034	CLA	C1D-ND	2.96	1.41	1.37
14	F	203	CLA	C4B-NB	2.96	1.41	1.37
14	b	3023	CLA	C4B-NB	2.96	1.41	1.37
14	B	3034	CLA	C1D-ND	2.96	1.41	1.37
14	2	3008	CLA	C1D-ND	2.96	1.41	1.37
16	l	210	BCR	C30-C25	-2.95	1.50	1.53
13	1	801	CL0	CMC-C2C	-2.95	1.46	1.50
14	1	816	CLA	C4B-NB	2.94	1.41	1.37
14	9	103	CLA	C4B-NB	2.94	1.41	1.37
14	2	3015	CLA	C4B-NB	2.94	1.41	1.37
14	B	3023	CLA	C4B-NB	2.94	1.41	1.37
14	a	820	CLA	C4B-NB	2.94	1.41	1.37
14	b	3008	CLA	C1D-ND	2.94	1.41	1.37
14	A	840	CLA	C1D-ND	2.94	1.41	1.37
14	1	821	CLA	C4B-NB	2.93	1.41	1.37
14	b	3015	CLA	C4B-NB	2.93	1.41	1.37
14	1	819	CLA	C4B-NB	2.93	1.41	1.37
13	A	801	CL0	CAC-C3C	-2.93	1.46	1.51
14	a	818	CLA	C4B-NB	2.93	1.41	1.37
14	A	834	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	835	CLA	C1D-ND	2.93	1.41	1.37
14	b	3010	CLA	C1D-ND	2.92	1.41	1.37
14	a	841	CLA	C4B-NB	2.92	1.41	1.37
14	6	203	CLA	C4B-NB	2.92	1.41	1.37
14	A	841	CLA	C1D-ND	2.92	1.41	1.37
14	b	3033	CLA	C1D-ND	2.92	1.41	1.37
14	A	842	CLA	C4B-NB	2.92	1.41	1.37
14	B	3030	CLA	C1D-ND	2.92	1.41	1.37
14	B	3015	CLA	C4B-NB	2.91	1.41	1.37
14	b	3030	CLA	C1D-ND	2.91	1.41	1.37
13	a	801	CL0	CMC-C2C	-2.91	1.46	1.50
14	A	811	CLA	C1B-C2B	2.91	1.50	1.43
14	1	818	CLA	C4B-NB	2.91	1.41	1.37
14	1	833	CLA	C1D-ND	2.91	1.41	1.37
14	A	821	CLA	C4B-NB	2.90	1.41	1.37
14	a	817	CLA	C4B-NB	2.90	1.41	1.37
14	A	843	CLA	CMD-C2D	-2.90	1.44	1.50
14	a	810	CLA	C1B-C2B	2.90	1.49	1.43
13	A	801	CL0	CMC-C2C	-2.90	1.46	1.50
14	f	203	CLA	C4B-NB	2.90	1.41	1.37
14	a	842	CLA	CMD-C2D	-2.90	1.44	1.50
14	1	843	CLA	CMD-C2D	-2.89	1.44	1.50
14	b	3010	CLA	CMC-C2C	-2.89	1.44	1.50
14	l	208	CLA	C1D-ND	2.89	1.41	1.37
14	0	209	CLA	C1D-ND	2.89	1.41	1.37
14	2	3019	CLA	C1D-ND	2.89	1.41	1.37
14	A	819	CLA	C4B-NB	2.89	1.41	1.37
14	2	3017	CLA	C1D-ND	2.89	1.41	1.37
14	2	3030	CLA	C1D-ND	2.89	1.41	1.37
14	2	3038	CLA	C4B-NB	2.89	1.41	1.37
14	1	834	CLA	C1D-ND	2.89	1.41	1.37
14	j	1102	CLA	C4B-NB	2.89	1.41	1.37
14	8	101	CLA	C4B-NB	2.89	1.41	1.37
14	1	803	CLA	C4B-NB	2.88	1.41	1.37
14	1	806	CLA	C1D-ND	2.88	1.41	1.37
13	1	801	CL0	CAC-C3C	-2.88	1.46	1.51
14	A	818	CLA	C4B-NB	2.88	1.41	1.37
14	1	811	CLA	C1B-C2B	2.88	1.49	1.43
13	a	801	CL0	CAC-C3C	-2.88	1.46	1.51
14	b	3019	CLA	C1D-ND	2.88	1.41	1.37
14	B	3008	CLA	C1D-ND	2.88	1.41	1.37
14	a	831	CLA	C1D-ND	2.87	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	0	211	BCR	C30-C25	-2.87	1.50	1.53
14	A	812	CLA	C4B-NB	2.87	1.41	1.37
14	1	823	CLA	C4B-NB	2.87	1.41	1.37
14	B	3010	CLA	CMC-C2C	-2.87	1.44	1.50
14	a	814	CLA	C4B-NB	2.87	1.41	1.37
14	B	3042	CLA	C4B-NB	2.87	1.41	1.37
14	B	3011	CLA	CMB-C2B	-2.87	1.44	1.50
14	A	832	CLA	C1D-ND	2.87	1.41	1.37
14	b	3024	CLA	C4B-NB	2.87	1.41	1.37
14	2	3033	CLA	C1D-ND	2.87	1.41	1.37
14	B	3038	CLA	C4B-NB	2.86	1.41	1.37
14	2	3010	CLA	C1D-ND	2.86	1.41	1.37
14	A	833	CLA	C1D-ND	2.86	1.41	1.37
14	B	3033	CLA	C1D-ND	2.86	1.41	1.37
14	L	205	CLA	C1D-ND	2.86	1.41	1.37
14	a	805	CLA	C1D-ND	2.86	1.41	1.37
14	2	3024	CLA	C4B-NB	2.86	1.41	1.37
14	2	3010	CLA	CMC-C2C	-2.86	1.44	1.50
14	a	833	CLA	C1D-ND	2.86	1.41	1.37
14	b	3011	CLA	CMB-C2B	-2.86	1.44	1.50
14	B	3010	CLA	C1D-ND	2.85	1.41	1.37
14	B	3019	CLA	C1D-ND	2.85	1.41	1.37
14	a	822	CLA	C4B-NB	2.85	1.41	1.37
14	B	3024	CLA	C4B-NB	2.85	1.41	1.37
14	B	3025	CLA	C4B-NB	2.85	1.41	1.37
14	a	803	CLA	C4B-NB	2.85	1.41	1.37
14	B	3017	CLA	C1D-ND	2.85	1.41	1.37
14	2	3011	CLA	CMB-C2B	-2.85	1.44	1.50
14	a	807	CLA	C4B-NB	2.85	1.41	1.37
14	1	802	CLA	CMD-C2D	-2.85	1.44	1.50
14	a	832	CLA	C1D-ND	2.85	1.41	1.37
20	2	3050	LMG	O1-C7	-2.85	1.38	1.43
16	L	206	BCR	C30-C25	-2.84	1.50	1.53
14	b	3017	CLA	C1D-ND	2.84	1.41	1.37
14	1	815	CLA	C4B-NB	2.84	1.41	1.37
14	b	3038	CLA	C4B-NB	2.84	1.41	1.37
20	B	3050	LMG	O1-C7	-2.84	1.38	1.43
14	1	812	CLA	C4B-NB	2.84	1.41	1.37
14	a	802	CLA	CMD-C2D	-2.84	1.45	1.50
14	b	3042	CLA	C4B-NB	2.84	1.41	1.37
14	2	3022	CLA	C4B-NB	2.84	1.41	1.37
14	A	829	CLA	C4B-NB	2.84	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	3042	CLA	C4B-NB	2.84	1.41	1.37
14	a	811	CLA	C4B-NB	2.84	1.41	1.37
14	1	832	CLA	C1D-ND	2.84	1.41	1.37
14	1	822	CLA	C4B-NB	2.83	1.41	1.37
14	A	811	CLA	C4B-NB	2.83	1.41	1.37
14	b	3029	CLA	CMD-C2D	-2.83	1.45	1.50
14	1	807	CLA	C1D-ND	2.83	1.41	1.37
14	A	802	CLA	CMD-C2D	-2.82	1.45	1.50
14	A	803	CLA	C4B-NB	2.82	1.41	1.37
14	A	823	CLA	C4B-NB	2.82	1.41	1.37
14	b	3025	CLA	C4B-NB	2.82	1.41	1.37
14	1	814	CLA	C4B-NB	2.82	1.41	1.37
14	J	101	CLA	C4B-NB	2.82	1.41	1.37
14	2	3029	CLA	CMD-C2D	-2.82	1.45	1.50
14	B	3020	CLA	CMC-C2C	-2.82	1.45	1.50
14	a	842	CLA	CMB-C2B	-2.82	1.45	1.50
14	B	3022	CLA	C4B-NB	2.82	1.41	1.37
14	A	814	CLA	C4B-NB	2.82	1.41	1.37
14	B	3026	CLA	C4B-NB	2.82	1.41	1.37
14	a	828	CLA	C4B-NB	2.82	1.41	1.37
14	1	829	CLA	C4B-NB	2.82	1.41	1.37
14	A	828	CLA	C4B-NB	2.82	1.41	1.37
14	b	3026	CLA	C4B-NB	2.82	1.41	1.37
14	A	807	CLA	C1D-ND	2.81	1.41	1.37
14	B	3029	CLA	CMD-C2D	-2.81	1.45	1.50
14	A	843	CLA	C4B-NB	2.81	1.41	1.37
14	A	822	CLA	C4B-NB	2.81	1.41	1.37
14	1	843	CLA	CMB-C2B	-2.80	1.45	1.50
14	b	3022	CLA	C4B-NB	2.80	1.41	1.37
14	B	3036	CLA	CMD-C2D	-2.80	1.45	1.50
14	B	3016	CLA	C1B-C2B	2.79	1.49	1.43
14	2	3037	CLA	C3B-C4B	2.79	1.50	1.42
14	b	3032	CLA	C4B-NB	2.79	1.41	1.37
14	f	204	CLA	C1B-C2B	2.79	1.49	1.43
14	b	3029	CLA	C1D-ND	2.79	1.41	1.37
14	2	3025	CLA	C4B-NB	2.79	1.41	1.37
14	B	3032	CLA	C4B-NB	2.79	1.41	1.37
14	a	813	CLA	C4B-NB	2.79	1.41	1.37
14	A	806	CLA	C1D-ND	2.79	1.41	1.37
14	a	842	CLA	C4B-NB	2.78	1.41	1.37
14	A	855	CLA	C1B-C2B	2.78	1.49	1.43
14	b	3016	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	824	CLA	C4B-NB	2.78	1.41	1.37
14	b	3020	CLA	CMC-C2C	-2.78	1.45	1.50
14	2	3029	CLA	C1D-ND	2.78	1.41	1.37
14	B	3029	CLA	C1D-ND	2.78	1.41	1.37
14	A	843	CLA	CMB-C2B	-2.78	1.45	1.50
14	A	803	CLA	CMC-C2C	-2.78	1.45	1.50
14	0	203	CLA	C1B-C2B	2.78	1.49	1.43
14	B	3005	CLA	C1D-ND	2.78	1.41	1.37
14	a	810	CLA	C4B-NB	2.78	1.41	1.37
14	b	3005	CLA	C1D-ND	2.78	1.41	1.37
14	a	812	CLA	C4B-NB	2.78	1.41	1.37
14	1	821	CLA	C3B-C4B	2.78	1.50	1.42
14	x	1701	CLA	C1B-C2B	2.78	1.49	1.43
14	l	206	CLA	C3B-C4B	2.78	1.50	1.42
14	L	203	CLA	C3B-C4B	2.77	1.50	1.42
14	2	3003	CLA	CMC-C2C	-2.77	1.45	1.50
14	2	3020	CLA	CMC-C2C	-2.77	1.45	1.50
14	2	3031	CLA	MG-NB	-2.77	2.00	2.05
14	A	808	CLA	C4B-NB	2.77	1.41	1.37
14	0	207	CLA	C3B-C4B	2.77	1.50	1.42
14	L	204	CLA	C1D-ND	2.77	1.41	1.37
14	B	3037	CLA	C3B-C4B	2.77	1.50	1.42
14	A	803	CLA	C1D-ND	2.77	1.41	1.37
14	1	811	CLA	C4B-NB	2.77	1.41	1.37
14	B	3003	CLA	CMC-C2C	-2.77	1.45	1.50
14	6	204	CLA	C1B-C2B	2.76	1.49	1.43
14	a	821	CLA	C4B-NB	2.76	1.41	1.37
14	a	829	CLA	C1D-ND	2.76	1.41	1.37
14	a	820	CLA	C3B-C4B	2.76	1.50	1.42
14	B	3013	CLA	C4B-NB	2.76	1.41	1.37
14	b	3037	CLA	C3B-C4B	2.76	1.50	1.42
14	2	3013	CLA	C4B-NB	2.76	1.41	1.37
20	b	3050	LMG	O1-C7	-2.76	1.39	1.43
14	X	1701	CLA	C1B-C2B	2.76	1.49	1.43
14	2	3016	CLA	C1B-C2B	2.76	1.49	1.43
14	A	830	CLA	CMD-C2D	-2.76	1.45	1.50
14	a	827	CLA	C4B-NB	2.76	1.41	1.37
14	1	830	CLA	C1D-ND	2.76	1.41	1.37
14	a	803	CLA	CMC-C2C	-2.76	1.45	1.50
14	a	829	CLA	CMD-C2D	-2.76	1.45	1.50
14	a	843	CLA	C4B-NB	2.75	1.41	1.37
14	2	3026	CLA	C4B-NB	2.75	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	830	CLA	C4B-NB	2.75	1.41	1.37
14	a	831	CLA	CMB-C2B	-2.75	1.45	1.50
14	A	821	CLA	C3B-C4B	2.75	1.50	1.42
14	0	208	CLA	C1D-ND	2.75	1.41	1.37
14	1	831	CLA	C4B-NB	2.75	1.41	1.37
14	A	808	CLA	C1B-C2B	2.75	1.49	1.43
14	B	3021	CLA	C1B-C2B	2.75	1.49	1.43
14	F	204	CLA	C1B-C2B	2.75	1.49	1.43
14	z	1701	CLA	C1B-C2B	2.75	1.49	1.43
14	a	823	CLA	C1B-C2B	2.75	1.49	1.43
14	A	832	CLA	CMB-C2B	-2.74	1.45	1.50
14	a	803	CLA	C1D-ND	2.74	1.41	1.37
14	b	3003	CLA	CMC-C2C	-2.74	1.45	1.50
14	b	3036	CLA	CMD-C2D	-2.74	1.45	1.50
14	2	3027	CLA	C4B-NB	2.74	1.41	1.37
14	b	3013	CLA	C4B-NB	2.74	1.41	1.37
14	1	808	CLA	C4B-NB	2.74	1.41	1.37
14	1	830	CLA	CMD-C2D	-2.74	1.45	1.50
14	2	3036	CLA	CMD-C2D	-2.74	1.45	1.50
14	M	1601	CLA	C1B-C2B	2.74	1.49	1.43
14	1	828	CLA	C4B-NB	2.74	1.41	1.37
14	2	3005	CLA	C1D-ND	2.73	1.41	1.37
14	2	3011	CLA	C1D-ND	2.73	1.41	1.37
14	1	803	CLA	CMC-C2C	-2.73	1.45	1.50
14	A	824	CLA	C4B-NB	2.73	1.41	1.37
14	b	3004	CLA	C1D-ND	2.73	1.41	1.37
14	b	3021	CLA	C1B-C2B	2.73	1.49	1.43
14	1	824	CLA	C1B-C2B	2.73	1.49	1.43
14	B	3041	CLA	C1D-ND	2.73	1.41	1.37
14	1	827	CLA	C1D-ND	2.73	1.41	1.37
14	A	831	CLA	CMD-C2D	-2.73	1.45	1.50
14	A	824	CLA	C1B-C2B	2.73	1.49	1.43
14	A	843	CLA	CMC-C2C	-2.73	1.45	1.50
14	b	3031	CLA	MG-NB	-2.73	2.00	2.05
14	2	3010	CLA	C4B-NB	2.73	1.41	1.37
14	2	3041	CLA	C1D-ND	2.73	1.41	1.37
14	a	806	CLA	C1D-ND	2.72	1.41	1.37
14	A	844	CLA	C4B-NB	2.72	1.41	1.37
14	B	3004	CLA	C1D-ND	2.72	1.41	1.37
14	1	803	CLA	C1D-ND	2.72	1.41	1.37
14	2	3004	CLA	C1D-ND	2.72	1.41	1.37
14	1	808	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3004	CLA	CMD-C2D	-2.72	1.45	1.50
14	2	3021	CLA	C1B-C2B	2.72	1.49	1.43
14	2	3032	CLA	C4B-NB	2.72	1.41	1.37
14	1	832	CLA	CMB-C2B	-2.72	1.45	1.50
14	a	803	CLA	CMB-C2B	-2.72	1.45	1.50
14	1	843	CLA	CMC-C2C	-2.72	1.45	1.50
14	B	3011	CLA	C1D-ND	2.71	1.41	1.37
14	a	807	CLA	C1B-C2B	2.71	1.49	1.43
14	b	3042	CLA	CMD-C2D	-2.71	1.45	1.50
14	1	844	CLA	C4B-NB	2.71	1.41	1.37
14	a	842	CLA	CMC-C2C	-2.71	1.45	1.50
14	A	830	CLA	C1D-ND	2.71	1.41	1.37
14	b	3022	CLA	C1B-C2B	2.71	1.49	1.43
14	A	803	CLA	CMB-C2B	-2.71	1.45	1.50
14	B	3031	CLA	MG-NB	-2.71	2.00	2.05
14	B	3017	CLA	C1B-C2B	2.71	1.49	1.43
14	2	3034	CLA	C4B-NB	2.71	1.41	1.37
14	B	3042	CLA	CMD-C2D	-2.71	1.45	1.50
14	a	823	CLA	C4B-NB	2.71	1.41	1.37
14	2	3042	CLA	CMD-C2D	-2.70	1.45	1.50
14	a	840	CLA	C4B-NB	2.70	1.41	1.37
14	2	3017	CLA	C4B-NB	2.70	1.41	1.37
14	b	3041	CLA	CMD-C2D	-2.70	1.45	1.50
14	2	3004	CLA	CMD-C2D	-2.70	1.45	1.50
14	A	813	CLA	C4B-NB	2.70	1.41	1.37
14	b	3034	CLA	C4B-NB	2.70	1.41	1.37
20	b	3050	LMG	O7-C8	-2.70	1.40	1.46
14	a	826	CLA	C1D-ND	2.70	1.41	1.37
14	b	3041	CLA	C1D-ND	2.70	1.41	1.37
14	1	843	CLA	C4B-NB	2.70	1.41	1.37
14	B	3030	CLA	CMD-C2D	-2.70	1.45	1.50
14	2	3041	CLA	CMD-C2D	-2.70	1.45	1.50
14	B	3017	CLA	C4B-NB	2.70	1.41	1.37
14	b	3017	CLA	C4B-NB	2.70	1.41	1.37
14	1	813	CLA	C4B-NB	2.70	1.41	1.37
14	B	3022	CLA	C1B-C2B	2.70	1.49	1.43
14	B	3033	CLA	C3B-C4B	2.69	1.50	1.42
14	1	831	CLA	CMD-C2D	-2.69	1.45	1.50
14	9	101	CLA	C1B-C2B	2.69	1.49	1.43
14	B	3041	CLA	CMD-C2D	-2.69	1.45	1.50
14	b	3004	CLA	CMD-C2D	-2.69	1.45	1.50
14	a	830	CLA	CMD-C2D	-2.69	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	3022	CLA	C1B-C2B	2.69	1.49	1.43
14	A	827	CLA	C1D-ND	2.69	1.41	1.37
14	b	3033	CLA	C3B-C4B	2.69	1.50	1.42
14	A	831	CLA	C4B-NB	2.69	1.41	1.37
14	2	3030	CLA	CMD-C2D	-2.69	1.45	1.50
14	1	803	CLA	CMB-C2B	-2.68	1.45	1.50
14	B	3027	CLA	C4B-NB	2.68	1.41	1.37
14	2	3033	CLA	C3B-C4B	2.68	1.50	1.42
14	l	207	CLA	C1D-ND	2.68	1.41	1.37
20	B	3050	LMG	O7-C8	-2.68	1.40	1.46
14	b	3010	CLA	C4B-NB	2.68	1.41	1.37
14	2	3028	CLA	C1D-ND	2.68	1.41	1.37
14	B	3028	CLA	C1D-ND	2.68	1.41	1.37
14	b	3014	CLA	C4B-NB	2.68	1.41	1.37
20	2	3050	LMG	O7-C8	-2.67	1.40	1.46
14	B	3034	CLA	C4B-NB	2.67	1.41	1.37
14	b	3030	CLA	CMB-C2B	-2.67	1.45	1.50
14	b	3028	CLA	C1D-ND	2.67	1.41	1.37
14	1	841	CLA	C4B-NB	2.67	1.41	1.37
14	2	3029	CLA	C4B-NB	2.67	1.41	1.37
14	b	3017	CLA	C1B-C2B	2.67	1.49	1.43
14	a	835	CLA	C4B-NB	2.67	1.41	1.37
14	1	836	CLA	C4B-NB	2.66	1.41	1.37
14	K	101	CLA	C1B-C2B	2.66	1.49	1.43
14	B	3031	CLA	CMB-C2B	-2.66	1.45	1.50
14	A	823	CLA	C1B-C2B	2.66	1.49	1.43
14	1	814	CLA	C1B-C2B	2.66	1.49	1.43
14	b	3011	CLA	C1D-ND	2.66	1.41	1.37
14	B	3010	CLA	C4B-NB	2.66	1.41	1.37
14	2	3017	CLA	C1B-C2B	2.66	1.49	1.43
14	a	813	CLA	C1B-C2B	2.66	1.49	1.43
14	2	3019	CLA	CMD-C2D	-2.66	1.45	1.50
14	B	3012	CLA	CMB-C2B	-2.66	1.45	1.50
14	b	3027	CLA	C4B-NB	2.66	1.41	1.37
14	A	842	CLA	CMD-C2D	-2.65	1.45	1.50
14	k	102	CLA	C1B-C2B	2.65	1.49	1.43
14	2	3015	CLA	C1B-C2B	2.65	1.49	1.43
14	b	3015	CLA	C1B-C2B	2.65	1.49	1.43
14	A	814	CLA	C1B-C2B	2.65	1.49	1.43
14	b	3031	CLA	CMB-C2B	-2.65	1.45	1.50
14	1	828	CLA	C1B-C2B	2.64	1.49	1.43
14	A	817	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	k	101	CLA	C1B-C2B	2.64	1.49	1.43
14	B	3028	CLA	C3B-C4B	2.64	1.50	1.42
14	B	3023	CLA	C3B-C4B	2.64	1.50	1.42
14	A	815	CLA	C1B-C2B	2.64	1.49	1.43
14	B	3014	CLA	C4B-NB	2.64	1.41	1.37
14	b	3005	CLA	C1B-C2B	2.64	1.49	1.43
14	1	823	CLA	C1B-C2B	2.64	1.49	1.43
14	b	3028	CLA	C3B-C4B	2.64	1.50	1.42
14	A	810	CLA	C4B-NB	2.64	1.41	1.37
14	b	3030	CLA	CMD-C2D	-2.64	1.45	1.50
14	b	3012	CLA	CMB-C2B	-2.64	1.45	1.50
14	2	3028	CLA	C3B-C4B	2.64	1.50	1.42
14	a	816	CLA	C1B-C2B	2.64	1.49	1.43
14	a	827	CLA	C1B-C2B	2.64	1.49	1.43
14	2	3012	CLA	CMB-C2B	-2.64	1.45	1.50
14	2	3023	CLA	C3B-C4B	2.64	1.50	1.42
14	2	3005	CLA	C1B-C2B	2.63	1.49	1.43
14	a	840	CLA	C1B-C2B	2.63	1.49	1.43
14	A	841	CLA	C4B-NB	2.63	1.41	1.37
14	1	842	CLA	CMD-C2D	-2.63	1.45	1.50
14	a	814	CLA	C1B-C2B	2.63	1.49	1.43
14	B	3005	CLA	C1B-C2B	2.63	1.49	1.43
14	2	3042	CLA	C1D-ND	2.63	1.41	1.37
14	A	836	CLA	C4B-NB	2.63	1.41	1.37
14	1	804	CLA	C4B-NB	2.63	1.41	1.37
14	B	3006	CLA	C4B-NB	2.63	1.41	1.37
14	B	3030	CLA	CMB-C2B	-2.63	1.45	1.50
14	1	821	CLA	C1B-C2B	2.62	1.49	1.43
14	b	3007	CLA	CMB-C2B	-2.62	1.45	1.50
14	K	102	CLA	C1B-C2B	2.62	1.49	1.43
14	2	3031	CLA	CMB-C2B	-2.62	1.45	1.50
14	a	819	CLA	C4B-NB	2.62	1.41	1.37
14	1	815	CLA	C1B-C2B	2.62	1.49	1.43
14	b	3023	CLA	C3B-C4B	2.62	1.50	1.42
14	b	3019	CLA	CMD-C2D	-2.62	1.45	1.50
14	b	3006	CLA	C4B-NB	2.62	1.41	1.37
14	B	3015	CLA	C1B-C2B	2.62	1.49	1.43
14	0	209	CLA	CMD-C2D	-2.62	1.45	1.50
14	2	3030	CLA	CMB-C2B	-2.62	1.45	1.50
14	a	842	CLA	C1D-ND	2.62	1.41	1.37
14	l	208	CLA	CMD-C2D	-2.62	1.45	1.50
14	A	828	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	809	CLA	C4B-NB	2.62	1.41	1.37
14	A	821	CLA	C1B-C2B	2.62	1.49	1.43
14	2	3006	CLA	C4B-NB	2.62	1.41	1.37
14	2	3014	CLA	C4B-NB	2.62	1.41	1.37
14	J	101	CLA	C1B-C2B	2.62	1.49	1.43
14	A	802	CLA	C1D-ND	2.62	1.41	1.37
14	A	841	CLA	C1B-C2B	2.62	1.49	1.43
14	B	3019	CLA	CMD-C2D	-2.61	1.45	1.50
14	a	822	CLA	C1B-C2B	2.61	1.49	1.43
14	l	207	CLA	CMD-C2D	-2.61	1.45	1.50
14	9	103	CLA	C1B-C2B	2.61	1.49	1.43
14	a	820	CLA	C1B-C2B	2.61	1.49	1.43
14	2	3003	CLA	C1D-ND	2.61	1.41	1.37
14	b	3035	CLA	C1B-C2B	2.61	1.49	1.43
14	1	817	CLA	C1B-C2B	2.61	1.49	1.43
14	b	3016	CLA	C4B-NB	2.61	1.41	1.37
14	2	3016	CLA	C4B-NB	2.61	1.41	1.37
14	L	205	CLA	CMD-C2D	-2.61	1.45	1.50
14	a	841	CLA	CMD-C2D	-2.61	1.45	1.50
14	1	841	CLA	C1B-C2B	2.60	1.49	1.43
14	1	820	CLA	C4B-NB	2.60	1.41	1.37
14	1	802	CLA	C1D-ND	2.60	1.41	1.37
14	1	810	CLA	C4B-NB	2.60	1.41	1.37
14	2	3035	CLA	C1B-C2B	2.60	1.49	1.43
14	2	3007	CLA	CMB-C2B	-2.60	1.45	1.50
14	B	3034	CLA	C1B-C2B	2.60	1.49	1.43
14	A	843	CLA	C1D-ND	2.60	1.41	1.37
14	B	3029	CLA	C4B-NB	2.60	1.41	1.37
14	B	3006	CLA	CMD-C2D	-2.60	1.45	1.50
14	6	203	CLA	C1B-C2B	2.60	1.49	1.43
14	B	3009	CLA	C4B-NB	2.60	1.41	1.37
14	2	3008	CLA	C4B-NB	2.60	1.41	1.37
14	b	3029	CLA	C4B-NB	2.60	1.41	1.37
14	a	835	CLA	CMB-C2B	-2.60	1.45	1.50
14	A	836	CLA	CMB-C2B	-2.60	1.45	1.50
14	B	3008	CLA	C4B-NB	2.60	1.41	1.37
14	1	826	CLA	C4B-NB	2.60	1.41	1.37
14	8	101	CLA	C1B-C2B	2.60	1.49	1.43
14	b	3023	CLA	C1B-C2B	2.59	1.49	1.43
14	a	802	CLA	C1D-ND	2.59	1.41	1.37
14	a	825	CLA	C4B-NB	2.59	1.41	1.37
14	j	1102	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	821	CLA	CHC-C1C	2.59	1.43	1.38
14	0	208	CLA	CMD-C2D	-2.59	1.45	1.50
14	B	3035	CLA	C1B-C2B	2.59	1.49	1.43
14	B	3007	CLA	CMB-C2B	-2.59	1.45	1.50
14	b	3034	CLA	C1B-C2B	2.59	1.49	1.43
14	2	3004	CLA	C1B-C2B	2.59	1.49	1.43
14	b	3029	CLA	CMB-C2B	-2.59	1.45	1.50
14	b	3042	CLA	C1D-ND	2.59	1.41	1.37
14	b	3019	CLA	C4B-NB	2.59	1.41	1.37
14	a	831	CLA	MG-NB	-2.58	2.00	2.05
17	A	854	LHG	O7-C5	-2.58	1.40	1.46
17	a	853	LHG	O7-C5	-2.58	1.40	1.46
14	a	818	CLA	CMC-C2C	-2.58	1.45	1.50
14	1	840	CLA	CMD-C2D	-2.58	1.45	1.50
14	2	3015	CLA	CMD-C2D	-2.58	1.45	1.50
14	1	819	CLA	CMC-C2C	-2.58	1.45	1.50
14	2	3029	CLA	CMB-C2B	-2.58	1.45	1.50
14	2	3034	CLA	C1B-C2B	2.58	1.49	1.43
14	B	3004	CLA	C1B-C2B	2.58	1.49	1.43
17	1	853	LHG	O7-C5	-2.58	1.40	1.46
14	B	3012	CLA	C1B-C2B	2.57	1.49	1.43
14	f	203	CLA	C1B-C2B	2.57	1.49	1.43
14	1	835	CLA	C1B-C2B	2.57	1.49	1.43
14	2	3035	CLA	C4B-NB	2.57	1.41	1.37
14	a	804	CLA	C4B-NB	2.57	1.41	1.37
14	1	840	CLA	C4B-NB	2.57	1.41	1.37
14	A	832	CLA	MG-NB	-2.57	2.00	2.05
14	1	839	CLA	CMB-C2B	-2.57	1.45	1.50
14	a	817	CLA	C1B-C2B	2.57	1.49	1.43
14	A	803	CLA	C3B-C4B	2.57	1.50	1.42
14	b	3004	CLA	C1B-C2B	2.57	1.49	1.43
14	b	3006	CLA	CMD-C2D	-2.57	1.45	1.50
14	B	3003	CLA	C1D-ND	2.57	1.41	1.37
14	1	818	CLA	C1B-C2B	2.57	1.49	1.43
14	F	203	CLA	C1B-C2B	2.57	1.49	1.43
14	l	203	CLA	C4B-NB	2.57	1.41	1.37
14	L	204	CLA	CMD-C2D	-2.57	1.45	1.50
14	b	3035	CLA	C4B-NB	2.57	1.41	1.37
14	B	3029	CLA	CMB-C2B	-2.57	1.45	1.50
14	A	818	CLA	C1B-C2B	2.57	1.49	1.43
14	1	803	CLA	C3B-C4B	2.57	1.50	1.42
14	1	812	CLA	C1B-C2B	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	807	CLA	C4B-NB	2.57	1.41	1.37
14	A	820	CLA	C4B-NB	2.57	1.41	1.37
14	B	3016	CLA	C4B-NB	2.57	1.41	1.37
14	A	809	CLA	C4B-NB	2.56	1.41	1.37
14	b	3009	CLA	CMD-C2D	-2.56	1.45	1.50
14	j	1101	CLA	C4B-NB	2.56	1.41	1.37
14	a	834	CLA	C1B-C2B	2.56	1.49	1.43
14	2	3009	CLA	CMD-C2D	-2.56	1.45	1.50
14	1	831	CLA	C1D-ND	2.56	1.41	1.37
14	2	3009	CLA	C4B-NB	2.56	1.41	1.37
14	a	806	CLA	C4B-NB	2.56	1.41	1.37
14	b	3008	CLA	C4B-NB	2.56	1.41	1.37
14	1	836	CLA	CMB-C2B	-2.56	1.45	1.50
14	2	3006	CLA	CMD-C2D	-2.56	1.45	1.50
14	A	826	CLA	C4B-NB	2.56	1.41	1.37
14	a	830	CLA	C1D-ND	2.56	1.41	1.37
14	B	3009	CLA	CMD-C2D	-2.56	1.45	1.50
14	A	834	CLA	C4B-NB	2.56	1.41	1.37
14	2	3012	CLA	C4B-NB	2.56	1.41	1.37
14	1	832	CLA	MG-NB	-2.56	2.00	2.05
14	1	805	CLA	C4B-NB	2.56	1.41	1.37
14	B	3015	CLA	CMD-C2D	-2.56	1.45	1.50
14	2	3030	CLA	C1B-C2B	2.56	1.49	1.43
14	a	839	CLA	C4B-NB	2.55	1.41	1.37
14	b	3012	CLA	C4B-NB	2.55	1.41	1.37
14	b	3009	CLA	C4B-NB	2.55	1.41	1.37
14	a	803	CLA	C3B-C4B	2.55	1.50	1.42
14	B	3023	CLA	C1B-C2B	2.55	1.49	1.43
14	1	806	CLA	C1B-C2B	2.55	1.49	1.43
14	0	204	CLA	C4B-NB	2.55	1.41	1.37
14	A	806	CLA	C1B-C2B	2.55	1.49	1.43
14	A	840	CLA	CMD-C2D	-2.55	1.45	1.50
14	A	821	CLA	CHC-C1C	2.55	1.43	1.38
14	A	805	CLA	C4B-NB	2.55	1.41	1.37
14	B	3042	CLA	C1D-ND	2.55	1.41	1.37
14	2	3025	CLA	C1B-C2B	2.55	1.49	1.43
14	1	820	CLA	CMB-C2B	-2.55	1.45	1.50
14	a	820	CLA	CHC-C1C	2.55	1.43	1.38
14	A	840	CLA	C4B-NB	2.55	1.41	1.37
14	B	3012	CLA	C4B-NB	2.55	1.41	1.37
14	A	835	CLA	C1B-C2B	2.55	1.49	1.43
14	j	1103	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	3012	CLA	C1B-C2B	2.55	1.49	1.43
14	A	819	CLA	CMC-C2C	-2.55	1.45	1.50
14	A	831	CLA	C1D-ND	2.55	1.41	1.37
14	1	843	CLA	C1D-ND	2.54	1.41	1.37
14	b	3025	CLA	C1B-C2B	2.54	1.49	1.43
14	a	805	CLA	C1B-C2B	2.54	1.49	1.43
14	2	3023	CLA	C1B-C2B	2.54	1.49	1.43
14	F	201	CLA	C3B-C4B	2.54	1.50	1.42
14	a	829	CLA	MG-NB	-2.54	2.00	2.05
14	b	3015	CLA	CMD-C2D	-2.54	1.45	1.50
14	B	3035	CLA	C4B-NB	2.54	1.41	1.37
14	1	807	CLA	C4B-NB	2.54	1.41	1.37
14	A	820	CLA	CMB-C2B	-2.54	1.45	1.50
14	B	3030	CLA	C1B-C2B	2.54	1.49	1.43
14	b	3030	CLA	C1B-C2B	2.54	1.49	1.43
14	1	816	CLA	CHC-C1C	2.54	1.43	1.38
14	a	838	CLA	CMB-C2B	-2.54	1.45	1.50
14	B	3008	CLA	C1B-C2B	2.54	1.49	1.43
14	b	3008	CLA	C1B-C2B	2.54	1.49	1.43
14	2	3008	CLA	C1B-C2B	2.54	1.49	1.43
14	a	805	CLA	CMB-C2B	-2.54	1.45	1.50
14	b	3012	CLA	C1B-C2B	2.54	1.49	1.43
14	a	803	CLA	CMD-C2D	-2.53	1.45	1.50
14	1	829	CLA	CMD-C2D	-2.53	1.45	1.50
14	1	842	CLA	C3B-C4B	2.53	1.50	1.42
14	1	825	CLA	C4B-NB	2.53	1.41	1.37
14	1	827	CLA	C4B-NB	2.53	1.41	1.37
14	B	3025	CLA	C1B-C2B	2.53	1.49	1.43
14	1	806	CLA	CMB-C2B	-2.53	1.45	1.50
14	A	810	CLA	CMD-C2D	-2.53	1.45	1.50
14	a	836	CLA	C3B-C4B	2.53	1.50	1.42
14	a	811	CLA	C1B-C2B	2.53	1.49	1.43
14	b	3015	CLA	C3B-C4B	2.53	1.50	1.42
14	b	3011	CLA	CMD-C2D	-2.53	1.45	1.50
14	A	804	CLA	C1B-C2B	2.53	1.49	1.43
14	1	830	CLA	MG-NB	-2.53	2.00	2.05
14	A	804	CLA	C4B-NB	2.53	1.41	1.37
14	1	834	CLA	C4B-NB	2.53	1.41	1.37
14	b	3011	CLA	MG-NB	-2.53	2.00	2.05
14	a	841	CLA	C3B-C4B	2.53	1.50	1.42
14	A	829	CLA	CMD-C2D	-2.53	1.45	1.50
14	0	204	CLA	CMD-C2D	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	839	CLA	CMB-C2B	-2.52	1.45	1.50
14	a	826	CLA	C4B-NB	2.52	1.41	1.37
14	A	842	CLA	C3B-C4B	2.52	1.50	1.42
14	A	825	CLA	C4B-NB	2.52	1.41	1.37
14	1	804	CLA	C1B-C2B	2.52	1.49	1.43
14	B	3011	CLA	CMD-C2D	-2.52	1.45	1.50
14	J	102	CLA	C1B-C2B	2.52	1.49	1.43
14	A	830	CLA	MG-NB	-2.52	2.00	2.05
14	b	3026	CLA	CMC-C2C	-2.52	1.45	1.50
14	b	3027	CLA	CMD-C2D	-2.52	1.45	1.50
14	a	839	CLA	CMD-C2D	-2.52	1.45	1.50
14	B	3039	CLA	C4B-NB	2.52	1.41	1.37
14	b	3039	CLA	C4B-NB	2.52	1.41	1.37
14	j	1101	CLA	C1B-C2B	2.52	1.49	1.43
14	a	809	CLA	CMD-C2D	-2.52	1.45	1.50
14	b	3042	CLA	CMB-C2B	-2.52	1.45	1.50
14	A	841	CLA	CMD-C2D	-2.52	1.45	1.50
14	2	3019	CLA	C4B-NB	2.51	1.41	1.37
14	B	3026	CLA	CMC-C2C	-2.51	1.45	1.50
14	B	3036	CLA	C3B-C4B	2.51	1.50	1.42
14	B	3042	CLA	CMB-C2B	-2.51	1.45	1.50
14	1	841	CLA	CMD-C2D	-2.51	1.45	1.50
14	B	3003	CLA	CMD-C2D	-2.51	1.45	1.50
14	a	802	CLA	C4B-NB	2.51	1.41	1.37
14	2	3039	CLA	C4B-NB	2.51	1.41	1.37
14	8	102	CLA	C1B-C2B	2.51	1.49	1.43
14	B	3036	CLA	CMB-C2B	-2.51	1.45	1.50
14	A	837	CLA	C3B-C4B	2.51	1.50	1.42
14	A	812	CLA	C1B-C2B	2.51	1.49	1.43
14	a	840	CLA	CMD-C2D	-2.51	1.45	1.50
14	b	3018	CLA	C1B-C2B	2.51	1.49	1.43
14	A	803	CLA	CMD-C2D	-2.51	1.45	1.50
14	b	3003	CLA	C1D-ND	2.51	1.41	1.37
14	B	3015	CLA	C3B-C4B	2.51	1.50	1.42
14	B	3018	CLA	C1B-C2B	2.51	1.49	1.43
14	1	809	CLA	C4B-NB	2.51	1.41	1.37
14	2	3015	CLA	C3B-C4B	2.51	1.50	1.42
14	2	3011	CLA	CMC-C2C	-2.51	1.45	1.50
14	2	3011	CLA	CMD-C2D	-2.51	1.45	1.50
14	2	3042	CLA	CMB-C2B	-2.51	1.45	1.50
14	a	819	CLA	CMB-C2B	-2.51	1.45	1.50
14	1	837	CLA	C3B-C4B	2.51	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	201	CLA	C3B-C4B	2.51	1.50	1.42
14	1	803	CLA	CMD-C2D	-2.51	1.45	1.50
14	a	815	CLA	CHC-C1C	2.51	1.43	1.38
14	L	201	CLA	C4B-NB	2.51	1.41	1.37
14	L	201	CLA	CMD-C2D	-2.51	1.45	1.50
14	B	3019	CLA	C4B-NB	2.50	1.41	1.37
14	b	3020	CLA	C1B-C2B	2.50	1.49	1.43
14	1	836	CLA	C1B-C2B	2.50	1.49	1.43
14	A	833	CLA	MG-NB	-2.50	2.00	2.05
14	b	3036	CLA	C3B-C4B	2.50	1.50	1.42
14	A	806	CLA	CMB-C2B	-2.50	1.45	1.50
14	B	3008	CLA	CMC-C2C	-2.50	1.45	1.50
14	A	836	CLA	C1B-C2B	2.50	1.49	1.43
14	1	832	CLA	CMD-C2D	-2.50	1.45	1.50
14	A	807	CLA	CMD-C2D	-2.50	1.45	1.50
14	b	3003	CLA	CMD-C2D	-2.50	1.45	1.50
14	l	203	CLA	CMD-C2D	-2.50	1.45	1.50
14	1	838	CLA	C4B-NB	2.50	1.41	1.37
14	0	207	CLA	CMD-C2D	-2.50	1.45	1.50
14	a	833	CLA	C4B-NB	2.50	1.41	1.37
14	a	831	CLA	CMD-C2D	-2.50	1.45	1.50
14	B	3011	CLA	MG-NB	-2.49	2.00	2.05
14	A	827	CLA	C4B-NB	2.49	1.41	1.37
14	b	3018	CLA	CMB-C2B	-2.49	1.45	1.50
14	a	828	CLA	CMD-C2D	-2.49	1.45	1.50
14	f	201	CLA	C3B-C4B	2.49	1.50	1.42
14	2	3024	CLA	C1B-C2B	2.49	1.49	1.43
14	a	824	CLA	C4B-NB	2.49	1.41	1.37
14	l	208	CLA	C4B-NB	2.49	1.41	1.37
14	b	3034	CLA	CMD-C2D	-2.49	1.45	1.50
14	a	832	CLA	MG-NB	-2.49	2.00	2.05
14	2	3011	CLA	MG-NB	-2.49	2.00	2.05
14	a	831	CLA	CMC-C2C	-2.49	1.45	1.50
14	b	3011	CLA	CMC-C2C	-2.49	1.45	1.50
14	b	3008	CLA	CMC-C2C	-2.49	1.45	1.50
14	2	3029	CLA	MG-NB	-2.49	2.00	2.05
14	1	802	CLA	C4B-NB	2.49	1.41	1.37
14	A	807	CLA	C1B-C2B	2.49	1.49	1.43
14	A	832	CLA	CMD-C2D	-2.49	1.45	1.50
14	2	3036	CLA	C3B-C4B	2.49	1.50	1.42
14	B	3007	CLA	C4B-NB	2.49	1.41	1.37
14	2	3036	CLA	CMB-C2B	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	837	CLA	C4B-NB	2.48	1.41	1.37
14	B	3039	CLA	MG-NB	-2.48	2.00	2.05
14	a	818	CLA	CMB-C2B	-2.48	1.45	1.50
14	b	3036	CLA	CMB-C2B	-2.48	1.45	1.50
14	A	810	CLA	C1B-C2B	2.48	1.49	1.43
14	1	810	CLA	C1B-C2B	2.48	1.49	1.43
14	B	3027	CLA	CMD-C2D	-2.48	1.45	1.50
14	2	3018	CLA	C1B-C2B	2.48	1.49	1.43
14	L	205	CLA	C4B-NB	2.48	1.41	1.37
14	a	808	CLA	C4B-NB	2.48	1.41	1.37
14	B	3018	CLA	CMB-C2B	-2.48	1.45	1.50
14	B	3011	CLA	CMC-C2C	-2.48	1.45	1.50
14	1	832	CLA	CMC-C2C	-2.48	1.45	1.50
14	B	3041	CLA	C4B-NB	2.48	1.41	1.37
14	B	3040	CLA	CMD-C2D	-2.48	1.45	1.50
14	2	3003	CLA	CMD-C2D	-2.48	1.45	1.50
14	1	819	CLA	C1B-C2B	2.48	1.48	1.43
14	2	3020	CLA	C1B-C2B	2.48	1.48	1.43
14	1	203	CLA	CMC-C2C	-2.48	1.45	1.50
14	b	3038	CLA	CMC-C2C	-2.48	1.45	1.50
14	a	835	CLA	C1B-C2B	2.48	1.48	1.43
14	B	3038	CLA	CMC-C2C	-2.48	1.45	1.50
14	b	3039	CLA	MG-NB	-2.48	2.00	2.05
14	2	3004	CLA	CMC-C2C	-2.48	1.45	1.50
14	1	807	CLA	C1B-C2B	2.47	1.48	1.43
14	2	3034	CLA	CMD-C2D	-2.47	1.45	1.50
14	B	3024	CLA	C1B-C2B	2.47	1.48	1.43
14	2	3041	CLA	C4B-NB	2.47	1.41	1.37
13	a	801	CL0	CHC-C4B	-2.47	1.35	1.39
14	a	832	CLA	CMD-C2D	-2.47	1.45	1.50
14	1	206	CLA	CMD-C2D	-2.47	1.45	1.50
14	L	201	CLA	CMC-C2C	-2.47	1.45	1.50
14	L	203	CLA	CMD-C2D	-2.47	1.45	1.50
14	1	807	CLA	CMD-C2D	-2.47	1.45	1.50
14	1	838	CLA	C1B-C2B	2.47	1.48	1.43
14	2	3026	CLA	CMC-C2C	-2.47	1.45	1.50
14	b	3040	CLA	CMD-C2D	-2.47	1.45	1.50
14	A	819	CLA	CMB-C2B	-2.47	1.45	1.50
14	a	828	CLA	CMC-C2C	-2.47	1.45	1.50
14	a	806	CLA	C1B-C2B	2.47	1.48	1.43
14	1	833	CLA	MG-NB	-2.47	2.00	2.05
14	A	816	CLA	CHC-C1C	2.47	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	CHC-C4B	-2.47	1.35	1.39
14	B	3034	CLA	CMD-C2D	-2.47	1.45	1.50
14	2	3030	CLA	C4B-NB	2.47	1.41	1.37
14	a	809	CLA	C1B-C2B	2.47	1.48	1.43
14	B	3042	CLA	C3B-C4B	2.47	1.49	1.42
14	a	812	CLA	C1B-C2B	2.47	1.48	1.43
14	1	829	CLA	CMC-C2C	-2.47	1.45	1.50
14	B	3006	CLA	CMC-C2C	-2.47	1.45	1.50
14	2	3042	CLA	C3B-C4B	2.47	1.49	1.42
14	a	818	CLA	C1B-C2B	2.47	1.48	1.43
14	1	208	CLA	MG-NB	-2.47	2.00	2.05
14	2	3007	CLA	C4B-NB	2.47	1.41	1.37
14	b	3004	CLA	CMC-C2C	-2.47	1.45	1.50
13	1	801	CL0	CHC-C4B	-2.47	1.35	1.39
14	b	3029	CLA	MG-NB	-2.46	2.00	2.05
14	1	810	CLA	CMD-C2D	-2.46	1.45	1.50
14	b	3042	CLA	C3B-C4B	2.46	1.49	1.42
14	2	3008	CLA	CMC-C2C	-2.46	1.45	1.50
14	A	819	CLA	C1B-C2B	2.46	1.48	1.43
14	b	3038	CLA	CMB-C2B	-2.46	1.45	1.50
14	L	205	CLA	MG-NB	-2.46	2.00	2.05
14	2	3007	CLA	CMD-C2D	-2.46	1.45	1.50
14	B	3004	CLA	CMC-C2C	-2.46	1.45	1.50
14	a	806	CLA	CMD-C2D	-2.46	1.45	1.50
14	2	3040	CLA	CMD-C2D	-2.46	1.45	1.50
14	0	204	CLA	CMC-C2C	-2.46	1.45	1.50
14	j	1103	CLA	C3B-C4B	2.46	1.49	1.42
14	A	833	CLA	CMD-C2D	-2.46	1.45	1.50
14	b	3024	CLA	C1B-C2B	2.46	1.48	1.43
14	2	3027	CLA	CMD-C2D	-2.46	1.45	1.50
14	A	818	CLA	CMD-C2D	-2.45	1.45	1.50
14	A	829	CLA	CMC-C2C	-2.45	1.45	1.50
14	A	832	CLA	CMC-C2C	-2.45	1.45	1.50
14	2	3038	CLA	CMC-C2C	-2.45	1.45	1.50
14	6	204	CLA	C3B-C4B	2.45	1.49	1.42
14	A	839	CLA	MG-NB	-2.45	2.00	2.05
14	A	838	CLA	C4B-NB	2.45	1.41	1.37
14	B	3014	CLA	C1B-C2B	2.45	1.48	1.43
14	2	3039	CLA	MG-NB	-2.45	2.00	2.05
14	A	816	CLA	C1B-C2B	2.45	1.48	1.43
14	B	3020	CLA	C1B-C2B	2.45	1.48	1.43
14	a	826	CLA	C3B-C4B	2.45	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	833	CLA	CMD-C2D	-2.45	1.45	1.50
14	2	3019	CLA	C1B-C2B	2.45	1.48	1.43
14	1	826	CLA	CMD-C2D	-2.45	1.45	1.50
14	A	844	CLA	C1B-C2B	2.45	1.48	1.43
14	K	102	CLA	C3B-C4B	2.45	1.49	1.42
14	2	3004	CLA	CMB-C2B	-2.45	1.45	1.50
14	b	3014	CLA	C1B-C2B	2.44	1.48	1.43
14	1	816	CLA	C1B-C2B	2.44	1.48	1.43
14	b	3030	CLA	C4B-NB	2.44	1.41	1.37
14	a	817	CLA	CMD-C2D	-2.44	1.45	1.50
14	2	3038	CLA	CMB-C2B	-2.44	1.45	1.50
14	a	815	CLA	C3B-C4B	2.44	1.49	1.42
14	2	3018	CLA	CMB-C2B	-2.44	1.45	1.50
14	B	3032	CLA	C1B-C2B	2.44	1.48	1.43
14	0	209	CLA	MG-NB	-2.44	2.01	2.05
14	B	3037	CLA	C1B-C2B	2.44	1.48	1.43
14	1	813	CLA	C1B-C2B	2.44	1.48	1.43
14	1	844	CLA	C1B-C2B	2.44	1.48	1.43
14	B	3029	CLA	MG-NB	-2.44	2.01	2.05
14	a	829	CLA	C1B-C2B	2.44	1.48	1.43
14	1	816	CLA	C3B-C4B	2.44	1.49	1.42
14	a	838	CLA	C1B-C2B	2.44	1.48	1.43
14	a	843	CLA	C1B-C2B	2.44	1.48	1.43
14	1	819	CLA	CMB-C2B	-2.44	1.45	1.50
14	b	3020	CLA	CMD-C2D	-2.43	1.45	1.50
14	2	3038	CLA	C1B-C2B	2.43	1.48	1.43
14	A	831	CLA	MG-NB	-2.43	2.01	2.05
14	A	822	CLA	CMB-C2B	-2.43	1.45	1.50
14	B	3030	CLA	C4B-NB	2.43	1.41	1.37
14	A	816	CLA	C3B-C4B	2.43	1.49	1.42
14	b	3003	CLA	C4B-NB	2.43	1.41	1.37
14	M	1601	CLA	CMD-C2D	-2.43	1.45	1.50
14	B	3014	CLA	CMC-C2C	-2.43	1.45	1.50
14	b	3007	CLA	C4B-NB	2.43	1.41	1.37
14	9	103	CLA	C3B-C4B	2.43	1.49	1.42
14	2	3014	CLA	C1B-C2B	2.43	1.48	1.43
16	B	3052	BCR	C33-C5	-2.43	1.47	1.50
14	a	821	CLA	CMB-C2B	-2.43	1.45	1.50
14	b	3019	CLA	MG-NB	-2.43	2.01	2.05
14	1	208	CLA	CMB-C2B	-2.43	1.45	1.50
14	8	102	CLA	C3B-C4B	2.43	1.49	1.42
14	1	827	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3007	CLA	CMD-C2D	-2.43	1.45	1.50
16	0	205	BCR	C33-C5	-2.43	1.47	1.50
14	F	204	CLA	C3B-C4B	2.43	1.49	1.42
14	a	825	CLA	CMD-C2D	-2.43	1.45	1.50
14	b	3037	CLA	C1B-C2B	2.43	1.48	1.43
14	B	3031	CLA	C4B-NB	2.43	1.41	1.37
13	A	801	CL0	MG-NB	-2.43	2.01	2.05
14	A	826	CLA	CMD-C2D	-2.43	1.45	1.50
14	2	3006	CLA	CMC-C2C	-2.42	1.45	1.50
14	f	204	CLA	C3B-C4B	2.42	1.49	1.42
14	a	828	CLA	C3B-C4B	2.42	1.49	1.42
14	A	813	CLA	C1B-C2B	2.42	1.48	1.43
14	1	839	CLA	MG-NB	-2.42	2.01	2.05
14	B	3003	CLA	C4B-NB	2.42	1.41	1.37
14	a	837	CLA	C1B-C2B	2.42	1.48	1.43
14	A	832	CLA	C4B-NB	2.42	1.41	1.37
14	b	3006	CLA	CMC-C2C	-2.42	1.45	1.50
14	1	822	CLA	CMB-C2B	-2.42	1.45	1.50
14	1	829	CLA	C3B-C4B	2.42	1.49	1.42
16	l	204	BCR	C33-C5	-2.42	1.47	1.50
14	b	3013	CLA	C1B-C2B	2.42	1.48	1.43
14	a	830	CLA	MG-NB	-2.42	2.01	2.05
14	b	3041	CLA	C4B-NB	2.42	1.41	1.37
14	J	102	CLA	C3B-C4B	2.42	1.49	1.42
14	A	837	CLA	C1B-C2B	2.42	1.48	1.43
14	2	3009	CLA	C1B-C2B	2.42	1.48	1.43
14	b	3024	CLA	C3B-C4B	2.42	1.49	1.42
14	0	203	CLA	C3B-C4B	2.42	1.49	1.42
14	2	3037	CLA	C1B-C2B	2.42	1.48	1.43
14	0	209	CLA	C4B-NB	2.42	1.41	1.37
14	0	203	CLA	CMD-C2D	-2.42	1.45	1.50
14	b	3014	CLA	CMC-C2C	-2.41	1.45	1.50
14	B	3004	CLA	MG-NB	-2.41	2.01	2.05
14	k	102	CLA	C3B-C4B	2.41	1.49	1.42
14	1	831	CLA	MG-NB	-2.41	2.01	2.05
14	A	825	CLA	MG-NB	-2.41	2.01	2.05
14	b	3010	CLA	C3B-C4B	2.41	1.49	1.42
14	B	3038	CLA	CMB-C2B	-2.41	1.45	1.50
14	A	829	CLA	C3B-C4B	2.41	1.49	1.42
14	B	3030	CLA	MG-NB	-2.41	2.01	2.05
14	B	3020	CLA	CMD-C2D	-2.41	1.45	1.50
14	A	839	CLA	C4B-NB	2.41	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	809	CLA	CMD-C2D	-2.41	1.45	1.50
14	A	826	CLA	C1B-C2B	2.41	1.48	1.43
14	B	3003	CLA	MG-NB	-2.41	2.01	2.05
14	B	3009	CLA	C1B-C2B	2.41	1.48	1.43
14	A	855	CLA	CMD-C2D	-2.41	1.45	1.50
14	b	3004	CLA	MG-NB	-2.41	2.01	2.05
14	b	3040	CLA	C1B-C2B	2.41	1.48	1.43
14	1	826	CLA	C1B-C2B	2.41	1.48	1.43
14	1	818	CLA	CMD-C2D	-2.41	1.45	1.50
14	a	836	CLA	C1B-C2B	2.41	1.48	1.43
14	2	3007	CLA	CMC-C2C	-2.41	1.45	1.50
14	a	838	CLA	C4B-NB	2.41	1.41	1.37
14	B	3013	CLA	C1B-C2B	2.41	1.48	1.43
13	1	801	CL0	MG-NB	-2.41	2.01	2.05
14	a	815	CLA	C1B-C2B	2.41	1.48	1.43
14	1	844	CLA	C3B-C4B	2.41	1.49	1.42
14	B	3007	CLA	CMC-C2C	-2.40	1.45	1.50
14	a	825	CLA	C1B-C2B	2.40	1.48	1.43
14	A	844	CLA	C3B-C4B	2.40	1.49	1.42
14	A	827	CLA	C3B-C4B	2.40	1.49	1.42
14	2	3041	CLA	C1B-C2B	2.40	1.48	1.43
14	A	839	CLA	C1B-C2B	2.40	1.48	1.43
14	B	3019	CLA	C1B-C2B	2.40	1.48	1.43
14	A	802	CLA	C4B-NB	2.40	1.41	1.37
14	1	832	CLA	C4B-NB	2.40	1.41	1.37
14	1	802	CLA	C3B-C4B	2.40	1.49	1.42
14	B	3004	CLA	CMB-C2B	-2.40	1.45	1.50
14	2	3026	CLA	C3B-C4B	2.40	1.49	1.42
14	2	3032	CLA	C1B-C2B	2.40	1.48	1.43
14	M	1601	CLA	C3B-C4B	2.40	1.49	1.42
14	b	3004	CLA	CMB-C2B	-2.40	1.45	1.50
14	A	802	CLA	C3B-C4B	2.40	1.49	1.42
14	a	802	CLA	MG-NB	-2.40	2.01	2.05
14	a	812	CLA	CMD-C2D	-2.40	1.45	1.50
14	a	843	CLA	C3B-C4B	2.40	1.49	1.42
14	2	3019	CLA	MG-NB	-2.40	2.01	2.05
14	2	3010	CLA	C3B-C4B	2.40	1.49	1.42
14	b	3007	CLA	CMC-C2C	-2.40	1.45	1.50
14	A	838	CLA	C1B-C2B	2.40	1.48	1.43
14	b	3009	CLA	C1B-C2B	2.40	1.48	1.43
14	b	3019	CLA	C1B-C2B	2.40	1.48	1.43
14	b	3039	CLA	CMB-C2B	-2.40	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	853	LHG	O8-C6	-2.40	1.39	1.45
14	A	802	CLA	MG-NB	-2.40	2.01	2.05
14	B	3010	CLA	C3B-C4B	2.40	1.49	1.42
14	A	855	CLA	C3B-C4B	2.40	1.49	1.42
14	l	207	CLA	MG-NB	-2.40	2.01	2.05
17	a	852	LHG	O8-C6	-2.40	1.39	1.45
13	a	801	CL0	MG-NB	-2.40	2.01	2.05
14	a	841	CLA	CMC-C2C	-2.40	1.45	1.50
14	1	839	CLA	C1B-C2B	2.40	1.48	1.43
14	1	818	CLA	C3B-C4B	2.40	1.49	1.42
14	0	209	CLA	CMB-C2B	-2.39	1.45	1.50
14	A	813	CLA	CMD-C2D	-2.39	1.45	1.50
14	a	802	CLA	C3B-C4B	2.39	1.49	1.42
14	2	3004	CLA	MG-NB	-2.39	2.01	2.05
14	b	3032	CLA	C1B-C2B	2.39	1.48	1.43
14	2	3024	CLA	C3B-C4B	2.39	1.49	1.42
14	b	3038	CLA	CMD-C2D	-2.39	1.45	1.50
14	B	3041	CLA	C1B-C2B	2.39	1.48	1.43
14	B	3024	CLA	C3B-C4B	2.39	1.49	1.42
14	1	826	CLA	MG-NB	-2.39	2.01	2.05
14	b	3007	CLA	CMD-C2D	-2.39	1.45	1.50
14	b	3030	CLA	MG-NB	-2.39	2.01	2.05
14	1	802	CLA	MG-NB	-2.39	2.01	2.05
17	2	3051	LHG	O7-C5	-2.39	1.41	1.46
14	a	817	CLA	C3B-C4B	2.39	1.49	1.42
14	b	3038	CLA	C1B-C2B	2.39	1.48	1.43
14	1	842	CLA	CMC-C2C	-2.39	1.45	1.50
14	2	3031	CLA	C4B-NB	2.39	1.41	1.37
14	2	3039	CLA	CMB-C2B	-2.39	1.45	1.50
14	2	3020	CLA	CMD-C2D	-2.39	1.45	1.50
14	2	3027	CLA	C1B-C2B	2.39	1.48	1.43
14	2	3042	CLA	MG-NB	-2.38	2.01	2.05
14	A	820	CLA	CMD-C2D	-2.38	1.45	1.50
14	2	3036	CLA	C1B-C2B	2.38	1.48	1.43
14	b	3027	CLA	C1B-C2B	2.38	1.48	1.43
14	b	3026	CLA	C3B-C4B	2.38	1.49	1.42
14	B	3036	CLA	C1B-C2B	2.38	1.48	1.43
14	1	834	CLA	C3B-C4B	2.38	1.49	1.42
14	a	824	CLA	MG-NB	-2.38	2.01	2.05
14	2	3038	CLA	CMD-C2D	-2.38	1.45	1.50
14	B	3027	CLA	MG-NB	-2.38	2.01	2.05
14	1	822	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	818	CLA	C3B-C4B	2.38	1.49	1.42
14	a	838	CLA	CMC-C2C	-2.38	1.45	1.50
14	F	203	CLA	C3B-C4B	2.38	1.49	1.42
16	2	3049	BCR	C38-C26	-2.38	1.47	1.50
14	b	3003	CLA	MG-NB	-2.38	2.01	2.05
14	B	3008	CLA	CMD-C2D	-2.38	1.45	1.50
14	1	830	CLA	C1B-C2B	2.38	1.48	1.43
14	A	839	CLA	CMC-C2C	-2.38	1.45	1.50
14	b	3032	CLA	CMD-C2D	-2.38	1.45	1.50
14	2	3032	CLA	CMD-C2D	-2.38	1.45	1.50
14	f	203	CLA	C3B-C4B	2.38	1.49	1.42
14	x	1701	CLA	CHC-C1C	2.38	1.43	1.38
14	a	830	CLA	C1B-C2B	2.38	1.48	1.43
14	B	3019	CLA	MG-NB	-2.38	2.01	2.05
14	a	838	CLA	MG-NB	-2.38	2.01	2.05
14	9	101	CLA	CMD-C2D	-2.38	1.45	1.50
14	1	813	CLA	CMD-C2D	-2.38	1.45	1.50
14	B	3027	CLA	C1B-C2B	2.38	1.48	1.43
14	B	3039	CLA	CMB-C2B	-2.38	1.45	1.50
14	2	3030	CLA	MG-NB	-2.38	2.01	2.05
14	B	3038	CLA	C1B-C2B	2.38	1.48	1.43
14	a	833	CLA	C3B-C4B	2.38	1.49	1.42
14	K	101	CLA	CMD-C2D	-2.38	1.45	1.50
14	b	3035	CLA	CMB-C2B	-2.38	1.45	1.50
14	A	834	CLA	C3B-C4B	2.38	1.49	1.42
14	L	205	CLA	CMB-C2B	-2.37	1.45	1.50
14	B	3032	CLA	CMD-C2D	-2.37	1.45	1.50
14	a	819	CLA	CMD-C2D	-2.37	1.45	1.50
14	1	838	CLA	CMD-C2D	-2.37	1.45	1.50
14	2	3035	CLA	CMB-C2B	-2.37	1.45	1.50
14	A	823	CLA	C3B-C4B	2.37	1.49	1.42
14	2	3014	CLA	CMC-C2C	-2.37	1.45	1.50
14	J	102	CLA	CHC-C1C	2.37	1.43	1.38
14	A	806	CLA	CMD-C2D	-2.37	1.45	1.50
14	L	204	CLA	MG-NB	-2.37	2.01	2.05
14	a	825	CLA	MG-NB	-2.37	2.01	2.05
14	b	3031	CLA	C4B-NB	2.37	1.41	1.37
14	1	820	CLA	CMD-C2D	-2.37	1.45	1.50
14	a	821	CLA	MG-NB	-2.37	2.01	2.05
14	6	203	CLA	CHC-C1C	2.37	1.43	1.38
14	A	831	CLA	C1B-C2B	2.37	1.48	1.43
14	0	208	CLA	CMB-C2B	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	3036	CLA	C1B-C2B	2.37	1.48	1.43
14	2	3003	CLA	MG-NB	-2.37	2.01	2.05
14	z	1701	CLA	C3B-C4B	2.37	1.49	1.42
14	A	822	CLA	C3B-C4B	2.37	1.49	1.42
14	l	203	CLA	C3B-C4B	2.37	1.49	1.42
17	1	852	LHG	O8-C6	-2.37	1.39	1.45
14	B	3027	CLA	CMC-C2C	-2.37	1.45	1.50
14	b	3012	CLA	CMC-C2C	-2.37	1.45	1.50
14	1	837	CLA	C1B-C2B	2.37	1.48	1.43
14	f	203	CLA	CHC-C1C	2.37	1.43	1.38
14	8	102	CLA	CHC-C1C	2.37	1.43	1.38
14	1	839	CLA	CMC-C2C	-2.37	1.45	1.50
14	b	3041	CLA	C1B-C2B	2.37	1.48	1.43
14	0	208	CLA	C1B-C2B	2.37	1.48	1.43
14	B	3014	CLA	CMD-C2D	-2.37	1.45	1.50
14	X	1701	CLA	C3B-C4B	2.37	1.49	1.42
14	a	837	CLA	CMD-C2D	-2.37	1.45	1.50
14	b	3008	CLA	CMD-C2D	-2.37	1.45	1.50
14	1	833	CLA	CMB-C2B	-2.37	1.45	1.50
14	a	826	CLA	CMD-C2D	-2.37	1.45	1.50
14	a	833	CLA	CMD-C2D	-2.37	1.45	1.50
14	A	805	CLA	C3B-C4B	2.36	1.49	1.42
14	A	834	CLA	CMD-C2D	-2.36	1.45	1.50
14	A	830	CLA	C1B-C2B	2.36	1.48	1.43
14	2	3003	CLA	C4B-NB	2.36	1.41	1.37
14	b	3014	CLA	CMD-C2D	-2.36	1.45	1.50
14	k	101	CLA	C3B-C4B	2.36	1.49	1.42
14	1	839	CLA	C4B-NB	2.36	1.41	1.37
14	A	826	CLA	CMB-C2B	-2.36	1.45	1.50
20	2	3050	LMG	O6-C5	-2.36	1.38	1.44
14	z	1701	CLA	CHC-C1C	2.36	1.43	1.38
14	a	805	CLA	CMD-C2D	-2.36	1.45	1.50
14	a	822	CLA	C3B-C4B	2.36	1.49	1.42
14	6	203	CLA	C3B-C4B	2.36	1.49	1.42
14	B	3040	CLA	C1B-C2B	2.36	1.48	1.43
17	b	3051	LHG	O7-C5	-2.36	1.41	1.46
14	1	825	CLA	CMD-C2D	-2.36	1.45	1.50
14	B	3026	CLA	CMD-C2D	-2.36	1.45	1.50
14	B	3035	CLA	CMB-C2B	-2.36	1.45	1.50
14	A	826	CLA	MG-NB	-2.36	2.01	2.05
14	B	3026	CLA	C3B-C4B	2.36	1.49	1.42
14	2	3040	CLA	C1B-C2B	2.36	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	3006	CLA	CMB-C2B	-2.36	1.45	1.50
14	A	822	CLA	MG-NB	-2.36	2.01	2.05
14	F	203	CLA	CMD-C2D	-2.36	1.45	1.50
14	1	802	CLA	CMC-C2C	-2.36	1.45	1.50
14	F	203	CLA	CHC-C1C	2.36	1.43	1.38
14	a	821	CLA	C3B-C4B	2.36	1.49	1.42
14	2	3013	CLA	C1B-C2B	2.36	1.48	1.43
14	a	802	CLA	CMC-C2C	-2.36	1.45	1.50
14	a	835	CLA	CMC-C2C	-2.36	1.45	1.50
14	a	804	CLA	C3B-C4B	2.36	1.49	1.42
14	A	842	CLA	CMC-C2C	-2.36	1.45	1.50
14	k	101	CLA	CMD-C2D	-2.36	1.45	1.50
14	1	831	CLA	C1B-C2B	2.36	1.48	1.43
14	A	843	CLA	MG-NB	-2.36	2.01	2.05
14	B	3041	CLA	CMB-C2B	-2.36	1.45	1.50
14	a	824	CLA	CMD-C2D	-2.36	1.45	1.50
14	2	3008	CLA	CMD-C2D	-2.36	1.45	1.50
14	1	822	CLA	MG-NB	-2.36	2.01	2.05
14	x	1701	CLA	C3B-C4B	2.36	1.49	1.42
14	l	208	CLA	CMC-C2C	-2.36	1.45	1.50
14	2	3033	CLA	CMD-C2D	-2.36	1.45	1.50
14	l	207	CLA	C1B-C2B	2.36	1.48	1.43
14	a	825	CLA	CMB-C2B	-2.36	1.45	1.50
14	2	3006	CLA	CMB-C2B	-2.36	1.45	1.50
17	B	3051	LHG	O7-C5	-2.36	1.41	1.46
14	b	3040	CLA	C3B-C4B	2.36	1.49	1.42
14	b	3034	CLA	CMC-C2C	-2.35	1.45	1.50
14	K	101	CLA	C3B-C4B	2.35	1.49	1.42
20	b	3050	LMG	O6-C5	-2.35	1.38	1.44
14	B	3040	CLA	CMB-C2B	-2.35	1.45	1.50
14	1	805	CLA	C3B-C4B	2.35	1.49	1.42
14	1	812	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	3010	CLA	CMB-C2B	-2.35	1.45	1.50
14	1	827	CLA	CMD-C2D	-2.35	1.45	1.50
14	6	203	CLA	CMD-C2D	-2.35	1.45	1.50
20	B	3050	LMG	O6-C5	-2.35	1.38	1.44
14	A	827	CLA	CMD-C2D	-2.35	1.46	1.50
14	2	3035	CLA	CMD-C2D	-2.35	1.46	1.50
14	2	3040	CLA	C3B-C4B	2.35	1.49	1.42
14	A	806	CLA	CMC-C2C	-2.35	1.46	1.50
14	A	838	CLA	CMD-C2D	-2.35	1.46	1.50
14	a	808	CLA	CMD-C2D	-2.35	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	806	CLA	CMD-C2D	-2.35	1.46	1.50
14	1	829	CLA	CMB-C2B	-2.35	1.46	1.50
14	B	3042	CLA	MG-NB	-2.35	2.01	2.05
14	a	831	CLA	C4B-NB	2.35	1.40	1.37
14	1	823	CLA	C3B-C4B	2.35	1.49	1.42
14	1	809	CLA	CMD-C2D	-2.35	1.46	1.50
14	B	3012	CLA	CMC-C2C	-2.35	1.46	1.50
14	A	825	CLA	C3B-C4B	2.35	1.49	1.42
14	B	3006	CLA	C1B-C2B	2.35	1.48	1.43
14	b	3026	CLA	MG-NB	-2.35	2.01	2.05
14	1	834	CLA	CMD-C2D	-2.35	1.46	1.50
14	B	3010	CLA	CMB-C2B	-2.35	1.46	1.50
14	a	828	CLA	CMB-C2B	-2.35	1.46	1.50
14	2	3012	CLA	CMC-C2C	-2.35	1.46	1.50
14	b	3042	CLA	MG-NB	-2.35	2.01	2.05
14	B	3033	CLA	CMD-C2D	-2.35	1.46	1.50
14	B	3034	CLA	C3B-C4B	2.35	1.49	1.42
14	0	209	CLA	CMC-C2C	-2.34	1.46	1.50
14	a	838	CLA	CMD-C2D	-2.34	1.46	1.50
14	1	805	CLA	CMD-C2D	-2.34	1.46	1.50
14	X	1701	CLA	CHC-C1C	2.34	1.43	1.38
16	B	3049	BCR	C38-C26	-2.34	1.47	1.50
14	b	3040	CLA	CMB-C2B	-2.34	1.46	1.50
14	B	3005	CLA	CMD-C2D	-2.34	1.46	1.50
14	2	3010	CLA	C1B-C2B	2.34	1.48	1.43
14	L	204	CLA	CMC-C2C	-2.34	1.46	1.50
14	2	3026	CLA	CMD-C2D	-2.34	1.46	1.50
14	0	208	CLA	MG-NB	-2.34	2.01	2.05
14	a	826	CLA	MG-NB	-2.34	2.01	2.05
14	L	201	CLA	C3B-C4B	2.34	1.49	1.42
14	A	825	CLA	CMD-C2D	-2.34	1.46	1.50
14	2	3010	CLA	CMB-C2B	-2.34	1.46	1.50
14	0	204	CLA	C3B-C4B	2.34	1.49	1.42
14	B	3026	CLA	MG-NB	-2.34	2.01	2.05
14	a	842	CLA	MG-NB	-2.34	2.01	2.05
14	2	3026	CLA	MG-NB	-2.34	2.01	2.05
14	b	3011	CLA	C4B-NB	2.34	1.40	1.37
14	A	828	CLA	CMC-C2C	-2.34	1.46	1.50
14	B	3038	CLA	CMD-C2D	-2.34	1.46	1.50
14	a	827	CLA	CMC-C2C	-2.34	1.46	1.50
14	B	3011	CLA	C4B-NB	2.34	1.40	1.37
14	a	811	CLA	CMD-C2D	-2.34	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	9	101	CLA	C3B-C4B	2.34	1.49	1.42
14	2	3027	CLA	MG-NB	-2.34	2.01	2.05
14	k	102	CLA	CHC-C1C	2.34	1.43	1.38
14	L	205	CLA	CMC-C2C	-2.34	1.46	1.50
14	2	3032	CLA	C3B-C4B	2.34	1.49	1.42
14	A	839	CLA	CMD-C2D	-2.34	1.46	1.50
16	b	3049	BCR	C38-C26	-2.34	1.47	1.50
14	B	3040	CLA	C3B-C4B	2.34	1.49	1.42
14	8	101	CLA	C3B-C4B	2.34	1.49	1.42
14	l	207	CLA	CMB-C2B	-2.33	1.46	1.50
14	2	3034	CLA	CMC-C2C	-2.33	1.46	1.50
16	a	849	BCR	C38-C26	-2.33	1.47	1.50
14	B	3035	CLA	CMD-C2D	-2.33	1.46	1.50
14	b	3026	CLA	CMD-C2D	-2.33	1.46	1.50
14	L	204	CLA	C1B-C2B	2.33	1.48	1.43
14	a	805	CLA	CMC-C2C	-2.33	1.46	1.50
14	A	834	CLA	MG-NB	-2.33	2.01	2.05
14	b	3027	CLA	MG-NB	-2.33	2.01	2.05
14	b	3027	CLA	CMC-C2C	-2.33	1.46	1.50
14	b	3006	CLA	C1B-C2B	2.33	1.48	1.43
14	1	825	CLA	MG-NB	-2.33	2.01	2.05
14	b	3022	CLA	C3B-C4B	2.33	1.49	1.42
14	2	3034	CLA	C3B-C4B	2.33	1.49	1.42
14	1	826	CLA	CMB-C2B	-2.33	1.46	1.50
14	2	3020	CLA	CMB-C2B	-2.33	1.46	1.50
14	b	3033	CLA	CMD-C2D	-2.33	1.46	1.50
14	2	3032	CLA	MG-NB	-2.33	2.01	2.05
14	F	201	CLA	CMD-C2D	-2.33	1.46	1.50
14	b	3020	CLA	CMB-C2B	-2.33	1.46	1.50
14	b	3035	CLA	CMD-C2D	-2.33	1.46	1.50
14	2	3027	CLA	CMC-C2C	-2.33	1.46	1.50
14	1	818	CLA	CHC-C1C	2.33	1.43	1.38
14	B	3012	CLA	MG-NB	-2.33	2.01	2.05
14	l	207	CLA	CMC-C2C	-2.33	1.46	1.50
14	1	841	CLA	MG-NB	-2.33	2.01	2.05
14	A	833	CLA	C1B-C2B	2.33	1.48	1.43
14	b	3034	CLA	C3B-C4B	2.33	1.49	1.42
14	j	1103	CLA	CHC-C1C	2.33	1.43	1.38
14	j	1102	CLA	C3B-C4B	2.33	1.49	1.42
14	A	835	CLA	CMD-C2D	-2.33	1.46	1.50
14	1	806	CLA	CMC-C2C	-2.33	1.46	1.50
14	2	3040	CLA	CMB-C2B	-2.33	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	834	CLA	CMD-C2D	-2.33	1.46	1.50
14	1	828	CLA	CMC-C2C	-2.33	1.46	1.50
14	2	3025	CLA	CMD-C2D	-2.33	1.46	1.50
14	B	3006	CLA	CMB-C2B	-2.33	1.46	1.50
14	2	3041	CLA	CMB-C2B	-2.33	1.46	1.50
14	a	824	CLA	C3B-C4B	2.33	1.49	1.42
14	b	3003	CLA	C3B-C4B	2.33	1.49	1.42
14	1	843	CLA	C3B-C4B	2.33	1.49	1.42
14	b	3032	CLA	MG-NB	-2.32	2.01	2.05
14	B	3003	CLA	C3B-C4B	2.32	1.49	1.42
14	2	3006	CLA	C1B-C2B	2.32	1.48	1.43
14	a	806	CLA	MG-NB	-2.32	2.01	2.05
14	1	807	CLA	C3B-C4B	2.32	1.49	1.42
14	1	810	CLA	MG-NB	-2.32	2.01	2.05
14	2	3014	CLA	CMD-C2D	-2.32	1.46	1.50
14	2	3003	CLA	C3B-C4B	2.32	1.49	1.42
14	A	833	CLA	CMB-C2B	-2.32	1.46	1.50
14	A	836	CLA	CMC-C2C	-2.32	1.46	1.50
14	f	203	CLA	CMD-C2D	-2.32	1.46	1.50
14	A	804	CLA	CMB-C2B	-2.32	1.46	1.50
14	B	3023	CLA	CHC-C1C	2.32	1.43	1.38
14	1	803	CLA	MG-NB	-2.32	2.01	2.05
14	A	843	CLA	C3B-C4B	2.32	1.49	1.42
14	a	832	CLA	CMB-C2B	-2.32	1.46	1.50
14	2	3028	CLA	CHC-C1C	2.32	1.43	1.38
14	B	3007	CLA	C1B-C2B	2.32	1.48	1.43
14	a	842	CLA	C3B-C4B	2.32	1.49	1.42
14	A	803	CLA	MG-NB	-2.32	2.01	2.05
14	B	3025	CLA	CMD-C2D	-2.32	1.46	1.50
14	b	3041	CLA	CMB-C2B	-2.32	1.46	1.50
14	L	204	CLA	CMB-C2B	-2.32	1.46	1.50
14	1	804	CLA	CMB-C2B	-2.32	1.46	1.50
14	1	830	CLA	C4B-NB	2.32	1.40	1.37
14	B	3022	CLA	C3B-C4B	2.32	1.49	1.42
14	B	3034	CLA	CMC-C2C	-2.32	1.46	1.50
14	1	843	CLA	MG-NB	-2.32	2.01	2.05
14	a	832	CLA	C4B-NB	2.32	1.40	1.37
14	K	102	CLA	CHC-C1C	2.32	1.43	1.38
14	f	201	CLA	CMD-C2D	-2.32	1.46	1.50
14	L	203	CLA	CMB-C2B	-2.32	1.46	1.50
14	1	836	CLA	CMC-C2C	-2.32	1.46	1.50
14	A	827	CLA	MG-NB	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	803	CLA	MG-NB	-2.31	2.01	2.05
14	B	3010	CLA	C1B-C2B	2.31	1.48	1.43
14	a	832	CLA	C1B-C2B	2.31	1.48	1.43
14	A	812	CLA	CMD-C2D	-2.31	1.46	1.50
14	a	829	CLA	C4B-NB	2.31	1.40	1.37
14	b	3023	CLA	CHC-C1C	2.31	1.43	1.38
16	7	101	BCR	C38-C26	-2.31	1.47	1.50
14	2	3011	CLA	C4B-NB	2.31	1.40	1.37
14	A	837	CLA	CMB-C2B	-2.31	1.46	1.50
14	B	3016	CLA	CMD-C2D	-2.31	1.46	1.50
14	0	208	CLA	CMC-C2C	-2.31	1.46	1.50
14	1	807	CLA	MG-NB	-2.31	2.01	2.05
14	b	3005	CLA	CMD-C2D	-2.31	1.46	1.50
14	A	838	CLA	C3B-C4B	2.31	1.49	1.42
14	a	840	CLA	MG-NB	-2.31	2.01	2.05
14	1	813	CLA	C3B-C4B	2.31	1.49	1.42
14	L	201	CLA	C1B-C2B	2.31	1.48	1.43
14	A	841	CLA	MG-NB	-2.31	2.01	2.05
14	A	823	CLA	CMD-C2D	-2.31	1.46	1.50
14	b	3019	CLA	CMB-C2B	-2.31	1.46	1.50
14	a	837	CLA	C3B-C4B	2.31	1.49	1.42
14	a	804	CLA	CMD-C2D	-2.31	1.46	1.50
14	2	3022	CLA	C3B-C4B	2.31	1.49	1.42
14	a	829	CLA	CMB-C2B	-2.31	1.46	1.50
14	a	840	CLA	CMB-C2B	-2.31	1.46	1.50
14	a	841	CLA	CMB-C2B	-2.31	1.46	1.50
14	b	3025	CLA	CMC-C2C	-2.31	1.46	1.50
14	1	835	CLA	CMD-C2D	-2.31	1.46	1.50
14	1	833	CLA	C1B-C2B	2.31	1.48	1.43
14	B	3032	CLA	C3B-C4B	2.31	1.49	1.42
14	b	3028	CLA	CHC-C1C	2.31	1.43	1.38
14	b	3039	CLA	C1B-C2B	2.31	1.48	1.43
14	1	839	CLA	CMD-C2D	-2.31	1.46	1.50
14	6	201	CLA	CMD-C2D	-2.31	1.46	1.50
16	B	3052	BCR	C38-C26	-2.31	1.47	1.50
14	b	3039	CLA	CMD-C2D	-2.31	1.46	1.50
14	A	840	CLA	C1B-C2B	2.31	1.48	1.43
14	a	806	CLA	C3B-C4B	2.31	1.49	1.42
14	1	840	CLA	C1B-C2B	2.31	1.48	1.43
14	A	805	CLA	MG-NB	-2.31	2.01	2.05
14	A	805	CLA	CMD-C2D	-2.31	1.46	1.50
14	F	203	CLA	CMC-C2C	-2.31	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3039	CLA	C1B-C2B	2.30	1.48	1.43
14	f	203	CLA	CMC-C2C	-2.30	1.46	1.50
14	2	3025	CLA	CMC-C2C	-2.30	1.46	1.50
14	a	839	CLA	C1B-C2B	2.30	1.48	1.43
14	b	3010	CLA	C1B-C2B	2.30	1.48	1.43
14	a	820	CLA	CMD-C2D	-2.30	1.46	1.50
14	b	3041	CLA	CMC-C2C	-2.30	1.46	1.50
14	A	818	CLA	CHC-C1C	2.30	1.43	1.38
14	J	101	CLA	C3B-C4B	2.30	1.49	1.42
14	A	802	CLA	CMC-C2C	-2.30	1.46	1.50
14	a	821	CLA	CMD-C2D	-2.30	1.46	1.50
14	A	810	CLA	MG-NB	-2.30	2.01	2.05
14	b	3007	CLA	C1B-C2B	2.30	1.48	1.43
14	l	203	CLA	C1B-C2B	2.30	1.48	1.43
14	2	3016	CLA	CMC-C2C	-2.30	1.46	1.50
14	1	827	CLA	MG-NB	-2.30	2.01	2.05
16	A	850	BCR	C38-C26	-2.30	1.47	1.50
14	2	3029	CLA	C1B-C2B	2.30	1.48	1.43
14	b	3005	CLA	CMC-C2C	-2.30	1.46	1.50
14	2	3005	CLA	CMC-C2C	-2.30	1.46	1.50
14	b	3012	CLA	MG-NB	-2.30	2.01	2.05
14	A	842	CLA	CMB-C2B	-2.30	1.46	1.50
14	b	3020	CLA	C3B-C4B	2.30	1.49	1.42
14	A	814	CLA	CMD-C2D	-2.30	1.46	1.50
14	B	3032	CLA	MG-NB	-2.30	2.01	2.05
14	A	830	CLA	CMB-C2B	-2.30	1.46	1.50
14	B	3025	CLA	CMC-C2C	-2.30	1.46	1.50
14	a	836	CLA	CMB-C2B	-2.30	1.46	1.50
14	a	805	CLA	MG-NB	-2.30	2.01	2.05
14	B	3009	CLA	CMC-C2C	-2.30	1.46	1.50
14	j	1101	CLA	CMB-C2B	-2.30	1.46	1.50
14	1	836	CLA	CMD-C2D	-2.30	1.46	1.50
14	2	3039	CLA	C1B-C2B	2.30	1.48	1.43
14	a	805	CLA	C4B-NB	2.30	1.40	1.37
14	1	824	CLA	CMC-C2C	-2.30	1.46	1.50
14	2	3011	CLA	C1B-NB	-2.30	1.34	1.37
14	B	3020	CLA	C3B-C4B	2.30	1.49	1.42
14	A	806	CLA	MG-NB	-2.30	2.01	2.05
17	L	207	LHG	O7-C5	-2.30	1.41	1.46
14	b	3032	CLA	C3B-C4B	2.29	1.49	1.42
14	a	811	CLA	CMB-C2B	-2.29	1.46	1.50
14	A	809	CLA	C1B-C2B	2.29	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	809	CLA	C1B-C2B	2.29	1.48	1.43
14	1	809	CLA	C3B-C4B	2.29	1.49	1.42
14	b	3029	CLA	C1B-C2B	2.29	1.48	1.43
14	A	824	CLA	CMC-C2C	-2.29	1.46	1.50
14	1	823	CLA	CMD-C2D	-2.29	1.46	1.50
14	0	207	CLA	CMB-C2B	-2.29	1.46	1.50
14	B	3020	CLA	CMB-C2B	-2.29	1.46	1.50
14	a	813	CLA	CMD-C2D	-2.29	1.46	1.50
14	a	823	CLA	CMC-C2C	-2.29	1.46	1.50
14	a	812	CLA	C3B-C4B	2.29	1.49	1.42
14	A	830	CLA	C4B-NB	2.29	1.40	1.37
16	l	204	BCR	C38-C26	-2.29	1.47	1.50
16	1	849	BCR	C38-C26	-2.29	1.47	1.50
14	a	808	CLA	C1B-C2B	2.29	1.48	1.43
14	6	201	CLA	MG-NB	-2.29	2.01	2.05
14	A	807	CLA	C3B-C4B	2.29	1.49	1.42
14	A	822	CLA	CMD-C2D	-2.29	1.46	1.50
14	2	3016	CLA	CMD-C2D	-2.29	1.46	1.50
14	F	201	CLA	CMB-C2B	-2.29	1.46	1.50
14	2	3025	CLA	CMB-C2B	-2.29	1.46	1.50
14	a	809	CLA	MG-NB	-2.29	2.01	2.05
14	2	3028	CLA	CMD-C2D	-2.29	1.46	1.50
14	b	3025	CLA	C3B-C4B	2.29	1.49	1.42
14	a	833	CLA	MG-NB	-2.29	2.01	2.05
14	a	817	CLA	CHC-C1C	2.29	1.43	1.38
14	b	3016	CLA	CMD-C2D	-2.29	1.46	1.50
14	2	3019	CLA	CMB-C2B	-2.29	1.46	1.50
14	b	3033	CLA	C1B-C2B	2.29	1.48	1.43
16	i	101	BCR	C38-C26	-2.29	1.47	1.50
14	b	3016	CLA	CMC-C2C	-2.29	1.46	1.50
14	A	809	CLA	CMC-C2C	-2.29	1.46	1.50
14	f	201	CLA	CMB-C2B	-2.29	1.46	1.50
14	B	3028	CLA	MG-NB	-2.29	2.01	2.05
14	1	814	CLA	CMD-C2D	-2.29	1.46	1.50
14	A	813	CLA	C3B-C4B	2.29	1.49	1.42
14	b	3035	CLA	MG-NB	-2.29	2.01	2.05
16	2	3046	BCR	C38-C26	-2.29	1.47	1.50
14	A	812	CLA	C3B-C4B	2.29	1.49	1.42
14	1	805	CLA	MG-NB	-2.29	2.01	2.05
14	1	825	CLA	C3B-C4B	2.29	1.49	1.42
14	6	203	CLA	CMC-C2C	-2.29	1.46	1.50
14	2	3007	CLA	C1B-C2B	2.29	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	3009	CLA	CMC-C2C	-2.28	1.46	1.50
14	1	812	CLA	CMB-C2B	-2.28	1.46	1.50
14	b	3025	CLA	CMB-C2B	-2.28	1.46	1.50
14	1	842	CLA	MG-NB	-2.28	2.01	2.05
14	a	816	CLA	CMB-C2B	-2.28	1.46	1.50
14	a	822	CLA	CMD-C2D	-2.28	1.46	1.50
14	A	814	CLA	MG-NB	-2.28	2.01	2.05
14	2	3012	CLA	MG-NB	-2.28	2.01	2.05
14	a	804	CLA	CMB-C2B	-2.28	1.46	1.50
14	2	3005	CLA	CMD-C2D	-2.28	1.46	1.50
14	2	3028	CLA	CMC-C2C	-2.28	1.46	1.50
14	B	3029	CLA	C1B-C2B	2.28	1.48	1.43
14	B	3025	CLA	CMB-C2B	-2.28	1.46	1.50
14	2	3016	CLA	MG-NB	-2.28	2.01	2.05
14	1	834	CLA	MG-NB	-2.28	2.01	2.05
14	1	841	CLA	CMB-C2B	-2.28	1.46	1.50
14	A	809	CLA	C3B-C4B	2.28	1.49	1.42
14	a	804	CLA	MG-NB	-2.28	2.01	2.05
14	A	805	CLA	CMB-C2B	-2.28	1.46	1.50
14	A	811	CLA	CMD-C2D	-2.28	1.46	1.50
14	A	824	CLA	CMB-C2B	-2.28	1.46	1.50
14	B	3039	CLA	CMD-C2D	-2.28	1.46	1.50
14	0	204	CLA	C1B-C2B	2.28	1.48	1.43
14	B	3024	CLA	CHC-C1C	2.28	1.43	1.38
14	1	822	CLA	CHC-C1C	2.28	1.43	1.38
14	A	805	CLA	C1B-C2B	2.28	1.48	1.43
14	B	3025	CLA	C3B-C4B	2.28	1.49	1.42
14	B	3030	CLA	CMC-C2C	-2.28	1.46	1.50
14	A	837	CLA	CHC-C1C	2.28	1.43	1.38
14	1	814	CLA	MG-NB	-2.28	2.01	2.05
14	A	812	CLA	CMB-C2B	-2.28	1.46	1.50
14	1	824	CLA	CMD-C2D	-2.28	1.46	1.50
17	l	201	LHG	O7-C5	-2.28	1.41	1.46
14	2	3035	CLA	MG-NB	-2.28	2.01	2.05
14	a	823	CLA	CMB-C2B	-2.28	1.46	1.50
14	B	3028	CLA	CHC-C1C	2.28	1.43	1.38
14	1	812	CLA	C3B-C4B	2.28	1.49	1.42
14	B	3008	CLA	MG-NB	-2.28	2.01	2.05
14	b	3028	CLA	MG-NB	-2.28	2.01	2.05
14	6	203	CLA	MG-NB	-2.28	2.01	2.05
14	1	805	CLA	C1B-C2B	2.28	1.48	1.43
14	B	3041	CLA	MG-NB	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	203	CLA	MG-NB	-2.28	2.01	2.05
14	2	3041	CLA	CMC-C2C	-2.28	1.46	1.50
14	1	838	CLA	C3B-C4B	2.28	1.49	1.42
14	b	3028	CLA	CMD-C2D	-2.28	1.46	1.50
14	1	820	CLA	C1B-C2B	2.28	1.48	1.43
14	B	3005	CLA	CMC-C2C	-2.27	1.46	1.50
16	A	847	BCR	C38-C26	-2.27	1.47	1.50
14	A	807	CLA	MG-NB	-2.27	2.01	2.05
14	b	3008	CLA	MG-NB	-2.27	2.01	2.05
14	A	829	CLA	CMB-C2B	-2.27	1.46	1.50
14	1	810	CLA	CMB-C2B	-2.27	1.46	1.50
14	2	3025	CLA	C3B-C4B	2.27	1.49	1.42
14	a	819	CLA	C1B-C2B	2.27	1.48	1.43
14	a	811	CLA	C3B-C4B	2.27	1.49	1.42
14	l	206	CLA	CMB-C2B	-2.27	1.46	1.50
14	1	835	CLA	CMC-C2C	-2.27	1.46	1.50
14	2	3039	CLA	CMD-C2D	-2.27	1.46	1.50
14	2	3023	CLA	CHC-C1C	2.27	1.43	1.38
14	0	209	CLA	C1B-C2B	2.27	1.48	1.43
14	B	3041	CLA	CMC-C2C	-2.27	1.46	1.50
14	B	3011	CLA	C1B-C2B	2.27	1.48	1.43
14	1	806	CLA	MG-NB	-2.27	2.01	2.05
14	2	3033	CLA	C1B-C2B	2.27	1.48	1.43
14	b	3025	CLA	CMD-C2D	-2.27	1.46	1.50
14	B	3019	CLA	CMB-C2B	-2.27	1.46	1.50
14	a	809	CLA	CMB-C2B	-2.27	1.46	1.50
14	A	836	CLA	MG-NB	-2.27	2.01	2.05
14	f	201	CLA	CHC-C1C	2.27	1.43	1.38
14	B	3014	CLA	C3B-C4B	2.27	1.49	1.42
14	L	203	CLA	CMC-C2C	-2.27	1.46	1.50
14	1	809	CLA	CMB-C2B	-2.27	1.46	1.50
14	b	3016	CLA	MG-NB	-2.27	2.01	2.05
16	I	101	BCR	C38-C26	-2.27	1.47	1.50
20	b	3050	LMG	O8-C9	-2.27	1.40	1.45
14	A	809	CLA	MG-NB	-2.27	2.01	2.05
14	A	813	CLA	MG-NB	-2.27	2.01	2.05
14	l	208	CLA	C1B-C2B	2.27	1.48	1.43
14	1	809	CLA	CMC-C2C	-2.27	1.46	1.50
14	1	835	CLA	CMB-C2B	-2.27	1.46	1.50
14	1	806	CLA	C4B-NB	2.27	1.40	1.37
14	A	828	CLA	MG-NB	-2.27	2.01	2.05
14	9	103	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	835	CLA	CMC-C2C	-2.27	1.46	1.50
14	a	819	CLA	MG-NB	-2.27	2.01	2.05
14	A	824	CLA	CMD-C2D	-2.27	1.46	1.50
14	2	3020	CLA	C3B-C4B	2.27	1.49	1.42
14	A	821	CLA	CMD-C2D	-2.27	1.46	1.50
14	A	836	CLA	CMD-C2D	-2.27	1.46	1.50
14	2	3028	CLA	MG-NB	-2.27	2.01	2.05
14	l	206	CLA	CMC-C2C	-2.27	1.46	1.50
14	F	201	CLA	MG-NB	-2.26	2.01	2.05
14	b	3031	CLA	CMC-C2C	-2.26	1.46	1.50
14	2	3030	CLA	CMC-C2C	-2.26	1.46	1.50
20	2	3050	LMG	O8-C9	-2.26	1.40	1.45
14	B	3031	CLA	CMC-C2C	-2.26	1.46	1.50
14	1	814	CLA	CMC-C2C	-2.26	1.46	1.50
14	b	3014	CLA	C3B-C4B	2.26	1.49	1.42
14	6	201	CLA	CMB-C2B	-2.26	1.46	1.50
14	a	804	CLA	C1B-C2B	2.26	1.48	1.43
14	a	813	CLA	MG-NB	-2.26	2.01	2.05
14	a	830	CLA	CMC-C2C	-2.26	1.46	1.50
14	1	821	CLA	CMD-C2D	-2.26	1.46	1.50
14	B	3011	CLA	C1B-NB	-2.26	1.34	1.37
14	A	840	CLA	MG-NB	-2.26	2.01	2.05
14	2	3014	CLA	C3B-C4B	2.26	1.49	1.42
14	2	3031	CLA	CMC-C2C	-2.26	1.46	1.50
14	B	3035	CLA	MG-NB	-2.26	2.01	2.05
14	a	827	CLA	MG-NB	-2.26	2.01	2.05
14	1	842	CLA	CMB-C2B	-2.26	1.46	1.50
14	2	3008	CLA	CMB-C2B	-2.26	1.46	1.50
14	2	3013	CLA	CMD-C2D	-2.26	1.46	1.50
14	b	3031	CLA	CMD-C2D	-2.26	1.46	1.50
14	L	205	CLA	C1B-C2B	2.26	1.48	1.43
16	0	205	BCR	C38-C26	-2.26	1.47	1.50
14	a	812	CLA	MG-NB	-2.26	2.01	2.05
14	a	839	CLA	MG-NB	-2.26	2.01	2.05
14	A	817	CLA	CMB-C2B	-2.26	1.46	1.50
14	a	823	CLA	CMD-C2D	-2.26	1.46	1.50
14	1	837	CLA	CMB-C2B	-2.26	1.46	1.50
14	1	840	CLA	MG-NB	-2.26	2.01	2.05
14	2	3021	CLA	CHC-C1C	2.26	1.43	1.38
14	B	3033	CLA	C1B-C2B	2.26	1.48	1.43
14	6	201	CLA	CHC-C1C	2.26	1.43	1.38
14	2	3011	CLA	C1B-C2B	2.26	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	824	CLA	CMB-C2B	-2.26	1.46	1.50
14	A	804	CLA	C3B-C4B	2.26	1.49	1.42
14	a	836	CLA	CHC-C1C	2.26	1.43	1.38
14	1	825	CLA	C1B-C2B	2.26	1.48	1.43
14	A	810	CLA	CMB-C2B	-2.26	1.46	1.50
14	f	203	CLA	MG-NB	-2.26	2.01	2.05
14	8	102	CLA	CBD-CAD	2.26	1.56	1.51
14	A	820	CLA	C1B-C2B	2.26	1.48	1.43
14	B	3008	CLA	CMB-C2B	-2.26	1.46	1.50
14	1	804	CLA	MG-NB	-2.26	2.01	2.05
14	2	3041	CLA	MG-NB	-2.26	2.01	2.05
16	a	846	BCR	C38-C26	-2.26	1.47	1.50
14	a	834	CLA	CMC-C2C	-2.26	1.46	1.50
14	a	810	CLA	C3B-C4B	2.26	1.49	1.42
14	b	3021	CLA	CHC-C1C	2.26	1.43	1.38
14	a	814	CLA	CHC-C1C	2.26	1.43	1.38
14	1	841	CLA	CMC-C2C	-2.26	1.46	1.50
14	A	835	CLA	MG-NB	-2.26	2.01	2.05
14	1	809	CLA	MG-NB	-2.26	2.01	2.05
14	B	3031	CLA	CMD-C2D	-2.25	1.46	1.50
14	1	822	CLA	CMD-C2D	-2.25	1.46	1.50
14	A	833	CLA	C4B-NB	2.25	1.40	1.37
14	B	3028	CLA	CMC-C2C	-2.25	1.46	1.50
14	1	802	CLA	CMB-C2B	-2.25	1.46	1.50
17	0	201	LHG	O7-C5	-2.25	1.41	1.46
14	B	3016	CLA	MG-NB	-2.25	2.01	2.05
14	1	833	CLA	CMC-C2C	-2.25	1.46	1.50
14	a	821	CLA	CHC-C1C	2.25	1.43	1.38
14	A	806	CLA	C4B-NB	2.25	1.40	1.37
14	A	802	CLA	CMB-C2B	-2.25	1.46	1.50
14	1	833	CLA	C4B-NB	2.25	1.40	1.37
14	B	3013	CLA	MG-NB	-2.25	2.01	2.05
14	a	829	CLA	C3B-C4B	2.25	1.49	1.42
14	B	3016	CLA	CMC-C2C	-2.25	1.46	1.50
14	1	822	CLA	CMC-C2C	-2.25	1.46	1.50
14	a	826	CLA	CMB-C2B	-2.25	1.46	1.50
14	b	3013	CLA	CMD-C2D	-2.25	1.46	1.50
14	a	810	CLA	CMD-C2D	-2.25	1.46	1.50
14	1	813	CLA	MG-NB	-2.25	2.01	2.05
14	1	827	CLA	CMB-C2B	-2.25	1.46	1.50
14	1	811	CLA	C3B-C4B	2.25	1.49	1.42
14	F	201	CLA	CHC-C1C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	3008	CLA	MG-NB	-2.25	2.01	2.05
16	a	847	BCR	C38-C26	-2.25	1.47	1.50
14	b	3041	CLA	MG-NB	-2.25	2.01	2.05
14	A	841	CLA	CMB-C2B	-2.25	1.46	1.50
14	a	832	CLA	CMC-C2C	-2.25	1.46	1.50
14	j	1101	CLA	C3B-C4B	2.25	1.49	1.42
14	a	835	CLA	MG-NB	-2.25	2.01	2.05
14	1	820	CLA	MG-NB	-2.25	2.01	2.05
14	a	824	CLA	C1B-C2B	2.25	1.48	1.43
14	b	3011	CLA	C1B-NB	-2.25	1.34	1.37
14	A	811	CLA	C3B-C4B	2.25	1.49	1.42
14	a	840	CLA	CMC-C2C	-2.25	1.46	1.50
16	1	846	BCR	C38-C26	-2.25	1.47	1.50
14	1	804	CLA	C3B-C4B	2.25	1.49	1.42
14	2	3009	CLA	CMC-C2C	-2.25	1.46	1.50
14	1	830	CLA	CMB-C2B	-2.24	1.46	1.50
14	B	3021	CLA	CHC-C1C	2.24	1.43	1.38
14	1	831	CLA	CMC-C2C	-2.24	1.46	1.50
14	b	3030	CLA	CMC-C2C	-2.24	1.46	1.50
14	0	204	CLA	CMB-C2B	-2.24	1.46	1.50
14	l	203	CLA	MG-NB	-2.24	2.01	2.05
14	A	841	CLA	CMC-C2C	-2.24	1.46	1.50
14	A	827	CLA	CMB-C2B	-2.24	1.46	1.50
14	B	3007	CLA	MG-NB	-2.24	2.01	2.05
14	0	204	CLA	MG-NB	-2.24	2.01	2.05
14	a	802	CLA	CMB-C2B	-2.24	1.46	1.50
14	B	3028	CLA	CMD-C2D	-2.24	1.46	1.50
14	A	804	CLA	MG-NB	-2.24	2.01	2.05
14	1	808	CLA	C3B-C4B	2.24	1.49	1.42
14	a	808	CLA	C3B-C4B	2.24	1.49	1.42
14	B	3026	CLA	CMB-C2B	-2.24	1.46	1.50
14	2	3024	CLA	CMD-C2D	-2.24	1.46	1.50
14	b	3008	CLA	CMB-C2B	-2.24	1.46	1.50
14	A	842	CLA	MG-NB	-2.24	2.01	2.05
14	l	203	CLA	CMB-C2B	-2.24	1.46	1.50
14	a	834	CLA	CMB-C2B	-2.24	1.46	1.50
14	b	3028	CLA	CMC-C2C	-2.24	1.46	1.50
14	f	201	CLA	C1B-C2B	2.24	1.48	1.43
14	b	3013	CLA	MG-NB	-2.24	2.01	2.05
14	1	817	CLA	CMB-C2B	-2.24	1.46	1.50
14	2	3031	CLA	CMD-C2D	-2.24	1.46	1.50
14	b	3021	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	3031	CLA	C1B-C2B	2.24	1.48	1.43
14	L	201	CLA	CMB-C2B	-2.24	1.46	1.50
14	2	3021	CLA	C3B-C4B	2.24	1.49	1.42
16	l	210	BCR	C38-C26	-2.24	1.47	1.50
14	b	3029	CLA	CMC-C2C	-2.24	1.46	1.50
14	J	102	CLA	CBD-CAD	2.24	1.56	1.51
14	A	810	CLA	CMC-C2C	-2.23	1.46	1.50
14	A	814	CLA	CMC-C2C	-2.23	1.46	1.50
14	b	3026	CLA	CHC-C1C	2.23	1.43	1.38
14	A	835	CLA	CMB-C2B	-2.23	1.46	1.50
14	1	805	CLA	CMB-C2B	-2.23	1.46	1.50
14	0	207	CLA	CMC-C2C	-2.23	1.46	1.50
14	b	3011	CLA	C1B-C2B	2.23	1.48	1.43
14	b	3034	CLA	CMB-C2B	-2.23	1.46	1.50
14	1	811	CLA	CMD-C2D	-2.23	1.46	1.50
14	1	837	CLA	CHC-C1C	2.23	1.43	1.38
14	B	3026	CLA	C1B-C2B	2.23	1.48	1.43
14	b	3007	CLA	MG-NB	-2.23	2.01	2.05
16	0	211	BCR	C38-C26	-2.23	1.47	1.50
14	j	1101	CLA	MG-NB	-2.23	2.01	2.05
14	a	808	CLA	CMB-C2B	-2.23	1.46	1.50
14	A	825	CLA	C1B-C2B	2.23	1.48	1.43
14	a	841	CLA	MG-NB	-2.23	2.01	2.05
14	A	822	CLA	CMC-C2C	-2.23	1.46	1.50
14	1	810	CLA	CMC-C2C	-2.23	1.46	1.50
14	a	809	CLA	CMC-C2C	-2.23	1.46	1.50
14	1	828	CLA	MG-NB	-2.23	2.01	2.05
14	a	827	CLA	C3B-C4B	2.23	1.49	1.42
14	1	829	CLA	C1B-C2B	2.23	1.48	1.43
14	A	813	CLA	CMB-C2B	-2.23	1.46	1.50
14	B	3024	CLA	CMD-C2D	-2.23	1.46	1.50
14	a	827	CLA	CMB-C2B	-2.23	1.46	1.50
14	1	836	CLA	MG-NB	-2.23	2.01	2.05
20	B	3050	LMG	O8-C9	-2.23	1.40	1.45
14	2	3031	CLA	C1B-C2B	2.23	1.48	1.43
16	b	3046	BCR	C38-C26	-2.23	1.47	1.50
14	A	822	CLA	CHC-C1C	2.23	1.42	1.38
14	A	820	CLA	MG-NB	-2.23	2.01	2.05
14	b	3017	CLA	C3B-C4B	2.23	1.49	1.42
14	a	808	CLA	CMC-C2C	-2.23	1.46	1.50
14	a	835	CLA	CMD-C2D	-2.23	1.46	1.50
14	b	3024	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	828	CLA	CMD-C2D	-2.23	1.46	1.50
14	B	3036	CLA	MG-NB	-2.23	2.01	2.05
14	B	3029	CLA	CMC-C2C	-2.23	1.46	1.50
14	1	828	CLA	CMB-C2B	-2.23	1.46	1.50
14	j	1103	CLA	CBD-CAD	2.23	1.56	1.51
14	a	807	CLA	CMC-C2C	-2.23	1.46	1.50
14	K	101	CLA	CMB-C2B	-2.22	1.46	1.50
14	a	827	CLA	CMD-C2D	-2.22	1.46	1.50
14	f	201	CLA	MG-NB	-2.22	2.01	2.05
14	1	838	CLA	CMB-C2B	-2.22	1.46	1.50
14	b	3036	CLA	MG-NB	-2.22	2.01	2.05
14	2	3024	CLA	CHC-C1C	2.22	1.42	1.38
14	a	807	CLA	C3B-C4B	2.22	1.49	1.42
14	b	3017	CLA	MG-NB	-2.22	2.01	2.05
14	2	3018	CLA	CMD-C2D	-2.22	1.46	1.50
14	1	812	CLA	CMC-C2C	-2.22	1.46	1.50
14	1	835	CLA	MG-NB	-2.22	2.01	2.05
14	2	3007	CLA	MG-NB	-2.22	2.01	2.05
14	2	3017	CLA	C3B-C4B	2.22	1.49	1.42
14	2	3006	CLA	C3B-C4B	2.22	1.49	1.42
14	1	830	CLA	C3B-C4B	2.22	1.49	1.42
14	b	3026	CLA	C1B-C2B	2.22	1.48	1.43
14	6	201	CLA	C1B-C2B	2.22	1.48	1.43
14	2	3013	CLA	MG-NB	-2.22	2.01	2.05
14	B	3017	CLA	C3B-C4B	2.22	1.49	1.42
14	a	837	CLA	CMB-C2B	-2.22	1.46	1.50
14	2	3026	CLA	CMB-C2B	-2.22	1.46	1.50
14	A	815	CLA	CHC-C1C	2.22	1.42	1.38
14	a	819	CLA	C1B-NB	-2.22	1.34	1.37
14	a	818	CLA	C3B-C4B	2.22	1.49	1.42
14	a	839	CLA	CMB-C2B	-2.22	1.46	1.50
14	2	3029	CLA	CMC-C2C	-2.22	1.46	1.50
14	B	3027	CLA	CMB-C2B	-2.22	1.46	1.50
14	b	3004	CLA	C4B-NB	2.22	1.40	1.37
14	A	809	CLA	CMB-C2B	-2.22	1.46	1.50
14	a	813	CLA	CMC-C2C	-2.22	1.46	1.50
14	b	3021	CLA	CMD-C2D	-2.22	1.46	1.50
14	1	840	CLA	CMB-C2B	-2.22	1.46	1.50
16	L	206	BCR	C38-C26	-2.22	1.47	1.50
14	B	3019	CLA	C3B-C4B	2.22	1.49	1.42
14	a	828	CLA	C1B-C2B	2.22	1.48	1.43
14	b	3028	CLA	CMB-C2B	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	813	CLA	CMB-C2B	-2.21	1.46	1.50
14	1	828	CLA	C3B-C4B	2.21	1.49	1.42
14	2	3028	CLA	CMB-C2B	-2.21	1.46	1.50
14	2	3026	CLA	CHC-C1C	2.21	1.42	1.38
14	B	3021	CLA	C3B-C4B	2.21	1.49	1.42
14	A	808	CLA	C3B-C4B	2.21	1.49	1.42
14	B	3013	CLA	CMD-C2D	-2.21	1.46	1.50
14	b	3026	CLA	CMB-C2B	-2.21	1.46	1.50
14	0	207	CLA	MG-NB	-2.21	2.01	2.05
14	b	3025	CLA	MG-NB	-2.21	2.01	2.05
14	B	3026	CLA	CHC-C1C	2.21	1.42	1.38
14	b	3024	CLA	CHC-C1C	2.21	1.42	1.38
14	1	815	CLA	C3B-C4B	2.21	1.49	1.42
14	L	201	CLA	MG-NB	-2.21	2.01	2.05
16	A	848	BCR	C38-C26	-2.21	1.47	1.50
14	a	839	CLA	C3B-C4B	2.21	1.49	1.42
14	2	3021	CLA	CMD-C2D	-2.21	1.46	1.50
14	a	834	CLA	MG-NB	-2.21	2.01	2.05
14	2	3003	CLA	MG-ND	-2.21	2.01	2.05
14	B	3017	CLA	MG-NB	-2.21	2.01	2.05
14	A	830	CLA	C3B-C4B	2.21	1.49	1.42
14	b	3038	CLA	C3B-C4B	2.21	1.49	1.42
14	1	820	CLA	C3B-C4B	2.21	1.49	1.42
14	1	834	CLA	CMC-C2C	-2.21	1.46	1.50
14	2	3032	CLA	CMB-C2B	-2.21	1.46	1.50
14	A	812	CLA	MG-NB	-2.21	2.01	2.05
14	0	207	CLA	CHC-C1C	2.21	1.42	1.38
14	A	820	CLA	C3B-C4B	2.21	1.49	1.42
14	B	3018	CLA	CMD-C2D	-2.21	1.46	1.50
14	B	3004	CLA	C4B-NB	2.21	1.40	1.37
14	B	3021	CLA	CMD-C2D	-2.21	1.46	1.50
14	A	828	CLA	CMB-C2B	-2.21	1.46	1.50
14	A	828	CLA	CMD-C2D	-2.21	1.46	1.50
16	1	847	BCR	C38-C26	-2.21	1.47	1.50
14	B	3005	CLA	MG-NB	-2.21	2.01	2.05
14	A	838	CLA	CMB-C2B	-2.21	1.46	1.50
14	b	3032	CLA	CMB-C2B	-2.21	1.46	1.50
14	1	815	CLA	CHC-C1C	2.21	1.42	1.38
14	B	3038	CLA	C3B-C4B	2.21	1.49	1.42
14	B	3013	CLA	CMC-C2C	-2.21	1.46	1.50
14	a	802	CLA	C1B-C2B	2.21	1.48	1.43
14	a	821	CLA	CMC-C2C	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3006	CLA	C3B-C4B	2.21	1.49	1.42
14	1	840	CLA	C3B-C4B	2.21	1.49	1.42
14	B	3032	CLA	CMB-C2B	-2.21	1.46	1.50
14	a	808	CLA	MG-NB	-2.21	2.01	2.05
14	a	814	CLA	C3B-C4B	2.21	1.49	1.42
14	2	3038	CLA	C3B-C4B	2.21	1.49	1.42
14	9	101	CLA	CMB-C2B	-2.21	1.46	1.50
14	2	3013	CLA	CMC-C2C	-2.20	1.46	1.50
14	A	835	CLA	C4B-NB	2.20	1.40	1.37
14	A	802	CLA	C1B-C2B	2.20	1.48	1.43
14	1	802	CLA	C1B-C2B	2.20	1.48	1.43
14	1	837	CLA	MG-NB	-2.20	2.01	2.05
14	B	3034	CLA	CMB-C2B	-2.20	1.46	1.50
14	1	844	CLA	CMB-C2B	-2.20	1.46	1.50
14	A	817	CLA	C3B-C4B	2.20	1.49	1.42
14	b	3006	CLA	C3B-C4B	2.20	1.49	1.42
14	b	3005	CLA	MG-NB	-2.20	2.01	2.05
14	b	3018	CLA	CMD-C2D	-2.20	1.46	1.50
14	2	3024	CLA	CMC-C2C	-2.20	1.46	1.50
14	A	844	CLA	CMC-C2C	-2.20	1.46	1.50
14	b	3009	CLA	C3B-C4B	2.20	1.49	1.42
14	2	3009	CLA	MG-NB	-2.20	2.01	2.05
14	b	3018	CLA	MG-NB	-2.20	2.01	2.05
14	1	831	CLA	MG-ND	-2.20	2.01	2.05
14	b	3010	CLA	MG-NB	-2.20	2.01	2.05
16	B	3049	BCR	C33-C5	-2.20	1.47	1.50
14	a	836	CLA	MG-NB	-2.20	2.01	2.05
14	B	3025	CLA	MG-NB	-2.20	2.01	2.05
14	A	833	CLA	CMC-C2C	-2.20	1.46	1.50
14	1	844	CLA	CMC-C2C	-2.20	1.46	1.50
14	l	206	CLA	CHC-C1C	2.20	1.42	1.38
14	B	3039	CLA	CMC-C2C	-2.20	1.46	1.50
14	L	203	CLA	CHC-C1C	2.20	1.42	1.38
14	A	832	CLA	C1B-C2B	2.20	1.48	1.43
14	A	834	CLA	CMB-C2B	-2.19	1.46	1.50
14	b	3039	CLA	CMC-C2C	-2.19	1.46	1.50
14	K	101	CLA	CHC-C1C	2.19	1.42	1.38
14	B	3040	CLA	MG-NB	-2.19	2.01	2.05
14	F	201	CLA	C1B-C2B	2.19	1.48	1.43
14	2	3005	CLA	MG-NB	-2.19	2.01	2.05
14	B	3010	CLA	MG-NB	-2.19	2.01	2.05
14	A	831	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	3017	CLA	CMB-C2B	-2.19	1.46	1.50
16	B	3046	BCR	C38-C26	-2.19	1.47	1.50
14	A	829	CLA	C1B-C2B	2.19	1.48	1.43
14	k	101	CLA	CHC-C1C	2.19	1.42	1.38
14	b	3040	CLA	MG-NB	-2.19	2.01	2.05
14	2	3036	CLA	MG-NB	-2.19	2.01	2.05
14	2	3038	CLA	MG-NB	-2.19	2.01	2.05
14	A	840	CLA	C3B-C4B	2.19	1.49	1.42
14	a	824	CLA	CMB-C2B	-2.19	1.46	1.50
14	A	831	CLA	MG-ND	-2.19	2.01	2.05
14	b	3013	CLA	CMC-C2C	-2.19	1.46	1.50
14	B	3024	CLA	CMC-C2C	-2.19	1.46	1.50
14	2	3018	CLA	MG-NB	-2.19	2.01	2.05
14	A	834	CLA	CMC-C2C	-2.19	1.46	1.50
14	1	838	CLA	CMC-C2C	-2.19	1.46	1.50
14	a	812	CLA	CMB-C2B	-2.19	1.46	1.50
14	B	3031	CLA	C1B-C2B	2.19	1.48	1.43
14	b	3003	CLA	CMB-C2B	-2.19	1.46	1.50
14	2	3026	CLA	C1B-C2B	2.19	1.48	1.43
14	B	3020	CLA	CHC-C1C	2.19	1.42	1.38
14	a	816	CLA	C3B-C4B	2.19	1.49	1.42
14	a	819	CLA	C3B-C4B	2.19	1.49	1.42
14	b	3003	CLA	MG-ND	-2.19	2.01	2.05
14	1	817	CLA	C3B-C4B	2.19	1.49	1.42
16	6	202	BCR	C38-C26	-2.19	1.47	1.50
14	A	819	CLA	C3B-C4B	2.19	1.49	1.42
14	2	3017	CLA	MG-NB	-2.19	2.01	2.05
14	B	3017	CLA	CMB-C2B	-2.19	1.46	1.50
14	2	3019	CLA	C3B-C4B	2.19	1.49	1.42
14	B	3009	CLA	MG-NB	-2.19	2.01	2.05
16	f	202	BCR	C38-C26	-2.19	1.47	1.50
14	b	3023	CLA	CMD-C2D	-2.19	1.46	1.50
14	a	830	CLA	MG-ND	-2.19	2.01	2.05
14	2	3010	CLA	MG-NB	-2.19	2.01	2.05
17	A	854	LHG	P-O6	2.19	1.68	1.59
14	A	815	CLA	C3B-C4B	2.19	1.49	1.42
14	2	3033	CLA	CMB-C2B	-2.19	1.46	1.50
14	2	3034	CLA	CMB-C2B	-2.19	1.46	1.50
14	B	3041	CLA	C3B-C4B	2.19	1.49	1.42
14	2	3039	CLA	CMC-C2C	-2.19	1.46	1.50
14	A	804	CLA	CMC-C2C	-2.18	1.46	1.50
14	B	3034	CLA	MG-NB	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	812	CLA	CMC-C2C	-2.18	1.46	1.50
14	2	3027	CLA	C3B-C4B	2.18	1.49	1.42
14	a	843	CLA	CMC-C2C	-2.18	1.46	1.50
14	9	101	CLA	CHC-C1C	2.18	1.42	1.38
14	a	843	CLA	CMB-C2B	-2.18	1.46	1.50
14	1	820	CLA	C1B-NB	-2.18	1.35	1.37
14	a	833	CLA	CMB-C2B	-2.18	1.46	1.50
14	b	3017	CLA	CMB-C2B	-2.18	1.46	1.50
17	1	853	LHG	P-O6	2.18	1.67	1.59
14	A	828	CLA	C3B-C4B	2.18	1.49	1.42
14	A	840	CLA	CMB-C2B	-2.18	1.46	1.50
16	F	202	BCR	C38-C26	-2.18	1.47	1.50
14	B	3003	CLA	MG-ND	-2.18	2.01	2.05
16	2	3049	BCR	C33-C5	-2.18	1.47	1.50
14	A	823	CLA	CHC-C1C	2.18	1.42	1.38
14	A	807	CLA	CMC-C2C	-2.18	1.46	1.50
14	a	817	CLA	CMB-C2B	-2.18	1.46	1.50
14	1	808	CLA	CMC-C2C	-2.18	1.46	1.50
14	2	3003	CLA	CMB-C2B	-2.18	1.46	1.50
14	2	3025	CLA	MG-NB	-2.18	2.01	2.05
17	a	853	LHG	P-O6	2.18	1.67	1.59
14	L	203	CLA	MG-NB	-2.18	2.01	2.05
14	1	832	CLA	C1B-C2B	2.18	1.48	1.43
14	a	841	CLA	CHC-C1C	2.18	1.42	1.38
14	B	3033	CLA	CMB-C2B	-2.18	1.46	1.50
14	a	822	CLA	MG-NB	-2.18	2.01	2.05
14	0	203	CLA	CHC-C1C	2.18	1.42	1.38
14	b	3041	CLA	C3B-C4B	2.18	1.49	1.42
14	1	819	CLA	C3B-C4B	2.18	1.49	1.42
14	B	3018	CLA	MG-NB	-2.18	2.01	2.05
14	A	824	CLA	C3B-C4B	2.18	1.49	1.42
14	2	3042	CLA	C1B-C2B	2.18	1.48	1.43
14	A	807	CLA	C1B-NB	-2.18	1.35	1.37
14	1	807	CLA	CMB-C2B	-2.17	1.46	1.50
14	B	3015	CLA	CHC-C1C	2.17	1.42	1.38
14	2	3020	CLA	CHC-C1C	2.17	1.42	1.38
14	A	820	CLA	C1B-NB	-2.17	1.35	1.37
14	1	206	CLA	MG-NB	-2.17	2.01	2.05
14	2	3034	CLA	MG-NB	-2.17	2.01	2.05
14	j	1101	CLA	CMD-C2D	-2.17	1.46	1.50
14	b	3027	CLA	C3B-C4B	2.17	1.49	1.42
14	B	3038	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	817	CLA	CMD-C2D	-2.17	1.46	1.50
14	A	807	CLA	CMB-C2B	-2.17	1.46	1.50
14	1	834	CLA	CMB-C2B	-2.17	1.46	1.50
14	1	823	CLA	MG-NB	-2.17	2.01	2.05
14	k	101	CLA	CMB-C2B	-2.17	1.46	1.50
14	M	1601	CLA	CHC-C1C	2.17	1.42	1.38
14	B	3014	CLA	MG-NB	-2.17	2.01	2.05
14	a	816	CLA	CMD-C2D	-2.17	1.46	1.50
14	b	3024	CLA	CMC-C2C	-2.17	1.46	1.50
14	A	823	CLA	MG-NB	-2.17	2.01	2.05
14	1	835	CLA	C4B-NB	2.17	1.40	1.37
14	B	3027	CLA	C3B-C4B	2.17	1.49	1.42
14	1	842	CLA	CHC-C1C	2.17	1.42	1.38
14	b	3034	CLA	MG-NB	-2.17	2.01	2.05
14	2	3041	CLA	C3B-C4B	2.17	1.49	1.42
14	a	826	CLA	C1B-NB	-2.17	1.35	1.37
14	a	807	CLA	MG-NB	-2.17	2.01	2.05
14	A	808	CLA	CHC-C1C	2.17	1.42	1.38
14	B	3022	CLA	CMB-C2B	-2.17	1.46	1.50
14	b	3017	CLA	CMD-C2D	-2.17	1.46	1.50
14	B	3028	CLA	CMB-C2B	-2.17	1.46	1.50
14	1	804	CLA	CMC-C2C	-2.17	1.46	1.50
14	B	3009	CLA	C3B-C4B	2.17	1.49	1.42
14	1	825	CLA	CMB-C2B	-2.17	1.46	1.50
14	1	827	CLA	C1B-NB	-2.17	1.35	1.37
14	A	844	CLA	CMB-C2B	-2.17	1.46	1.50
14	a	811	CLA	CMC-C2C	-2.17	1.46	1.50
14	a	831	CLA	C1B-C2B	2.17	1.48	1.43
14	A	808	CLA	CMC-C2C	-2.17	1.46	1.50
14	b	3027	CLA	CMB-C2B	-2.16	1.46	1.50
14	1	820	CLA	CMC-C2C	-2.16	1.46	1.50
14	A	837	CLA	MG-NB	-2.16	2.01	2.05
14	2	3037	CLA	CHC-C1C	2.16	1.42	1.38
14	1	810	CLA	C3B-C4B	2.16	1.49	1.42
14	a	823	CLA	C3B-C4B	2.16	1.49	1.42
14	A	842	CLA	CHC-C1C	2.16	1.42	1.38
14	B	3010	CLA	CMD-C2D	-2.16	1.46	1.50
14	0	209	CLA	C3B-C4B	2.16	1.49	1.42
14	2	3008	CLA	C3B-C4B	2.16	1.49	1.42
14	1	805	CLA	CHC-C1C	2.16	1.42	1.38
14	b	3010	CLA	CMD-C2D	-2.16	1.46	1.50
14	1	837	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	0	210	BCR	C38-C26	-2.16	1.47	1.50
14	b	3009	CLA	MG-NB	-2.16	2.01	2.05
14	A	838	CLA	CMC-C2C	-2.16	1.46	1.50
14	1	817	CLA	CMD-C2D	-2.16	1.46	1.50
14	1	827	CLA	CHC-C1C	2.16	1.42	1.38
14	a	806	CLA	CMC-C2C	-2.16	1.46	1.50
14	2	3022	CLA	CMB-C2B	-2.16	1.46	1.50
14	B	3013	CLA	CMB-C2B	-2.16	1.46	1.50
14	a	834	CLA	C4B-NB	2.16	1.40	1.37
16	I	102	BCR	C38-C26	-2.16	1.47	1.50
14	2	3027	CLA	CMB-C2B	-2.16	1.46	1.50
14	1	833	CLA	MG-ND	-2.16	2.01	2.05
14	2	3014	CLA	MG-NB	-2.16	2.01	2.05
14	A	825	CLA	CMB-C2B	-2.16	1.46	1.50
14	B	3003	CLA	CMB-C2B	-2.16	1.46	1.50
14	b	3005	CLA	CMB-C2B	-2.16	1.46	1.50
16	b	3049	BCR	C33-C5	-2.16	1.47	1.50
14	b	3042	CLA	C1B-C2B	2.16	1.48	1.43
14	1	808	CLA	MG-NB	-2.16	2.01	2.05
14	b	3033	CLA	CMB-C2B	-2.16	1.46	1.50
14	2	3040	CLA	MG-NB	-2.16	2.01	2.05
14	a	833	CLA	CMC-C2C	-2.16	1.46	1.50
14	1	834	CLA	C1B-NB	-2.16	1.35	1.37
14	6	203	CLA	CMB-C2B	-2.15	1.46	1.50
14	a	804	CLA	CHC-C1C	2.15	1.42	1.38
14	a	837	CLA	CMC-C2C	-2.15	1.46	1.50
14	2	3004	CLA	C4B-NB	2.15	1.40	1.37
14	b	3019	CLA	C3B-C4B	2.15	1.49	1.42
14	2	3018	CLA	C3B-C4B	2.15	1.49	1.42
14	2	3014	CLA	CHC-C1C	2.15	1.42	1.38
14	a	809	CLA	C3B-C4B	2.15	1.49	1.42
14	a	813	CLA	CMB-C2B	-2.15	1.46	1.50
14	b	3013	CLA	CMB-C2B	-2.15	1.46	1.50
14	B	3042	CLA	C1B-C2B	2.15	1.48	1.43
14	a	824	CLA	CHC-C1C	2.15	1.42	1.38
14	a	810	CLA	CMB-C2B	-2.15	1.46	1.50
14	a	807	CLA	CHC-C1C	2.15	1.42	1.38
14	b	3020	CLA	CHC-C1C	2.15	1.42	1.38
14	1	843	CLA	C1B-C2B	2.15	1.48	1.43
14	1	807	CLA	CMC-C2C	-2.15	1.46	1.50
14	b	3014	CLA	MG-NB	-2.15	2.01	2.05
14	A	817	CLA	MG-NB	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	813	CLA	CHC-C1C	2.15	1.42	1.38
14	a	816	CLA	MG-NB	-2.15	2.01	2.05
14	1	818	CLA	MG-NB	-2.15	2.01	2.05
14	A	844	CLA	MG-NB	-2.15	2.01	2.05
14	2	3023	CLA	CMD-C2D	-2.15	1.46	1.50
14	a	836	CLA	CMD-C2D	-2.15	1.46	1.50
14	A	843	CLA	MG-ND	-2.15	2.01	2.05
14	B	3031	CLA	MG-ND	-2.15	2.01	2.05
14	A	855	CLA	CHC-C1C	2.15	1.42	1.38
14	2	3009	CLA	C3B-C4B	2.15	1.49	1.42
14	A	810	CLA	C3B-C4B	2.15	1.49	1.42
14	1	824	CLA	C3B-C4B	2.15	1.49	1.42
14	b	3037	CLA	CHC-C1C	2.14	1.42	1.38
14	a	822	CLA	CHC-C1C	2.14	1.42	1.38
14	A	843	CLA	C1B-C2B	2.14	1.48	1.43
14	2	3031	CLA	MG-ND	-2.14	2.01	2.05
14	A	820	CLA	CMC-C2C	-2.14	1.46	1.50
14	B	3017	CLA	CMC-C2C	-2.14	1.46	1.50
14	A	805	CLA	CHC-C1C	2.14	1.42	1.38
13	1	801	CL0	MG-ND	-2.14	2.01	2.05
14	B	3006	CLA	MG-NB	-2.14	2.01	2.05
14	a	811	CLA	MG-NB	-2.14	2.01	2.05
14	B	3015	CLA	CMB-C2B	-2.14	1.46	1.50
14	2	3017	CLA	CMC-C2C	-2.14	1.46	1.50
14	b	3018	CLA	C3B-C4B	2.14	1.49	1.42
14	b	3008	CLA	C3B-C4B	2.14	1.49	1.42
14	A	825	CLA	CHC-C1C	2.14	1.42	1.38
14	A	837	CLA	CMD-C2D	-2.14	1.46	1.50
14	B	3017	CLA	CMD-C2D	-2.14	1.46	1.50
14	1	814	CLA	CMB-C2B	-2.14	1.46	1.50
14	1	817	CLA	MG-NB	-2.14	2.01	2.05
14	B	3007	CLA	C3B-C4B	2.14	1.49	1.42
14	b	3022	CLA	CMB-C2B	-2.14	1.46	1.50
14	2	3038	CLA	CHC-C1C	2.14	1.42	1.38
14	b	3007	CLA	C3B-C4B	2.14	1.49	1.42
14	0	203	CLA	CMB-C2B	-2.14	1.46	1.50
16	j	1105	BCR	C38-C26	-2.14	1.47	1.50
14	2	3014	CLA	CMB-C2B	-2.14	1.46	1.50
16	M	1602	BCR	C33-C5	-2.14	1.47	1.50
14	1	811	CLA	CHC-C1C	2.14	1.42	1.38
14	B	3024	CLA	CMB-C2B	-2.14	1.46	1.50
14	b	3031	CLA	MG-ND	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	3024	CLA	CMB-C2B	-2.14	1.46	1.50
14	b	3014	CLA	CMB-C2B	-2.14	1.46	1.50
14	1	818	CLA	CMB-C2B	-2.14	1.46	1.50
14	1	813	CLA	CHC-C1C	2.14	1.42	1.38
14	1	812	CLA	MG-NB	-2.14	2.01	2.05
14	b	3017	CLA	CMC-C2C	-2.14	1.46	1.50
14	B	3005	CLA	CMB-C2B	-2.14	1.46	1.50
14	a	806	CLA	CMB-C2B	-2.14	1.46	1.50
14	j	1101	CLA	CMC-C2C	-2.14	1.46	1.50
14	b	3038	CLA	MG-NB	-2.14	2.01	2.05
14	A	818	CLA	CMB-C2B	-2.13	1.46	1.50
14	B	3014	CLA	CMB-C2B	-2.13	1.46	1.50
14	b	3015	CLA	CHC-C1C	2.13	1.42	1.38
14	b	3003	CLA	C1B-C2B	2.13	1.48	1.43
14	A	811	CLA	CMB-C2B	-2.13	1.46	1.50
14	b	3039	CLA	C3B-C4B	2.13	1.49	1.42
14	1	843	CLA	MG-ND	-2.13	2.01	2.05
14	L	205	CLA	C3B-C4B	2.13	1.49	1.42
14	a	842	CLA	MG-ND	-2.13	2.01	2.05
14	A	804	CLA	CMD-C2D	-2.13	1.46	1.50
14	a	842	CLA	C1B-C2B	2.13	1.48	1.43
14	b	3036	CLA	CHC-C1C	2.13	1.42	1.38
14	b	3013	CLA	C3B-C4B	2.13	1.49	1.42
14	f	203	CLA	CMB-C2B	-2.13	1.46	1.50
14	2	3010	CLA	CMD-C2D	-2.13	1.46	1.50
14	B	3037	CLA	CHC-C1C	2.13	1.42	1.38
14	2	3015	CLA	CMB-C2B	-2.13	1.46	1.50
14	1	808	CLA	CHC-C1C	2.13	1.42	1.38
14	1	823	CLA	CHC-C1C	2.13	1.42	1.38
14	b	3014	CLA	CHC-C1C	2.13	1.42	1.38
16	8	104	BCR	C38-C26	-2.13	1.47	1.50
14	B	3018	CLA	C3B-C4B	2.13	1.48	1.42
14	A	809	CLA	CHC-C1C	2.13	1.42	1.38
14	a	825	CLA	CMC-C2C	-2.13	1.46	1.50
14	b	3012	CLA	CMD-C2D	-2.13	1.46	1.50
14	a	826	CLA	CMC-C2C	-2.13	1.46	1.50
14	2	3007	CLA	C3B-C4B	2.13	1.48	1.42
14	1	842	CLA	C1B-C2B	2.13	1.48	1.43
14	b	3006	CLA	MG-NB	-2.13	2.01	2.05
16	b	3048	BCR	C38-C26	-2.13	1.47	1.50
14	2	3005	CLA	CMB-C2B	-2.13	1.46	1.50
16	b	3048	BCR	C33-C5	-2.13	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	826	CLA	CHC-C1C	2.13	1.42	1.38
13	1	801	CL0	CBD-CGD	-2.13	1.49	1.52
14	a	818	CLA	CMD-C2D	-2.13	1.46	1.50
14	A	818	CLA	MG-NB	-2.13	2.01	2.05
16	B	3045	BCR	C38-C26	-2.13	1.47	1.50
14	2	3006	CLA	MG-NB	-2.13	2.01	2.05
14	b	3025	CLA	CHC-C1C	2.12	1.42	1.38
14	2	3032	CLA	CHC-C1C	2.12	1.42	1.38
16	y	101	BCR	C33-C5	-2.12	1.47	1.50
14	B	3023	CLA	CMD-C2D	-2.12	1.46	1.50
14	2	3017	CLA	CMD-C2D	-2.12	1.46	1.50
14	a	837	CLA	MG-NB	-2.12	2.01	2.05
14	2	3013	CLA	CMB-C2B	-2.12	1.46	1.50
14	M	1601	CLA	CMB-C2B	-2.12	1.46	1.50
14	B	3037	CLA	CMD-C2D	-2.12	1.46	1.50
14	1	844	CLA	MG-NB	-2.12	2.01	2.05
14	a	810	CLA	CHC-C1C	2.12	1.42	1.38
14	B	3032	CLA	CMC-C2C	-2.12	1.46	1.50
14	B	3003	CLA	C1B-C2B	2.12	1.48	1.43
14	1	827	CLA	CMC-C2C	-2.12	1.46	1.50
14	1	808	CLA	CMD-C2D	-2.12	1.46	1.50
14	a	812	CLA	CHC-C1C	2.12	1.42	1.38
14	8	101	CLA	CHC-C1C	2.12	1.42	1.38
14	B	3012	CLA	CMD-C2D	-2.12	1.46	1.50
14	a	841	CLA	C1B-C2B	2.12	1.48	1.43
14	a	827	CLA	CHC-C1C	2.12	1.42	1.38
14	1	834	CLA	CHC-C1C	2.12	1.42	1.38
14	2	3039	CLA	C3B-C4B	2.12	1.48	1.42
13	a	801	CL0	MG-ND	-2.12	2.01	2.05
14	2	3003	CLA	C1B-C2B	2.12	1.48	1.43
14	A	802	CLA	CHC-C1C	2.12	1.42	1.38
14	l	208	CLA	C3B-C4B	2.12	1.48	1.42
16	A	851	BCR	C38-C26	-2.12	1.47	1.50
14	x	1701	CLA	CMD-C2D	-2.12	1.46	1.50
14	K	101	CLA	MG-NB	-2.12	2.01	2.05
14	a	843	CLA	MG-NB	-2.12	2.01	2.05
14	1	807	CLA	C1B-NB	-2.12	1.35	1.37
14	A	827	CLA	CMC-C2C	-2.12	1.46	1.50
13	A	801	CL0	MG-ND	-2.12	2.01	2.05
14	1	802	CLA	C1B-NB	-2.12	1.35	1.37
14	A	830	CLA	CMC-C2C	-2.12	1.46	1.50
13	A	801	CL0	CBD-CGD	-2.12	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3039	CLA	C3B-C4B	2.12	1.48	1.42
14	a	823	CLA	MG-NB	-2.12	2.01	2.05
14	a	829	CLA	MG-ND	-2.12	2.01	2.05
14	a	829	CLA	CMC-C2C	-2.12	1.46	1.50
14	1	830	CLA	CMC-C2C	-2.12	1.46	1.50
14	A	834	CLA	CHC-C1C	2.12	1.42	1.38
14	2	3037	CLA	CMD-C2D	-2.11	1.46	1.50
14	a	833	CLA	CHC-C1C	2.11	1.42	1.38
14	a	832	CLA	C3B-C4B	2.11	1.48	1.42
14	X	1701	CLA	CMD-C2D	-2.11	1.46	1.50
14	A	808	CLA	MG-NB	-2.11	2.01	2.05
14	6	204	CLA	CMD-C2D	-2.11	1.46	1.50
14	1	824	CLA	MG-NB	-2.11	2.01	2.05
14	A	855	CLA	CMB-C2B	-2.11	1.46	1.50
14	1	804	CLA	CMD-C2D	-2.11	1.46	1.50
16	0	210	BCR	C33-C5	-2.11	1.47	1.50
14	1	828	CLA	CHC-C1C	2.11	1.42	1.38
14	a	806	CLA	C1B-NB	-2.11	1.35	1.37
14	A	814	CLA	CMB-C2B	-2.11	1.46	1.50
14	1	811	CLA	CMB-C2B	-2.11	1.46	1.50
16	2	3045	BCR	C38-C26	-2.11	1.47	1.50
14	B	3009	CLA	CMB-C2B	-2.11	1.46	1.50
14	a	819	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	830	CLA	MG-ND	-2.11	2.01	2.05
14	B	3036	CLA	CHC-C1C	2.11	1.42	1.38
14	j	1102	CLA	CHC-C1C	2.11	1.42	1.38
14	1	841	CLA	C3B-C4B	2.11	1.48	1.42
14	b	3032	CLA	CMC-C2C	-2.11	1.46	1.50
14	2	3012	CLA	CMD-C2D	-2.11	1.46	1.50
14	B	3039	CLA	C1B-NB	-2.11	1.35	1.37
14	A	827	CLA	CHC-C1C	2.11	1.42	1.38
16	B	3048	BCR	C38-C26	-2.11	1.47	1.50
16	b	3045	BCR	C38-C26	-2.11	1.47	1.50
14	1	834	CLA	C1B-C2B	2.11	1.48	1.43
14	A	805	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	833	CLA	C3B-C4B	2.11	1.48	1.42
14	2	3013	CLA	C3B-C4B	2.11	1.48	1.42
14	a	832	CLA	MG-ND	-2.11	2.01	2.05
16	a	849	BCR	C33-C5	-2.11	1.47	1.50
14	f	204	CLA	CMD-C2D	-2.11	1.46	1.50
14	A	816	CLA	MG-NB	-2.11	2.01	2.05
14	F	203	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	3024	CLA	CMB-C2B	-2.11	1.46	1.50
14	b	3037	CLA	CMD-C2D	-2.11	1.46	1.50
14	B	3032	CLA	CHC-C1C	2.10	1.42	1.38
14	J	101	CLA	CHC-C1C	2.10	1.42	1.38
14	a	808	CLA	CHC-C1C	2.10	1.42	1.38
14	A	819	CLA	CMD-C2D	-2.10	1.46	1.50
16	I	102	BCR	C33-C5	-2.10	1.47	1.50
16	2	3048	BCR	C38-C26	-2.10	1.47	1.50
14	a	817	CLA	MG-NB	-2.10	2.01	2.05
14	k	101	CLA	MG-NB	-2.10	2.01	2.05
14	2	3032	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	842	CLA	C1B-C2B	2.10	1.48	1.43
14	b	3019	CLA	CMC-C2C	-2.10	1.46	1.50
14	j	1103	CLA	CMC-C2C	-2.10	1.46	1.50
14	B	3014	CLA	CHC-C1C	2.10	1.42	1.38
14	A	824	CLA	MG-NB	-2.10	2.01	2.05
14	A	833	CLA	MG-ND	-2.10	2.01	2.05
14	B	3006	CLA	CHC-C1C	2.10	1.42	1.38
14	b	3032	CLA	CHC-C1C	2.10	1.42	1.38
14	B	3013	CLA	C3B-C4B	2.10	1.48	1.42
14	a	802	CLA	MG-ND	-2.10	2.01	2.05
14	1	819	CLA	CMD-C2D	-2.10	1.46	1.50
14	1	816	CLA	MG-NB	-2.10	2.01	2.05
14	2	3009	CLA	CMB-C2B	-2.10	1.46	1.50
14	L	203	CLA	C1B-C2B	2.10	1.48	1.43
14	9	101	CLA	MG-NB	-2.10	2.01	2.05
14	A	838	CLA	MG-NB	-2.10	2.01	2.05
14	1	805	CLA	CMC-C2C	-2.10	1.46	1.50
14	a	833	CLA	C1B-C2B	2.10	1.48	1.43
14	1	833	CLA	C3B-C4B	2.10	1.48	1.42
14	B	3008	CLA	C3B-C4B	2.10	1.48	1.42
14	1	815	CLA	CMB-C2B	-2.10	1.46	1.50
16	1	209	BCR	C38-C26	-2.10	1.47	1.50
14	F	204	CLA	CMD-C2D	-2.10	1.46	1.50
14	2	3039	CLA	C1B-NB	-2.10	1.35	1.37
14	1	809	CLA	CHC-C1C	2.10	1.42	1.38
14	1	825	CLA	CHC-C1C	2.10	1.42	1.38
14	2	3015	CLA	CHC-C1C	2.10	1.42	1.38
14	1	830	CLA	MG-ND	-2.10	2.01	2.05
14	0	207	CLA	C1B-C2B	2.10	1.48	1.43
14	8	102	CLA	CMD-C2D	-2.10	1.46	1.50
14	L	204	CLA	MG-ND	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	838	CLA	MG-NB	-2.10	2.01	2.05
14	1	822	CLA	C1B-C2B	2.10	1.48	1.43
14	a	802	CLA	CHC-C1C	2.09	1.42	1.38
14	b	3034	CLA	CHC-C1C	2.09	1.42	1.38
14	a	833	CLA	C1B-NB	-2.09	1.35	1.37
16	1	849	BCR	C33-C5	-2.09	1.47	1.50
14	8	102	CLA	CMC-C2C	-2.09	1.46	1.50
14	k	101	CLA	CMC-C2C	-2.09	1.46	1.50
14	A	834	CLA	C1B-C2B	2.09	1.48	1.43
14	A	811	CLA	CHC-C1C	2.09	1.42	1.38
14	9	101	CLA	CMC-C2C	-2.09	1.46	1.50
16	1	850	BCR	C33-C5	-2.09	1.47	1.50
14	B	3025	CLA	CHC-C1C	2.09	1.42	1.38
14	b	3038	CLA	CHC-C1C	2.09	1.42	1.38
14	2	3013	CLA	CHC-C1C	2.09	1.42	1.38
13	a	801	CL0	CBD-CGD	-2.09	1.49	1.52
14	2	3019	CLA	CMC-C2C	-2.09	1.46	1.50
14	2	3025	CLA	CHC-C1C	2.09	1.42	1.38
14	b	3003	CLA	C1B-NB	-2.09	1.35	1.37
14	b	3015	CLA	CMB-C2B	-2.09	1.46	1.50
14	B	3016	CLA	C3B-C4B	2.09	1.48	1.42
14	a	804	CLA	CMC-C2C	-2.09	1.46	1.50
14	B	3038	CLA	CHC-C1C	2.09	1.42	1.38
14	A	832	CLA	MG-ND	-2.09	2.01	2.05
14	J	102	CLA	CMC-C2C	-2.09	1.46	1.50
14	0	208	CLA	MG-ND	-2.09	2.01	2.05
14	a	842	CLA	C1B-NB	-2.09	1.35	1.37
14	A	827	CLA	C1B-NB	-2.09	1.35	1.37
14	B	3033	CLA	MG-NB	-2.09	2.01	2.05
14	z	1701	CLA	CMD-C2D	-2.09	1.46	1.50
16	2	3048	BCR	C33-C5	-2.09	1.47	1.50
14	1	815	CLA	CMD-C2D	-2.08	1.46	1.50
14	A	844	CLA	CMD-C2D	-2.08	1.46	1.50
14	1	826	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	808	CLA	CMD-C2D	-2.08	1.46	1.50
14	a	840	CLA	C3B-C4B	2.08	1.48	1.42
14	A	815	CLA	CMB-C2B	-2.08	1.46	1.50
14	b	3006	CLA	CHC-C1C	2.08	1.42	1.38
14	1	802	CLA	CHC-C1C	2.08	1.42	1.38
14	2	3036	CLA	CHC-C1C	2.08	1.42	1.38
14	B	3016	CLA	CMB-C2B	-2.08	1.46	1.50
14	2	3033	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	l	209	BCR	C33-C5	-2.08	1.47	1.50
14	a	843	CLA	CMD-C2D	-2.08	1.46	1.50
16	1	850	BCR	C38-C26	-2.08	1.47	1.50
14	B	3019	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	841	CLA	C3B-C4B	2.08	1.48	1.42
14	2	3024	CLA	MG-NB	-2.08	2.01	2.05
14	J	102	CLA	CMD-C2D	-2.08	1.46	1.50
16	m	101	BCR	C33-C5	-2.08	1.47	1.50
14	j	1103	CLA	CMD-C2D	-2.08	1.46	1.50
14	A	817	CLA	CMC-C2C	-2.08	1.46	1.50
14	B	3033	CLA	CHC-C1C	2.08	1.42	1.38
14	A	802	CLA	MG-ND	-2.08	2.01	2.05
14	1	832	CLA	MG-ND	-2.08	2.01	2.05
14	A	836	CLA	C3B-C4B	2.08	1.48	1.42
14	2	3034	CLA	CHC-C1C	2.08	1.42	1.38
14	a	807	CLA	CMD-C2D	-2.07	1.46	1.50
14	2	3021	CLA	CMB-C2B	-2.07	1.46	1.50
14	A	814	CLA	CHC-C1C	2.07	1.42	1.38
14	a	815	CLA	MG-NB	-2.07	2.01	2.05
14	b	3009	CLA	CMB-C2B	-2.07	1.46	1.50
16	0	205	BCR	C27-C26	-2.07	1.47	1.51
14	2	3023	CLA	CMC-C2C	-2.07	1.46	1.50
14	A	828	CLA	CHC-C1C	2.07	1.42	1.38
14	b	3027	CLA	CHC-C1C	2.07	1.42	1.38
14	1	844	CLA	CHC-C1C	2.07	1.42	1.38
14	A	832	CLA	C1B-NB	-2.07	1.35	1.37
14	l	203	CLA	C1B-NB	-2.07	1.35	1.37
14	2	3003	CLA	C1B-NB	-2.07	1.35	1.37
14	b	3024	CLA	MG-NB	-2.07	2.01	2.05
14	b	3029	CLA	MG-ND	-2.07	2.01	2.05
14	b	3033	CLA	CMC-C2C	-2.07	1.46	1.50
14	B	3027	CLA	CHC-C1C	2.07	1.42	1.38
14	1	802	CLA	MG-ND	-2.07	2.01	2.05
14	B	3034	CLA	CHC-C1C	2.07	1.42	1.38
14	K	101	CLA	CMC-C2C	-2.07	1.46	1.50
14	6	201	CLA	CMC-C2C	-2.07	1.46	1.50
14	a	825	CLA	MG-ND	-2.07	2.01	2.05
14	2	3033	CLA	MG-NB	-2.07	2.01	2.05
14	2	3022	CLA	CMD-C2D	-2.07	1.46	1.50
16	2	3047	BCR	C38-C26	-2.07	1.47	1.50
14	A	834	CLA	C1B-NB	-2.07	1.35	1.37
14	1	838	CLA	C1B-NB	-2.07	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	826	CLA	CMC-C2C	-2.07	1.46	1.50
14	B	3022	CLA	CMD-C2D	-2.07	1.46	1.50
14	2	3033	CLA	CHC-C1C	2.07	1.42	1.38
14	2	3022	CLA	MG-NB	-2.07	2.01	2.05
14	a	813	CLA	C3B-C4B	2.07	1.48	1.42
14	A	843	CLA	C1B-NB	-2.07	1.35	1.37
14	B	3021	CLA	CMB-C2B	-2.07	1.46	1.50
14	a	814	CLA	CMD-C2D	-2.07	1.46	1.50
14	1	826	CLA	MG-ND	-2.07	2.01	2.05
14	a	814	CLA	CMB-C2B	-2.07	1.46	1.50
14	1	814	CLA	C3B-C4B	2.06	1.48	1.42
16	B	3047	BCR	C38-C26	-2.06	1.47	1.50
14	a	821	CLA	C1B-C2B	2.06	1.48	1.43
13	1	801	CL0	C3B-C2B	-2.06	1.37	1.40
14	b	3033	CLA	CHC-C1C	2.06	1.42	1.38
16	B	3048	BCR	C33-C5	-2.06	1.47	1.50
14	A	826	CLA	MG-ND	-2.06	2.01	2.05
14	1	832	CLA	C1B-NB	-2.06	1.35	1.37
14	B	3030	CLA	MG-ND	-2.06	2.01	2.05
14	1	819	CLA	MG-NB	-2.06	2.01	2.05
14	A	822	CLA	C1B-C2B	2.06	1.48	1.43
14	2	3006	CLA	CHC-C1C	2.06	1.42	1.38
14	F	201	CLA	CMC-C2C	-2.06	1.46	1.50
14	B	3029	CLA	MG-ND	-2.06	2.01	2.05
14	b	3021	CLA	CMB-C2B	-2.06	1.46	1.50
16	B	3052	BCR	C27-C26	-2.06	1.47	1.51
14	a	831	CLA	MG-ND	-2.06	2.01	2.05
14	A	829	CLA	MG-NB	-2.06	2.01	2.05
14	B	3024	CLA	MG-NB	-2.06	2.01	2.05
14	1	836	CLA	C3B-C4B	2.06	1.48	1.42
13	A	801	CL0	C3B-C2B	-2.06	1.37	1.40
14	B	3035	CLA	CMC-C2C	-2.06	1.46	1.50
14	2	3030	CLA	MG-ND	-2.06	2.01	2.05
14	1	824	CLA	CHC-C1C	2.06	1.42	1.38
14	b	3016	CLA	CMB-C2B	-2.06	1.46	1.50
14	0	208	CLA	C4B-NB	2.06	1.40	1.37
16	A	851	BCR	C33-C5	-2.06	1.47	1.50
14	B	3003	CLA	C1B-NB	-2.06	1.35	1.37
14	a	831	CLA	C3B-C4B	2.06	1.48	1.42
14	2	3016	CLA	C3B-C4B	2.06	1.48	1.42
14	l	206	CLA	C1B-C2B	2.06	1.48	1.43
14	b	3035	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	K	102	CLA	MG-NB	-2.06	2.01	2.05
14	b	3033	CLA	MG-NB	-2.06	2.01	2.05
16	a	850	BCR	C38-C26	-2.06	1.47	1.50
14	a	813	CLA	CHC-C1C	2.06	1.42	1.38
14	l	814	CLA	CHC-C1C	2.05	1.42	1.38
14	b	3023	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	3022	CLA	MG-NB	-2.05	2.01	2.05
14	f	201	CLA	CMC-C2C	-2.05	1.46	1.50
14	A	802	CLA	C1B-NB	-2.05	1.35	1.37
14	8	101	CLA	CMC-C2C	-2.05	1.46	1.50
14	a	818	CLA	MG-NB	-2.05	2.01	2.05
14	1	810	CLA	CHC-C1C	2.05	1.42	1.38
14	1	817	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	3016	CLA	C3B-C4B	2.05	1.48	1.42
14	a	816	CLA	CMC-C2C	-2.05	1.46	1.50
16	l	204	BCR	C27-C26	-2.05	1.47	1.51
14	2	3040	CLA	CMC-C2C	-2.05	1.46	1.50
14	A	819	CLA	MG-NB	-2.05	2.01	2.05
14	j	1103	CLA	MG-NB	-2.05	2.01	2.05
14	2	3027	CLA	CHC-C1C	2.05	1.42	1.38
16	A	850	BCR	C33-C5	-2.05	1.47	1.50
14	a	828	CLA	MG-NB	-2.05	2.01	2.05
14	b	3030	CLA	MG-ND	-2.05	2.01	2.05
14	a	811	CLA	CHC-C1C	2.05	1.42	1.38
14	b	3013	CLA	CHC-C1C	2.05	1.42	1.38
14	a	817	CLA	CMC-C2C	-2.05	1.46	1.50
14	x	1701	CLA	CMB-C2B	-2.05	1.46	1.50
16	L	206	BCR	C33-C5	-2.05	1.47	1.50
14	a	822	CLA	CMC-C2C	-2.05	1.46	1.50
14	A	811	CLA	MG-NB	-2.05	2.01	2.05
14	A	855	CLA	MG-NB	-2.05	2.01	2.05
14	2	3039	CLA	CHC-C1C	2.05	1.42	1.38
16	a	850	BCR	C33-C5	-2.05	1.47	1.50
16	9	102	BCR	C38-C26	-2.05	1.47	1.50
16	y	101	BCR	C38-C26	-2.05	1.47	1.50
14	b	3004	CLA	MG-ND	-2.04	2.01	2.05
14	8	101	CLA	CMD-C2D	-2.04	1.46	1.50
14	B	3040	CLA	CMC-C2C	-2.04	1.46	1.50
14	1	813	CLA	CMC-C2C	-2.04	1.46	1.50
16	J	104	BCR	C38-C26	-2.04	1.47	1.50
14	2	3029	CLA	MG-ND	-2.04	2.01	2.05
14	f	204	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	204	CLA	C4B-NB	2.04	1.40	1.37
14	A	815	CLA	MG-NB	-2.04	2.01	2.05
14	a	835	CLA	C3B-C4B	2.04	1.48	1.42
14	b	3022	CLA	CMD-C2D	-2.04	1.46	1.50
14	0	204	CLA	C1B-NB	-2.04	1.35	1.37
14	J	102	CLA	MG-NB	-2.04	2.01	2.05
14	X	1701	CLA	MG-NB	-2.04	2.01	2.05
14	1	843	CLA	C1B-NB	-2.04	1.35	1.37
14	A	832	CLA	C3B-C4B	2.04	1.48	1.42
16	M	1602	BCR	C38-C26	-2.04	1.47	1.50
16	i	101	BCR	C33-C5	-2.04	1.47	1.50
14	a	843	CLA	CHC-C1C	2.04	1.42	1.38
14	1	829	CLA	MG-NB	-2.03	2.01	2.05
14	a	802	CLA	C1B-NB	-2.03	1.35	1.37
14	B	3033	CLA	CMC-C2C	-2.03	1.46	1.50
14	l	207	CLA	MG-ND	-2.03	2.01	2.05
14	A	814	CLA	C3B-C4B	2.03	1.48	1.42
14	b	3020	CLA	MG-NB	-2.03	2.01	2.05
16	a	845	BCR	C38-C26	-2.03	1.47	1.50
14	1	832	CLA	C3B-C4B	2.03	1.48	1.42
14	1	844	CLA	CMD-C2D	-2.03	1.46	1.50
14	a	823	CLA	CHC-C1C	2.03	1.42	1.38
14	L	201	CLA	C1B-NB	-2.03	1.35	1.37
14	1	806	CLA	MG-ND	-2.03	2.01	2.05
14	b	3037	CLA	CMB-C2B	-2.03	1.46	1.50
16	7	101	BCR	C33-C5	-2.03	1.47	1.50
16	I	101	BCR	C33-C5	-2.03	1.47	1.50
14	A	815	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	3020	CLA	MG-NB	-2.03	2.01	2.05
14	B	3023	CLA	CMB-C2B	-2.03	1.46	1.50
14	2	3016	CLA	CMB-C2B	-2.03	1.46	1.50
16	l	209	BCR	C27-C26	-2.03	1.47	1.51
14	F	204	CLA	MG-NB	-2.03	2.01	2.05
14	A	823	CLA	CMC-C2C	-2.03	1.46	1.50
14	k	102	CLA	MG-NB	-2.03	2.01	2.05
14	2	3004	CLA	MG-ND	-2.03	2.01	2.05
14	A	812	CLA	CHC-C1C	2.03	1.42	1.38
14	b	3039	CLA	CHC-C1C	2.03	1.42	1.38
14	B	3031	CLA	C3B-C4B	2.03	1.48	1.42
14	A	805	CLA	C1B-NB	-2.03	1.35	1.37
17	B	3051	LHG	P-O6	2.03	1.67	1.59
14	1	803	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	3022	CLA	MG-NB	-2.03	2.01	2.05
14	a	803	CLA	MG-ND	-2.03	2.01	2.05
14	B	3013	CLA	CHC-C1C	2.03	1.42	1.38
14	b	3021	CLA	MG-NB	-2.03	2.01	2.05
14	J	101	CLA	CMD-C2D	-2.02	1.46	1.50
14	a	825	CLA	C3B-C4B	2.02	1.48	1.42
14	B	3039	CLA	CHC-C1C	2.02	1.42	1.38
14	1	811	CLA	MG-NB	-2.02	2.01	2.05
14	b	3015	CLA	CMC-C2C	-2.02	1.46	1.50
14	1	803	CLA	MG-ND	-2.02	2.01	2.05
14	f	204	CLA	CMB-C2B	-2.02	1.46	1.50
16	b	3047	BCR	C38-C26	-2.02	1.47	1.50
14	l	207	CLA	C4B-NB	2.02	1.40	1.37
14	a	814	CLA	MG-NB	-2.02	2.01	2.05
14	8	101	CLA	MG-NB	-2.02	2.01	2.05
14	1	839	CLA	C3B-C4B	2.02	1.48	1.42
14	1	837	CLA	CMC-C2C	-2.02	1.46	1.50
14	6	204	CLA	CMB-C2B	-2.02	1.46	1.50
14	1	805	CLA	C1B-NB	-2.02	1.35	1.37
14	1	823	CLA	CMC-C2C	-2.02	1.46	1.50
13	a	801	CL0	C3B-C2B	-2.02	1.37	1.40
14	A	844	CLA	CHC-C1C	2.02	1.42	1.38
14	a	837	CLA	C1B-NB	-2.02	1.35	1.37
16	m	101	BCR	C38-C26	-2.02	1.47	1.50
14	M	1601	CLA	CBD-CAD	2.02	1.56	1.51
14	1	811	CLA	CMC-C2C	-2.02	1.46	1.50
14	a	838	CLA	C3B-C4B	2.02	1.48	1.42
14	j	1102	CLA	CMB-C2B	-2.02	1.46	1.50
14	1	826	CLA	C3B-C4B	2.02	1.48	1.42
14	B	3021	CLA	MG-NB	-2.02	2.01	2.05
14	F	204	CLA	CMB-C2B	-2.02	1.46	1.50
14	A	803	CLA	CHC-C1C	2.02	1.42	1.38
14	9	103	CLA	CMD-C2D	-2.02	1.46	1.50
14	2	3031	CLA	C3B-C4B	2.02	1.48	1.42
14	b	3029	CLA	CHC-C1C	2.02	1.42	1.38
14	a	836	CLA	CMC-C2C	-2.02	1.46	1.50
14	A	818	CLA	CMC-C2C	-2.02	1.46	1.50
14	J	101	CLA	CMC-C2C	-2.02	1.46	1.50
14	X	1701	CLA	CMB-C2B	-2.02	1.46	1.50
14	a	824	CLA	CMC-C2C	-2.01	1.46	1.50
16	I	102	BCR	C27-C26	-2.01	1.47	1.51
14	b	3023	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	z	1701	CLA	MG-NB	-2.01	2.01	2.05
14	a	809	CLA	CHC-C1C	2.01	1.42	1.38
14	b	3039	CLA	C1B-NB	-2.01	1.35	1.37
14	1	818	CLA	CMC-C2C	-2.01	1.46	1.50
14	A	831	CLA	C3B-C4B	2.01	1.48	1.42
14	0	203	CLA	MG-NB	-2.01	2.01	2.05
14	b	3031	CLA	CHC-C1C	2.01	1.42	1.38
14	a	830	CLA	C3B-C4B	2.01	1.48	1.42
16	0	210	BCR	C27-C26	-2.01	1.47	1.51
17	b	3051	LHG	P-O6	2.01	1.67	1.59
14	9	103	CLA	MG-NB	-2.01	2.01	2.05
14	A	825	CLA	CMC-C2C	-2.01	1.46	1.50
14	2	3042	CLA	CMC-C2C	-2.01	1.46	1.50
14	b	3040	CLA	CHC-C1C	2.01	1.42	1.38
14	2	3035	CLA	CMC-C2C	-2.01	1.46	1.50
14	2	3021	CLA	MG-NB	-2.01	2.01	2.05
14	B	3042	CLA	CMC-C2C	-2.01	1.46	1.50
14	a	810	CLA	CMC-C2C	-2.01	1.46	1.50
14	A	840	CLA	CHC-C1C	2.01	1.42	1.38
14	z	1701	CLA	CMB-C2B	-2.01	1.46	1.50
14	0	203	CLA	CBD-CAD	2.01	1.56	1.51
17	2	3051	LHG	P-O6	2.01	1.67	1.59
14	a	822	CLA	CMB-C2B	-2.01	1.46	1.50
14	a	826	CLA	C1B-C2B	2.01	1.47	1.43
14	B	3023	CLA	CMC-C2C	-2.01	1.46	1.50
14	j	1103	CLA	CMB-C2B	-2.01	1.46	1.50
14	A	810	CLA	CHC-C1C	2.01	1.42	1.38
14	9	103	CLA	CMC-C2C	-2.01	1.46	1.50
14	1	815	CLA	MG-NB	-2.01	2.01	2.05
14	1	827	CLA	C1B-C2B	2.01	1.47	1.43
14	a	831	CLA	C1B-NB	-2.01	1.35	1.37
14	a	812	CLA	CMC-C2C	-2.01	1.46	1.50
14	J	101	CLA	CMB-C2B	-2.00	1.46	1.50
14	A	813	CLA	CMC-C2C	-2.00	1.46	1.50
14	a	805	CLA	MG-ND	-2.00	2.01	2.05
14	L	201	CLA	MG-ND	-2.00	2.01	2.05
14	8	101	CLA	CMB-C2B	-2.00	1.46	1.50
14	A	838	CLA	C1B-NB	-2.00	1.35	1.37
14	2	3023	CLA	CMB-C2B	-2.00	1.46	1.50
14	1	806	CLA	C1B-NB	-2.00	1.35	1.37
14	K	102	CLA	CMB-C2B	-2.00	1.46	1.50
14	1	817	CLA	CHC-C1C	2.00	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	k	102	CLA	CMB-C2B	-2.00	1.46	1.50
14	1	807	CLA	MG-ND	-2.00	2.01	2.05

All (2506) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3005	CLA	C4A-NA-C1A	8.23	110.43	106.68
14	B	3005	CLA	C4A-NA-C1A	8.22	110.43	106.68
14	2	3005	CLA	C4A-NA-C1A	8.21	110.42	106.68
14	a	805	CLA	C4A-NA-C1A	8.12	110.38	106.68
14	A	806	CLA	C4A-NA-C1A	8.01	110.33	106.68
14	1	806	CLA	C4A-NA-C1A	8.00	110.33	106.68
14	2	3011	CLA	C4A-NA-C1A	7.97	110.31	106.68
14	1	835	CLA	C4A-NA-C1A	7.95	110.31	106.68
14	A	835	CLA	C4A-NA-C1A	7.93	110.30	106.68
14	b	3011	CLA	C4A-NA-C1A	7.92	110.29	106.68
14	a	834	CLA	C4A-NA-C1A	7.88	110.27	106.68
14	B	3011	CLA	C4A-NA-C1A	7.84	110.25	106.68
14	1	841	CLA	C4A-NA-C1A	7.72	110.20	106.68
14	b	3041	CLA	C4A-NA-C1A	7.70	110.19	106.68
14	B	3008	CLA	C4A-NA-C1A	7.68	110.18	106.68
14	A	841	CLA	C4A-NA-C1A	7.67	110.18	106.68
14	2	3010	CLA	C4A-NA-C1A	7.65	110.17	106.68
14	a	840	CLA	C4A-NA-C1A	7.65	110.17	106.68
14	B	3010	CLA	C4A-NA-C1A	7.62	110.16	106.68
14	B	3041	CLA	C4A-NA-C1A	7.59	110.14	106.68
14	2	3008	CLA	C4A-NA-C1A	7.58	110.14	106.68
14	b	3010	CLA	C4A-NA-C1A	7.57	110.13	106.68
14	2	3041	CLA	C4A-NA-C1A	7.55	110.12	106.68
14	1	831	CLA	C4A-NA-C1A	7.53	110.11	106.68
14	2	3004	CLA	C4A-NA-C1A	7.52	110.11	106.68
14	A	831	CLA	C4A-NA-C1A	7.51	110.11	106.68
14	b	3008	CLA	C4A-NA-C1A	7.51	110.11	106.68
14	1	829	CLA	C4A-NA-C1A	7.51	110.10	106.68
14	1	804	CLA	C4A-NA-C1A	7.47	110.09	106.68
14	B	3020	CLA	C4A-NA-C1A	7.47	110.09	106.68
14	a	830	CLA	C4A-NA-C1A	7.46	110.08	106.68
14	A	804	CLA	C4A-NA-C1A	7.45	110.08	106.68
14	2	3020	CLA	C4A-NA-C1A	7.45	110.08	106.68
14	B	3004	CLA	C4A-NA-C1A	7.44	110.07	106.68
14	A	829	CLA	C4A-NA-C1A	7.43	110.07	106.68
14	a	828	CLA	C4A-NA-C1A	7.42	110.07	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3004	CLA	C4A-NA-C1A	7.40	110.06	106.68
14	A	836	CLA	C4A-NA-C1A	7.40	110.06	106.68
14	b	3020	CLA	C4A-NA-C1A	7.39	110.05	106.68
14	j	1101	CLA	C4A-NA-C1A	7.38	110.05	106.68
14	l	207	CLA	C4A-NA-C1A	7.38	110.05	106.68
14	A	807	CLA	C4A-NA-C1A	7.38	110.05	106.68
14	B	3009	CLA	C4A-NA-C1A	7.38	110.04	106.68
14	a	806	CLA	C4A-NA-C1A	7.36	110.04	106.68
14	0	208	CLA	C4A-NA-C1A	7.35	110.03	106.68
14	b	3022	CLA	C4A-NA-C1A	7.35	110.03	106.68
14	1	843	CLA	C4A-NA-C1A	7.33	110.03	106.68
14	B	3034	CLA	C4A-NA-C1A	7.33	110.02	106.68
14	1	807	CLA	C4A-NA-C1A	7.32	110.02	106.68
14	2	3034	CLA	C4A-NA-C1A	7.30	110.01	106.68
14	L	204	CLA	C4A-NA-C1A	7.29	110.01	106.68
14	a	842	CLA	C4A-NA-C1A	7.28	110.00	106.68
14	1	836	CLA	C4A-NA-C1A	7.28	110.00	106.68
14	b	3016	CLA	C4A-NA-C1A	7.27	109.99	106.68
14	2	3009	CLA	C4A-NA-C1A	7.26	109.99	106.68
14	2	3022	CLA	C4A-NA-C1A	7.26	109.99	106.68
14	2	3007	CLA	C4A-NA-C1A	7.25	109.99	106.68
14	A	843	CLA	C4A-NA-C1A	7.25	109.99	106.68
14	B	3022	CLA	C4A-NA-C1A	7.24	109.98	106.68
14	B	3016	CLA	C4A-NA-C1A	7.24	109.98	106.68
14	2	3016	CLA	C4A-NA-C1A	7.23	109.98	106.68
14	a	835	CLA	C4A-NA-C1A	7.23	109.98	106.68
14	b	3009	CLA	C4A-NA-C1A	7.23	109.98	106.68
14	B	3007	CLA	C4A-NA-C1A	7.21	109.97	106.68
14	B	3012	CLA	C4A-NA-C1A	7.20	109.97	106.68
14	b	3034	CLA	C4A-NA-C1A	7.20	109.97	106.68
14	b	3012	CLA	C4A-NA-C1A	7.20	109.96	106.68
13	1	801	CL0	C1B-CHB-C4A	7.19	125.94	121.32
14	2	3038	CLA	C4A-NA-C1A	7.18	109.96	106.68
14	A	838	CLA	C4A-NA-C1A	7.17	109.95	106.68
14	2	3006	CLA	C4A-NA-C1A	7.16	109.95	106.68
14	b	3017	CLA	C4A-NA-C1A	7.15	109.94	106.68
13	A	801	CL0	C1B-CHB-C4A	7.14	125.92	121.32
14	b	3007	CLA	C4A-NA-C1A	7.14	109.94	106.68
14	2	3012	CLA	C4A-NA-C1A	7.13	109.93	106.68
14	B	3038	CLA	C4A-NA-C1A	7.13	109.93	106.68
14	L	201	CLA	C4A-NA-C1A	7.11	109.92	106.68
14	a	837	CLA	C4A-NA-C1A	7.11	109.92	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	3017	CLA	C4A-NA-C1A	7.11	109.92	106.68
13	a	801	CL0	C1B-CHB-C4A	7.11	125.90	121.32
14	A	809	CLA	C4A-NA-C1A	7.10	109.92	106.68
14	a	808	CLA	C4A-NA-C1A	7.10	109.92	106.68
14	b	3038	CLA	C4A-NA-C1A	7.10	109.92	106.68
14	1	838	CLA	C4A-NA-C1A	7.09	109.92	106.68
14	0	204	CLA	C4A-NA-C1A	7.09	109.91	106.68
14	A	824	CLA	C4A-NA-C1A	7.08	109.91	106.68
14	B	3006	CLA	C4A-NA-C1A	7.07	109.91	106.68
14	1	809	CLA	C4A-NA-C1A	7.07	109.91	106.68
14	a	823	CLA	C4A-NA-C1A	7.07	109.90	106.68
14	B	3017	CLA	C4A-NA-C1A	7.04	109.89	106.68
14	b	3006	CLA	C4A-NA-C1A	7.04	109.89	106.68
14	l	203	CLA	C4A-NA-C1A	7.03	109.89	106.68
14	A	826	CLA	C4A-NA-C1A	7.02	109.88	106.68
14	a	822	CLA	C4A-NA-C1A	7.01	109.88	106.68
14	a	827	CLA	C4A-NA-C1A	6.99	109.87	106.68
14	1	824	CLA	C4A-NA-C1A	6.98	109.86	106.68
14	A	828	CLA	C4A-NA-C1A	6.97	109.86	106.68
14	B	3030	CLA	C4A-NA-C1A	6.96	109.85	106.68
14	a	825	CLA	C4A-NA-C1A	6.96	109.85	106.68
14	2	3030	CLA	C4A-NA-C1A	6.96	109.85	106.68
14	1	823	CLA	C4A-NA-C1A	6.95	109.85	106.68
14	1	826	CLA	C4A-NA-C1A	6.95	109.85	106.68
14	b	3030	CLA	C4A-NA-C1A	6.93	109.84	106.68
14	b	3035	CLA	C4A-NA-C1A	6.93	109.84	106.68
14	6	204	CLA	C4A-NA-C1A	6.92	109.84	106.68
14	B	3035	CLA	C4A-NA-C1A	6.90	109.83	106.68
14	1	828	CLA	C4A-NA-C1A	6.89	109.82	106.68
14	2	3035	CLA	C4A-NA-C1A	6.89	109.82	106.68
14	A	811	CLA	C4A-NA-C1A	6.89	109.82	106.68
14	F	204	CLA	C4A-NA-C1A	6.89	109.82	106.68
14	K	101	CLA	C4A-NA-C1A	6.88	109.82	106.68
14	f	204	CLA	C4A-NA-C1A	6.87	109.81	106.68
14	B	3025	CLA	C4A-NA-C1A	6.86	109.81	106.68
14	k	101	CLA	C4A-NA-C1A	6.86	109.81	106.68
14	b	3039	CLA	C4A-NA-C1A	6.85	109.80	106.68
14	A	823	CLA	C4A-NA-C1A	6.85	109.80	106.68
14	9	101	CLA	C4A-NA-C1A	6.83	109.80	106.68
14	1	802	CLA	C4A-NA-C1A	6.82	109.79	106.68
14	B	3039	CLA	C4A-NA-C1A	6.82	109.79	106.68
14	1	811	CLA	C4A-NA-C1A	6.81	109.79	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	810	CLA	C4A-NA-C1A	6.81	109.78	106.68
14	b	3042	CLA	C4A-NA-C1A	6.80	109.78	106.68
14	a	802	CLA	C4A-NA-C1A	6.80	109.78	106.68
14	1	830	CLA	C4A-NA-C1A	6.80	109.78	106.68
14	2	3025	CLA	C4A-NA-C1A	6.80	109.78	106.68
14	2	3039	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	1	817	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	B	3042	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	2	3042	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	A	802	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	a	829	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	A	830	CLA	C4A-NA-C1A	6.78	109.77	106.68
14	F	201	CLA	C4A-NA-C1A	6.76	109.76	106.68
14	1	814	CLA	C4A-NA-C1A	6.76	109.76	106.68
14	b	3025	CLA	C4A-NA-C1A	6.76	109.76	106.68
14	a	804	CLA	C4A-NA-C1A	6.75	109.76	106.68
14	z	1701	CLA	C4A-NA-C1A	6.75	109.76	106.68
14	1	840	CLA	C4A-NA-C1A	6.74	109.76	106.68
14	2	3015	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	6	201	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	a	819	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	A	817	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	a	814	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	a	839	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	1	820	CLA	C4A-NA-C1A	6.72	109.75	106.68
14	b	3026	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	1	834	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	f	201	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	A	834	CLA	C4A-NA-C1A	6.70	109.73	106.68
14	A	805	CLA	C4A-NA-C1A	6.70	109.73	106.68
14	1	822	CLA	C4A-NA-C1A	6.70	109.73	106.68
14	A	814	CLA	C4A-NA-C1A	6.69	109.73	106.68
14	A	820	CLA	C4A-NA-C1A	6.69	109.73	106.68
14	B	3015	CLA	C4A-NA-C1A	6.69	109.73	106.68
14	X	1701	CLA	C4A-NA-C1A	6.68	109.73	106.68
14	A	812	CLA	C4A-NA-C1A	6.68	109.73	106.68
14	b	3027	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	b	3015	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	1	805	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	A	840	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	a	816	CLA	C4A-NA-C1A	6.66	109.72	106.68
14	1	818	CLA	C4A-NA-C1A	6.65	109.71	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	833	CLA	C4A-NA-C1A	6.64	109.71	106.68
14	x	1701	CLA	C4A-NA-C1A	6.63	109.71	106.68
14	a	813	CLA	C4A-NA-C1A	6.63	109.70	106.68
14	f	203	CLA	C4A-NA-C1A	6.63	109.70	106.68
14	a	817	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	a	811	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	B	3026	CLA	C4A-NA-C1A	6.61	109.69	106.68
14	B	3027	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	F	203	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	1	815	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	B	3033	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	6	203	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	b	3033	CLA	C4A-NA-C1A	6.59	109.69	106.68
14	2	3026	CLA	C4A-NA-C1A	6.59	109.69	106.68
14	A	855	CLA	C4A-NA-C1A	6.58	109.68	106.68
14	a	831	CLA	C4A-NA-C1A	6.58	109.68	106.68
14	a	821	CLA	C4A-NA-C1A	6.57	109.68	106.68
14	1	832	CLA	C4A-NA-C1A	6.57	109.67	106.68
14	A	844	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	1	812	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	A	832	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	2	3027	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	A	818	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	a	843	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	a	838	CLA	C4A-NA-C1A	6.54	109.66	106.68
14	1	844	CLA	C4A-NA-C1A	6.54	109.66	106.68
14	A	815	CLA	C4A-NA-C1A	6.52	109.66	106.68
14	M	1601	CLA	C4A-NA-C1A	6.52	109.66	106.68
14	A	822	CLA	C4A-NA-C1A	6.52	109.65	106.68
14	a	818	CLA	C4A-NA-C1A	6.52	109.65	106.68
14	l	206	CLA	C4A-NA-C1A	6.51	109.65	106.68
14	1	839	CLA	C4A-NA-C1A	6.51	109.65	106.68
14	A	842	CLA	C4A-NA-C1A	6.50	109.64	106.68
14	2	3014	CLA	C4A-NA-C1A	6.50	109.64	106.68
14	B	3014	CLA	C4A-NA-C1A	6.50	109.64	106.68
14	A	827	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	0	207	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	a	826	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	0	203	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	1	819	CLA	C4A-NA-C1A	6.48	109.64	106.68
14	b	3019	CLA	C4A-NA-C1A	6.48	109.63	106.68
14	2	3033	CLA	C4A-NA-C1A	6.47	109.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	3024	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	2	3019	CLA	C4A-NA-C1A	6.46	109.63	106.68
14	A	839	CLA	C4A-NA-C1A	6.46	109.63	106.68
14	a	824	CLA	C4A-NA-C1A	6.46	109.63	106.68
14	b	3014	CLA	C4A-NA-C1A	6.45	109.62	106.68
14	a	841	CLA	C4A-NA-C1A	6.45	109.62	106.68
14	a	809	CLA	C4A-NA-C1A	6.44	109.62	106.68
14	J	101	CLA	C4A-NA-C1A	6.43	109.61	106.68
14	b	3024	CLA	C4A-NA-C1A	6.43	109.61	106.68
14	2	3032	CLA	C4A-NA-C1A	6.43	109.61	106.68
14	A	816	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	a	815	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	A	810	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	j	1102	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	a	807	CLA	C4A-NA-C1A	6.41	109.60	106.68
14	l	208	CLA	C4A-NA-C1A	6.41	109.60	106.68
14	A	821	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	1	842	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	1	825	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	0	209	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	A	819	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	1	821	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	B	3024	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	1	813	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	2	3013	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	a	812	CLA	C4A-NA-C1A	6.38	109.59	106.68
14	1	816	CLA	C4A-NA-C1A	6.38	109.59	106.68
14	B	3019	CLA	C4A-NA-C1A	6.37	109.58	106.68
14	L	203	CLA	C4A-NA-C1A	6.37	109.58	106.68
14	1	827	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	A	808	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	A	825	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	B	3032	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	L	205	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	b	3021	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	b	3032	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	8	101	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	1	810	CLA	C4A-NA-C1A	6.33	109.57	106.68
14	a	820	CLA	C4A-NA-C1A	6.32	109.56	106.68
14	b	3013	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	A	813	CLA	C4A-NA-C1A	6.30	109.55	106.68
14	b	3023	CLA	C4A-NA-C1A	6.29	109.55	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3021	CLA	C4A-NA-C1A	6.29	109.55	106.68
14	1	808	CLA	C4A-NA-C1A	6.28	109.55	106.68
14	2	3021	CLA	C4A-NA-C1A	6.28	109.54	106.68
14	2	3023	CLA	C4A-NA-C1A	6.26	109.54	106.68
14	1	833	CLA	C4A-NA-C1A	6.22	109.52	106.68
14	B	3023	CLA	C4A-NA-C1A	6.21	109.51	106.68
14	B	3013	CLA	C4A-NA-C1A	6.19	109.50	106.68
14	2	3040	CLA	C4A-NA-C1A	6.17	109.49	106.68
14	B	3040	CLA	C4A-NA-C1A	6.15	109.48	106.68
14	a	832	CLA	C4A-NA-C1A	6.15	109.48	106.68
14	b	3029	CLA	C4A-NA-C1A	6.09	109.46	106.68
14	b	3040	CLA	C4A-NA-C1A	6.09	109.46	106.68
14	a	803	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	j	1103	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	J	102	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	8	102	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	A	803	CLA	C4A-NA-C1A	6.04	109.43	106.68
14	A	833	CLA	C4A-NA-C1A	6.03	109.43	106.68
14	B	3029	CLA	C4A-NA-C1A	6.01	109.42	106.68
14	K	102	CLA	C4A-NA-C1A	5.98	109.41	106.68
14	1	837	CLA	C4A-NA-C1A	5.97	109.40	106.68
14	b	3003	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	1	803	CLA	C4A-NA-C1A	5.93	109.38	106.68
14	B	3037	CLA	C4A-NA-C1A	5.92	109.38	106.68
14	9	103	CLA	C4A-NA-C1A	5.92	109.38	106.68
14	2	3029	CLA	C4A-NA-C1A	5.91	109.37	106.68
14	B	3003	CLA	C4A-NA-C1A	5.90	109.37	106.68
14	2	3037	CLA	C4A-NA-C1A	5.89	109.37	106.68
14	a	836	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	k	102	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	A	837	CLA	C4A-NA-C1A	5.87	109.36	106.68
14	2	3003	CLA	C4A-NA-C1A	5.85	109.35	106.68
14	B	3018	CLA	C4A-NA-C1A	5.83	109.34	106.68
14	b	3037	CLA	C4A-NA-C1A	5.81	109.33	106.68
14	b	3028	CLA	C4A-NA-C1A	5.78	109.32	106.68
14	B	3028	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	B	3036	CLA	C4A-NA-C1A	5.70	109.28	106.68
14	b	3018	CLA	C4A-NA-C1A	5.70	109.28	106.68
14	2	3028	CLA	C4A-NA-C1A	5.67	109.27	106.68
14	2	3018	CLA	C4A-NA-C1A	5.67	109.27	106.68
14	b	3036	CLA	C4A-NA-C1A	5.65	109.26	106.68
14	2	3036	CLA	C4A-NA-C1A	5.61	109.24	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	3031	CLA	C4A-NA-C1A	5.58	109.22	106.68
14	b	3031	CLA	C4A-NA-C1A	5.47	109.18	106.68
14	B	3031	CLA	C4A-NA-C1A	5.45	109.17	106.68
14	b	3017	CLA	CAC-C3C-C4C	5.08	131.40	124.79
14	B	3017	CLA	CAC-C3C-C4C	5.05	131.36	124.79
14	2	3017	CLA	CAC-C3C-C4C	5.04	131.35	124.79
17	0	202	LHG	O4-P-O5	4.49	133.35	112.44
17	l	202	LHG	O4-P-O5	4.49	133.33	112.44
17	L	208	LHG	O4-P-O5	4.49	133.33	112.44
17	a	852	LHG	O4-P-O5	4.46	133.21	112.44
17	A	853	LHG	O4-P-O5	4.46	133.17	112.44
17	1	852	LHG	O4-P-O5	4.45	133.16	112.44
17	1	853	LHG	O4-P-O5	4.41	132.96	112.44
17	l	201	LHG	O4-P-O5	4.41	132.95	112.44
17	0	201	LHG	O4-P-O5	4.41	132.94	112.44
17	A	854	LHG	O4-P-O5	4.40	132.94	112.44
17	L	207	LHG	O4-P-O5	4.40	132.93	112.44
17	a	853	LHG	O4-P-O5	4.40	132.91	112.44
17	2	3051	LHG	O4-P-O5	4.35	132.66	112.44
14	B	3016	CLA	C4-C3-C5	4.34	122.77	115.23
14	2	3016	CLA	C4-C3-C5	4.34	122.77	115.23
17	b	3051	LHG	O4-P-O5	4.34	132.64	112.44
17	B	3051	LHG	O4-P-O5	4.34	132.64	112.44
14	b	3016	CLA	C4-C3-C5	4.33	122.75	115.23
13	1	801	CL0	C4D-CHA-CBD	-4.18	104.75	108.97
13	a	801	CL0	C4D-CHA-CBD	-4.16	104.77	108.97
13	A	801	CL0	C4D-CHA-CBD	-4.15	104.78	108.97
14	a	838	CLA	O2D-CGD-O1D	-4.12	115.83	123.85
14	A	839	CLA	O2D-CGD-O1D	-4.11	115.85	123.85
14	B	3003	CLA	CMB-C2B-C1B	-4.09	119.20	125.42
14	1	839	CLA	O2D-CGD-O1D	-4.08	115.91	123.85
14	b	3003	CLA	CMB-C2B-C1B	-4.08	119.21	125.42
14	2	3003	CLA	CMB-C2B-C1B	-4.06	119.23	125.42
14	A	802	CLA	C4-C3-C5	4.01	122.18	115.23
14	a	802	CLA	C4-C3-C5	4.01	122.18	115.23
14	1	802	CLA	C4-C3-C5	4.00	122.17	115.23
16	9	104	BCR	C2-C1-C6	3.96	116.20	110.44
16	k	103	BCR	C2-C1-C6	3.95	116.17	110.44
16	K	103	BCR	C2-C1-C6	3.93	116.15	110.44
14	b	3026	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
14	2	3026	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
14	B	3026	CLA	O2D-CGD-O1D	-3.91	116.23	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	j	1106	BCR	C7-C8-C9	-3.88	120.50	126.23
14	b	3003	CLA	C4-C3-C5	3.87	121.94	115.23
14	B	3003	CLA	C4-C3-C5	3.86	121.93	115.23
16	2	3052	BCR	C7-C8-C9	-3.86	120.52	126.23
16	B	3053	BCR	C7-C8-C9	-3.86	120.53	126.23
14	2	3003	CLA	C4-C3-C5	3.82	121.86	115.23
14	b	3012	CLA	O2D-CGD-O1D	-3.80	116.44	123.85
14	2	3012	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
14	B	3012	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
14	a	826	CLA	CMB-C2B-C1B	-3.74	119.73	125.42
14	b	3039	CLA	C1-C2-C3	-3.73	120.08	126.20
14	A	827	CLA	CMB-C2B-C1B	-3.73	119.74	125.42
14	B	3039	CLA	C1-C2-C3	-3.73	120.09	126.20
14	1	829	CLA	CMB-C2B-C1B	-3.73	119.75	125.42
14	2	3039	CLA	C1-C2-C3	-3.72	120.10	126.20
14	1	827	CLA	CMB-C2B-C1B	-3.72	119.75	125.42
16	m	101	BCR	C24-C23-C22	-3.72	120.73	126.23
14	A	829	CLA	CMB-C2B-C1B	-3.72	119.76	125.42
14	a	828	CLA	CMB-C2B-C1B	-3.72	119.76	125.42
16	0	205	BCR	C15-C16-C17	-3.71	115.94	123.52
16	B	3052	BCR	C15-C16-C17	-3.70	115.94	123.52
16	y	101	BCR	C24-C23-C22	-3.70	120.76	126.23
16	l	204	BCR	C15-C16-C17	-3.70	115.95	123.52
14	b	3033	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
16	M	1602	BCR	C24-C23-C22	-3.69	120.77	126.23
14	B	3033	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
14	2	3009	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
14	2	3033	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
14	L	204	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
14	0	208	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
14	l	207	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
14	A	844	CLA	CMB-C2B-C1B	-3.67	119.83	125.42
14	B	3009	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
14	a	843	CLA	CMB-C2B-C1B	-3.66	119.84	125.42
14	A	822	CLA	CMB-C2B-C1B	-3.66	119.85	125.42
14	b	3009	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
14	a	821	CLA	CMB-C2B-C1B	-3.65	119.86	125.42
14	F	201	CLA	C3B-C4B-NB	-3.64	107.28	110.53
14	1	822	CLA	CMB-C2B-C1B	-3.64	119.87	125.42
14	6	201	CLA	C3B-C4B-NB	-3.64	107.28	110.53
14	2	3019	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
14	1	844	CLA	CMB-C2B-C1B	-3.63	119.89	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3019	CLA	O2D-CGD-O1D	-3.61	116.81	123.85
14	b	3019	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
14	f	201	CLA	C3B-C4B-NB	-3.61	107.31	110.53
14	A	806	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
14	1	806	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
14	1	819	CLA	C4-C3-C5	3.60	121.48	115.23
13	1	801	CL0	O2D-CGD-O1D	-3.60	116.84	123.85
13	A	801	CL0	O2D-CGD-O1D	-3.60	116.85	123.85
16	f	205	BCR	C2-C1-C6	3.59	115.66	110.44
13	a	801	CL0	O2D-CGD-O1D	-3.58	116.88	123.85
14	A	819	CLA	C4-C3-C5	3.58	121.44	115.23
14	A	834	CLA	C1-C2-C3	-3.57	120.34	126.20
14	1	834	CLA	C1-C2-C3	-3.56	120.36	126.20
14	a	818	CLA	C4-C3-C5	3.56	121.41	115.23
14	a	805	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
14	A	821	CLA	CMB-C2B-C1B	-3.56	120.00	125.42
14	a	833	CLA	C1-C2-C3	-3.56	120.37	126.20
16	F	205	BCR	C2-C1-C6	3.56	115.60	110.44
14	a	820	CLA	CMB-C2B-C1B	-3.55	120.01	125.42
16	6	205	BCR	C2-C1-C6	3.55	115.59	110.44
14	B	3005	CLA	CAC-C3C-C4C	3.54	129.40	124.79
14	1	821	CLA	CMB-C2B-C1B	-3.54	120.03	125.42
14	1	206	CLA	C3B-C4B-NB	-3.53	107.38	110.53
14	L	203	CLA	C3B-C4B-NB	-3.53	107.38	110.53
14	0	207	CLA	C3B-C4B-NB	-3.53	107.38	110.53
16	A	848	BCR	C15-C16-C17	-3.53	116.30	123.52
14	2	3005	CLA	CAC-C3C-C4C	3.53	129.38	124.79
14	b	3005	CLA	CAC-C3C-C4C	3.53	129.38	124.79
16	a	847	BCR	C15-C16-C17	-3.52	116.31	123.52
13	a	801	CL0	O2D-CGD-CBD	3.52	114.81	110.95
14	a	815	CLA	C3B-C4B-NB	-3.52	107.39	110.53
13	1	801	CL0	O2D-CGD-CBD	3.51	114.80	110.95
16	1	847	BCR	C15-C16-C17	-3.50	116.35	123.52
14	1	816	CLA	C3B-C4B-NB	-3.50	107.40	110.53
13	A	801	CL0	O2D-CGD-CBD	3.50	114.79	110.95
14	L	203	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
14	b	3003	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
16	1	846	BCR	C27-C26-C25	3.49	127.42	122.70
14	2	3003	CLA	O2D-CGD-O1D	-3.48	117.06	123.85
14	0	207	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
14	1	817	CLA	C4-C3-C5	3.48	121.27	115.23
16	a	846	BCR	C27-C26-C25	3.48	127.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	817	CLA	C4-C3-C5	3.48	121.26	115.23
14	B	3003	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
14	l	206	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
14	1	808	CLA	O2D-CGD-O1D	-3.47	117.08	123.85
14	a	816	CLA	C4-C3-C5	3.47	121.26	115.23
16	A	847	BCR	C2-C1-C6	3.47	115.48	110.44
14	A	808	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
14	A	816	CLA	C3B-C4B-NB	-3.47	107.44	110.53
14	L	205	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
16	a	846	BCR	C2-C1-C6	3.46	115.47	110.44
16	1	846	BCR	C2-C1-C6	3.46	115.46	110.44
14	a	807	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
14	0	209	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
14	l	208	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
14	b	3032	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
16	A	847	BCR	C27-C26-C25	3.45	127.36	122.70
14	2	3032	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
14	B	3032	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
14	A	841	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
14	1	841	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
14	a	840	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
14	B	3026	CLA	O2D-CGD-CBD	3.41	117.19	111.23
14	2	3026	CLA	O2D-CGD-CBD	3.41	117.19	111.23
14	2	3013	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
14	A	813	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
14	B	3030	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
14	B	3013	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
14	b	3030	CLA	O2D-CGD-O1D	-3.39	117.26	123.85
14	b	3026	CLA	O2D-CGD-CBD	3.38	117.14	111.23
14	b	3013	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
14	1	825	CLA	C3B-C4B-NB	-3.38	107.52	110.53
14	a	812	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
14	1	813	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
14	1	825	CLA	C1-C2-C3	-3.37	120.67	126.20
14	A	825	CLA	C1-C2-C3	-3.37	120.68	126.20
14	a	824	CLA	C1-C2-C3	-3.37	120.68	126.20
14	2	3030	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
14	B	3042	CLA	C3B-C4B-NB	-3.36	107.53	110.53
14	2	3017	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
14	B	3018	CLA	C4-C3-C5	3.36	121.05	115.23
14	A	842	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
14	2	3018	CLA	C4-C3-C5	3.35	121.05	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	842	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
14	a	829	CLA	CMB-C2B-C1B	-3.35	120.32	125.42
14	b	3018	CLA	C4-C3-C5	3.35	121.04	115.23
14	B	3017	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
14	2	3022	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
14	A	825	CLA	C3B-C4B-NB	-3.34	107.55	110.53
14	1	830	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
14	a	824	CLA	C3B-C4B-NB	-3.33	107.56	110.53
14	2	3026	CLA	C3B-C4B-NB	-3.33	107.56	110.53
14	b	3017	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
14	A	830	CLA	CMB-C2B-C1B	-3.33	120.36	125.42
14	a	841	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
14	B	3026	CLA	C3B-C4B-NB	-3.32	107.57	110.53
14	1	840	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
14	A	842	CLA	C3B-C4B-NB	-3.31	107.57	110.53
14	b	3003	CLA	CMB-C2B-C3B	3.31	134.34	126.55
14	B	3022	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
14	a	841	CLA	C3B-C4B-NB	-3.31	107.58	110.53
14	1	842	CLA	C3B-C4B-NB	-3.31	107.58	110.53
14	A	832	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
14	2	3003	CLA	CMB-C2B-C3B	3.30	134.32	126.55
14	2	3042	CLA	C3B-C4B-NB	-3.30	107.58	110.53
14	b	3010	CLA	C1-C2-C3	-3.30	120.79	126.20
14	b	3022	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
14	B	3003	CLA	CMB-C2B-C3B	3.30	134.30	126.55
14	b	3026	CLA	C3B-C4B-NB	-3.30	107.59	110.53
14	b	3042	CLA	C3B-C4B-NB	-3.29	107.59	110.53
14	B	3007	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
14	B	3031	CLA	C3B-C4B-NB	-3.29	107.60	110.53
14	b	3023	CLA	CMB-C2B-C1B	-3.28	120.42	125.42
14	a	832	CLA	C3B-C4B-NB	-3.28	107.60	110.53
14	2	3010	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
14	B	3010	CLA	C1-C2-C3	-3.28	120.83	126.20
14	2	3007	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
14	a	839	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
14	A	840	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
14	B	3010	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
16	A	848	BCR	C27-C26-C25	3.27	127.12	122.70
14	2	3010	CLA	C1-C2-C3	-3.27	120.85	126.20
14	a	831	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
14	2	3026	CLA	CAA-C2A-C1A	-3.26	101.28	111.97
14	b	3031	CLA	C3B-C4B-NB	-3.26	107.62	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3007	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
14	a	805	CLA	CHB-C4A-NA	3.26	129.11	124.40
14	1	832	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
16	1	847	BCR	C27-C26-C25	3.26	127.11	122.70
14	b	3010	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
14	1	806	CLA	CHB-C4A-NA	3.26	129.10	124.40
14	b	3033	CLA	C3B-C4B-NB	-3.25	107.63	110.53
14	B	3026	CLA	CAA-C2A-C1A	-3.25	101.31	111.97
14	B	3023	CLA	CMB-C2B-C1B	-3.25	120.47	125.42
14	b	3026	CLA	CAA-C2A-C1A	-3.25	101.32	111.97
14	1	822	CLA	C3B-C4B-NB	-3.25	107.63	110.53
16	a	847	BCR	C27-C26-C25	3.25	127.09	122.70
14	a	802	CLA	CMB-C2B-C1B	-3.25	120.47	125.42
14	A	806	CLA	CHB-C4A-NA	3.25	129.08	124.40
14	2	3023	CLA	CMB-C2B-C1B	-3.24	120.48	125.42
14	A	802	CLA	CMB-C2B-C1B	-3.24	120.48	125.42
14	2	3039	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
14	1	802	CLA	C3B-C4B-NB	-3.23	107.64	110.53
14	1	802	CLA	CMB-C2B-C1B	-3.23	120.50	125.42
14	B	3039	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
14	1	818	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
14	b	3039	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	1	835	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	2	3031	CLA	C3B-C4B-NB	-3.22	107.66	110.53
14	A	818	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	2	3033	CLA	C3B-C4B-NB	-3.22	107.66	110.53
14	a	836	CLA	C3B-C4B-NB	-3.22	107.66	110.53
14	A	835	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
14	a	834	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
14	1	837	CLA	C3B-C4B-NB	-3.21	107.66	110.53
14	A	833	CLA	C3B-C4B-NB	-3.21	107.66	110.53
14	a	837	CLA	CMB-C2B-C1B	-3.21	120.54	125.42
14	a	817	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
14	1	833	CLA	C3B-C4B-NB	-3.20	107.67	110.53
14	1	838	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
14	A	805	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
14	A	822	CLA	C3B-C4B-NB	-3.20	107.68	110.53
14	A	838	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
14	1	805	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
14	B	3033	CLA	C3B-C4B-NB	-3.19	107.68	110.53
14	a	804	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
14	9	103	CLA	O2D-CGD-O1D	-3.18	117.65	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	836	CLA	C4-C3-C5	3.18	120.75	115.23
14	k	102	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
14	1	832	CLA	C3B-C4B-NB	-3.17	107.70	110.53
14	A	832	CLA	C3B-C4B-NB	-3.17	107.70	110.53
14	a	821	CLA	C3B-C4B-NB	-3.17	107.70	110.53
16	B	3044	BCR	C15-C16-C17	-3.17	117.04	123.52
14	K	102	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
16	b	3044	BCR	C15-C16-C17	-3.17	117.04	123.52
14	A	837	CLA	C3B-C4B-NB	-3.16	107.70	110.53
14	2	3011	CLA	C4-C3-C5	3.16	120.71	115.23
14	a	842	CLA	C3B-C4B-NB	-3.15	107.72	110.53
16	2	3044	BCR	C15-C16-C17	-3.15	117.08	123.52
16	l	209	BCR	C2-C1-C6	3.14	115.01	110.44
14	b	3011	CLA	C4-C3-C5	3.14	120.68	115.23
14	a	835	CLA	C4-C3-C5	3.14	120.68	115.23
14	a	802	CLA	C3B-C4B-NB	-3.14	107.73	110.53
14	a	831	CLA	C3B-C4B-NB	-3.14	107.73	110.53
14	B	3011	CLA	C4-C3-C5	3.14	120.67	115.23
16	l	209	BCR	C24-C23-C22	-3.14	121.60	126.23
14	A	843	CLA	C3B-C4B-NB	-3.13	107.73	110.53
14	1	836	CLA	C4-C3-C5	3.13	120.67	115.23
16	0	210	BCR	C24-C23-C22	-3.13	121.60	126.23
14	B	3023	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
16	I	102	BCR	C2-C1-C6	3.13	114.99	110.44
14	A	817	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
16	0	210	BCR	C2-C1-C6	3.13	114.98	110.44
14	2	3023	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
14	1	843	CLA	C3B-C4B-NB	-3.13	107.74	110.53
14	2	3008	CLA	C3B-C4B-NB	-3.12	107.74	110.53
14	1	804	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	A	804	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	A	844	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
16	I	102	BCR	C24-C23-C22	-3.12	121.62	126.23
14	A	802	CLA	C3B-C4B-NB	-3.12	107.75	110.53
14	a	810	CLA	C3B-C4B-NB	-3.12	107.75	110.53
14	1	817	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	b	3023	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	j	1101	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	a	819	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	a	816	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	2	3028	CLA	C3B-C4B-NB	-3.10	107.76	110.53
14	a	826	CLA	O2D-CGD-O1D	-3.09	117.83	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3028	CLA	C3B-C4B-NB	-3.09	107.77	110.53
14	B	3028	CLA	C3B-C4B-NB	-3.09	107.77	110.53
16	F	205	BCR	C16-C15-C14	-3.09	117.20	123.52
14	A	820	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
16	f	205	BCR	C16-C15-C14	-3.08	117.21	123.52
14	1	811	CLA	C3B-C4B-NB	-3.08	107.78	110.53
14	1	844	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
14	a	830	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
14	1	827	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	a	843	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	A	811	CLA	C3B-C4B-NB	-3.07	107.79	110.53
14	K	101	CLA	C3B-C4B-NB	-3.07	107.79	110.53
14	1	831	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
16	6	205	BCR	C16-C15-C14	-3.07	117.24	123.52
14	1	803	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
14	1	805	CLA	CMB-C2B-C1B	-3.06	120.75	125.42
14	a	803	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	a	804	CLA	CMB-C2B-C1B	-3.06	120.76	125.42
14	b	3039	CLA	CMB-C2B-C1B	-3.06	120.76	125.42
14	A	838	CLA	C1-C2-C3	-3.06	121.19	126.20
14	2	3036	CLA	C3B-C4B-NB	-3.06	107.80	110.53
14	A	805	CLA	CMB-C2B-C1B	-3.06	120.77	125.42
14	A	827	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
14	A	831	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
14	1	820	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
14	b	3036	CLA	C3B-C4B-NB	-3.05	107.81	110.53
14	A	843	CLA	C4-C3-C5	3.05	120.52	115.23
14	1	838	CLA	C1-C2-C3	-3.05	121.20	126.20
16	a	849	BCR	C15-C16-C17	-3.05	117.28	123.52
14	a	842	CLA	C4-C3-C5	3.05	120.52	115.23
14	a	837	CLA	C1-C2-C3	-3.05	121.21	126.20
14	A	825	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
14	b	3027	CLA	C3B-C4B-NB	-3.04	107.81	110.53
14	9	101	CLA	C3B-C4B-NB	-3.04	107.81	110.53
16	A	850	BCR	C15-C16-C17	-3.04	117.30	123.52
14	1	827	CLA	CMB-C2B-C3B	3.04	133.70	126.55
16	1	849	BCR	C15-C16-C17	-3.04	117.30	123.52
14	k	101	CLA	C3B-C4B-NB	-3.04	107.82	110.53
14	A	803	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
14	1	825	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
14	2	3027	CLA	C3B-C4B-NB	-3.04	107.82	110.53
14	a	808	CLA	CHB-C4A-NA	3.04	128.78	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	3035	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
14	B	3036	CLA	C3B-C4B-NB	-3.03	107.82	110.53
14	B	3039	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
14	a	824	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
14	2	3039	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
14	a	826	CLA	CMB-C2B-C3B	3.02	133.66	126.55
14	A	809	CLA	C3B-C4B-NB	-3.02	107.83	110.53
14	1	809	CLA	C3B-C4B-NB	-3.02	107.83	110.53
16	6	205	BCR	C35-C13-C14	-3.02	117.92	122.82
14	1	829	CLA	CMB-C2B-C3B	3.02	133.66	126.55
14	1	843	CLA	C4-C3-C5	3.02	120.47	115.23
14	a	828	CLA	CMB-C2B-C3B	3.02	133.66	126.55
14	a	838	CLA	O2D-CGD-CBD	3.02	116.51	111.23
14	A	833	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	B	3035	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	A	827	CLA	CMB-C2B-C3B	3.02	133.65	126.55
16	F	205	BCR	C35-C13-C14	-3.02	117.93	122.82
14	1	809	CLA	CHB-C4A-NA	3.02	128.75	124.40
14	a	806	CLA	CHB-C4A-NA	3.01	128.75	124.40
14	A	829	CLA	CMB-C2B-C3B	3.01	133.64	126.55
14	B	3024	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	b	3024	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	b	3040	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	2	3038	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	b	3024	CLA	CMB-C2B-C1B	-3.01	120.84	125.42
14	A	809	CLA	CHB-C4A-NA	3.01	128.74	124.40
14	B	3038	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
14	b	3008	CLA	C3B-C4B-NB	-3.01	107.85	110.53
14	B	3027	CLA	C3B-C4B-NB	-3.01	107.85	110.53
14	A	834	CLA	CHB-C4A-NA	3.01	128.74	124.40
14	B	3041	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	a	832	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
16	f	205	BCR	C35-C13-C14	-3.00	117.95	122.82
14	2	3040	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	B	3008	CLA	C3B-C4B-NB	-3.00	107.85	110.53
14	A	839	CLA	O2D-CGD-CBD	3.00	116.48	111.23
14	A	807	CLA	CHB-C4A-NA	3.00	128.73	124.40
14	B	3040	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
16	2	3048	BCR	C27-C26-C25	3.00	126.76	122.70
14	2	3010	CLA	C3A-C2A-C1A	3.00	105.83	101.34
14	b	3010	CLA	C3B-C4B-NB	-3.00	107.85	110.53
14	2	3024	CLA	CMB-C2B-C1B	-3.00	120.86	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	828	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
14	2	3042	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
14	B	3024	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
14	2	3010	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	b	3042	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
14	2	3041	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
14	b	3035	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	1	839	CLA	O2D-CGD-CBD	2.99	116.46	111.23
14	1	840	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	1	807	CLA	CHB-C4A-NA	2.99	128.71	124.40
14	B	3042	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	b	3038	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	6	204	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	1	833	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	2	3024	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
14	1	834	CLA	CHB-C4A-NA	2.99	128.71	124.40
14	a	839	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	B	3048	BCR	C15-C16-C17	-2.98	117.41	123.52
14	a	833	CLA	CHB-C4A-NA	2.98	128.71	124.40
16	b	3048	BCR	C27-C26-C25	2.98	126.73	122.70
14	b	3010	CLA	C3A-C2A-C1A	2.98	105.81	101.34
16	2	3048	BCR	C15-C16-C17	-2.98	117.42	123.52
16	b	3048	BCR	C15-C16-C17	-2.98	117.42	123.52
14	B	3006	CLA	C1-C2-C3	-2.98	121.31	126.20
14	L	201	CLA	CHB-C4A-NA	2.98	128.70	124.40
16	B	3048	BCR	C27-C26-C25	2.98	126.73	122.70
14	a	827	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
14	b	3041	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
14	2	3006	CLA	C1-C2-C3	-2.97	121.33	126.20
14	0	204	CLA	CHB-C4A-NA	2.97	128.69	124.40
14	A	843	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	F	204	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	l	203	CLA	CHB-C4A-NA	2.97	128.68	124.40
14	B	3010	CLA	C3A-C2A-C1A	2.97	105.78	101.34
14	A	809	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
14	1	809	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
13	1	801	CL0	C3D-C4D-CHA	2.96	113.05	108.54
14	a	808	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	1	843	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	a	842	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
16	A	852	BCR	C15-C16-C17	-2.95	117.47	123.52
14	1	828	CLA	O2D-CGD-O1D	-2.95	118.10	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	814	CLA	C3B-C4B-NB	-2.95	107.89	110.53
14	a	808	CLA	C3B-C4B-NB	-2.95	107.89	110.53
14	b	3017	CLA	CAC-C3C-C2C	-2.95	122.14	127.56
14	a	828	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
14	0	208	CLA	C3B-C4B-NB	-2.95	107.90	110.53
16	a	851	BCR	C15-C16-C17	-2.95	117.48	123.52
14	A	834	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	f	204	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	1	834	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	a	813	CLA	C3B-C4B-NB	-2.95	107.90	110.53
14	2	3017	CLA	CAC-C3C-C2C	-2.95	122.14	127.56
14	L	204	CLA	C3B-C4B-NB	-2.95	107.90	110.53
13	a	801	CL0	C3D-C4D-CHA	2.94	113.02	108.54
16	1	851	BCR	C15-C16-C17	-2.94	117.50	123.52
14	b	3006	CLA	C1-C2-C3	-2.94	121.38	126.20
13	A	801	CL0	C3D-C4D-CHA	2.94	113.01	108.54
14	A	840	CLA	C3B-C4B-NB	-2.94	107.90	110.53
14	1	813	CLA	C3B-C4B-NB	-2.94	107.90	110.53
14	1	830	CLA	C3B-C4B-NB	-2.94	107.90	110.53
14	A	855	CLA	C3A-C2A-C1A	-2.94	103.29	106.30
14	B	3017	CLA	O2D-CGD-CBD	2.94	116.36	111.23
14	1	841	CLA	C3B-C4B-NB	-2.94	107.91	110.53
14	b	3021	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	A	813	CLA	C3B-C4B-NB	-2.93	107.91	110.53
14	1	836	CLA	C3B-C4B-NB	-2.93	107.91	110.53
14	B	3021	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	B	3010	CLA	C3B-C4B-NB	-2.93	107.91	110.53
14	B	3017	CLA	CAC-C3C-C2C	-2.93	122.17	127.56
14	a	812	CLA	C3B-C4B-NB	-2.93	107.91	110.53
14	A	821	CLA	CMB-C2B-C3B	2.93	133.44	126.55
14	2	3017	CLA	O2D-CGD-CBD	2.93	116.35	111.23
16	B	3053	BCR	C2-C1-C6	2.93	114.69	110.44
14	A	829	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	A	812	CLA	C3B-C4B-NB	-2.92	107.92	110.53
14	a	835	CLA	C3B-C4B-NB	-2.92	107.92	110.53
14	1	829	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	a	821	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	a	840	CLA	C3B-C4B-NB	-2.92	107.92	110.53
14	1	826	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	B	3033	CLA	CAC-C3C-C4C	2.92	128.59	124.79
14	A	841	CLA	CHB-C4A-NA	2.92	128.62	124.40
14	1	812	CLA	C3B-C4B-NB	-2.92	107.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3012	CLA	C4-C3-C5	2.92	120.29	115.23
14	1	821	CLA	CMB-C2B-C3B	2.92	133.41	126.55
14	A	826	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	2	3021	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	a	820	CLA	CMB-C2B-C3B	2.92	133.41	126.55
14	a	811	CLA	C3B-C4B-NB	-2.91	107.93	110.53
14	B	3032	CLA	C3B-C4B-NB	-2.91	107.93	110.53
14	0	207	CLA	CHB-C4A-NA	2.91	128.60	124.40
14	F	203	CLA	CMB-C2B-C1B	-2.91	120.98	125.42
14	a	833	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
14	j	1101	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
14	a	840	CLA	CHB-C4A-NA	2.91	128.60	124.40
14	A	835	CLA	CHB-C4A-NA	2.91	128.60	124.40
14	j	1103	CLA	C3B-C4B-NB	-2.91	107.94	110.53
14	2	3032	CLA	C3B-C4B-NB	-2.91	107.94	110.53
14	a	825	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
14	a	838	CLA	C3B-C4B-NB	-2.91	107.94	110.53
14	b	3014	CLA	C3B-C4B-NB	-2.91	107.94	110.53
14	l	207	CLA	C3B-C4B-NB	-2.91	107.94	110.53
14	A	822	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
14	B	3014	CLA	C3B-C4B-NB	-2.90	107.94	110.53
16	j	1106	BCR	C2-C1-C6	2.90	114.65	110.44
14	B	3014	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	l	206	CLA	CHB-C4A-NA	2.90	128.59	124.40
14	1	839	CLA	C3B-C4B-NB	-2.90	107.94	110.53
14	b	3037	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	b	3010	CLA	O2A-CGA-O1A	-2.90	116.38	123.63
14	b	3017	CLA	O2D-CGD-CBD	2.90	116.30	111.23
14	2	3012	CLA	C4-C3-C5	2.90	120.26	115.23
16	a	850	BCR	C2-C1-C6	2.90	114.65	110.44
14	b	3014	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
16	B	3044	BCR	C24-C23-C22	-2.90	121.95	126.23
14	a	819	CLA	CHB-C4A-NA	2.90	128.58	124.40
14	2	3033	CLA	CAC-C3C-C4C	2.90	128.56	124.79
14	f	203	CLA	CMB-C2B-C1B	-2.90	121.01	125.42
14	A	804	CLA	CMB-C2B-C1B	-2.90	121.01	125.42
14	a	829	CLA	C3B-C4B-NB	-2.90	107.94	110.53
14	b	3032	CLA	C3B-C4B-NB	-2.90	107.94	110.53
16	b	3047	BCR	C27-C26-C25	2.90	126.62	122.70
14	2	3014	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
14	b	3033	CLA	CAC-C3C-C4C	2.90	128.56	124.79
14	2	3010	CLA	O2A-CGA-O1A	-2.89	116.39	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	0	203	CLA	C3A-C2A-C1A	-2.89	103.34	106.30
14	1	820	CLA	CHB-C4A-NA	2.89	128.58	124.40
14	A	839	CLA	C3B-C4B-NB	-2.89	107.95	110.53
14	A	841	CLA	C3B-C4B-NB	-2.89	107.95	110.53
14	b	3012	CLA	C4-C3-C5	2.89	120.25	115.23
14	B	3037	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
16	2	3052	BCR	C2-C1-C6	2.89	114.64	110.44
17	2	3051	LHG	O8-C23-C24	2.89	120.65	111.83
14	A	810	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
16	2	3047	BCR	C27-C26-C25	2.89	126.61	122.70
17	b	3051	LHG	O8-C23-C24	2.89	120.65	111.83
14	1	822	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	a	809	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
14	2	3037	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
14	1	835	CLA	CHB-C4A-NA	2.89	128.57	124.40
14	2	3036	CLA	C1-C2-C3	-2.89	122.09	126.76
14	1	841	CLA	CHB-C4A-NA	2.89	128.56	124.40
14	a	834	CLA	CHB-C4A-NA	2.88	128.56	124.40
16	1	850	BCR	C2-C1-C6	2.88	114.63	110.44
14	A	827	CLA	CAA-C2A-C1A	-2.88	102.53	111.97
14	L	203	CLA	CHB-C4A-NA	2.88	128.56	124.40
16	B	3047	BCR	C27-C26-C25	2.88	126.60	122.70
14	a	826	CLA	CAA-C2A-C1A	-2.88	102.53	111.97
14	a	813	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
14	b	3036	CLA	C1-C2-C3	-2.88	122.10	126.76
14	B	3010	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
14	6	203	CLA	CMB-C2B-C1B	-2.88	121.03	125.42
16	b	3044	BCR	C24-C23-C22	-2.88	121.97	126.23
14	1	827	CLA	CAA-C2A-C1A	-2.88	102.54	111.97
14	A	830	CLA	C3B-C4B-NB	-2.88	107.96	110.53
14	1	810	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	B	3051	LHG	O8-C23-C24	2.88	120.61	111.83
14	8	102	CLA	C3B-C4B-NB	-2.87	107.96	110.53
14	M	1601	CLA	C3A-C2A-C1A	-2.87	103.36	106.30
14	2	3014	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	A	836	CLA	C3B-C4B-NB	-2.87	107.97	110.53
16	2	3044	BCR	C24-C23-C22	-2.87	121.99	126.23
14	A	814	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	1	814	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	A	820	CLA	CHB-C4A-NA	2.87	128.54	124.40
14	A	814	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	b	3006	CLA	C3B-C4B-NB	-2.87	107.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	203	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
14	a	829	CLA	CMB-C2B-C3B	2.87	133.29	126.55
16	2	3049	BCR	C27-C26-C25	2.87	126.58	122.70
14	f	203	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
14	B	3041	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	2	3041	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	1	804	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
14	1	830	CLA	CMB-C2B-C3B	2.86	133.29	126.55
14	A	826	CLA	C6-C5-C3	2.86	120.43	113.47
14	B	3006	CLA	C3B-C4B-NB	-2.86	107.98	110.53
14	a	807	CLA	C3B-C4B-NB	-2.86	107.98	110.53
14	a	817	CLA	C3B-C4B-NB	-2.86	107.98	110.53
16	B	3049	BCR	C27-C26-C25	2.86	126.57	122.70
14	A	841	CLA	C1-C2-C3	-2.86	121.51	126.20
14	A	844	CLA	CMB-C2B-C3B	2.86	133.27	126.55
17	a	852	LHG	O8-C23-C24	2.86	120.55	111.83
14	A	830	CLA	CMB-C2B-C3B	2.86	133.27	126.55
16	A	851	BCR	C2-C1-C6	2.86	114.59	110.44
14	1	826	CLA	C6-C5-C3	2.86	120.42	113.47
14	a	806	CLA	CMB-C2B-C1B	-2.86	121.07	125.42
14	B	3008	CLA	CHB-C4A-NA	2.86	128.52	124.40
14	A	803	CLA	C3B-C4B-NB	-2.86	107.98	110.53
14	a	825	CLA	C6-C5-C3	2.86	120.42	113.47
17	A	853	LHG	O8-C23-C24	2.85	120.54	111.83
16	b	3049	BCR	C27-C26-C25	2.85	126.56	122.70
14	2	3008	CLA	CHB-C4A-NA	2.85	128.52	124.40
14	1	841	CLA	C1-C2-C3	-2.85	121.52	126.20
14	B	3005	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
14	1	818	CLA	C3B-C4B-NB	-2.85	107.98	110.53
14	a	803	CLA	C3B-C4B-NB	-2.85	107.99	110.53
14	B	3036	CLA	C1-C2-C3	-2.85	122.16	126.76
17	1	852	LHG	O8-C23-C24	2.85	120.52	111.83
14	2	3025	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
14	1	834	CLA	C3B-C4B-NB	-2.85	107.99	110.53
14	B	3004	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	k	101	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	1	807	CLA	CMB-C2B-C1B	-2.84	121.09	125.42
14	b	3005	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	2	3011	CLA	CHB-C4A-NA	2.84	128.50	124.40
14	A	807	CLA	CMB-C2B-C1B	-2.84	121.09	125.42
14	A	808	CLA	C3B-C4B-NB	-2.84	107.99	110.53
14	1	823	CLA	CMB-C2B-C1B	-2.84	121.09	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	0	201	LHG	O8-C23-C24	2.84	120.48	111.83
14	F	203	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
14	a	840	CLA	C1-C2-C3	-2.84	121.55	126.20
14	a	843	CLA	CMB-C2B-C3B	2.84	133.22	126.55
20	2	3050	LMG	O6-C1-O1	-2.83	103.34	110.04
14	2	3005	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
17	L	207	LHG	O8-C23-C24	2.83	120.47	111.83
14	9	101	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
14	1	844	CLA	CMB-C2B-C3B	2.83	133.21	126.55
14	A	823	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
14	2	3006	CLA	C3B-C4B-NB	-2.82	108.01	110.53
14	a	818	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
14	b	3030	CLA	O2D-CGD-CBD	2.82	116.17	111.23
14	b	3041	CLA	C3B-C4B-NB	-2.82	108.01	110.53
20	B	3050	LMG	O6-C1-O1	-2.82	103.38	110.04
14	1	803	CLA	C3B-C4B-NB	-2.82	108.01	110.53
14	1	822	CLA	CMB-C2B-C3B	2.82	133.18	126.55
14	A	822	CLA	CMB-C2B-C3B	2.82	133.18	126.55
14	6	201	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	a	822	CLA	CMB-C2B-C1B	-2.82	121.13	125.42
17	l	201	LHG	O8-C23-C24	2.82	120.43	111.83
14	A	819	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	A	834	CLA	C3B-C4B-NB	-2.82	108.02	110.53
20	b	3050	LMG	O6-C1-O1	-2.82	103.39	110.04
14	1	819	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
14	b	3004	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
14	b	3011	CLA	CHB-C4A-NA	2.81	128.46	124.40
14	a	821	CLA	CMB-C2B-C3B	2.81	133.17	126.55
14	a	823	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	B	3025	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	B	3030	CLA	O2D-CGD-CBD	2.81	116.14	111.23
14	b	3025	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	J	102	CLA	C3B-C4B-NB	-2.81	108.02	110.53
14	2	3030	CLA	O2D-CGD-CBD	2.81	116.14	111.23
14	1	827	CLA	C3B-C4B-NB	-2.81	108.03	110.53
14	2	3004	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
14	b	3008	CLA	CHB-C4A-NA	2.80	128.44	124.40
14	1	808	CLA	C3B-C4B-NB	-2.80	108.03	110.53
14	B	3034	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	B	3015	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	A	824	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	x	1701	CLA	O2D-CGD-O1D	-2.80	118.40	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	801	CL0	C1C-CHC-C4B	2.80	126.08	116.07
14	z	1701	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	K	101	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
13	A	801	CL0	C1C-CHC-C4B	2.80	126.07	116.07
14	1	824	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
14	B	3011	CLA	CHB-C4A-NA	2.80	128.43	124.40
14	b	3022	CLA	CHB-C4A-NA	2.79	128.43	124.40
14	b	3015	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
14	1	807	CLA	O1D-CGD-CBD	2.79	130.03	124.52
14	f	201	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
16	B	3046	BCR	C24-C23-C22	-2.79	122.11	126.23
14	2	3037	CLA	C3B-C4B-NB	-2.79	108.04	110.53
14	X	1701	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
16	b	3046	BCR	C27-C26-C25	2.79	126.47	122.70
14	a	833	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	2	3048	BCR	C38-C26-C25	-2.79	121.44	124.48
14	L	203	CLA	O2D-CGD-CBD	2.79	116.10	111.23
13	1	801	CL0	C1C-CHC-C4B	2.78	126.03	116.07
14	a	819	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
16	B	3046	BCR	C27-C26-C25	2.78	126.47	122.70
14	J	101	CLA	CHB-C4A-NA	2.78	128.41	124.40
14	1	820	CLA	CMB-C2B-C1B	-2.78	121.19	125.42
14	l	206	CLA	O2D-CGD-CBD	2.78	116.09	111.23
14	A	818	CLA	C3B-C4B-NB	-2.78	108.05	110.53
16	m	101	BCR	C27-C26-C25	2.78	126.46	122.70
14	2	3022	CLA	CHB-C4A-NA	2.78	128.41	124.40
14	b	3037	CLA	C3B-C4B-NB	-2.78	108.05	110.53
14	f	203	CLA	C3B-C4B-NB	-2.77	108.05	110.53
14	0	207	CLA	O2D-CGD-CBD	2.77	116.08	111.23
14	a	826	CLA	C3B-C4B-NB	-2.77	108.06	110.53
16	j	1106	BCR	C38-C26-C25	-2.77	121.46	124.48
14	F	201	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
14	b	3034	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
14	2	3034	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
14	2	3028	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
14	j	1102	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	l	209	BCR	C29-C30-C25	2.77	114.46	110.44
14	A	820	CLA	CMB-C2B-C1B	-2.77	121.20	125.42
14	2	3009	CLA	CHB-C4A-NA	2.77	128.39	124.40
14	2	3015	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
16	b	3046	BCR	C24-C23-C22	-2.77	122.14	126.23
14	B	3031	CLA	O2D-CGD-O1D	-2.77	118.47	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	3053	BCR	C38-C26-C25	-2.76	121.47	124.48
16	2	3052	BCR	C38-C26-C25	-2.76	121.47	124.48
14	F	203	CLA	C3B-C4B-NB	-2.76	108.06	110.53
14	a	806	CLA	O1D-CGD-CBD	2.76	129.97	124.52
14	8	101	CLA	CHB-C4A-NA	2.76	128.39	124.40
14	A	838	CLA	CHB-C4A-NA	2.76	128.39	124.40
16	2	3049	BCR	C15-C16-C17	-2.76	117.87	123.52
14	B	3007	CLA	CHB-C4A-NA	2.76	128.38	124.40
16	1	849	BCR	C2-C1-C6	2.76	114.45	110.44
14	b	3028	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	b	3031	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	b	3049	BCR	C15-C16-C17	-2.76	117.88	123.52
14	B	3022	CLA	CHB-C4A-NA	2.76	128.38	124.40
14	a	820	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	B	3048	BCR	C38-C26-C25	-2.76	121.48	124.48
16	0	210	BCR	C29-C30-C25	2.76	114.44	110.44
14	A	807	CLA	O1D-CGD-CBD	2.75	129.95	124.52
16	2	3046	BCR	C24-C23-C22	-2.75	122.16	126.23
14	1	805	CLA	CHB-C4A-NA	2.75	128.37	124.40
14	1	842	CLA	C1-C2-C3	-2.75	121.69	126.20
14	J	101	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
14	B	3028	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	8	101	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
16	a	849	BCR	C2-C1-C6	2.75	114.43	110.44
14	2	3007	CLA	CHB-C4A-NA	2.75	128.37	124.40
14	B	3037	CLA	C3B-C4B-NB	-2.75	108.08	110.53
16	I	102	BCR	C29-C30-C25	2.75	114.43	110.44
14	l	203	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	B	3009	CLA	CHB-C4A-NA	2.74	128.36	124.40
14	a	841	CLA	C1-C2-C3	-2.74	121.70	126.20
14	j	1102	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
14	M	1601	CLA	C3B-C4B-NB	-2.74	108.08	110.53
14	j	1102	CLA	C3B-C4B-NB	-2.74	108.08	110.53
14	B	3042	CLA	C1-C2-C3	-2.74	121.70	126.20
14	b	3007	CLA	CHB-C4A-NA	2.74	128.36	124.40
14	2	3020	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
14	2	3031	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
16	M	1602	BCR	C27-C26-C25	2.74	126.41	122.70
14	B	3020	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
14	A	827	CLA	C3B-C4B-NB	-2.74	108.08	110.53
14	b	3042	CLA	C1-C2-C3	-2.74	121.71	126.20
14	a	804	CLA	CHB-C4A-NA	2.74	128.35	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	852	BCR	C7-C8-C9	-2.74	122.18	126.23
14	8	101	CLA	C3B-C4B-NB	-2.74	108.09	110.53
14	1	816	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	1	821	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
16	A	850	BCR	C2-C1-C6	2.74	114.42	110.44
16	B	3049	BCR	C15-C16-C17	-2.74	117.92	123.52
14	2	3029	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
16	y	101	BCR	C27-C26-C25	2.73	126.40	122.70
16	2	3046	BCR	C27-C26-C25	2.73	126.40	122.70
14	L	201	CLA	C3B-C4B-NB	-2.73	108.09	110.53
16	a	851	BCR	C7-C8-C9	-2.73	122.19	126.23
16	1	851	BCR	C7-C8-C9	-2.73	122.19	126.23
16	2	3049	BCR	C16-C15-C14	-2.73	117.93	123.52
14	0	204	CLA	C3B-C4B-NB	-2.73	108.09	110.53
14	A	816	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
16	b	3048	BCR	C38-C26-C25	-2.73	121.51	124.48
14	1	836	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
14	A	842	CLA	C1-C2-C3	-2.72	121.73	126.20
14	2	3042	CLA	C1-C2-C3	-2.72	121.73	126.20
16	b	3049	BCR	C16-C15-C14	-2.72	117.95	123.52
14	B	3025	CLA	CHB-C4A-NA	2.72	128.33	124.40
14	a	837	CLA	CHB-C4A-NA	2.72	128.33	124.40
14	B	3025	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	A	821	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	a	822	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	a	815	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	a	835	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	1	818	CLA	O2D-CGD-CBD	2.72	115.99	111.23
14	1	838	CLA	CHB-C4A-NA	2.72	128.33	124.40
14	a	827	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	6	203	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	A	818	CLA	O2D-CGD-CBD	2.72	115.98	111.23
14	1	828	CLA	C3B-C4B-NB	-2.72	108.10	110.53
14	1	815	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
14	A	831	CLA	CHB-C4A-NA	2.71	128.32	124.40
14	b	3009	CLA	CHB-C4A-NA	2.71	128.32	124.40
14	A	805	CLA	CHB-C4A-NA	2.71	128.32	124.40
14	B	3016	CLA	C6-C5-C3	2.71	120.08	113.47
14	b	3017	CLA	CHB-C4A-NA	2.71	128.31	124.40
16	6	205	BCR	C27-C26-C25	2.71	126.37	122.70
14	1	804	CLA	CHB-C4A-NA	2.71	128.31	124.40
14	A	802	CLA	CHB-C4A-NA	2.71	128.31	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	0	203	CLA	C3B-C4B-NB	-2.71	108.11	110.53
14	B	3026	CLA	C1-C2-C3	-2.71	121.76	126.20
14	1	823	CLA	C3B-C4B-NB	-2.71	108.11	110.53
14	A	836	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
14	b	3029	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
14	f	204	CLA	C1-C2-C3	-2.71	122.39	126.76
14	b	3038	CLA	C3B-C4B-NB	-2.71	108.11	110.53
14	A	828	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	J	101	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	b	3013	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	a	817	CLA	O2D-CGD-CBD	2.70	115.96	111.23
14	b	3016	CLA	C6-C5-C3	2.70	120.05	113.47
14	B	3038	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	0	209	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	A	804	CLA	CHB-C4A-NA	2.70	128.30	124.40
16	B	3049	BCR	C16-C15-C14	-2.70	117.99	123.52
14	1	802	CLA	CHB-C4A-NA	2.70	128.30	124.40
14	A	805	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	A	855	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	1	810	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	A	815	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
14	b	3020	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
14	B	3029	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
14	A	810	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	2	3016	CLA	C6-C5-C3	2.70	120.03	113.47
14	2	3025	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	1	831	CLA	CHB-C4A-NA	2.69	128.29	124.40
14	B	3017	CLA	CHB-C4A-NA	2.69	128.29	124.40
14	B	3013	CLA	C3B-C4B-NB	-2.69	108.13	110.53
14	2	3013	CLA	C3B-C4B-NB	-2.69	108.13	110.53
14	2	3042	CLA	CHB-C4A-NA	2.69	128.29	124.40
14	2	3011	CLA	O1D-CGD-CBD	2.69	129.82	124.52
14	2	3025	CLA	CHB-C4A-NA	2.69	128.28	124.40
14	A	823	CLA	C3B-C4B-NB	-2.69	108.13	110.53
14	2	3006	CLA	CHB-C4A-NA	2.69	128.28	124.40
16	F	202	BCR	C15-C16-C17	-2.69	118.02	123.52
16	f	202	BCR	C15-C16-C17	-2.69	118.02	123.52
14	b	3025	CLA	C3B-C4B-NB	-2.69	108.13	110.53
14	j	1101	CLA	CHB-C4A-NA	2.69	128.28	124.40
14	2	3017	CLA	CHB-C4A-NA	2.68	128.27	124.40
14	B	3019	CLA	C3B-C4B-NB	-2.68	108.13	110.53
14	a	804	CLA	C3B-C4B-NB	-2.68	108.13	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	3026	CLA	C1-C2-C3	-2.68	121.80	126.20
16	6	202	BCR	C15-C16-C17	-2.68	118.03	123.52
14	B	3042	CLA	CHB-C4A-NA	2.68	128.27	124.40
14	b	3025	CLA	CHB-C4A-NA	2.68	128.27	124.40
14	a	830	CLA	CHB-C4A-NA	2.68	128.26	124.40
14	b	3006	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	2	3006	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	1	808	CLA	O2D-CGD-CBD	2.68	115.91	111.23
14	a	837	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
14	a	814	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
13	A	801	CL0	CMD-C2D-C3D	2.67	130.02	124.68
16	F	205	BCR	C27-C26-C25	2.67	126.31	122.70
14	B	3016	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
14	a	802	CLA	CHB-C4A-NA	2.67	128.25	124.40
14	b	3023	CLA	CMB-C2B-C3B	2.67	132.83	126.55
14	2	3026	CLA	C1-O2A-CGA	-2.67	110.19	116.65
14	2	3038	CLA	C3B-C4B-NB	-2.67	108.15	110.53
14	2	3019	CLA	C3B-C4B-NB	-2.67	108.15	110.53
14	b	3011	CLA	O1D-CGD-CBD	2.67	129.78	124.52
14	L	205	CLA	C3B-C4B-NB	-2.67	108.15	110.53
14	B	3011	CLA	O1D-CGD-CBD	2.67	129.78	124.52
13	a	801	CL0	CMD-C2D-C3D	2.67	130.01	124.68
14	b	3026	CLA	C1-C2-C3	-2.67	121.83	126.20
14	b	3015	CLA	C6-C5-C3	2.67	119.96	113.47
16	A	848	BCR	C37-C22-C21	-2.67	118.50	122.82
14	b	3006	CLA	CHB-C4A-NA	2.66	128.25	124.40
13	1	801	CL0	CMD-C2D-C3D	2.66	130.01	124.68
14	F	204	CLA	C1-C2-C3	-2.66	122.45	126.76
14	6	204	CLA	C1-C2-C3	-2.66	122.45	126.76
14	a	819	CLA	C1-C2-C3	-2.66	121.84	126.20
14	2	3038	CLA	CHB-C4A-NA	2.66	128.24	124.40
14	l	208	CLA	C3B-C4B-NB	-2.66	108.16	110.53
16	1	849	BCR	C27-C26-C25	2.66	126.30	122.70
14	B	3006	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	b	3042	CLA	CHB-C4A-NA	2.66	128.24	124.40
14	L	205	CLA	O2D-CGD-CBD	2.66	115.88	111.23
14	A	834	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
16	f	205	BCR	C27-C26-C25	2.66	126.30	122.70
14	A	838	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
14	b	3026	CLA	C1-O2A-CGA	-2.66	110.22	116.65
14	a	809	CLA	C3B-C4B-NB	-2.66	108.16	110.53
16	2	3052	BCR	C27-C26-C25	2.66	126.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	834	CLA	CMB-C2B-C1B	-2.66	121.38	125.42
16	i	101	BCR	C15-C16-C17	-2.66	118.08	123.52
14	a	807	CLA	O2D-CGD-CBD	2.65	115.87	111.23
14	l	208	CLA	O2D-CGD-CBD	2.65	115.87	111.23
14	b	3019	CLA	C3B-C4B-NB	-2.65	108.16	110.53
14	B	3006	CLA	CHB-C4A-NA	2.65	128.23	124.40
14	1	838	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	A	808	CLA	O2D-CGD-CBD	2.65	115.87	111.23
14	A	841	CLA	O2D-CGD-CBD	2.65	115.86	111.23
14	B	3015	CLA	C6-C5-C3	2.65	119.92	113.47
16	I	101	BCR	C15-C16-C17	-2.65	118.10	123.52
14	B	3026	CLA	C1-O2A-CGA	-2.65	110.23	116.65
14	b	3008	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	2	3016	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	A	820	CLA	C1-C2-C3	-2.65	121.86	126.20
14	a	833	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
14	b	3036	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
14	1	830	CLA	CHB-C4A-NA	2.65	128.22	124.40
16	1	847	BCR	C37-C22-C21	-2.65	118.53	122.82
14	B	3023	CLA	CMB-C2B-C3B	2.65	132.77	126.55
16	A	849	BCR	C15-C16-C17	-2.64	118.11	123.52
14	b	3016	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
14	2	3012	CLA	CHB-C4A-NA	2.64	128.21	124.40
14	K	102	CLA	C3B-C4B-NB	-2.64	108.17	110.53
14	b	3038	CLA	CHB-C4A-NA	2.64	128.21	124.40
14	a	829	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
14	a	840	CLA	O2D-CGD-CBD	2.64	115.84	111.23
14	B	3008	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
14	0	209	CLA	O2D-CGD-CBD	2.64	115.84	111.23
14	B	3036	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
16	j	1106	BCR	C27-C26-C25	2.64	126.27	122.70
14	2	3008	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
14	2	3036	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
14	1	805	CLA	C3B-C4B-NB	-2.63	108.18	110.53
16	B	3049	BCR	C2-C1-C6	2.63	114.27	110.44
16	B	3053	BCR	C27-C26-C25	2.63	126.26	122.70
14	2	3005	CLA	CHB-C4A-NA	2.63	128.20	124.40
14	A	821	CLA	CHB-C4A-NA	2.63	128.20	124.40
14	a	802	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
16	j	1106	BCR	C15-C16-C17	-2.63	118.13	123.52
14	2	3023	CLA	CMB-C2B-C3B	2.63	132.74	126.55
16	a	847	BCR	C37-C22-C21	-2.63	118.55	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	3039	CLA	C3B-C4B-NB	-2.63	108.18	110.53
14	1	841	CLA	O2D-CGD-CBD	2.63	115.83	111.23
14	b	3033	CLA	CHB-C4A-NA	2.63	128.20	124.40
16	7	101	BCR	C15-C16-C17	-2.63	118.14	123.52
14	b	3005	CLA	CHB-C4A-NA	2.63	128.19	124.40
16	1	848	BCR	C15-C16-C17	-2.63	118.14	123.52
14	A	830	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
14	2	3015	CLA	C6-C5-C3	2.63	119.87	113.47
16	a	848	BCR	C15-C16-C17	-2.63	118.14	123.52
14	b	3031	CLA	CMB-C2B-C1B	-2.63	121.42	125.42
14	B	3038	CLA	CHB-C4A-NA	2.63	128.19	124.40
16	b	3049	BCR	C2-C1-C6	2.63	114.25	110.44
16	a	849	BCR	C27-C26-C25	2.63	126.25	122.70
14	1	821	CLA	CHB-C4A-NA	2.63	128.19	124.40
14	A	802	CLA	CMB-C2B-C3B	2.63	132.73	126.55
14	B	3039	CLA	C3B-C4B-NB	-2.63	108.19	110.53
17	l	202	LHG	O8-C23-C24	2.63	119.84	111.83
14	b	3018	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
16	j	1106	BCR	C11-C10-C9	-2.62	123.60	127.28
16	2	3052	BCR	C11-C10-C9	-2.62	123.60	127.28
14	2	3018	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
16	B	3053	BCR	C15-C16-C17	-2.62	118.15	123.52
14	B	3013	CLA	O2D-CGD-CBD	2.62	115.81	111.23
14	1	820	CLA	C1-C2-C3	-2.62	121.90	126.20
16	B	3053	BCR	C11-C10-C9	-2.62	123.60	127.28
14	1	830	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
16	2	3049	BCR	C2-C1-C6	2.62	114.25	110.44
17	0	202	LHG	O8-C23-C24	2.62	119.83	111.83
14	a	823	CLA	CHB-C4A-NA	2.62	128.18	124.40
14	1	802	CLA	CMB-C2B-C3B	2.62	132.71	126.55
14	B	3024	CLA	CHB-C4A-NA	2.62	128.18	124.40
14	a	802	CLA	CMB-C2B-C3B	2.62	132.71	126.55
16	A	850	BCR	C27-C26-C25	2.62	126.24	122.70
16	k	103	BCR	C15-C16-C17	-2.62	118.16	123.52
16	2	3052	BCR	C15-C16-C17	-2.62	118.16	123.52
14	2	3031	CLA	CMB-C2B-C1B	-2.62	121.44	125.42
14	a	814	CLA	CHB-C4A-NA	2.62	128.18	124.40
14	a	820	CLA	CHB-C4A-NA	2.62	128.18	124.40
14	2	3040	CLA	C3B-C4B-NB	-2.62	108.19	110.53
17	L	208	LHG	O8-C23-C24	2.61	119.81	111.83
14	A	824	CLA	CHB-C4A-NA	2.61	128.17	124.40
14	B	3005	CLA	CHB-C4A-NA	2.61	128.17	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	802	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
14	2	3013	CLA	O2D-CGD-CBD	2.61	115.80	111.23
14	b	3039	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	2	3024	CLA	CHB-C4A-NA	2.61	128.17	124.40
14	B	3020	CLA	CHB-C4A-NA	2.61	128.17	124.40
14	b	3040	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	9	103	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	B	3033	CLA	CHB-C4A-NA	2.61	128.16	124.40
14	a	820	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	B	3018	CLA	CHB-C4A-NA	2.61	128.16	124.40
14	B	3004	CLA	C3B-C4B-NB	-2.60	108.20	110.53
14	b	3004	CLA	C3B-C4B-NB	-2.60	108.20	110.53
14	b	3024	CLA	CHB-C4A-NA	2.60	128.16	124.40
14	B	3018	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
14	b	3012	CLA	CHB-C4A-NA	2.60	128.16	124.40
14	b	3013	CLA	O2D-CGD-CBD	2.60	115.78	111.23
14	B	3012	CLA	CHB-C4A-NA	2.60	128.15	124.40
16	9	104	BCR	C15-C16-C17	-2.60	118.20	123.52
14	A	812	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
16	f	202	BCR	C2-C1-C6	2.60	114.21	110.44
14	1	838	CLA	CMB-C2B-C3B	2.60	132.66	126.55
14	B	3009	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	F	202	BCR	C2-C1-C6	2.59	114.21	110.44
14	A	802	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
16	K	103	BCR	C15-C16-C17	-2.59	118.22	123.52
16	I	101	BCR	C27-C26-C25	2.59	126.21	122.70
16	7	101	BCR	C27-C26-C25	2.59	126.21	122.70
14	a	829	CLA	CHB-C4A-NA	2.59	128.14	124.40
14	a	812	CLA	CHB-C4A-NA	2.59	128.14	124.40
14	A	821	CLA	C3B-C4B-NB	-2.59	108.22	110.53
14	B	3040	CLA	C3B-C4B-NB	-2.59	108.22	110.53
14	B	3027	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
14	2	3020	CLA	CHB-C4A-NA	2.59	128.13	124.40
14	2	3007	CLA	C3B-C4B-NB	-2.59	108.22	110.53
14	A	802	CLA	C1-C2-C3	-2.59	121.96	126.20
14	1	802	CLA	C1-C2-C3	-2.59	121.96	126.20
14	A	830	CLA	CHB-C4A-NA	2.59	128.13	124.40
14	a	822	CLA	CHB-C4A-NA	2.59	128.13	124.40
14	1	813	CLA	CHB-C4A-NA	2.59	128.13	124.40
14	1	812	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	1	824	CLA	CHB-C4A-NA	2.58	128.13	124.40
14	A	813	CLA	CHB-C4A-NA	2.58	128.13	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	6	202	BCR	C2-C1-C6	2.58	114.19	110.44
14	2	3033	CLA	CHB-C4A-NA	2.58	128.13	124.40
14	1	821	CLA	C3B-C4B-NB	-2.58	108.22	110.53
14	2	3022	CLA	O2D-CGD-CBD	2.58	115.74	111.23
14	a	811	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	k	102	CLA	C3B-C4B-NB	-2.58	108.23	110.53
14	1	802	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
14	b	3009	CLA	C1-C2-C3	-2.58	121.97	126.20
14	a	837	CLA	CMB-C2B-C3B	2.58	132.61	126.55
14	b	3009	CLA	C3B-C4B-NB	-2.58	108.23	110.53
14	B	3031	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
14	b	3026	CLA	CAA-CBA-CGA	-2.58	105.89	113.21
16	A	846	BCR	C24-C23-C22	-2.58	122.42	126.23
14	a	802	CLA	O2A-CGA-O1A	-2.58	117.19	123.63
14	2	3016	CLA	C3B-C4B-NB	-2.58	108.23	110.53
14	b	3018	CLA	CHB-C4A-NA	2.57	128.12	124.40
14	b	3022	CLA	O2D-CGD-CBD	2.57	115.73	111.23
14	2	3009	CLA	C1-C2-C3	-2.57	121.98	126.20
20	B	3050	LMG	C1-O6-C5	-2.57	108.70	113.72
14	B	3022	CLA	O2D-CGD-CBD	2.57	115.73	111.23
14	1	823	CLA	CHB-C4A-NA	2.57	128.11	124.40
14	2	3033	CLA	C1-C2-C3	-2.57	121.98	126.20
14	A	805	CLA	CMB-C2B-C3B	2.57	132.60	126.55
16	i	101	BCR	C27-C26-C25	2.57	126.18	122.70
14	b	3027	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
14	2	3035	CLA	C3B-C4B-NB	-2.57	108.24	110.53
16	j	1105	BCR	C20-C21-C22	-2.57	123.67	127.28
14	A	823	CLA	CHB-C4A-NA	2.57	128.11	124.40
14	B	3026	CLA	CAA-CBA-CGA	-2.57	105.92	113.21
14	B	3009	CLA	C1-C2-C3	-2.57	121.99	126.20
14	0	204	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
16	a	845	BCR	C24-C23-C22	-2.57	122.44	126.23
14	2	3027	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
14	1	805	CLA	CMB-C2B-C3B	2.57	132.59	126.55
14	B	3033	CLA	C1-C2-C3	-2.57	121.99	126.20
14	2	3026	CLA	CAA-CBA-CGA	-2.57	105.92	113.21
14	b	3033	CLA	C1-C2-C3	-2.57	121.99	126.20
14	A	815	CLA	CHB-C4A-NA	2.57	128.10	124.40
14	a	804	CLA	CMB-C2B-C3B	2.56	132.58	126.55
14	A	802	CLA	O2A-CGA-O1A	-2.56	117.21	123.63
16	j	1105	BCR	C15-C16-C17	-2.56	118.27	123.52
14	2	3018	CLA	CHB-C4A-NA	2.56	128.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	203	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
20	2	3050	LMG	C1-O6-C5	-2.56	108.72	113.72
14	1	815	CLA	CHB-C4A-NA	2.56	128.10	124.40
16	J	104	BCR	C15-C16-C17	-2.56	118.28	123.52
16	8	104	BCR	C15-C16-C17	-2.56	118.28	123.52
14	a	815	CLA	CHB-C4A-NA	2.56	128.09	124.40
14	A	838	CLA	CMB-C2B-C3B	2.56	132.57	126.55
16	A	846	BCR	C15-C14-C13	-2.56	123.69	127.28
16	B	3045	BCR	C15-C16-C17	-2.56	118.29	123.52
14	1	818	CLA	CHB-C4A-NA	2.56	128.09	124.40
20	b	3050	LMG	C1-O6-C5	-2.56	108.73	113.72
14	b	3020	CLA	CHB-C4A-NA	2.56	128.09	124.40
14	l	207	CLA	CHB-C4A-NA	2.56	128.09	124.40
14	2	3019	CLA	CMB-C2B-C1B	-2.56	121.53	125.42
14	B	3016	CLA	C3B-C4B-NB	-2.56	108.25	110.53
14	B	3035	CLA	C3B-C4B-NB	-2.56	108.25	110.53
14	l	207	CLA	C1-C2-C3	-2.55	122.01	126.20
16	a	846	BCR	C30-C25-C26	-2.55	119.14	122.64
14	0	208	CLA	CHB-C4A-NA	2.55	128.09	124.40
14	B	3007	CLA	C3B-C4B-NB	-2.55	108.25	110.53
14	b	3035	CLA	C3B-C4B-NB	-2.55	108.25	110.53
16	J	104	BCR	C20-C21-C22	-2.55	123.70	127.28
16	8	104	BCR	C20-C21-C22	-2.55	123.70	127.28
16	9	102	BCR	C24-C23-C22	-2.55	122.46	126.23
14	a	817	CLA	CHB-C4A-NA	2.55	128.08	124.40
14	1	816	CLA	CHB-C4A-NA	2.55	128.08	124.40
13	A	801	CL0	CMB-C2B-C3B	2.55	129.78	124.68
16	2	3052	BCR	C33-C5-C6	-2.55	121.70	124.48
14	A	816	CLA	CHB-C4A-NA	2.55	128.08	124.40
14	b	3007	CLA	C3B-C4B-NB	-2.55	108.25	110.53
14	z	1701	CLA	C3B-C4B-NB	-2.55	108.25	110.53
14	1	822	CLA	CHB-C4A-NA	2.55	128.08	124.40
16	2	3045	BCR	C15-C16-C17	-2.55	118.30	123.52
14	B	3011	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
14	b	3011	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
16	1	850	BCR	C15-C16-C17	-2.55	118.31	123.52
14	b	3003	CLA	C3B-C4B-NB	-2.55	108.26	110.53
13	a	801	CL0	C4C-CHD-C1D	2.55	125.18	116.07
14	L	204	CLA	C1-C2-C3	-2.55	122.02	126.20
14	L	204	CLA	CHB-C4A-NA	2.55	128.07	124.40
13	1	801	CL0	CMB-C2B-C3B	2.55	129.77	124.68
16	1	846	BCR	C30-C25-C26	-2.54	119.16	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	201	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
16	0	210	BCR	C15-C16-C17	-2.54	118.31	123.52
14	a	802	CLA	C1-C2-C3	-2.54	122.03	126.20
14	2	3004	CLA	C3B-C4B-NB	-2.54	108.26	110.53
16	a	850	BCR	C15-C16-C17	-2.54	118.32	123.52
13	1	801	CL0	C4C-CHD-C1D	2.54	125.17	116.07
17	0	201	LHG	C27-C26-C25	-2.54	101.52	114.37
16	b	3045	BCR	C15-C16-C17	-2.54	118.32	123.52
14	0	209	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
13	A	801	CL0	C4C-CHD-C1D	2.54	125.16	116.07
14	1	840	CLA	CHB-C4A-NA	2.54	128.07	124.40
14	2	3024	CLA	CMB-C2B-C3B	2.54	132.53	126.55
16	j	1104	BCR	C15-C16-C17	-2.54	118.32	123.52
14	X	1701	CLA	C3B-C4B-NB	-2.54	108.26	110.53
16	a	845	BCR	C15-C14-C13	-2.54	123.72	127.28
16	9	102	BCR	C20-C21-C22	-2.54	123.72	127.28
16	I	102	BCR	C15-C16-C17	-2.54	118.33	123.52
14	b	3024	CLA	CMB-C2B-C3B	2.54	132.52	126.55
17	L	207	LHG	C27-C26-C25	-2.54	101.54	114.37
17	l	201	LHG	C27-C26-C25	-2.54	101.54	114.37
16	a	845	BCR	C20-C21-C22	-2.54	123.72	127.28
14	2	3011	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
16	9	102	BCR	C15-C14-C13	-2.53	123.72	127.28
16	A	851	BCR	C15-C16-C17	-2.53	118.33	123.52
14	B	3037	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
16	8	103	BCR	C15-C16-C17	-2.53	118.33	123.52
14	A	822	CLA	CHB-C4A-NA	2.53	128.06	124.40
14	2	3034	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
14	b	3034	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
14	b	3019	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
16	j	1106	BCR	C33-C5-C6	-2.53	121.72	124.48
16	B	3053	BCR	C33-C5-C6	-2.53	121.72	124.48
14	b	3016	CLA	C3B-C4B-NB	-2.53	108.27	110.53
14	B	3034	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
16	2	3047	BCR	C15-C14-C13	-2.53	123.73	127.28
14	B	3024	CLA	CMB-C2B-C3B	2.53	132.50	126.55
14	0	208	CLA	C1-C2-C3	-2.53	122.06	126.20
14	b	3027	CLA	CHB-C4A-NA	2.53	128.05	124.40
14	L	205	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
14	a	839	CLA	CHB-C4A-NA	2.53	128.04	124.40
16	A	846	BCR	C20-C21-C22	-2.52	123.74	127.28
16	J	103	BCR	C15-C16-C17	-2.52	118.35	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	821	CLA	CHB-C4A-NA	2.52	128.04	124.40
16	1	850	BCR	C27-C26-C25	2.52	126.11	122.70
16	l	209	BCR	C15-C16-C17	-2.52	118.36	123.52
14	k	101	CLA	CHB-C4A-NA	2.52	128.04	124.40
14	b	3015	CLA	C1-C2-C3	-2.52	122.06	126.20
14	A	811	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
14	1	825	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
16	a	850	BCR	C27-C26-C25	2.52	126.11	122.70
14	B	3015	CLA	C1-C2-C3	-2.52	122.07	126.20
14	a	810	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
14	B	3003	CLA	C3B-C4B-NB	-2.51	108.28	110.53
13	a	801	CL0	CMB-C2B-C3B	2.51	129.71	124.68
14	A	825	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
14	2	3015	CLA	C1-C2-C3	-2.51	122.08	126.20
14	1	833	CLA	CHB-C4A-NA	2.51	128.03	124.40
16	A	847	BCR	C30-C25-C26	-2.51	119.20	122.64
14	A	820	CLA	O2D-CGD-CBD	2.51	115.62	111.23
14	a	819	CLA	O2D-CGD-CBD	2.51	115.62	111.23
14	a	810	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	1	811	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
14	a	842	CLA	C6-C7-C8	-2.51	107.63	115.97
14	1	826	CLA	C3B-C4B-NB	-2.51	108.29	110.53
14	B	3019	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
14	A	840	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	2	3037	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
16	B	3047	BCR	C15-C14-C13	-2.50	123.77	127.28
14	a	809	CLA	CHB-C4A-NA	2.50	128.01	124.40
16	b	3046	BCR	C7-C8-C9	-2.50	122.53	126.23
14	1	820	CLA	O2D-CGD-CBD	2.50	115.61	111.23
14	A	811	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	1	811	CLA	CHB-C4A-NA	2.50	128.01	124.40
16	8	103	BCR	C2-C1-C6	2.50	114.07	110.44
14	2	3032	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	1	208	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
16	0	205	BCR	C8-C7-C6	-2.50	120.33	127.00
14	B	3027	CLA	CHB-C4A-NA	2.50	128.00	124.40
14	9	101	CLA	CHB-C4A-NA	2.50	128.00	124.40
14	2	3009	CLA	C3B-C4B-NB	-2.50	108.30	110.53
14	1	843	CLA	C6-C7-C8	-2.50	107.67	115.97
14	a	825	CLA	C3B-C4B-NB	-2.49	108.30	110.53
14	A	826	CLA	CHB-C4A-NA	2.49	128.00	124.40
16	A	851	BCR	C27-C26-C25	2.49	126.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	804	CLA	O2D-CGD-CBD	2.49	115.59	111.23
16	a	849	BCR	C16-C15-C14	-2.49	118.42	123.52
14	a	824	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
14	b	3037	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
14	A	818	CLA	CHB-C4A-NA	2.49	127.99	124.40
16	b	3047	BCR	C15-C14-C13	-2.49	123.79	127.28
14	A	810	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	A	843	CLA	C6-C7-C8	-2.49	107.70	115.97
16	j	1104	BCR	C2-C1-C6	2.49	114.05	110.44
14	1	805	CLA	O2D-CGD-CBD	2.49	115.58	111.23
14	1	838	CLA	CAC-C3C-C4C	2.49	128.02	124.79
16	A	850	BCR	C16-C15-C14	-2.49	118.43	123.52
14	1	837	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
16	l	204	BCR	C8-C7-C6	-2.48	120.36	127.00
14	b	3032	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	2	3023	CLA	CHB-C4A-NA	2.48	127.98	124.40
16	1	849	BCR	C16-C15-C14	-2.48	118.44	123.52
16	B	3052	BCR	C8-C7-C6	-2.48	120.37	127.00
14	2	3003	CLA	C3B-C4B-NB	-2.48	108.32	110.53
14	b	3023	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	K	101	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	A	805	CLA	O2D-CGD-CBD	2.48	115.56	111.23
14	B	3023	CLA	CHB-C4A-NA	2.48	127.97	124.40
14	A	837	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
14	A	806	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
14	a	834	CLA	C3B-C4B-NB	-2.48	108.32	110.53
14	a	832	CLA	CHB-C4A-NA	2.48	127.97	124.40
14	1	826	CLA	CHB-C4A-NA	2.47	127.97	124.40
16	6	205	BCR	C38-C26-C25	-2.47	121.78	124.48
16	J	103	BCR	C2-C1-C6	2.47	114.03	110.44
14	a	831	CLA	CHB-C4A-NA	2.47	127.97	124.40
14	x	1701	CLA	C3B-C4B-NB	-2.47	108.32	110.53
16	B	3046	BCR	C7-C8-C9	-2.47	122.58	126.23
14	b	3034	CLA	C3B-C4B-NB	-2.47	108.32	110.53
14	1	835	CLA	C3B-C4B-NB	-2.47	108.32	110.53
14	1	806	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
14	A	807	CLA	C3B-C4B-NB	-2.47	108.33	110.53
14	A	838	CLA	CAC-C3C-C4C	2.47	128.00	124.79
16	B	3044	BCR	C27-C26-C25	2.47	126.04	122.70
14	1	832	CLA	CHB-C4A-NA	2.47	127.96	124.40
14	A	831	CLA	C3B-C4B-NB	-2.47	108.33	110.53
14	a	830	CLA	C3B-C4B-NB	-2.47	108.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	832	CLA	CHB-C4A-NA	2.47	127.96	124.40
14	2	3019	CLA	CHB-C4A-NA	2.47	127.96	124.40
14	B	3007	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
14	1	810	CLA	CHB-C4A-NA	2.47	127.96	124.40
14	1	831	CLA	C3B-C4B-NB	-2.46	108.33	110.53
14	2	3011	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
14	b	3039	CLA	CMB-C2B-C3B	2.46	132.35	126.55
14	B	3032	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	2	3027	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	B	3042	CLA	CMC-C2C-C1C	-2.46	121.19	125.03
14	b	3042	CLA	CMC-C2C-C1C	-2.46	121.19	125.03
14	A	826	CLA	C3B-C4B-NB	-2.46	108.33	110.53
14	A	836	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	a	825	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	B	3004	CLA	O1D-CGD-CBD	2.46	129.36	124.52
14	B	3011	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
14	A	833	CLA	CHB-C4A-NA	2.46	127.94	124.40
14	a	836	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
16	2	3046	BCR	C7-C8-C9	-2.45	122.61	126.23
14	b	3006	CLA	O1D-CGD-CBD	2.45	129.36	124.52
14	B	3039	CLA	CMB-C2B-C3B	2.45	132.32	126.55
14	2	3006	CLA	O1D-CGD-CBD	2.45	129.35	124.52
14	a	837	CLA	CAC-C3C-C4C	2.45	127.98	124.79
20	b	3050	LMG	O3-C3-C2	-2.45	104.60	110.38
16	b	3044	BCR	C27-C26-C25	2.45	126.01	122.70
16	2	3044	BCR	C27-C26-C25	2.45	126.01	122.70
14	b	3004	CLA	O1D-CGD-CBD	2.45	129.34	124.52
14	2	3009	CLA	O2D-CGD-CBD	2.45	115.51	111.23
14	B	3019	CLA	CHB-C4A-NA	2.45	127.93	124.40
16	1	204	BCR	C27-C26-C25	2.45	126.01	122.70
16	7	101	BCR	C2-C1-C6	2.44	113.99	110.44
14	2	3034	CLA	C3B-C4B-NB	-2.44	108.35	110.53
16	F	205	BCR	C38-C26-C25	-2.44	121.82	124.48
14	1	843	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	A	835	CLA	C3B-C4B-NB	-2.44	108.35	110.53
14	a	805	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
14	2	3039	CLA	CMB-C2B-C3B	2.44	132.29	126.55
14	b	3019	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	B	3041	CLA	C3A-C2A-C1A	2.44	104.99	101.34
14	a	818	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	B	3009	CLA	O2D-CGD-CBD	2.44	115.49	111.23
14	1	807	CLA	C3B-C4B-NB	-2.44	108.36	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	3007	CLA	CMB-C2B-C1B	-2.43	121.71	125.42
14	A	807	CLA	CMB-C2B-C3B	2.43	132.27	126.55
20	2	3050	LMG	O3-C3-C2	-2.43	104.64	110.38
14	B	3005	CLA	O1D-CGD-CBD	2.43	129.31	124.52
14	a	826	CLA	CHB-C4A-NA	2.43	127.91	124.40
16	l	209	BCR	C7-C8-C9	-2.43	122.64	126.23
14	2	3042	CLA	CMC-C2C-C1C	-2.43	121.23	125.03
14	B	3034	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	I	102	BCR	C7-C8-C9	-2.43	122.64	126.23
14	b	3011	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
20	B	3050	LMG	O3-C3-C2	-2.43	104.65	110.38
14	B	3006	CLA	O1D-CGD-CBD	2.43	129.31	124.52
16	0	205	BCR	C27-C26-C25	2.43	125.99	122.70
14	2	3005	CLA	O1D-CGD-CBD	2.43	129.31	124.52
14	b	3009	CLA	O2D-CGD-CBD	2.43	115.48	111.23
14	b	3005	CLA	O1D-CGD-CBD	2.43	129.31	124.52
16	f	205	BCR	C38-C26-C25	-2.43	121.84	124.48
14	2	3004	CLA	O1D-CGD-CBD	2.43	129.30	124.52
14	A	819	CLA	CHB-C4A-NA	2.43	127.90	124.40
14	b	3028	CLA	CHB-C4A-NA	2.43	127.90	124.40
16	B	3052	BCR	C27-C26-C25	2.43	125.98	122.70
17	0	202	LHG	C11-C10-C9	-2.43	102.11	114.37
14	A	834	CLA	CMB-C2B-C3B	2.43	132.25	126.55
16	I	101	BCR	C2-C1-C6	2.43	113.96	110.44
14	1	834	CLA	CMB-C2B-C3B	2.42	132.25	126.55
17	l	202	LHG	C11-C10-C9	-2.42	102.11	114.37
14	2	3041	CLA	C3A-C2A-C1A	2.42	104.97	101.34
14	2	3029	CLA	C3B-C4B-NB	-2.42	108.37	110.53
16	A	846	BCR	C29-C30-C25	2.42	113.96	110.44
14	1	819	CLA	CHB-C4A-NA	2.42	127.90	124.40
14	b	3028	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
14	a	806	CLA	C3B-C4B-NB	-2.42	108.37	110.53
14	a	833	CLA	CMB-C2B-C3B	2.42	132.25	126.55
17	L	208	LHG	C11-C10-C9	-2.42	102.12	114.37
14	A	827	CLA	CHB-C4A-NA	2.42	127.90	124.40
14	2	3028	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
14	B	3028	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
14	2	3013	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	1	807	CLA	CMB-C2B-C3B	2.42	132.24	126.55
14	0	208	CLA	O2D-CGD-CBD	2.42	115.46	111.23
14	6	204	CLA	C3B-C4B-NB	-2.42	108.37	110.53
14	2	3028	CLA	CHB-C4A-NA	2.42	127.89	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3041	CLA	C3A-C2A-C1A	2.42	104.96	101.34
14	B	3032	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
14	L	204	CLA	O2D-CGD-CBD	2.42	115.45	111.23
16	a	845	BCR	C29-C30-C25	2.42	113.95	110.44
16	9	102	BCR	C29-C30-C25	2.42	113.95	110.44
14	a	842	CLA	CHB-C4A-NA	2.41	127.89	124.40
16	a	845	BCR	C15-C16-C17	-2.41	118.58	123.52
14	a	835	CLA	CHB-C4A-NA	2.41	127.88	124.40
14	k	102	CLA	CHB-C4A-NA	2.41	127.88	124.40
14	B	3028	CLA	CHB-C4A-NA	2.41	127.88	124.40
16	i	101	BCR	C2-C1-C6	2.41	113.94	110.44
14	9	103	CLA	CHB-C4A-NA	2.41	127.88	124.40
14	2	3019	CLA	C4-C3-C5	2.41	119.41	115.23
16	J	104	BCR	C29-C30-C25	2.41	113.94	110.44
14	2	3023	CLA	C3B-C4B-NB	-2.41	108.38	110.53
14	b	3007	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
14	l	207	CLA	O2D-CGD-CBD	2.41	115.44	111.23
14	A	828	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
14	a	819	CLA	C3B-C4B-NB	-2.41	108.38	110.53
14	b	3019	CLA	C4-C3-C5	2.41	119.41	115.23
14	a	806	CLA	CMB-C2B-C3B	2.41	132.21	126.55
14	2	3004	CLA	CHB-C4A-NA	2.41	127.87	124.40
14	1	836	CLA	CHB-C4A-NA	2.41	127.87	124.40
14	A	828	CLA	CHB-C4A-NA	2.40	127.87	124.40
14	K	102	CLA	CHB-C4A-NA	2.40	127.87	124.40
16	9	102	BCR	C15-C16-C17	-2.40	118.60	123.52
14	B	3019	CLA	C4-C3-C5	2.40	119.40	115.23
14	A	814	CLA	CHB-C4A-NA	2.40	127.87	124.40
16	0	210	BCR	C7-C8-C9	-2.40	122.68	126.23
16	8	104	BCR	C29-C30-C25	2.40	113.93	110.44
14	B	3035	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	b	3004	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	b	3013	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	1	814	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	A	843	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	2	3035	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	B	3017	CLA	C3B-C4B-NB	-2.40	108.39	110.53
14	a	827	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	A	823	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
14	1	840	CLA	CAA-CBA-CGA	-2.40	106.40	113.21
13	A	801	CL0	O1D-CGD-CBD	2.40	128.36	124.72
16	a	849	BCR	C8-C7-C6	-2.40	120.59	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3023	CLA	C3B-C4B-NB	-2.40	108.39	110.53
14	2	3021	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	A	850	BCR	C8-C7-C6	-2.40	120.59	127.00
17	a	852	LHG	C20-C19-C18	-2.40	102.25	114.37
13	1	801	CL0	O1D-CGD-CBD	2.40	128.36	124.72
14	1	828	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
17	A	853	LHG	C20-C19-C18	-2.40	102.26	114.37
14	b	3035	CLA	CHB-C4A-NA	2.39	127.86	124.40
14	2	3017	CLA	C3B-C4B-NB	-2.39	108.39	110.53
14	2	3018	CLA	C6-C5-C3	2.39	119.29	113.47
14	b	3041	CLA	CHB-C4A-NA	2.39	127.85	124.40
17	1	852	LHG	C20-C19-C18	-2.39	102.28	114.37
14	1	823	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
14	b	3034	CLA	C4-C3-C5	2.39	119.38	115.23
14	b	3041	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
16	j	1105	BCR	C29-C30-C25	2.39	113.91	110.44
14	1	823	CLA	CMB-C2B-C3B	2.39	132.17	126.55
16	1	849	BCR	C8-C7-C6	-2.39	120.62	127.00
14	b	3032	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
16	A	846	BCR	C15-C16-C17	-2.39	118.63	123.52
14	a	822	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
14	B	3004	CLA	CHB-C4A-NA	2.39	127.84	124.40
14	A	823	CLA	CMB-C2B-C3B	2.39	132.16	126.55
14	b	3029	CLA	C3B-C4B-NB	-2.38	108.40	110.53
14	B	3018	CLA	C6-C5-C3	2.38	119.28	113.47
14	A	818	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
14	2	3041	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
14	a	839	CLA	CAA-CBA-CGA	-2.38	106.44	113.21
14	1	827	CLA	CHB-C4A-NA	2.38	127.84	124.40
14	a	827	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
16	B	3046	BCR	C15-C16-C17	-2.38	118.64	123.52
16	a	851	BCR	C15-C14-C13	-2.38	123.94	127.28
14	B	3034	CLA	C4-C3-C5	2.38	119.36	115.23
14	a	822	CLA	CMB-C2B-C3B	2.38	132.15	126.55
14	A	840	CLA	CAA-CBA-CGA	-2.38	106.44	113.21
16	0	211	BCR	C8-C7-C6	-2.38	120.64	127.00
14	a	810	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
14	1	826	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
14	2	3032	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
14	0	204	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
16	l	210	BCR	C8-C7-C6	-2.38	120.64	127.00
16	B	3053	BCR	C37-C22-C23	2.38	121.72	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	813	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	b	3014	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	A	839	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	B	3013	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	A	810	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
14	2	3018	CLA	C3B-C4B-NB	-2.38	108.41	110.53
14	b	3026	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
14	A	811	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
14	b	3018	CLA	C6-C5-C3	2.38	119.25	113.47
16	y	101	BCR	C15-C16-C17	-2.38	118.66	123.52
14	B	3041	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
14	a	817	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
16	J	103	BCR	C29-C30-C25	2.38	113.89	110.44
14	1	810	CLA	CMB-C2B-C1B	-2.37	121.80	125.42
16	L	206	BCR	C27-C26-C25	2.37	125.91	122.70
14	b	3021	CLA	CHB-C4A-NA	2.37	127.83	124.40
14	1	839	CLA	CHB-C4A-NA	2.37	127.83	124.40
14	L	201	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
14	2	3034	CLA	C4-C3-C5	2.37	119.35	115.23
14	a	825	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
14	2	3021	CLA	CHB-C4A-NA	2.37	127.82	124.40
14	1	820	CLA	C3B-C4B-NB	-2.37	108.41	110.53
14	1	811	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
14	B	3014	CLA	CHB-C4A-NA	2.37	127.82	124.40
16	b	3046	BCR	C15-C16-C17	-2.37	118.67	123.52
14	b	3017	CLA	C3B-C4B-NB	-2.37	108.42	110.53
14	1	828	CLA	CHB-C4A-NA	2.37	127.82	124.40
16	j	1104	BCR	C29-C30-C25	2.37	113.88	110.44
13	a	801	CL0	O1D-CGD-CBD	2.37	128.31	124.72
14	2	3014	CLA	CHB-C4A-NA	2.37	127.82	124.40
14	b	3021	CLA	C3B-C4B-NB	-2.37	108.42	110.53
14	1	825	CLA	CHB-C4A-NA	2.37	127.81	124.40
16	2	3046	BCR	C15-C16-C17	-2.37	118.68	123.52
16	j	1106	BCR	C37-C22-C23	2.37	121.70	118.09
14	2	3026	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
14	b	3024	CLA	C3B-C4B-NB	-2.36	108.42	110.53
16	1	851	BCR	C15-C14-C13	-2.36	123.97	127.28
14	1	825	CLA	CMB-C2B-C3B	2.36	132.10	126.55
14	B	3023	CLA	C3B-C4B-NB	-2.36	108.42	110.53
14	A	855	CLA	CHB-C4A-NA	2.36	127.81	124.40
16	F	202	BCR	C8-C7-C6	-2.36	120.70	127.00
14	a	809	CLA	CMB-C2B-C1B	-2.36	121.83	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	203	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
14	1	818	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
16	8	103	BCR	C29-C30-C25	2.36	113.86	110.44
14	M	1601	CLA	CHB-C4A-NA	2.36	127.80	124.40
14	B	3028	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
14	B	3029	CLA	C3B-C4B-NB	-2.36	108.43	110.53
16	m	101	BCR	C15-C16-C17	-2.35	118.70	123.52
16	0	211	BCR	C27-C26-C25	2.35	125.89	122.70
16	2	3047	BCR	C38-C26-C25	-2.35	121.92	124.48
14	B	3021	CLA	CHB-C4A-NA	2.35	127.79	124.40
17	A	854	LHG	O8-C23-C24	2.35	119.00	111.83
16	f	202	BCR	C8-C7-C6	-2.35	120.72	127.00
16	2	3052	BCR	C37-C22-C23	2.35	121.68	118.09
14	0	203	CLA	CHB-C4A-NA	2.35	127.79	124.40
14	B	3021	CLA	C3B-C4B-NB	-2.35	108.43	110.53
14	b	3011	CLA	C3B-C4B-NB	-2.35	108.43	110.53
14	a	824	CLA	CHB-C4A-NA	2.35	127.79	124.40
16	B	3047	BCR	C38-C26-C25	-2.35	121.92	124.48
14	B	3041	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	2	3015	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	A	832	CLA	O2D-CGD-CBD	2.34	115.33	111.23
14	2	3028	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
16	L	206	BCR	C8-C7-C6	-2.34	120.74	127.00
14	a	838	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	B	3026	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
14	B	3011	CLA	C3B-C4B-NB	-2.34	108.44	110.53
16	2	3047	BCR	C8-C7-C6	-2.34	120.74	127.00
16	M	1602	BCR	C15-C16-C17	-2.34	118.73	123.52
14	b	3017	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
14	A	804	CLA	CMB-C2B-C3B	2.34	132.05	126.55
16	b	3047	BCR	C8-C7-C6	-2.34	120.75	127.00
14	f	204	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	b	3015	CLA	CHB-C4A-NA	2.34	127.77	124.40
17	1	853	LHG	O8-C23-C24	2.34	118.96	111.83
17	a	853	LHG	O8-C23-C24	2.34	118.96	111.83
14	A	820	CLA	C3B-C4B-NB	-2.34	108.44	110.53
14	F	204	CLA	CHB-C4A-NA	2.33	127.77	124.40
14	A	826	CLA	CMB-C2B-C1B	-2.33	121.86	125.42
16	6	202	BCR	C8-C7-C6	-2.33	120.76	127.00
16	a	848	BCR	C24-C23-C22	-2.33	122.78	126.23
14	B	3018	CLA	C3B-C4B-NB	-2.33	108.45	110.53
14	A	825	CLA	CHB-C4A-NA	2.33	127.77	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	3047	BCR	C2-C1-C6	2.33	113.83	110.44
14	b	3018	CLA	C3B-C4B-NB	-2.33	108.45	110.53
14	2	3011	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	A	849	BCR	C24-C23-C22	-2.33	122.78	126.23
14	1	832	CLA	O2D-CGD-CBD	2.33	115.30	111.23
14	f	204	CLA	C3B-C4B-NB	-2.33	108.45	110.53
14	j	1101	CLA	CMB-C2B-C3B	2.33	132.03	126.55
16	B	3047	BCR	C8-C7-C6	-2.33	120.79	127.00
14	2	3041	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	6	204	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	b	3003	CLA	O2D-CGD-CBD	2.32	115.29	111.23
16	A	852	BCR	C15-C14-C13	-2.32	124.02	127.28
16	b	3047	BCR	C38-C26-C25	-2.32	121.95	124.48
14	b	3028	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
14	A	810	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
14	2	3003	CLA	O2D-CGD-CBD	2.32	115.29	111.23
16	b	3047	BCR	C2-C1-C6	2.32	113.81	110.44
14	A	825	CLA	CMB-C2B-C3B	2.32	132.00	126.55
16	1	848	BCR	C24-C23-C22	-2.32	122.81	126.23
14	a	807	CLA	CHB-C4A-NA	2.32	127.74	124.40
14	B	3017	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
14	a	824	CLA	CMB-C2B-C3B	2.32	132.00	126.55
13	1	801	CL0	CHA-C1A-C2A	-2.32	127.87	133.31
14	1	804	CLA	CMB-C2B-C3B	2.32	132.00	126.55
14	2	3017	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
13	a	801	CL0	CHA-C1A-C2A	-2.31	127.87	133.31
14	B	3015	CLA	CHB-C4A-NA	2.31	127.74	124.40
14	l	208	CLA	CHB-C4A-NA	2.31	127.74	124.40
14	a	831	CLA	O2D-CGD-CBD	2.31	115.27	111.23
15	1	845	PQN	C11-C3-C2	-2.31	120.93	124.89
14	f	201	CLA	CHB-C4A-NA	2.31	127.73	124.40
15	a	844	PQN	C11-C3-C2	-2.31	120.93	124.89
14	B	3003	CLA	O2D-CGD-CBD	2.31	115.26	111.23
14	A	808	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	A	812	CLA	CHB-C4A-NA	2.30	127.73	124.40
14	0	209	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	A	834	CLA	O1D-CGD-CBD	2.30	129.06	124.52
16	l	210	BCR	C27-C26-C25	2.30	125.81	122.70
17	l	201	LHG	C20-C19-C18	-2.30	102.73	114.37
14	b	3027	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
17	0	201	LHG	C20-C19-C18	-2.30	102.73	114.37
13	A	801	CL0	CHA-C1A-C2A	-2.30	127.90	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3033	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
14	1	808	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	1	810	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
14	2	3033	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
16	B	3047	BCR	C2-C1-C6	2.30	113.78	110.44
14	a	843	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	F	204	CLA	C3B-C4B-NB	-2.30	108.48	110.53
16	I	101	BCR	C8-C7-C6	-2.30	120.86	127.00
16	i	101	BCR	C8-C7-C6	-2.30	120.87	127.00
14	B	3042	CLA	CMC-C2C-C3C	2.29	132.36	126.15
14	1	203	CLA	CAC-C3C-C4C	2.29	127.77	124.79
14	2	3018	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
14	0	204	CLA	CAC-C3C-C4C	2.29	127.77	124.79
14	b	3029	CLA	CHB-C4A-NA	2.29	127.71	124.40
17	L	207	LHG	C20-C19-C18	-2.29	102.79	114.37
14	b	3008	CLA	O1D-CGD-CBD	2.29	129.04	124.52
14	b	3042	CLA	CMC-C2C-C3C	2.29	132.34	126.15
14	B	3035	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
14	2	3035	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
14	6	203	CLA	CMB-C2B-C3B	2.29	131.93	126.55
14	a	843	CLA	C3B-C4B-NB	-2.29	108.49	110.53
14	L	201	CLA	CAC-C3C-C4C	2.29	127.77	124.79
14	A	844	CLA	C3B-C4B-NB	-2.29	108.49	110.53
14	b	3015	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
14	f	203	CLA	CMB-C2B-C3B	2.29	131.93	126.55
14	F	201	CLA	CHB-C4A-NA	2.29	127.70	124.40
14	2	3024	CLA	C3B-C4B-NB	-2.29	108.49	110.53
14	2	3042	CLA	CMC-C2C-C3C	2.28	132.33	126.15
20	b	3050	LMG	O1-C7-C8	-2.28	105.26	110.82
14	b	3018	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
14	1	812	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	1	817	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
20	B	3050	LMG	O1-C7-C8	-2.28	105.27	110.82
14	A	844	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	a	816	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
16	1	847	BCR	C8-C7-C6	-2.28	120.91	127.00
14	2	3008	CLA	O1D-CGD-CBD	2.28	129.01	124.52
14	8	102	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	F	203	CLA	CMB-C2B-C3B	2.28	131.91	126.55
14	J	102	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	a	809	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
14	6	201	CLA	CHB-C4A-NA	2.27	127.68	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	820	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
14	B	3018	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
16	A	849	BCR	C28-C27-C26	-2.27	110.00	114.06
16	a	848	BCR	C28-C27-C26	-2.27	110.00	114.06
16	7	101	BCR	C8-C7-C6	-2.27	120.92	127.00
14	A	809	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
15	A	845	PQN	C11-C3-C2	-2.27	120.99	124.89
14	L	205	CLA	CHB-C4A-NA	2.27	127.68	124.40
16	A	851	BCR	C8-C7-C6	-2.27	120.93	127.00
20	2	3050	LMG	O1-C7-C8	-2.27	105.29	110.82
14	b	3035	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
14	B	3008	CLA	O1D-CGD-CBD	2.27	129.00	124.52
14	1	834	CLA	O1D-CGD-CBD	2.27	129.00	124.52
14	2	3027	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
14	a	811	CLA	CHB-C4A-NA	2.27	127.68	124.40
16	1	850	BCR	C8-C7-C6	-2.27	120.94	127.00
16	A	848	BCR	C8-C7-C6	-2.27	120.94	127.00
14	1	844	CLA	C3B-C4B-NB	-2.27	108.50	110.53
14	a	808	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
14	B	3015	CLA	C5-C3-C2	2.27	126.25	121.17
14	2	3015	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
16	a	847	BCR	C15-C14-C13	-2.27	124.10	127.28
14	A	817	CLA	C3B-C4B-NB	-2.27	108.51	110.53
14	j	1103	CLA	CHB-C4A-NA	2.26	127.67	124.40
14	B	3033	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
14	2	3015	CLA	C5-C3-C2	2.26	126.25	121.17
14	A	817	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
16	A	848	BCR	C15-C14-C13	-2.26	124.11	127.28
14	a	819	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
14	B	3006	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
16	1	848	BCR	C28-C27-C26	-2.26	110.03	114.06
14	A	815	CLA	C3B-C4B-NB	-2.26	108.51	110.53
14	B	3027	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
14	a	816	CLA	CHB-C4A-NA	2.26	127.66	124.40
16	1	847	BCR	C15-C14-C13	-2.26	124.11	127.28
14	b	3006	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
14	l	207	CLA	C7-C6-C5	-2.25	107.25	113.26
16	a	847	BCR	C8-C7-C6	-2.25	120.97	127.00
14	B	3029	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	b	3022	CLA	C3B-C4B-NB	-2.25	108.52	110.53
14	1	837	CLA	O1A-CGA-CBA	2.25	130.24	123.09
14	2	3019	CLA	CMB-C2B-C3B	2.25	131.85	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	844	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	1	840	CLA	O2D-CGD-CBD	2.25	115.17	111.23
16	1	849	BCR	C38-C26-C25	-2.25	122.03	124.48
16	y	101	BCR	C37-C22-C21	-2.25	119.17	122.82
16	b	3048	BCR	C8-C7-C6	-2.25	120.98	127.00
16	6	205	BCR	C8-C7-C6	-2.25	120.98	127.00
14	B	3024	CLA	C3B-C4B-NB	-2.25	108.52	110.53
16	B	3048	BCR	C8-C7-C6	-2.25	120.98	127.00
14	1	817	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	A	837	CLA	O1A-CGA-CBA	2.25	130.23	123.09
14	a	833	CLA	O1D-CGD-CBD	2.25	128.96	124.52
16	a	849	BCR	C38-C26-C25	-2.25	122.03	124.48
16	a	850	BCR	C8-C7-C6	-2.25	120.99	127.00
14	A	804	CLA	C3B-C4B-NB	-2.25	108.52	110.53
14	X	1701	CLA	CHB-C4A-NA	2.25	127.64	124.40
14	b	3019	CLA	CMB-C2B-C3B	2.25	131.84	126.55
16	f	202	BCR	C16-C15-C14	-2.25	118.92	123.52
20	B	3050	LMG	C40-C39-C38	-2.25	103.01	114.37
14	2	3012	CLA	O2D-CGD-CBD	2.25	115.16	111.23
20	b	3050	LMG	C40-C39-C38	-2.25	103.01	114.37
14	1	842	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
16	F	202	BCR	C16-C15-C14	-2.25	118.92	123.52
16	1	846	BCR	C15-C16-C17	-2.25	118.92	123.52
16	a	846	BCR	C38-C26-C25	-2.25	122.03	124.48
14	L	204	CLA	C7-C6-C5	-2.25	107.28	113.26
14	B	3015	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
14	2	3006	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
14	A	817	CLA	CHB-C4A-NA	2.24	127.64	124.40
14	2	3040	CLA	CHB-C4A-NA	2.24	127.64	124.40
16	2	3048	BCR	C8-C7-C6	-2.24	121.00	127.00
14	z	1701	CLA	CHB-C4A-NA	2.24	127.64	124.40
13	A	801	CL0	O2A-CGA-O1A	-2.24	118.02	123.63
20	2	3050	LMG	C40-C39-C38	-2.24	103.03	114.37
14	K	102	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
14	f	203	CLA	CHB-C4A-NA	2.24	127.63	124.40
16	0	205	BCR	C37-C22-C21	-2.24	119.19	122.82
14	b	3015	CLA	C5-C3-C2	2.24	126.19	121.17
13	a	801	CL0	O2A-CGA-O1A	-2.24	118.03	123.63
14	1	809	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
16	B	3048	BCR	C2-C1-C6	2.24	113.69	110.44
13	1	801	CL0	O2A-CGA-O1A	-2.24	118.03	123.63
14	a	836	CLA	O1A-CGA-CBA	2.24	130.19	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	809	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
14	B	3036	CLA	CHB-C4A-NA	2.24	127.63	124.40
14	a	819	CLA	CMB-C2B-C3B	2.24	131.81	126.55
14	a	808	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
14	1	809	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
16	b	3048	BCR	C2-C1-C6	2.23	113.69	110.44
14	A	837	CLA	O2A-CGA-O1A	-2.23	117.58	123.33
14	1	820	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
16	a	846	BCR	C15-C16-C17	-2.23	118.95	123.52
14	A	842	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
14	B	3010	CLA	CHB-C4A-NA	2.23	127.62	124.40
16	A	847	BCR	C15-C16-C17	-2.23	118.95	123.52
14	B	3031	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
14	1	817	CLA	C3B-C4B-NB	-2.23	108.54	110.53
14	k	102	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
14	2	3014	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
16	6	202	BCR	C16-C15-C14	-2.23	118.96	123.52
14	1	826	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
14	9	103	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
14	0	208	CLA	C7-C6-C5	-2.23	107.32	113.26
14	b	3040	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	x	1701	CLA	CHB-C4A-NA	2.23	127.61	124.40
16	f	205	BCR	C8-C7-C6	-2.23	121.05	127.00
14	1	820	CLA	CMB-C2B-C3B	2.23	131.79	126.55
16	2	3044	BCR	C8-C7-C6	-2.23	121.05	127.00
14	1	827	CLA	O2D-CGD-CBD	2.23	115.12	111.23
16	B	3044	BCR	C8-C7-C6	-2.23	121.05	127.00
17	2	3051	LHG	C20-C19-C18	-2.23	103.12	114.37
14	B	3012	CLA	O2D-CGD-CBD	2.22	115.12	111.23
14	2	3031	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
14	2	3003	CLA	CMD-C2D-C1D	-2.22	120.81	124.73
14	b	3014	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
14	1	804	CLA	C3B-C4B-NB	-2.22	108.55	110.53
14	1	831	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
16	F	205	BCR	C8-C7-C6	-2.22	121.06	127.00
14	a	830	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
14	B	3019	CLA	CMB-C2B-C3B	2.22	131.78	126.55
14	b	3012	CLA	O2D-CGD-CBD	2.22	115.11	111.23
16	b	3044	BCR	C8-C7-C6	-2.22	121.06	127.00
14	b	3031	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
14	2	3029	CLA	CHB-C4A-NA	2.22	127.61	124.40
17	b	3051	LHG	C20-C19-C18	-2.22	103.14	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	841	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
14	a	836	CLA	O2A-CGA-O1A	-2.22	117.62	123.33
16	2	3048	BCR	C2-C1-C6	2.22	113.67	110.44
14	b	3036	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
14	a	816	CLA	C3B-C4B-NB	-2.22	108.55	110.53
14	1	815	CLA	C3B-C4B-NB	-2.22	108.55	110.53
17	B	3051	LHG	C20-C19-C18	-2.22	103.15	114.37
14	B	3040	CLA	CHB-C4A-NA	2.22	127.60	124.40
14	A	840	CLA	O2D-CGD-CBD	2.22	115.11	111.23
14	a	814	CLA	C3B-C4B-NB	-2.22	108.55	110.53
14	b	3036	CLA	CHB-C4A-NA	2.22	127.60	124.40
16	8	104	BCR	C37-C22-C23	2.22	121.47	118.09
16	l	204	BCR	C37-C22-C21	-2.22	119.23	122.82
14	B	3014	CLA	CMB-C2B-C1B	-2.22	122.05	125.42
14	1	837	CLA	O2A-CGA-O1A	-2.22	117.64	123.33
14	A	827	CLA	O2D-CGD-CBD	2.21	115.10	111.23
14	j	1103	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
14	b	3010	CLA	CHB-C4A-NA	2.21	127.59	124.40
14	2	3034	CLA	CHB-C4A-NA	2.21	127.59	124.40
17	1	853	LHG	C11-C10-C9	-2.21	103.18	114.37
14	2	3038	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
14	A	820	CLA	CMB-C2B-C3B	2.21	131.75	126.55
14	2	3036	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
14	2	3030	CLA	CHB-C4A-NA	2.21	127.59	124.40
16	B	3046	BCR	C38-C26-C25	-2.21	122.07	124.48
16	b	3045	BCR	C28-C27-C26	-2.21	110.11	114.06
17	a	853	LHG	C11-C10-C9	-2.21	103.20	114.37
14	1	842	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
14	B	3022	CLA	C3B-C4B-NB	-2.21	108.56	110.53
14	A	826	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
14	B	3036	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
14	b	3036	CLA	C2D-C1D-ND	-2.21	107.94	110.13
14	A	831	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
14	a	825	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
17	A	854	LHG	C11-C10-C9	-2.21	103.22	114.37
16	1	846	BCR	C38-C26-C25	-2.20	122.08	124.48
14	2	3019	CLA	O2D-CGD-CBD	2.20	115.08	111.23
16	A	850	BCR	C38-C26-C25	-2.20	122.08	124.48
16	M	1602	BCR	C37-C22-C21	-2.20	119.25	122.82
14	b	3019	CLA	O2D-CGD-CBD	2.20	115.08	111.23
14	0	209	CLA	CMB-C2B-C3B	2.20	131.73	126.55
14	b	3031	CLA	CMB-C2B-C3B	2.20	131.73	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3034	CLA	CHB-C4A-NA	2.20	127.58	124.40
14	2	3010	CLA	CHB-C4A-NA	2.20	127.58	124.40
14	a	826	CLA	O2D-CGD-CBD	2.20	115.07	111.23
16	B	3052	BCR	C37-C22-C21	-2.20	119.25	122.82
14	l	208	CLA	CMB-C2B-C3B	2.20	131.72	126.55
16	A	852	BCR	C11-C10-C9	-2.20	124.19	127.28
14	A	842	CLA	CHB-C4A-NA	2.20	127.57	124.40
14	2	3036	CLA	C2D-C1D-ND	-2.20	107.95	110.13
14	l	207	CLA	CAC-C3C-C4C	2.20	127.65	124.79
16	2	3045	BCR	C28-C27-C26	-2.20	110.14	114.06
16	m	101	BCR	C37-C22-C21	-2.20	119.26	122.82
14	L	205	CLA	CMB-C2B-C3B	2.20	131.72	126.55
14	a	839	CLA	O2D-CGD-CBD	2.20	115.07	111.23
14	2	3036	CLA	CHB-C4A-NA	2.19	127.57	124.40
14	L	204	CLA	CAC-C3C-C4C	2.19	127.64	124.79
16	I	102	BCR	C28-C27-C26	-2.19	110.14	114.06
14	B	3026	CLA	CMB-C2B-C3B	2.19	131.71	126.55
14	0	207	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
16	0	210	BCR	C28-C27-C26	-2.19	110.15	114.06
16	J	104	BCR	C37-C22-C23	2.19	121.44	118.09
14	l	208	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
16	l	210	BCR	C16-C15-C14	-2.19	119.03	123.52
20	b	3050	LMG	C42-C41-C40	-2.19	103.29	114.37
14	B	3038	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
14	B	3003	CLA	CMD-C2D-C1D	-2.19	120.87	124.73
14	B	3036	CLA	C2D-C1D-ND	-2.19	107.96	110.13
14	B	3019	CLA	O2D-CGD-CBD	2.19	115.06	111.23
14	j	1101	CLA	C3B-C4B-NB	-2.19	108.58	110.53
14	0	209	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
14	6	203	CLA	CHB-C4A-NA	2.19	127.56	124.40
16	b	3045	BCR	C27-C26-C25	2.19	125.66	122.70
16	A	847	BCR	C38-C26-C25	-2.19	122.09	124.48
14	b	3038	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
14	0	204	CLA	C2A-C1A-CHA	2.19	127.67	123.87
14	F	203	CLA	CHB-C4A-NA	2.19	127.56	124.40
16	B	3045	BCR	C28-C27-C26	-2.19	110.15	114.06
20	B	3050	LMG	C42-C41-C40	-2.19	103.31	114.37
16	l	209	BCR	C28-C27-C26	-2.19	110.16	114.06
14	a	841	CLA	CHB-C4A-NA	2.18	127.55	124.40
14	1	837	CLA	CHB-C4A-NA	2.18	127.55	124.40
16	A	849	BCR	C2-C1-C6	2.18	113.61	110.44
20	2	3050	LMG	C42-C41-C40	-2.18	103.33	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	206	BCR	C16-C15-C14	-2.18	119.05	123.52
14	A	842	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
14	2	3022	CLA	C3B-C4B-NB	-2.18	108.58	110.53
14	l	206	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	b	3026	CLA	CHB-C4A-NA	2.18	127.55	124.40
14	a	825	CLA	C1-C2-C3	-2.18	122.62	126.20
14	2	3031	CLA	CMB-C2B-C3B	2.18	131.68	126.55
14	B	3030	CLA	CHB-C4A-NA	2.18	127.55	124.40
14	B	3033	CLA	O2D-CGD-CBD	2.18	115.04	111.23
14	L	205	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
16	1	848	BCR	C2-C1-C6	2.18	113.60	110.44
16	b	3046	BCR	C38-C26-C25	-2.18	122.11	124.48
16	b	3047	BCR	C24-C23-C22	-2.18	123.01	126.23
16	j	1106	BCR	C20-C21-C22	-2.18	124.22	127.28
14	b	3026	CLA	CMB-C2B-C3B	2.18	131.67	126.55
14	L	201	CLA	C2A-C1A-CHA	2.18	127.64	123.87
14	b	3003	CLA	CMD-C2D-C1D	-2.17	120.90	124.73
14	a	816	CLA	O2D-CGD-CBD	2.17	115.03	111.23
16	2	3052	BCR	C15-C14-C13	-2.17	124.23	127.28
14	J	102	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
14	1	842	CLA	CHB-C4A-NA	2.17	127.54	124.40
14	L	203	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
16	1	851	BCR	C11-C10-C9	-2.17	124.23	127.28
14	a	841	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
14	A	827	CLA	C1-C2-C3	-2.17	122.64	126.20
14	b	3030	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	1	829	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	b	3011	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
14	b	3026	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
14	a	815	CLA	C3A-C2A-C1A	2.17	104.59	101.34
14	l	203	CLA	C2A-C1A-CHA	2.17	127.64	123.87
14	A	826	CLA	C1-C2-C3	-2.17	122.64	126.20
14	B	3011	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	2	3045	BCR	C27-C26-C25	2.17	125.64	122.70
14	1	838	CLA	C3B-C4B-NB	-2.17	108.59	110.53
20	B	3050	LMG	C3-C4-C5	-2.17	106.30	110.23
14	B	3017	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
14	b	3010	CLA	C7-C6-C5	-2.17	107.48	113.26
14	2	3028	CLA	CMB-C2B-C3B	2.17	131.65	126.55
14	b	3034	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	2	3011	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
14	B	3010	CLA	C7-C6-C5	-2.17	107.48	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	3026	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	8	102	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
14	l	203	CLA	O1D-CGD-CBD	2.17	128.79	124.52
14	A	817	CLA	O2D-CGD-CBD	2.17	115.02	111.23
14	1	817	CLA	O2D-CGD-CBD	2.17	115.02	111.23
14	b	3028	CLA	CMB-C2B-C3B	2.17	131.64	126.55
14	L	203	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
14	B	3003	CLA	CHB-C4A-NA	2.16	127.52	124.40
14	B	3026	CLA	CHB-C4A-NA	2.16	127.52	124.40
16	j	1105	BCR	C37-C22-C23	2.16	121.39	118.09
14	b	3033	CLA	O2D-CGD-CBD	2.16	115.01	111.23
14	2	3021	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
14	l	206	CLA	CMB-C2B-C1B	-2.16	122.12	125.42
16	B	3045	BCR	C27-C26-C25	2.16	125.63	122.70
14	b	3016	CLA	CHB-C4A-NA	2.16	127.52	124.40
14	b	3003	CLA	CHB-C4A-NA	2.16	127.52	124.40
14	1	822	CLA	CHB-C1B-NB	2.16	127.29	124.05
16	0	211	BCR	C16-C15-C14	-2.16	119.09	123.52
14	B	3009	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	F	202	BCR	C38-C26-C25	-2.16	122.13	124.48
14	a	805	CLA	C1-O2A-CGA	2.16	121.88	116.65
16	a	851	BCR	C11-C10-C9	-2.16	124.25	127.28
14	2	3026	CLA	CMB-C2B-C3B	2.16	131.63	126.55
14	2	3003	CLA	CMD-C2D-C3D	2.16	132.64	127.69
14	0	208	CLA	CAC-C3C-C4C	2.16	127.60	124.79
16	2	3047	BCR	C24-C23-C22	-2.16	123.04	126.23
14	2	3010	CLA	C7-C6-C5	-2.16	107.51	113.26
14	2	3033	CLA	O2D-CGD-CBD	2.16	115.00	111.23
16	a	848	BCR	C2-C1-C6	2.16	113.57	110.44
20	b	3050	LMG	C3-C4-C5	-2.16	106.32	110.23
14	b	3021	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	1	806	CLA	C3B-C4B-NB	-2.16	108.61	110.53
14	B	3028	CLA	CMB-C2B-C3B	2.16	131.62	126.55
14	b	3034	CLA	CMB-C2B-C3B	2.16	131.62	126.55
14	B	3003	CLA	CMD-C2D-C3D	2.16	132.63	127.69
14	B	3026	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
14	B	3032	CLA	CMB-C2B-C3B	2.15	131.62	126.55
16	F	202	BCR	C27-C26-C25	2.15	125.61	122.70
14	b	3003	CLA	CMD-C2D-C3D	2.15	132.63	127.69
14	a	836	CLA	CHB-C4A-NA	2.15	127.51	124.40
14	0	204	CLA	O1D-CGD-CBD	2.15	128.77	124.52
17	2	3051	LHG	C27-C26-C25	-2.15	103.48	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	805	CLA	C3B-C4B-NB	-2.15	108.61	110.53
14	2	3039	CLA	C5-C3-C2	2.15	126.00	121.17
14	2	3009	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
17	b	3051	LHG	C27-C26-C25	-2.15	103.49	114.37
14	b	3040	CLA	O2D-CGD-CBD	2.15	114.99	111.23
14	B	3031	CLA	CMB-C2B-C3B	2.15	131.61	126.55
14	a	809	CLA	C1-C2-C3	-2.15	122.67	126.20
14	1	810	CLA	C1-C2-C3	-2.15	122.67	126.20
14	A	839	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
14	b	3009	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
16	B	3047	BCR	C24-C23-C22	-2.15	123.05	126.23
14	b	3017	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
14	2	3010	CLA	C11-C12-C13	-2.15	108.82	115.97
17	B	3051	LHG	C27-C26-C25	-2.15	103.50	114.37
14	a	821	CLA	CHB-C1B-NB	2.15	127.27	124.05
20	2	3050	LMG	C3-C4-C5	-2.15	106.34	110.23
14	a	828	CLA	CHB-C4A-NA	2.15	127.50	124.40
14	B	3034	CLA	CMB-C2B-C3B	2.15	131.60	126.55
14	B	3039	CLA	C5-C3-C2	2.15	125.99	121.17
14	0	207	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
14	j	1101	CLA	O2D-CGD-CBD	2.15	114.98	111.23
14	1	804	CLA	O2D-CGD-CBD	2.15	114.98	111.23
14	2	3010	CLA	O2D-CGD-CBD	2.15	114.98	111.23
14	A	810	CLA	C1-C2-C3	-2.15	122.68	126.20
14	B	3021	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	2	3048	BCR	C33-C5-C6	-2.15	122.14	124.48
14	a	826	CLA	C1-C2-C3	-2.14	122.68	126.20
14	1	826	CLA	C1-C2-C3	-2.14	122.68	126.20
16	2	3052	BCR	C20-C21-C22	-2.14	124.27	127.28
14	a	837	CLA	C3B-C4B-NB	-2.14	108.62	110.53
16	f	202	BCR	C27-C26-C25	2.14	125.60	122.70
14	1	824	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	2	3046	BCR	C38-C26-C25	-2.14	122.15	124.48
14	A	824	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	2	3003	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	2	3016	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	a	841	CLA	CHB-C1B-NB	2.14	127.26	124.05
16	6	202	BCR	C27-C26-C25	2.14	125.60	122.70
16	L	206	BCR	C24-C23-C22	-2.14	123.07	126.23
16	A	846	BCR	C38-C26-C25	-2.14	122.15	124.48
14	2	3026	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	b	3039	CLA	C5-C3-C2	2.14	125.97	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	j	1106	BCR	C15-C14-C13	-2.14	124.28	127.28
14	b	3022	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
14	L	201	CLA	O1D-CGD-CBD	2.14	128.73	124.52
16	2	3049	BCR	C8-C7-C6	-2.14	121.29	127.00
14	B	3010	CLA	O2D-CGD-CBD	2.14	114.97	111.23
14	1	827	CLA	C1-C2-C3	-2.14	122.70	126.20
14	2	3034	CLA	CMB-C2B-C3B	2.14	131.58	126.55
14	1	839	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	A	837	CLA	CHB-C4A-NA	2.14	127.48	124.40
14	b	3010	CLA	C11-C12-C13	-2.13	108.87	115.97
16	B	3048	BCR	C33-C5-C6	-2.13	122.16	124.48
16	B	3053	BCR	C20-C21-C22	-2.13	124.29	127.28
16	B	3049	BCR	C8-C7-C6	-2.13	121.30	127.00
14	1	835	CLA	O2D-CGD-CBD	2.13	114.96	111.23
14	a	823	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
14	a	802	CLA	O1D-CGD-CBD	2.13	128.72	124.52
13	a	801	CL0	C3C-C4C-NC	-2.13	109.44	114.65
14	1	807	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
14	A	807	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
14	B	3010	CLA	C11-C12-C13	-2.13	108.88	115.97
14	A	804	CLA	O2D-CGD-CBD	2.13	114.95	111.23
14	A	808	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	A	801	CL0	C3C-C4C-NC	-2.13	109.45	114.65
14	b	3010	CLA	O2D-CGD-CBD	2.13	114.95	111.23
14	A	806	CLA	C3B-C4B-NB	-2.13	108.63	110.53
14	b	3032	CLA	CMB-C2B-C3B	2.13	131.56	126.55
16	0	211	BCR	C24-C23-C22	-2.13	123.09	126.23
16	a	848	BCR	C8-C7-C6	-2.13	121.31	127.00
14	1	816	CLA	C3A-C2A-C1A	2.13	104.53	101.34
14	2	3017	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
13	1	801	CL0	C3C-C4C-NC	-2.13	109.45	114.65
14	A	816	CLA	C3A-C2A-C1A	2.13	104.52	101.34
14	a	806	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
14	A	835	CLA	O2D-CGD-CBD	2.13	114.95	111.23
14	B	3016	CLA	CHB-C4A-NA	2.13	127.47	124.40
14	B	3008	CLA	CBC-CAC-C3C	-2.13	106.66	112.42
14	B	3007	CLA	O1D-CGD-CBD	2.13	128.71	124.52
16	a	847	BCR	C38-C26-C25	-2.13	122.17	124.48
14	b	3029	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
16	l	210	BCR	C24-C23-C22	-2.13	123.09	126.23
14	A	806	CLA	C1-O2A-CGA	2.12	121.79	116.65
16	A	849	BCR	C8-C7-C6	-2.12	121.32	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	806	CLA	O1D-CGD-CBD	2.12	128.71	124.52
16	j	1105	BCR	C2-C1-C6	2.12	113.52	110.44
14	1	806	CLA	C1-O2A-CGA	2.12	121.79	116.65
16	B	3053	BCR	C15-C14-C13	-2.12	124.30	127.28
16	l	204	BCR	C1-C6-C5	-2.12	119.74	122.64
14	2	3029	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
16	1	848	BCR	C8-C7-C6	-2.12	121.33	127.00
14	2	3040	CLA	O2D-CGD-CBD	2.12	114.94	111.23
16	a	845	BCR	C38-C26-C25	-2.12	122.17	124.48
14	A	838	CLA	C3B-C4B-NB	-2.12	108.64	110.53
14	2	3008	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
14	A	822	CLA	CHB-C1B-NB	2.12	127.23	124.05
14	a	834	CLA	O2D-CGD-CBD	2.12	114.93	111.23
16	B	3049	BCR	C37-C22-C23	2.12	121.32	118.09
16	A	848	BCR	C38-C26-C25	-2.12	122.17	124.48
14	B	3012	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
16	b	3048	BCR	C33-C5-C6	-2.12	122.17	124.48
16	2	3049	BCR	C37-C22-C23	2.12	121.32	118.09
14	2	3032	CLA	CMB-C2B-C3B	2.12	131.53	126.55
14	B	3040	CLA	O2D-CGD-CBD	2.12	114.93	111.23
16	b	3049	BCR	C37-C22-C23	2.12	121.32	118.09
16	b	3045	BCR	C8-C7-C6	-2.11	121.35	127.00
14	1	842	CLA	CHB-C1B-NB	2.11	127.22	124.05
16	9	102	BCR	C38-C26-C25	-2.11	122.18	124.48
14	b	3008	CLA	CBC-CAC-C3C	-2.11	106.69	112.42
14	a	816	CLA	C6-C5-C3	2.11	118.61	113.47
14	2	3012	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
14	A	829	CLA	CHB-C4A-NA	2.11	127.45	124.40
14	A	817	CLA	C6-C5-C3	2.11	118.61	113.47
14	a	838	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
14	b	3039	CLA	CHB-C4A-NA	2.11	127.44	124.40
16	0	205	BCR	C1-C6-C5	-2.11	119.75	122.64
14	b	3018	CLA	C5-C3-C2	-2.11	116.44	121.17
16	j	1104	BCR	C27-C26-C25	2.11	125.55	122.70
14	1	802	CLA	O1D-CGD-CBD	2.11	128.68	124.52
14	1	829	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	2	3045	BCR	C8-C7-C6	-2.11	121.37	127.00
14	l	203	CLA	C1-C2-C3	-2.11	122.75	126.20
14	1	808	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
14	2	3007	CLA	O1D-CGD-CBD	2.11	128.67	124.52
14	1	817	CLA	C6-C5-C3	2.11	118.60	113.47
16	b	3049	BCR	C8-C7-C6	-2.11	121.37	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3029	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	B	3052	BCR	C1-C6-C5	-2.11	119.76	122.64
14	B	3005	CLA	C3B-C4B-NB	-2.10	108.65	110.53
14	2	3011	CLA	C2A-C1A-CHA	2.10	127.52	123.87
14	A	842	CLA	CHB-C1B-NB	2.10	127.20	124.05
16	f	202	BCR	C38-C26-C25	-2.10	122.19	124.48
14	A	829	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	B	3045	BCR	C8-C7-C6	-2.10	121.38	127.00
14	a	807	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	J	103	BCR	C8-C7-C6	-2.10	121.38	127.00
14	B	3018	CLA	C5-C3-C2	-2.10	116.45	121.17
14	B	3034	CLA	CAA-CBA-CGA	-2.10	107.25	113.21
14	B	3012	CLA	C3B-C4B-NB	-2.10	108.66	110.53
14	2	3039	CLA	CHB-C4A-NA	2.10	127.43	124.40
14	A	809	CLA	CMB-C2B-C3B	2.10	131.49	126.55
17	A	853	LHG	C18-C17-C16	-2.10	103.76	114.37
14	b	3011	CLA	C2A-C1A-CHA	2.10	127.51	123.87
16	A	851	BCR	C38-C26-C25	-2.10	122.20	124.48
16	l	204	BCR	C15-C14-C13	-2.10	124.34	127.28
14	B	3020	CLA	C3B-C4B-NB	-2.10	108.66	110.53
14	a	808	CLA	CMB-C2B-C3B	2.10	131.48	126.55
16	j	1104	BCR	C8-C7-C6	-2.10	121.40	127.00
14	2	3022	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
16	f	205	BCR	C37-C22-C23	2.09	121.29	118.09
14	B	3022	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
14	A	806	CLA	O1D-CGD-CBD	2.09	128.65	124.52
17	1	852	LHG	C18-C17-C16	-2.09	103.79	114.37
16	8	103	BCR	C8-C7-C6	-2.09	121.41	127.00
14	a	828	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
14	2	3016	CLA	C1-C2-C3	-2.09	122.77	126.20
14	A	830	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
14	b	3012	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
14	f	204	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
14	2	3034	CLA	CAA-CBA-CGA	-2.09	107.28	113.21
16	a	850	BCR	C38-C26-C25	-2.09	122.20	124.48
14	a	820	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
14	A	821	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
14	0	204	CLA	C1-C2-C3	-2.09	122.78	126.20
14	a	829	CLA	O1D-CGD-CBD	2.09	128.64	124.52
16	B	3049	BCR	C7-C8-C9	-2.09	123.15	126.23
14	b	3034	CLA	CAA-CBA-CGA	-2.09	107.28	113.21
14	2	3030	CLA	C3B-C4B-NB	-2.09	108.67	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	837	CLA	O1D-CGD-CBD	2.09	128.63	124.52
16	1	847	BCR	C38-C26-C25	-2.09	122.21	124.48
14	1	830	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
14	2	3018	CLA	C5-C3-C2	-2.09	116.49	121.17
14	A	838	CLA	O1D-CGD-CBD	2.08	128.63	124.52
16	8	104	BCR	C2-C1-C6	2.08	113.47	110.44
16	B	3053	BCR	C37-C22-C21	-2.08	119.44	122.82
16	f	205	BCR	C20-C21-C22	-2.08	124.36	127.28
16	0	205	BCR	C15-C14-C13	-2.08	124.36	127.28
16	2	3049	BCR	C7-C8-C9	-2.08	123.15	126.23
14	9	103	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
14	1	809	CLA	CMB-C2B-C3B	2.08	131.45	126.55
14	b	3012	CLA	C3B-C4B-NB	-2.08	108.67	110.53
14	a	811	CLA	O1D-CGD-CBD	2.08	128.63	124.52
14	2	3005	CLA	C3B-C4B-NB	-2.08	108.67	110.53
17	a	852	LHG	C18-C17-C16	-2.08	103.84	114.37
14	b	3007	CLA	O1D-CGD-CBD	2.08	128.62	124.52
16	B	3052	BCR	C15-C14-C13	-2.08	124.36	127.28
17	l	201	LHG	C11-C10-C9	-2.08	103.85	114.37
16	a	845	BCR	C16-C15-C14	-2.08	119.26	123.52
14	A	802	CLA	O1D-CGD-CBD	2.08	128.62	124.52
16	A	846	BCR	C16-C15-C14	-2.08	119.26	123.52
14	1	812	CLA	O1D-CGD-CBD	2.08	128.62	124.52
16	1	850	BCR	C38-C26-C25	-2.08	122.22	124.48
16	a	850	BCR	C24-C23-C22	-2.08	123.16	126.23
14	B	3039	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	1	830	CLA	O1D-CGD-CBD	2.08	128.62	124.52
16	6	202	BCR	C38-C26-C25	-2.08	122.22	124.48
14	f	201	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
14	a	829	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	1	838	CLA	O1D-CGD-CBD	2.08	128.61	124.52
14	B	3039	CLA	CHB-C4A-NA	2.08	127.40	124.40
17	0	201	LHG	C11-C10-C9	-2.08	103.88	114.37
14	2	3026	CLA	CHD-C1D-ND	-2.08	121.88	124.80
16	1	850	BCR	C24-C23-C22	-2.08	123.17	126.23
14	1	821	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
14	b	3015	CLA	C3B-C4B-NB	-2.07	108.68	110.53
14	A	830	CLA	O1D-CGD-CBD	2.07	128.61	124.52
14	2	3020	CLA	C3B-C4B-NB	-2.07	108.68	110.53
14	a	825	CLA	CMB-C2B-C3B	2.07	131.43	126.55
14	1	826	CLA	CMB-C2B-C3B	2.07	131.43	126.55
17	L	207	LHG	C11-C10-C9	-2.07	103.89	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	3049	BCR	C7-C8-C9	-2.07	123.17	126.23
14	2	3037	CLA	CHB-C4A-NA	2.07	127.39	124.40
16	A	848	BCR	C36-C18-C17	-2.07	119.46	122.82
16	f	202	BCR	C29-C30-C25	2.07	113.45	110.44
16	9	102	BCR	C16-C15-C14	-2.07	119.28	123.52
16	F	205	BCR	C37-C22-C23	2.07	121.25	118.09
16	A	851	BCR	C24-C23-C22	-2.07	123.17	126.23
14	B	3020	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
16	J	104	BCR	C16-C15-C14	-2.07	119.28	123.52
14	L	201	CLA	C1-C2-C3	-2.07	122.81	126.20
16	6	205	BCR	C20-C21-C22	-2.07	124.38	127.28
16	j	1106	BCR	C37-C22-C21	-2.07	119.46	122.82
14	A	826	CLA	CMB-C2B-C3B	2.07	131.42	126.55
14	k	102	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
14	b	3020	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	1	847	BCR	C36-C18-C17	-2.07	119.47	122.82
14	b	3027	CLA	CMB-C2B-C3B	2.07	131.41	126.55
20	b	3050	LMG	O1-C1-C2	-2.07	105.14	108.27
14	B	3016	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	A	812	CLA	O1D-CGD-CBD	2.06	128.59	124.52
16	M	1602	BCR	C7-C8-C9	-2.06	123.18	126.23
14	a	805	CLA	O1D-CGD-CBD	2.06	128.59	124.52
14	2	3032	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
14	b	3032	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
14	f	201	CLA	CHB-C1B-NB	2.06	127.14	124.05
14	6	201	CLA	CHB-C1B-NB	2.06	127.14	124.05
16	a	845	BCR	C16-C17-C18	-2.06	124.39	127.28
14	B	3027	CLA	CMB-C2B-C3B	2.06	131.40	126.55
14	b	3026	CLA	CHD-C1D-ND	-2.06	121.90	124.80
14	B	3011	CLA	C2A-C1A-CHA	2.06	127.44	123.87
14	B	3032	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
14	K	102	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
16	8	103	BCR	C27-C26-C25	2.06	125.49	122.70
16	j	1105	BCR	C16-C15-C14	-2.06	119.30	123.52
16	B	3047	BCR	C16-C17-C18	-2.06	124.39	127.28
14	8	101	CLA	O1D-CGD-CBD	2.06	128.58	124.52
14	b	3016	CLA	C1-C2-C3	-2.06	122.82	126.20
16	J	104	BCR	C2-C1-C6	2.06	113.43	110.44
16	6	205	BCR	C37-C22-C23	2.06	121.23	118.09
16	2	3047	BCR	C16-C17-C18	-2.06	124.39	127.28
14	2	3015	CLA	C3B-C4B-NB	-2.06	108.69	110.53
14	b	3005	CLA	C3B-C4B-NB	-2.05	108.70	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	3050	LMG	O1-C1-C2	-2.05	105.15	108.27
14	B	3037	CLA	CHB-C4A-NA	2.05	127.36	124.40
16	a	845	BCR	C8-C7-C6	-2.05	121.51	127.00
14	L	203	CLA	CHB-C1B-NB	2.05	127.13	124.05
14	2	3020	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
14	b	3020	CLA	C3B-C4B-NB	-2.05	108.70	110.53
16	F	202	BCR	C29-C30-C25	2.05	113.42	110.44
16	2	3052	BCR	C37-C22-C21	-2.05	119.49	122.82
14	2	3039	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
14	6	201	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
16	j	1105	BCR	C28-C27-C26	-2.05	110.40	114.06
14	B	3012	CLA	C1-C2-C3	-2.05	122.84	126.20
14	A	810	CLA	CMB-C2B-C3B	2.05	131.37	126.55
14	b	3030	CLA	C3B-C4B-NB	-2.05	108.70	110.53
16	y	101	BCR	C7-C8-C9	-2.05	123.20	126.23
16	6	202	BCR	C29-C30-C25	2.05	113.41	110.44
14	b	3039	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
16	9	102	BCR	C16-C17-C18	-2.05	124.41	127.28
14	B	3030	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
14	6	204	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
14	A	828	CLA	O1D-CGD-CBD	2.05	128.56	124.52
16	8	104	BCR	C28-C27-C26	-2.05	110.41	114.06
14	b	3016	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
13	A	801	CL0	C4D-ND-C1D	2.05	106.77	105.22
14	2	3016	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
16	F	205	BCR	C20-C21-C22	-2.05	124.41	127.28
14	b	3037	CLA	CHB-C4A-NA	2.05	127.35	124.40
16	J	104	BCR	C28-C27-C26	-2.04	110.41	114.06
14	2	3030	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
16	8	104	BCR	C16-C15-C14	-2.04	119.34	123.52
14	b	3007	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	B	3026	CLA	CHD-C1D-ND	-2.04	121.93	124.80
14	2	3012	CLA	C3B-C4B-NB	-2.04	108.71	110.53
14	j	1102	CLA	O1D-CGD-CBD	2.04	128.55	124.52
14	B	3031	CLA	CHB-C4A-NA	2.04	127.35	124.40
14	2	3005	CLA	C6-C7-C8	-2.04	109.17	115.97
14	a	809	CLA	CMB-C2B-C3B	2.04	131.35	126.55
14	f	204	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	b	3005	CLA	C6-C7-C8	-2.04	109.18	115.97
14	F	204	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
14	b	3031	CLA	CHB-C4A-NA	2.04	127.35	124.40
14	J	101	CLA	O1D-CGD-CBD	2.04	128.54	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	834	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	2	3027	CLA	CMB-C2B-C3B	2.04	131.35	126.55
14	1	810	CLA	CMB-C2B-C3B	2.04	131.35	126.55
14	B	3016	CLA	C1-C2-C3	-2.04	122.86	126.20
20	B	3050	LMG	O1-C1-C2	-2.04	105.18	108.27
14	F	204	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	2	3007	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	L	203	CLA	C1-C2-C3	-2.04	122.86	126.20
16	a	846	BCR	C15-C14-C13	-2.04	124.42	127.28
14	6	204	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
14	1	826	CLA	O1D-CGD-CBD	2.04	128.54	124.52
16	A	846	BCR	C28-C27-C26	-2.04	110.42	114.06
14	1	827	CLA	CHD-C1D-ND	-2.04	121.94	124.80
14	B	3030	CLA	C3B-C4B-NB	-2.04	108.71	110.53
14	1	834	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
14	2	3025	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
16	m	101	BCR	C7-C8-C9	-2.03	123.23	126.23
14	B	3005	CLA	C6-C7-C8	-2.03	109.21	115.97
14	1	824	CLA	C3B-C4B-NB	-2.03	108.72	110.53
14	A	826	CLA	O1D-CGD-CBD	2.03	128.53	124.52
14	B	3007	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
14	B	3017	CLA	C11-C10-C8	-2.03	109.21	115.97
14	2	3015	CLA	CMB-C2B-C3B	2.03	131.33	126.55
16	a	845	BCR	C28-C27-C26	-2.03	110.43	114.06
14	2	3031	CLA	CHB-C4A-NA	2.03	127.33	124.40
14	b	3017	CLA	C11-C10-C8	-2.03	109.21	115.97
14	a	827	CLA	O1D-CGD-CBD	2.03	128.52	124.52
20	b	3050	LMG	C22-C21-C20	-2.03	104.10	114.37
14	0	207	CLA	CHB-C1B-NB	2.03	127.09	124.05
14	b	3028	CLA	CBA-CAA-C2A	2.03	119.83	113.79
14	A	842	CLA	O2D-CGD-CBD	2.03	114.78	111.23
16	a	847	BCR	C36-C18-C17	-2.03	119.53	122.82
16	A	846	BCR	C8-C7-C6	-2.03	121.58	127.00
17	b	3051	LHG	C11-C10-C9	-2.03	104.12	114.37
14	a	833	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
16	A	846	BCR	C16-C17-C18	-2.03	124.44	127.28
14	2	3017	CLA	C11-C10-C8	-2.03	109.23	115.97
14	b	3010	CLA	C11-C10-C8	-2.03	109.23	115.97
14	1	825	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
14	l	206	CLA	CHB-C1B-NB	2.03	127.09	124.05
14	b	3015	CLA	CMB-C2B-C3B	2.02	131.31	126.55
14	A	827	CLA	CHD-C1D-ND	-2.02	121.95	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	3050	LMG	C22-C21-C20	-2.02	104.14	114.37
14	1	831	CLA	O2D-CGD-CBD	2.02	114.77	111.23
14	B	3028	CLA	CBA-CAA-C2A	2.02	119.81	113.79
14	A	825	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
14	A	815	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
14	B	3007	CLA	CMB-C2B-C3B	2.02	131.30	126.55
14	2	3028	CLA	CBA-CAA-C2A	2.02	119.81	113.79
14	b	3031	CLA	CHB-C1B-NB	2.02	127.08	124.05
17	B	3051	LHG	C11-C10-C9	-2.02	104.16	114.37
14	F	201	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
14	B	3010	CLA	C11-C10-C8	-2.02	109.25	115.97
16	a	845	BCR	C7-C8-C9	-2.02	123.25	126.23
14	2	3030	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
14	a	814	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
14	1	828	CLA	O1D-CGD-CBD	2.02	128.50	124.52
14	0	207	CLA	C1-C2-C3	-2.02	122.89	126.20
20	B	3050	LMG	C22-C21-C20	-2.02	104.17	114.37
14	j	1103	CLA	CMB-C2B-C3B	2.02	131.29	126.55
14	a	824	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
14	B	3026	CLA	CED-O2D-CGD	-2.02	111.34	115.92
17	2	3051	LHG	C11-C10-C9	-2.02	104.17	114.37
17	l	202	LHG	C20-C19-C18	-2.02	104.18	114.37
16	J	103	BCR	C27-C26-C25	2.02	125.43	122.70
14	B	3015	CLA	CMB-C2B-C3B	2.01	131.29	126.55
14	b	3007	CLA	CMB-C2B-C3B	2.01	131.29	126.55
16	J	104	BCR	C8-C7-C6	-2.01	121.62	127.00
14	F	201	CLA	CHB-C1B-NB	2.01	127.07	124.05
16	7	101	BCR	C36-C18-C19	2.01	121.17	118.09
14	2	3010	CLA	C11-C10-C8	-2.01	109.27	115.97
17	0	202	LHG	C20-C19-C18	-2.01	104.19	114.37
13	1	801	CL0	C4D-ND-C1D	2.01	106.75	105.22
14	l	206	CLA	C1-C2-C3	-2.01	122.90	126.20
14	b	3026	CLA	CED-O2D-CGD	-2.01	111.35	115.92
17	L	208	LHG	C20-C19-C18	-2.01	104.19	114.37
14	b	3012	CLA	C1-C2-C3	-2.01	122.90	126.20
14	b	3030	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	1	849	BCR	C21-C20-C19	-2.01	117.37	123.20
16	i	101	BCR	C36-C18-C19	2.01	121.16	118.09
14	A	824	CLA	C3B-C4B-NB	-2.01	108.73	110.53
14	a	830	CLA	O2D-CGD-CBD	2.01	114.75	111.23
14	a	825	CLA	O1D-CGD-CBD	2.01	128.48	124.52
14	a	832	CLA	O1D-CGD-CBD	2.01	128.48	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	9	102	BCR	C8-C7-C6	-2.01	121.63	127.00
14	2	3007	CLA	CMB-C2B-C3B	2.01	131.28	126.55
14	2	3014	CLA	CMB-C2B-C3B	2.01	131.28	126.55
14	B	3036	CLA	CHB-C1B-NB	2.01	127.06	124.05
14	b	3033	CLA	CHB-C1B-NB	2.01	127.06	124.05
16	9	102	BCR	C28-C27-C26	-2.01	110.47	114.06
14	b	3014	CLA	CMB-C2B-C3B	2.01	131.28	126.55
16	1	846	BCR	C15-C14-C13	-2.01	124.46	127.28
14	a	812	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
16	b	3047	BCR	C16-C17-C18	-2.01	124.46	127.28
16	a	849	BCR	C21-C20-C19	-2.01	117.38	123.20
14	B	3015	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
14	b	3025	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
14	1	842	CLA	O2D-CGD-CBD	2.01	114.74	111.23
14	B	3025	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
13	a	801	CL0	C4D-ND-C1D	2.01	106.74	105.22
16	k	103	BCR	C16-C15-C14	-2.01	119.41	123.52
14	B	3014	CLA	CMB-C2B-C3B	2.01	131.27	126.55
14	J	102	CLA	CMB-C2B-C3B	2.01	131.27	126.55
16	j	1105	BCR	C8-C7-C6	-2.00	121.64	127.00
16	2	3047	BCR	C7-C8-C9	-2.00	123.27	126.23
14	b	3015	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
14	1	815	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
14	k	101	CLA	O1D-CGD-CBD	2.00	128.47	124.52
14	a	828	CLA	O1D-CGD-CBD	2.00	128.47	124.52
14	B	3031	CLA	CHB-C1B-NB	2.00	127.05	124.05
14	2	3036	CLA	CHB-C1B-NB	2.00	127.05	124.05
16	A	850	BCR	C21-C20-C19	-2.00	117.40	123.20
16	l	204	BCR	C2-C1-C6	2.00	113.35	110.44
14	2	3026	CLA	CED-O2D-CGD	-2.00	111.37	115.92
14	A	839	CLA	C1-C2-C3	-2.00	122.92	126.20
14	B	3021	CLA	C7-C6-C5	-2.00	107.93	113.26
14	A	833	CLA	O1D-CGD-CBD	2.00	128.47	124.52
14	B	3005	CLA	C3A-C2A-C1A	2.00	104.33	101.34

All (285) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NC
13	A	801	CL0	NA
13	A	801	CL0	ND
13	a	801	CL0	NC

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Mol	Chain	Res	Type	Atom
13	a	801	CL0	NA
13	a	801	CL0	ND
13	1	801	CL0	NC
13	1	801	CL0	NA
13	1	801	CL0	ND
14	A	802	CLA	ND
14	A	803	CLA	ND
14	A	804	CLA	ND
14	A	805	CLA	ND
14	A	806	CLA	ND
14	A	807	CLA	ND
14	A	808	CLA	ND
14	A	809	CLA	ND
14	A	810	CLA	ND
14	A	811	CLA	ND
14	A	812	CLA	ND
14	A	813	CLA	ND
14	A	814	CLA	ND
14	A	815	CLA	ND
14	A	816	CLA	ND
14	A	817	CLA	ND
14	A	818	CLA	ND
14	A	819	CLA	ND
14	A	820	CLA	ND
14	A	821	CLA	ND
14	A	822	CLA	ND
14	A	823	CLA	ND
14	A	824	CLA	ND
14	A	825	CLA	ND
14	A	826	CLA	ND
14	A	827	CLA	ND
14	A	828	CLA	ND
14	A	829	CLA	ND
14	A	830	CLA	ND
14	A	831	CLA	ND
14	A	832	CLA	ND
14	A	833	CLA	ND
14	A	834	CLA	ND
14	A	835	CLA	ND
14	A	836	CLA	ND
14	A	837	CLA	ND
14	A	838	CLA	ND

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Mol	Chain	Res	Type	Atom
14	A	839	CLA	ND
14	A	840	CLA	ND
14	A	841	CLA	ND
14	A	842	CLA	ND
14	A	843	CLA	ND
14	A	844	CLA	ND
14	A	855	CLA	ND
14	B	3003	CLA	ND
14	B	3004	CLA	ND
14	B	3005	CLA	ND
14	B	3006	CLA	ND
14	B	3007	CLA	ND
14	B	3008	CLA	ND
14	B	3009	CLA	ND
14	B	3010	CLA	ND
14	B	3011	CLA	ND
14	B	3012	CLA	ND
14	B	3014	CLA	ND
14	B	3015	CLA	ND
14	B	3016	CLA	ND
14	B	3017	CLA	ND
14	B	3019	CLA	ND
14	B	3020	CLA	ND
14	B	3021	CLA	ND
14	B	3022	CLA	ND
14	B	3023	CLA	ND
14	B	3025	CLA	ND
14	B	3026	CLA	ND
14	B	3027	CLA	ND
14	B	3028	CLA	ND
14	B	3029	CLA	ND
14	B	3030	CLA	ND
14	B	3031	CLA	ND
14	B	3032	CLA	ND
14	B	3033	CLA	ND
14	B	3034	CLA	ND
14	B	3035	CLA	ND
14	B	3036	CLA	ND
14	B	3037	CLA	ND
14	B	3038	CLA	ND
14	B	3039	CLA	ND
14	B	3041	CLA	ND

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Mol	Chain	Res	Type	Atom
14	B	3042	CLA	ND
14	F	201	CLA	ND
14	F	203	CLA	ND
14	F	204	CLA	ND
14	J	101	CLA	ND
14	J	102	CLA	ND
14	K	101	CLA	ND
14	K	102	CLA	ND
14	L	201	CLA	ND
14	L	203	CLA	ND
14	L	204	CLA	ND
14	L	205	CLA	ND
14	M	1601	CLA	ND
14	X	1701	CLA	ND
14	a	802	CLA	ND
14	a	803	CLA	ND
14	a	804	CLA	ND
14	a	805	CLA	ND
14	a	806	CLA	ND
14	a	807	CLA	ND
14	a	808	CLA	ND
14	a	809	CLA	ND
14	a	810	CLA	ND
14	a	811	CLA	ND
14	a	812	CLA	ND
14	a	813	CLA	ND
14	a	814	CLA	ND
14	a	815	CLA	ND
14	a	816	CLA	ND
14	a	817	CLA	ND
14	a	818	CLA	ND
14	a	819	CLA	ND
14	a	820	CLA	ND
14	a	821	CLA	ND
14	a	822	CLA	ND
14	a	823	CLA	ND
14	a	824	CLA	ND
14	a	825	CLA	ND
14	a	826	CLA	ND
14	a	827	CLA	ND
14	a	828	CLA	ND
14	a	829	CLA	ND

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Mol	Chain	Res	Type	Atom
14	a	830	CLA	ND
14	a	831	CLA	ND
14	a	832	CLA	ND
14	a	833	CLA	ND
14	a	834	CLA	ND
14	a	835	CLA	ND
14	a	836	CLA	ND
14	a	837	CLA	ND
14	a	838	CLA	ND
14	a	839	CLA	ND
14	a	840	CLA	ND
14	a	841	CLA	ND
14	a	842	CLA	ND
14	a	843	CLA	ND
14	b	3003	CLA	ND
14	b	3004	CLA	ND
14	b	3005	CLA	ND
14	b	3006	CLA	ND
14	b	3007	CLA	ND
14	b	3008	CLA	ND
14	b	3009	CLA	ND
14	b	3010	CLA	ND
14	b	3011	CLA	ND
14	b	3012	CLA	ND
14	b	3014	CLA	ND
14	b	3015	CLA	ND
14	b	3016	CLA	ND
14	b	3017	CLA	ND
14	b	3019	CLA	ND
14	b	3020	CLA	ND
14	b	3021	CLA	ND
14	b	3022	CLA	ND
14	b	3023	CLA	ND
14	b	3025	CLA	ND
14	b	3026	CLA	ND
14	b	3027	CLA	ND
14	b	3028	CLA	ND
14	b	3029	CLA	ND
14	b	3030	CLA	ND
14	b	3031	CLA	ND
14	b	3032	CLA	ND
14	b	3033	CLA	ND

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Mol	Chain	Res	Type	Atom
14	b	3034	CLA	ND
14	b	3035	CLA	ND
14	b	3036	CLA	ND
14	b	3037	CLA	ND
14	b	3038	CLA	ND
14	b	3039	CLA	ND
14	b	3041	CLA	ND
14	b	3042	CLA	ND
14	f	201	CLA	ND
14	f	203	CLA	ND
14	f	204	CLA	ND
14	j	1101	CLA	ND
14	j	1102	CLA	ND
14	j	1103	CLA	ND
14	k	101	CLA	ND
14	k	102	CLA	ND
14	l	203	CLA	ND
14	l	206	CLA	ND
14	l	207	CLA	ND
14	l	208	CLA	ND
14	x	1701	CLA	ND
14	1	802	CLA	ND
14	1	803	CLA	ND
14	1	804	CLA	ND
14	1	805	CLA	ND
14	1	806	CLA	ND
14	1	807	CLA	ND
14	1	808	CLA	ND
14	1	809	CLA	ND
14	1	810	CLA	ND
14	1	811	CLA	ND
14	1	812	CLA	ND
14	1	813	CLA	ND
14	1	814	CLA	ND
14	1	815	CLA	ND
14	1	816	CLA	ND
14	1	817	CLA	ND
14	1	818	CLA	ND
14	1	819	CLA	ND
14	1	820	CLA	ND
14	1	821	CLA	ND
14	1	822	CLA	ND

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Mol	Chain	Res	Type	Atom
14	1	823	CLA	ND
14	1	824	CLA	ND
14	1	825	CLA	ND
14	1	826	CLA	ND
14	1	827	CLA	ND
14	1	828	CLA	ND
14	1	829	CLA	ND
14	1	830	CLA	ND
14	1	831	CLA	ND
14	1	832	CLA	ND
14	1	833	CLA	ND
14	1	834	CLA	ND
14	1	835	CLA	ND
14	1	836	CLA	ND
14	1	837	CLA	ND
14	1	838	CLA	ND
14	1	839	CLA	ND
14	1	840	CLA	ND
14	1	841	CLA	ND
14	1	842	CLA	ND
14	1	843	CLA	ND
14	1	844	CLA	ND
14	2	3003	CLA	ND
14	2	3004	CLA	ND
14	2	3005	CLA	ND
14	2	3006	CLA	ND
14	2	3007	CLA	ND
14	2	3008	CLA	ND
14	2	3009	CLA	ND
14	2	3010	CLA	ND
14	2	3011	CLA	ND
14	2	3012	CLA	ND
14	2	3014	CLA	ND
14	2	3015	CLA	ND
14	2	3016	CLA	ND
14	2	3017	CLA	ND
14	2	3019	CLA	ND
14	2	3020	CLA	ND
14	2	3021	CLA	ND
14	2	3022	CLA	ND
14	2	3023	CLA	ND
14	2	3025	CLA	ND

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Mol	Chain	Res	Type	Atom
14	2	3026	CLA	ND
14	2	3027	CLA	ND
14	2	3028	CLA	ND
14	2	3029	CLA	ND
14	2	3030	CLA	ND
14	2	3031	CLA	ND
14	2	3032	CLA	ND
14	2	3033	CLA	ND
14	2	3034	CLA	ND
14	2	3035	CLA	ND
14	2	3036	CLA	ND
14	2	3037	CLA	ND
14	2	3038	CLA	ND
14	2	3039	CLA	ND
14	2	3041	CLA	ND
14	2	3042	CLA	ND
14	6	201	CLA	ND
14	6	203	CLA	ND
14	6	204	CLA	ND
14	8	101	CLA	ND
14	8	102	CLA	ND
14	9	101	CLA	ND
14	9	103	CLA	ND
14	0	203	CLA	ND
14	0	204	CLA	ND
14	0	207	CLA	ND
14	0	208	CLA	ND
14	0	209	CLA	ND
14	z	1701	CLA	ND

All (4318) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	CLA	C14-C13-C15-C16
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA
14	A	805	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	806	CLA	CAD-CBD-CGD-O1D
14	A	806	CLA	CAD-CBD-CGD-O2D
14	A	806	CLA	C6-C7-C8-C9
14	A	807	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C3A-C2A-CAA-CBA
14	A	809	CLA	CHA-CBD-CGD-O1D
14	A	809	CLA	CHA-CBD-CGD-O2D
14	A	810	CLA	CBD-CGD-O2D-CED
14	A	812	CLA	CBD-CGD-O2D-CED
14	A	814	CLA	CAD-CBD-CGD-O1D
14	A	814	CLA	CAD-CBD-CGD-O2D
14	A	815	CLA	CBD-CGD-O2D-CED
14	A	816	CLA	CAD-CBD-CGD-O1D
14	A	816	CLA	CAD-CBD-CGD-O2D
14	A	817	CLA	C1A-C2A-CAA-CBA
14	A	817	CLA	C3A-C2A-CAA-CBA
14	A	817	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C3A-C2A-CAA-CBA
14	A	820	CLA	CHA-CBD-CGD-O1D
14	A	820	CLA	CHA-CBD-CGD-O2D
14	A	821	CLA	C1A-C2A-CAA-CBA
14	A	821	CLA	C3A-C2A-CAA-CBA
14	A	824	CLA	C3A-C2A-CAA-CBA
14	A	826	CLA	CHA-CBD-CGD-O1D
14	A	826	CLA	CHA-CBD-CGD-O2D
14	A	829	CLA	O2A-C1-C2-C3
14	A	831	CLA	CHA-CBD-CGD-O1D
14	A	831	CLA	CHA-CBD-CGD-O2D
14	A	834	CLA	C2B-C3B-CAB-CBB
14	A	834	CLA	C4B-C3B-CAB-CBB
14	A	835	CLA	CHA-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O2D
14	A	839	CLA	CAD-CBD-CGD-O1D
14	A	839	CLA	CAD-CBD-CGD-O2D
14	B	3003	CLA	CAD-CBD-CGD-O1D
14	B	3003	CLA	CAD-CBD-CGD-O2D
14	B	3005	CLA	C4C-C3C-CAC-CBC
14	B	3005	CLA	CBD-CGD-O2D-CED
14	B	3006	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	B	3007	CLA	C3A-C2A-CAA-CBA
14	B	3007	CLA	CAD-CBD-CGD-O1D
14	B	3007	CLA	CAD-CBD-CGD-O2D
14	B	3010	CLA	CHA-CBD-CGD-O1D
14	B	3010	CLA	CHA-CBD-CGD-O2D
14	B	3011	CLA	C1A-C2A-CAA-CBA
14	B	3012	CLA	CAD-CBD-CGD-O1D
14	B	3012	CLA	CAD-CBD-CGD-O2D
14	B	3014	CLA	C1A-C2A-CAA-CBA
14	B	3014	CLA	C3A-C2A-CAA-CBA
14	B	3016	CLA	CHA-CBD-CGD-O2D
14	B	3016	CLA	C4-C3-C5-C6
14	B	3016	CLA	C11-C10-C8-C7
14	B	3017	CLA	C2C-C3C-CAC-CBC
14	B	3017	CLA	C4C-C3C-CAC-CBC
14	B	3018	CLA	C1A-C2A-CAA-CBA
14	B	3018	CLA	C3A-C2A-CAA-CBA
14	B	3018	CLA	C2B-C3B-CAB-CBB
14	B	3018	CLA	C4B-C3B-CAB-CBB
14	B	3019	CLA	C3A-C2A-CAA-CBA
14	B	3019	CLA	C4-C3-C5-C6
14	B	3020	CLA	C2B-C3B-CAB-CBB
14	B	3020	CLA	C4B-C3B-CAB-CBB
14	B	3020	CLA	CBD-CGD-O2D-CED
14	B	3021	CLA	C4B-C3B-CAB-CBB
14	B	3025	CLA	CHA-CBD-CGD-O2D
14	B	3028	CLA	C1A-C2A-CAA-CBA
14	B	3028	CLA	C3A-C2A-CAA-CBA
14	B	3031	CLA	C1A-C2A-CAA-CBA
14	B	3031	CLA	C3A-C2A-CAA-CBA
14	B	3033	CLA	CAD-CBD-CGD-O1D
14	B	3033	CLA	CAD-CBD-CGD-O2D
14	B	3034	CLA	CHA-CBD-CGD-O1D
14	B	3034	CLA	CHA-CBD-CGD-O2D
14	B	3035	CLA	CBD-CGD-O2D-CED
14	B	3036	CLA	CBD-CGD-O2D-CED
14	B	3037	CLA	C1A-C2A-CAA-CBA
14	B	3037	CLA	C3A-C2A-CAA-CBA
14	B	3038	CLA	CHA-CBD-CGD-O1D
14	B	3038	CLA	CHA-CBD-CGD-O2D
14	B	3042	CLA	C1A-C2A-CAA-CBA
14	B	3042	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	F	203	CLA	CBD-CGD-O2D-CED
14	F	204	CLA	CBD-CGD-O2D-CED
14	K	101	CLA	CAD-CBD-CGD-O1D
14	K	101	CLA	CAD-CBD-CGD-O2D
14	K	101	CLA	CBD-CGD-O2D-CED
14	K	102	CLA	CAD-CBD-CGD-O1D
14	K	102	CLA	CAD-CBD-CGD-O2D
14	L	203	CLA	C1A-C2A-CAA-CBA
14	L	203	CLA	C3A-C2A-CAA-CBA
14	X	1701	CLA	CBD-CGD-O2D-CED
14	a	802	CLA	C14-C13-C15-C16
14	a	804	CLA	C1A-C2A-CAA-CBA
14	a	804	CLA	C3A-C2A-CAA-CBA
14	a	804	CLA	CHA-CBD-CGD-O1D
14	a	804	CLA	CHA-CBD-CGD-O2D
14	a	805	CLA	C1A-C2A-CAA-CBA
14	a	805	CLA	C3A-C2A-CAA-CBA
14	a	805	CLA	CAD-CBD-CGD-O1D
14	a	805	CLA	CAD-CBD-CGD-O2D
14	a	806	CLA	C1A-C2A-CAA-CBA
14	a	808	CLA	C3A-C2A-CAA-CBA
14	a	808	CLA	CHA-CBD-CGD-O1D
14	a	808	CLA	CHA-CBD-CGD-O2D
14	a	809	CLA	CBD-CGD-O2D-CED
14	a	811	CLA	CBD-CGD-O2D-CED
14	a	813	CLA	CAD-CBD-CGD-O1D
14	a	813	CLA	CAD-CBD-CGD-O2D
14	a	814	CLA	CBD-CGD-O2D-CED
14	a	815	CLA	CAD-CBD-CGD-O1D
14	a	815	CLA	CAD-CBD-CGD-O2D
14	a	816	CLA	C1A-C2A-CAA-CBA
14	a	816	CLA	C3A-C2A-CAA-CBA
14	a	816	CLA	CBD-CGD-O2D-CED
14	a	819	CLA	C1A-C2A-CAA-CBA
14	a	819	CLA	C3A-C2A-CAA-CBA
14	a	819	CLA	CHA-CBD-CGD-O1D
14	a	819	CLA	CHA-CBD-CGD-O2D
14	a	820	CLA	C1A-C2A-CAA-CBA
14	a	820	CLA	C3A-C2A-CAA-CBA
14	a	823	CLA	C3A-C2A-CAA-CBA
14	a	825	CLA	CHA-CBD-CGD-O1D
14	a	825	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	a	828	CLA	O2A-C1-C2-C3
14	a	830	CLA	CHA-CBD-CGD-O1D
14	a	830	CLA	CHA-CBD-CGD-O2D
14	a	833	CLA	C2B-C3B-CAB-CBB
14	a	833	CLA	C4B-C3B-CAB-CBB
14	a	834	CLA	CHA-CBD-CGD-O1D
14	a	834	CLA	CHA-CBD-CGD-O2D
14	a	838	CLA	CAD-CBD-CGD-O1D
14	a	838	CLA	CAD-CBD-CGD-O2D
14	b	3003	CLA	CAD-CBD-CGD-O1D
14	b	3003	CLA	CAD-CBD-CGD-O2D
14	b	3005	CLA	C4C-C3C-CAC-CBC
14	b	3005	CLA	CBD-CGD-O2D-CED
14	b	3006	CLA	CHA-CBD-CGD-O2D
14	b	3007	CLA	C3A-C2A-CAA-CBA
14	b	3007	CLA	CAD-CBD-CGD-O1D
14	b	3007	CLA	CAD-CBD-CGD-O2D
14	b	3010	CLA	CHA-CBD-CGD-O1D
14	b	3010	CLA	CHA-CBD-CGD-O2D
14	b	3011	CLA	C1A-C2A-CAA-CBA
14	b	3012	CLA	CAD-CBD-CGD-O1D
14	b	3012	CLA	CAD-CBD-CGD-O2D
14	b	3014	CLA	C1A-C2A-CAA-CBA
14	b	3014	CLA	C3A-C2A-CAA-CBA
14	b	3016	CLA	CHA-CBD-CGD-O2D
14	b	3016	CLA	C4-C3-C5-C6
14	b	3016	CLA	C11-C10-C8-C7
14	b	3017	CLA	C2C-C3C-CAC-CBC
14	b	3017	CLA	C4C-C3C-CAC-CBC
14	b	3018	CLA	C1A-C2A-CAA-CBA
14	b	3018	CLA	C3A-C2A-CAA-CBA
14	b	3018	CLA	C2B-C3B-CAB-CBB
14	b	3018	CLA	C4B-C3B-CAB-CBB
14	b	3019	CLA	C3A-C2A-CAA-CBA
14	b	3019	CLA	C4-C3-C5-C6
14	b	3020	CLA	C2B-C3B-CAB-CBB
14	b	3020	CLA	C4B-C3B-CAB-CBB
14	b	3020	CLA	CBD-CGD-O2D-CED
14	b	3021	CLA	C4B-C3B-CAB-CBB
14	b	3025	CLA	CHA-CBD-CGD-O2D
14	b	3028	CLA	C1A-C2A-CAA-CBA
14	b	3028	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	3031	CLA	C1A-C2A-CAA-CBA
14	b	3031	CLA	C3A-C2A-CAA-CBA
14	b	3033	CLA	CAD-CBD-CGD-O1D
14	b	3033	CLA	CAD-CBD-CGD-O2D
14	b	3034	CLA	CHA-CBD-CGD-O1D
14	b	3034	CLA	CHA-CBD-CGD-O2D
14	b	3035	CLA	CBD-CGD-O2D-CED
14	b	3036	CLA	CBD-CGD-O2D-CED
14	b	3037	CLA	C1A-C2A-CAA-CBA
14	b	3037	CLA	C3A-C2A-CAA-CBA
14	b	3038	CLA	CHA-CBD-CGD-O1D
14	b	3038	CLA	CHA-CBD-CGD-O2D
14	b	3042	CLA	C1A-C2A-CAA-CBA
14	b	3042	CLA	C3A-C2A-CAA-CBA
14	f	203	CLA	CBD-CGD-O2D-CED
14	f	204	CLA	CBD-CGD-O2D-CED
14	j	1101	CLA	C1A-C2A-CAA-CBA
14	j	1101	CLA	C3A-C2A-CAA-CBA
14	j	1101	CLA	CHA-CBD-CGD-O1D
14	j	1101	CLA	CHA-CBD-CGD-O2D
14	k	101	CLA	CAD-CBD-CGD-O1D
14	k	101	CLA	CAD-CBD-CGD-O2D
14	k	101	CLA	CBD-CGD-O2D-CED
14	k	102	CLA	CAD-CBD-CGD-O1D
14	k	102	CLA	CAD-CBD-CGD-O2D
14	l	206	CLA	C1A-C2A-CAA-CBA
14	l	206	CLA	C3A-C2A-CAA-CBA
14	x	1701	CLA	CBD-CGD-O2D-CED
14	1	802	CLA	C14-C13-C15-C16
14	1	804	CLA	C1A-C2A-CAA-CBA
14	1	804	CLA	C3A-C2A-CAA-CBA
14	1	804	CLA	CHA-CBD-CGD-O1D
14	1	804	CLA	CHA-CBD-CGD-O2D
14	1	805	CLA	C1A-C2A-CAA-CBA
14	1	805	CLA	C3A-C2A-CAA-CBA
14	1	805	CLA	CHA-CBD-CGD-O1D
14	1	805	CLA	CHA-CBD-CGD-O2D
14	1	806	CLA	C1A-C2A-CAA-CBA
14	1	806	CLA	C3A-C2A-CAA-CBA
14	1	806	CLA	CAD-CBD-CGD-O1D
14	1	806	CLA	CAD-CBD-CGD-O2D
14	1	807	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	1	809	CLA	C3A-C2A-CAA-CBA
14	1	809	CLA	CHA-CBD-CGD-O1D
14	1	809	CLA	CHA-CBD-CGD-O2D
14	1	810	CLA	CBD-CGD-O2D-CED
14	1	812	CLA	CBD-CGD-O2D-CED
14	1	814	CLA	CAD-CBD-CGD-O1D
14	1	814	CLA	CAD-CBD-CGD-O2D
14	1	815	CLA	CBD-CGD-O2D-CED
14	1	816	CLA	CAD-CBD-CGD-O1D
14	1	816	CLA	CAD-CBD-CGD-O2D
14	1	817	CLA	C1A-C2A-CAA-CBA
14	1	817	CLA	C3A-C2A-CAA-CBA
14	1	817	CLA	CBD-CGD-O2D-CED
14	1	820	CLA	C1A-C2A-CAA-CBA
14	1	820	CLA	C3A-C2A-CAA-CBA
14	1	820	CLA	CHA-CBD-CGD-O1D
14	1	820	CLA	CHA-CBD-CGD-O2D
14	1	821	CLA	C1A-C2A-CAA-CBA
14	1	821	CLA	C3A-C2A-CAA-CBA
14	1	824	CLA	C3A-C2A-CAA-CBA
14	1	826	CLA	CHA-CBD-CGD-O1D
14	1	826	CLA	CHA-CBD-CGD-O2D
14	1	829	CLA	O2A-C1-C2-C3
14	1	831	CLA	CHA-CBD-CGD-O1D
14	1	831	CLA	CHA-CBD-CGD-O2D
14	1	834	CLA	C2B-C3B-CAB-CBB
14	1	834	CLA	C4B-C3B-CAB-CBB
14	1	835	CLA	CHA-CBD-CGD-O1D
14	1	835	CLA	CHA-CBD-CGD-O2D
14	1	839	CLA	CAD-CBD-CGD-O1D
14	1	839	CLA	CAD-CBD-CGD-O2D
14	2	3003	CLA	CAD-CBD-CGD-O1D
14	2	3003	CLA	CAD-CBD-CGD-O2D
14	2	3005	CLA	C4C-C3C-CAC-CBC
14	2	3005	CLA	CBD-CGD-O2D-CED
14	2	3006	CLA	CHA-CBD-CGD-O2D
14	2	3007	CLA	C3A-C2A-CAA-CBA
14	2	3007	CLA	CAD-CBD-CGD-O1D
14	2	3007	CLA	CAD-CBD-CGD-O2D
14	2	3010	CLA	CHA-CBD-CGD-O1D
14	2	3010	CLA	CHA-CBD-CGD-O2D
14	2	3011	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	2	3012	CLA	CAD-CBD-CGD-O1D
14	2	3012	CLA	CAD-CBD-CGD-O2D
14	2	3014	CLA	C1A-C2A-CAA-CBA
14	2	3014	CLA	C3A-C2A-CAA-CBA
14	2	3016	CLA	CHA-CBD-CGD-O2D
14	2	3016	CLA	C4-C3-C5-C6
14	2	3016	CLA	C11-C10-C8-C7
14	2	3017	CLA	C2C-C3C-CAC-CBC
14	2	3017	CLA	C4C-C3C-CAC-CBC
14	2	3018	CLA	C1A-C2A-CAA-CBA
14	2	3018	CLA	C3A-C2A-CAA-CBA
14	2	3018	CLA	C2B-C3B-CAB-CBB
14	2	3018	CLA	C4B-C3B-CAB-CBB
14	2	3019	CLA	C3A-C2A-CAA-CBA
14	2	3019	CLA	C4-C3-C5-C6
14	2	3020	CLA	C2B-C3B-CAB-CBB
14	2	3020	CLA	C4B-C3B-CAB-CBB
14	2	3020	CLA	CBD-CGD-O2D-CED
14	2	3021	CLA	C4B-C3B-CAB-CBB
14	2	3025	CLA	CHA-CBD-CGD-O2D
14	2	3028	CLA	C1A-C2A-CAA-CBA
14	2	3028	CLA	C3A-C2A-CAA-CBA
14	2	3031	CLA	C1A-C2A-CAA-CBA
14	2	3031	CLA	C3A-C2A-CAA-CBA
14	2	3033	CLA	CAD-CBD-CGD-O1D
14	2	3033	CLA	CAD-CBD-CGD-O2D
14	2	3034	CLA	CHA-CBD-CGD-O1D
14	2	3034	CLA	CHA-CBD-CGD-O2D
14	2	3035	CLA	CBD-CGD-O2D-CED
14	2	3036	CLA	CBD-CGD-O2D-CED
14	2	3037	CLA	C1A-C2A-CAA-CBA
14	2	3037	CLA	C3A-C2A-CAA-CBA
14	2	3038	CLA	CHA-CBD-CGD-O1D
14	2	3038	CLA	CHA-CBD-CGD-O2D
14	2	3042	CLA	C1A-C2A-CAA-CBA
14	2	3042	CLA	C3A-C2A-CAA-CBA
14	6	203	CLA	CBD-CGD-O2D-CED
14	6	204	CLA	CBD-CGD-O2D-CED
14	9	101	CLA	C1A-C2A-CAA-CBA
14	9	101	CLA	CAD-CBD-CGD-O1D
14	9	101	CLA	CAD-CBD-CGD-O2D
14	9	101	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	9	103	CLA	CAD-CBD-CGD-O1D
14	9	103	CLA	CAD-CBD-CGD-O2D
14	0	207	CLA	C1A-C2A-CAA-CBA
14	0	207	CLA	C3A-C2A-CAA-CBA
14	z	1701	CLA	CBD-CGD-O2D-CED
16	A	846	BCR	C7-C8-C9-C34
16	A	846	BCR	C9-C10-C11-C12
16	A	846	BCR	C10-C11-C12-C13
16	A	847	BCR	C7-C8-C9-C34
16	A	847	BCR	C11-C12-C13-C35
16	A	847	BCR	C16-C17-C18-C36
16	A	847	BCR	C17-C18-C19-C20
16	A	847	BCR	C22-C23-C24-C25
16	A	848	BCR	C6-C7-C8-C9
16	A	848	BCR	C11-C12-C13-C35
16	A	848	BCR	C14-C15-C16-C17
16	A	848	BCR	C16-C17-C18-C19
16	A	848	BCR	C16-C17-C18-C36
16	A	848	BCR	C20-C21-C22-C23
16	A	848	BCR	C20-C21-C22-C37
16	A	849	BCR	C20-C21-C22-C37
16	A	849	BCR	C23-C24-C25-C26
16	A	849	BCR	C23-C24-C25-C30
16	A	850	BCR	C37-C22-C23-C24
16	A	851	BCR	C7-C8-C9-C34
16	A	851	BCR	C11-C10-C9-C8
16	A	851	BCR	C35-C13-C14-C15
16	A	851	BCR	C16-C17-C18-C19
16	A	851	BCR	C18-C19-C20-C21
16	A	851	BCR	C20-C21-C22-C23
16	A	851	BCR	C20-C21-C22-C37
16	A	851	BCR	C37-C22-C23-C24
16	A	851	BCR	C22-C23-C24-C25
16	A	852	BCR	C5-C6-C7-C8
16	A	852	BCR	C7-C8-C9-C34
16	A	852	BCR	C10-C11-C12-C13
16	A	852	BCR	C11-C12-C13-C14
16	A	852	BCR	C16-C17-C18-C36
16	B	3044	BCR	C7-C8-C9-C10
16	B	3044	BCR	C17-C18-C19-C20
16	B	3044	BCR	C21-C22-C23-C24
16	B	3045	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	B	3045	BCR	C7-C8-C9-C10
16	B	3045	BCR	C7-C8-C9-C34
16	B	3045	BCR	C21-C22-C23-C24
16	B	3046	BCR	C17-C18-C19-C20
16	B	3046	BCR	C18-C19-C20-C21
16	B	3046	BCR	C20-C21-C22-C23
16	B	3046	BCR	C20-C21-C22-C37
16	B	3046	BCR	C37-C22-C23-C24
16	B	3046	BCR	C22-C23-C24-C25
16	B	3047	BCR	C11-C10-C9-C34
16	B	3047	BCR	C12-C13-C14-C15
16	B	3047	BCR	C35-C13-C14-C15
16	B	3048	BCR	C6-C7-C8-C9
16	B	3048	BCR	C10-C11-C12-C13
16	B	3048	BCR	C11-C12-C13-C14
16	B	3048	BCR	C11-C12-C13-C35
16	B	3052	BCR	C7-C8-C9-C34
16	B	3052	BCR	C20-C21-C22-C23
16	B	3052	BCR	C20-C21-C22-C37
16	B	3053	BCR	C16-C17-C18-C19
16	B	3053	BCR	C16-C17-C18-C36
16	B	3053	BCR	C18-C19-C20-C21
16	B	3053	BCR	C20-C21-C22-C23
16	B	3053	BCR	C20-C21-C22-C37
16	B	3053	BCR	C23-C24-C25-C26
16	F	202	BCR	C11-C12-C13-C35
16	F	202	BCR	C20-C21-C22-C37
16	F	202	BCR	C37-C22-C23-C24
16	F	205	BCR	C12-C13-C14-C15
16	I	102	BCR	C7-C8-C9-C10
16	I	102	BCR	C21-C22-C23-C24
16	I	102	BCR	C23-C24-C25-C26
16	I	102	BCR	C23-C24-C25-C30
16	J	103	BCR	C6-C7-C8-C9
16	J	103	BCR	C7-C8-C9-C10
16	J	103	BCR	C7-C8-C9-C34
16	J	104	BCR	C14-C15-C16-C17
16	J	104	BCR	C20-C21-C22-C23
16	J	104	BCR	C20-C21-C22-C37
16	L	206	BCR	C11-C12-C13-C14
16	L	206	BCR	C11-C12-C13-C35
16	M	1602	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
16	M	1602	BCR	C36-C18-C19-C20
16	M	1602	BCR	C20-C21-C22-C37
16	M	1602	BCR	C21-C22-C23-C24
16	M	1602	BCR	C22-C23-C24-C25
16	a	845	BCR	C7-C8-C9-C34
16	a	845	BCR	C9-C10-C11-C12
16	a	845	BCR	C10-C11-C12-C13
16	a	846	BCR	C7-C8-C9-C34
16	a	846	BCR	C11-C12-C13-C35
16	a	846	BCR	C16-C17-C18-C36
16	a	846	BCR	C17-C18-C19-C20
16	a	846	BCR	C22-C23-C24-C25
16	a	847	BCR	C6-C7-C8-C9
16	a	847	BCR	C11-C12-C13-C35
16	a	847	BCR	C14-C15-C16-C17
16	a	847	BCR	C16-C17-C18-C19
16	a	847	BCR	C16-C17-C18-C36
16	a	847	BCR	C20-C21-C22-C23
16	a	847	BCR	C20-C21-C22-C37
16	a	848	BCR	C20-C21-C22-C37
16	a	848	BCR	C23-C24-C25-C26
16	a	848	BCR	C23-C24-C25-C30
16	a	849	BCR	C37-C22-C23-C24
16	a	850	BCR	C7-C8-C9-C34
16	a	850	BCR	C11-C10-C9-C8
16	a	850	BCR	C35-C13-C14-C15
16	a	850	BCR	C16-C17-C18-C19
16	a	850	BCR	C18-C19-C20-C21
16	a	850	BCR	C20-C21-C22-C23
16	a	850	BCR	C20-C21-C22-C37
16	a	850	BCR	C37-C22-C23-C24
16	a	850	BCR	C22-C23-C24-C25
16	a	851	BCR	C5-C6-C7-C8
16	a	851	BCR	C7-C8-C9-C34
16	a	851	BCR	C10-C11-C12-C13
16	a	851	BCR	C11-C12-C13-C14
16	a	851	BCR	C16-C17-C18-C36
16	b	3044	BCR	C7-C8-C9-C10
16	b	3044	BCR	C17-C18-C19-C20
16	b	3044	BCR	C21-C22-C23-C24
16	b	3045	BCR	C6-C7-C8-C9
16	b	3045	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
16	b	3045	BCR	C7-C8-C9-C34
16	b	3045	BCR	C21-C22-C23-C24
16	b	3046	BCR	C17-C18-C19-C20
16	b	3046	BCR	C18-C19-C20-C21
16	b	3046	BCR	C20-C21-C22-C23
16	b	3046	BCR	C20-C21-C22-C37
16	b	3046	BCR	C37-C22-C23-C24
16	b	3046	BCR	C22-C23-C24-C25
16	b	3047	BCR	C11-C10-C9-C34
16	b	3047	BCR	C12-C13-C14-C15
16	b	3047	BCR	C35-C13-C14-C15
16	b	3048	BCR	C6-C7-C8-C9
16	b	3048	BCR	C10-C11-C12-C13
16	b	3048	BCR	C11-C12-C13-C14
16	b	3048	BCR	C11-C12-C13-C35
16	f	202	BCR	C11-C12-C13-C35
16	f	202	BCR	C20-C21-C22-C37
16	f	202	BCR	C37-C22-C23-C24
16	f	205	BCR	C12-C13-C14-C15
16	j	1104	BCR	C6-C7-C8-C9
16	j	1104	BCR	C7-C8-C9-C10
16	j	1104	BCR	C7-C8-C9-C34
16	j	1105	BCR	C14-C15-C16-C17
16	j	1105	BCR	C20-C21-C22-C23
16	j	1105	BCR	C20-C21-C22-C37
16	j	1106	BCR	C16-C17-C18-C19
16	j	1106	BCR	C16-C17-C18-C36
16	j	1106	BCR	C18-C19-C20-C21
16	j	1106	BCR	C20-C21-C22-C23
16	j	1106	BCR	C20-C21-C22-C37
16	j	1106	BCR	C23-C24-C25-C26
16	l	204	BCR	C7-C8-C9-C34
16	l	204	BCR	C20-C21-C22-C23
16	l	204	BCR	C20-C21-C22-C37
16	l	209	BCR	C7-C8-C9-C10
16	l	209	BCR	C21-C22-C23-C24
16	l	209	BCR	C23-C24-C25-C26
16	l	209	BCR	C23-C24-C25-C30
16	l	210	BCR	C11-C12-C13-C14
16	l	210	BCR	C11-C12-C13-C35
16	m	101	BCR	C35-C13-C14-C15
16	m	101	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
16	m	101	BCR	C20-C21-C22-C37
16	m	101	BCR	C21-C22-C23-C24
16	m	101	BCR	C22-C23-C24-C25
16	1	846	BCR	C7-C8-C9-C34
16	1	846	BCR	C11-C12-C13-C35
16	1	846	BCR	C16-C17-C18-C36
16	1	846	BCR	C17-C18-C19-C20
16	1	846	BCR	C22-C23-C24-C25
16	1	847	BCR	C6-C7-C8-C9
16	1	847	BCR	C11-C12-C13-C35
16	1	847	BCR	C14-C15-C16-C17
16	1	847	BCR	C16-C17-C18-C19
16	1	847	BCR	C16-C17-C18-C36
16	1	847	BCR	C20-C21-C22-C23
16	1	847	BCR	C20-C21-C22-C37
16	1	848	BCR	C20-C21-C22-C37
16	1	848	BCR	C23-C24-C25-C26
16	1	848	BCR	C23-C24-C25-C30
16	1	849	BCR	C37-C22-C23-C24
16	1	850	BCR	C7-C8-C9-C34
16	1	850	BCR	C11-C10-C9-C8
16	1	850	BCR	C35-C13-C14-C15
16	1	850	BCR	C16-C17-C18-C19
16	1	850	BCR	C18-C19-C20-C21
16	1	850	BCR	C20-C21-C22-C23
16	1	850	BCR	C20-C21-C22-C37
16	1	850	BCR	C37-C22-C23-C24
16	1	850	BCR	C22-C23-C24-C25
16	1	851	BCR	C5-C6-C7-C8
16	1	851	BCR	C7-C8-C9-C34
16	1	851	BCR	C10-C11-C12-C13
16	1	851	BCR	C11-C12-C13-C14
16	1	851	BCR	C16-C17-C18-C36
16	2	3044	BCR	C7-C8-C9-C10
16	2	3044	BCR	C17-C18-C19-C20
16	2	3044	BCR	C21-C22-C23-C24
16	2	3045	BCR	C6-C7-C8-C9
16	2	3045	BCR	C7-C8-C9-C10
16	2	3045	BCR	C7-C8-C9-C34
16	2	3045	BCR	C21-C22-C23-C24
16	2	3046	BCR	C17-C18-C19-C20
16	2	3046	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
16	2	3046	BCR	C20-C21-C22-C23
16	2	3046	BCR	C20-C21-C22-C37
16	2	3046	BCR	C37-C22-C23-C24
16	2	3046	BCR	C22-C23-C24-C25
16	2	3047	BCR	C11-C10-C9-C34
16	2	3047	BCR	C12-C13-C14-C15
16	2	3047	BCR	C35-C13-C14-C15
16	2	3048	BCR	C6-C7-C8-C9
16	2	3048	BCR	C10-C11-C12-C13
16	2	3048	BCR	C11-C12-C13-C14
16	2	3048	BCR	C11-C12-C13-C35
16	2	3052	BCR	C16-C17-C18-C19
16	2	3052	BCR	C16-C17-C18-C36
16	2	3052	BCR	C18-C19-C20-C21
16	2	3052	BCR	C20-C21-C22-C23
16	2	3052	BCR	C20-C21-C22-C37
16	2	3052	BCR	C23-C24-C25-C26
16	6	202	BCR	C11-C12-C13-C35
16	6	202	BCR	C20-C21-C22-C37
16	6	202	BCR	C37-C22-C23-C24
16	6	205	BCR	C12-C13-C14-C15
16	8	103	BCR	C6-C7-C8-C9
16	8	103	BCR	C7-C8-C9-C10
16	8	103	BCR	C7-C8-C9-C34
16	8	104	BCR	C14-C15-C16-C17
16	8	104	BCR	C20-C21-C22-C23
16	8	104	BCR	C20-C21-C22-C37
16	9	102	BCR	C7-C8-C9-C34
16	9	102	BCR	C9-C10-C11-C12
16	9	102	BCR	C10-C11-C12-C13
16	0	205	BCR	C7-C8-C9-C34
16	0	205	BCR	C20-C21-C22-C23
16	0	205	BCR	C20-C21-C22-C37
16	0	210	BCR	C7-C8-C9-C10
16	0	210	BCR	C21-C22-C23-C24
16	0	210	BCR	C23-C24-C25-C26
16	0	210	BCR	C23-C24-C25-C30
16	0	211	BCR	C11-C12-C13-C14
16	0	211	BCR	C11-C12-C13-C35
16	y	101	BCR	C35-C13-C14-C15
16	y	101	BCR	C36-C18-C19-C20
16	y	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
16	y	101	BCR	C21-C22-C23-C24
16	y	101	BCR	C22-C23-C24-C25
17	A	853	LHG	O1-C1-C2-C3
17	A	853	LHG	C3-O3-P-O5
17	A	854	LHG	C3-O3-P-O4
17	A	854	LHG	C4-O6-P-O3
17	A	854	LHG	C4-O6-P-O5
17	B	3051	LHG	C3-O3-P-O5
17	B	3051	LHG	O6-C4-C5-O7
17	B	3051	LHG	O9-C7-O7-C5
17	B	3051	LHG	C8-C7-O7-C5
17	L	207	LHG	C3-O3-P-O4
17	L	207	LHG	C3-O3-P-O6
17	L	207	LHG	O10-C23-O8-C6
17	L	207	LHG	C24-C23-O8-C6
17	L	208	LHG	O1-C1-C2-C3
17	L	208	LHG	C1-C2-C3-O3
17	L	208	LHG	C2-C3-O3-P
17	L	208	LHG	C3-O3-P-O6
17	L	208	LHG	C4-O6-P-O3
17	L	208	LHG	C4-O6-P-O4
17	a	852	LHG	O1-C1-C2-C3
17	a	852	LHG	C3-O3-P-O5
17	a	853	LHG	C3-O3-P-O4
17	a	853	LHG	C4-O6-P-O3
17	a	853	LHG	C4-O6-P-O5
17	b	3051	LHG	C3-O3-P-O5
17	b	3051	LHG	O6-C4-C5-O7
17	b	3051	LHG	O9-C7-O7-C5
17	b	3051	LHG	C8-C7-O7-C5
17	l	201	LHG	C3-O3-P-O4
17	l	201	LHG	C3-O3-P-O6
17	l	201	LHG	O10-C23-O8-C6
17	l	201	LHG	C24-C23-O8-C6
17	l	202	LHG	O1-C1-C2-C3
17	l	202	LHG	C1-C2-C3-O3
17	l	202	LHG	C2-C3-O3-P
17	l	202	LHG	C3-O3-P-O6
17	l	202	LHG	C4-O6-P-O3
17	l	202	LHG	C4-O6-P-O4
17	1	852	LHG	O1-C1-C2-C3
17	1	852	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
17	1	853	LHG	C3-O3-P-O4
17	1	853	LHG	C4-O6-P-O3
17	1	853	LHG	C4-O6-P-O5
17	2	3051	LHG	C3-O3-P-O5
17	2	3051	LHG	O6-C4-C5-O7
17	2	3051	LHG	O9-C7-O7-C5
17	2	3051	LHG	C8-C7-O7-C5
17	0	201	LHG	C3-O3-P-O4
17	0	201	LHG	C3-O3-P-O6
17	0	201	LHG	O10-C23-O8-C6
17	0	201	LHG	C24-C23-O8-C6
17	0	202	LHG	O1-C1-C2-C3
17	0	202	LHG	C1-C2-C3-O3
17	0	202	LHG	C2-C3-O3-P
17	0	202	LHG	C3-O3-P-O6
17	0	202	LHG	C4-O6-P-O3
17	0	202	LHG	C4-O6-P-O4
14	B	3005	CLA	C2C-C3C-CAC-CBC
14	b	3005	CLA	C2C-C3C-CAC-CBC
14	2	3005	CLA	C2C-C3C-CAC-CBC
14	A	829	CLA	O1D-CGD-O2D-CED
14	a	828	CLA	O1D-CGD-O2D-CED
14	1	829	CLA	O1D-CGD-O2D-CED
14	B	3033	CLA	C2C-C3C-CAC-CBC
14	b	3033	CLA	C2C-C3C-CAC-CBC
14	2	3033	CLA	C2C-C3C-CAC-CBC
14	A	810	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	O1D-CGD-O2D-CED
14	A	821	CLA	O1D-CGD-O2D-CED
14	A	841	CLA	O1D-CGD-O2D-CED
14	B	3035	CLA	O1D-CGD-O2D-CED
14	B	3036	CLA	O1D-CGD-O2D-CED
14	F	201	CLA	O1D-CGD-O2D-CED
14	F	203	CLA	O1D-CGD-O2D-CED
14	F	204	CLA	O1D-CGD-O2D-CED
14	a	809	CLA	O1D-CGD-O2D-CED
14	a	816	CLA	O1D-CGD-O2D-CED
14	a	820	CLA	O1D-CGD-O2D-CED
14	a	840	CLA	O1D-CGD-O2D-CED
14	b	3035	CLA	O1D-CGD-O2D-CED
14	b	3036	CLA	O1D-CGD-O2D-CED
14	f	201	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	f	203	CLA	O1D-CGD-O2D-CED
14	f	204	CLA	O1D-CGD-O2D-CED
14	1	810	CLA	O1D-CGD-O2D-CED
14	1	817	CLA	O1D-CGD-O2D-CED
14	1	821	CLA	O1D-CGD-O2D-CED
14	1	841	CLA	O1D-CGD-O2D-CED
14	2	3035	CLA	O1D-CGD-O2D-CED
14	2	3036	CLA	O1D-CGD-O2D-CED
14	6	201	CLA	O1D-CGD-O2D-CED
14	6	203	CLA	O1D-CGD-O2D-CED
14	6	204	CLA	O1D-CGD-O2D-CED
14	A	816	CLA	CBD-CGD-O2D-CED
14	A	821	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	CBD-CGD-O2D-CED
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	829	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	CBD-CGD-O2D-CED
14	B	3004	CLA	CBD-CGD-O2D-CED
14	B	3014	CLA	CBD-CGD-O2D-CED
14	B	3037	CLA	CBD-CGD-O2D-CED
14	F	201	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CBD-CGD-O2D-CED
14	a	815	CLA	CBD-CGD-O2D-CED
14	a	820	CLA	CBD-CGD-O2D-CED
14	a	821	CLA	CBD-CGD-O2D-CED
14	a	822	CLA	CBD-CGD-O2D-CED
14	a	828	CLA	CBD-CGD-O2D-CED
14	a	840	CLA	CBD-CGD-O2D-CED
14	b	3004	CLA	CBD-CGD-O2D-CED
14	b	3014	CLA	CBD-CGD-O2D-CED
14	b	3037	CLA	CBD-CGD-O2D-CED
14	f	201	CLA	CBD-CGD-O2D-CED
14	j	1102	CLA	CBD-CGD-O2D-CED
14	1	816	CLA	CBD-CGD-O2D-CED
14	1	821	CLA	CBD-CGD-O2D-CED
14	1	822	CLA	CBD-CGD-O2D-CED
14	1	823	CLA	CBD-CGD-O2D-CED
14	1	829	CLA	CBD-CGD-O2D-CED
14	1	841	CLA	CBD-CGD-O2D-CED
14	2	3004	CLA	CBD-CGD-O2D-CED
14	2	3014	CLA	CBD-CGD-O2D-CED
14	2	3037	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	6	201	CLA	CBD-CGD-O2D-CED
14	8	101	CLA	CBD-CGD-O2D-CED
14	A	806	CLA	O1A-CGA-O2A-C1
14	B	3021	CLA	O1A-CGA-O2A-C1
14	a	805	CLA	O1A-CGA-O2A-C1
14	b	3021	CLA	O1A-CGA-O2A-C1
14	1	806	CLA	O1A-CGA-O2A-C1
14	2	3021	CLA	O1A-CGA-O2A-C1
14	B	3042	CLA	C4C-C3C-CAC-CBC
14	b	3042	CLA	C4C-C3C-CAC-CBC
14	2	3042	CLA	C4C-C3C-CAC-CBC
14	B	3033	CLA	C4C-C3C-CAC-CBC
14	b	3033	CLA	C4C-C3C-CAC-CBC
14	2	3033	CLA	C4C-C3C-CAC-CBC
14	A	823	CLA	O1D-CGD-O2D-CED
14	J	101	CLA	O1D-CGD-O2D-CED
14	a	822	CLA	O1D-CGD-O2D-CED
14	j	1102	CLA	O1D-CGD-O2D-CED
14	1	823	CLA	O1D-CGD-O2D-CED
14	8	101	CLA	O1D-CGD-O2D-CED
14	B	3018	CLA	CBA-CGA-O2A-C1
14	B	3021	CLA	CBA-CGA-O2A-C1
14	b	3018	CLA	CBA-CGA-O2A-C1
14	b	3021	CLA	CBA-CGA-O2A-C1
14	2	3018	CLA	CBA-CGA-O2A-C1
14	2	3021	CLA	CBA-CGA-O2A-C1
14	A	802	CLA	O1A-CGA-O2A-C1
14	A	817	CLA	O1A-CGA-O2A-C1
14	A	818	CLA	O1A-CGA-O2A-C1
14	A	820	CLA	O1A-CGA-O2A-C1
14	A	833	CLA	O1A-CGA-O2A-C1
14	B	3018	CLA	O1A-CGA-O2A-C1
14	a	802	CLA	O1A-CGA-O2A-C1
14	a	816	CLA	O1A-CGA-O2A-C1
14	a	817	CLA	O1A-CGA-O2A-C1
14	a	819	CLA	O1A-CGA-O2A-C1
14	a	832	CLA	O1A-CGA-O2A-C1
14	b	3018	CLA	O1A-CGA-O2A-C1
14	1	802	CLA	O1A-CGA-O2A-C1
14	1	817	CLA	O1A-CGA-O2A-C1
14	1	818	CLA	O1A-CGA-O2A-C1
14	1	820	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	1	833	CLA	O1A-CGA-O2A-C1
14	2	3018	CLA	O1A-CGA-O2A-C1
14	A	815	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	O1D-CGD-O2D-CED
14	a	814	CLA	O1D-CGD-O2D-CED
14	x	1701	CLA	O1D-CGD-O2D-CED
14	1	815	CLA	O1D-CGD-O2D-CED
14	z	1701	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	O1D-CGD-O2D-CED
14	B	3005	CLA	O1D-CGD-O2D-CED
14	B	3020	CLA	O1D-CGD-O2D-CED
14	K	101	CLA	O1D-CGD-O2D-CED
14	a	811	CLA	O1D-CGD-O2D-CED
14	b	3005	CLA	O1D-CGD-O2D-CED
14	b	3020	CLA	O1D-CGD-O2D-CED
14	k	101	CLA	O1D-CGD-O2D-CED
14	1	812	CLA	O1D-CGD-O2D-CED
14	2	3005	CLA	O1D-CGD-O2D-CED
14	2	3020	CLA	O1D-CGD-O2D-CED
14	9	101	CLA	O1D-CGD-O2D-CED
14	B	3042	CLA	C2C-C3C-CAC-CBC
14	b	3042	CLA	C2C-C3C-CAC-CBC
14	2	3042	CLA	C2C-C3C-CAC-CBC
14	K	101	CLA	O1A-CGA-O2A-C1
14	k	101	CLA	O1A-CGA-O2A-C1
14	9	101	CLA	O1A-CGA-O2A-C1
14	A	810	CLA	C3-C5-C6-C7
14	A	818	CLA	C3-C5-C6-C7
14	A	826	CLA	C3-C5-C6-C7
14	A	841	CLA	C3-C5-C6-C7
14	A	842	CLA	C3-C5-C6-C7
14	B	3006	CLA	C3-C5-C6-C7
14	B	3012	CLA	C3-C5-C6-C7
14	B	3016	CLA	C3-C5-C6-C7
14	B	3020	CLA	C3-C5-C6-C7
14	B	3039	CLA	C3-C5-C6-C7
14	F	201	CLA	C3-C5-C6-C7
14	L	205	CLA	C3-C5-C6-C7
14	a	809	CLA	C3-C5-C6-C7
14	a	817	CLA	C3-C5-C6-C7
14	a	825	CLA	C3-C5-C6-C7
14	a	840	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	a	841	CLA	C3-C5-C6-C7
14	b	3006	CLA	C3-C5-C6-C7
14	b	3012	CLA	C3-C5-C6-C7
14	b	3016	CLA	C3-C5-C6-C7
14	b	3020	CLA	C3-C5-C6-C7
14	b	3039	CLA	C3-C5-C6-C7
14	f	201	CLA	C3-C5-C6-C7
14	l	208	CLA	C3-C5-C6-C7
14	1	810	CLA	C3-C5-C6-C7
14	1	818	CLA	C3-C5-C6-C7
14	1	826	CLA	C3-C5-C6-C7
14	1	841	CLA	C3-C5-C6-C7
14	1	842	CLA	C3-C5-C6-C7
14	2	3006	CLA	C3-C5-C6-C7
14	2	3012	CLA	C3-C5-C6-C7
14	2	3016	CLA	C3-C5-C6-C7
14	2	3020	CLA	C3-C5-C6-C7
14	2	3039	CLA	C3-C5-C6-C7
14	6	201	CLA	C3-C5-C6-C7
14	0	209	CLA	C3-C5-C6-C7
14	A	802	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	CBA-CGA-O2A-C1
14	A	817	CLA	CBA-CGA-O2A-C1
14	A	833	CLA	CBA-CGA-O2A-C1
14	B	3019	CLA	CBA-CGA-O2A-C1
14	a	802	CLA	CBA-CGA-O2A-C1
14	a	805	CLA	CBA-CGA-O2A-C1
14	a	816	CLA	CBA-CGA-O2A-C1
14	a	832	CLA	CBA-CGA-O2A-C1
14	b	3019	CLA	CBA-CGA-O2A-C1
14	1	802	CLA	CBA-CGA-O2A-C1
14	1	806	CLA	CBA-CGA-O2A-C1
14	1	817	CLA	CBA-CGA-O2A-C1
14	1	833	CLA	CBA-CGA-O2A-C1
14	2	3019	CLA	CBA-CGA-O2A-C1
14	A	824	CLA	CBD-CGD-O2D-CED
14	A	825	CLA	CBD-CGD-O2D-CED
14	A	830	CLA	CBD-CGD-O2D-CED
14	A	838	CLA	CBD-CGD-O2D-CED
14	B	3008	CLA	CBD-CGD-O2D-CED
14	B	3022	CLA	CBD-CGD-O2D-CED
14	B	3023	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	3031	CLA	CBD-CGD-O2D-CED
14	B	3039	CLA	CBD-CGD-O2D-CED
14	B	3042	CLA	CBD-CGD-O2D-CED
14	L	203	CLA	CBD-CGD-O2D-CED
14	a	823	CLA	CBD-CGD-O2D-CED
14	a	824	CLA	CBD-CGD-O2D-CED
14	a	829	CLA	CBD-CGD-O2D-CED
14	a	837	CLA	CBD-CGD-O2D-CED
14	b	3008	CLA	CBD-CGD-O2D-CED
14	b	3022	CLA	CBD-CGD-O2D-CED
14	b	3023	CLA	CBD-CGD-O2D-CED
14	b	3031	CLA	CBD-CGD-O2D-CED
14	b	3039	CLA	CBD-CGD-O2D-CED
14	b	3042	CLA	CBD-CGD-O2D-CED
14	l	206	CLA	CBD-CGD-O2D-CED
14	1	824	CLA	CBD-CGD-O2D-CED
14	1	825	CLA	CBD-CGD-O2D-CED
14	1	830	CLA	CBD-CGD-O2D-CED
14	1	838	CLA	CBD-CGD-O2D-CED
14	2	3008	CLA	CBD-CGD-O2D-CED
14	2	3022	CLA	CBD-CGD-O2D-CED
14	2	3023	CLA	CBD-CGD-O2D-CED
14	2	3031	CLA	CBD-CGD-O2D-CED
14	2	3039	CLA	CBD-CGD-O2D-CED
14	2	3042	CLA	CBD-CGD-O2D-CED
14	0	207	CLA	CBD-CGD-O2D-CED
17	L	207	LHG	C8-C7-O7-C5
17	l	201	LHG	C8-C7-O7-C5
17	0	201	LHG	C8-C7-O7-C5
14	A	802	CLA	C4-C3-C5-C6
14	A	836	CLA	C4-C3-C5-C6
14	B	3018	CLA	C4-C3-C5-C6
14	a	802	CLA	C4-C3-C5-C6
14	a	835	CLA	C4-C3-C5-C6
14	b	3018	CLA	C4-C3-C5-C6
14	1	802	CLA	C4-C3-C5-C6
14	1	836	CLA	C4-C3-C5-C6
14	2	3018	CLA	C4-C3-C5-C6
14	A	802	CLA	C2-C3-C5-C6
14	B	3016	CLA	C2-C3-C5-C6
14	B	3018	CLA	C2-C3-C5-C6
14	B	3019	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	a	802	CLA	C2-C3-C5-C6
14	b	3016	CLA	C2-C3-C5-C6
14	b	3018	CLA	C2-C3-C5-C6
14	b	3019	CLA	C2-C3-C5-C6
14	1	802	CLA	C2-C3-C5-C6
14	2	3016	CLA	C2-C3-C5-C6
14	2	3018	CLA	C2-C3-C5-C6
14	2	3019	CLA	C2-C3-C5-C6
14	K	101	CLA	CBA-CGA-O2A-C1
14	k	101	CLA	CBA-CGA-O2A-C1
14	9	101	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	C2A-CAA-CBA-CGA
14	B	3011	CLA	C2A-CAA-CBA-CGA
14	a	824	CLA	C2A-CAA-CBA-CGA
14	b	3011	CLA	C2A-CAA-CBA-CGA
14	1	825	CLA	C2A-CAA-CBA-CGA
14	2	3011	CLA	C2A-CAA-CBA-CGA
14	A	834	CLA	C3-C5-C6-C7
14	B	3034	CLA	C3-C5-C6-C7
14	a	833	CLA	C3-C5-C6-C7
14	b	3034	CLA	C3-C5-C6-C7
14	1	834	CLA	C3-C5-C6-C7
14	2	3034	CLA	C3-C5-C6-C7
14	A	818	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	CBA-CGA-O2A-C1
14	B	3017	CLA	CBA-CGA-O2A-C1
14	B	3026	CLA	CBA-CGA-O2A-C1
14	B	3031	CLA	CBA-CGA-O2A-C1
14	a	817	CLA	CBA-CGA-O2A-C1
14	a	819	CLA	CBA-CGA-O2A-C1
14	b	3017	CLA	CBA-CGA-O2A-C1
14	b	3026	CLA	CBA-CGA-O2A-C1
14	b	3031	CLA	CBA-CGA-O2A-C1
14	1	818	CLA	CBA-CGA-O2A-C1
14	1	820	CLA	CBA-CGA-O2A-C1
14	2	3017	CLA	CBA-CGA-O2A-C1
14	2	3026	CLA	CBA-CGA-O2A-C1
14	2	3031	CLA	CBA-CGA-O2A-C1
17	B	3051	LHG	C24-C23-O8-C6
17	L	208	LHG	C24-C23-O8-C6
17	b	3051	LHG	C24-C23-O8-C6
17	l	202	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
17	2	3051	LHG	C24-C23-O8-C6
17	0	202	LHG	C24-C23-O8-C6
16	A	852	BCR	C9-C10-C11-C12
16	B	3048	BCR	C15-C16-C17-C18
16	a	851	BCR	C9-C10-C11-C12
16	b	3048	BCR	C15-C16-C17-C18
16	1	851	BCR	C9-C10-C11-C12
16	2	3048	BCR	C15-C16-C17-C18
14	B	3019	CLA	O1A-CGA-O2A-C1
14	B	3026	CLA	O1A-CGA-O2A-C1
14	b	3019	CLA	O1A-CGA-O2A-C1
14	b	3026	CLA	O1A-CGA-O2A-C1
14	2	3019	CLA	O1A-CGA-O2A-C1
14	2	3026	CLA	O1A-CGA-O2A-C1
17	L	208	LHG	O10-C23-O8-C6
17	l	202	LHG	O10-C23-O8-C6
17	0	202	LHG	O10-C23-O8-C6
14	B	3037	CLA	O1D-CGD-O2D-CED
14	b	3037	CLA	O1D-CGD-O2D-CED
14	2	3037	CLA	O1D-CGD-O2D-CED
14	A	816	CLA	C3-C5-C6-C7
14	B	3015	CLA	C3-C5-C6-C7
14	B	3018	CLA	C3-C5-C6-C7
14	a	815	CLA	C3-C5-C6-C7
14	b	3015	CLA	C3-C5-C6-C7
14	b	3018	CLA	C3-C5-C6-C7
14	1	816	CLA	C3-C5-C6-C7
14	2	3015	CLA	C3-C5-C6-C7
14	2	3018	CLA	C3-C5-C6-C7
14	A	818	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	CBD-CGD-O2D-CED
14	B	3012	CLA	CBD-CGD-O2D-CED
14	B	3040	CLA	CBD-CGD-O2D-CED
14	a	817	CLA	CBD-CGD-O2D-CED
14	a	841	CLA	CBD-CGD-O2D-CED
14	b	3012	CLA	CBD-CGD-O2D-CED
14	b	3040	CLA	CBD-CGD-O2D-CED
14	1	818	CLA	CBD-CGD-O2D-CED
14	1	842	CLA	CBD-CGD-O2D-CED
14	2	3012	CLA	CBD-CGD-O2D-CED
14	2	3040	CLA	CBD-CGD-O2D-CED
14	A	809	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	L	203	CLA	CBA-CGA-O2A-C1
14	l	206	CLA	CBA-CGA-O2A-C1
14	0	207	CLA	CBA-CGA-O2A-C1
14	B	3003	CLA	CBD-CGD-O2D-CED
14	b	3003	CLA	CBD-CGD-O2D-CED
14	2	3003	CLA	CBD-CGD-O2D-CED
14	A	816	CLA	O1D-CGD-O2D-CED
14	a	815	CLA	O1D-CGD-O2D-CED
14	1	816	CLA	O1D-CGD-O2D-CED
14	B	3017	CLA	O1A-CGA-O2A-C1
14	B	3031	CLA	O1A-CGA-O2A-C1
14	b	3017	CLA	O1A-CGA-O2A-C1
14	b	3031	CLA	O1A-CGA-O2A-C1
14	2	3017	CLA	O1A-CGA-O2A-C1
14	2	3031	CLA	O1A-CGA-O2A-C1
14	B	3028	CLA	C3-C5-C6-C7
14	b	3028	CLA	C3-C5-C6-C7
14	2	3028	CLA	C3-C5-C6-C7
14	A	811	CLA	CBD-CGD-O2D-CED
14	a	810	CLA	CBD-CGD-O2D-CED
14	1	811	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	O1D-CGD-O2D-CED
14	a	821	CLA	O1D-CGD-O2D-CED
14	1	822	CLA	O1D-CGD-O2D-CED
14	a	808	CLA	CBA-CGA-O2A-C1
14	1	809	CLA	CBA-CGA-O2A-C1
14	A	817	CLA	C4-C3-C5-C6
14	A	833	CLA	C4-C3-C5-C6
14	A	843	CLA	C4-C3-C5-C6
14	B	3003	CLA	C4-C3-C5-C6
14	B	3012	CLA	C4-C3-C5-C6
14	B	3034	CLA	C4-C3-C5-C6
14	a	816	CLA	C4-C3-C5-C6
14	a	832	CLA	C4-C3-C5-C6
14	a	842	CLA	C4-C3-C5-C6
14	b	3003	CLA	C4-C3-C5-C6
14	b	3012	CLA	C4-C3-C5-C6
14	b	3034	CLA	C4-C3-C5-C6
14	1	817	CLA	C4-C3-C5-C6
14	1	833	CLA	C4-C3-C5-C6
14	1	843	CLA	C4-C3-C5-C6
14	2	3003	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	2	3012	CLA	C4-C3-C5-C6
14	2	3034	CLA	C4-C3-C5-C6
14	A	817	CLA	C2-C3-C5-C6
14	A	843	CLA	C2-C3-C5-C6
14	B	3003	CLA	C2-C3-C5-C6
14	a	816	CLA	C2-C3-C5-C6
14	a	842	CLA	C2-C3-C5-C6
14	b	3003	CLA	C2-C3-C5-C6
14	1	817	CLA	C2-C3-C5-C6
14	1	843	CLA	C2-C3-C5-C6
14	2	3003	CLA	C2-C3-C5-C6
14	B	3034	CLA	CBD-CGD-O2D-CED
14	b	3034	CLA	CBD-CGD-O2D-CED
14	2	3034	CLA	CBD-CGD-O2D-CED
14	L	203	CLA	O1A-CGA-O2A-C1
14	l	206	CLA	O1A-CGA-O2A-C1
14	0	207	CLA	O1A-CGA-O2A-C1
17	B	3051	LHG	O10-C23-O8-C6
17	b	3051	LHG	O10-C23-O8-C6
17	2	3051	LHG	O10-C23-O8-C6
14	A	833	CLA	C3-C5-C6-C7
14	b	3014	CLA	O1D-CGD-O2D-CED
14	L	205	CLA	CBA-CGA-O2A-C1
14	l	208	CLA	CBA-CGA-O2A-C1
14	0	209	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	CBD-CGD-O2D-CED
14	B	3024	CLA	CBD-CGD-O2D-CED
14	B	3028	CLA	CBD-CGD-O2D-CED
14	a	805	CLA	CBD-CGD-O2D-CED
14	b	3024	CLA	CBD-CGD-O2D-CED
14	b	3028	CLA	CBD-CGD-O2D-CED
14	1	806	CLA	CBD-CGD-O2D-CED
14	2	3024	CLA	CBD-CGD-O2D-CED
14	2	3028	CLA	CBD-CGD-O2D-CED
20	B	3050	LMG	O6-C5-C6-O5
20	b	3050	LMG	O6-C5-C6-O5
20	2	3050	LMG	O6-C5-C6-O5
14	A	838	CLA	C2C-C3C-CAC-CBC
14	a	837	CLA	C2C-C3C-CAC-CBC
14	1	838	CLA	C2C-C3C-CAC-CBC
17	B	3051	LHG	C27-C28-C29-C30
17	b	3051	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
17	2	3051	LHG	C27-C28-C29-C30
14	B	3014	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	O1A-CGA-O2A-C1
14	a	808	CLA	O1A-CGA-O2A-C1
14	1	809	CLA	O1A-CGA-O2A-C1
14	B	3004	CLA	O1D-CGD-O2D-CED
14	b	3004	CLA	O1D-CGD-O2D-CED
14	2	3004	CLA	O1D-CGD-O2D-CED
14	2	3014	CLA	O1D-CGD-O2D-CED
14	a	832	CLA	C3-C5-C6-C7
14	1	833	CLA	C3-C5-C6-C7
16	A	848	BCR	C15-C16-C17-C18
16	a	847	BCR	C15-C16-C17-C18
16	1	847	BCR	C15-C16-C17-C18
14	L	205	CLA	O1A-CGA-O2A-C1
14	l	208	CLA	O1A-CGA-O2A-C1
14	0	209	CLA	O1A-CGA-O2A-C1
14	B	3006	CLA	CBA-CGA-O2A-C1
14	B	3029	CLA	CBA-CGA-O2A-C1
14	B	3032	CLA	CBA-CGA-O2A-C1
14	B	3036	CLA	CBA-CGA-O2A-C1
14	b	3006	CLA	CBA-CGA-O2A-C1
14	b	3029	CLA	CBA-CGA-O2A-C1
14	b	3032	CLA	CBA-CGA-O2A-C1
14	b	3036	CLA	CBA-CGA-O2A-C1
14	2	3006	CLA	CBA-CGA-O2A-C1
14	2	3029	CLA	CBA-CGA-O2A-C1
14	2	3032	CLA	CBA-CGA-O2A-C1
14	2	3036	CLA	CBA-CGA-O2A-C1
20	B	3050	LMG	C29-C28-O8-C9
20	b	3050	LMG	C29-C28-O8-C9
20	2	3050	LMG	C29-C28-O8-C9
14	B	3015	CLA	CBD-CGD-O2D-CED
20	2	3050	LMG	C4-C5-C6-O5
14	A	819	CLA	C4-C3-C5-C6
14	B	3011	CLA	C4-C3-C5-C6
14	a	818	CLA	C4-C3-C5-C6
14	b	3011	CLA	C4-C3-C5-C6
14	1	819	CLA	C4-C3-C5-C6
14	2	3011	CLA	C4-C3-C5-C6
14	A	819	CLA	C2-C3-C5-C6
14	A	833	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	836	CLA	C2-C3-C5-C6
14	B	3011	CLA	C2-C3-C5-C6
14	B	3012	CLA	C2-C3-C5-C6
14	a	818	CLA	C2-C3-C5-C6
14	a	832	CLA	C2-C3-C5-C6
14	a	835	CLA	C2-C3-C5-C6
14	b	3011	CLA	C2-C3-C5-C6
14	b	3012	CLA	C2-C3-C5-C6
14	b	3034	CLA	C2-C3-C5-C6
14	1	819	CLA	C2-C3-C5-C6
14	1	833	CLA	C2-C3-C5-C6
14	1	836	CLA	C2-C3-C5-C6
14	2	3011	CLA	C2-C3-C5-C6
14	2	3012	CLA	C2-C3-C5-C6
14	A	812	CLA	C3-C5-C6-C7
14	a	811	CLA	C3-C5-C6-C7
14	1	812	CLA	C3-C5-C6-C7
14	b	3015	CLA	CBD-CGD-O2D-CED
14	2	3015	CLA	CBD-CGD-O2D-CED
14	A	803	CLA	C6-C7-C8-C9
14	A	817	CLA	C6-C7-C8-C9
14	A	819	CLA	C6-C7-C8-C9
14	A	825	CLA	C11-C12-C13-C14
14	A	833	CLA	C11-C12-C13-C14
14	A	841	CLA	C11-C12-C13-C14
14	B	3005	CLA	C11-C12-C13-C14
14	B	3006	CLA	C11-C10-C8-C9
14	B	3006	CLA	C11-C12-C13-C14
14	B	3009	CLA	C11-C12-C13-C14
14	B	3014	CLA	C11-C12-C13-C14
14	B	3028	CLA	C14-C13-C15-C16
14	B	3035	CLA	C14-C13-C15-C16
14	B	3039	CLA	C11-C10-C8-C9
14	B	3041	CLA	C14-C13-C15-C16
14	L	204	CLA	C6-C7-C8-C9
14	L	205	CLA	C6-C7-C8-C9
14	a	803	CLA	C6-C7-C8-C9
14	a	805	CLA	C6-C7-C8-C9
14	a	816	CLA	C6-C7-C8-C9
14	a	818	CLA	C6-C7-C8-C9
14	a	824	CLA	C11-C12-C13-C14
14	a	832	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	a	840	CLA	C11-C12-C13-C14
14	b	3005	CLA	C11-C12-C13-C14
14	b	3006	CLA	C11-C10-C8-C9
14	b	3006	CLA	C11-C12-C13-C14
14	b	3009	CLA	C11-C12-C13-C14
14	b	3014	CLA	C11-C12-C13-C14
14	b	3028	CLA	C14-C13-C15-C16
14	b	3035	CLA	C14-C13-C15-C16
14	b	3039	CLA	C11-C10-C8-C9
14	b	3041	CLA	C14-C13-C15-C16
14	l	207	CLA	C6-C7-C8-C9
14	l	208	CLA	C6-C7-C8-C9
14	1	803	CLA	C6-C7-C8-C9
14	1	806	CLA	C6-C7-C8-C9
14	1	817	CLA	C6-C7-C8-C9
14	1	819	CLA	C6-C7-C8-C9
14	1	825	CLA	C11-C12-C13-C14
14	1	833	CLA	C11-C12-C13-C14
14	1	841	CLA	C11-C12-C13-C14
14	2	3005	CLA	C11-C12-C13-C14
14	2	3006	CLA	C11-C10-C8-C9
14	2	3006	CLA	C11-C12-C13-C14
14	2	3009	CLA	C11-C12-C13-C14
14	2	3014	CLA	C11-C12-C13-C14
14	2	3028	CLA	C14-C13-C15-C16
14	2	3035	CLA	C14-C13-C15-C16
14	2	3039	CLA	C11-C10-C8-C9
14	2	3041	CLA	C14-C13-C15-C16
14	0	208	CLA	C6-C7-C8-C9
14	0	209	CLA	C6-C7-C8-C9
20	B	3050	LMG	C4-C5-C6-O5
20	b	3050	LMG	C4-C5-C6-O5
14	a	823	CLA	O1D-CGD-O2D-CED
17	A	854	LHG	O2-C2-C3-O3
17	L	208	LHG	O2-C2-C3-O3
17	a	853	LHG	O2-C2-C3-O3
17	l	202	LHG	O2-C2-C3-O3
17	1	853	LHG	O2-C2-C3-O3
17	0	202	LHG	O2-C2-C3-O3
14	A	824	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	O1D-CGD-O2D-CED
14	a	829	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	1	824	CLA	O1D-CGD-O2D-CED
14	1	830	CLA	O1D-CGD-O2D-CED
14	B	3031	CLA	O1D-CGD-O2D-CED
14	b	3031	CLA	O1D-CGD-O2D-CED
14	2	3031	CLA	O1D-CGD-O2D-CED
16	B	3044	BCR	C7-C8-C9-C34
16	B	3044	BCR	C36-C18-C19-C20
16	B	3046	BCR	C7-C8-C9-C34
16	B	3047	BCR	C7-C8-C9-C34
16	B	3048	BCR	C36-C18-C19-C20
16	B	3052	BCR	C11-C12-C13-C35
16	F	202	BCR	C7-C8-C9-C34
16	I	101	BCR	C7-C8-C9-C34
16	I	102	BCR	C7-C8-C9-C34
16	I	102	BCR	C37-C22-C23-C24
16	J	103	BCR	C37-C22-C23-C24
16	J	104	BCR	C7-C8-C9-C34
16	M	1602	BCR	C7-C8-C9-C34
16	M	1602	BCR	C37-C22-C23-C24
16	b	3044	BCR	C7-C8-C9-C34
16	b	3044	BCR	C36-C18-C19-C20
16	b	3046	BCR	C7-C8-C9-C34
16	b	3047	BCR	C7-C8-C9-C34
16	b	3048	BCR	C36-C18-C19-C20
16	f	202	BCR	C7-C8-C9-C34
16	i	101	BCR	C7-C8-C9-C34
16	j	1104	BCR	C37-C22-C23-C24
16	j	1105	BCR	C7-C8-C9-C34
16	l	204	BCR	C11-C12-C13-C35
16	l	209	BCR	C7-C8-C9-C34
16	l	209	BCR	C37-C22-C23-C24
16	m	101	BCR	C7-C8-C9-C34
16	m	101	BCR	C37-C22-C23-C24
16	2	3044	BCR	C7-C8-C9-C34
16	2	3044	BCR	C36-C18-C19-C20
16	2	3046	BCR	C7-C8-C9-C34
16	2	3047	BCR	C7-C8-C9-C34
16	2	3048	BCR	C36-C18-C19-C20
16	6	202	BCR	C7-C8-C9-C34
16	7	101	BCR	C7-C8-C9-C34
16	8	103	BCR	C37-C22-C23-C24
16	8	104	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
16	0	205	BCR	C11-C12-C13-C35
16	0	210	BCR	C7-C8-C9-C34
16	0	210	BCR	C37-C22-C23-C24
16	y	101	BCR	C7-C8-C9-C34
16	y	101	BCR	C37-C22-C23-C24
16	A	851	BCR	C21-C22-C23-C24
16	A	852	BCR	C7-C8-C9-C10
16	a	850	BCR	C21-C22-C23-C24
16	a	851	BCR	C7-C8-C9-C10
16	1	850	BCR	C21-C22-C23-C24
16	1	851	BCR	C7-C8-C9-C10
14	A	843	CLA	C2A-CAA-CBA-CGA
14	B	3041	CLA	C2A-CAA-CBA-CGA
14	a	842	CLA	C2A-CAA-CBA-CGA
14	b	3041	CLA	C2A-CAA-CBA-CGA
14	1	843	CLA	C2A-CAA-CBA-CGA
14	2	3041	CLA	C2A-CAA-CBA-CGA
14	B	3032	CLA	O1A-CGA-O2A-C1
14	B	3036	CLA	O1A-CGA-O2A-C1
14	b	3032	CLA	O1A-CGA-O2A-C1
14	b	3036	CLA	O1A-CGA-O2A-C1
14	2	3032	CLA	O1A-CGA-O2A-C1
14	2	3036	CLA	O1A-CGA-O2A-C1
14	A	829	CLA	CBA-CGA-O2A-C1
14	B	3004	CLA	CBA-CGA-O2A-C1
14	B	3035	CLA	CBA-CGA-O2A-C1
14	a	828	CLA	CBA-CGA-O2A-C1
14	b	3004	CLA	CBA-CGA-O2A-C1
14	b	3035	CLA	CBA-CGA-O2A-C1
14	1	829	CLA	CBA-CGA-O2A-C1
14	2	3004	CLA	CBA-CGA-O2A-C1
14	2	3035	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	O1D-CGD-O2D-CED
14	B	3023	CLA	O1D-CGD-O2D-CED
14	L	203	CLA	O1D-CGD-O2D-CED
14	a	837	CLA	O1D-CGD-O2D-CED
14	b	3023	CLA	O1D-CGD-O2D-CED
14	1	206	CLA	O1D-CGD-O2D-CED
14	1	838	CLA	O1D-CGD-O2D-CED
14	2	3023	CLA	O1D-CGD-O2D-CED
14	0	207	CLA	O1D-CGD-O2D-CED
14	A	834	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	a	833	CLA	CBD-CGD-O2D-CED
14	1	834	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C13-C15-C16-C17
14	A	824	CLA	C10-C11-C12-C13
14	B	3018	CLA	C5-C6-C7-C8
14	a	806	CLA	C13-C15-C16-C17
14	a	823	CLA	C10-C11-C12-C13
14	b	3018	CLA	C5-C6-C7-C8
14	1	807	CLA	C13-C15-C16-C17
14	1	824	CLA	C10-C11-C12-C13
14	2	3018	CLA	C5-C6-C7-C8
14	B	3008	CLA	O1D-CGD-O2D-CED
14	B	3039	CLA	O1D-CGD-O2D-CED
14	b	3008	CLA	O1D-CGD-O2D-CED
14	b	3039	CLA	O1D-CGD-O2D-CED
14	2	3008	CLA	O1D-CGD-O2D-CED
14	2	3039	CLA	O1D-CGD-O2D-CED
14	B	3006	CLA	O1A-CGA-O2A-C1
14	b	3006	CLA	O1A-CGA-O2A-C1
14	2	3006	CLA	O1A-CGA-O2A-C1
14	A	802	CLA	CBD-CGD-O2D-CED
14	1	802	CLA	CBD-CGD-O2D-CED
14	B	3003	CLA	C11-C12-C13-C15
14	B	3012	CLA	C12-C13-C15-C16
14	B	3027	CLA	C11-C10-C8-C7
14	b	3003	CLA	C11-C12-C13-C15
14	b	3012	CLA	C12-C13-C15-C16
14	b	3027	CLA	C11-C10-C8-C7
14	2	3003	CLA	C11-C12-C13-C15
14	2	3012	CLA	C12-C13-C15-C16
14	2	3027	CLA	C11-C10-C8-C7
14	A	832	CLA	CBA-CGA-O2A-C1
14	1	832	CLA	CBA-CGA-O2A-C1
14	B	3017	CLA	C13-C15-C16-C17
14	B	3017	CLA	C15-C16-C17-C18
14	b	3017	CLA	C15-C16-C17-C18
14	2	3017	CLA	C15-C16-C17-C18
14	2	3042	CLA	O1D-CGD-O2D-CED
14	B	3028	CLA	C2C-C3C-CAC-CBC
14	b	3028	CLA	C2C-C3C-CAC-CBC
14	2	3028	CLA	C2C-C3C-CAC-CBC
14	a	802	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	3042	CLA	O1D-CGD-O2D-CED
14	b	3042	CLA	O1D-CGD-O2D-CED
14	b	3017	CLA	C13-C15-C16-C17
14	2	3017	CLA	C13-C15-C16-C17
14	a	831	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	C10-C11-C12-C13
14	B	3006	CLA	C15-C16-C17-C18
14	B	3010	CLA	C13-C15-C16-C17
14	b	3006	CLA	C15-C16-C17-C18
14	1	828	CLA	C8-C10-C11-C12
14	1	838	CLA	C10-C11-C12-C13
14	2	3006	CLA	C15-C16-C17-C18
15	B	3043	PQN	C18-C20-C21-C22
15	b	3043	PQN	C18-C20-C21-C22
15	2	3043	PQN	C18-C20-C21-C22
14	A	816	CLA	C2A-CAA-CBA-CGA
14	A	830	CLA	C2A-CAA-CBA-CGA
14	B	3003	CLA	C2A-CAA-CBA-CGA
14	B	3015	CLA	C2A-CAA-CBA-CGA
14	a	815	CLA	C2A-CAA-CBA-CGA
14	a	829	CLA	C2A-CAA-CBA-CGA
14	b	3003	CLA	C2A-CAA-CBA-CGA
14	b	3015	CLA	C2A-CAA-CBA-CGA
14	1	816	CLA	C2A-CAA-CBA-CGA
14	1	830	CLA	C2A-CAA-CBA-CGA
14	2	3003	CLA	C2A-CAA-CBA-CGA
14	2	3015	CLA	C2A-CAA-CBA-CGA
14	A	812	CLA	C10-C11-C12-C13
14	A	828	CLA	C8-C10-C11-C12
14	A	833	CLA	C10-C11-C12-C13
14	A	833	CLA	C15-C16-C17-C18
14	B	3008	CLA	C8-C10-C11-C12
14	B	3026	CLA	C5-C6-C7-C8
14	B	3033	CLA	C15-C16-C17-C18
14	a	811	CLA	C10-C11-C12-C13
14	a	827	CLA	C8-C10-C11-C12
14	a	832	CLA	C10-C11-C12-C13
14	a	832	CLA	C15-C16-C17-C18
14	a	837	CLA	C10-C11-C12-C13
14	b	3008	CLA	C8-C10-C11-C12
14	b	3010	CLA	C13-C15-C16-C17
14	b	3026	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	b	3033	CLA	C15-C16-C17-C18
14	1	812	CLA	C10-C11-C12-C13
14	1	833	CLA	C10-C11-C12-C13
14	1	833	CLA	C15-C16-C17-C18
14	2	3008	CLA	C8-C10-C11-C12
14	2	3010	CLA	C13-C15-C16-C17
14	2	3026	CLA	C5-C6-C7-C8
14	2	3033	CLA	C15-C16-C17-C18
16	B	3052	BCR	C22-C23-C24-C25
16	l	204	BCR	C22-C23-C24-C25
16	0	205	BCR	C22-C23-C24-C25
17	B	3051	LHG	C29-C30-C31-C32
17	b	3051	LHG	C29-C30-C31-C32
17	2	3051	LHG	C29-C30-C31-C32
14	A	825	CLA	O1D-CGD-O2D-CED
14	B	3022	CLA	O1D-CGD-O2D-CED
14	a	824	CLA	O1D-CGD-O2D-CED
14	b	3022	CLA	O1D-CGD-O2D-CED
14	1	825	CLA	O1D-CGD-O2D-CED
14	2	3022	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	C5-C6-C7-C8
14	A	819	CLA	C13-C15-C16-C17
14	A	839	CLA	C8-C10-C11-C12
14	A	839	CLA	C15-C16-C17-C18
14	B	3003	CLA	C13-C15-C16-C17
14	B	3009	CLA	C15-C16-C17-C18
14	B	3014	CLA	C15-C16-C17-C18
14	B	3015	CLA	C10-C11-C12-C13
14	B	3015	CLA	C15-C16-C17-C18
14	B	3027	CLA	C13-C15-C16-C17
14	L	205	CLA	C5-C6-C7-C8
14	a	806	CLA	C5-C6-C7-C8
14	a	818	CLA	C13-C15-C16-C17
14	a	838	CLA	C8-C10-C11-C12
14	a	838	CLA	C15-C16-C17-C18
14	b	3003	CLA	C13-C15-C16-C17
14	b	3009	CLA	C15-C16-C17-C18
14	b	3014	CLA	C15-C16-C17-C18
14	b	3015	CLA	C10-C11-C12-C13
14	b	3015	CLA	C15-C16-C17-C18
14	b	3027	CLA	C13-C15-C16-C17
14	l	208	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	1	807	CLA	C5-C6-C7-C8
14	1	819	CLA	C13-C15-C16-C17
14	1	839	CLA	C8-C10-C11-C12
14	1	839	CLA	C15-C16-C17-C18
14	2	3003	CLA	C13-C15-C16-C17
14	2	3009	CLA	C15-C16-C17-C18
14	2	3014	CLA	C15-C16-C17-C18
14	2	3015	CLA	C10-C11-C12-C13
14	2	3015	CLA	C15-C16-C17-C18
14	2	3027	CLA	C13-C15-C16-C17
14	0	209	CLA	C5-C6-C7-C8
17	B	3051	LHG	O2-C2-C3-O3
17	b	3051	LHG	O2-C2-C3-O3
17	2	3051	LHG	O2-C2-C3-O3
14	A	825	CLA	CBA-CGA-O2A-C1
14	a	824	CLA	CBA-CGA-O2A-C1
14	1	825	CLA	CBA-CGA-O2A-C1
14	B	3004	CLA	C8-C10-C11-C12
14	b	3004	CLA	C8-C10-C11-C12
14	2	3004	CLA	C8-C10-C11-C12
14	A	838	CLA	C3-C5-C6-C7
14	a	837	CLA	C3-C5-C6-C7
14	1	838	CLA	C3-C5-C6-C7
13	A	801	CL0	C8-C10-C11-C12
13	a	801	CL0	C8-C10-C11-C12
13	1	801	CL0	C8-C10-C11-C12
14	A	804	CLA	C15-C16-C17-C18
14	A	826	CLA	C13-C15-C16-C17
14	A	832	CLA	C5-C6-C7-C8
14	A	843	CLA	C13-C15-C16-C17
14	B	3025	CLA	C15-C16-C17-C18
14	B	3039	CLA	C13-C15-C16-C17
14	L	203	CLA	C8-C10-C11-C12
14	a	825	CLA	C13-C15-C16-C17
14	a	831	CLA	C5-C6-C7-C8
14	a	842	CLA	C13-C15-C16-C17
14	b	3025	CLA	C15-C16-C17-C18
14	b	3039	CLA	C13-C15-C16-C17
14	j	1101	CLA	C15-C16-C17-C18
14	l	206	CLA	C8-C10-C11-C12
14	1	804	CLA	C15-C16-C17-C18
14	1	826	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	1	832	CLA	C5-C6-C7-C8
14	1	843	CLA	C13-C15-C16-C17
14	2	3025	CLA	C15-C16-C17-C18
14	2	3039	CLA	C13-C15-C16-C17
14	0	207	CLA	C8-C10-C11-C12
14	A	829	CLA	O1A-CGA-O2A-C1
14	B	3029	CLA	O1A-CGA-O2A-C1
14	a	828	CLA	O1A-CGA-O2A-C1
14	b	3029	CLA	O1A-CGA-O2A-C1
14	1	829	CLA	O1A-CGA-O2A-C1
14	2	3029	CLA	O1A-CGA-O2A-C1
14	B	3034	CLA	C2-C3-C5-C6
14	2	3034	CLA	C2-C3-C5-C6
14	B	3040	CLA	O1D-CGD-O2D-CED
14	b	3040	CLA	O1D-CGD-O2D-CED
14	2	3040	CLA	O1D-CGD-O2D-CED
14	B	3034	CLA	C13-C15-C16-C17
14	b	3034	CLA	C13-C15-C16-C17
14	2	3034	CLA	C13-C15-C16-C17
14	B	3004	CLA	O1A-CGA-O2A-C1
14	b	3004	CLA	O1A-CGA-O2A-C1
14	b	3035	CLA	O1A-CGA-O2A-C1
14	2	3004	CLA	O1A-CGA-O2A-C1
14	A	842	CLA	O1D-CGD-O2D-CED
14	a	841	CLA	O1D-CGD-O2D-CED
14	1	842	CLA	O1D-CGD-O2D-CED
14	B	3035	CLA	O1A-CGA-O2A-C1
14	2	3035	CLA	O1A-CGA-O2A-C1
14	L	204	CLA	C2C-C3C-CAC-CBC
14	l	207	CLA	C2C-C3C-CAC-CBC
14	0	208	CLA	C2C-C3C-CAC-CBC
17	L	207	LHG	C32-C33-C34-C35
17	l	201	LHG	C32-C33-C34-C35
17	0	201	LHG	C32-C33-C34-C35
17	B	3051	LHG	C1-C2-C3-O3
17	b	3051	LHG	C1-C2-C3-O3
17	2	3051	LHG	C1-C2-C3-O3
14	B	3028	CLA	C2A-CAA-CBA-CGA
14	b	3028	CLA	C2A-CAA-CBA-CGA
14	2	3028	CLA	C2A-CAA-CBA-CGA
14	A	812	CLA	CBA-CGA-O2A-C1
14	A	824	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	839	CLA	CBA-CGA-O2A-C1
14	B	3030	CLA	CBA-CGA-O2A-C1
14	a	811	CLA	CBA-CGA-O2A-C1
14	a	823	CLA	CBA-CGA-O2A-C1
14	a	838	CLA	CBA-CGA-O2A-C1
14	b	3030	CLA	CBA-CGA-O2A-C1
14	1	812	CLA	CBA-CGA-O2A-C1
14	1	824	CLA	CBA-CGA-O2A-C1
14	1	839	CLA	CBA-CGA-O2A-C1
14	2	3030	CLA	CBA-CGA-O2A-C1
16	F	202	BCR	C14-C15-C16-C17
16	f	202	BCR	C14-C15-C16-C17
16	6	202	BCR	C14-C15-C16-C17
14	A	818	CLA	C10-C11-C12-C13
14	B	3006	CLA	C8-C10-C11-C12
14	B	3012	CLA	C13-C15-C16-C17
14	B	3017	CLA	C5-C6-C7-C8
14	B	3035	CLA	C15-C16-C17-C18
14	a	817	CLA	C10-C11-C12-C13
14	b	3006	CLA	C8-C10-C11-C12
14	b	3012	CLA	C13-C15-C16-C17
14	b	3017	CLA	C5-C6-C7-C8
14	b	3035	CLA	C15-C16-C17-C18
14	1	818	CLA	C10-C11-C12-C13
14	2	3006	CLA	C8-C10-C11-C12
14	2	3012	CLA	C13-C15-C16-C17
14	2	3017	CLA	C5-C6-C7-C8
14	2	3026	CLA	C10-C11-C12-C13
14	2	3035	CLA	C15-C16-C17-C18
14	A	826	CLA	CBD-CGD-O2D-CED
14	a	825	CLA	CBD-CGD-O2D-CED
14	1	826	CLA	CBD-CGD-O2D-CED
14	A	818	CLA	O1D-CGD-O2D-CED
14	B	3012	CLA	O1D-CGD-O2D-CED
14	a	817	CLA	O1D-CGD-O2D-CED
14	b	3012	CLA	O1D-CGD-O2D-CED
14	1	818	CLA	O1D-CGD-O2D-CED
14	2	3012	CLA	O1D-CGD-O2D-CED
14	B	3026	CLA	C10-C11-C12-C13
14	b	3026	CLA	C10-C11-C12-C13
14	A	809	CLA	C15-C16-C17-C18
14	A	838	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	A	841	CLA	C5-C6-C7-C8
14	B	3007	CLA	C15-C16-C17-C18
14	a	808	CLA	C15-C16-C17-C18
14	a	837	CLA	C13-C15-C16-C17
14	a	840	CLA	C5-C6-C7-C8
14	b	3007	CLA	C15-C16-C17-C18
14	1	809	CLA	C15-C16-C17-C18
14	1	838	CLA	C13-C15-C16-C17
14	1	841	CLA	C5-C6-C7-C8
14	2	3007	CLA	C15-C16-C17-C18
14	A	840	CLA	C13-C15-C16-C17
14	a	839	CLA	C13-C15-C16-C17
14	1	840	CLA	C13-C15-C16-C17
14	L	204	CLA	C3-C5-C6-C7
14	l	207	CLA	C3-C5-C6-C7
14	0	208	CLA	C3-C5-C6-C7
14	B	3007	CLA	CBA-CGA-O2A-C1
14	b	3007	CLA	CBA-CGA-O2A-C1
14	2	3007	CLA	CBA-CGA-O2A-C1
16	A	846	BCR	C11-C10-C9-C34
16	A	849	BCR	C35-C13-C14-C15
16	A	852	BCR	C35-C13-C14-C15
16	B	3052	BCR	C16-C17-C18-C36
16	B	3053	BCR	C35-C13-C14-C15
16	I	101	BCR	C35-C13-C14-C15
16	I	101	BCR	C16-C17-C18-C36
16	L	206	BCR	C11-C10-C9-C34
16	L	206	BCR	C16-C17-C18-C36
16	M	1602	BCR	C16-C17-C18-C36
16	a	845	BCR	C11-C10-C9-C34
16	a	848	BCR	C35-C13-C14-C15
16	a	851	BCR	C35-C13-C14-C15
16	i	101	BCR	C35-C13-C14-C15
16	i	101	BCR	C16-C17-C18-C36
16	j	1106	BCR	C35-C13-C14-C15
16	l	204	BCR	C16-C17-C18-C36
16	l	210	BCR	C11-C10-C9-C34
16	l	210	BCR	C16-C17-C18-C36
16	m	101	BCR	C16-C17-C18-C36
16	1	848	BCR	C35-C13-C14-C15
16	1	851	BCR	C35-C13-C14-C15
16	2	3052	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
16	7	101	BCR	C35-C13-C14-C15
16	7	101	BCR	C16-C17-C18-C36
16	9	102	BCR	C11-C10-C9-C34
16	0	205	BCR	C16-C17-C18-C36
16	0	211	BCR	C11-C10-C9-C34
16	0	211	BCR	C16-C17-C18-C36
16	y	101	BCR	C16-C17-C18-C36
14	b	3003	CLA	O1D-CGD-O2D-CED
16	A	848	BCR	C7-C8-C9-C34
16	A	852	BCR	C11-C12-C13-C35
16	B	3044	BCR	C37-C22-C23-C24
16	a	847	BCR	C7-C8-C9-C34
16	a	851	BCR	C11-C12-C13-C35
16	b	3044	BCR	C37-C22-C23-C24
16	1	847	BCR	C7-C8-C9-C34
16	1	851	BCR	C11-C12-C13-C35
16	2	3044	BCR	C37-C22-C23-C24
14	A	825	CLA	O1A-CGA-O2A-C1
14	a	824	CLA	O1A-CGA-O2A-C1
14	1	825	CLA	O1A-CGA-O2A-C1
14	A	802	CLA	C2A-CAA-CBA-CGA
14	A	818	CLA	C2A-CAA-CBA-CGA
14	A	823	CLA	C2A-CAA-CBA-CGA
14	A	832	CLA	C2A-CAA-CBA-CGA
14	B	3024	CLA	C2A-CAA-CBA-CGA
14	a	802	CLA	C2A-CAA-CBA-CGA
14	a	817	CLA	C2A-CAA-CBA-CGA
14	a	822	CLA	C2A-CAA-CBA-CGA
14	a	831	CLA	C2A-CAA-CBA-CGA
14	b	3024	CLA	C2A-CAA-CBA-CGA
14	1	802	CLA	C2A-CAA-CBA-CGA
14	1	818	CLA	C2A-CAA-CBA-CGA
14	1	823	CLA	C2A-CAA-CBA-CGA
14	1	832	CLA	C2A-CAA-CBA-CGA
14	2	3024	CLA	C2A-CAA-CBA-CGA
14	A	838	CLA	C15-C16-C17-C18
14	B	3016	CLA	C13-C15-C16-C17
14	a	806	CLA	C8-C10-C11-C12
14	a	837	CLA	C15-C16-C17-C18
14	b	3016	CLA	C13-C15-C16-C17
14	1	807	CLA	C8-C10-C11-C12
14	1	838	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	A	806	CLA	O2A-C1-C2-C3
14	a	805	CLA	O2A-C1-C2-C3
14	1	806	CLA	O2A-C1-C2-C3
14	A	816	CLA	C16-C17-C18-C19
14	B	3016	CLA	C16-C17-C18-C20
14	B	3019	CLA	C16-C17-C18-C20
14	b	3016	CLA	C16-C17-C18-C20
14	b	3019	CLA	C16-C17-C18-C20
14	1	816	CLA	C16-C17-C18-C19
14	2	3016	CLA	C16-C17-C18-C20
14	2	3019	CLA	C16-C17-C18-C20
17	A	854	LHG	C29-C30-C31-C32
17	a	853	LHG	C29-C30-C31-C32
14	B	3003	CLA	O1D-CGD-O2D-CED
14	2	3003	CLA	O1D-CGD-O2D-CED
14	A	832	CLA	O1A-CGA-O2A-C1
14	a	831	CLA	O1A-CGA-O2A-C1
14	1	832	CLA	O1A-CGA-O2A-C1
14	A	803	CLA	C3-C5-C6-C7
14	a	803	CLA	C3-C5-C6-C7
14	1	803	CLA	C3-C5-C6-C7
14	A	807	CLA	C8-C10-C11-C12
14	2	3016	CLA	C13-C15-C16-C17
16	A	847	BCR	C12-C13-C14-C15
16	A	851	BCR	C12-C13-C14-C15
16	A	852	BCR	C11-C10-C9-C8
16	B	3053	BCR	C12-C13-C14-C15
16	F	202	BCR	C11-C10-C9-C8
16	I	101	BCR	C16-C17-C18-C19
16	I	102	BCR	C20-C21-C22-C23
16	J	103	BCR	C11-C10-C9-C8
16	L	206	BCR	C12-C13-C14-C15
16	M	1602	BCR	C11-C10-C9-C8
16	a	846	BCR	C12-C13-C14-C15
16	a	850	BCR	C12-C13-C14-C15
16	a	851	BCR	C11-C10-C9-C8
16	f	202	BCR	C11-C10-C9-C8
16	i	101	BCR	C16-C17-C18-C19
16	j	1104	BCR	C11-C10-C9-C8
16	j	1106	BCR	C12-C13-C14-C15
16	l	209	BCR	C20-C21-C22-C23
16	l	210	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
16	m	101	BCR	C11-C10-C9-C8
16	1	846	BCR	C12-C13-C14-C15
16	1	850	BCR	C12-C13-C14-C15
16	1	851	BCR	C11-C10-C9-C8
16	2	3052	BCR	C12-C13-C14-C15
16	6	202	BCR	C11-C10-C9-C8
16	7	101	BCR	C16-C17-C18-C19
16	8	103	BCR	C11-C10-C9-C8
16	0	210	BCR	C20-C21-C22-C23
16	0	211	BCR	C12-C13-C14-C15
16	y	101	BCR	C11-C10-C9-C8
17	1	853	LHG	C29-C30-C31-C32
17	L	208	LHG	C8-C7-O7-C5
17	l	202	LHG	C8-C7-O7-C5
17	0	202	LHG	C8-C7-O7-C5
14	A	811	CLA	O1D-CGD-O2D-CED
14	B	3034	CLA	O1D-CGD-O2D-CED
14	a	810	CLA	O1D-CGD-O2D-CED
14	b	3034	CLA	O1D-CGD-O2D-CED
14	1	811	CLA	O1D-CGD-O2D-CED
14	2	3034	CLA	O1D-CGD-O2D-CED
14	A	822	CLA	C15-C16-C17-C18
14	A	829	CLA	C10-C11-C12-C13
14	B	3025	CLA	C10-C11-C12-C13
14	B	3035	CLA	C10-C11-C12-C13
14	B	3039	CLA	C15-C16-C17-C18
14	a	821	CLA	C15-C16-C17-C18
14	a	828	CLA	C10-C11-C12-C13
14	b	3025	CLA	C10-C11-C12-C13
14	b	3035	CLA	C10-C11-C12-C13
14	b	3039	CLA	C15-C16-C17-C18
14	1	822	CLA	C15-C16-C17-C18
14	1	829	CLA	C10-C11-C12-C13
14	2	3025	CLA	C10-C11-C12-C13
14	2	3035	CLA	C10-C11-C12-C13
14	2	3039	CLA	C15-C16-C17-C18
14	A	805	CLA	C2C-C3C-CAC-CBC
14	a	804	CLA	C2C-C3C-CAC-CBC
14	1	805	CLA	C2C-C3C-CAC-CBC
14	A	821	CLA	C16-C17-C18-C19
14	A	836	CLA	C16-C17-C18-C19
14	A	843	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	B	3031	CLA	C6-C7-C8-C9
14	B	3031	CLA	C6-C7-C8-C10
14	a	815	CLA	C16-C17-C18-C19
14	a	820	CLA	C16-C17-C18-C19
14	a	835	CLA	C16-C17-C18-C19
14	a	842	CLA	C16-C17-C18-C19
14	b	3031	CLA	C6-C7-C8-C9
14	b	3031	CLA	C6-C7-C8-C10
14	1	821	CLA	C16-C17-C18-C19
14	1	836	CLA	C16-C17-C18-C19
14	1	843	CLA	C16-C17-C18-C19
14	2	3031	CLA	C6-C7-C8-C10
14	A	812	CLA	O1A-CGA-O2A-C1
14	a	811	CLA	O1A-CGA-O2A-C1
14	1	812	CLA	O1A-CGA-O2A-C1
14	a	824	CLA	C13-C15-C16-C17
14	A	825	CLA	C13-C15-C16-C17
14	1	825	CLA	C13-C15-C16-C17
14	A	821	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	CBA-CGA-O2A-C1
14	a	820	CLA	CBA-CGA-O2A-C1
14	a	837	CLA	CBA-CGA-O2A-C1
14	1	821	CLA	CBA-CGA-O2A-C1
14	1	838	CLA	CBA-CGA-O2A-C1
17	A	853	LHG	C10-C11-C12-C13
17	a	852	LHG	C10-C11-C12-C13
17	1	852	LHG	C10-C11-C12-C13
17	L	208	LHG	O1-C1-C2-O2
17	l	202	LHG	O1-C1-C2-O2
17	0	202	LHG	O1-C1-C2-O2
17	A	853	LHG	C9-C10-C11-C12
17	a	852	LHG	C9-C10-C11-C12
14	A	827	CLA	C8-C10-C11-C12
14	a	820	CLA	C15-C16-C17-C18
14	a	826	CLA	C8-C10-C11-C12
14	1	827	CLA	C8-C10-C11-C12
14	A	813	CLA	C4B-C3B-CAB-CBB
14	A	815	CLA	C4B-C3B-CAB-CBB
14	A	819	CLA	C4B-C3B-CAB-CBB
14	A	824	CLA	C4B-C3B-CAB-CBB
14	A	835	CLA	C4B-C3B-CAB-CBB
14	a	812	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	a	814	CLA	C4B-C3B-CAB-CBB
14	a	818	CLA	C4B-C3B-CAB-CBB
14	a	823	CLA	C4B-C3B-CAB-CBB
14	1	813	CLA	C4B-C3B-CAB-CBB
14	1	815	CLA	C4B-C3B-CAB-CBB
14	1	819	CLA	C4B-C3B-CAB-CBB
14	1	824	CLA	C4B-C3B-CAB-CBB
17	1	852	LHG	C9-C10-C11-C12
14	A	816	CLA	C16-C17-C18-C20
14	A	819	CLA	C16-C17-C18-C19
14	A	819	CLA	C16-C17-C18-C20
14	A	824	CLA	C16-C17-C18-C20
14	A	839	CLA	C16-C17-C18-C20
14	B	3006	CLA	C16-C17-C18-C19
14	B	3016	CLA	C16-C17-C18-C19
14	B	3019	CLA	C16-C17-C18-C19
14	a	815	CLA	C16-C17-C18-C20
14	a	818	CLA	C16-C17-C18-C19
14	a	818	CLA	C16-C17-C18-C20
14	a	823	CLA	C16-C17-C18-C20
14	a	838	CLA	C16-C17-C18-C20
14	b	3006	CLA	C16-C17-C18-C19
14	b	3016	CLA	C16-C17-C18-C19
14	b	3019	CLA	C16-C17-C18-C19
14	1	816	CLA	C16-C17-C18-C20
14	1	819	CLA	C16-C17-C18-C19
14	1	819	CLA	C16-C17-C18-C20
14	1	824	CLA	C16-C17-C18-C20
14	1	839	CLA	C16-C17-C18-C20
14	2	3006	CLA	C16-C17-C18-C19
14	2	3016	CLA	C16-C17-C18-C19
14	2	3019	CLA	C16-C17-C18-C19
14	2	3031	CLA	C6-C7-C8-C9
14	A	813	CLA	C2A-CAA-CBA-CGA
14	A	822	CLA	C2A-CAA-CBA-CGA
14	a	812	CLA	C2A-CAA-CBA-CGA
14	a	821	CLA	C2A-CAA-CBA-CGA
14	1	813	CLA	C2A-CAA-CBA-CGA
14	1	822	CLA	C2A-CAA-CBA-CGA
14	A	821	CLA	C15-C16-C17-C18
14	A	842	CLA	C10-C11-C12-C13
14	B	3007	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	a	841	CLA	C10-C11-C12-C13
14	b	3007	CLA	C10-C11-C12-C13
14	1	821	CLA	C15-C16-C17-C18
14	1	842	CLA	C10-C11-C12-C13
14	2	3007	CLA	C10-C11-C12-C13
20	B	3050	LMG	C11-C10-O7-C8
20	b	3050	LMG	C11-C10-O7-C8
20	2	3050	LMG	C11-C10-O7-C8
14	A	809	CLA	C6-C7-C8-C10
14	B	3011	CLA	C11-C12-C13-C15
14	B	3018	CLA	C11-C12-C13-C15
14	B	3027	CLA	C12-C13-C15-C16
14	a	808	CLA	C6-C7-C8-C10
14	b	3011	CLA	C11-C12-C13-C15
14	b	3018	CLA	C11-C12-C13-C15
14	b	3027	CLA	C12-C13-C15-C16
14	1	809	CLA	C6-C7-C8-C10
14	2	3011	CLA	C11-C12-C13-C15
14	2	3018	CLA	C11-C12-C13-C15
14	2	3027	CLA	C12-C13-C15-C16
17	B	3051	LHG	C32-C33-C34-C35
17	b	3051	LHG	C32-C33-C34-C35
17	2	3051	LHG	C32-C33-C34-C35
14	A	806	CLA	C13-C15-C16-C17
14	A	819	CLA	C8-C10-C11-C12
14	a	805	CLA	C13-C15-C16-C17
14	a	818	CLA	C8-C10-C11-C12
14	1	806	CLA	C13-C15-C16-C17
14	1	819	CLA	C8-C10-C11-C12
14	2	3015	CLA	C8-C10-C11-C12
14	a	838	CLA	O1A-CGA-O2A-C1
14	1	839	CLA	O1A-CGA-O2A-C1
14	A	809	CLA	C3-C5-C6-C7
14	A	817	CLA	C3-C5-C6-C7
14	B	3010	CLA	C3-C5-C6-C7
14	a	808	CLA	C3-C5-C6-C7
14	a	816	CLA	C3-C5-C6-C7
14	b	3010	CLA	C3-C5-C6-C7
14	1	809	CLA	C3-C5-C6-C7
14	1	817	CLA	C3-C5-C6-C7
14	2	3010	CLA	C3-C5-C6-C7
14	A	807	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	B	3011	CLA	C3A-C2A-CAA-CBA
14	B	3038	CLA	C3A-C2A-CAA-CBA
14	a	806	CLA	C3A-C2A-CAA-CBA
14	b	3011	CLA	C3A-C2A-CAA-CBA
14	b	3038	CLA	C3A-C2A-CAA-CBA
14	1	807	CLA	C3A-C2A-CAA-CBA
14	2	3011	CLA	C3A-C2A-CAA-CBA
14	2	3038	CLA	C3A-C2A-CAA-CBA
14	A	806	CLA	O1D-CGD-O2D-CED
14	B	3028	CLA	O1D-CGD-O2D-CED
14	a	805	CLA	O1D-CGD-O2D-CED
14	1	806	CLA	O1D-CGD-O2D-CED
17	A	853	LHG	C27-C28-C29-C30
17	L	207	LHG	C34-C35-C36-C37
17	a	852	LHG	C27-C28-C29-C30
17	1	852	LHG	C27-C28-C29-C30
17	A	853	LHG	C32-C33-C34-C35
17	a	852	LHG	C32-C33-C34-C35
17	1	201	LHG	C34-C35-C36-C37
17	1	852	LHG	C32-C33-C34-C35
17	0	201	LHG	C34-C35-C36-C37
14	A	804	CLA	C10-C11-C12-C13
14	B	3015	CLA	C8-C10-C11-C12
14	b	3015	CLA	C8-C10-C11-C12
14	2	3030	CLA	C13-C15-C16-C17
14	b	3028	CLA	O1D-CGD-O2D-CED
14	2	3028	CLA	O1D-CGD-O2D-CED
16	A	848	BCR	C19-C20-C21-C22
16	a	847	BCR	C19-C20-C21-C22
16	1	847	BCR	C19-C20-C21-C22
14	A	824	CLA	O1A-CGA-O2A-C1
14	A	839	CLA	O1A-CGA-O2A-C1
14	B	3007	CLA	O1A-CGA-O2A-C1
14	B	3030	CLA	O1A-CGA-O2A-C1
14	a	823	CLA	O1A-CGA-O2A-C1
14	b	3007	CLA	O1A-CGA-O2A-C1
14	b	3030	CLA	O1A-CGA-O2A-C1
14	1	824	CLA	O1A-CGA-O2A-C1
14	2	3007	CLA	O1A-CGA-O2A-C1
14	2	3030	CLA	O1A-CGA-O2A-C1
14	B	3030	CLA	C13-C15-C16-C17
14	b	3030	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	1	804	CLA	C10-C11-C12-C13
17	L	208	LHG	C4-C5-C6-O8
17	l	202	LHG	C4-C5-C6-O8
17	0	202	LHG	C4-C5-C6-O8
17	A	853	LHG	C11-C10-C9-C8
17	L	208	LHG	C12-C13-C14-C15
17	a	852	LHG	C11-C10-C9-C8
17	l	202	LHG	C12-C13-C14-C15
17	1	852	LHG	C11-C10-C9-C8
17	0	202	LHG	C12-C13-C14-C15
14	A	827	CLA	C3-C5-C6-C7
14	a	826	CLA	C3-C5-C6-C7
14	1	827	CLA	C3-C5-C6-C7
17	L	208	LHG	C23-C24-C25-C26
17	l	202	LHG	C23-C24-C25-C26
17	0	202	LHG	C23-C24-C25-C26
14	j	1101	CLA	C10-C11-C12-C13
17	B	3051	LHG	C13-C14-C15-C16
17	b	3051	LHG	C13-C14-C15-C16
17	2	3051	LHG	C13-C14-C15-C16
20	b	3050	LMG	C35-C36-C37-C38
20	2	3050	LMG	C35-C36-C37-C38
14	B	3030	CLA	C8-C10-C11-C12
14	2	3030	CLA	C8-C10-C11-C12
14	B	3024	CLA	O1D-CGD-O2D-CED
14	b	3024	CLA	O1D-CGD-O2D-CED
14	2	3024	CLA	O1D-CGD-O2D-CED
17	b	3051	LHG	C15-C16-C17-C18
17	2	3051	LHG	C15-C16-C17-C18
20	B	3050	LMG	C35-C36-C37-C38
14	A	836	CLA	C16-C17-C18-C20
14	a	835	CLA	C16-C17-C18-C20
14	1	836	CLA	C16-C17-C18-C20
14	A	813	CLA	C2B-C3B-CAB-CBB
14	A	815	CLA	C2B-C3B-CAB-CBB
14	B	3021	CLA	C2B-C3B-CAB-CBB
14	a	812	CLA	C2B-C3B-CAB-CBB
14	a	814	CLA	C2B-C3B-CAB-CBB
14	b	3021	CLA	C2B-C3B-CAB-CBB
14	1	813	CLA	C2B-C3B-CAB-CBB
14	1	815	CLA	C2B-C3B-CAB-CBB
14	2	3021	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	A	851	BCR	C1-C6-C7-C8
16	A	851	BCR	C5-C6-C7-C8
16	A	851	BCR	C23-C24-C25-C26
16	A	851	BCR	C23-C24-C25-C30
16	A	852	BCR	C1-C6-C7-C8
16	B	3048	BCR	C23-C24-C25-C26
16	B	3048	BCR	C23-C24-C25-C30
16	B	3053	BCR	C23-C24-C25-C30
16	J	103	BCR	C1-C6-C7-C8
16	J	103	BCR	C5-C6-C7-C8
16	J	104	BCR	C23-C24-C25-C30
16	M	1602	BCR	C1-C6-C7-C8
16	M	1602	BCR	C5-C6-C7-C8
16	a	850	BCR	C1-C6-C7-C8
16	a	850	BCR	C5-C6-C7-C8
16	a	850	BCR	C23-C24-C25-C26
16	a	850	BCR	C23-C24-C25-C30
16	a	851	BCR	C1-C6-C7-C8
16	b	3048	BCR	C23-C24-C25-C26
16	b	3048	BCR	C23-C24-C25-C30
16	j	1104	BCR	C1-C6-C7-C8
16	j	1104	BCR	C5-C6-C7-C8
16	j	1105	BCR	C23-C24-C25-C30
16	j	1106	BCR	C23-C24-C25-C30
16	m	101	BCR	C1-C6-C7-C8
16	m	101	BCR	C5-C6-C7-C8
16	1	850	BCR	C1-C6-C7-C8
16	1	850	BCR	C5-C6-C7-C8
16	1	850	BCR	C23-C24-C25-C26
16	1	850	BCR	C23-C24-C25-C30
16	1	851	BCR	C1-C6-C7-C8
16	2	3048	BCR	C23-C24-C25-C26
16	2	3048	BCR	C23-C24-C25-C30
16	2	3052	BCR	C23-C24-C25-C30
16	8	103	BCR	C1-C6-C7-C8
16	8	103	BCR	C5-C6-C7-C8
16	8	104	BCR	C23-C24-C25-C30
16	y	101	BCR	C1-C6-C7-C8
16	y	101	BCR	C5-C6-C7-C8
17	B	3051	LHG	C15-C16-C17-C18
17	A	853	LHG	C8-C7-O7-C5
17	a	852	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
17	1	852	LHG	C8-C7-O7-C5
14	A	802	CLA	C8-C10-C11-C12
14	a	802	CLA	C8-C10-C11-C12
14	b	3030	CLA	C8-C10-C11-C12
14	1	802	CLA	C8-C10-C11-C12
13	A	801	CL0	C3-C5-C6-C7
13	a	801	CL0	C3-C5-C6-C7
13	1	801	CL0	C3-C5-C6-C7
14	B	3023	CLA	C3-C5-C6-C7
14	b	3023	CLA	C3-C5-C6-C7
14	2	3023	CLA	C3-C5-C6-C7
17	a	853	LHG	C10-C11-C12-C13
17	1	853	LHG	C10-C11-C12-C13
17	A	854	LHG	C10-C11-C12-C13
14	B	3031	CLA	C2A-CAA-CBA-CGA
14	b	3031	CLA	C2A-CAA-CBA-CGA
14	2	3031	CLA	C2A-CAA-CBA-CGA
14	b	3021	CLA	C10-C11-C12-C13
14	2	3021	CLA	C10-C11-C12-C13
17	l	202	LHG	C15-C16-C17-C18
14	A	821	CLA	C4-C3-C5-C6
14	a	820	CLA	C4-C3-C5-C6
14	1	821	CLA	C4-C3-C5-C6
17	L	208	LHG	C15-C16-C17-C18
17	0	202	LHG	C15-C16-C17-C18
16	A	847	BCR	C10-C11-C12-C13
16	A	848	BCR	C18-C19-C20-C21
16	a	846	BCR	C10-C11-C12-C13
16	a	847	BCR	C18-C19-C20-C21
16	1	846	BCR	C10-C11-C12-C13
16	1	847	BCR	C18-C19-C20-C21
14	B	3007	CLA	C13-C15-C16-C17
14	B	3021	CLA	C10-C11-C12-C13
14	2	3007	CLA	C13-C15-C16-C17
17	A	853	LHG	C24-C25-C26-C27
14	A	840	CLA	CBA-CGA-O2A-C1
14	B	3023	CLA	CBA-CGA-O2A-C1
14	a	839	CLA	CBA-CGA-O2A-C1
14	b	3023	CLA	CBA-CGA-O2A-C1
14	1	840	CLA	CBA-CGA-O2A-C1
14	2	3023	CLA	CBA-CGA-O2A-C1
14	B	3041	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	b	3041	CLA	C6-C7-C8-C9
14	2	3041	CLA	C6-C7-C8-C9
17	A	854	LHG	C26-C27-C28-C29
17	a	852	LHG	C24-C25-C26-C27
17	a	853	LHG	C26-C27-C28-C29
17	1	853	LHG	C26-C27-C28-C29
17	1	852	LHG	C24-C25-C26-C27
16	A	851	BCR	C14-C15-C16-C17
16	a	850	BCR	C14-C15-C16-C17
16	1	850	BCR	C14-C15-C16-C17
14	A	830	CLA	C8-C10-C11-C12
14	a	829	CLA	C8-C10-C11-C12
14	b	3007	CLA	C13-C15-C16-C17
14	1	830	CLA	C8-C10-C11-C12
14	A	830	CLA	C13-C15-C16-C17
14	a	829	CLA	C13-C15-C16-C17
14	1	830	CLA	C13-C15-C16-C17
14	2	3026	CLA	C3-C5-C6-C7
14	A	821	CLA	C16-C17-C18-C20
14	a	820	CLA	C16-C17-C18-C20
14	1	821	CLA	C16-C17-C18-C20
14	a	837	CLA	O1A-CGA-O2A-C1
14	1	838	CLA	O1A-CGA-O2A-C1
14	A	810	CLA	C15-C16-C17-C18
14	B	3030	CLA	C5-C6-C7-C8
14	a	809	CLA	C15-C16-C17-C18
14	b	3030	CLA	C5-C6-C7-C8
14	1	810	CLA	C15-C16-C17-C18
14	2	3030	CLA	C5-C6-C7-C8
17	L	207	LHG	O9-C7-O7-C5
17	l	201	LHG	O9-C7-O7-C5
17	0	201	LHG	O9-C7-O7-C5
20	B	3050	LMG	C31-C32-C33-C34
20	b	3050	LMG	C31-C32-C33-C34
20	2	3050	LMG	C31-C32-C33-C34
14	A	838	CLA	O1A-CGA-O2A-C1
14	B	3029	CLA	C13-C15-C16-C17
14	b	3029	CLA	C13-C15-C16-C17
14	2	3029	CLA	C13-C15-C16-C17
14	B	3026	CLA	C3-C5-C6-C7
14	b	3026	CLA	C3-C5-C6-C7
16	A	847	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	a	846	BCR	C11-C12-C13-C14
16	1	846	BCR	C11-C12-C13-C14
17	l	201	LHG	C33-C34-C35-C36
14	A	807	CLA	C16-C17-C18-C19
14	A	824	CLA	C16-C17-C18-C19
14	A	838	CLA	C16-C17-C18-C20
14	B	3017	CLA	C16-C17-C18-C19
14	B	3017	CLA	C16-C17-C18-C20
14	a	806	CLA	C16-C17-C18-C19
14	a	823	CLA	C16-C17-C18-C19
14	a	837	CLA	C16-C17-C18-C20
14	b	3017	CLA	C16-C17-C18-C19
14	b	3017	CLA	C16-C17-C18-C20
14	1	807	CLA	C16-C17-C18-C19
14	1	824	CLA	C16-C17-C18-C19
14	1	838	CLA	C16-C17-C18-C20
14	2	3017	CLA	C16-C17-C18-C19
14	2	3017	CLA	C16-C17-C18-C20
17	L	207	LHG	C33-C34-C35-C36
17	0	201	LHG	C33-C34-C35-C36
14	A	803	CLA	C4-C3-C5-C6
14	a	803	CLA	C4-C3-C5-C6
14	1	803	CLA	C4-C3-C5-C6
14	a	820	CLA	C2-C3-C5-C6
20	B	3050	LMG	C12-C13-C14-C15
20	b	3050	LMG	C12-C13-C14-C15
20	2	3050	LMG	C12-C13-C14-C15
14	A	821	CLA	O1A-CGA-O2A-C1
14	a	820	CLA	O1A-CGA-O2A-C1
14	1	821	CLA	O1A-CGA-O2A-C1
14	A	827	CLA	C15-C16-C17-C18
14	B	3028	CLA	C8-C10-C11-C12
14	a	826	CLA	C15-C16-C17-C18
14	b	3028	CLA	C8-C10-C11-C12
14	1	827	CLA	C15-C16-C17-C18
14	2	3028	CLA	C8-C10-C11-C12
14	2	3035	CLA	C13-C15-C16-C17
20	B	3050	LMG	C16-C17-C18-C19
20	b	3050	LMG	C16-C17-C18-C19
20	2	3050	LMG	C16-C17-C18-C19
14	B	3035	CLA	C13-C15-C16-C17
14	b	3035	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	A	838	CLA	C16-C17-C18-C19
14	B	3006	CLA	C16-C17-C18-C20
14	a	837	CLA	C16-C17-C18-C19
14	b	3006	CLA	C16-C17-C18-C20
14	1	838	CLA	C16-C17-C18-C19
14	2	3006	CLA	C16-C17-C18-C20
14	B	3003	CLA	C15-C16-C17-C18
14	b	3003	CLA	C15-C16-C17-C18
14	1	203	CLA	C5-C6-C7-C8
14	2	3003	CLA	C15-C16-C17-C18
20	B	3050	LMG	C18-C19-C20-C21
14	B	3021	CLA	C8-C10-C11-C12
14	L	201	CLA	C5-C6-C7-C8
14	b	3021	CLA	C8-C10-C11-C12
14	b	3035	CLA	C8-C10-C11-C12
14	2	3021	CLA	C8-C10-C11-C12
14	0	204	CLA	C5-C6-C7-C8
17	A	854	LHG	C32-C33-C34-C35
20	2	3050	LMG	C18-C19-C20-C21
14	A	837	CLA	CBD-CGD-O2D-CED
17	a	853	LHG	C32-C33-C34-C35
17	1	853	LHG	C32-C33-C34-C35
20	b	3050	LMG	C18-C19-C20-C21
14	A	807	CLA	C16-C17-C18-C20
14	a	806	CLA	C16-C17-C18-C20
14	1	807	CLA	C16-C17-C18-C20
14	B	3035	CLA	C8-C10-C11-C12
14	2	3035	CLA	C8-C10-C11-C12
14	A	805	CLA	C2-C3-C5-C6
14	A	812	CLA	C2-C3-C5-C6
14	A	821	CLA	C2-C3-C5-C6
14	a	804	CLA	C2-C3-C5-C6
14	a	811	CLA	C2-C3-C5-C6
14	1	805	CLA	C2-C3-C5-C6
14	1	812	CLA	C2-C3-C5-C6
14	1	821	CLA	C2-C3-C5-C6
14	A	803	CLA	C2A-CAA-CBA-CGA
14	B	3005	CLA	C2A-CAA-CBA-CGA
14	a	803	CLA	C2A-CAA-CBA-CGA
14	b	3005	CLA	C2A-CAA-CBA-CGA
14	1	803	CLA	C2A-CAA-CBA-CGA
14	2	3005	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	A	814	CLA	CBD-CGD-O2D-CED
14	a	813	CLA	CBD-CGD-O2D-CED
14	a	836	CLA	CBD-CGD-O2D-CED
14	1	814	CLA	CBD-CGD-O2D-CED
14	1	837	CLA	CBD-CGD-O2D-CED
14	A	812	CLA	C8-C10-C11-C12
14	a	811	CLA	C8-C10-C11-C12
14	1	812	CLA	C8-C10-C11-C12
17	A	853	LHG	O1-C1-C2-O2
17	L	207	LHG	O1-C1-C2-O2
17	a	852	LHG	O1-C1-C2-O2
17	l	201	LHG	O1-C1-C2-O2
17	1	852	LHG	O1-C1-C2-O2
17	0	201	LHG	O1-C1-C2-O2
14	A	840	CLA	O1A-CGA-O2A-C1
14	B	3023	CLA	O1A-CGA-O2A-C1
14	a	839	CLA	O1A-CGA-O2A-C1
14	b	3023	CLA	O1A-CGA-O2A-C1
14	1	840	CLA	O1A-CGA-O2A-C1
14	2	3023	CLA	O1A-CGA-O2A-C1
14	A	809	CLA	C1A-C2A-CAA-CBA
14	A	824	CLA	C1A-C2A-CAA-CBA
14	A	830	CLA	C1A-C2A-CAA-CBA
14	B	3007	CLA	C1A-C2A-CAA-CBA
14	B	3019	CLA	C1A-C2A-CAA-CBA
14	B	3026	CLA	C1A-C2A-CAA-CBA
14	B	3033	CLA	C1A-C2A-CAA-CBA
14	B	3038	CLA	C1A-C2A-CAA-CBA
14	K	101	CLA	C1A-C2A-CAA-CBA
14	a	808	CLA	C1A-C2A-CAA-CBA
14	a	823	CLA	C1A-C2A-CAA-CBA
14	a	829	CLA	C1A-C2A-CAA-CBA
14	b	3007	CLA	C1A-C2A-CAA-CBA
14	b	3019	CLA	C1A-C2A-CAA-CBA
14	b	3026	CLA	C1A-C2A-CAA-CBA
14	b	3033	CLA	C1A-C2A-CAA-CBA
14	b	3038	CLA	C1A-C2A-CAA-CBA
14	k	101	CLA	C1A-C2A-CAA-CBA
14	1	809	CLA	C1A-C2A-CAA-CBA
14	1	824	CLA	C1A-C2A-CAA-CBA
14	1	830	CLA	C1A-C2A-CAA-CBA
14	2	3007	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	2	3019	CLA	C1A-C2A-CAA-CBA
14	2	3026	CLA	C1A-C2A-CAA-CBA
14	2	3033	CLA	C1A-C2A-CAA-CBA
14	2	3038	CLA	C1A-C2A-CAA-CBA
14	B	3015	CLA	O1D-CGD-O2D-CED
14	B	3004	CLA	C15-C16-C17-C18
14	b	3004	CLA	C15-C16-C17-C18
14	2	3004	CLA	C15-C16-C17-C18
14	a	830	CLA	C5-C6-C7-C8
14	1	831	CLA	C5-C6-C7-C8
14	b	3015	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	C12-C13-C15-C16
13	a	801	CL0	C12-C13-C15-C16
13	1	801	CL0	C12-C13-C15-C16
14	A	806	CLA	C11-C12-C13-C15
14	A	807	CLA	C11-C12-C13-C15
14	A	810	CLA	C11-C12-C13-C15
14	A	818	CLA	C12-C13-C15-C16
14	A	827	CLA	C12-C13-C15-C16
14	A	843	CLA	C12-C13-C15-C16
14	B	3005	CLA	C11-C10-C8-C7
14	B	3035	CLA	C12-C13-C15-C16
14	B	3041	CLA	C11-C12-C13-C15
14	L	201	CLA	C6-C7-C8-C10
14	a	805	CLA	C11-C12-C13-C15
14	a	806	CLA	C11-C12-C13-C15
14	a	809	CLA	C11-C12-C13-C15
14	a	817	CLA	C12-C13-C15-C16
14	a	826	CLA	C12-C13-C15-C16
14	a	842	CLA	C12-C13-C15-C16
14	b	3005	CLA	C11-C10-C8-C7
14	b	3035	CLA	C12-C13-C15-C16
14	b	3041	CLA	C11-C12-C13-C15
14	l	203	CLA	C6-C7-C8-C10
14	1	806	CLA	C11-C12-C13-C15
14	1	807	CLA	C11-C12-C13-C15
14	1	810	CLA	C11-C12-C13-C15
14	1	818	CLA	C12-C13-C15-C16
14	1	827	CLA	C12-C13-C15-C16
14	1	843	CLA	C12-C13-C15-C16
14	2	3005	CLA	C11-C10-C8-C7
14	2	3035	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	2	3041	CLA	C11-C12-C13-C15
14	0	204	CLA	C6-C7-C8-C10
14	A	835	CLA	C16-C17-C18-C20
14	B	3023	CLA	C6-C7-C8-C10
14	a	834	CLA	C16-C17-C18-C20
14	b	3023	CLA	C6-C7-C8-C10
14	1	835	CLA	C16-C17-C18-C20
14	2	3023	CLA	C6-C7-C8-C10
14	A	831	CLA	C5-C6-C7-C8
14	2	3015	CLA	O1D-CGD-O2D-CED
17	b	3051	LHG	C16-C17-C18-C19
17	2	3051	LHG	C16-C17-C18-C19
14	A	834	CLA	C4-C3-C5-C6
14	a	833	CLA	C4-C3-C5-C6
14	1	834	CLA	C4-C3-C5-C6
14	A	803	CLA	C2-C3-C5-C6
14	a	803	CLA	C2-C3-C5-C6
14	1	803	CLA	C2-C3-C5-C6
17	B	3051	LHG	C16-C17-C18-C19
17	L	207	LHG	C16-C17-C18-C19
17	l	201	LHG	C16-C17-C18-C19
14	A	814	CLA	C2A-CAA-CBA-CGA
14	A	819	CLA	C2A-CAA-CBA-CGA
14	L	204	CLA	C2A-CAA-CBA-CGA
14	X	1701	CLA	C2A-CAA-CBA-CGA
14	a	813	CLA	C2A-CAA-CBA-CGA
14	a	818	CLA	C2A-CAA-CBA-CGA
14	l	207	CLA	C2A-CAA-CBA-CGA
14	x	1701	CLA	C2A-CAA-CBA-CGA
14	1	814	CLA	C2A-CAA-CBA-CGA
14	1	819	CLA	C2A-CAA-CBA-CGA
14	0	208	CLA	C2A-CAA-CBA-CGA
14	z	1701	CLA	C2A-CAA-CBA-CGA
14	A	816	CLA	C11-C10-C8-C9
14	A	818	CLA	C14-C13-C15-C16
14	A	827	CLA	C11-C10-C8-C9
14	B	3004	CLA	C14-C13-C15-C16
14	B	3006	CLA	C6-C7-C8-C9
14	B	3010	CLA	C11-C10-C8-C9
14	B	3015	CLA	C6-C7-C8-C9
14	B	3015	CLA	C11-C12-C13-C14
14	B	3027	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	L	204	CLA	C14-C13-C15-C16
14	a	815	CLA	C11-C10-C8-C9
14	a	817	CLA	C14-C13-C15-C16
14	a	826	CLA	C11-C10-C8-C9
14	b	3004	CLA	C14-C13-C15-C16
14	b	3006	CLA	C6-C7-C8-C9
14	b	3010	CLA	C11-C10-C8-C9
14	b	3015	CLA	C6-C7-C8-C9
14	b	3015	CLA	C11-C12-C13-C14
14	b	3027	CLA	C6-C7-C8-C9
14	l	207	CLA	C14-C13-C15-C16
14	1	816	CLA	C11-C10-C8-C9
14	1	818	CLA	C14-C13-C15-C16
14	1	827	CLA	C11-C10-C8-C9
14	2	3004	CLA	C14-C13-C15-C16
14	2	3006	CLA	C6-C7-C8-C9
14	2	3010	CLA	C11-C10-C8-C9
14	2	3015	CLA	C6-C7-C8-C9
14	2	3015	CLA	C11-C12-C13-C14
14	2	3027	CLA	C6-C7-C8-C9
14	0	208	CLA	C14-C13-C15-C16
17	L	207	LHG	C10-C11-C12-C13
17	l	201	LHG	C10-C11-C12-C13
17	0	201	LHG	C16-C17-C18-C19
17	0	201	LHG	C10-C11-C12-C13
14	L	204	CLA	C4C-C3C-CAC-CBC
14	B	3026	CLA	C8-C10-C11-C12
14	b	3026	CLA	C8-C10-C11-C12
14	2	3026	CLA	C8-C10-C11-C12
17	L	207	LHG	C4-C5-C6-O8
17	l	201	LHG	C4-C5-C6-O8
17	0	201	LHG	C4-C5-C6-O8
14	l	207	CLA	C4C-C3C-CAC-CBC
14	0	208	CLA	C4C-C3C-CAC-CBC
17	A	854	LHG	C31-C32-C33-C34
17	a	853	LHG	C31-C32-C33-C34
17	1	853	LHG	C31-C32-C33-C34
17	0	202	LHG	C14-C15-C16-C17
14	B	3015	CLA	C5-C6-C7-C8
14	b	3015	CLA	C5-C6-C7-C8
14	2	3015	CLA	C5-C6-C7-C8
17	L	208	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	l	202	LHG	C14-C15-C16-C17
14	A	834	CLA	O1D-CGD-O2D-CED
14	1	834	CLA	O1D-CGD-O2D-CED
14	A	831	CLA	CBA-CGA-O2A-C1
14	a	830	CLA	CBA-CGA-O2A-C1
14	1	805	CLA	CBA-CGA-O2A-C1
14	1	831	CLA	CBA-CGA-O2A-C1
14	k	102	CLA	C2C-C3C-CAC-CBC
14	9	103	CLA	C2C-C3C-CAC-CBC
14	a	833	CLA	O1D-CGD-O2D-CED
16	I	102	BCR	C35-C13-C14-C15
16	J	104	BCR	C11-C10-C9-C34
16	j	1105	BCR	C11-C10-C9-C34
16	l	209	BCR	C35-C13-C14-C15
16	8	104	BCR	C11-C10-C9-C34
16	0	210	BCR	C35-C13-C14-C15
14	A	817	CLA	C8-C10-C11-C12
14	a	816	CLA	C8-C10-C11-C12
14	1	817	CLA	C8-C10-C11-C12
14	A	805	CLA	C4-C3-C5-C6
14	A	812	CLA	C4-C3-C5-C6
14	a	804	CLA	C4-C3-C5-C6
14	a	811	CLA	C4-C3-C5-C6
14	1	805	CLA	C4-C3-C5-C6
14	1	812	CLA	C4-C3-C5-C6
14	K	102	CLA	C2C-C3C-CAC-CBC
14	A	834	CLA	C2-C3-C5-C6
14	a	833	CLA	C2-C3-C5-C6
14	1	834	CLA	C2-C3-C5-C6
14	A	828	CLA	C15-C16-C17-C18
14	a	827	CLA	C15-C16-C17-C18
14	1	828	CLA	C15-C16-C17-C18
17	a	853	LHG	C11-C10-C9-C8
14	A	835	CLA	C16-C17-C18-C19
14	a	834	CLA	C16-C17-C18-C19
14	1	835	CLA	C16-C17-C18-C19
17	A	854	LHG	C11-C10-C9-C8
17	1	853	LHG	C11-C10-C9-C8
14	B	3028	CLA	C10-C11-C12-C13
14	b	3028	CLA	C10-C11-C12-C13
14	2	3028	CLA	C10-C11-C12-C13
14	A	805	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	804	CLA	CBA-CGA-O2A-C1
14	A	816	CLA	O2A-C1-C2-C3
14	a	815	CLA	O2A-C1-C2-C3
14	1	816	CLA	O2A-C1-C2-C3
16	B	3047	BCR	C10-C11-C12-C13
16	b	3047	BCR	C10-C11-C12-C13
16	2	3047	BCR	C10-C11-C12-C13
14	B	3006	CLA	C13-C15-C16-C17
14	b	3006	CLA	C13-C15-C16-C17
14	2	3006	CLA	C13-C15-C16-C17
17	A	853	LHG	C13-C14-C15-C16
17	a	852	LHG	C13-C14-C15-C16
17	1	852	LHG	C13-C14-C15-C16
16	B	3053	BCR	C19-C20-C21-C22
16	j	1106	BCR	C19-C20-C21-C22
16	2	3052	BCR	C19-C20-C21-C22
14	A	839	CLA	C16-C17-C18-C19
14	B	3012	CLA	C16-C17-C18-C20
14	a	838	CLA	C16-C17-C18-C19
14	b	3012	CLA	C16-C17-C18-C20
14	1	839	CLA	C16-C17-C18-C19
14	2	3012	CLA	C16-C17-C18-C20
16	A	848	BCR	C12-C13-C14-C15
16	B	3047	BCR	C11-C10-C9-C8
16	J	103	BCR	C12-C13-C14-C15
16	a	847	BCR	C12-C13-C14-C15
16	b	3047	BCR	C11-C10-C9-C8
16	j	1104	BCR	C12-C13-C14-C15
16	1	847	BCR	C12-C13-C14-C15
16	2	3047	BCR	C11-C10-C9-C8
16	8	103	BCR	C12-C13-C14-C15
16	B	3049	BCR	C22-C23-C24-C25
16	b	3049	BCR	C22-C23-C24-C25
16	2	3049	BCR	C22-C23-C24-C25
20	b	3050	LMG	C22-C23-C24-C25
20	2	3050	LMG	C22-C23-C24-C25
14	A	804	CLA	CBA-CGA-O2A-C1
14	A	807	CLA	CBA-CGA-O2A-C1
14	K	102	CLA	CBA-CGA-O2A-C1
14	a	806	CLA	CBA-CGA-O2A-C1
14	j	1101	CLA	CBA-CGA-O2A-C1
14	k	102	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	1	804	CLA	CBA-CGA-O2A-C1
14	1	807	CLA	CBA-CGA-O2A-C1
14	9	103	CLA	CBA-CGA-O2A-C1
20	B	3050	LMG	C22-C23-C24-C25
14	B	3009	CLA	C2-C3-C5-C6
14	b	3009	CLA	C2-C3-C5-C6
14	2	3009	CLA	C2-C3-C5-C6
17	A	853	LHG	C30-C31-C32-C33
17	a	852	LHG	C30-C31-C32-C33
17	1	852	LHG	C30-C31-C32-C33
17	L	208	LHG	C19-C20-C21-C22
17	l	202	LHG	C19-C20-C21-C22
17	0	202	LHG	C19-C20-C21-C22
14	A	808	CLA	CBA-CGA-O2A-C1
14	A	815	CLA	CBA-CGA-O2A-C1
14	A	819	CLA	CBA-CGA-O2A-C1
14	B	3039	CLA	CBA-CGA-O2A-C1
14	a	807	CLA	CBA-CGA-O2A-C1
14	a	818	CLA	CBA-CGA-O2A-C1
14	b	3033	CLA	CBA-CGA-O2A-C1
14	b	3039	CLA	CBA-CGA-O2A-C1
14	1	808	CLA	CBA-CGA-O2A-C1
14	1	815	CLA	CBA-CGA-O2A-C1
14	1	819	CLA	CBA-CGA-O2A-C1
14	2	3033	CLA	CBA-CGA-O2A-C1
14	2	3039	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	C4C-C3C-CAC-CBC
14	a	837	CLA	C4C-C3C-CAC-CBC
14	1	838	CLA	C4C-C3C-CAC-CBC
17	a	853	LHG	C27-C28-C29-C30
14	B	3021	CLA	C3-C5-C6-C7
14	b	3021	CLA	C3-C5-C6-C7
14	2	3021	CLA	C3-C5-C6-C7
17	A	854	LHG	C27-C28-C29-C30
17	1	853	LHG	C27-C28-C29-C30
14	A	802	CLA	O1D-CGD-O2D-CED
14	a	802	CLA	O1D-CGD-O2D-CED
14	1	802	CLA	O1D-CGD-O2D-CED
14	L	201	CLA	C16-C17-C18-C20
14	l	203	CLA	C16-C17-C18-C20
14	A	822	CLA	C4-C3-C5-C6
14	A	830	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	B	3038	CLA	C4-C3-C5-C6
14	a	821	CLA	C4-C3-C5-C6
14	a	829	CLA	C4-C3-C5-C6
14	b	3038	CLA	C4-C3-C5-C6
14	1	822	CLA	C4-C3-C5-C6
14	1	830	CLA	C4-C3-C5-C6
14	2	3038	CLA	C4-C3-C5-C6
14	A	814	CLA	CBA-CGA-O2A-C1
14	A	827	CLA	CBA-CGA-O2A-C1
14	A	843	CLA	CBA-CGA-O2A-C1
14	B	3033	CLA	CBA-CGA-O2A-C1
14	a	813	CLA	CBA-CGA-O2A-C1
14	a	814	CLA	CBA-CGA-O2A-C1
14	a	826	CLA	CBA-CGA-O2A-C1
14	a	842	CLA	CBA-CGA-O2A-C1
14	1	814	CLA	CBA-CGA-O2A-C1
14	1	827	CLA	CBA-CGA-O2A-C1
14	1	843	CLA	CBA-CGA-O2A-C1
20	B	3050	LMG	C11-C12-C13-C14
20	2	3050	LMG	C11-C12-C13-C14
14	A	806	CLA	C11-C12-C13-C14
14	A	807	CLA	C11-C12-C13-C14
14	A	810	CLA	C11-C12-C13-C14
14	A	818	CLA	C11-C12-C13-C14
14	A	825	CLA	C11-C10-C8-C9
14	A	827	CLA	C14-C13-C15-C16
14	A	835	CLA	C14-C13-C15-C16
14	A	843	CLA	C14-C13-C15-C16
14	B	3003	CLA	C11-C12-C13-C14
14	B	3027	CLA	C14-C13-C15-C16
14	B	3033	CLA	C14-C13-C15-C16
14	B	3041	CLA	C11-C12-C13-C14
14	L	201	CLA	C6-C7-C8-C9
14	a	805	CLA	C11-C12-C13-C14
14	a	806	CLA	C11-C12-C13-C14
14	a	809	CLA	C11-C12-C13-C14
14	a	817	CLA	C11-C12-C13-C14
14	a	824	CLA	C11-C10-C8-C9
14	a	826	CLA	C14-C13-C15-C16
14	a	834	CLA	C14-C13-C15-C16
14	a	842	CLA	C14-C13-C15-C16
14	b	3003	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	b	3027	CLA	C14-C13-C15-C16
14	b	3033	CLA	C14-C13-C15-C16
14	b	3041	CLA	C11-C12-C13-C14
14	l	203	CLA	C6-C7-C8-C9
14	1	806	CLA	C11-C12-C13-C14
14	1	807	CLA	C11-C12-C13-C14
14	1	810	CLA	C11-C12-C13-C14
14	1	818	CLA	C11-C12-C13-C14
14	1	825	CLA	C11-C10-C8-C9
14	1	827	CLA	C14-C13-C15-C16
14	1	835	CLA	C14-C13-C15-C16
14	1	843	CLA	C14-C13-C15-C16
14	2	3003	CLA	C11-C12-C13-C14
14	2	3027	CLA	C14-C13-C15-C16
14	2	3033	CLA	C14-C13-C15-C16
14	2	3041	CLA	C11-C12-C13-C14
14	0	204	CLA	C6-C7-C8-C9
20	b	3050	LMG	C11-C12-C13-C14
14	A	826	CLA	O1D-CGD-O2D-CED
14	a	825	CLA	O1D-CGD-O2D-CED
14	1	817	CLA	C10-C11-C12-C13
17	L	208	LHG	C5-C4-O6-P
17	l	202	LHG	C5-C4-O6-P
17	0	202	LHG	C5-C4-O6-P
14	B	3008	CLA	C4B-C3B-CAB-CBB
14	B	3013	CLA	C4B-C3B-CAB-CBB
14	a	834	CLA	C4B-C3B-CAB-CBB
14	b	3008	CLA	C4B-C3B-CAB-CBB
14	b	3013	CLA	C4B-C3B-CAB-CBB
14	1	835	CLA	C4B-C3B-CAB-CBB
14	2	3008	CLA	C4B-C3B-CAB-CBB
14	2	3013	CLA	C4B-C3B-CAB-CBB
14	1	826	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	C10-C11-C12-C13
14	A	829	CLA	C5-C6-C7-C8
14	A	840	CLA	C10-C11-C12-C13
14	a	816	CLA	C10-C11-C12-C13
14	a	828	CLA	C5-C6-C7-C8
14	a	839	CLA	C10-C11-C12-C13
14	1	829	CLA	C5-C6-C7-C8
14	1	840	CLA	C10-C11-C12-C13
14	L	201	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	l	203	CLA	C16-C17-C18-C19
14	0	204	CLA	C16-C17-C18-C19
14	0	204	CLA	C16-C17-C18-C20
17	L	208	LHG	C25-C26-C27-C28
17	l	202	LHG	C25-C26-C27-C28
17	0	202	LHG	C25-C26-C27-C28
14	B	3029	CLA	C2A-CAA-CBA-CGA
14	b	3029	CLA	C2A-CAA-CBA-CGA
14	2	3029	CLA	C2A-CAA-CBA-CGA
17	2	3051	LHG	O6-C4-C5-C6
14	A	802	CLA	C12-C13-C15-C16
14	A	814	CLA	C11-C10-C8-C7
14	A	816	CLA	C11-C10-C8-C7
14	A	816	CLA	C11-C12-C13-C15
14	A	818	CLA	C11-C12-C13-C15
14	A	825	CLA	C11-C10-C8-C7
14	A	826	CLA	C11-C10-C8-C7
14	A	827	CLA	C11-C10-C8-C7
14	A	834	CLA	C12-C13-C15-C16
14	A	839	CLA	C12-C13-C15-C16
14	B	3004	CLA	C12-C13-C15-C16
14	B	3009	CLA	C11-C12-C13-C15
14	B	3015	CLA	C6-C7-C8-C10
14	B	3015	CLA	C11-C12-C13-C15
14	B	3020	CLA	C11-C12-C13-C15
14	B	3027	CLA	C6-C7-C8-C10
14	B	3028	CLA	C12-C13-C15-C16
14	B	3033	CLA	C12-C13-C15-C16
14	L	204	CLA	C12-C13-C15-C16
14	a	802	CLA	C12-C13-C15-C16
14	a	813	CLA	C11-C10-C8-C7
14	a	814	CLA	C12-C13-C15-C16
14	a	815	CLA	C11-C10-C8-C7
14	a	815	CLA	C11-C12-C13-C15
14	a	817	CLA	C11-C12-C13-C15
14	a	824	CLA	C11-C10-C8-C7
14	a	825	CLA	C11-C10-C8-C7
14	a	826	CLA	C11-C10-C8-C7
14	a	833	CLA	C12-C13-C15-C16
14	a	838	CLA	C12-C13-C15-C16
14	b	3004	CLA	C12-C13-C15-C16
14	b	3009	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	b	3015	CLA	C6-C7-C8-C10
14	b	3015	CLA	C11-C12-C13-C15
14	b	3020	CLA	C11-C12-C13-C15
14	b	3027	CLA	C6-C7-C8-C10
14	b	3028	CLA	C12-C13-C15-C16
14	b	3033	CLA	C12-C13-C15-C16
14	l	207	CLA	C12-C13-C15-C16
14	1	802	CLA	C12-C13-C15-C16
14	1	814	CLA	C11-C10-C8-C7
14	1	815	CLA	C12-C13-C15-C16
14	1	816	CLA	C11-C10-C8-C7
14	1	816	CLA	C11-C12-C13-C15
14	1	818	CLA	C11-C12-C13-C15
14	1	825	CLA	C11-C10-C8-C7
14	1	826	CLA	C11-C10-C8-C7
14	1	827	CLA	C11-C10-C8-C7
14	1	834	CLA	C12-C13-C15-C16
14	1	839	CLA	C12-C13-C15-C16
14	2	3004	CLA	C12-C13-C15-C16
14	2	3009	CLA	C11-C12-C13-C15
14	2	3015	CLA	C6-C7-C8-C10
14	2	3015	CLA	C11-C12-C13-C15
14	2	3020	CLA	C11-C12-C13-C15
14	2	3027	CLA	C6-C7-C8-C10
14	2	3028	CLA	C12-C13-C15-C16
14	2	3033	CLA	C12-C13-C15-C16
14	0	208	CLA	C12-C13-C15-C16
17	L	207	LHG	C9-C10-C11-C12
17	l	201	LHG	C9-C10-C11-C12
17	0	201	LHG	C9-C10-C11-C12
14	A	814	CLA	C3A-C2A-CAA-CBA
14	B	3010	CLA	C4-C3-C5-C6
14	B	3026	CLA	C3A-C2A-CAA-CBA
14	K	101	CLA	C3A-C2A-CAA-CBA
14	L	205	CLA	C4-C3-C5-C6
14	a	813	CLA	C3A-C2A-CAA-CBA
14	b	3010	CLA	C4-C3-C5-C6
14	b	3026	CLA	C3A-C2A-CAA-CBA
14	k	101	CLA	C3A-C2A-CAA-CBA
14	l	208	CLA	C4-C3-C5-C6
14	1	814	CLA	C3A-C2A-CAA-CBA
14	2	3010	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	2	3026	CLA	C3A-C2A-CAA-CBA
14	9	101	CLA	C3A-C2A-CAA-CBA
14	0	209	CLA	C4-C3-C5-C6
14	A	825	CLA	C2-C3-C5-C6
14	a	824	CLA	C2-C3-C5-C6
14	1	825	CLA	C2-C3-C5-C6
14	A	805	CLA	O1A-CGA-O2A-C1
14	a	804	CLA	O1A-CGA-O2A-C1
14	1	805	CLA	O1A-CGA-O2A-C1
20	B	3050	LMG	O10-C28-O8-C9
20	b	3050	LMG	O10-C28-O8-C9
20	2	3050	LMG	O10-C28-O8-C9
14	b	3038	CLA	C10-C11-C12-C13
14	j	1101	CLA	C8-C10-C11-C12
14	1	804	CLA	C8-C10-C11-C12
14	B	3028	CLA	CBA-CGA-O2A-C1
14	b	3028	CLA	CBA-CGA-O2A-C1
16	B	3052	BCR	C13-C14-C15-C16
16	J	104	BCR	C19-C20-C21-C22
16	j	1105	BCR	C19-C20-C21-C22
16	l	204	BCR	C13-C14-C15-C16
16	8	104	BCR	C19-C20-C21-C22
16	0	205	BCR	C13-C14-C15-C16
14	A	804	CLA	C8-C10-C11-C12
14	B	3038	CLA	C10-C11-C12-C13
14	2	3038	CLA	C10-C11-C12-C13
16	A	848	BCR	C37-C22-C23-C24
16	J	103	BCR	C36-C18-C19-C20
16	a	847	BCR	C37-C22-C23-C24
16	j	1104	BCR	C36-C18-C19-C20
16	1	847	BCR	C37-C22-C23-C24
16	8	103	BCR	C36-C18-C19-C20
14	A	831	CLA	O1A-CGA-O2A-C1
14	a	830	CLA	O1A-CGA-O2A-C1
14	1	831	CLA	O1A-CGA-O2A-C1
17	l	201	LHG	C14-C15-C16-C17
16	B	3053	BCR	C7-C8-C9-C10
16	j	1106	BCR	C7-C8-C9-C10
16	2	3052	BCR	C7-C8-C9-C10
17	L	207	LHG	C14-C15-C16-C17
17	0	201	LHG	C14-C15-C16-C17
20	2	3050	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
20	b	3050	LMG	C38-C39-C40-C41
14	A	835	CLA	C2A-CAA-CBA-CGA
14	a	834	CLA	C2A-CAA-CBA-CGA
14	1	835	CLA	C2A-CAA-CBA-CGA
14	2	3028	CLA	CBA-CGA-O2A-C1
14	A	836	CLA	C15-C16-C17-C18
14	1	836	CLA	C15-C16-C17-C18
20	B	3050	LMG	C38-C39-C40-C41
14	a	835	CLA	C15-C16-C17-C18
14	A	825	CLA	C4-C3-C5-C6
14	B	3009	CLA	C4-C3-C5-C6
14	a	824	CLA	C4-C3-C5-C6
14	b	3009	CLA	C4-C3-C5-C6
14	1	825	CLA	C4-C3-C5-C6
14	2	3009	CLA	C4-C3-C5-C6
14	A	822	CLA	C2-C3-C5-C6
14	A	830	CLA	C2-C3-C5-C6
14	B	3010	CLA	C2-C3-C5-C6
14	B	3038	CLA	C2-C3-C5-C6
14	L	205	CLA	C2-C3-C5-C6
14	a	821	CLA	C2-C3-C5-C6
14	a	829	CLA	C2-C3-C5-C6
14	b	3010	CLA	C2-C3-C5-C6
14	b	3038	CLA	C2-C3-C5-C6
14	l	208	CLA	C2-C3-C5-C6
14	1	822	CLA	C2-C3-C5-C6
14	1	830	CLA	C2-C3-C5-C6
14	2	3010	CLA	C2-C3-C5-C6
14	2	3038	CLA	C2-C3-C5-C6
14	0	209	CLA	C2-C3-C5-C6
14	B	3020	CLA	C16-C17-C18-C20
14	b	3020	CLA	C16-C17-C18-C20
14	2	3020	CLA	C16-C17-C18-C20
17	L	208	LHG	O9-C7-O7-C5
17	l	202	LHG	O9-C7-O7-C5
17	0	202	LHG	O9-C7-O7-C5
16	A	848	BCR	C1-C6-C7-C8
16	B	3045	BCR	C1-C6-C7-C8
16	B	3046	BCR	C1-C6-C7-C8
16	B	3047	BCR	C23-C24-C25-C30
16	B	3053	BCR	C1-C6-C7-C8
16	F	202	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
16	F	205	BCR	C23-C24-C25-C30
16	J	104	BCR	C1-C6-C7-C8
16	a	847	BCR	C1-C6-C7-C8
16	b	3045	BCR	C1-C6-C7-C8
16	b	3046	BCR	C1-C6-C7-C8
16	b	3047	BCR	C23-C24-C25-C30
16	f	202	BCR	C23-C24-C25-C30
16	f	205	BCR	C23-C24-C25-C30
16	j	1105	BCR	C1-C6-C7-C8
16	j	1106	BCR	C1-C6-C7-C8
16	1	847	BCR	C1-C6-C7-C8
16	2	3045	BCR	C1-C6-C7-C8
16	2	3046	BCR	C1-C6-C7-C8
16	2	3047	BCR	C23-C24-C25-C30
16	2	3052	BCR	C1-C6-C7-C8
16	6	202	BCR	C23-C24-C25-C30
16	6	205	BCR	C23-C24-C25-C30
16	8	104	BCR	C1-C6-C7-C8
14	2	3038	CLA	CBA-CGA-O2A-C1
14	a	806	CLA	O1A-CGA-O2A-C1
14	1	807	CLA	O1A-CGA-O2A-C1
14	B	3023	CLA	C6-C7-C8-C9
14	b	3023	CLA	C6-C7-C8-C9
14	2	3023	CLA	C6-C7-C8-C9
14	A	828	CLA	C5-C6-C7-C8
14	a	827	CLA	C5-C6-C7-C8
14	1	828	CLA	C5-C6-C7-C8
14	A	807	CLA	O1A-CGA-O2A-C1
14	B	3039	CLA	C4-C3-C5-C6
14	b	3039	CLA	C4-C3-C5-C6
14	2	3039	CLA	C4-C3-C5-C6
15	A	845	PQN	C23-C25-C26-C27
15	a	844	PQN	C23-C25-C26-C27
15	1	845	PQN	C23-C25-C26-C27
14	A	809	CLA	C16-C17-C18-C19
14	a	808	CLA	C16-C17-C18-C19
14	1	809	CLA	C16-C17-C18-C19
14	2	3012	CLA	C5-C6-C7-C8
14	B	3038	CLA	CBA-CGA-O2A-C1
14	b	3038	CLA	CBA-CGA-O2A-C1
14	K	102	CLA	O1A-CGA-O2A-C1
14	A	815	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	A	826	CLA	C11-C10-C8-C9
14	A	836	CLA	C11-C12-C13-C14
14	B	3007	CLA	C11-C10-C8-C9
14	a	814	CLA	C11-C10-C8-C9
14	a	825	CLA	C11-C10-C8-C9
14	a	835	CLA	C11-C12-C13-C14
14	b	3007	CLA	C11-C10-C8-C9
14	1	815	CLA	C11-C10-C8-C9
14	1	826	CLA	C11-C10-C8-C9
14	1	836	CLA	C11-C12-C13-C14
14	2	3007	CLA	C11-C10-C8-C9
16	A	846	BCR	C22-C23-C24-C25
16	A	849	BCR	C22-C23-C24-C25
16	A	852	BCR	C6-C7-C8-C9
16	B	3053	BCR	C22-C23-C24-C25
16	F	205	BCR	C6-C7-C8-C9
16	a	845	BCR	C22-C23-C24-C25
16	a	848	BCR	C22-C23-C24-C25
16	a	851	BCR	C6-C7-C8-C9
16	f	205	BCR	C6-C7-C8-C9
16	j	1106	BCR	C22-C23-C24-C25
16	1	848	BCR	C22-C23-C24-C25
16	1	851	BCR	C6-C7-C8-C9
16	2	3052	BCR	C22-C23-C24-C25
16	6	205	BCR	C6-C7-C8-C9
16	9	102	BCR	C22-C23-C24-C25
14	k	102	CLA	O1A-CGA-O2A-C1
14	9	103	CLA	O1A-CGA-O2A-C1
14	b	3012	CLA	C5-C6-C7-C8
16	B	3047	BCR	C14-C15-C16-C17
16	b	3047	BCR	C14-C15-C16-C17
16	2	3047	BCR	C14-C15-C16-C17
14	A	843	CLA	C16-C17-C18-C20
14	L	203	CLA	C16-C17-C18-C20
14	a	842	CLA	C16-C17-C18-C20
14	l	206	CLA	C16-C17-C18-C20
14	1	843	CLA	C16-C17-C18-C20
14	0	207	CLA	C16-C17-C18-C20
14	B	3012	CLA	C5-C6-C7-C8
14	1	835	CLA	C5-C6-C7-C8
14	A	835	CLA	C5-C6-C7-C8
14	a	834	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	l	202	LHG	C18-C19-C20-C21
14	B	3014	CLA	CBA-CGA-O2A-C1
14	B	3020	CLA	CBA-CGA-O2A-C1
14	b	3014	CLA	CBA-CGA-O2A-C1
14	b	3020	CLA	CBA-CGA-O2A-C1
14	2	3020	CLA	CBA-CGA-O2A-C1
14	B	3039	CLA	C2-C3-C5-C6
14	b	3039	CLA	C2-C3-C5-C6
14	2	3039	CLA	C2-C3-C5-C6
14	B	3020	CLA	C16-C17-C18-C19
14	2	3020	CLA	C16-C17-C18-C19
17	L	208	LHG	C18-C19-C20-C21
17	0	202	LHG	C18-C19-C20-C21
17	a	853	LHG	O9-C7-O7-C5
16	A	847	BCR	C11-C10-C9-C34
16	A	849	BCR	C16-C17-C18-C36
16	A	850	BCR	C35-C13-C14-C15
16	B	3045	BCR	C20-C21-C22-C37
16	B	3048	BCR	C35-C13-C14-C15
16	B	3052	BCR	C35-C13-C14-C15
16	B	3053	BCR	C11-C10-C9-C34
16	F	202	BCR	C35-C13-C14-C15
16	F	205	BCR	C16-C17-C18-C36
16	M	1602	BCR	C11-C10-C9-C34
16	a	846	BCR	C11-C10-C9-C34
16	a	848	BCR	C16-C17-C18-C36
16	a	849	BCR	C35-C13-C14-C15
16	b	3045	BCR	C20-C21-C22-C37
16	b	3048	BCR	C35-C13-C14-C15
16	f	202	BCR	C35-C13-C14-C15
16	f	205	BCR	C16-C17-C18-C36
16	j	1106	BCR	C11-C10-C9-C34
16	l	204	BCR	C35-C13-C14-C15
16	m	101	BCR	C11-C10-C9-C34
16	1	846	BCR	C11-C10-C9-C34
16	1	848	BCR	C16-C17-C18-C36
16	1	849	BCR	C35-C13-C14-C15
16	2	3045	BCR	C20-C21-C22-C37
16	2	3048	BCR	C35-C13-C14-C15
16	2	3052	BCR	C11-C10-C9-C34
16	6	202	BCR	C35-C13-C14-C15
16	6	205	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
16	0	205	BCR	C35-C13-C14-C15
14	2	3014	CLA	CBA-CGA-O2A-C1
14	B	3004	CLA	C13-C15-C16-C17
14	b	3004	CLA	C13-C15-C16-C17
17	l	202	LHG	C11-C12-C13-C14
17	B	3051	LHG	O6-C4-C5-C6
17	b	3051	LHG	O6-C4-C5-C6
14	b	3020	CLA	C16-C17-C18-C19
17	0	202	LHG	C11-C12-C13-C14
14	a	818	CLA	O1A-CGA-O2A-C1
14	a	826	CLA	O1A-CGA-O2A-C1
14	b	3028	CLA	O1A-CGA-O2A-C1
14	2	3028	CLA	O1A-CGA-O2A-C1
14	A	836	CLA	C5-C6-C7-C8
14	1	836	CLA	C5-C6-C7-C8
14	2	3004	CLA	C13-C15-C16-C17
17	L	208	LHG	C11-C12-C13-C14
14	A	803	CLA	C6-C7-C8-C10
14	A	807	CLA	C11-C10-C8-C7
14	A	815	CLA	C11-C10-C8-C7
14	A	815	CLA	C12-C13-C15-C16
14	A	824	CLA	C11-C10-C8-C7
14	A	824	CLA	C12-C13-C15-C16
14	A	826	CLA	C12-C13-C15-C16
14	A	830	CLA	C12-C13-C15-C16
14	A	831	CLA	C11-C10-C8-C7
14	A	834	CLA	C6-C7-C8-C10
14	A	835	CLA	C12-C13-C15-C16
14	A	836	CLA	C11-C12-C13-C15
14	A	838	CLA	C11-C10-C8-C7
14	B	3005	CLA	C6-C7-C8-C10
14	B	3006	CLA	C6-C7-C8-C10
14	B	3007	CLA	C11-C10-C8-C7
14	B	3010	CLA	C11-C10-C8-C7
14	B	3012	CLA	C11-C12-C13-C15
14	B	3020	CLA	C12-C13-C15-C16
14	B	3039	CLA	C6-C7-C8-C10
14	B	3039	CLA	C11-C10-C8-C7
14	L	203	CLA	C11-C10-C8-C7
14	L	205	CLA	C6-C7-C8-C10
14	a	803	CLA	C6-C7-C8-C10
14	a	806	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	a	814	CLA	C11-C10-C8-C7
14	a	823	CLA	C11-C10-C8-C7
14	a	823	CLA	C12-C13-C15-C16
14	a	825	CLA	C12-C13-C15-C16
14	a	830	CLA	C11-C10-C8-C7
14	a	833	CLA	C6-C7-C8-C10
14	a	834	CLA	C12-C13-C15-C16
14	a	835	CLA	C11-C12-C13-C15
14	a	837	CLA	C11-C10-C8-C7
14	b	3005	CLA	C6-C7-C8-C10
14	b	3006	CLA	C6-C7-C8-C10
14	b	3007	CLA	C11-C10-C8-C7
14	b	3010	CLA	C11-C10-C8-C7
14	b	3012	CLA	C11-C12-C13-C15
14	b	3020	CLA	C12-C13-C15-C16
14	b	3039	CLA	C6-C7-C8-C10
14	b	3039	CLA	C11-C10-C8-C7
14	l	206	CLA	C11-C10-C8-C7
14	l	208	CLA	C6-C7-C8-C10
14	1	803	CLA	C6-C7-C8-C10
14	1	807	CLA	C11-C10-C8-C7
14	1	815	CLA	C11-C10-C8-C7
14	1	824	CLA	C11-C10-C8-C7
14	1	824	CLA	C12-C13-C15-C16
14	1	831	CLA	C11-C10-C8-C7
14	1	834	CLA	C6-C7-C8-C10
14	1	835	CLA	C12-C13-C15-C16
14	1	836	CLA	C11-C12-C13-C15
14	1	838	CLA	C11-C10-C8-C7
14	2	3005	CLA	C6-C7-C8-C10
14	2	3007	CLA	C11-C10-C8-C7
14	2	3010	CLA	C11-C10-C8-C7
14	2	3012	CLA	C11-C12-C13-C15
14	2	3020	CLA	C12-C13-C15-C16
14	2	3039	CLA	C6-C7-C8-C10
14	2	3042	CLA	C6-C7-C8-C10
14	0	207	CLA	C11-C10-C8-C7
14	0	209	CLA	C6-C7-C8-C10
15	B	3043	PQN	C17-C18-C20-C21
15	b	3043	PQN	C17-C18-C20-C21
15	2	3043	PQN	C17-C18-C20-C21
14	A	824	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	a	823	CLA	C13-C15-C16-C17
14	a	835	CLA	C5-C6-C7-C8
14	1	824	CLA	C13-C15-C16-C17
16	A	848	BCR	C11-C12-C13-C14
16	A	851	BCR	C7-C8-C9-C10
16	I	101	BCR	C7-C8-C9-C10
16	M	1602	BCR	C7-C8-C9-C10
16	a	847	BCR	C11-C12-C13-C14
16	a	850	BCR	C7-C8-C9-C10
16	i	101	BCR	C7-C8-C9-C10
16	m	101	BCR	C7-C8-C9-C10
16	1	847	BCR	C11-C12-C13-C14
16	1	850	BCR	C7-C8-C9-C10
16	7	101	BCR	C7-C8-C9-C10
16	y	101	BCR	C7-C8-C9-C10
14	B	3003	CLA	CBA-CGA-O2A-C1
14	b	3003	CLA	CBA-CGA-O2A-C1
14	2	3003	CLA	CBA-CGA-O2A-C1
14	A	815	CLA	O1A-CGA-O2A-C1
14	A	819	CLA	O1A-CGA-O2A-C1
14	A	827	CLA	O1A-CGA-O2A-C1
14	B	3028	CLA	O1A-CGA-O2A-C1
14	B	3033	CLA	O1A-CGA-O2A-C1
14	a	814	CLA	O1A-CGA-O2A-C1
14	b	3033	CLA	O1A-CGA-O2A-C1
14	1	819	CLA	O1A-CGA-O2A-C1
14	1	827	CLA	O1A-CGA-O2A-C1
14	2	3033	CLA	O1A-CGA-O2A-C1
16	A	852	BCR	C16-C17-C18-C19
16	a	851	BCR	C16-C17-C18-C19
16	1	851	BCR	C16-C17-C18-C19
14	L	203	CLA	C15-C16-C17-C18
14	A	810	CLA	C2A-CAA-CBA-CGA
14	A	842	CLA	C2A-CAA-CBA-CGA
14	a	809	CLA	C2A-CAA-CBA-CGA
14	a	841	CLA	C2A-CAA-CBA-CGA
14	1	810	CLA	C2A-CAA-CBA-CGA
14	1	842	CLA	C2A-CAA-CBA-CGA
17	A	854	LHG	O9-C7-O7-C5
17	1	853	LHG	O9-C7-O7-C5
14	A	843	CLA	O1A-CGA-O2A-C1
14	a	813	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	842	CLA	O1A-CGA-O2A-C1
14	1	814	CLA	O1A-CGA-O2A-C1
14	1	815	CLA	O1A-CGA-O2A-C1
14	1	843	CLA	O1A-CGA-O2A-C1
14	l	206	CLA	C15-C16-C17-C18
14	0	207	CLA	C15-C16-C17-C18
14	A	822	CLA	CBA-CGA-O2A-C1
14	a	821	CLA	CBA-CGA-O2A-C1
14	1	822	CLA	CBA-CGA-O2A-C1
14	B	3019	CLA	O2A-C1-C2-C3
14	b	3019	CLA	O2A-C1-C2-C3
14	2	3019	CLA	O2A-C1-C2-C3
14	A	814	CLA	O1A-CGA-O2A-C1
14	B	3039	CLA	O1A-CGA-O2A-C1
14	b	3039	CLA	O1A-CGA-O2A-C1
14	1	808	CLA	O1A-CGA-O2A-C1
17	2	3051	LHG	C14-C15-C16-C17
17	B	3051	LHG	C14-C15-C16-C17
17	b	3051	LHG	C14-C15-C16-C17
14	A	809	CLA	C16-C17-C18-C20
14	B	3012	CLA	C16-C17-C18-C19
14	b	3012	CLA	C16-C17-C18-C19
14	1	809	CLA	C16-C17-C18-C20
14	2	3012	CLA	C16-C17-C18-C19
14	A	804	CLA	O1A-CGA-O2A-C1
14	A	808	CLA	O1A-CGA-O2A-C1
14	a	807	CLA	O1A-CGA-O2A-C1
14	j	1101	CLA	O1A-CGA-O2A-C1
14	1	804	CLA	O1A-CGA-O2A-C1
14	2	3039	CLA	O1A-CGA-O2A-C1
14	A	810	CLA	C8-C10-C11-C12
14	a	809	CLA	C8-C10-C11-C12
14	1	810	CLA	C8-C10-C11-C12
16	B	3052	BCR	C11-C10-C9-C8
16	l	204	BCR	C11-C10-C9-C8
16	0	205	BCR	C11-C10-C9-C8
14	B	3016	CLA	C5-C6-C7-C8
14	b	3016	CLA	C5-C6-C7-C8
14	A	811	CLA	O2A-C1-C2-C3
14	a	810	CLA	O2A-C1-C2-C3
14	1	811	CLA	O2A-C1-C2-C3
20	B	3050	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
14	a	808	CLA	C8-C10-C11-C12
14	1	809	CLA	C8-C10-C11-C12
20	b	3050	LMG	C17-C18-C19-C20
20	b	3050	LMG	C30-C31-C32-C33
20	b	3050	LMG	C24-C25-C26-C27
14	A	814	CLA	O1D-CGD-O2D-CED
17	A	854	LHG	C24-C23-O8-C6
17	1	853	LHG	C24-C23-O8-C6
14	A	809	CLA	C8-C10-C11-C12
14	2	3016	CLA	C5-C6-C7-C8
20	2	3050	LMG	C17-C18-C19-C20
20	2	3050	LMG	C30-C31-C32-C33
14	a	812	CLA	C2C-C3C-CAC-CBC
20	B	3050	LMG	C24-C25-C26-C27
20	2	3050	LMG	C24-C25-C26-C27
20	B	3050	LMG	C17-C18-C19-C20
14	B	3018	CLA	C8-C10-C11-C12
14	B	3029	CLA	C10-C11-C12-C13
14	B	3034	CLA	C5-C6-C7-C8
14	b	3018	CLA	C8-C10-C11-C12
14	b	3029	CLA	C10-C11-C12-C13
14	b	3034	CLA	C5-C6-C7-C8
14	2	3018	CLA	C8-C10-C11-C12
14	2	3029	CLA	C10-C11-C12-C13
14	2	3034	CLA	C5-C6-C7-C8
14	1	814	CLA	O1D-CGD-O2D-CED
17	L	207	LHG	O7-C5-C6-O8
17	l	201	LHG	O7-C5-C6-O8
17	0	201	LHG	O7-C5-C6-O8
14	A	816	CLA	C11-C12-C13-C14
14	A	824	CLA	C11-C10-C8-C9
14	A	827	CLA	C11-C12-C13-C14
14	B	3012	CLA	C11-C12-C13-C14
14	B	3012	CLA	C14-C13-C15-C16
14	B	3016	CLA	C11-C10-C8-C9
14	B	3039	CLA	C6-C7-C8-C9
14	a	815	CLA	C11-C12-C13-C14
14	a	823	CLA	C11-C10-C8-C9
14	a	826	CLA	C11-C12-C13-C14
14	b	3012	CLA	C11-C12-C13-C14
14	b	3012	CLA	C14-C13-C15-C16
14	b	3016	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	b	3039	CLA	C6-C7-C8-C9
14	1	816	CLA	C11-C12-C13-C14
14	1	824	CLA	C11-C10-C8-C9
14	1	827	CLA	C11-C12-C13-C14
14	2	3012	CLA	C11-C12-C13-C14
14	2	3012	CLA	C14-C13-C15-C16
14	2	3016	CLA	C11-C10-C8-C9
14	2	3039	CLA	C6-C7-C8-C9
14	A	830	CLA	C16-C17-C18-C20
14	a	808	CLA	C16-C17-C18-C20
14	a	829	CLA	C16-C17-C18-C20
14	1	830	CLA	C16-C17-C18-C20
14	a	813	CLA	O1D-CGD-O2D-CED
17	a	853	LHG	C24-C23-O8-C6
14	A	822	CLA	O1A-CGA-O2A-C1
14	B	3003	CLA	O1A-CGA-O2A-C1
14	B	3014	CLA	O1A-CGA-O2A-C1
14	B	3038	CLA	O1A-CGA-O2A-C1
14	a	821	CLA	O1A-CGA-O2A-C1
14	b	3003	CLA	O1A-CGA-O2A-C1
14	b	3014	CLA	O1A-CGA-O2A-C1
14	b	3038	CLA	O1A-CGA-O2A-C1
14	1	822	CLA	O1A-CGA-O2A-C1
14	2	3003	CLA	O1A-CGA-O2A-C1
14	2	3014	CLA	O1A-CGA-O2A-C1
14	2	3038	CLA	O1A-CGA-O2A-C1
14	1	813	CLA	C2C-C3C-CAC-CBC
17	L	207	LHG	C26-C27-C28-C29
17	l	201	LHG	C26-C27-C28-C29
14	A	832	CLA	C10-C11-C12-C13
14	B	3039	CLA	C10-C11-C12-C13
14	B	3042	CLA	C8-C10-C11-C12
14	a	831	CLA	C10-C11-C12-C13
14	b	3039	CLA	C10-C11-C12-C13
14	b	3042	CLA	C8-C10-C11-C12
14	1	832	CLA	C10-C11-C12-C13
14	2	3039	CLA	C10-C11-C12-C13
14	2	3042	CLA	C8-C10-C11-C12
14	B	3009	CLA	CBD-CGD-O2D-CED
14	2	3009	CLA	CBD-CGD-O2D-CED
17	0	201	LHG	C26-C27-C28-C29
14	A	819	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	B	3021	CLA	C2-C1-O2A-CGA
14	a	818	CLA	C2-C1-O2A-CGA
14	b	3021	CLA	C2-C1-O2A-CGA
14	1	819	CLA	C2-C1-O2A-CGA
14	2	3021	CLA	C2-C1-O2A-CGA
14	A	820	CLA	C15-C16-C17-C18
14	a	819	CLA	C15-C16-C17-C18
14	1	820	CLA	C15-C16-C17-C18
14	A	813	CLA	C2C-C3C-CAC-CBC
14	B	3028	CLA	C4-C3-C5-C6
14	b	3028	CLA	C4-C3-C5-C6
14	2	3028	CLA	C4-C3-C5-C6
14	1	835	CLA	C2C-C3C-CAC-CBC
14	b	3009	CLA	CBD-CGD-O2D-CED
14	0	207	CLA	C16-C17-C18-C19
16	B	3053	BCR	C14-C15-C16-C17
16	j	1106	BCR	C14-C15-C16-C17
16	2	3052	BCR	C14-C15-C16-C17
14	a	834	CLA	C2C-C3C-CAC-CBC
14	A	805	CLA	C4C-C3C-CAC-CBC
14	a	804	CLA	C4C-C3C-CAC-CBC
14	1	805	CLA	C4C-C3C-CAC-CBC
14	A	835	CLA	C2C-C3C-CAC-CBC
14	1	811	CLA	C2C-C3C-CAC-CBC
17	a	852	LHG	C29-C30-C31-C32
17	1	852	LHG	C29-C30-C31-C32
17	A	853	LHG	C29-C30-C31-C32
14	L	203	CLA	C16-C17-C18-C19
14	l	206	CLA	C16-C17-C18-C19
14	A	811	CLA	C2C-C3C-CAC-CBC
14	A	840	CLA	C3-C5-C6-C7
14	a	839	CLA	C3-C5-C6-C7
14	1	840	CLA	C3-C5-C6-C7
14	a	810	CLA	C2C-C3C-CAC-CBC
14	A	811	CLA	C4B-C3B-CAB-CBB
14	A	814	CLA	C1A-C2A-CAA-CBA
14	A	838	CLA	C1A-C2A-CAA-CBA
14	B	3036	CLA	C1A-C2A-CAA-CBA
14	B	3041	CLA	C4B-C3B-CAB-CBB
14	a	810	CLA	C4B-C3B-CAB-CBB
14	a	813	CLA	C1A-C2A-CAA-CBA
14	a	837	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	3036	CLA	C1A-C2A-CAA-CBA
14	b	3041	CLA	C4B-C3B-CAB-CBB
14	1	811	CLA	C4B-C3B-CAB-CBB
14	1	814	CLA	C1A-C2A-CAA-CBA
14	1	838	CLA	C1A-C2A-CAA-CBA
14	2	3036	CLA	C1A-C2A-CAA-CBA
14	2	3041	CLA	C4B-C3B-CAB-CBB
14	A	837	CLA	O1D-CGD-O2D-CED
14	a	836	CLA	O1D-CGD-O2D-CED
14	1	837	CLA	O1D-CGD-O2D-CED
16	A	849	BCR	C6-C7-C8-C9
16	a	848	BCR	C6-C7-C8-C9
16	j	1105	BCR	C22-C23-C24-C25
16	1	848	BCR	C6-C7-C8-C9
16	A	847	BCR	C7-C8-C9-C10
16	a	846	BCR	C7-C8-C9-C10
16	1	846	BCR	C7-C8-C9-C10
14	a	828	CLA	C16-C17-C18-C20
14	1	829	CLA	C16-C17-C18-C20
14	A	826	CLA	C2C-C3C-CAC-CBC
14	1	826	CLA	C2C-C3C-CAC-CBC
14	A	819	CLA	C6-C7-C8-C10
14	A	828	CLA	C6-C7-C8-C10
14	A	833	CLA	C11-C10-C8-C7
14	A	833	CLA	C11-C12-C13-C15
14	A	833	CLA	C12-C13-C15-C16
14	A	841	CLA	C11-C10-C8-C7
14	A	843	CLA	C6-C7-C8-C10
14	B	3003	CLA	C12-C13-C15-C16
14	B	3006	CLA	C11-C10-C8-C7
14	B	3006	CLA	C11-C12-C13-C15
14	B	3026	CLA	C6-C7-C8-C10
14	B	3027	CLA	C11-C12-C13-C15
14	B	3038	CLA	C11-C10-C8-C7
14	B	3042	CLA	C6-C7-C8-C10
14	L	204	CLA	C6-C7-C8-C10
14	a	818	CLA	C6-C7-C8-C10
14	a	827	CLA	C6-C7-C8-C10
14	a	829	CLA	C12-C13-C15-C16
14	a	832	CLA	C11-C10-C8-C7
14	a	832	CLA	C11-C12-C13-C15
14	a	832	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	a	840	CLA	C11-C10-C8-C7
14	a	842	CLA	C6-C7-C8-C10
14	b	3003	CLA	C12-C13-C15-C16
14	b	3006	CLA	C11-C10-C8-C7
14	b	3006	CLA	C11-C12-C13-C15
14	b	3026	CLA	C6-C7-C8-C10
14	b	3027	CLA	C11-C12-C13-C15
14	b	3038	CLA	C11-C10-C8-C7
14	b	3042	CLA	C6-C7-C8-C10
14	l	207	CLA	C6-C7-C8-C10
14	1	819	CLA	C6-C7-C8-C10
14	1	826	CLA	C12-C13-C15-C16
14	1	828	CLA	C6-C7-C8-C10
14	1	830	CLA	C12-C13-C15-C16
14	1	833	CLA	C11-C10-C8-C7
14	1	833	CLA	C11-C12-C13-C15
14	1	833	CLA	C12-C13-C15-C16
14	1	841	CLA	C11-C10-C8-C7
14	1	843	CLA	C6-C7-C8-C10
14	2	3003	CLA	C12-C13-C15-C16
14	2	3006	CLA	C6-C7-C8-C10
14	2	3006	CLA	C11-C10-C8-C7
14	2	3026	CLA	C6-C7-C8-C10
14	2	3027	CLA	C11-C12-C13-C15
14	2	3038	CLA	C11-C10-C8-C7
14	2	3039	CLA	C11-C10-C8-C7
14	0	208	CLA	C6-C7-C8-C10
14	a	825	CLA	C2C-C3C-CAC-CBC
14	A	829	CLA	C16-C17-C18-C20
14	A	840	CLA	C16-C17-C18-C20
14	a	839	CLA	C16-C17-C18-C20
14	1	840	CLA	C16-C17-C18-C20
14	B	3020	CLA	O1A-CGA-O2A-C1
14	b	3020	CLA	O1A-CGA-O2A-C1
14	2	3020	CLA	O1A-CGA-O2A-C1
17	B	3051	LHG	C11-C10-C9-C8
17	l	201	LHG	C17-C18-C19-C20
14	A	820	CLA	C4-C3-C5-C6
14	B	3025	CLA	C3A-C2A-CAA-CBA
14	a	819	CLA	C4-C3-C5-C6
14	b	3025	CLA	C3A-C2A-CAA-CBA
14	1	820	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	2	3025	CLA	C3A-C2A-CAA-CBA
17	b	3051	LHG	C11-C10-C9-C8
17	0	201	LHG	C17-C18-C19-C20
17	L	208	LHG	O6-C4-C5-O7
17	l	202	LHG	O6-C4-C5-O7
17	0	202	LHG	O6-C4-C5-O7
17	2	3051	LHG	C11-C10-C9-C8
17	A	853	LHG	C31-C32-C33-C34
17	L	207	LHG	C17-C18-C19-C20
14	A	829	CLA	C2A-CAA-CBA-CGA
14	a	828	CLA	C2A-CAA-CBA-CGA
14	1	829	CLA	C2A-CAA-CBA-CGA
14	A	807	CLA	C11-C10-C8-C9
14	A	815	CLA	C14-C13-C15-C16
14	A	824	CLA	C14-C13-C15-C16
14	A	831	CLA	C11-C10-C8-C9
14	A	833	CLA	C11-C10-C8-C9
14	A	834	CLA	C6-C7-C8-C9
14	A	834	CLA	C14-C13-C15-C16
14	A	839	CLA	C14-C13-C15-C16
14	B	3017	CLA	C11-C10-C8-C9
14	B	3025	CLA	C11-C12-C13-C14
14	B	3027	CLA	C11-C10-C8-C9
14	a	806	CLA	C11-C10-C8-C9
14	a	814	CLA	C14-C13-C15-C16
14	a	823	CLA	C14-C13-C15-C16
14	a	830	CLA	C11-C10-C8-C9
14	a	832	CLA	C11-C10-C8-C9
14	a	833	CLA	C6-C7-C8-C9
14	a	833	CLA	C14-C13-C15-C16
14	a	838	CLA	C14-C13-C15-C16
14	b	3017	CLA	C11-C10-C8-C9
14	b	3025	CLA	C11-C12-C13-C14
14	b	3027	CLA	C11-C10-C8-C9
14	1	807	CLA	C11-C10-C8-C9
14	1	815	CLA	C14-C13-C15-C16
14	1	831	CLA	C11-C10-C8-C9
14	1	833	CLA	C11-C10-C8-C9
14	1	834	CLA	C6-C7-C8-C9
14	1	834	CLA	C14-C13-C15-C16
14	1	839	CLA	C14-C13-C15-C16
14	2	3017	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	2	3025	CLA	C11-C12-C13-C14
14	2	3027	CLA	C11-C10-C8-C9
17	a	852	LHG	C31-C32-C33-C34
16	L	206	BCR	C15-C16-C17-C18
16	b	3048	BCR	C13-C14-C15-C16
16	l	210	BCR	C15-C16-C17-C18
16	2	3048	BCR	C13-C14-C15-C16
16	0	211	BCR	C15-C16-C17-C18
14	A	812	CLA	C5-C6-C7-C8
14	B	3034	CLA	C8-C10-C11-C12
14	a	811	CLA	C5-C6-C7-C8
14	b	3034	CLA	C8-C10-C11-C12
14	1	810	CLA	C10-C11-C12-C13
14	1	812	CLA	C5-C6-C7-C8
14	2	3019	CLA	C5-C6-C7-C8
14	2	3034	CLA	C8-C10-C11-C12
14	B	3032	CLA	C1-C2-C3-C4
14	b	3032	CLA	C1-C2-C3-C4
14	2	3032	CLA	C1-C2-C3-C4
17	1	852	LHG	C31-C32-C33-C34
14	A	810	CLA	C10-C11-C12-C13
17	L	208	LHG	O7-C5-C6-O8
17	l	202	LHG	O7-C5-C6-O8
17	0	202	LHG	O7-C5-C6-O8
14	B	3019	CLA	C5-C6-C7-C8
14	a	809	CLA	C10-C11-C12-C13
14	b	3019	CLA	C5-C6-C7-C8
14	B	3025	CLA	C3-C5-C6-C7
14	b	3025	CLA	C3-C5-C6-C7
14	2	3025	CLA	C3-C5-C6-C7
14	A	810	CLA	CAD-CBD-CGD-O2D
14	A	832	CLA	CAD-CBD-CGD-O2D
14	A	844	CLA	CAD-CBD-CGD-O2D
14	B	3014	CLA	CAD-CBD-CGD-O2D
14	B	3019	CLA	CAD-CBD-CGD-O2D
14	B	3027	CLA	CAD-CBD-CGD-O2D
14	B	3032	CLA	CAD-CBD-CGD-O2D
14	a	809	CLA	CAD-CBD-CGD-O2D
14	a	831	CLA	CAD-CBD-CGD-O2D
14	a	843	CLA	CAD-CBD-CGD-O2D
14	b	3014	CLA	CAD-CBD-CGD-O2D
14	b	3019	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	b	3027	CLA	CAD-CBD-CGD-O2D
14	b	3032	CLA	CAD-CBD-CGD-O2D
14	1	810	CLA	CAD-CBD-CGD-O2D
14	1	832	CLA	CAD-CBD-CGD-O2D
14	1	844	CLA	CAD-CBD-CGD-O2D
14	2	3014	CLA	CAD-CBD-CGD-O2D
14	2	3019	CLA	CAD-CBD-CGD-O2D
14	2	3027	CLA	CAD-CBD-CGD-O2D
14	2	3032	CLA	CAD-CBD-CGD-O2D
14	A	839	CLA	C5-C6-C7-C8
14	B	3023	CLA	C5-C6-C7-C8
14	a	838	CLA	C5-C6-C7-C8
14	b	3023	CLA	C5-C6-C7-C8
14	1	839	CLA	C5-C6-C7-C8
14	2	3023	CLA	C5-C6-C7-C8
14	A	810	CLA	CAD-CBD-CGD-O1D
14	A	832	CLA	CAD-CBD-CGD-O1D
14	A	844	CLA	CAD-CBD-CGD-O1D
14	B	3006	CLA	CHA-CBD-CGD-O1D
14	B	3014	CLA	CAD-CBD-CGD-O1D
14	B	3015	CLA	CHA-CBD-CGD-O1D
14	B	3015	CLA	CHA-CBD-CGD-O2D
14	B	3016	CLA	CHA-CBD-CGD-O1D
14	B	3019	CLA	CAD-CBD-CGD-O1D
14	B	3025	CLA	CHA-CBD-CGD-O1D
14	B	3027	CLA	CAD-CBD-CGD-O1D
14	B	3030	CLA	CHA-CBD-CGD-O1D
14	B	3030	CLA	CHA-CBD-CGD-O2D
14	B	3032	CLA	CAD-CBD-CGD-O1D
14	a	809	CLA	CAD-CBD-CGD-O1D
14	a	831	CLA	CAD-CBD-CGD-O1D
14	a	843	CLA	CAD-CBD-CGD-O1D
14	b	3006	CLA	CHA-CBD-CGD-O1D
14	b	3014	CLA	CAD-CBD-CGD-O1D
14	b	3015	CLA	CHA-CBD-CGD-O1D
14	b	3015	CLA	CHA-CBD-CGD-O2D
14	b	3016	CLA	CHA-CBD-CGD-O1D
14	b	3019	CLA	CAD-CBD-CGD-O1D
14	b	3025	CLA	CHA-CBD-CGD-O1D
14	b	3027	CLA	CAD-CBD-CGD-O1D
14	b	3030	CLA	CHA-CBD-CGD-O1D
14	b	3030	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	b	3032	CLA	CAD-CBD-CGD-O1D
14	1	810	CLA	CAD-CBD-CGD-O1D
14	1	832	CLA	CAD-CBD-CGD-O1D
14	1	844	CLA	CAD-CBD-CGD-O1D
14	2	3006	CLA	CHA-CBD-CGD-O1D
14	2	3014	CLA	CAD-CBD-CGD-O1D
14	2	3015	CLA	CHA-CBD-CGD-O1D
14	2	3015	CLA	CHA-CBD-CGD-O2D
14	2	3016	CLA	CHA-CBD-CGD-O1D
14	2	3019	CLA	CAD-CBD-CGD-O1D
14	2	3025	CLA	CHA-CBD-CGD-O1D
14	2	3027	CLA	CAD-CBD-CGD-O1D
14	2	3030	CLA	CHA-CBD-CGD-O1D
14	2	3030	CLA	CHA-CBD-CGD-O2D
14	2	3032	CLA	CAD-CBD-CGD-O1D
16	A	847	BCR	C9-C10-C11-C12
16	A	848	BCR	C13-C14-C15-C16
16	B	3047	BCR	C19-C20-C21-C22
16	B	3048	BCR	C13-C14-C15-C16
16	a	846	BCR	C9-C10-C11-C12
16	a	847	BCR	C13-C14-C15-C16
16	b	3047	BCR	C19-C20-C21-C22
16	1	846	BCR	C9-C10-C11-C12
16	1	847	BCR	C13-C14-C15-C16
16	2	3047	BCR	C19-C20-C21-C22
16	y	101	BCR	C11-C10-C9-C34
17	A	854	LHG	C3-O3-P-O5
17	A	854	LHG	C3-O3-P-O6
17	A	854	LHG	C4-O6-P-O4
17	B	3051	LHG	C3-O3-P-O6
17	L	207	LHG	C3-O3-P-O5
17	L	208	LHG	C3-O3-P-O5
17	L	208	LHG	C4-O6-P-O5
17	a	853	LHG	C3-O3-P-O5
17	a	853	LHG	C3-O3-P-O6
17	a	853	LHG	C4-O6-P-O4
17	b	3051	LHG	C3-O3-P-O6
17	l	201	LHG	C3-O3-P-O5
17	l	202	LHG	C3-O3-P-O5
17	l	202	LHG	C4-O6-P-O5
17	1	853	LHG	C3-O3-P-O5
17	1	853	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
17	1	853	LHG	C4-O6-P-O4
17	2	3051	LHG	C3-O3-P-O6
17	0	201	LHG	C3-O3-P-O5
17	0	202	LHG	C3-O3-P-O5
17	0	202	LHG	C4-O6-P-O5
14	X	1701	CLA	C2C-C3C-CAC-CBC
14	A	817	CLA	C2B-C3B-CAB-CBB
14	A	819	CLA	C2B-C3B-CAB-CBB
14	A	824	CLA	C2B-C3B-CAB-CBB
14	A	835	CLA	C2B-C3B-CAB-CBB
14	a	816	CLA	C2B-C3B-CAB-CBB
14	a	818	CLA	C2B-C3B-CAB-CBB
14	a	823	CLA	C2B-C3B-CAB-CBB
14	a	834	CLA	C2B-C3B-CAB-CBB
14	1	817	CLA	C2B-C3B-CAB-CBB
14	1	819	CLA	C2B-C3B-CAB-CBB
14	1	824	CLA	C2B-C3B-CAB-CBB
14	1	835	CLA	C2B-C3B-CAB-CBB
16	I	101	BCR	C1-C6-C7-C8
16	i	101	BCR	C1-C6-C7-C8
16	7	101	BCR	C1-C6-C7-C8
14	a	825	CLA	C8-C10-C11-C12
14	1	826	CLA	C8-C10-C11-C12
16	A	851	BCR	C11-C12-C13-C35
16	A	851	BCR	C36-C18-C19-C20
16	F	205	BCR	C37-C22-C23-C24
16	a	850	BCR	C11-C12-C13-C35
16	a	850	BCR	C36-C18-C19-C20
16	f	205	BCR	C37-C22-C23-C24
16	1	850	BCR	C11-C12-C13-C35
16	1	850	BCR	C36-C18-C19-C20
16	6	205	BCR	C37-C22-C23-C24
17	B	3051	LHG	C2-C3-O3-P
17	b	3051	LHG	C2-C3-O3-P
17	2	3051	LHG	C2-C3-O3-P
14	x	1701	CLA	C2C-C3C-CAC-CBC
14	z	1701	CLA	C2C-C3C-CAC-CBC
14	A	826	CLA	C8-C10-C11-C12
14	L	205	CLA	C16-C17-C18-C20
14	l	208	CLA	C16-C17-C18-C20
14	B	3036	CLA	C2C-C3C-CAC-CBC
14	b	3036	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	2	3036	CLA	C2C-C3C-CAC-CBC
14	a	817	CLA	C5-C6-C7-C8
14	B	3003	CLA	C3-C5-C6-C7
14	b	3003	CLA	C3-C5-C6-C7
14	A	818	CLA	C5-C6-C7-C8
14	1	818	CLA	C5-C6-C7-C8
14	0	209	CLA	C16-C17-C18-C20
14	A	825	CLA	C8-C10-C11-C12
14	a	824	CLA	C8-C10-C11-C12
14	b	3034	CLA	C10-C11-C12-C13
14	1	825	CLA	C8-C10-C11-C12
14	2	3034	CLA	C10-C11-C12-C13
17	2	3051	LHG	C24-C25-C26-C27
14	f	201	CLA	C10-C11-C12-C13
14	B	3034	CLA	C10-C11-C12-C13
14	A	820	CLA	C2-C3-C5-C6
14	a	819	CLA	C2-C3-C5-C6
14	1	820	CLA	C2-C3-C5-C6
17	B	3051	LHG	C24-C25-C26-C27
17	b	3051	LHG	C24-C25-C26-C27
14	F	201	CLA	C10-C11-C12-C13
14	6	201	CLA	C10-C11-C12-C13
14	L	204	CLA	C16-C17-C18-C20
14	l	207	CLA	C16-C17-C18-C20
14	0	208	CLA	C16-C17-C18-C20
20	B	3050	LMG	C42-C43-C44-C45
20	2	3050	LMG	C42-C43-C44-C45
14	2	3003	CLA	C3-C5-C6-C7
20	b	3050	LMG	C42-C43-C44-C45
14	A	806	CLA	C14-C13-C15-C16
14	A	809	CLA	C14-C13-C15-C16
14	A	814	CLA	C11-C10-C8-C9
14	A	819	CLA	C11-C12-C13-C14
14	A	828	CLA	C6-C7-C8-C9
14	A	830	CLA	C14-C13-C15-C16
14	B	3005	CLA	C6-C7-C8-C9
14	B	3017	CLA	C11-C12-C13-C14
14	B	3020	CLA	C11-C12-C13-C14
14	B	3020	CLA	C14-C13-C15-C16
14	B	3026	CLA	C11-C12-C13-C14
14	L	203	CLA	C11-C10-C8-C9
14	L	205	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	a	805	CLA	C14-C13-C15-C16
14	a	808	CLA	C14-C13-C15-C16
14	a	813	CLA	C11-C10-C8-C9
14	a	818	CLA	C11-C12-C13-C14
14	a	827	CLA	C6-C7-C8-C9
14	a	829	CLA	C14-C13-C15-C16
14	b	3005	CLA	C6-C7-C8-C9
14	b	3017	CLA	C11-C12-C13-C14
14	b	3020	CLA	C11-C12-C13-C14
14	b	3020	CLA	C14-C13-C15-C16
14	b	3026	CLA	C11-C12-C13-C14
14	l	206	CLA	C11-C10-C8-C9
14	l	208	CLA	C14-C13-C15-C16
14	1	806	CLA	C14-C13-C15-C16
14	1	809	CLA	C14-C13-C15-C16
14	1	814	CLA	C11-C10-C8-C9
14	1	819	CLA	C11-C12-C13-C14
14	1	824	CLA	C14-C13-C15-C16
14	1	828	CLA	C6-C7-C8-C9
14	1	830	CLA	C14-C13-C15-C16
14	2	3005	CLA	C6-C7-C8-C9
14	2	3017	CLA	C11-C12-C13-C14
14	2	3020	CLA	C11-C12-C13-C14
14	2	3020	CLA	C14-C13-C15-C16
14	2	3026	CLA	C11-C12-C13-C14
14	0	207	CLA	C11-C10-C8-C9
14	0	209	CLA	C14-C13-C15-C16
17	a	852	LHG	C15-C16-C17-C18
14	A	819	CLA	C11-C12-C13-C15
14	A	827	CLA	C11-C12-C13-C15
14	A	829	CLA	C11-C12-C13-C15
14	B	3005	CLA	C11-C12-C13-C15
14	B	3025	CLA	C11-C12-C13-C15
14	a	818	CLA	C11-C12-C13-C15
14	a	826	CLA	C11-C12-C13-C15
14	a	828	CLA	C11-C12-C13-C15
14	b	3005	CLA	C11-C12-C13-C15
14	b	3025	CLA	C11-C12-C13-C15
14	1	819	CLA	C11-C12-C13-C15
14	1	827	CLA	C11-C12-C13-C15
14	1	829	CLA	C11-C12-C13-C15
14	2	3005	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	2	3006	CLA	C11-C12-C13-C15
14	2	3025	CLA	C11-C12-C13-C15
14	2	3033	CLA	C11-C10-C8-C7
17	A	853	LHG	C15-C16-C17-C18
17	1	852	LHG	C15-C16-C17-C18
16	J	104	BCR	C22-C23-C24-C25
16	8	104	BCR	C22-C23-C24-C25
14	L	204	CLA	C16-C17-C18-C19
14	l	207	CLA	C16-C17-C18-C19
14	0	208	CLA	C16-C17-C18-C19
13	A	801	CL0	CAA-CBA-CGA-O2A
13	a	801	CL0	CAA-CBA-CGA-O2A
13	1	801	CL0	CAA-CBA-CGA-O2A
17	A	853	LHG	O7-C5-C6-O8
17	a	852	LHG	O7-C5-C6-O8
17	1	852	LHG	O7-C5-C6-O8
16	b	3047	BCR	C9-C10-C11-C12
14	A	806	CLA	C16-C17-C18-C19
17	l	202	LHG	C16-C17-C18-C19
14	B	3004	CLA	CAA-CBA-CGA-O2A
14	b	3004	CLA	CAA-CBA-CGA-O2A
14	2	3004	CLA	CAA-CBA-CGA-O2A
17	L	208	LHG	C16-C17-C18-C19
17	0	202	LHG	C16-C17-C18-C19
14	A	826	CLA	C2-C1-O2A-CGA
14	a	825	CLA	C2-C1-O2A-CGA
14	1	826	CLA	C2-C1-O2A-CGA
20	B	3050	LMG	C34-C35-C36-C37
20	b	3050	LMG	C34-C35-C36-C37
20	2	3050	LMG	C34-C35-C36-C37
14	a	805	CLA	C16-C17-C18-C19
14	1	806	CLA	C16-C17-C18-C19
14	1	803	CLA	C13-C15-C16-C17
14	B	3018	CLA	C2C-C3C-CAC-CBC
14	2	3018	CLA	C2C-C3C-CAC-CBC
14	2	3011	CLA	O1D-CGD-O2D-CED
14	b	3018	CLA	C2C-C3C-CAC-CBC
14	A	803	CLA	C13-C15-C16-C17
14	a	803	CLA	C13-C15-C16-C17
14	A	834	CLA	C2A-CAA-CBA-CGA
14	A	839	CLA	C2A-CAA-CBA-CGA
14	F	203	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	a	833	CLA	C2A-CAA-CBA-CGA
14	a	838	CLA	C2A-CAA-CBA-CGA
14	f	203	CLA	C2A-CAA-CBA-CGA
14	1	834	CLA	C2A-CAA-CBA-CGA
14	1	839	CLA	C2A-CAA-CBA-CGA
14	6	203	CLA	C2A-CAA-CBA-CGA
14	B	3011	CLA	O1D-CGD-O2D-CED
16	B	3047	BCR	C9-C10-C11-C12
16	2	3047	BCR	C9-C10-C11-C12
14	A	806	CLA	C16-C17-C18-C20
14	a	805	CLA	C16-C17-C18-C20
14	1	806	CLA	C16-C17-C18-C20
14	b	3011	CLA	O1D-CGD-O2D-CED
14	b	3028	CLA	C2-C3-C5-C6
17	1	853	LHG	C28-C29-C30-C31
14	1	840	CLA	C2C-C3C-CAC-CBC
17	A	854	LHG	C28-C29-C30-C31
17	a	853	LHG	C28-C29-C30-C31
14	A	840	CLA	C2C-C3C-CAC-CBC
14	A	817	CLA	C16-C17-C18-C20
14	a	816	CLA	C16-C17-C18-C20
14	1	817	CLA	C16-C17-C18-C20
14	B	3026	CLA	C6-C7-C8-C9
14	b	3026	CLA	C6-C7-C8-C9
14	2	3026	CLA	C6-C7-C8-C9
14	a	816	CLA	C13-C15-C16-C17
14	a	839	CLA	C2C-C3C-CAC-CBC
14	A	817	CLA	C13-C15-C16-C17
14	B	3021	CLA	C15-C16-C17-C18
14	1	817	CLA	C13-C15-C16-C17
14	2	3021	CLA	C15-C16-C17-C18
14	A	810	CLA	C4-C3-C5-C6
14	K	102	CLA	C4-C3-C5-C6
14	a	809	CLA	C4-C3-C5-C6
14	k	102	CLA	C4-C3-C5-C6
14	1	810	CLA	C4-C3-C5-C6
14	9	103	CLA	C4-C3-C5-C6
14	B	3028	CLA	C2-C3-C5-C6
14	2	3028	CLA	C2-C3-C5-C6
17	A	854	LHG	O6-C4-C5-O7
17	a	853	LHG	O6-C4-C5-O7
17	1	853	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
14	B	3032	CLA	O2A-C1-C2-C3
14	b	3032	CLA	O2A-C1-C2-C3
14	2	3032	CLA	O2A-C1-C2-C3
14	b	3021	CLA	C15-C16-C17-C18
14	A	830	CLA	C11-C12-C13-C15
14	B	3033	CLA	C11-C10-C8-C7
14	a	829	CLA	C11-C12-C13-C15
14	b	3033	CLA	C11-C10-C8-C7
14	l	206	CLA	C12-C13-C15-C16
14	1	830	CLA	C11-C12-C13-C15
14	0	207	CLA	C12-C13-C15-C16
14	A	829	CLA	C16-C17-C18-C19
14	a	828	CLA	C16-C17-C18-C19
14	1	829	CLA	C16-C17-C18-C19
14	B	3018	CLA	C4C-C3C-CAC-CBC
14	b	3018	CLA	C4C-C3C-CAC-CBC
14	2	3018	CLA	C4C-C3C-CAC-CBC
14	A	804	CLA	C13-C15-C16-C17
14	A	806	CLA	C10-C11-C12-C13
14	a	805	CLA	C10-C11-C12-C13
14	j	1101	CLA	C13-C15-C16-C17
14	1	804	CLA	C13-C15-C16-C17
14	1	806	CLA	C10-C11-C12-C13
14	A	830	CLA	C3A-C2A-CAA-CBA
14	a	829	CLA	C3A-C2A-CAA-CBA
14	1	830	CLA	C3A-C2A-CAA-CBA
14	b	3009	CLA	O1D-CGD-O2D-CED
14	2	3009	CLA	O1D-CGD-O2D-CED
14	A	834	CLA	C16-C17-C18-C20
14	B	3009	CLA	O1D-CGD-O2D-CED
16	A	847	BCR	C6-C7-C8-C9
16	B	3046	BCR	C11-C10-C9-C34
16	B	3047	BCR	C6-C7-C8-C9
16	F	202	BCR	C16-C17-C18-C36
16	F	205	BCR	C35-C13-C14-C15
16	a	846	BCR	C6-C7-C8-C9
16	b	3046	BCR	C11-C10-C9-C34
16	b	3047	BCR	C6-C7-C8-C9
16	f	202	BCR	C16-C17-C18-C36
16	f	205	BCR	C35-C13-C14-C15
16	1	846	BCR	C6-C7-C8-C9
16	2	3046	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
16	2	3047	BCR	C6-C7-C8-C9
16	6	202	BCR	C16-C17-C18-C36
16	6	205	BCR	C35-C13-C14-C15
16	9	104	BCR	C6-C7-C8-C9
14	b	3008	CLA	C3-C5-C6-C7
14	A	802	CLA	C2-C1-O2A-CGA
14	B	3006	CLA	C2-C1-O2A-CGA
14	B	3029	CLA	C2-C1-O2A-CGA
14	B	3036	CLA	C2-C1-O2A-CGA
14	a	802	CLA	C2-C1-O2A-CGA
14	b	3006	CLA	C2-C1-O2A-CGA
14	b	3029	CLA	C2-C1-O2A-CGA
14	b	3036	CLA	C2-C1-O2A-CGA
14	1	802	CLA	C2-C1-O2A-CGA
14	2	3006	CLA	C2-C1-O2A-CGA
14	2	3029	CLA	C2-C1-O2A-CGA
14	2	3036	CLA	C2-C1-O2A-CGA
14	B	3008	CLA	C3-C5-C6-C7
14	2	3008	CLA	C3-C5-C6-C7
14	a	833	CLA	C16-C17-C18-C20
14	1	834	CLA	C16-C17-C18-C20
14	B	3026	CLA	C13-C15-C16-C17
14	b	3026	CLA	C13-C15-C16-C17
14	2	3026	CLA	C13-C15-C16-C17
14	F	203	CLA	CAA-CBA-CGA-O1A
14	f	203	CLA	CAA-CBA-CGA-O1A
14	6	203	CLA	CAA-CBA-CGA-O1A
14	B	3028	CLA	C4C-C3C-CAC-CBC
14	2	3028	CLA	C4C-C3C-CAC-CBC
14	b	3028	CLA	C4C-C3C-CAC-CBC
14	A	805	CLA	C6-C7-C8-C9
14	A	810	CLA	C11-C10-C8-C9
14	A	815	CLA	C11-C12-C13-C14
14	A	821	CLA	C11-C12-C13-C14
14	A	822	CLA	C11-C10-C8-C9
14	A	830	CLA	C11-C12-C13-C14
14	A	840	CLA	C11-C12-C13-C14
14	B	3025	CLA	C11-C10-C8-C9
14	B	3027	CLA	C11-C12-C13-C14
14	B	3028	CLA	C11-C12-C13-C14
14	a	804	CLA	C6-C7-C8-C9
14	a	809	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	a	814	CLA	C11-C12-C13-C14
14	a	820	CLA	C11-C12-C13-C14
14	a	821	CLA	C11-C10-C8-C9
14	a	829	CLA	C11-C12-C13-C14
14	a	839	CLA	C11-C12-C13-C14
14	b	3025	CLA	C11-C10-C8-C9
14	b	3027	CLA	C11-C12-C13-C14
14	b	3028	CLA	C11-C12-C13-C14
14	1	805	CLA	C6-C7-C8-C9
14	1	810	CLA	C11-C10-C8-C9
14	1	815	CLA	C11-C12-C13-C14
14	1	821	CLA	C11-C12-C13-C14
14	1	822	CLA	C11-C10-C8-C9
14	1	830	CLA	C11-C12-C13-C14
14	1	840	CLA	C11-C12-C13-C14
14	2	3025	CLA	C11-C10-C8-C9
14	2	3027	CLA	C11-C12-C13-C14
14	2	3028	CLA	C11-C12-C13-C14
14	2	3042	CLA	C6-C7-C8-C9
14	A	802	CLA	C16-C17-C18-C20
14	A	830	CLA	C16-C17-C18-C19
14	a	802	CLA	C16-C17-C18-C20
14	a	829	CLA	C16-C17-C18-C19
14	1	802	CLA	C16-C17-C18-C20
14	1	830	CLA	C16-C17-C18-C19
17	A	853	LHG	C14-C15-C16-C17
17	1	852	LHG	C14-C15-C16-C17
20	B	3050	LMG	O9-C10-O7-C8
20	b	3050	LMG	O9-C10-O7-C8
20	2	3050	LMG	O9-C10-O7-C8
17	a	852	LHG	C14-C15-C16-C17
13	a	801	CL0	C15-C16-C17-C18
16	A	852	BCR	C13-C14-C15-C16
16	a	851	BCR	C13-C14-C15-C16
16	1	851	BCR	C13-C14-C15-C16
14	6	203	CLA	CAA-CBA-CGA-O2A
14	f	203	CLA	CAA-CBA-CGA-O2A
14	A	827	CLA	C1A-C2A-CAA-CBA
14	A	843	CLA	C1A-C2A-CAA-CBA
14	B	3032	CLA	C1A-C2A-CAA-CBA
14	a	826	CLA	C1A-C2A-CAA-CBA
14	a	835	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	a	842	CLA	C1A-C2A-CAA-CBA
14	b	3032	CLA	C1A-C2A-CAA-CBA
14	1	827	CLA	C1A-C2A-CAA-CBA
14	1	843	CLA	C1A-C2A-CAA-CBA
14	2	3032	CLA	C1A-C2A-CAA-CBA
16	B	3046	BCR	C11-C10-C9-C8
16	b	3046	BCR	C11-C10-C9-C8
16	2	3046	BCR	C11-C10-C9-C8
14	F	204	CLA	C2C-C3C-CAC-CBC
14	F	203	CLA	CAA-CBA-CGA-O2A
14	B	3038	CLA	C5-C6-C7-C8
13	A	801	CL0	C15-C16-C17-C18
14	b	3038	CLA	C5-C6-C7-C8
14	A	811	CLA	C2B-C3B-CAB-CBB
14	A	836	CLA	C2B-C3B-CAB-CBB
14	B	3008	CLA	C2B-C3B-CAB-CBB
14	B	3041	CLA	C2B-C3B-CAB-CBB
14	a	810	CLA	C2B-C3B-CAB-CBB
14	a	835	CLA	C2B-C3B-CAB-CBB
14	b	3008	CLA	C2B-C3B-CAB-CBB
14	b	3041	CLA	C2B-C3B-CAB-CBB
14	1	811	CLA	C2B-C3B-CAB-CBB
14	1	836	CLA	C2B-C3B-CAB-CBB
14	2	3008	CLA	C2B-C3B-CAB-CBB
14	2	3041	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C1-C6-C7-C8
16	A	847	BCR	C23-C24-C25-C30
16	A	850	BCR	C1-C6-C7-C8
16	B	3045	BCR	C5-C6-C7-C8
16	B	3046	BCR	C5-C6-C7-C8
16	B	3047	BCR	C23-C24-C25-C26
16	B	3052	BCR	C23-C24-C25-C30
16	B	3053	BCR	C5-C6-C7-C8
16	F	202	BCR	C23-C24-C25-C26
16	F	205	BCR	C23-C24-C25-C26
16	I	101	BCR	C5-C6-C7-C8
16	J	104	BCR	C5-C6-C7-C8
16	J	104	BCR	C23-C24-C25-C26
16	a	846	BCR	C1-C6-C7-C8
16	a	846	BCR	C23-C24-C25-C30
16	a	849	BCR	C1-C6-C7-C8
16	b	3045	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	b	3046	BCR	C5-C6-C7-C8
16	b	3047	BCR	C23-C24-C25-C26
16	f	202	BCR	C23-C24-C25-C26
16	f	205	BCR	C23-C24-C25-C26
16	i	101	BCR	C5-C6-C7-C8
16	j	1105	BCR	C5-C6-C7-C8
16	j	1105	BCR	C23-C24-C25-C26
16	j	1106	BCR	C5-C6-C7-C8
16	l	204	BCR	C23-C24-C25-C30
16	1	846	BCR	C1-C6-C7-C8
16	1	846	BCR	C23-C24-C25-C30
16	1	849	BCR	C1-C6-C7-C8
16	2	3045	BCR	C5-C6-C7-C8
16	2	3046	BCR	C5-C6-C7-C8
16	2	3047	BCR	C23-C24-C25-C26
16	2	3052	BCR	C5-C6-C7-C8
16	6	202	BCR	C23-C24-C25-C26
16	6	205	BCR	C23-C24-C25-C26
16	7	101	BCR	C5-C6-C7-C8
16	8	104	BCR	C5-C6-C7-C8
16	8	104	BCR	C23-C24-C25-C26
16	0	205	BCR	C23-C24-C25-C30
13	1	801	CL0	C15-C16-C17-C18
17	L	207	LHG	C25-C26-C27-C28
17	l	201	LHG	C25-C26-C27-C28
17	0	201	LHG	C25-C26-C27-C28
14	6	204	CLA	C2C-C3C-CAC-CBC
14	B	3011	CLA	CBD-CGD-O2D-CED
14	2	3038	CLA	C5-C6-C7-C8
14	B	3022	CLA	CAA-CBA-CGA-O2A
14	J	101	CLA	CAA-CBA-CGA-O1A
14	b	3022	CLA	CAA-CBA-CGA-O2A
14	j	1102	CLA	CAA-CBA-CGA-O1A
14	2	3022	CLA	CAA-CBA-CGA-O2A
14	8	101	CLA	CAA-CBA-CGA-O1A
17	0	201	LHG	C12-C13-C14-C15
17	L	207	LHG	C12-C13-C14-C15
17	l	201	LHG	C12-C13-C14-C15
14	A	844	CLA	CAA-CBA-CGA-O2A
14	a	843	CLA	CAA-CBA-CGA-O2A
14	1	844	CLA	CAA-CBA-CGA-O2A
14	f	204	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	A	806	CLA	C6-C7-C8-C10
14	A	817	CLA	C6-C7-C8-C10
14	A	821	CLA	C11-C12-C13-C15
14	A	825	CLA	C12-C13-C15-C16
14	A	836	CLA	C11-C10-C8-C7
14	B	3018	CLA	C6-C7-C8-C10
14	B	3034	CLA	C11-C10-C8-C7
14	B	3042	CLA	C12-C13-C15-C16
14	L	203	CLA	C12-C13-C15-C16
14	a	805	CLA	C6-C7-C8-C10
14	a	816	CLA	C6-C7-C8-C10
14	a	820	CLA	C11-C12-C13-C15
14	a	824	CLA	C12-C13-C15-C16
14	a	835	CLA	C11-C10-C8-C7
14	b	3018	CLA	C6-C7-C8-C10
14	b	3034	CLA	C11-C10-C8-C7
14	b	3042	CLA	C12-C13-C15-C16
14	1	806	CLA	C6-C7-C8-C10
14	1	817	CLA	C6-C7-C8-C10
14	1	821	CLA	C11-C12-C13-C15
14	1	825	CLA	C12-C13-C15-C16
14	1	836	CLA	C11-C10-C8-C7
14	2	3018	CLA	C6-C7-C8-C10
14	2	3034	CLA	C11-C10-C8-C7
14	2	3042	CLA	C12-C13-C15-C16
14	2	3011	CLA	CBD-CGD-O2D-CED
14	a	840	CLA	C16-C17-C18-C20
14	2	3005	CLA	C15-C16-C17-C18
14	b	3011	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	C16-C17-C18-C20
14	1	841	CLA	C16-C17-C18-C20
14	b	3005	CLA	C15-C16-C17-C18
16	B	3052	BCR	C37-C22-C23-C24
16	J	104	BCR	C36-C18-C19-C20
16	l	204	BCR	C37-C22-C23-C24
16	0	205	BCR	C37-C22-C23-C24
14	B	3031	CLA	C4-C3-C5-C6
14	b	3031	CLA	C4-C3-C5-C6
14	2	3031	CLA	C4-C3-C5-C6
14	B	3005	CLA	C15-C16-C17-C18
14	A	810	CLA	C2-C3-C5-C6
14	K	102	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	a	809	CLA	C2-C3-C5-C6
14	k	102	CLA	C2-C3-C5-C6
14	1	810	CLA	C2-C3-C5-C6
14	9	103	CLA	C2-C3-C5-C6
14	B	3025	CLA	C2-C1-O2A-CGA
14	b	3025	CLA	C2-C1-O2A-CGA
14	2	3025	CLA	C2-C1-O2A-CGA
16	F	202	BCR	C7-C8-C9-C10
16	f	202	BCR	C7-C8-C9-C10
16	6	202	BCR	C7-C8-C9-C10
14	B	3028	CLA	C5-C6-C7-C8
14	A	844	CLA	CAA-CBA-CGA-O1A
14	a	843	CLA	CAA-CBA-CGA-O1A
14	j	1102	CLA	CAA-CBA-CGA-O2A
14	1	844	CLA	CAA-CBA-CGA-O1A
14	8	101	CLA	CAA-CBA-CGA-O2A
14	A	842	CLA	C6-C7-C8-C9
14	B	3042	CLA	C6-C7-C8-C9
14	B	3042	CLA	C14-C13-C15-C16
14	a	841	CLA	C6-C7-C8-C9
14	b	3042	CLA	C6-C7-C8-C9
14	b	3042	CLA	C14-C13-C15-C16
14	1	842	CLA	C6-C7-C8-C9
14	2	3042	CLA	C14-C13-C15-C16
14	J	101	CLA	CAA-CBA-CGA-O2A
14	b	3028	CLA	C5-C6-C7-C8
14	2	3028	CLA	C5-C6-C7-C8
16	J	104	BCR	C6-C7-C8-C9
16	K	103	BCR	C6-C7-C8-C9
16	j	1105	BCR	C6-C7-C8-C9
16	k	103	BCR	C6-C7-C8-C9
16	8	104	BCR	C6-C7-C8-C9
14	2	3014	CLA	C4-C3-C5-C6
16	B	3052	BCR	C14-C15-C16-C17
16	l	204	BCR	C14-C15-C16-C17
16	0	205	BCR	C14-C15-C16-C17
14	A	806	CLA	C5-C6-C7-C8
14	a	805	CLA	C5-C6-C7-C8
14	1	806	CLA	C5-C6-C7-C8
14	A	802	CLA	C16-C17-C18-C19
14	a	802	CLA	C16-C17-C18-C19
14	1	802	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	B	3022	CLA	CAA-CBA-CGA-O1A
14	b	3022	CLA	CAA-CBA-CGA-O1A
14	2	3022	CLA	CAA-CBA-CGA-O1A
14	B	3009	CLA	C2A-CAA-CBA-CGA
14	b	3009	CLA	C2A-CAA-CBA-CGA
14	2	3009	CLA	C2A-CAA-CBA-CGA
17	A	854	LHG	C24-C25-C26-C27
17	B	3051	LHG	C23-C24-C25-C26
17	0	201	LHG	C29-C30-C31-C32
14	B	3014	CLA	C4-C3-C5-C6
14	L	201	CLA	C4-C3-C5-C6
14	b	3014	CLA	C4-C3-C5-C6
14	l	203	CLA	C4-C3-C5-C6
14	0	204	CLA	C4-C3-C5-C6
17	a	853	LHG	C24-C25-C26-C27
17	b	3051	LHG	C23-C24-C25-C26
17	L	207	LHG	C29-C30-C31-C32
17	1	853	LHG	C24-C25-C26-C27
14	B	3035	CLA	C16-C17-C18-C19
14	b	3035	CLA	C16-C17-C18-C19
14	2	3035	CLA	C16-C17-C18-C19
17	l	201	LHG	C29-C30-C31-C32
14	B	3024	CLA	CAA-CBA-CGA-O2A
14	b	3024	CLA	CAA-CBA-CGA-O2A
14	2	3024	CLA	CAA-CBA-CGA-O2A
17	2	3051	LHG	C23-C24-C25-C26
17	b	3051	LHG	C31-C32-C33-C34
17	2	3051	LHG	C31-C32-C33-C34
17	A	854	LHG	C1-C2-C3-O3
17	a	853	LHG	C1-C2-C3-O3
17	1	853	LHG	C1-C2-C3-O3
13	A	801	CL0	CHA-CBD-CGD-O1D
13	A	801	CL0	CHA-CBD-CGD-O2D
13	a	801	CL0	CHA-CBD-CGD-O1D
13	a	801	CL0	CHA-CBD-CGD-O2D
13	1	801	CL0	CHA-CBD-CGD-O1D
13	1	801	CL0	CHA-CBD-CGD-O2D
16	A	851	BCR	C11-C10-C9-C34
16	A	851	BCR	C16-C17-C18-C36
16	I	102	BCR	C16-C17-C18-C36
16	a	850	BCR	C11-C10-C9-C34
16	a	850	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
16	l	209	BCR	C16-C17-C18-C36
16	1	850	BCR	C11-C10-C9-C34
16	1	850	BCR	C16-C17-C18-C36
16	0	210	BCR	C16-C17-C18-C36
14	B	3033	CLA	CAA-CBA-CGA-O2A
14	b	3033	CLA	CAA-CBA-CGA-O2A
14	2	3033	CLA	CAA-CBA-CGA-O2A
17	B	3051	LHG	C31-C32-C33-C34
14	b	3004	CLA	C5-C6-C7-C8
14	A	840	CLA	C11-C12-C13-C15
14	a	839	CLA	C11-C12-C13-C15
14	1	840	CLA	C11-C12-C13-C15
14	B	3004	CLA	C5-C6-C7-C8
13	A	801	CL0	C11-C12-C13-C14
13	a	801	CL0	C11-C12-C13-C14
13	1	801	CL0	C11-C12-C13-C14
14	A	804	CLA	C11-C10-C8-C9
14	A	816	CLA	C6-C7-C8-C9
14	A	821	CLA	C14-C13-C15-C16
14	A	839	CLA	C11-C12-C13-C14
14	B	3003	CLA	C14-C13-C15-C16
14	B	3004	CLA	C11-C12-C13-C14
14	B	3008	CLA	C11-C12-C13-C14
14	B	3008	CLA	C14-C13-C15-C16
14	a	815	CLA	C6-C7-C8-C9
14	a	820	CLA	C14-C13-C15-C16
14	a	838	CLA	C11-C12-C13-C14
14	b	3003	CLA	C14-C13-C15-C16
14	b	3004	CLA	C11-C12-C13-C14
14	b	3008	CLA	C11-C12-C13-C14
14	b	3008	CLA	C14-C13-C15-C16
14	j	1101	CLA	C11-C10-C8-C9
14	1	804	CLA	C11-C10-C8-C9
14	1	816	CLA	C6-C7-C8-C9
14	1	821	CLA	C14-C13-C15-C16
14	1	839	CLA	C11-C12-C13-C14
14	2	3003	CLA	C14-C13-C15-C16
14	2	3004	CLA	C11-C12-C13-C14
14	2	3008	CLA	C11-C12-C13-C14
14	2	3008	CLA	C14-C13-C15-C16
14	2	3004	CLA	C5-C6-C7-C8
14	A	825	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	B	3018	CLA	C2-C1-O2A-CGA
14	B	3019	CLA	C2-C1-O2A-CGA
14	a	824	CLA	C2-C1-O2A-CGA
14	b	3018	CLA	C2-C1-O2A-CGA
14	b	3019	CLA	C2-C1-O2A-CGA
14	1	825	CLA	C2-C1-O2A-CGA
14	2	3018	CLA	C2-C1-O2A-CGA
14	2	3019	CLA	C2-C1-O2A-CGA
14	A	815	CLA	C3A-C2A-CAA-CBA
14	A	827	CLA	C3A-C2A-CAA-CBA
14	A	838	CLA	C3A-C2A-CAA-CBA
14	A	843	CLA	C3A-C2A-CAA-CBA
14	B	3032	CLA	C3A-C2A-CAA-CBA
14	a	814	CLA	C3A-C2A-CAA-CBA
14	a	826	CLA	C3A-C2A-CAA-CBA
14	a	837	CLA	C3A-C2A-CAA-CBA
14	a	842	CLA	C3A-C2A-CAA-CBA
14	b	3032	CLA	C3A-C2A-CAA-CBA
14	1	815	CLA	C3A-C2A-CAA-CBA
14	1	827	CLA	C3A-C2A-CAA-CBA
14	1	838	CLA	C3A-C2A-CAA-CBA
14	1	843	CLA	C3A-C2A-CAA-CBA
14	2	3032	CLA	C3A-C2A-CAA-CBA
16	B	3045	BCR	C18-C19-C20-C21
14	B	3024	CLA	CAA-CBA-CGA-O1A
14	a	805	CLA	C15-C16-C17-C18
14	1	806	CLA	C15-C16-C17-C18
16	A	852	BCR	C12-C13-C14-C15
16	K	103	BCR	C11-C10-C9-C8
16	a	851	BCR	C12-C13-C14-C15
16	k	103	BCR	C11-C10-C9-C8
16	1	851	BCR	C12-C13-C14-C15
16	9	104	BCR	C11-C10-C9-C8
14	b	3024	CLA	CAA-CBA-CGA-O1A
14	2	3024	CLA	CAA-CBA-CGA-O1A
16	2	3044	BCR	C22-C23-C24-C25
14	A	806	CLA	C15-C16-C17-C18
14	B	3019	CLA	C13-C15-C16-C17
14	b	3019	CLA	C13-C15-C16-C17
14	2	3019	CLA	C13-C15-C16-C17
14	a	815	CLA	C2C-C3C-CAC-CBC
14	b	3037	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	B	3037	CLA	CAA-CBA-CGA-O2A
14	2	3037	CLA	CAA-CBA-CGA-O2A
14	B	3032	CLA	C2C-C3C-CAC-CBC
14	B	3035	CLA	C5-C6-C7-C8
14	b	3035	CLA	C5-C6-C7-C8
14	2	3035	CLA	C5-C6-C7-C8
14	A	813	CLA	CAA-CBA-CGA-O2A
14	B	3037	CLA	CAA-CBA-CGA-O1A
14	b	3037	CLA	CAA-CBA-CGA-O1A
14	2	3037	CLA	CAA-CBA-CGA-O1A
14	B	3008	CLA	CAA-CBA-CGA-O2A
14	b	3008	CLA	CAA-CBA-CGA-O2A
14	2	3008	CLA	CAA-CBA-CGA-O2A
17	A	854	LHG	C8-C7-O7-C5
17	a	853	LHG	C8-C7-O7-C5
17	1	853	LHG	C8-C7-O7-C5
14	a	805	CLA	C2C-C3C-CAC-CBC
14	b	3032	CLA	C2C-C3C-CAC-CBC
14	a	812	CLA	CAA-CBA-CGA-O2A
14	1	824	CLA	C5-C6-C7-C8
14	A	802	CLA	C11-C12-C13-C14
14	A	809	CLA	C6-C7-C8-C9
14	A	838	CLA	C11-C10-C8-C9
14	A	841	CLA	C11-C10-C8-C9
14	A	843	CLA	C6-C7-C8-C9
14	L	203	CLA	C14-C13-C15-C16
14	a	802	CLA	C11-C12-C13-C14
14	a	808	CLA	C6-C7-C8-C9
14	a	837	CLA	C11-C10-C8-C9
14	a	840	CLA	C11-C10-C8-C9
14	a	842	CLA	C6-C7-C8-C9
14	l	206	CLA	C14-C13-C15-C16
14	1	802	CLA	C11-C12-C13-C14
14	1	809	CLA	C6-C7-C8-C9
14	1	838	CLA	C11-C10-C8-C9
14	1	841	CLA	C11-C10-C8-C9
14	1	843	CLA	C6-C7-C8-C9
14	0	207	CLA	C14-C13-C15-C16
14	1	816	CLA	C2C-C3C-CAC-CBC
14	2	3032	CLA	C2C-C3C-CAC-CBC
17	L	207	LHG	O6-C4-C5-C6
17	l	201	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
17	0	201	LHG	O6-C4-C5-C6
14	1	813	CLA	CAA-CBA-CGA-O2A
14	A	824	CLA	C5-C6-C7-C8
14	A	816	CLA	C2C-C3C-CAC-CBC
14	b	3011	CLA	CAA-CBA-CGA-O2A
14	b	3036	CLA	CAA-CBA-CGA-O2A
14	A	806	CLA	C2C-C3C-CAC-CBC
14	1	806	CLA	C2C-C3C-CAC-CBC
14	F	204	CLA	C2A-CAA-CBA-CGA
14	f	204	CLA	C2A-CAA-CBA-CGA
14	6	204	CLA	C2A-CAA-CBA-CGA
14	A	804	CLA	C11-C10-C8-C7
14	A	821	CLA	C12-C13-C15-C16
14	A	839	CLA	C11-C12-C13-C15
14	B	3004	CLA	C11-C12-C13-C15
14	B	3008	CLA	C11-C12-C13-C15
14	B	3008	CLA	C12-C13-C15-C16
14	B	3014	CLA	C11-C12-C13-C15
14	B	3020	CLA	C11-C10-C8-C7
14	B	3025	CLA	C11-C10-C8-C7
14	B	3028	CLA	C11-C12-C13-C15
14	B	3042	CLA	C11-C12-C13-C15
14	a	820	CLA	C12-C13-C15-C16
14	a	838	CLA	C11-C12-C13-C15
14	b	3004	CLA	C11-C12-C13-C15
14	b	3008	CLA	C11-C12-C13-C15
14	b	3008	CLA	C12-C13-C15-C16
14	b	3014	CLA	C11-C12-C13-C15
14	b	3020	CLA	C11-C10-C8-C7
14	b	3025	CLA	C11-C10-C8-C7
14	b	3028	CLA	C11-C12-C13-C15
14	b	3042	CLA	C11-C12-C13-C15
14	j	1101	CLA	C11-C10-C8-C7
14	1	804	CLA	C11-C10-C8-C7
14	1	821	CLA	C12-C13-C15-C16
14	1	839	CLA	C11-C12-C13-C15
14	2	3004	CLA	C11-C12-C13-C15
14	2	3008	CLA	C11-C12-C13-C15
14	2	3008	CLA	C12-C13-C15-C16
14	2	3014	CLA	C11-C12-C13-C15
14	2	3020	CLA	C11-C10-C8-C7
14	2	3025	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	2	3028	CLA	C11-C12-C13-C15
14	2	3042	CLA	C11-C12-C13-C15
14	B	3013	CLA	C2B-C3B-CAB-CBB
14	b	3013	CLA	C2B-C3B-CAB-CBB
14	2	3013	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C5-C6-C7-C8
16	A	847	BCR	C23-C24-C25-C26
16	A	848	BCR	C5-C6-C7-C8
16	A	850	BCR	C5-C6-C7-C8
16	B	3047	BCR	C1-C6-C7-C8
16	B	3052	BCR	C23-C24-C25-C26
16	a	846	BCR	C5-C6-C7-C8
16	a	846	BCR	C23-C24-C25-C26
16	a	847	BCR	C5-C6-C7-C8
16	a	849	BCR	C5-C6-C7-C8
16	b	3047	BCR	C1-C6-C7-C8
16	l	204	BCR	C23-C24-C25-C26
16	1	846	BCR	C5-C6-C7-C8
16	1	846	BCR	C23-C24-C25-C26
16	1	847	BCR	C5-C6-C7-C8
16	1	849	BCR	C5-C6-C7-C8
16	2	3047	BCR	C1-C6-C7-C8
16	0	205	BCR	C23-C24-C25-C26
14	B	3036	CLA	CAA-CBA-CGA-O2A
14	2	3011	CLA	CAA-CBA-CGA-O2A
14	2	3036	CLA	CAA-CBA-CGA-O2A
14	A	815	CLA	C2-C1-O2A-CGA
14	a	814	CLA	C2-C1-O2A-CGA
14	1	815	CLA	C2-C1-O2A-CGA
14	a	823	CLA	C5-C6-C7-C8
14	f	204	CLA	C4C-C3C-CAC-CBC
14	B	3011	CLA	CAA-CBA-CGA-O2A
14	6	204	CLA	C4C-C3C-CAC-CBC
14	F	204	CLA	C4C-C3C-CAC-CBC
14	B	3014	CLA	CAA-CBA-CGA-O2A
14	b	3014	CLA	CAA-CBA-CGA-O2A
14	2	3014	CLA	CAA-CBA-CGA-O2A
14	B	3035	CLA	C16-C17-C18-C20
14	b	3025	CLA	C13-C15-C16-C17
14	2	3025	CLA	C13-C15-C16-C17
14	B	3025	CLA	C13-C15-C16-C17
16	b	3045	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
16	2	3045	BCR	C18-C19-C20-C21
14	B	3017	CLA	CAA-CBA-CGA-O2A
14	b	3017	CLA	CAA-CBA-CGA-O2A
14	2	3017	CLA	CAA-CBA-CGA-O2A
14	A	814	CLA	C15-C16-C17-C18
20	b	3050	LMG	C21-C22-C23-C24
20	2	3050	LMG	C21-C22-C23-C24
14	A	832	CLA	C3-C5-C6-C7
14	a	831	CLA	C3-C5-C6-C7
14	1	832	CLA	C3-C5-C6-C7
20	B	3050	LMG	C21-C22-C23-C24
14	b	3035	CLA	C16-C17-C18-C20
14	a	813	CLA	C15-C16-C17-C18
14	1	814	CLA	C15-C16-C17-C18
14	0	207	CLA	C5-C6-C7-C8
14	a	812	CLA	CAA-CBA-CGA-O1A
14	1	813	CLA	CAA-CBA-CGA-O1A
13	A	801	CL0	C14-C13-C15-C16
13	a	801	CL0	C14-C13-C15-C16
13	1	801	CL0	C14-C13-C15-C16
14	A	807	CLA	C6-C7-C8-C9
14	A	826	CLA	C6-C7-C8-C9
14	A	826	CLA	C14-C13-C15-C16
14	B	3005	CLA	C11-C10-C8-C9
14	B	3021	CLA	C14-C13-C15-C16
14	B	3033	CLA	C11-C10-C8-C9
14	a	806	CLA	C6-C7-C8-C9
14	a	825	CLA	C6-C7-C8-C9
14	a	825	CLA	C14-C13-C15-C16
14	b	3005	CLA	C11-C10-C8-C9
14	b	3021	CLA	C14-C13-C15-C16
14	b	3033	CLA	C11-C10-C8-C9
14	1	807	CLA	C6-C7-C8-C9
14	1	826	CLA	C6-C7-C8-C9
14	1	826	CLA	C14-C13-C15-C16
14	2	3005	CLA	C11-C10-C8-C9
14	2	3021	CLA	C14-C13-C15-C16
14	2	3033	CLA	C11-C10-C8-C9
15	B	3043	PQN	C19-C18-C20-C21
15	b	3043	PQN	C19-C18-C20-C21
15	2	3043	PQN	C19-C18-C20-C21
16	j	1105	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
16	8	104	BCR	C36-C18-C19-C20
14	K	102	CLA	CAA-CBA-CGA-O2A
14	k	102	CLA	CAA-CBA-CGA-O2A
14	9	103	CLA	CAA-CBA-CGA-O2A
14	2	3035	CLA	C16-C17-C18-C20
14	l	206	CLA	C5-C6-C7-C8
14	A	815	CLA	C1A-C2A-CAA-CBA
14	A	817	CLA	C4B-C3B-CAB-CBB
14	A	836	CLA	C1A-C2A-CAA-CBA
14	A	836	CLA	C4B-C3B-CAB-CBB
14	A	855	CLA	C4B-C3B-CAB-CBB
14	B	3025	CLA	C1A-C2A-CAA-CBA
14	K	101	CLA	C4B-C3B-CAB-CBB
14	M	1601	CLA	C4B-C3B-CAB-CBB
14	a	814	CLA	C1A-C2A-CAA-CBA
14	a	816	CLA	C4B-C3B-CAB-CBB
14	a	835	CLA	C4B-C3B-CAB-CBB
14	b	3025	CLA	C1A-C2A-CAA-CBA
14	k	101	CLA	C4B-C3B-CAB-CBB
14	1	815	CLA	C1A-C2A-CAA-CBA
14	1	817	CLA	C4B-C3B-CAB-CBB
14	1	836	CLA	C1A-C2A-CAA-CBA
14	1	836	CLA	C4B-C3B-CAB-CBB
14	2	3025	CLA	C1A-C2A-CAA-CBA
14	9	101	CLA	C4B-C3B-CAB-CBB
14	0	203	CLA	C4B-C3B-CAB-CBB
14	L	203	CLA	C5-C6-C7-C8
16	B	3044	BCR	C22-C23-C24-C25
16	b	3044	BCR	C22-C23-C24-C25
14	A	802	CLA	CAA-CBA-CGA-O2A
14	A	809	CLA	CAA-CBA-CGA-O2A
14	A	840	CLA	CAA-CBA-CGA-O2A
14	a	808	CLA	CAA-CBA-CGA-O2A
14	a	839	CLA	CAA-CBA-CGA-O2A
14	1	809	CLA	CAA-CBA-CGA-O2A
14	A	813	CLA	CAA-CBA-CGA-O1A
16	A	847	BCR	C21-C22-C23-C24
16	J	104	BCR	C21-C22-C23-C24
16	a	846	BCR	C21-C22-C23-C24
16	j	1105	BCR	C21-C22-C23-C24
16	1	846	BCR	C21-C22-C23-C24
16	8	104	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	B	3049	BCR	C9-C10-C11-C12
16	b	3049	BCR	C9-C10-C11-C12
16	2	3049	BCR	C9-C10-C11-C12
14	A	804	CLA	C16-C17-C18-C20
14	A	816	CLA	CAA-CBA-CGA-O2A
14	a	802	CLA	CAA-CBA-CGA-O2A
14	a	815	CLA	CAA-CBA-CGA-O2A
14	1	802	CLA	CAA-CBA-CGA-O2A
14	1	816	CLA	CAA-CBA-CGA-O2A
14	1	840	CLA	CAA-CBA-CGA-O2A
14	A	804	CLA	C2A-CAA-CBA-CGA
14	A	824	CLA	C2A-CAA-CBA-CGA
14	a	823	CLA	C2A-CAA-CBA-CGA
14	j	1101	CLA	C2A-CAA-CBA-CGA
14	1	804	CLA	C2A-CAA-CBA-CGA
14	1	824	CLA	C2A-CAA-CBA-CGA
14	j	1101	CLA	C16-C17-C18-C20
14	1	804	CLA	C16-C17-C18-C20
14	F	204	CLA	CAA-CBA-CGA-O2A
14	f	204	CLA	CAA-CBA-CGA-O2A
14	6	204	CLA	CAA-CBA-CGA-O2A
14	B	3003	CLA	C2-C1-O2A-CGA
14	B	3042	CLA	C2-C1-O2A-CGA
14	b	3003	CLA	C2-C1-O2A-CGA
14	b	3042	CLA	C2-C1-O2A-CGA
14	2	3003	CLA	C2-C1-O2A-CGA
14	2	3007	CLA	C2-C1-O2A-CGA
14	2	3042	CLA	C2-C1-O2A-CGA
14	A	836	CLA	CAA-CBA-CGA-O2A
14	a	835	CLA	CAA-CBA-CGA-O2A
14	1	836	CLA	CAA-CBA-CGA-O2A
14	A	816	CLA	C6-C7-C8-C10
14	A	841	CLA	C11-C12-C13-C15
14	a	815	CLA	C6-C7-C8-C10
14	a	840	CLA	C11-C12-C13-C15
14	1	816	CLA	C6-C7-C8-C10
14	1	841	CLA	C11-C12-C13-C15
15	A	845	PQN	C17-C18-C20-C21
15	a	844	PQN	C17-C18-C20-C21
15	1	845	PQN	C17-C18-C20-C21
14	A	807	CLA	C10-C11-C12-C13
14	a	806	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	1	807	CLA	C10-C11-C12-C13
14	a	813	CLA	C16-C17-C18-C20
14	1	814	CLA	C16-C17-C18-C20
17	L	208	LHG	C4-C5-O7-C7
17	l	202	LHG	C4-C5-O7-C7
17	0	202	LHG	C4-C5-O7-C7
14	a	839	CLA	C4C-C3C-CAC-CBC
14	1	840	CLA	C4C-C3C-CAC-CBC
20	B	3050	LMG	O9-C10-C11-C12
14	A	814	CLA	C16-C17-C18-C20
14	A	842	CLA	C16-C17-C18-C20
14	a	841	CLA	C16-C17-C18-C20
14	1	842	CLA	C16-C17-C18-C20
14	A	821	CLA	CAA-CBA-CGA-O2A
14	a	820	CLA	CAA-CBA-CGA-O2A
14	1	821	CLA	CAA-CBA-CGA-O2A
14	b	3036	CLA	CAA-CBA-CGA-O1A
20	b	3050	LMG	O9-C10-C11-C12
20	2	3050	LMG	O9-C10-C11-C12
17	a	852	LHG	C23-C24-C25-C26
17	1	852	LHG	C23-C24-C25-C26
14	A	840	CLA	C4C-C3C-CAC-CBC
14	B	3017	CLA	CAA-CBA-CGA-O1A
14	B	3036	CLA	CAA-CBA-CGA-O1A
14	2	3017	CLA	CAA-CBA-CGA-O1A
17	A	853	LHG	C23-C24-C25-C26
14	b	3017	CLA	CAA-CBA-CGA-O1A
14	2	3036	CLA	CAA-CBA-CGA-O1A
14	0	209	CLA	CBD-CGD-O2D-CED
14	B	3010	CLA	C5-C6-C7-C8
14	A	841	CLA	C2A-CAA-CBA-CGA
14	B	3023	CLA	C2A-CAA-CBA-CGA
14	b	3023	CLA	C2A-CAA-CBA-CGA
14	2	3023	CLA	C2A-CAA-CBA-CGA
14	B	3015	CLA	CBA-CGA-O2A-C1
14	2	3015	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	C11-C12-C13-C14
14	A	833	CLA	C6-C7-C8-C9
14	A	833	CLA	C14-C13-C15-C16
14	B	3034	CLA	C11-C10-C8-C9
14	B	3038	CLA	C11-C10-C8-C9
14	B	3042	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	a	828	CLA	C11-C12-C13-C14
14	a	832	CLA	C6-C7-C8-C9
14	a	832	CLA	C14-C13-C15-C16
14	b	3034	CLA	C11-C10-C8-C9
14	b	3038	CLA	C11-C10-C8-C9
14	1	812	CLA	C6-C7-C8-C9
14	1	829	CLA	C11-C12-C13-C14
14	1	833	CLA	C6-C7-C8-C9
14	1	833	CLA	C14-C13-C15-C16
14	2	3034	CLA	C11-C10-C8-C9
14	2	3038	CLA	C11-C10-C8-C9
17	B	3051	LHG	O7-C7-C8-C9
17	b	3051	LHG	O7-C7-C8-C9
17	2	3051	LHG	O7-C7-C8-C9
14	b	3010	CLA	C5-C6-C7-C8
14	2	3010	CLA	C5-C6-C7-C8
14	A	815	CLA	C5-C6-C7-C8
14	a	814	CLA	C5-C6-C7-C8
14	a	820	CLA	C8-C10-C11-C12
14	1	825	CLA	C15-C16-C17-C18
14	A	836	CLA	CAA-CBA-CGA-O1A
14	B	3014	CLA	CAA-CBA-CGA-O1A
14	a	835	CLA	CAA-CBA-CGA-O1A
14	b	3014	CLA	CAA-CBA-CGA-O1A
14	2	3014	CLA	CAA-CBA-CGA-O1A
14	b	3015	CLA	CBA-CGA-O2A-C1
14	1	821	CLA	C8-C10-C11-C12
14	l	208	CLA	O1D-CGD-O2D-CED
14	K	102	CLA	CAA-CBA-CGA-O1A
14	b	3008	CLA	CAA-CBA-CGA-O1A
14	k	102	CLA	CAA-CBA-CGA-O1A
14	1	836	CLA	CAA-CBA-CGA-O1A
14	2	3008	CLA	CAA-CBA-CGA-O1A
14	9	103	CLA	CAA-CBA-CGA-O1A
14	L	205	CLA	O1D-CGD-O2D-CED
14	A	821	CLA	C8-C10-C11-C12
14	A	826	CLA	C15-C16-C17-C18
14	B	3031	CLA	C5-C6-C7-C8
14	a	825	CLA	C15-C16-C17-C18
14	b	3031	CLA	C5-C6-C7-C8
14	1	815	CLA	C5-C6-C7-C8
14	2	3031	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	L	201	CLA	CAA-CBA-CGA-O2A
14	l	203	CLA	CAA-CBA-CGA-O2A
14	0	204	CLA	CAA-CBA-CGA-O2A
14	A	825	CLA	C15-C16-C17-C18
14	1	826	CLA	C15-C16-C17-C18
14	l	208	CLA	CBD-CGD-O2D-CED
16	F	205	BCR	C21-C22-C23-C24
16	f	205	BCR	C21-C22-C23-C24
16	6	205	BCR	C21-C22-C23-C24
14	B	3008	CLA	CAA-CBA-CGA-O1A
14	a	824	CLA	C15-C16-C17-C18
14	F	204	CLA	CAA-CBA-CGA-O1A
14	f	204	CLA	CAA-CBA-CGA-O1A
14	6	204	CLA	CAA-CBA-CGA-O1A
14	A	818	CLA	C8-C10-C11-C12
14	a	817	CLA	C8-C10-C11-C12
14	a	840	CLA	C2A-CAA-CBA-CGA
14	1	841	CLA	C2A-CAA-CBA-CGA
14	1	818	CLA	C8-C10-C11-C12
17	B	3051	LHG	O9-C7-C8-C9
17	b	3051	LHG	O9-C7-C8-C9
17	2	3051	LHG	O9-C7-C8-C9
14	A	831	CLA	C15-C16-C17-C18
14	a	830	CLA	C15-C16-C17-C18
14	1	831	CLA	C15-C16-C17-C18
14	b	3013	CLA	CAA-CBA-CGA-O2A
17	A	853	LHG	O9-C7-C8-C9
17	1	852	LHG	O9-C7-C8-C9
14	B	3013	CLA	CAA-CBA-CGA-O2A
14	2	3013	CLA	CAA-CBA-CGA-O2A
14	a	815	CLA	CAA-CBA-CGA-O1A
14	1	816	CLA	CAA-CBA-CGA-O1A
17	a	852	LHG	O9-C7-C8-C9
14	0	204	CLA	O1A-CGA-O2A-C1
17	L	208	LHG	O6-C4-C5-C6
17	l	202	LHG	O6-C4-C5-C6
17	0	202	LHG	O6-C4-C5-C6
14	A	821	CLA	C2-C1-O2A-CGA
14	B	3007	CLA	C2-C1-O2A-CGA
14	a	820	CLA	C2-C1-O2A-CGA
14	b	3007	CLA	C2-C1-O2A-CGA
14	1	821	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	1	840	CLA	CAA-CBA-CGA-O1A
14	L	201	CLA	O1A-CGA-O2A-C1
14	l	203	CLA	O1A-CGA-O2A-C1
17	L	207	LHG	C31-C32-C33-C34
17	l	201	LHG	C31-C32-C33-C34
15	b	3043	PQN	C13-C15-C16-C17
14	L	205	CLA	CBD-CGD-O2D-CED
14	A	816	CLA	CAA-CBA-CGA-O1A
14	A	840	CLA	CAA-CBA-CGA-O1A
14	a	839	CLA	CAA-CBA-CGA-O1A
14	B	3015	CLA	C13-C15-C16-C17
14	2	3015	CLA	C13-C15-C16-C17
14	0	209	CLA	O1D-CGD-O2D-CED
15	B	3043	PQN	C13-C15-C16-C17
15	2	3043	PQN	C13-C15-C16-C17
14	b	3015	CLA	C13-C15-C16-C17
14	F	201	CLA	CAA-CBA-CGA-O2A
14	f	201	CLA	CAA-CBA-CGA-O2A
17	0	201	LHG	C31-C32-C33-C34
14	b	3013	CLA	CAA-CBA-CGA-O1A
14	2	3013	CLA	CAA-CBA-CGA-O1A
14	A	802	CLA	CAA-CBA-CGA-O1A
14	A	809	CLA	CAA-CBA-CGA-O1A
14	a	808	CLA	CAA-CBA-CGA-O1A
14	1	809	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

266 monomers are involved in 501 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	802	CLA	3	0
14	b	3009	CLA	1	0
14	a	838	CLA	1	0
14	B	3009	CLA	1	0
14	B	3016	CLA	2	0
14	a	823	CLA	1	0
16	0	210	BCR	1	0
14	a	826	CLA	1	0
14	a	815	CLA	3	0
14	A	827	CLA	1	0
14	L	204	CLA	1	0
14	A	817	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	9	102	BCR	1	0
14	A	828	CLA	2	0
14	1	813	CLA	1	0
14	f	203	CLA	2	0
14	a	817	CLA	1	0
17	2	3051	LHG	3	0
14	f	201	CLA	2	0
14	1	839	CLA	2	0
14	1	817	CLA	2	0
14	b	3036	CLA	4	0
16	j	1106	BCR	10	0
14	2	3003	CLA	5	0
16	A	848	BCR	2	0
14	l	203	CLA	1	0
16	b	3045	BCR	1	0
14	2	3005	CLA	4	0
14	B	3018	CLA	4	0
14	2	3019	CLA	2	0
14	b	3017	CLA	2	0
14	2	3025	CLA	1	0
14	2	3004	CLA	1	0
14	1	821	CLA	6	0
14	B	3042	CLA	1	0
14	2	3041	CLA	1	0
16	b	3047	BCR	3	0
14	2	3024	CLA	1	0
16	1	847	BCR	2	0
14	a	808	CLA	2	0
14	F	204	CLA	3	0
14	A	821	CLA	4	0
16	k	103	BCR	2	0
14	b	3004	CLA	1	0
16	l	209	BCR	1	0
14	b	3031	CLA	6	0
15	a	844	PQN	3	0
14	2	3036	CLA	4	0
14	b	3012	CLA	3	0
15	1	845	PQN	1	0
14	1	814	CLA	1	0
14	2	3038	CLA	2	0
14	1	803	CLA	2	0
14	2	3033	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3028	CLA	3	0
14	A	815	CLA	2	0
13	a	801	CL0	1	0
14	A	814	CLA	1	0
14	1	826	CLA	1	0
14	1	815	CLA	2	0
14	b	3025	CLA	2	0
16	A	847	BCR	1	0
14	A	803	CLA	2	0
14	2	3020	CLA	2	0
14	2	3040	CLA	4	0
14	L	201	CLA	2	0
14	1	806	CLA	3	0
14	2	3039	CLA	2	0
14	l	206	CLA	1	0
17	L	207	LHG	1	0
14	B	3035	CLA	3	0
14	A	838	CLA	1	0
14	1	809	CLA	3	0
14	b	3040	CLA	4	0
14	1	828	CLA	2	0
16	b	3046	BCR	1	0
14	a	842	CLA	2	0
14	A	812	CLA	1	0
14	A	833	CLA	1	0
14	L	203	CLA	1	0
14	6	203	CLA	2	0
14	2	3006	CLA	4	0
14	1	812	CLA	1	0
14	A	816	CLA	2	0
14	a	837	CLA	1	0
17	B	3051	LHG	5	0
14	b	3033	CLA	3	0
16	B	3053	BCR	3	0
14	A	842	CLA	1	0
16	9	104	BCR	2	0
16	A	851	BCR	7	0
16	B	3045	BCR	1	0
15	A	845	PQN	1	0
14	2	3035	CLA	3	0
16	a	849	BCR	1	0
14	l	208	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3004	CLA	1	0
14	2	3034	CLA	4	0
16	K	103	BCR	2	0
16	8	103	BCR	4	0
16	j	1104	BCR	3	0
14	1	843	CLA	2	0
14	2	3022	CLA	1	0
16	2	3045	BCR	1	0
14	1	833	CLA	1	0
14	A	820	CLA	2	0
17	b	3051	LHG	3	0
14	a	841	CLA	1	0
16	J	103	BCR	3	0
14	1	825	CLA	2	0
14	a	813	CLA	1	0
14	B	3015	CLA	2	0
14	a	820	CLA	5	0
13	1	801	CL0	1	0
14	F	203	CLA	3	0
14	L	205	CLA	3	0
16	a	847	BCR	1	0
14	b	3024	CLA	1	0
16	a	850	BCR	6	0
14	2	3037	CLA	1	0
16	y	101	BCR	4	0
14	b	3003	CLA	6	0
14	a	827	CLA	2	0
14	1	838	CLA	1	0
14	b	3038	CLA	2	0
14	0	209	CLA	2	0
14	z	1701	CLA	2	0
16	B	3046	BCR	1	0
16	m	101	BCR	1	0
16	I	102	BCR	1	0
17	A	853	LHG	2	0
14	b	3022	CLA	1	0
14	b	3026	CLA	3	0
17	l	202	LHG	1	0
14	j	1101	CLA	4	0
14	a	824	CLA	2	0
14	A	843	CLA	2	0
14	2	3009	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	3028	CLA	4	0
14	2	3016	CLA	2	0
14	A	832	CLA	2	0
14	1	819	CLA	3	0
14	b	3005	CLA	4	0
16	b	3048	BCR	3	0
14	A	829	CLA	2	0
16	B	3048	BCR	2	0
14	a	840	CLA	1	0
13	A	801	CL0	1	0
14	1	820	CLA	1	0
14	A	825	CLA	2	0
14	a	805	CLA	3	0
14	A	819	CLA	3	0
14	b	3039	CLA	3	0
14	b	3014	CLA	1	0
14	1	842	CLA	1	0
14	a	829	CLA	3	0
16	1	850	BCR	7	0
14	2	3042	CLA	1	0
14	1	824	CLA	1	0
14	1	827	CLA	1	0
16	M	1602	BCR	1	0
14	a	828	CLA	2	0
14	1	841	CLA	1	0
14	2	3015	CLA	1	0
14	a	816	CLA	2	0
14	A	855	CLA	1	0
14	b	3034	CLA	2	0
14	F	201	CLA	1	0
14	B	3040	CLA	3	0
14	b	3015	CLA	1	0
16	A	846	BCR	1	0
17	a	852	LHG	2	0
14	B	3003	CLA	6	0
14	B	3037	CLA	1	0
14	b	3016	CLA	2	0
14	b	3019	CLA	1	0
14	B	3019	CLA	1	0
16	1	846	BCR	1	0
16	1	848	BCR	1	0
14	B	3005	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3036	CLA	3	0
14	A	809	CLA	2	0
14	B	3026	CLA	2	0
14	2	3017	CLA	2	0
14	A	826	CLA	1	0
14	f	204	CLA	3	0
14	a	818	CLA	3	0
14	b	3037	CLA	1	0
17	0	202	LHG	1	0
14	A	830	CLA	3	0
14	1	805	CLA	1	0
14	a	831	CLA	2	0
14	2	3028	CLA	4	0
14	A	806	CLA	3	0
14	l	207	CLA	1	0
14	A	824	CLA	1	0
14	6	201	CLA	1	0
14	K	101	CLA	2	0
14	B	3017	CLA	2	0
14	B	3041	CLA	1	0
14	A	841	CLA	1	0
14	b	3035	CLA	3	0
14	a	825	CLA	1	0
14	A	807	CLA	3	0
14	B	3024	CLA	1	0
16	A	849	BCR	2	0
16	2	3047	BCR	2	0
14	a	804	CLA	1	0
20	2	3050	LMG	1	0
14	A	839	CLA	1	0
14	b	3018	CLA	3	0
14	B	3033	CLA	4	0
14	a	811	CLA	1	0
14	B	3034	CLA	5	0
14	B	3006	CLA	2	0
14	B	3031	CLA	6	0
14	1	816	CLA	2	0
14	a	832	CLA	2	0
14	A	810	CLA	1	0
16	a	845	BCR	1	0
16	B	3047	BCR	3	0
14	B	3022	CLA	1	0

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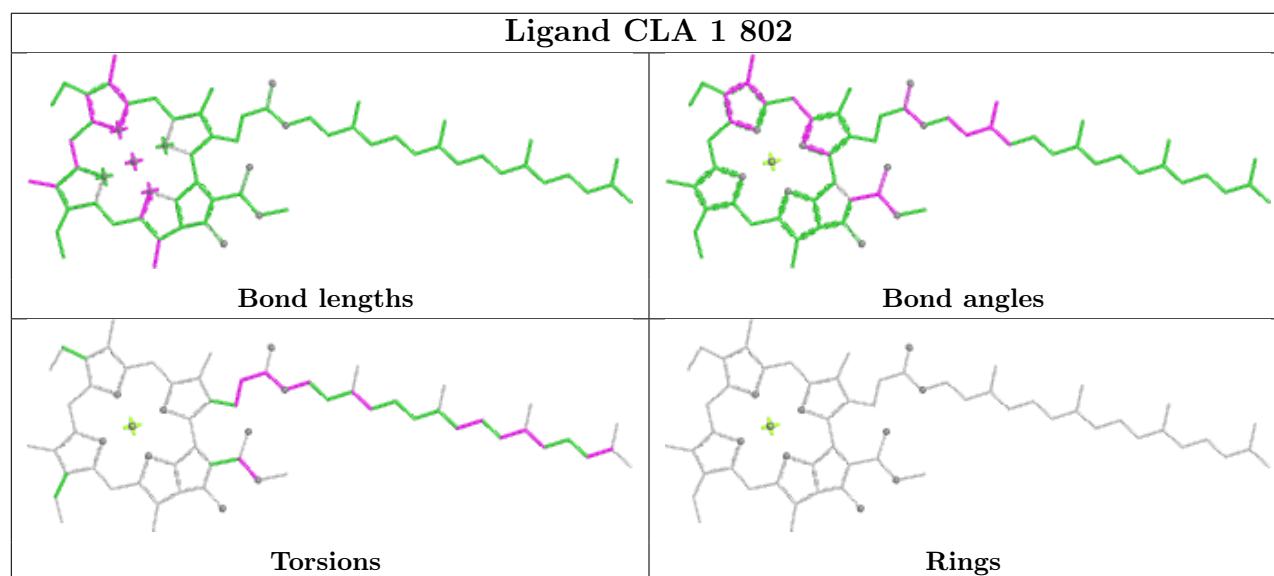
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3038	CLA	3	0
14	B	3012	CLA	3	0
14	1	810	CLA	1	0
14	2	3010	CLA	3	0
16	a	848	BCR	2	0
14	a	819	CLA	1	0
17	l	201	LHG	1	0
14	b	3010	CLA	3	0
14	B	3010	CLA	3	0
14	b	3020	CLA	2	0
14	2	3032	CLA	1	0
14	a	814	CLA	3	0
14	B	3020	CLA	2	0
14	B	3025	CLA	1	0
14	2	3031	CLA	6	0
14	2	3026	CLA	3	0
14	A	818	CLA	2	0
16	8	104	BCR	2	0
14	A	844	CLA	1	0
14	0	208	CLA	1	0
14	1	830	CLA	3	0
14	2	3018	CLA	3	0
14	a	802	CLA	3	0
14	2	3012	CLA	3	0
14	0	204	CLA	2	0
14	b	3041	CLA	1	0
14	a	803	CLA	2	0
14	1	818	CLA	2	0
14	b	3042	CLA	1	0
16	2	3048	BCR	4	0
16	2	3052	BCR	3	0
14	B	3039	CLA	2	0
14	1	829	CLA	3	0
14	6	204	CLA	3	0
17	1	852	LHG	2	0
14	a	806	CLA	4	0
14	a	812	CLA	1	0
14	A	802	CLA	3	0
14	1	807	CLA	3	0
16	2	3046	BCR	1	0
14	0	207	CLA	1	0
16	a	846	BCR	1	0

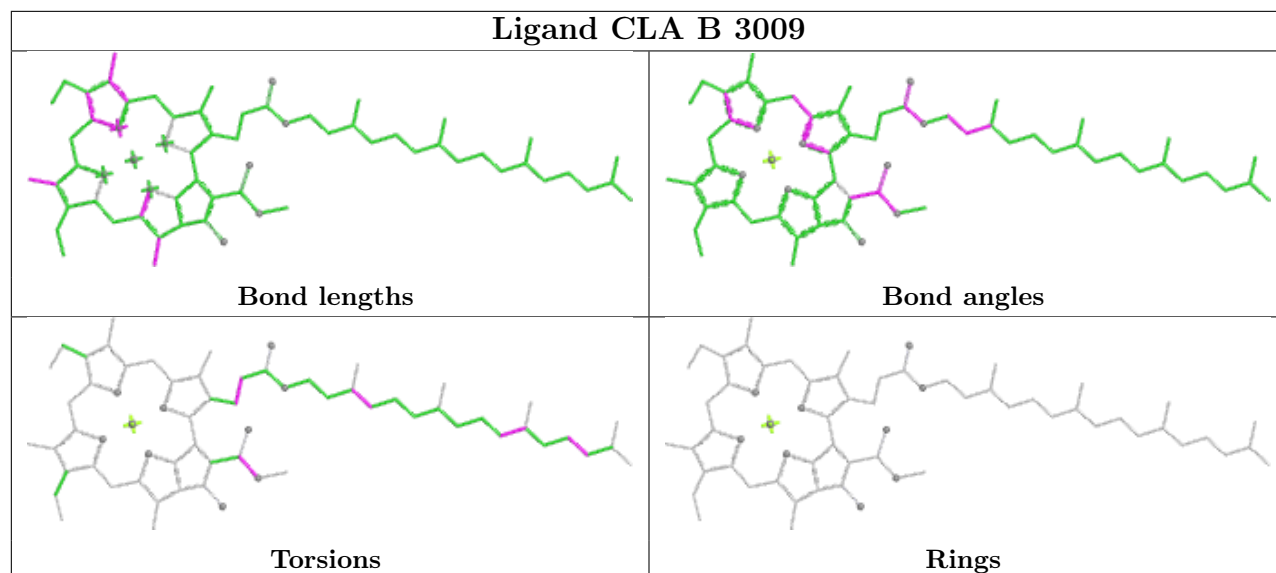
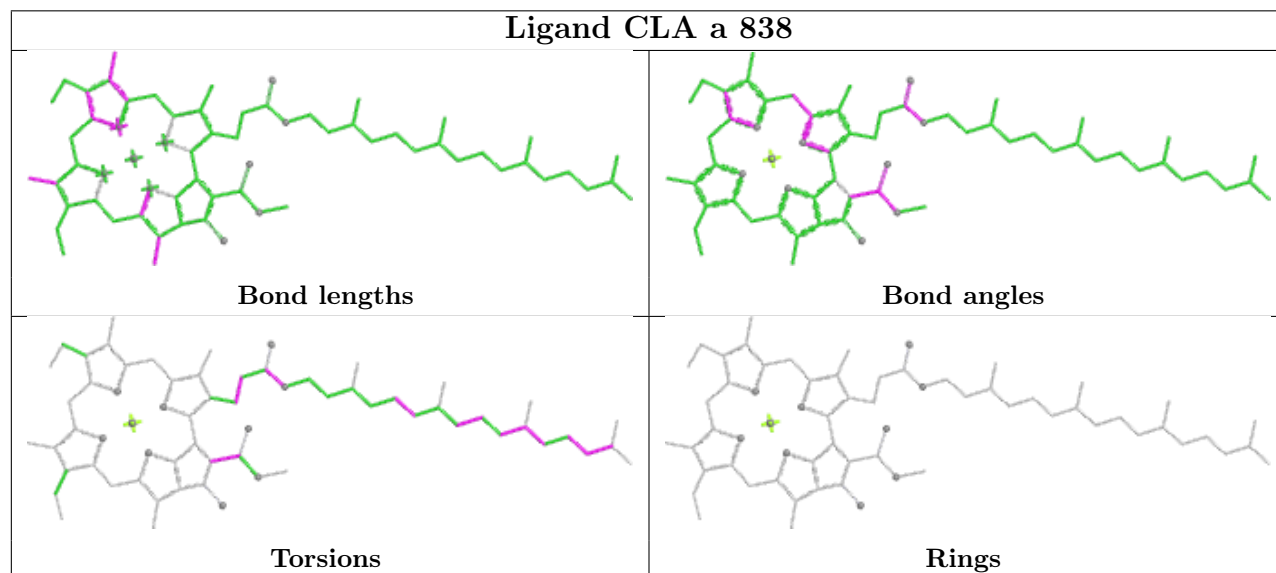
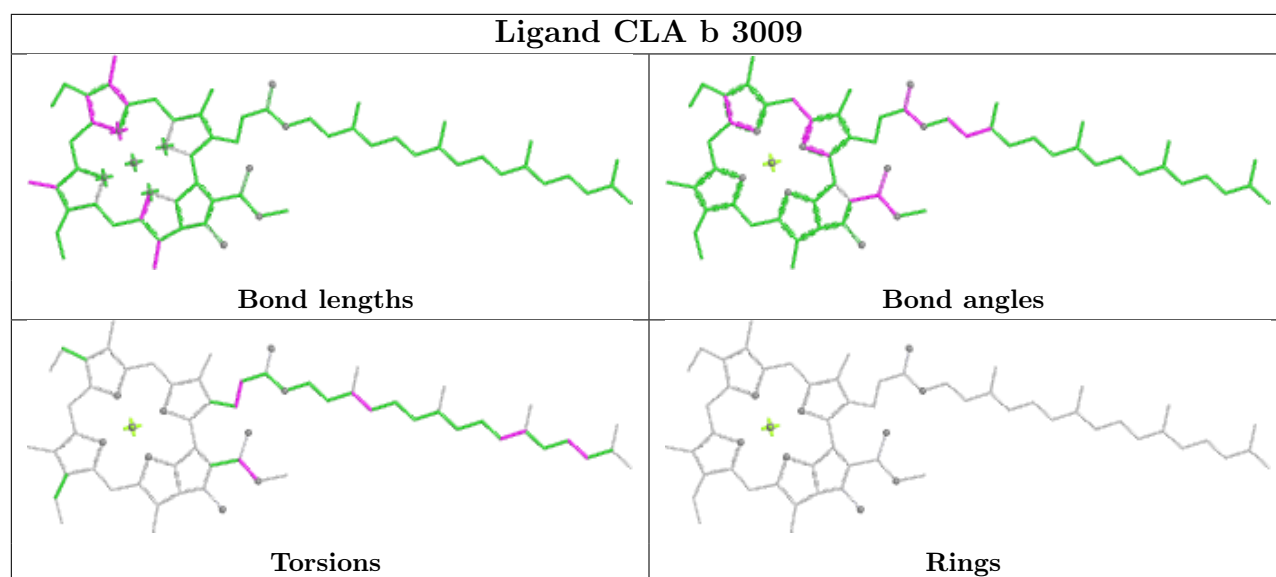
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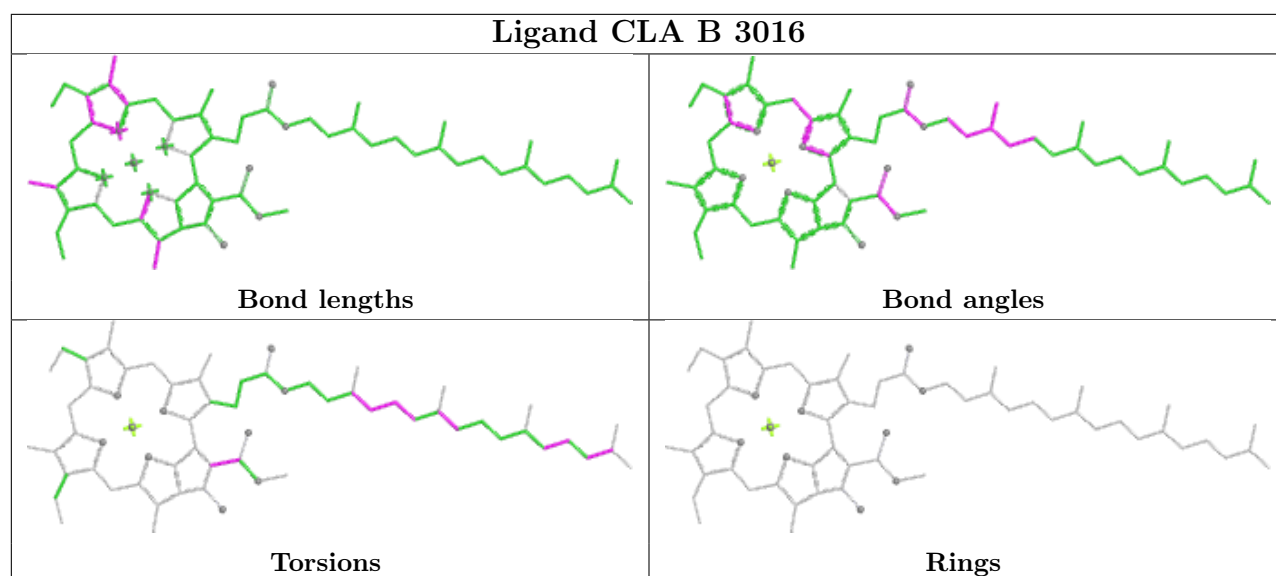
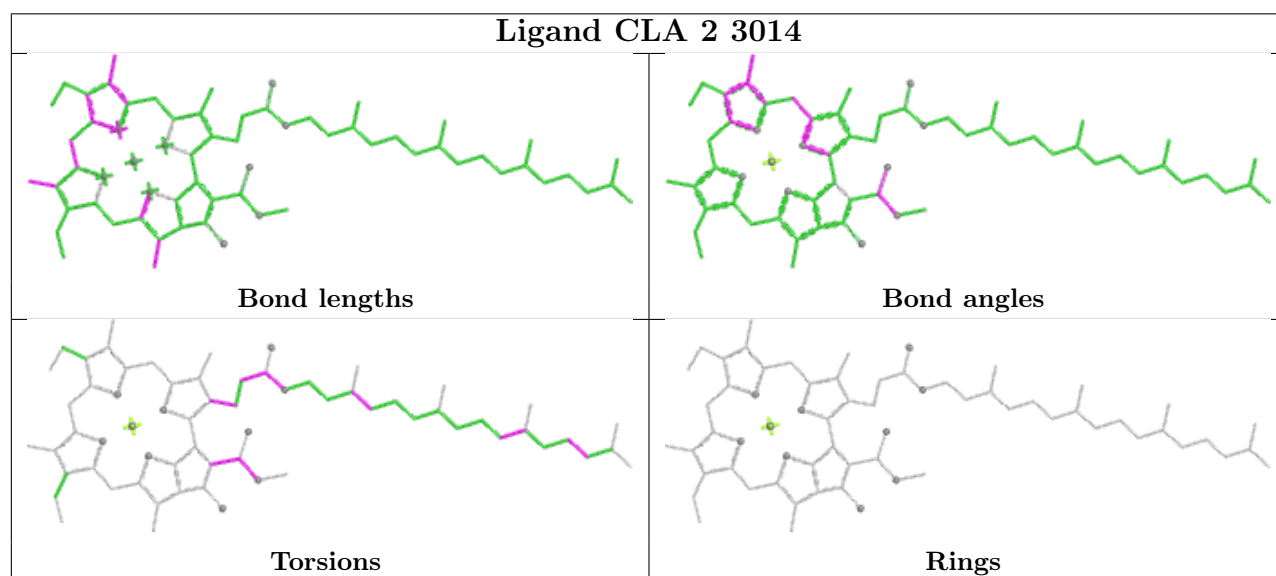
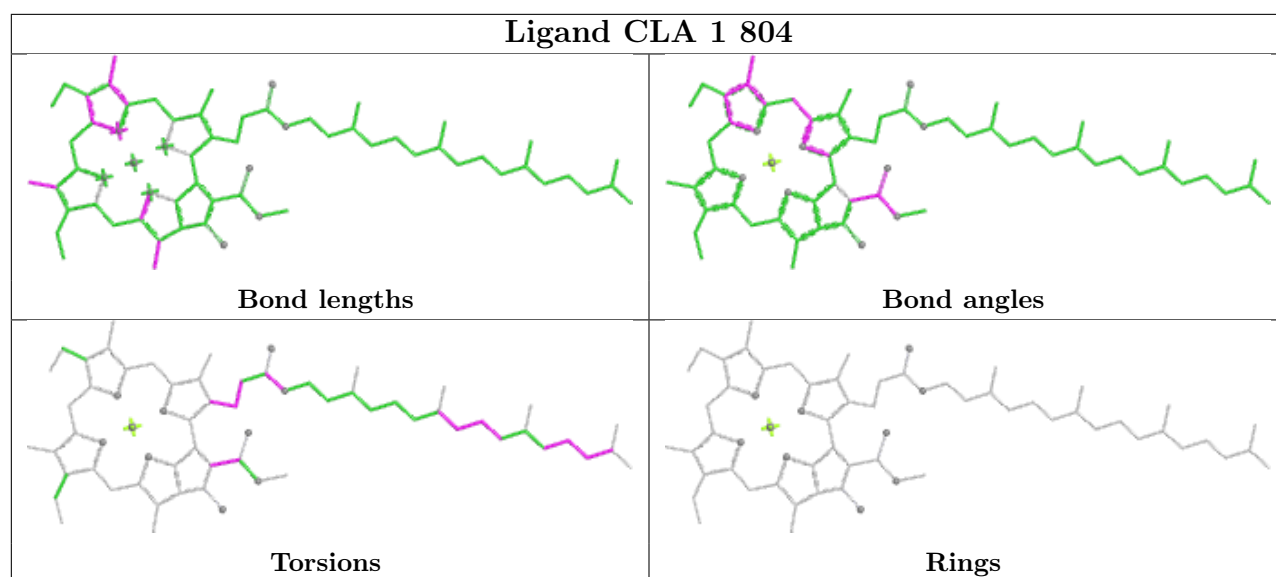
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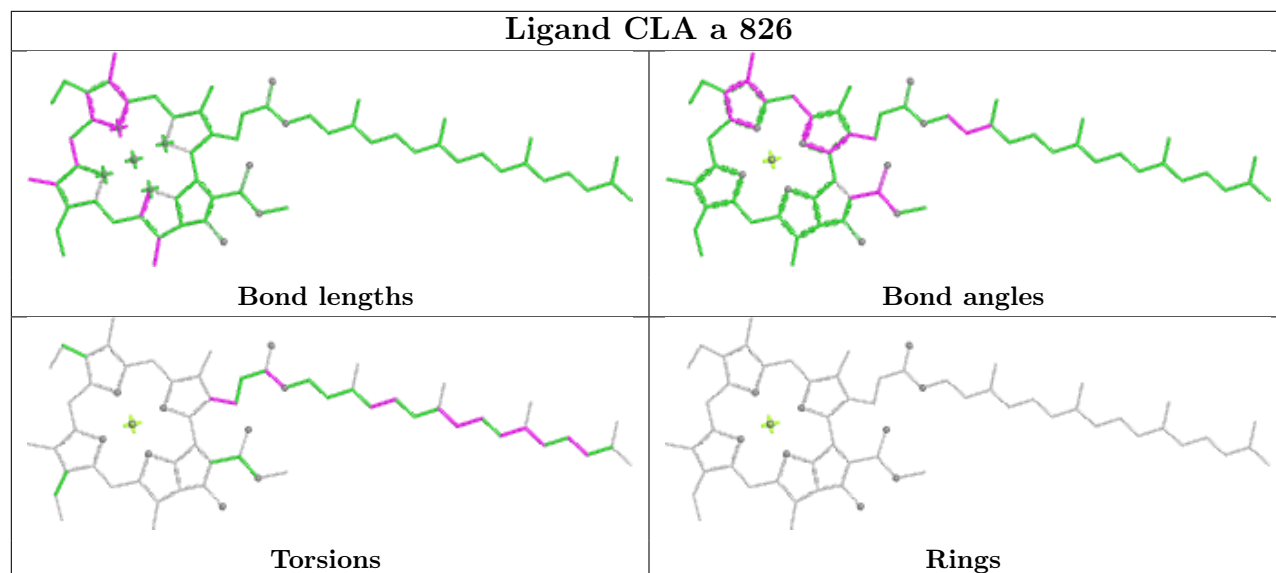
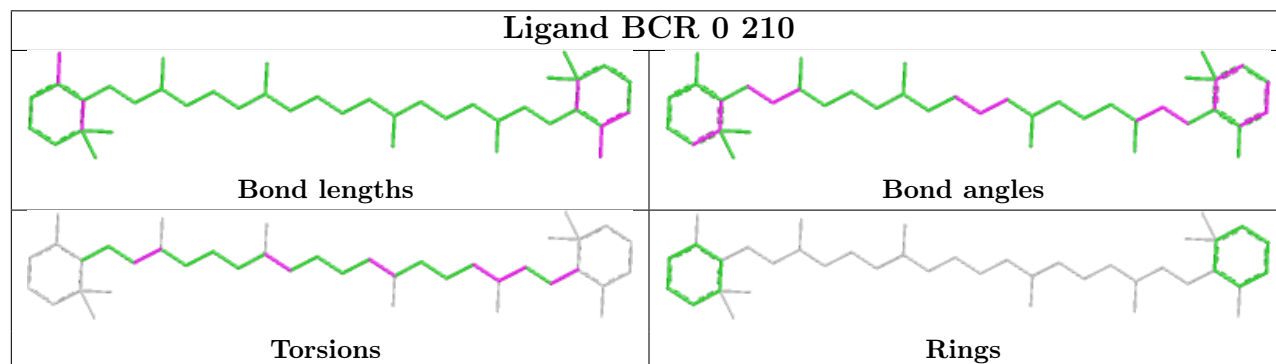
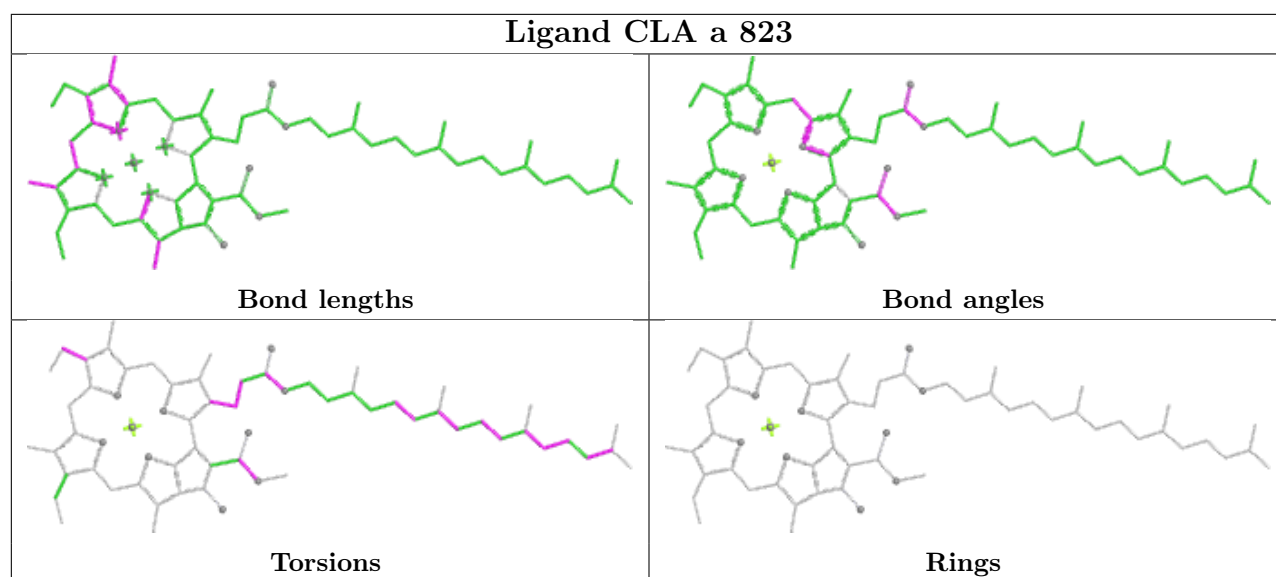
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	208	LHG	1	0
14	1	832	CLA	1	0

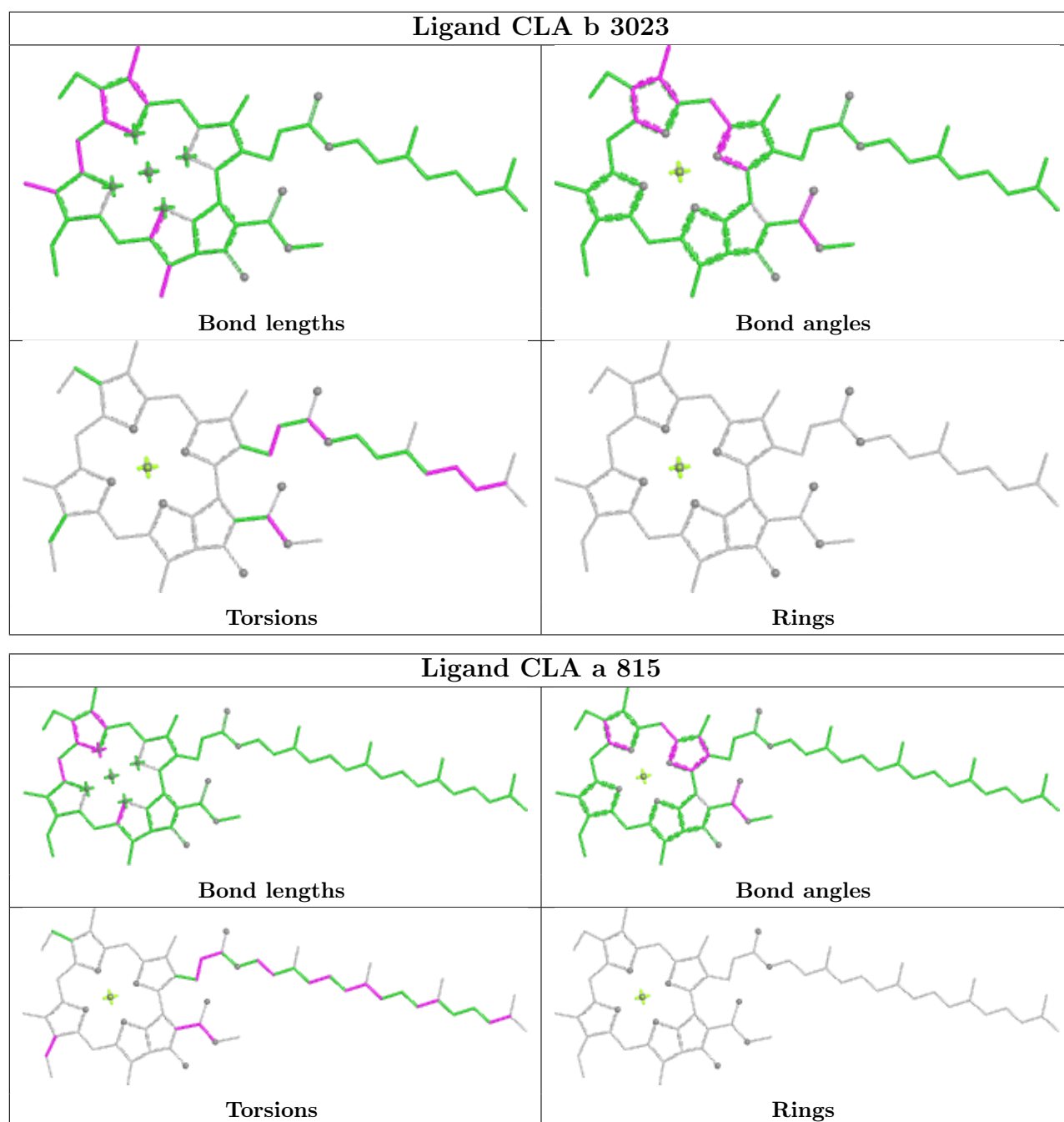
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

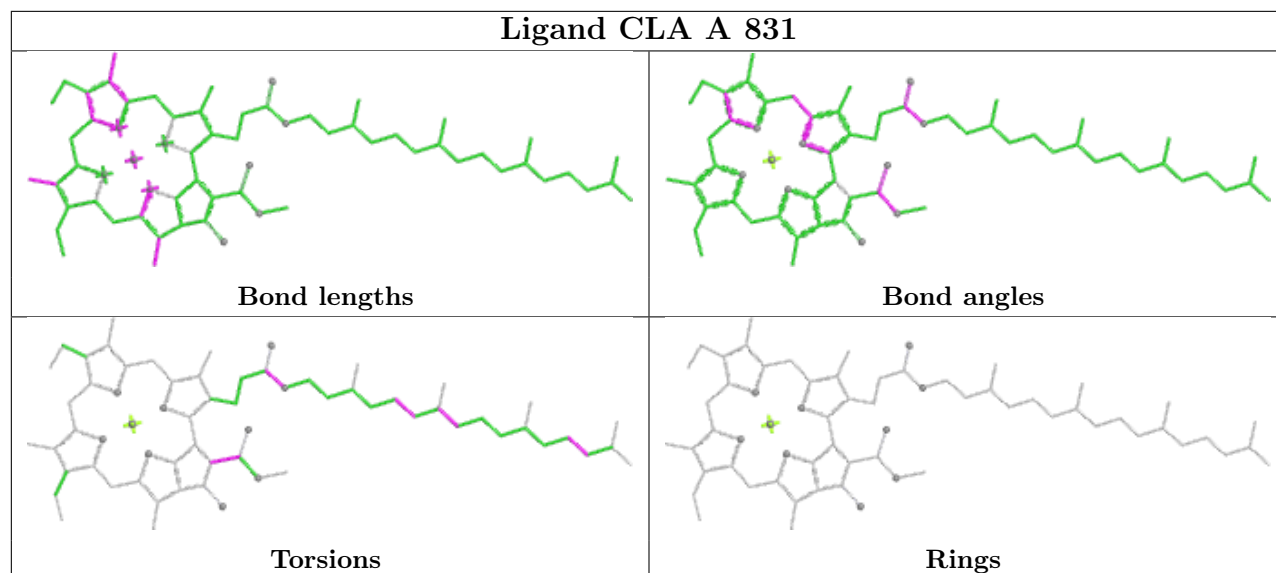
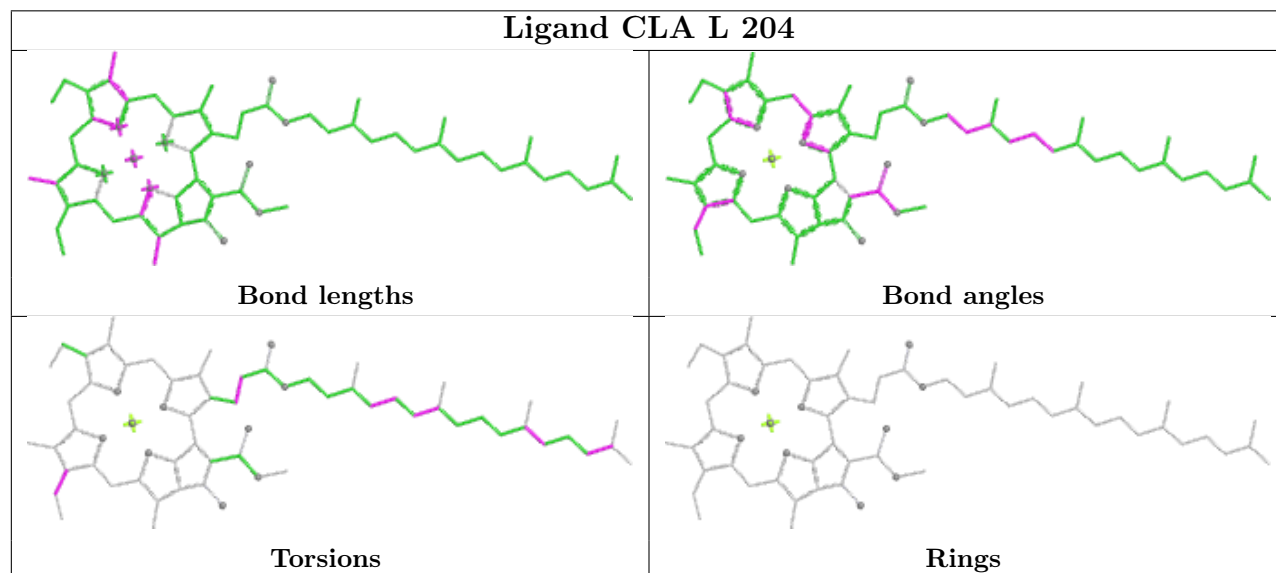
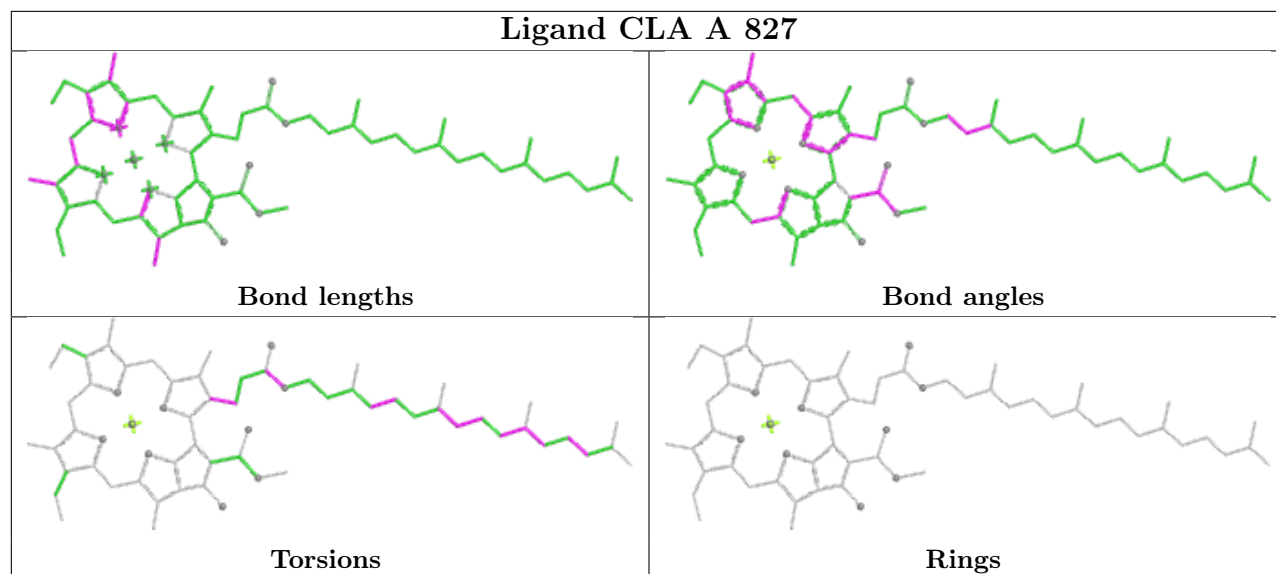




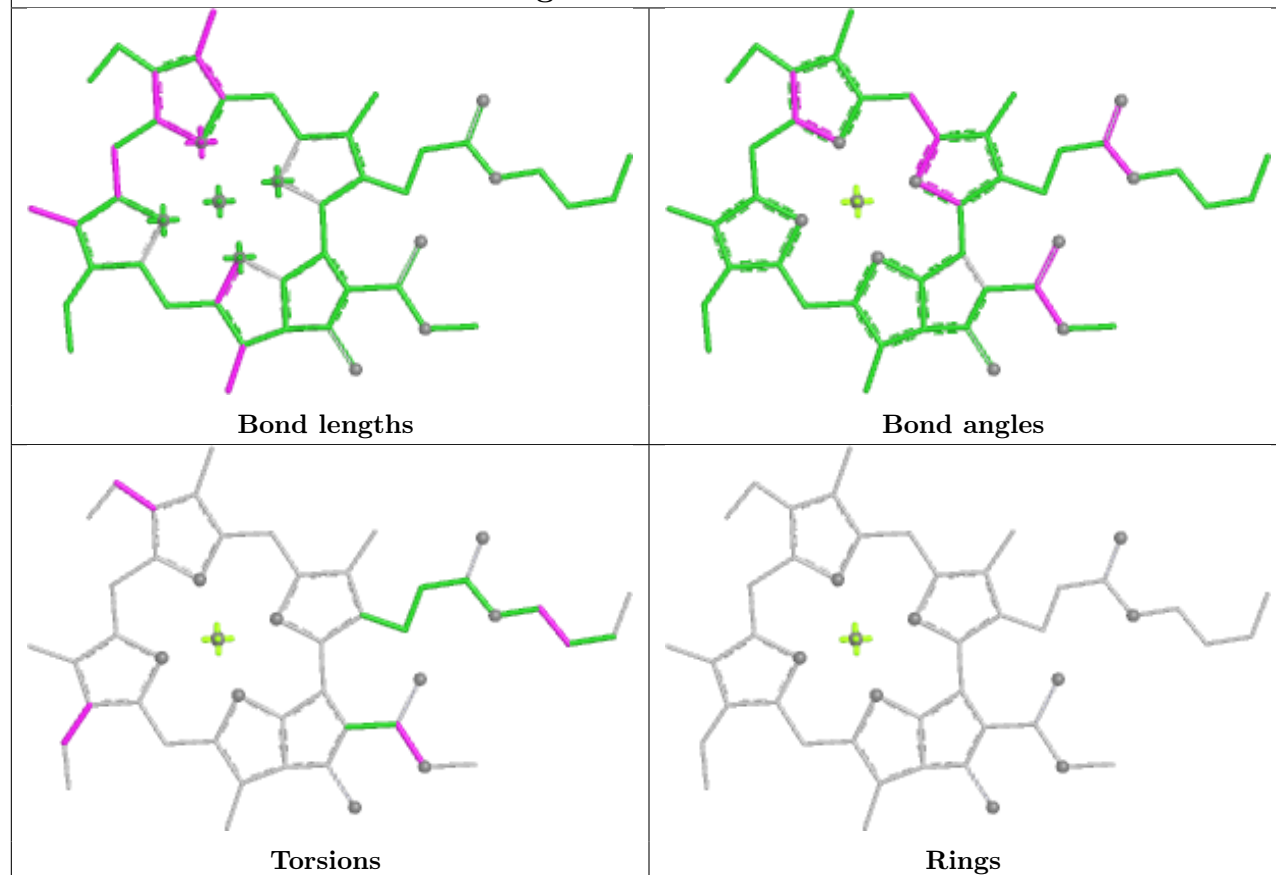




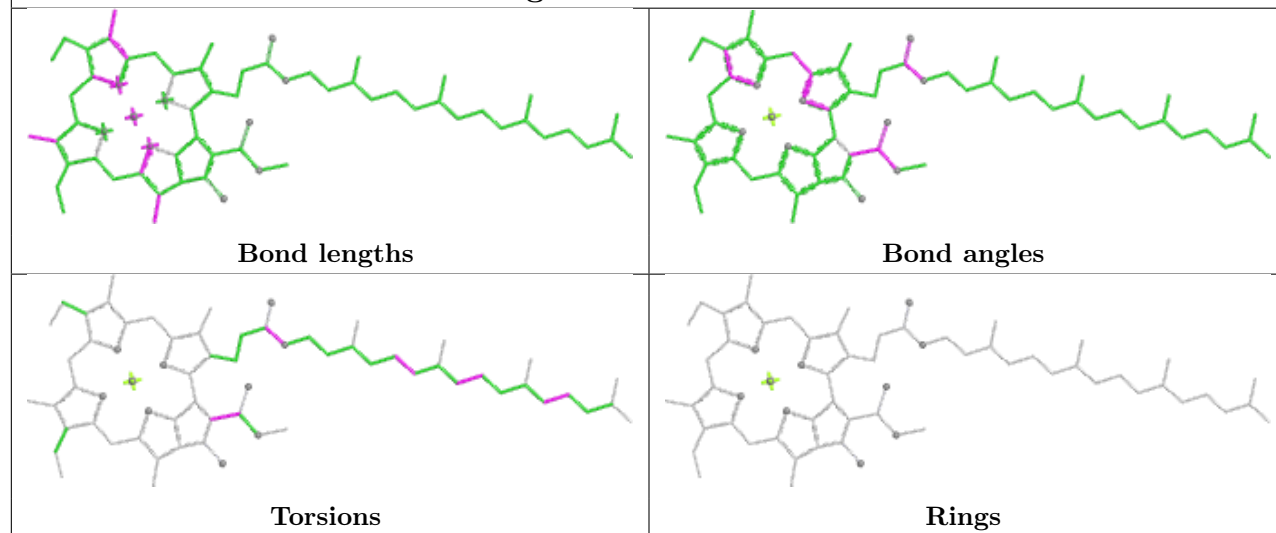


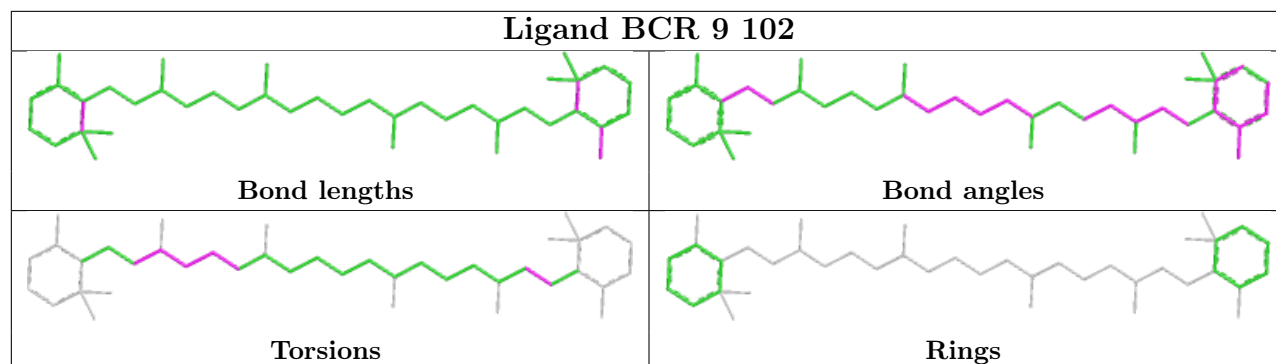
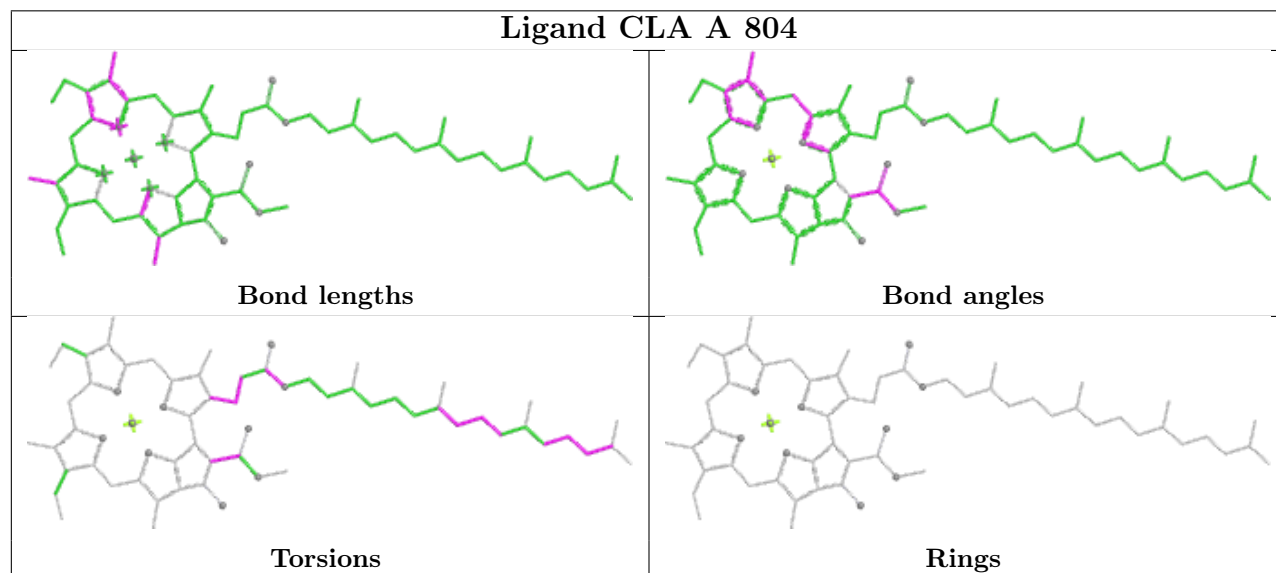
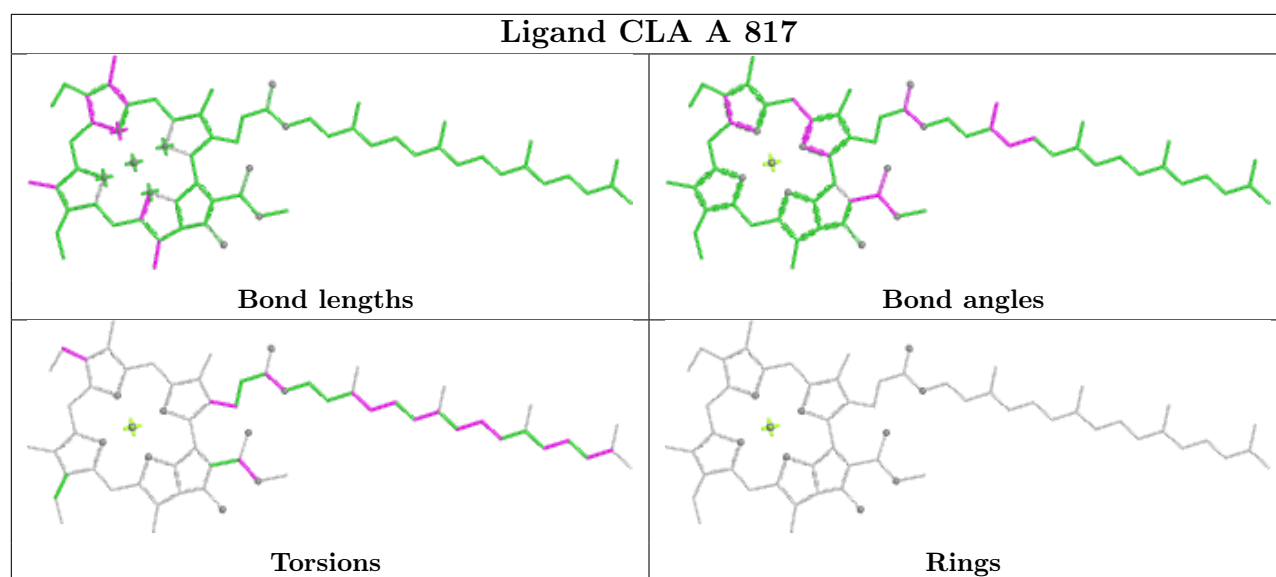


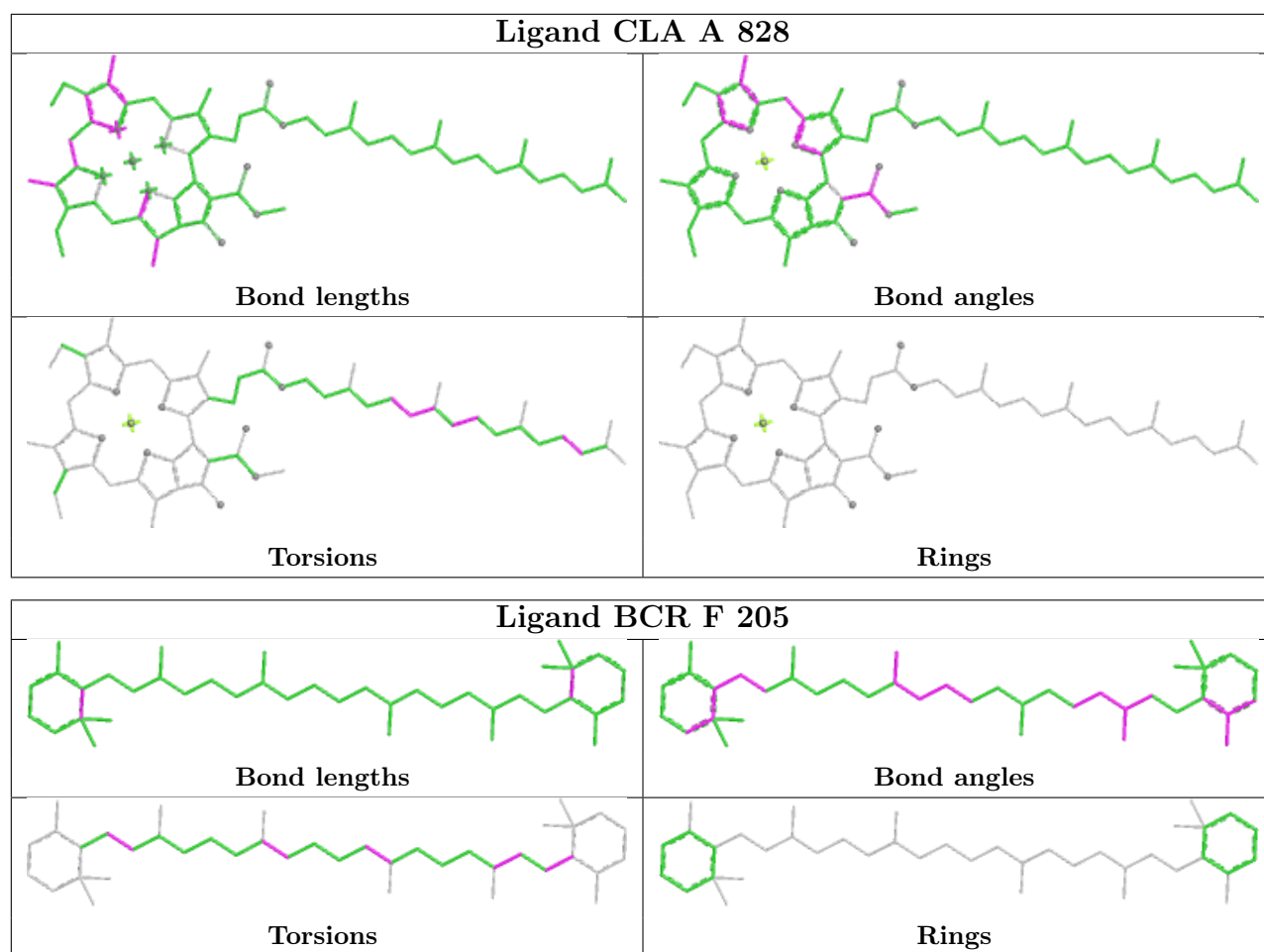
Ligand CLA 1 811



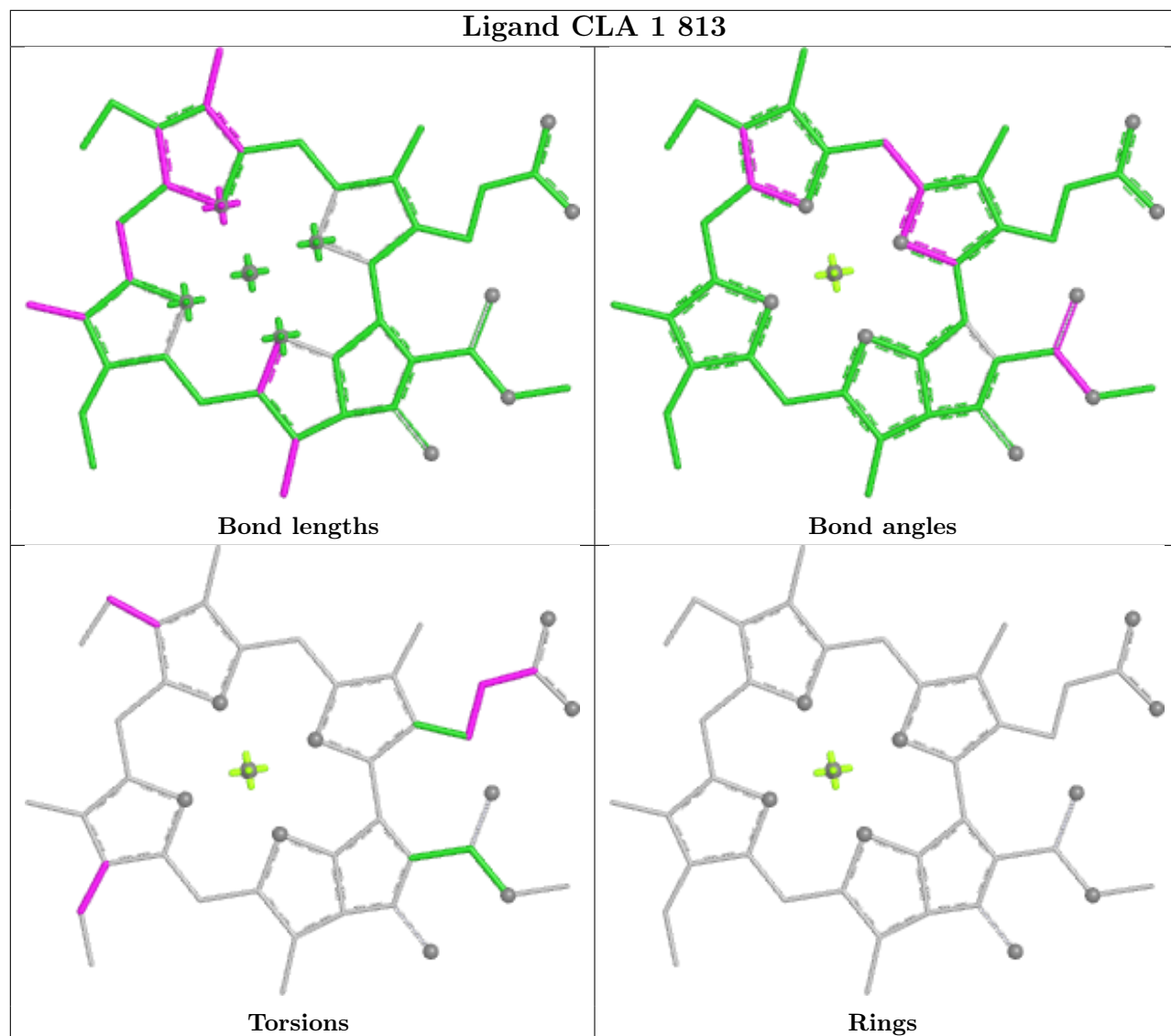
Ligand CLA b 3030



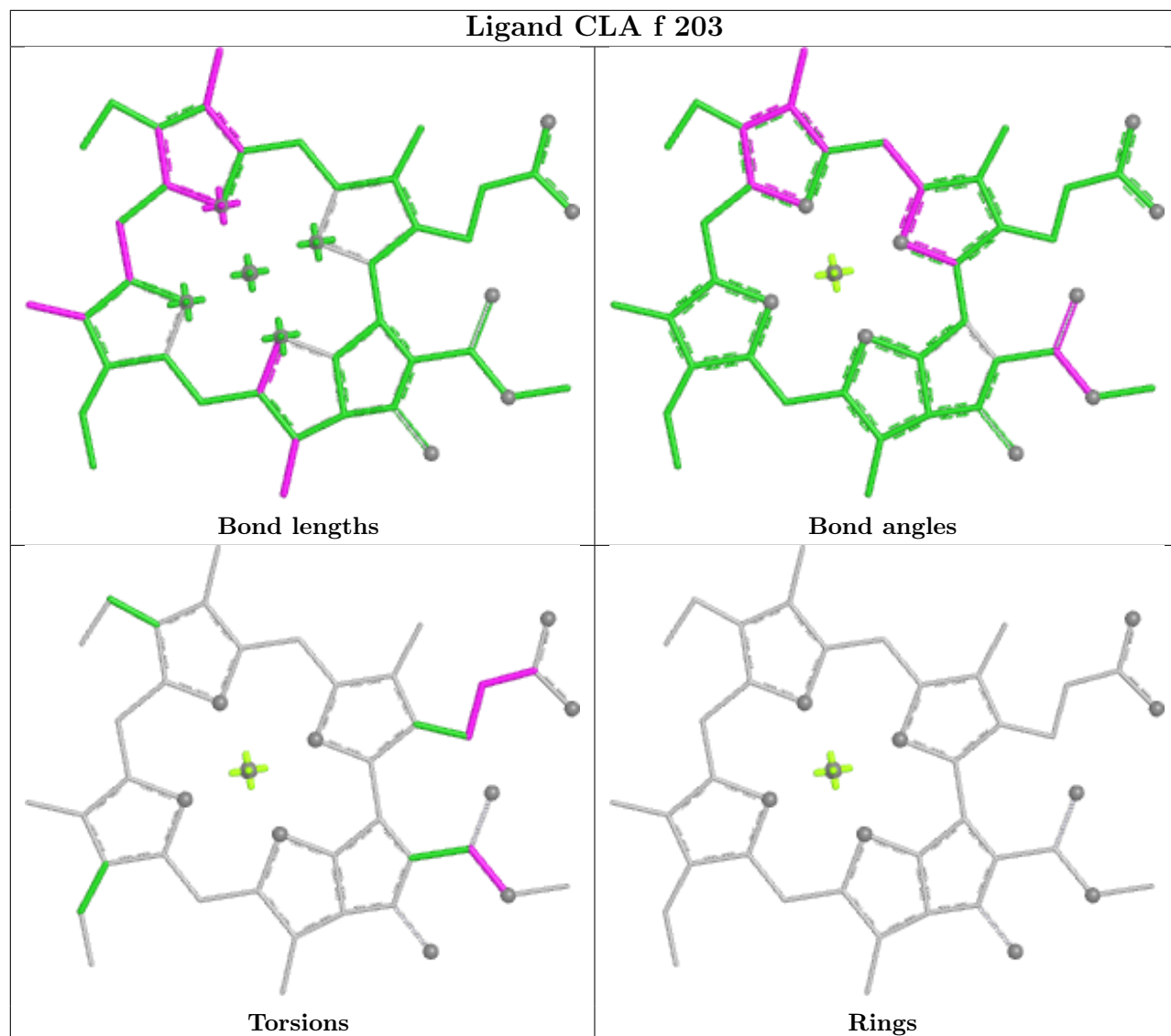




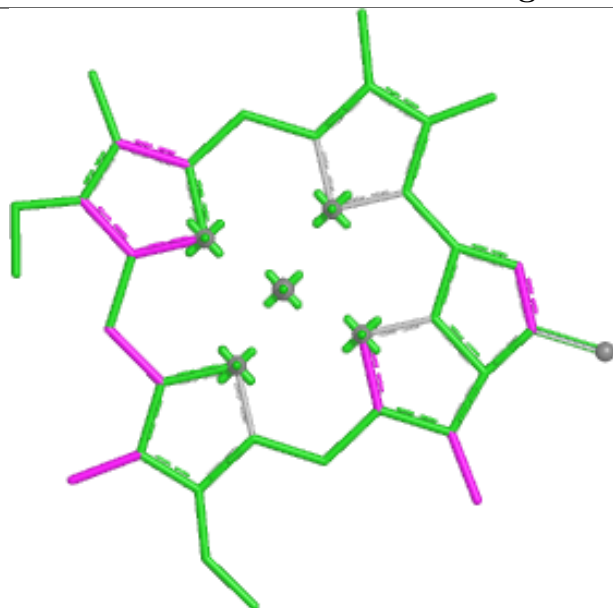
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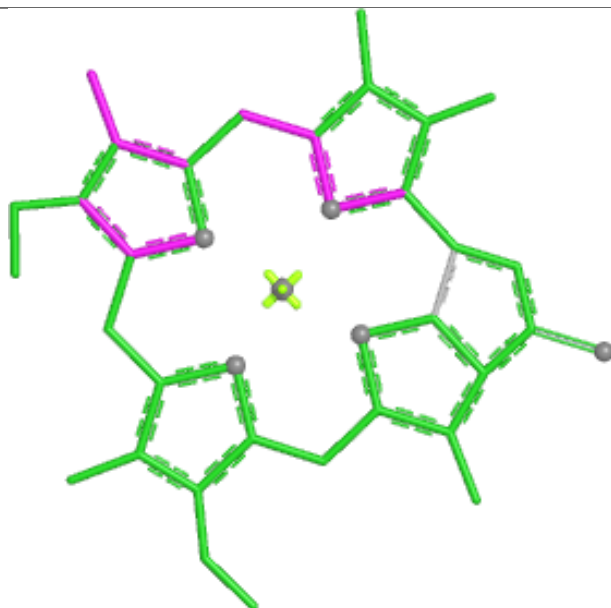
Ligand CLA f 203



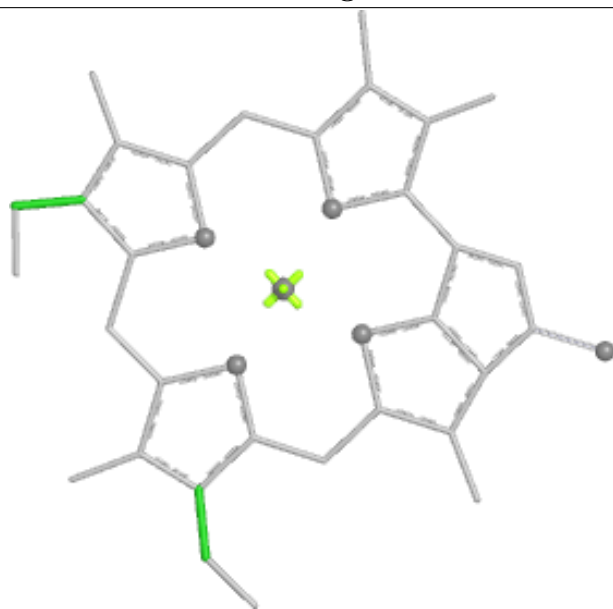
Ligand CLA 8 102



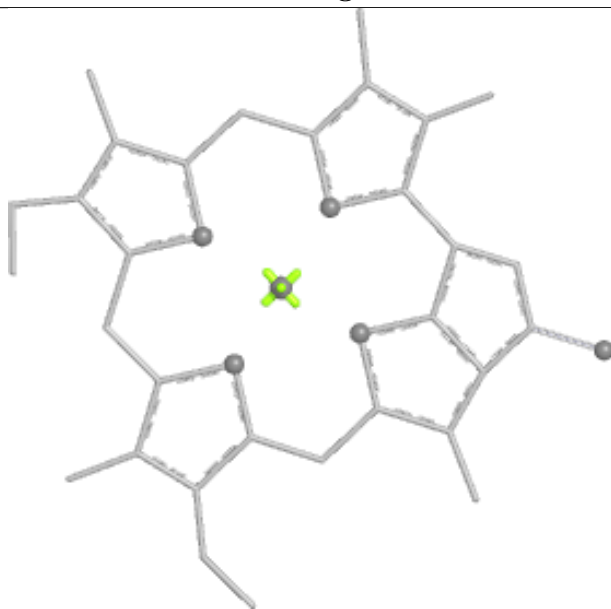
Bond lengths



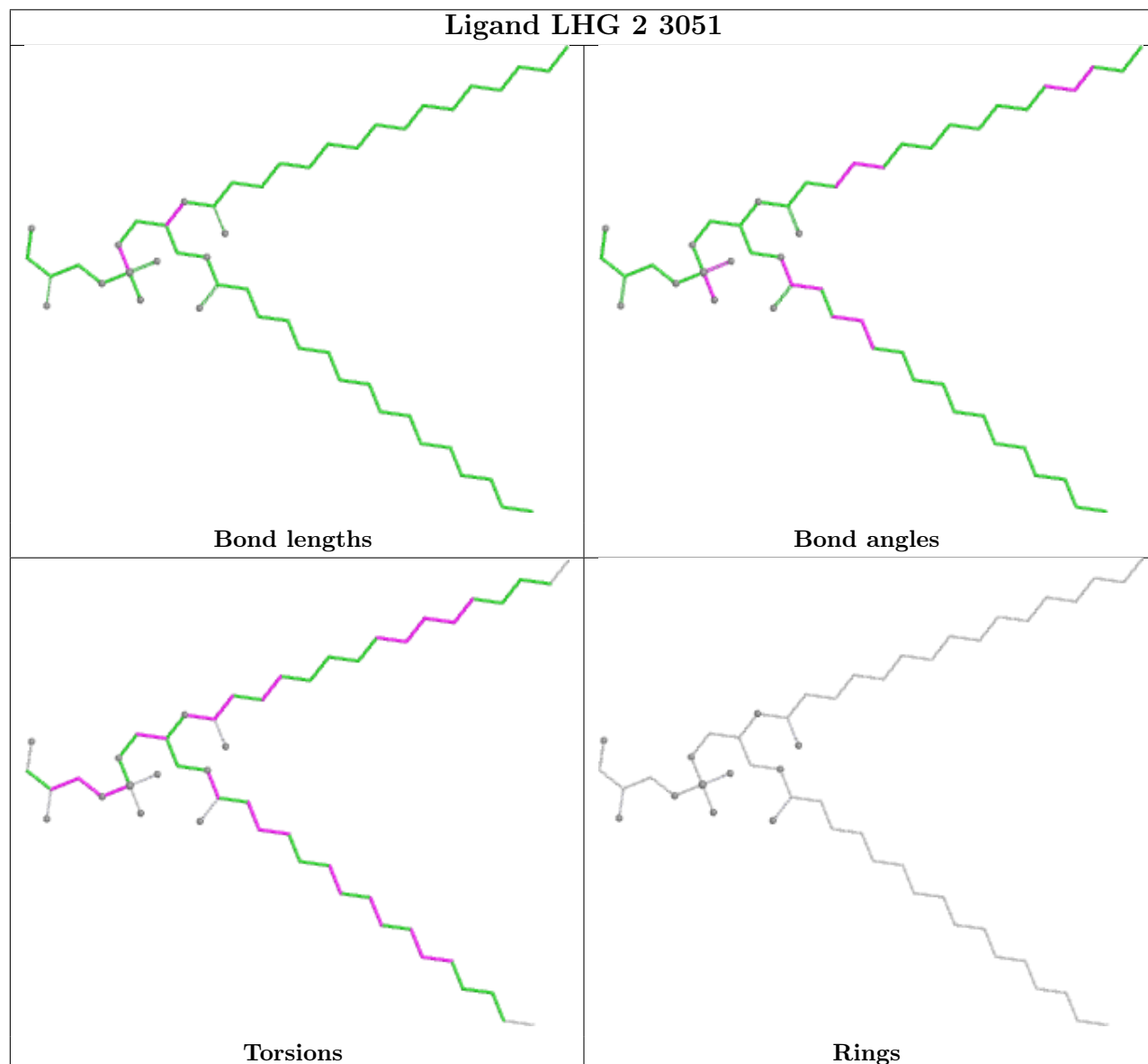
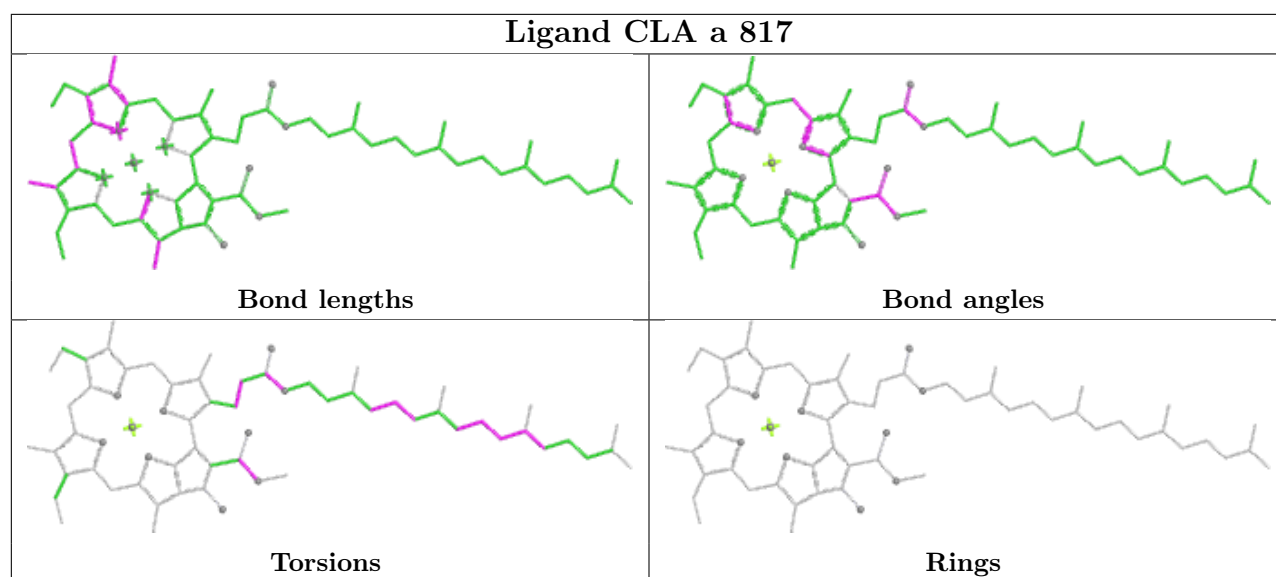
Bond angles

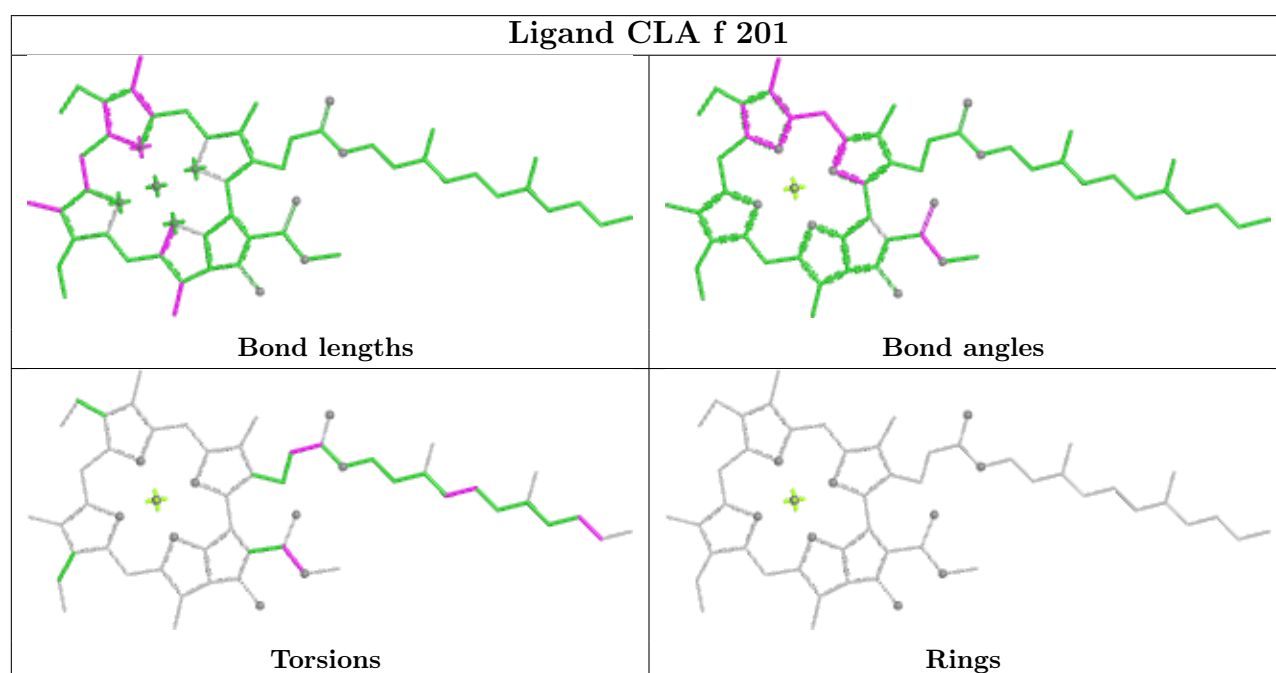
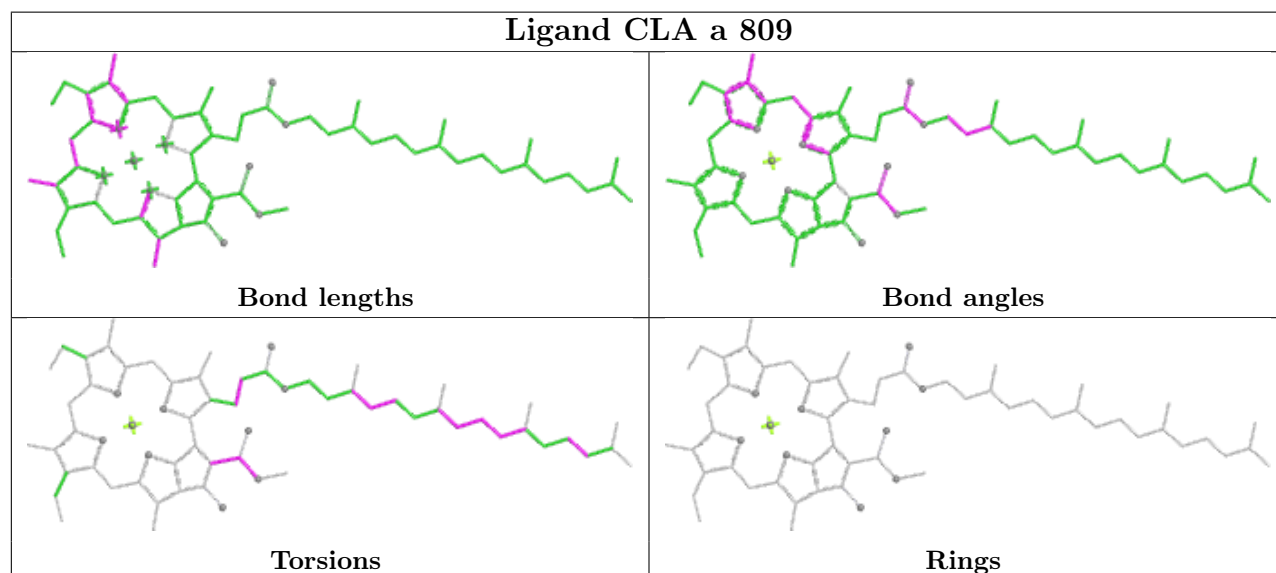
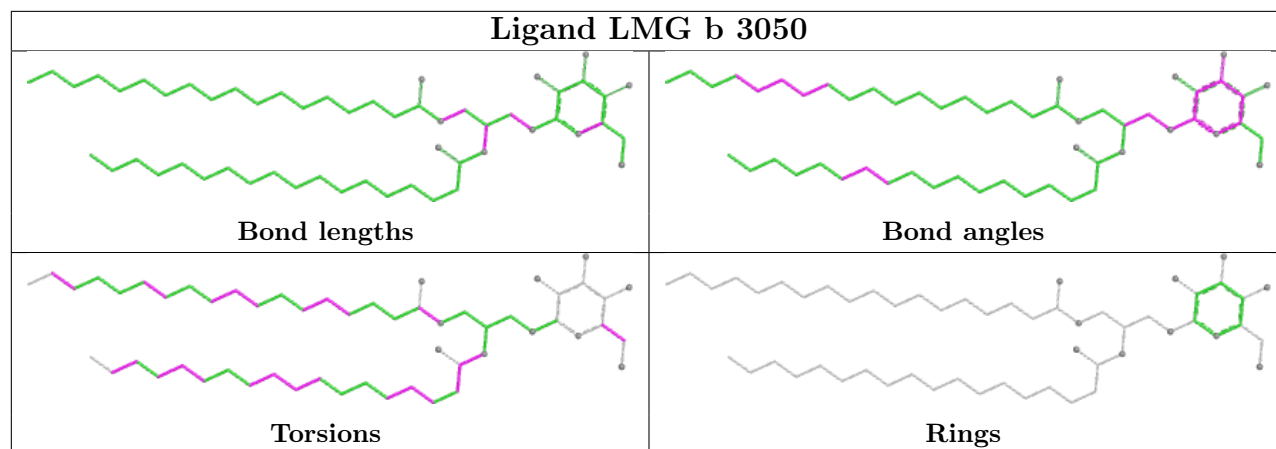


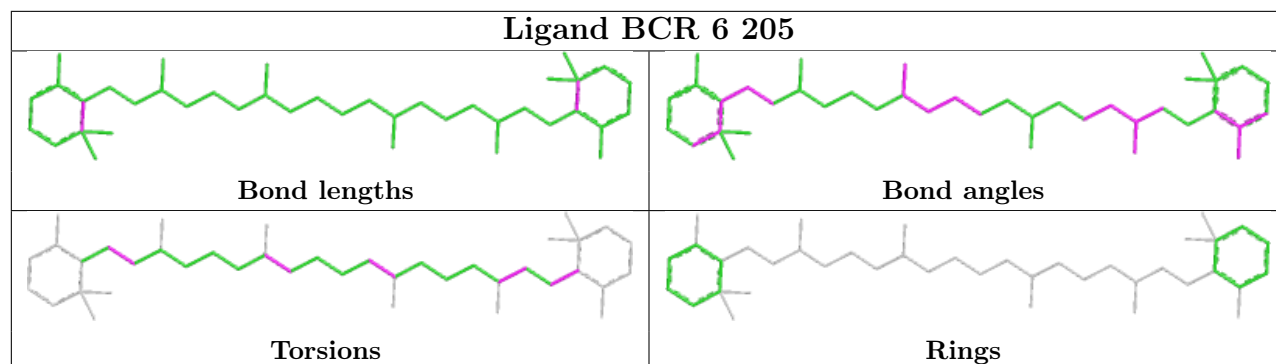
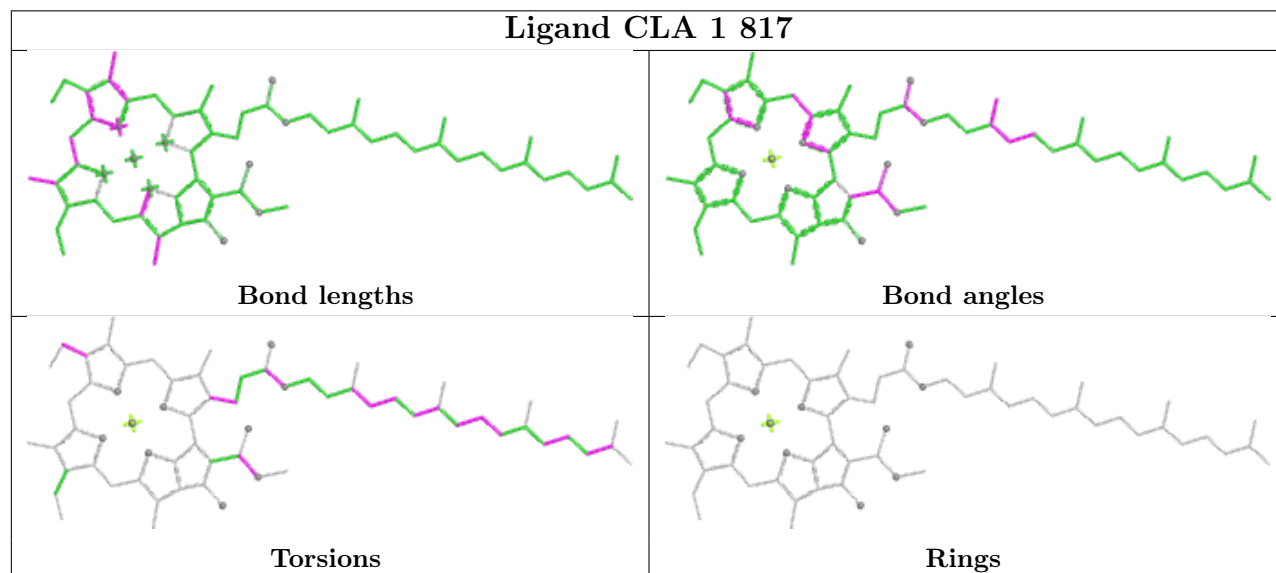
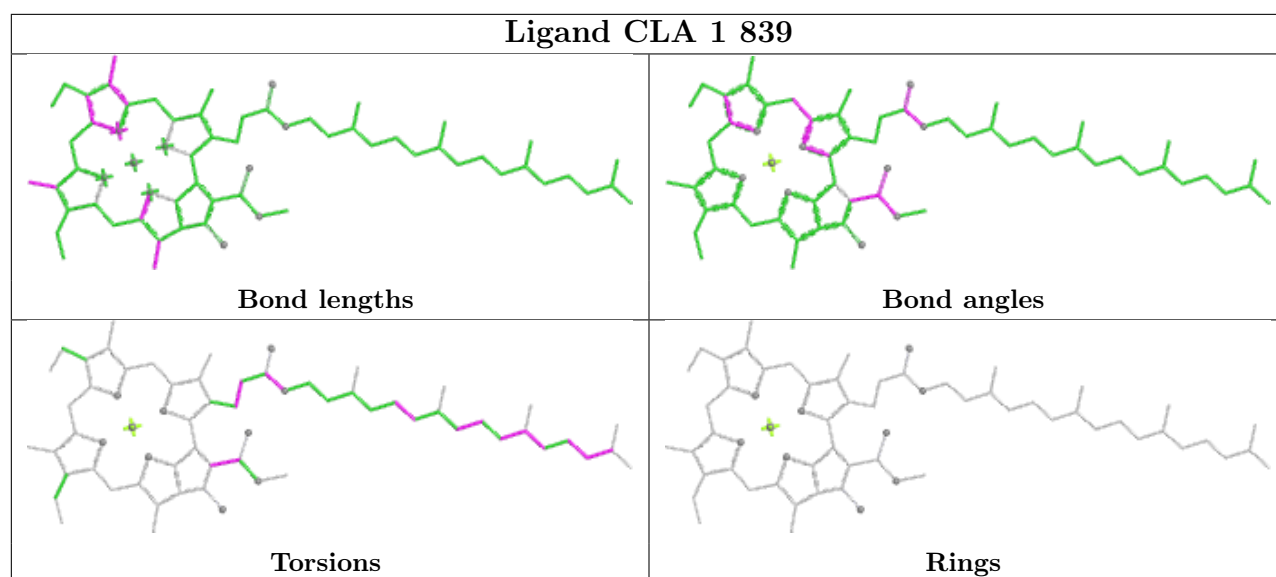
Torsions

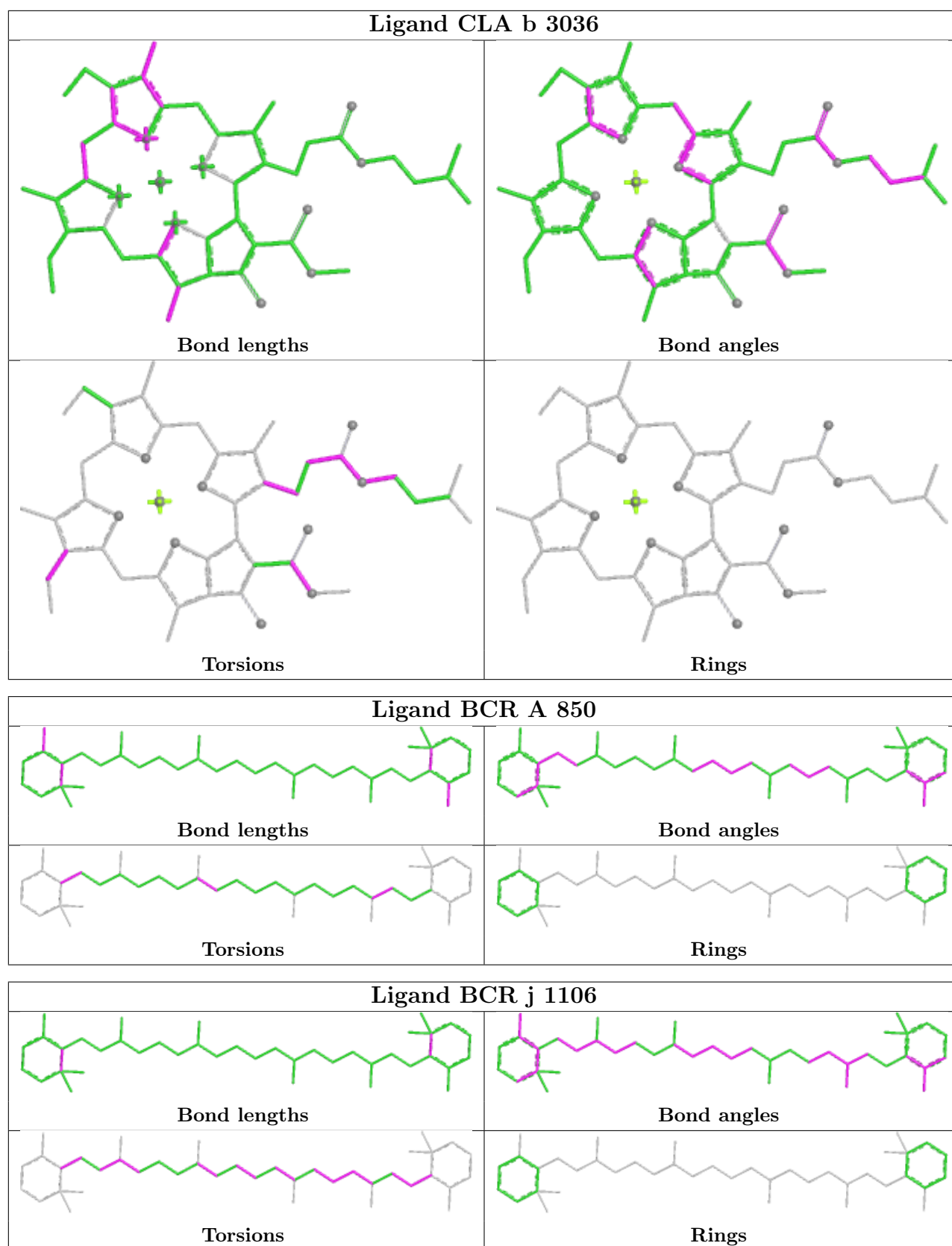


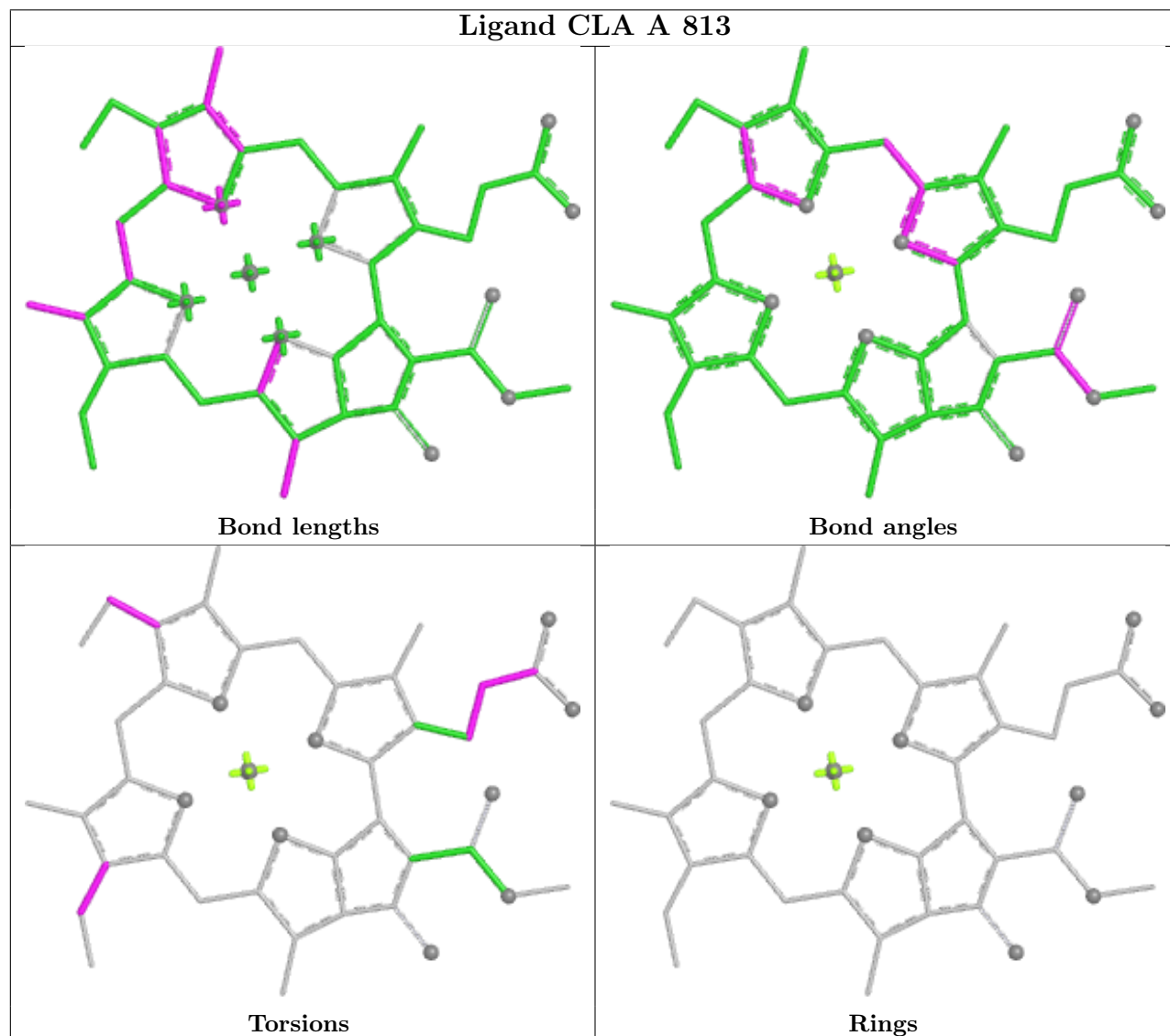
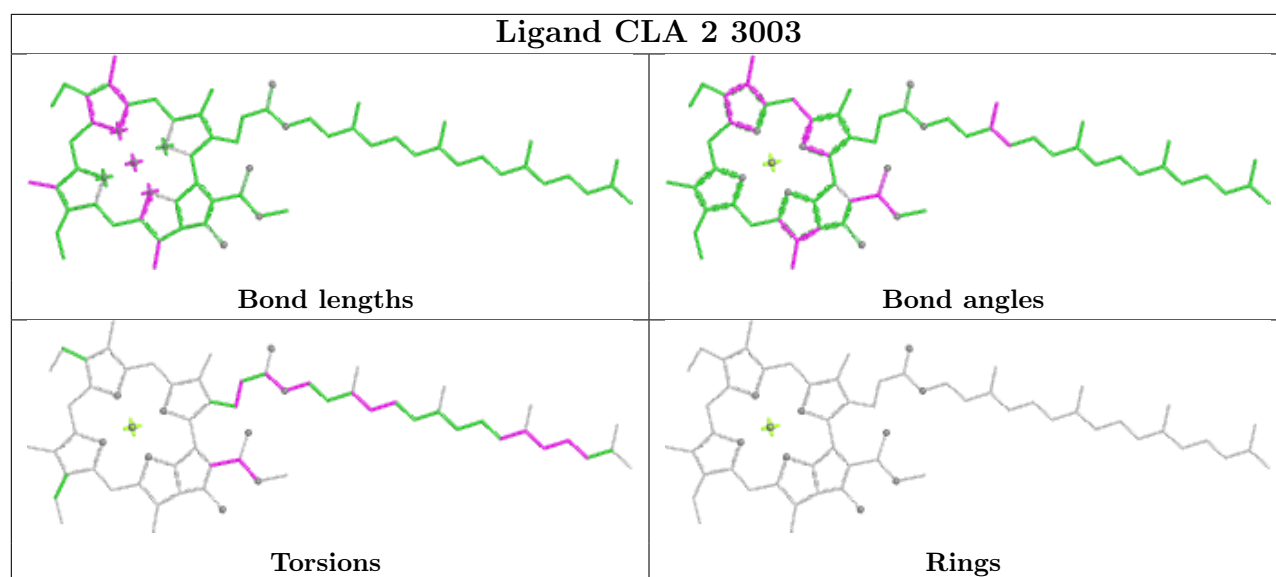
Rings

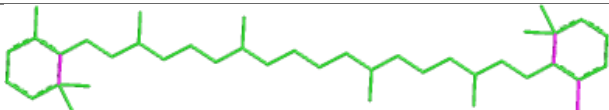
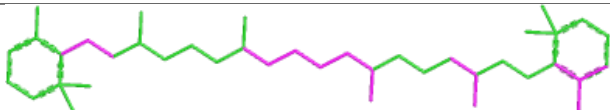
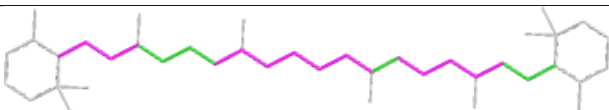
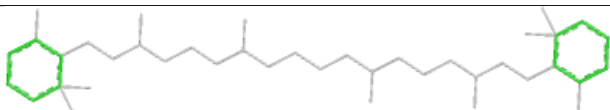


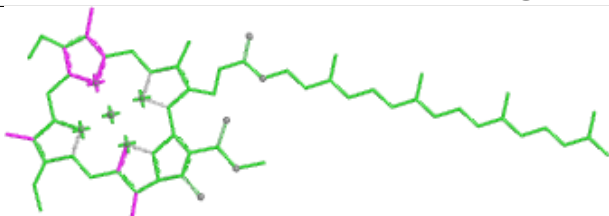
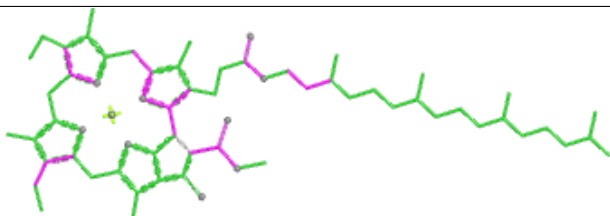
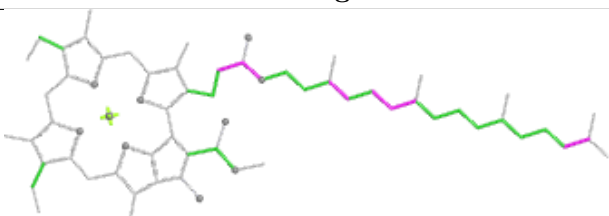
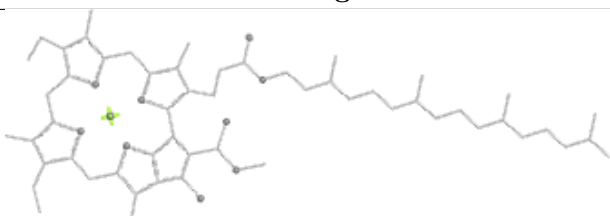


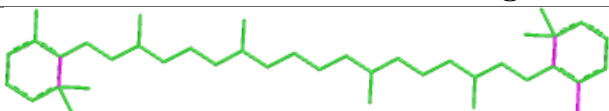
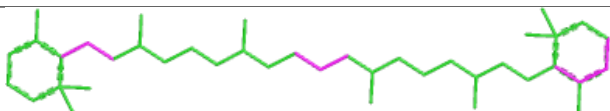
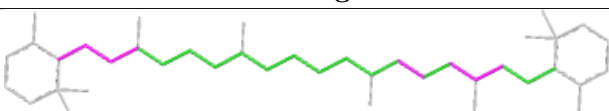
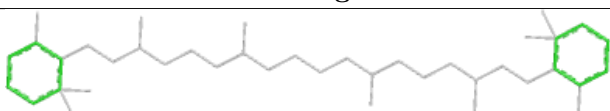


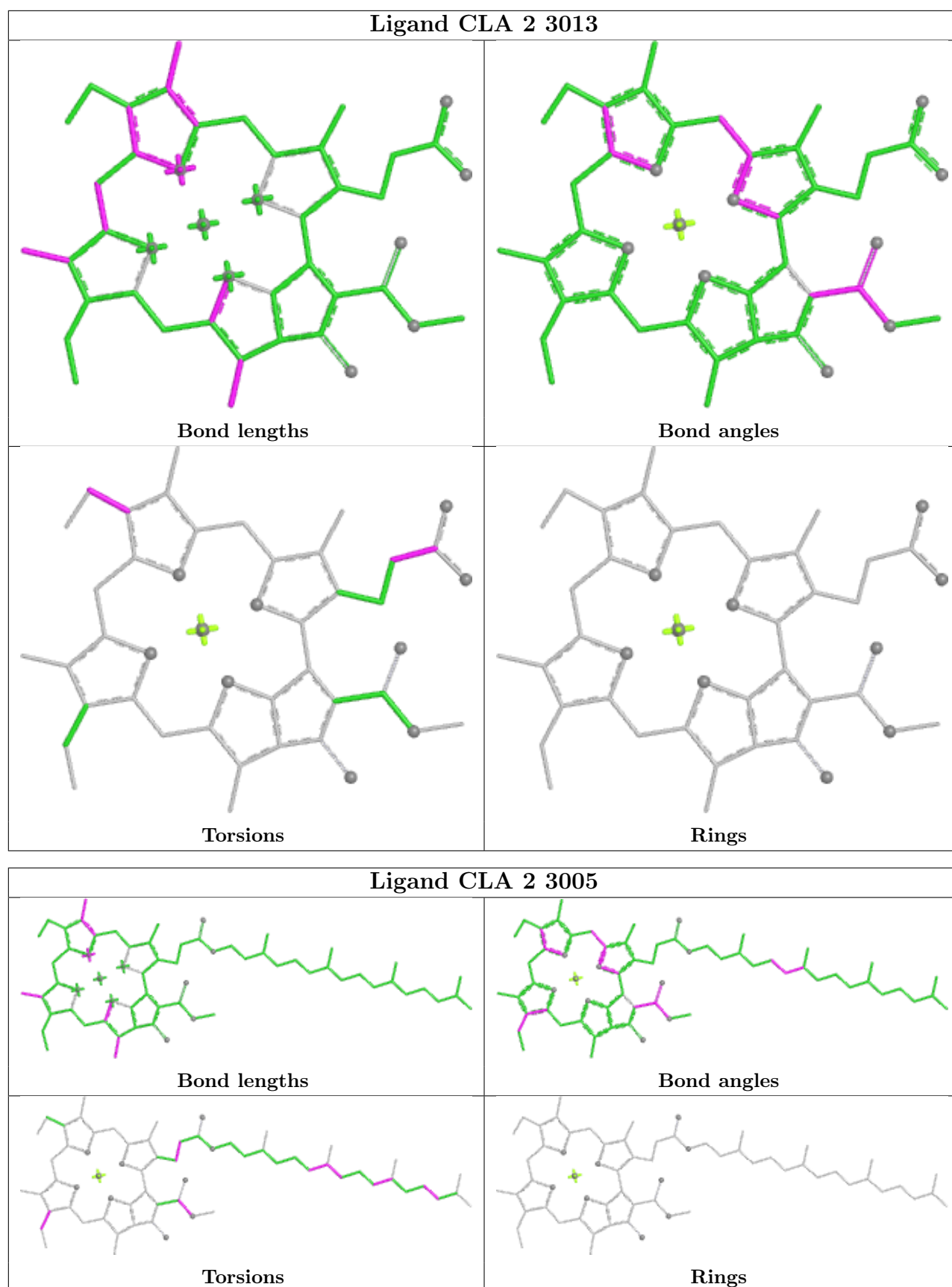




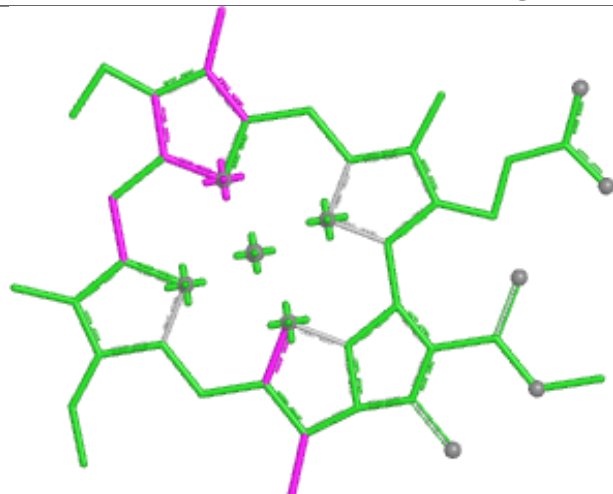
Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

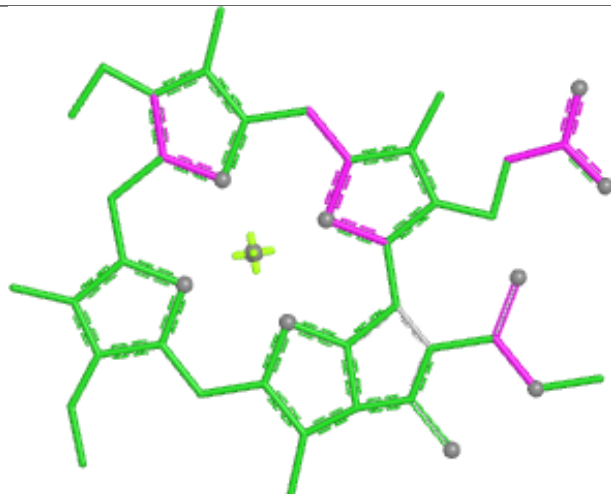
Ligand BCR b 3045	
	
Bond lengths	Bond angles
	
Torsions	Rings



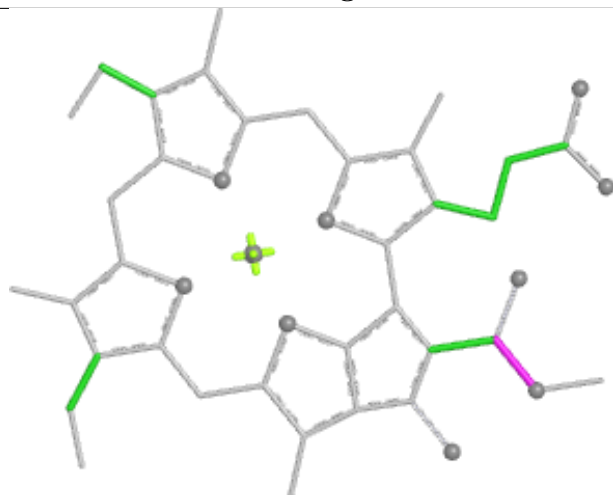
Ligand CLA A 837



Bond lengths



Bond angles

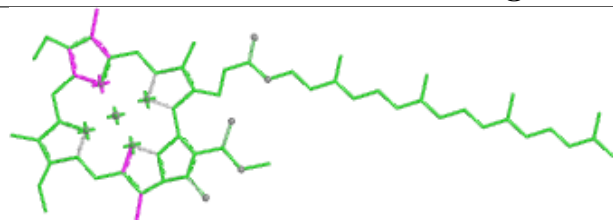


Torsions

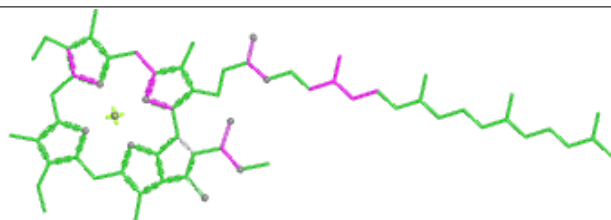


Rings

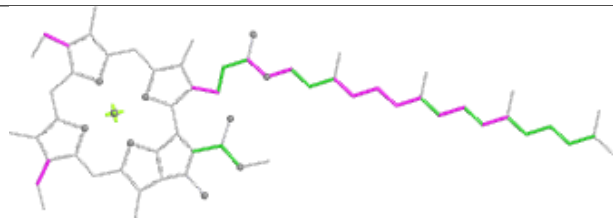
Ligand CLA B 3018



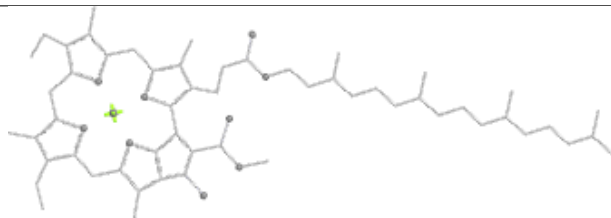
Bond lengths



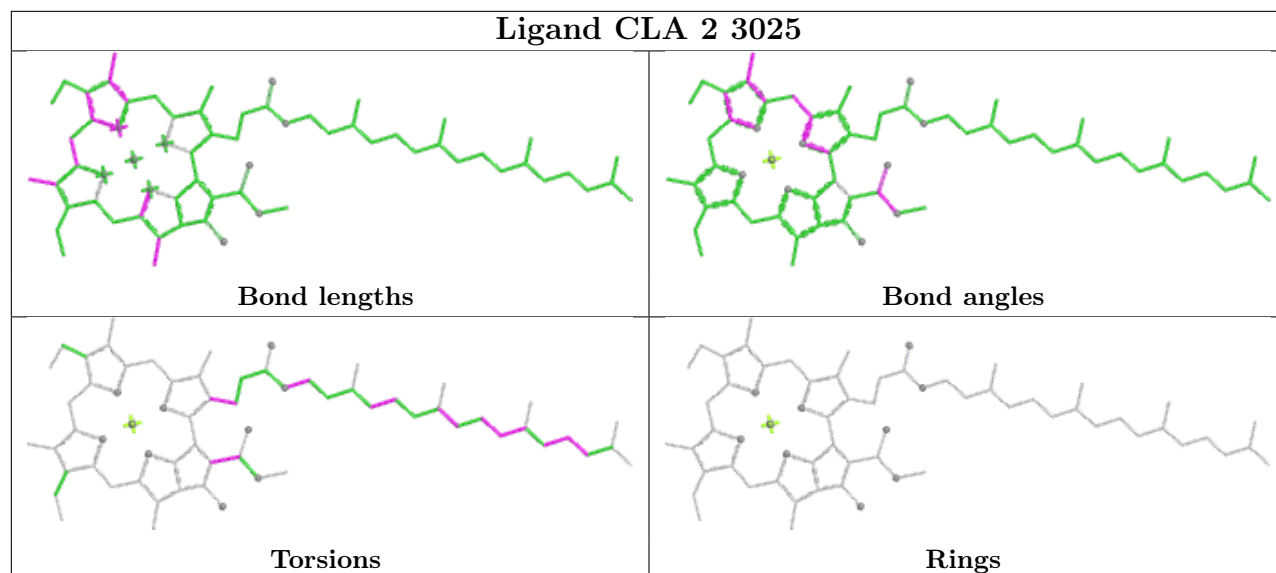
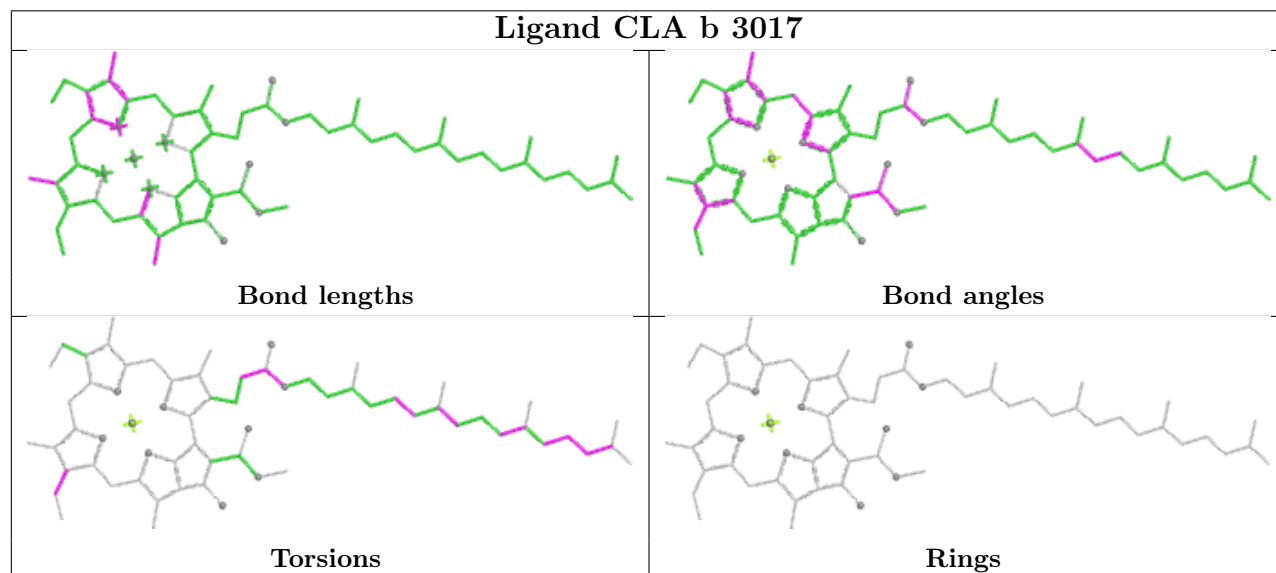
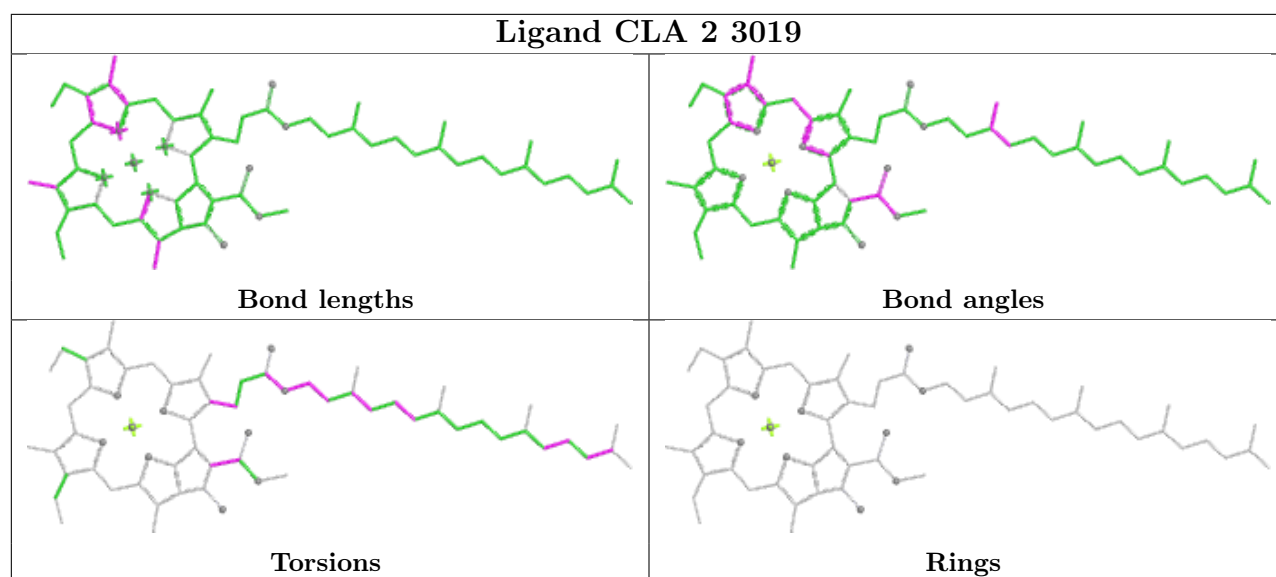
Bond angles

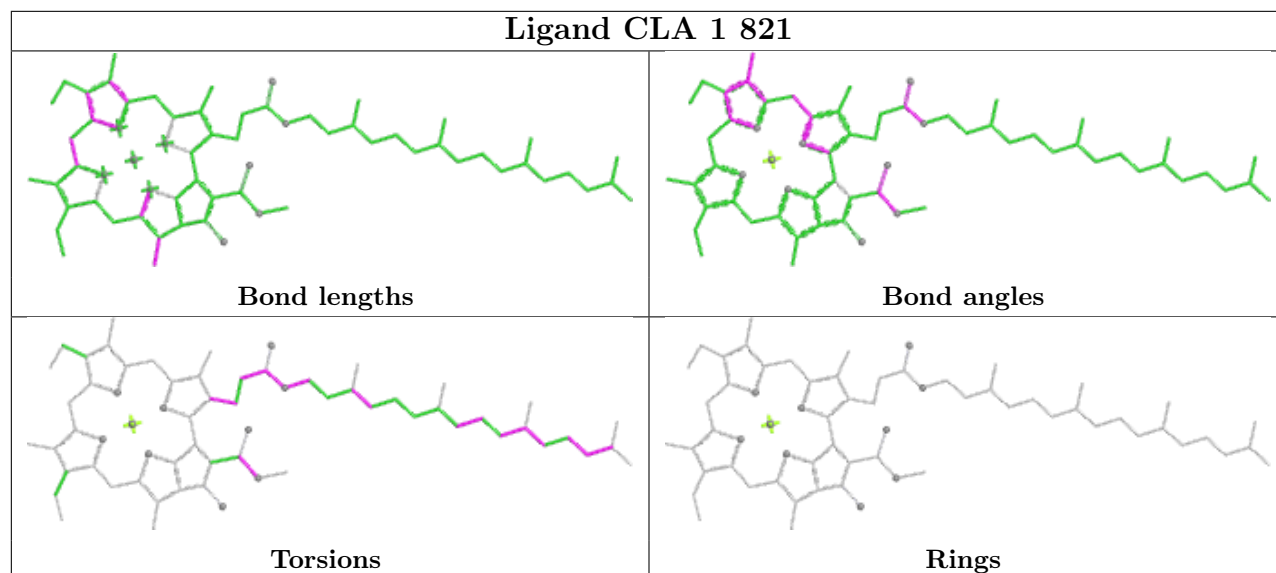
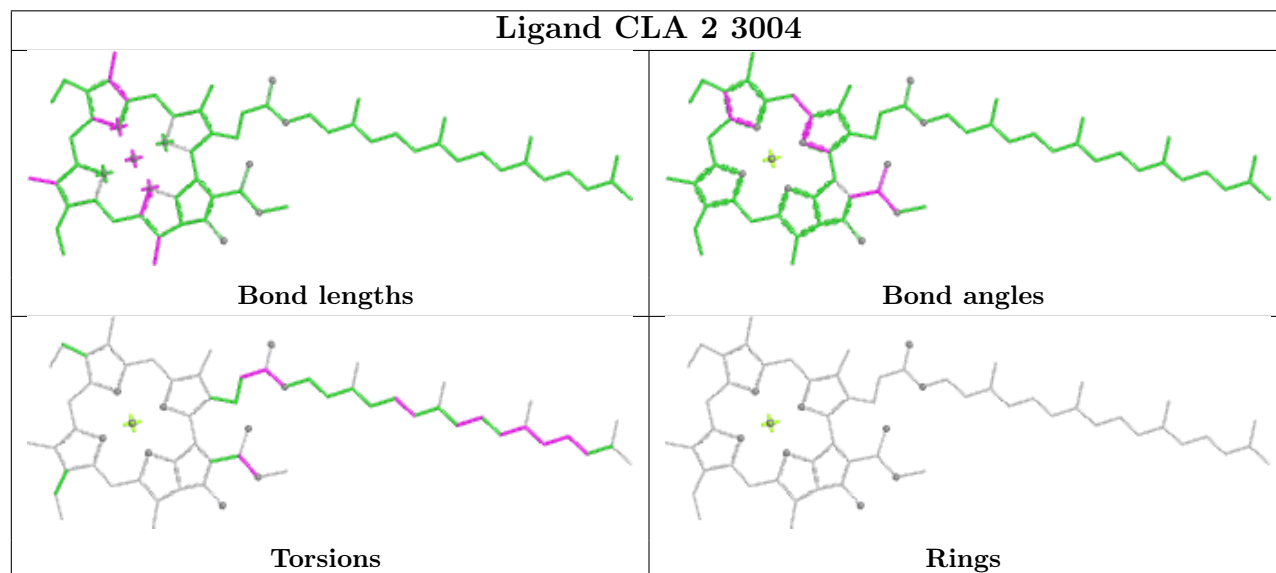
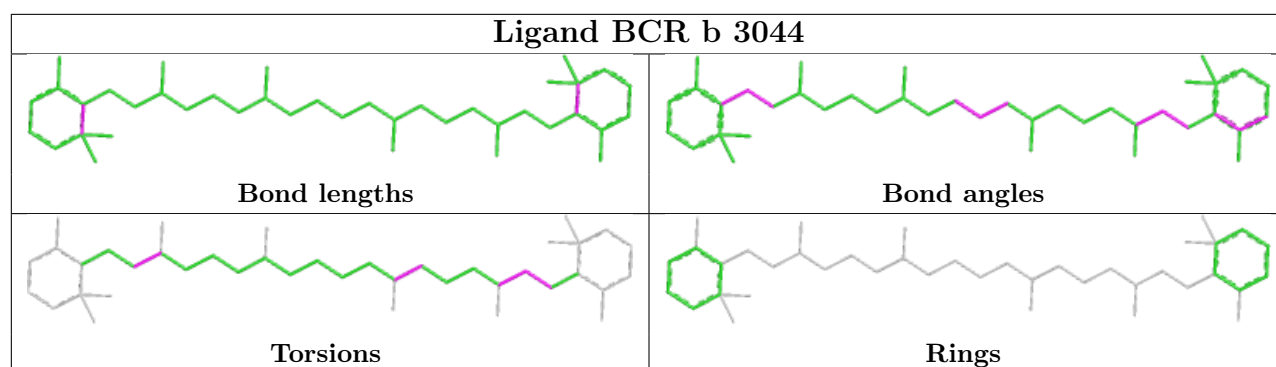


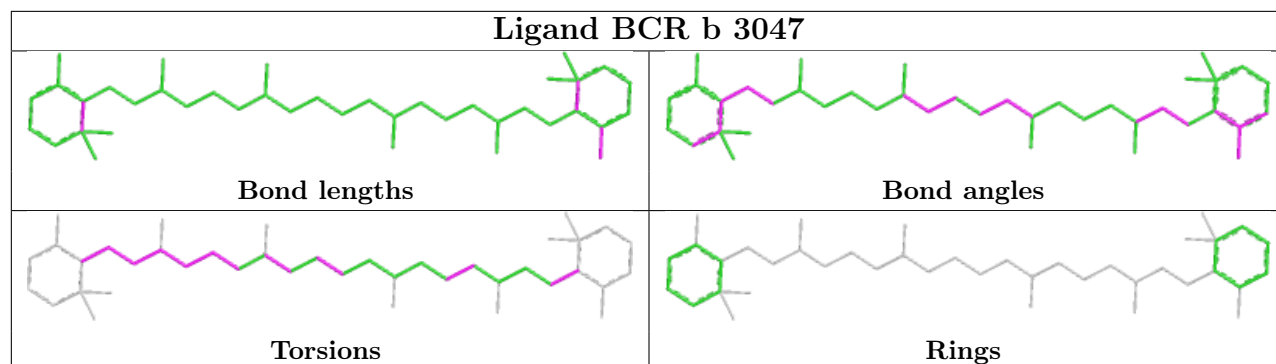
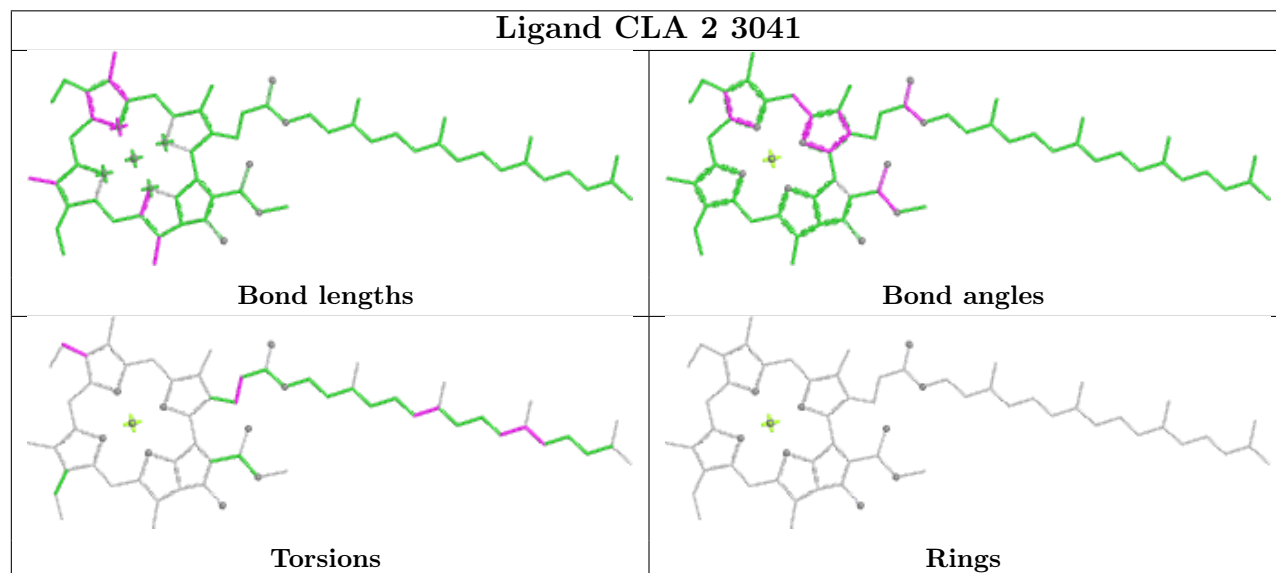
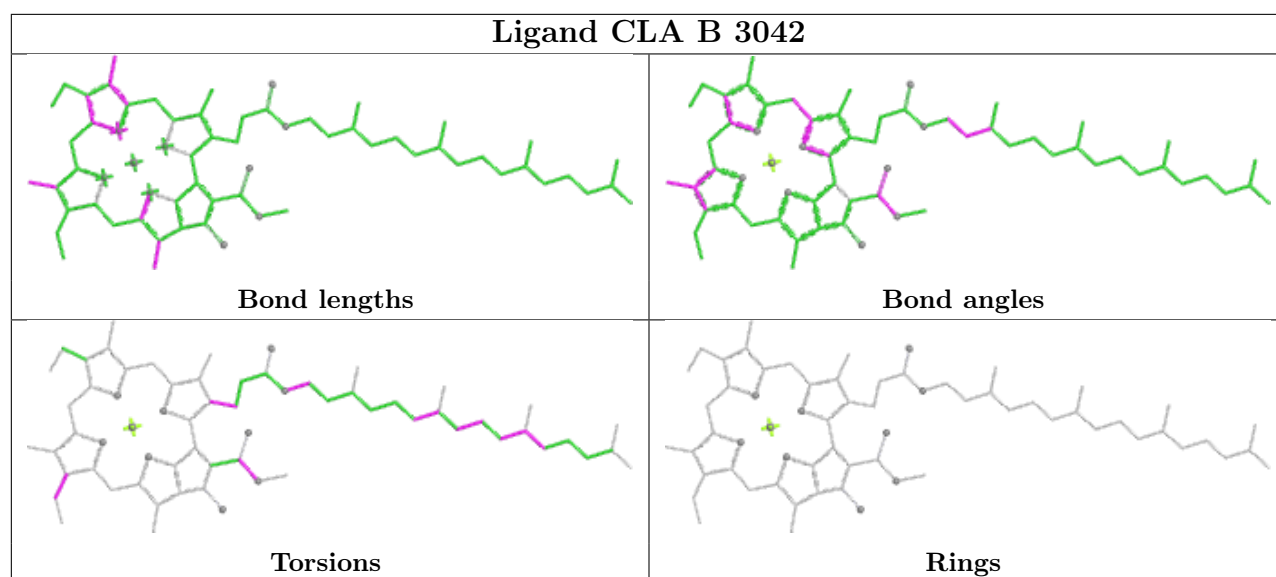
Torsions

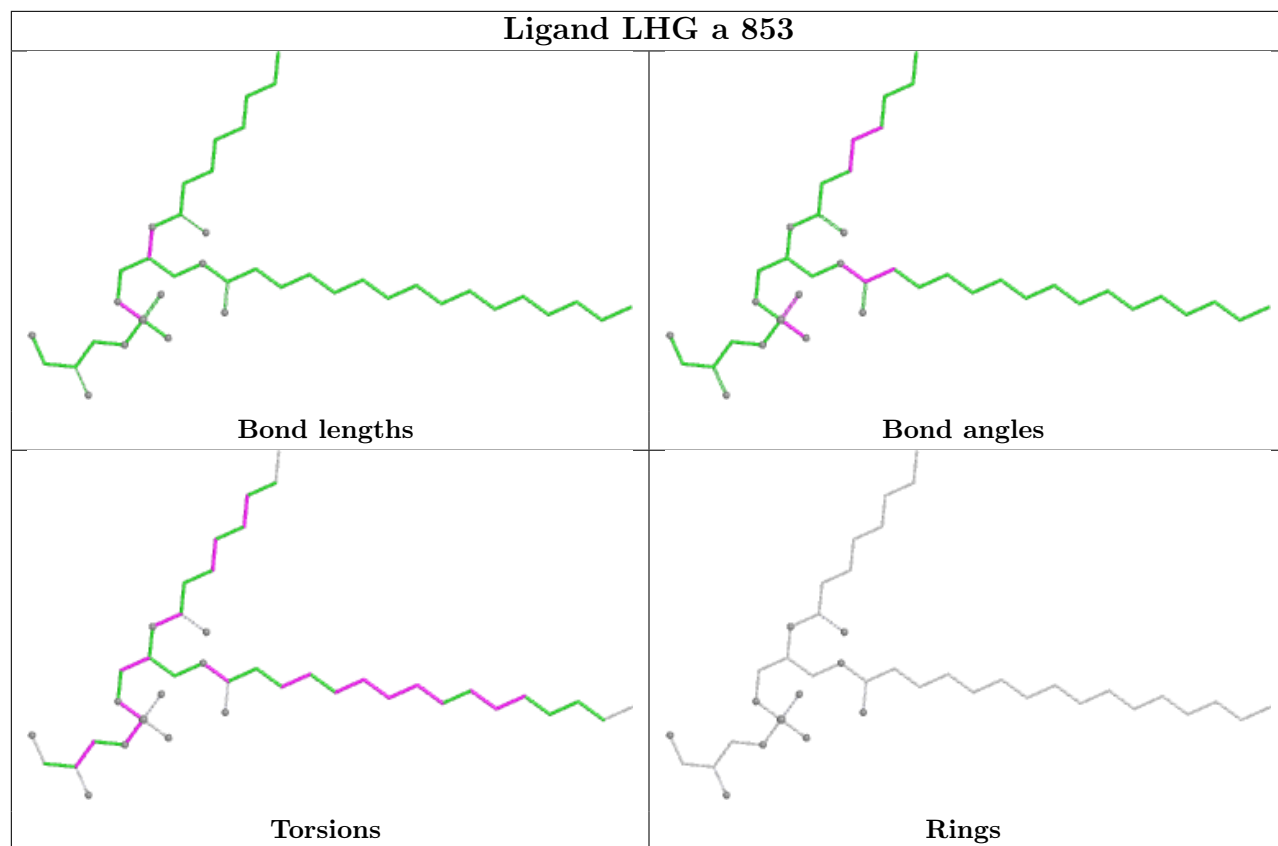


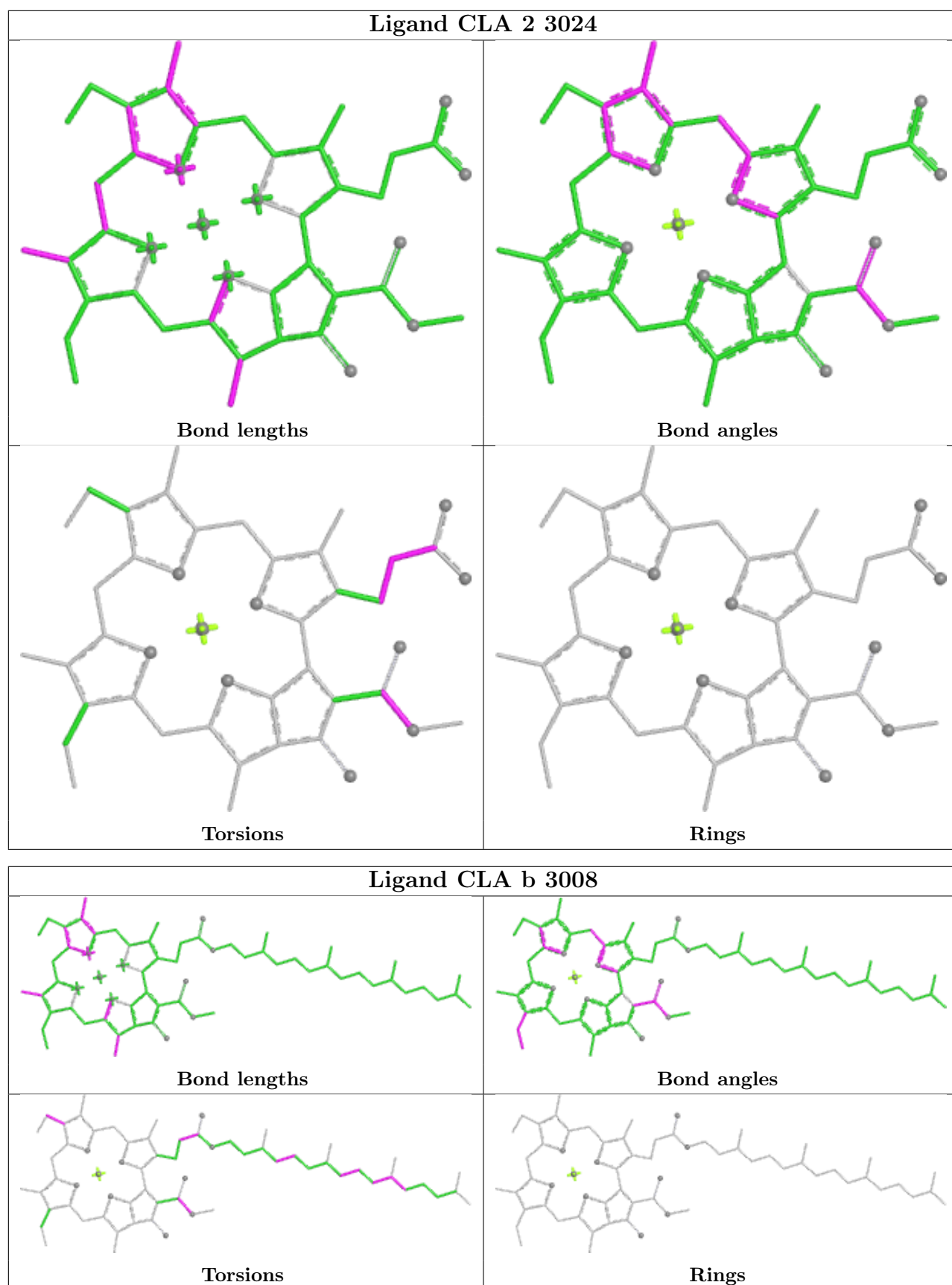
Rings

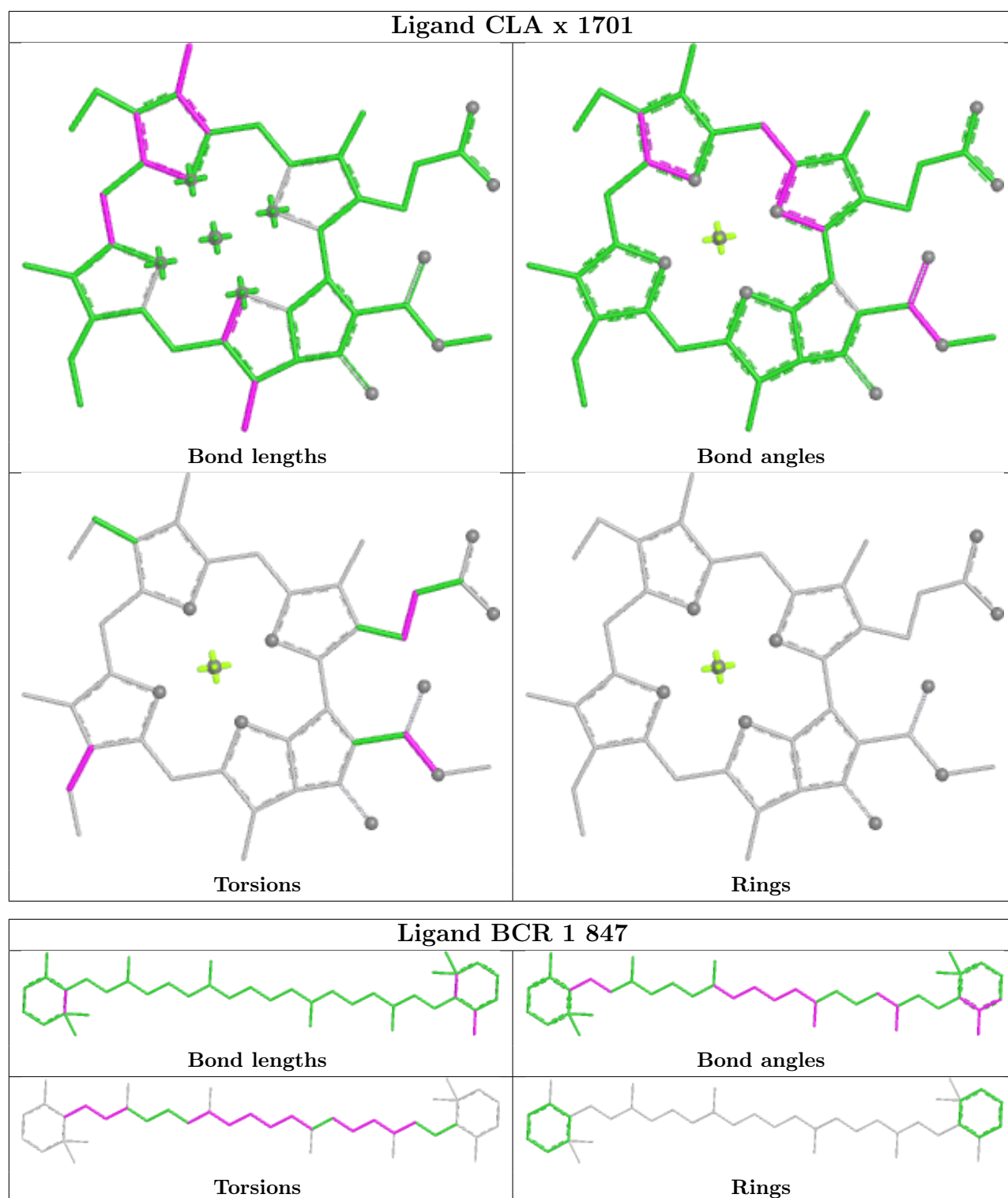




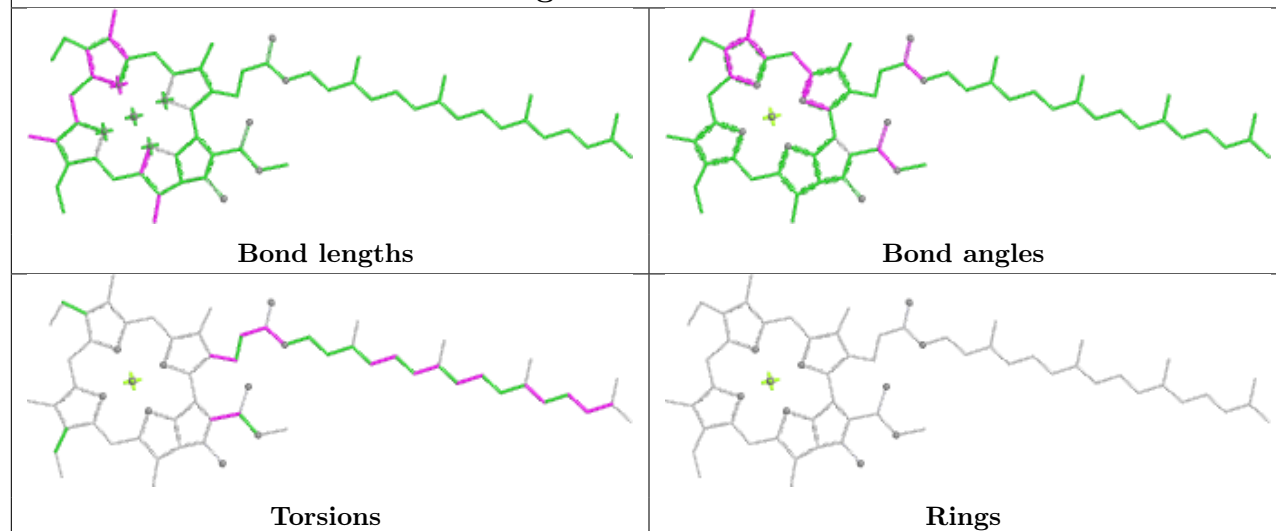




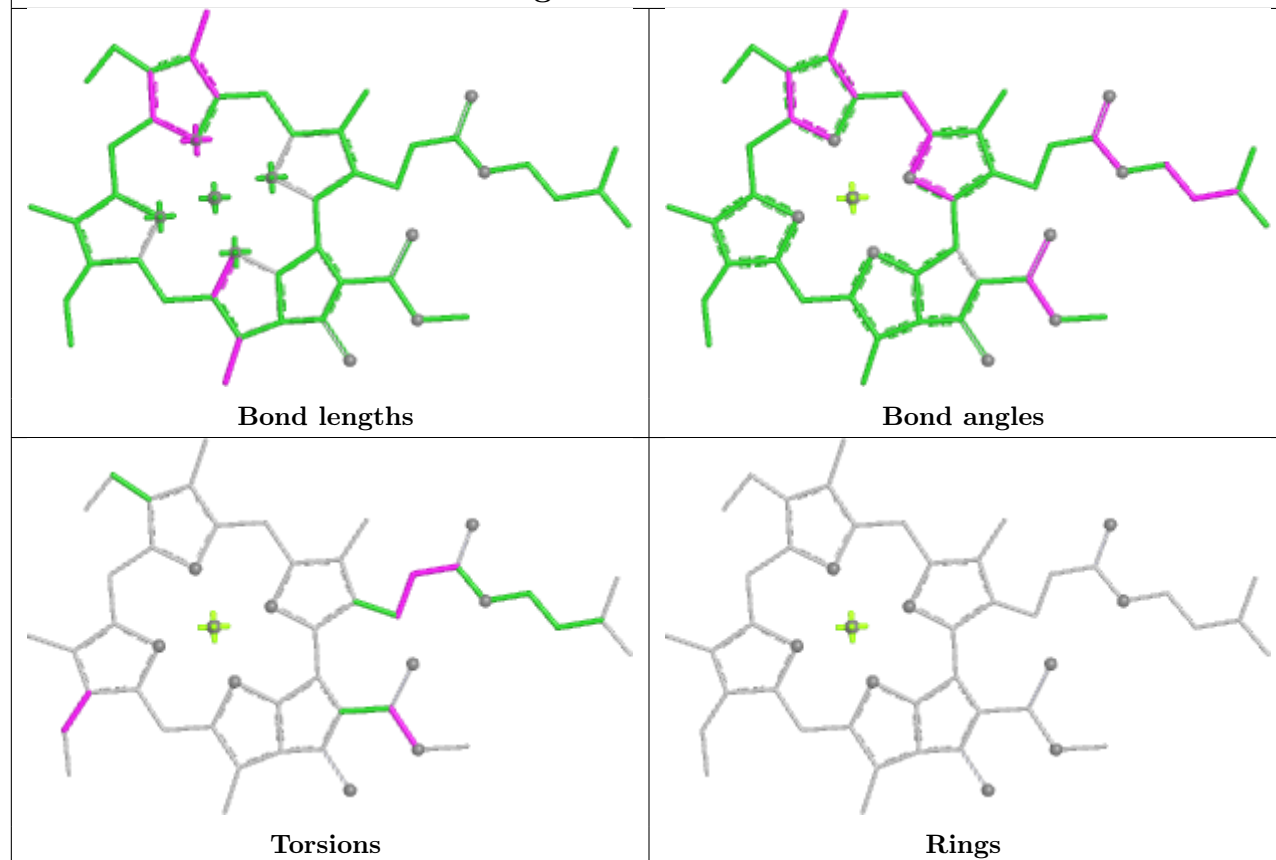


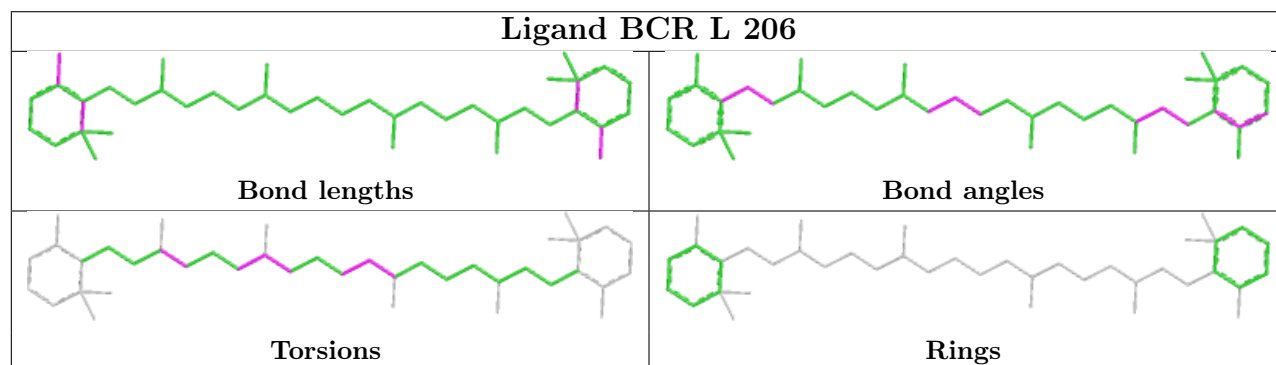
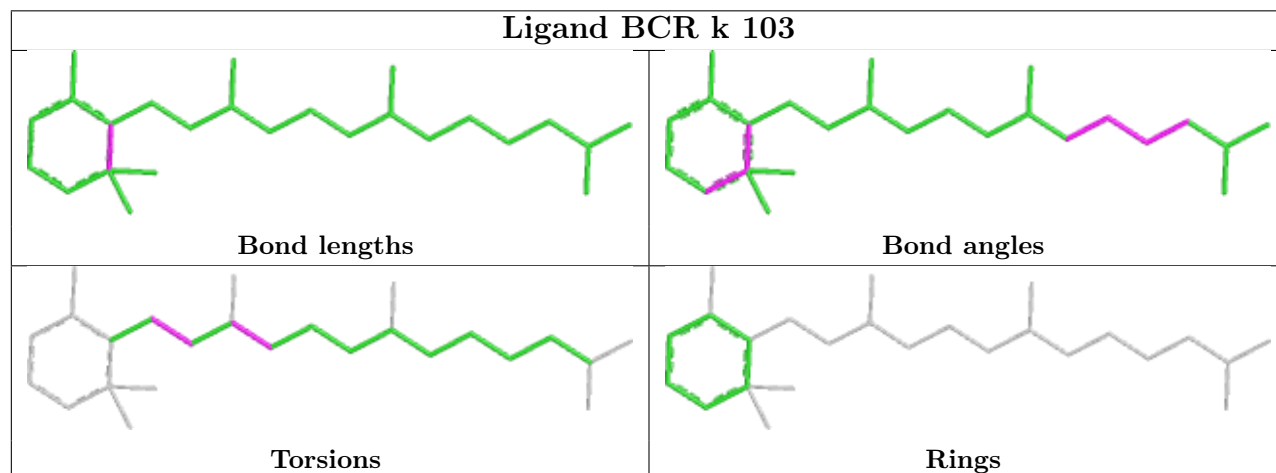
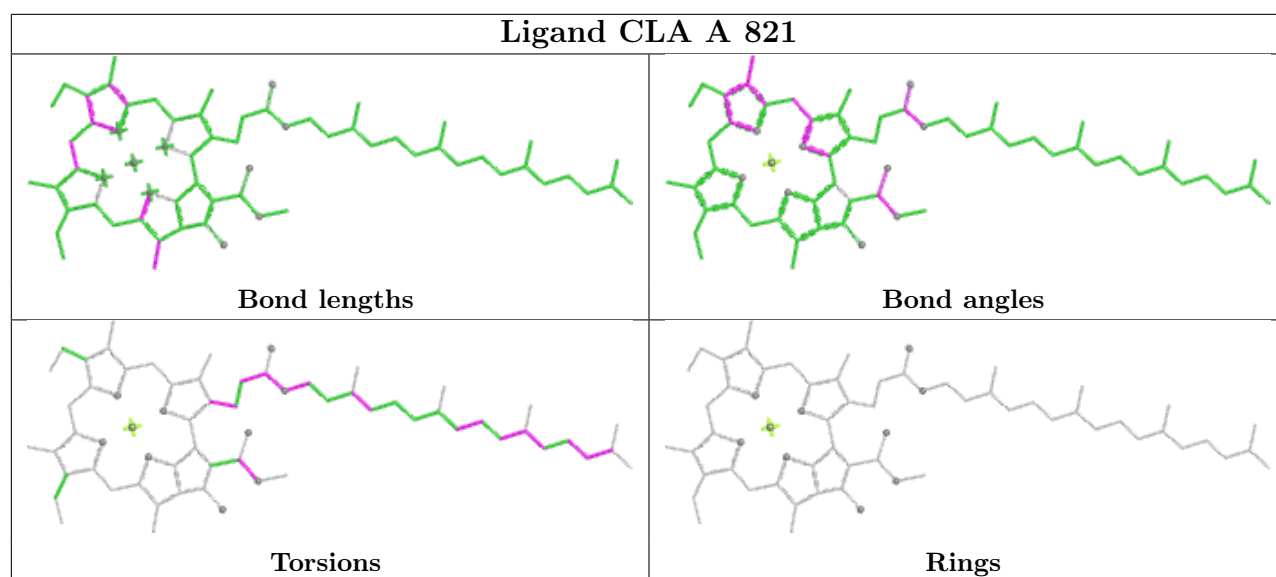


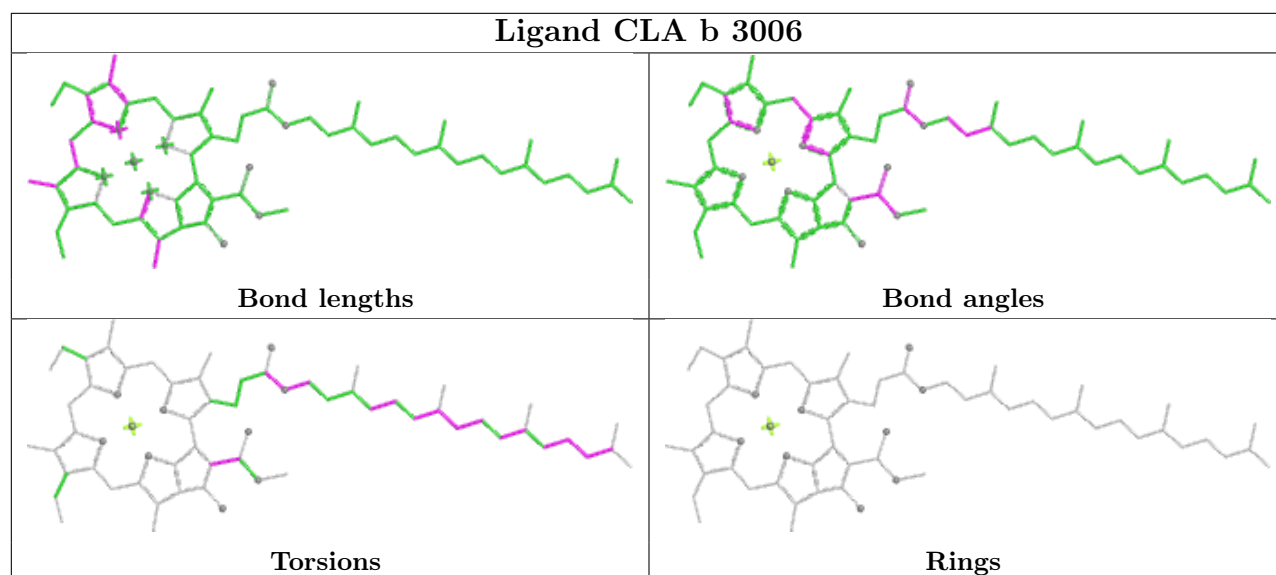
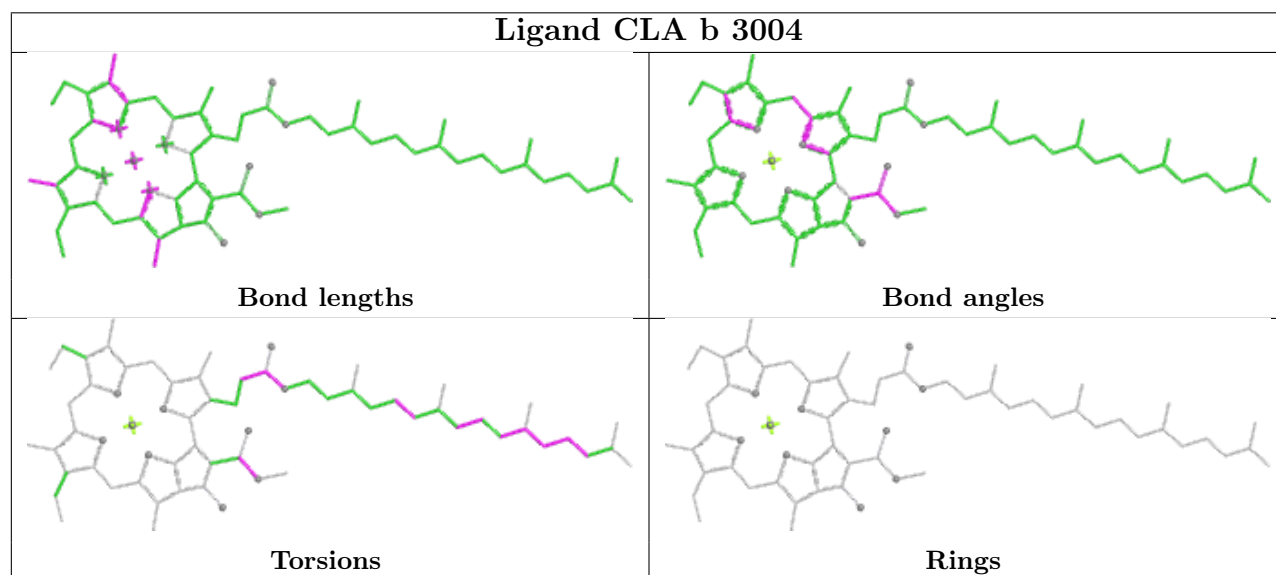
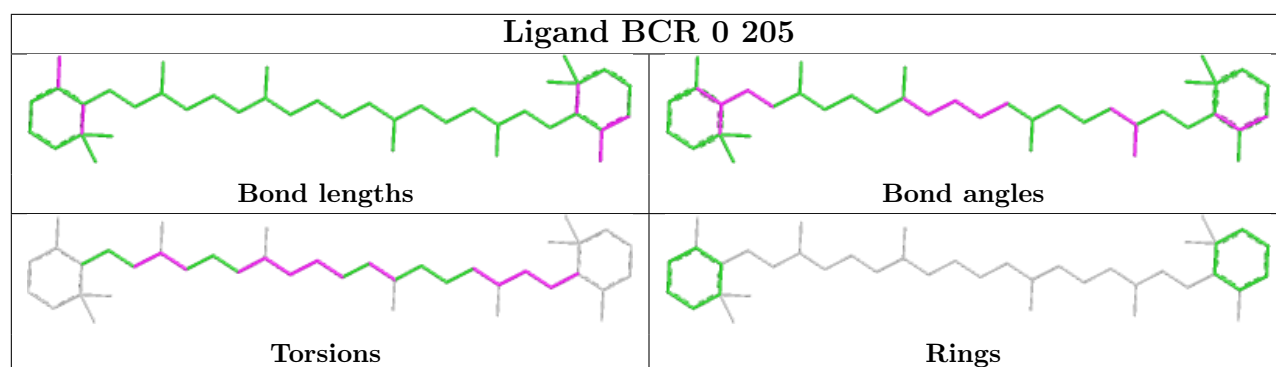
Ligand CLA a 808

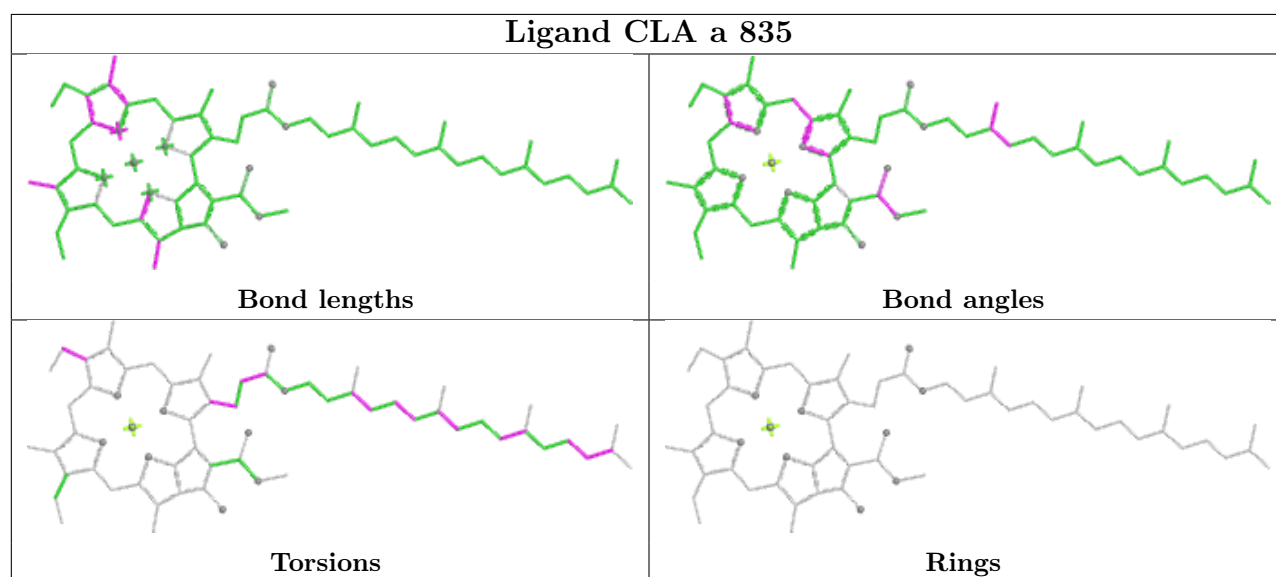
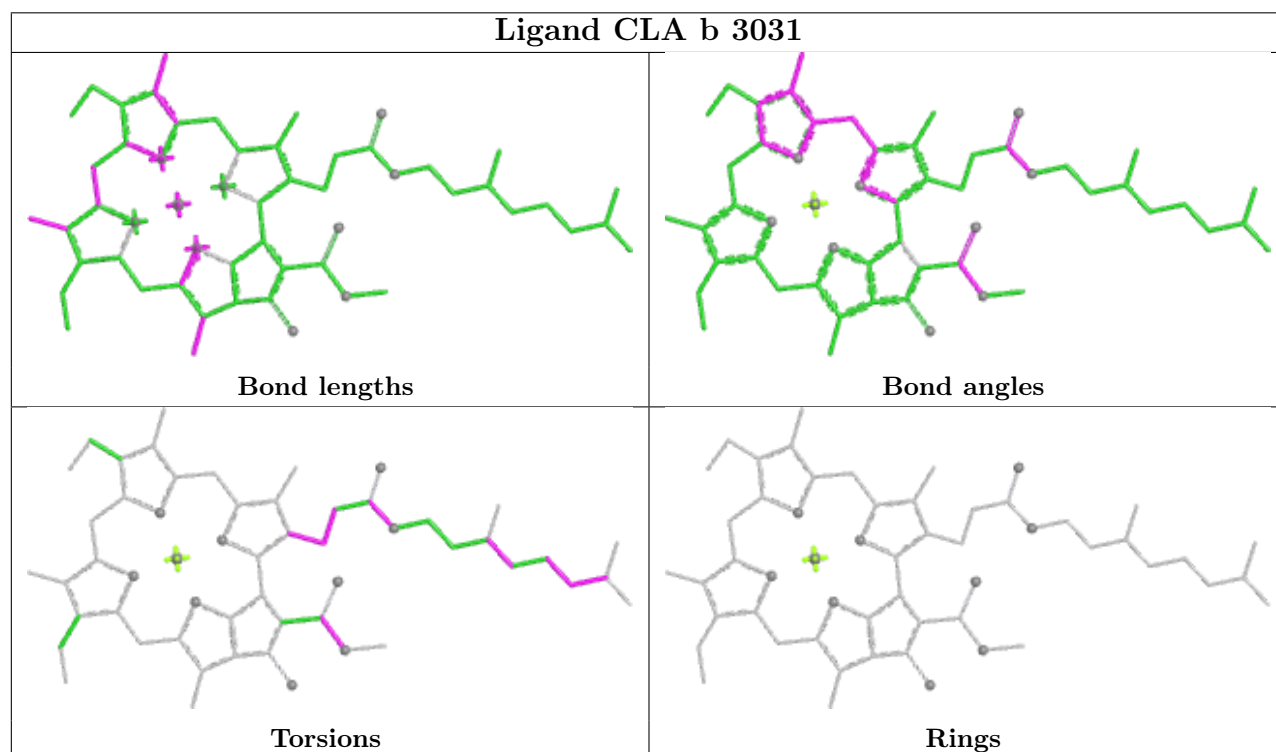
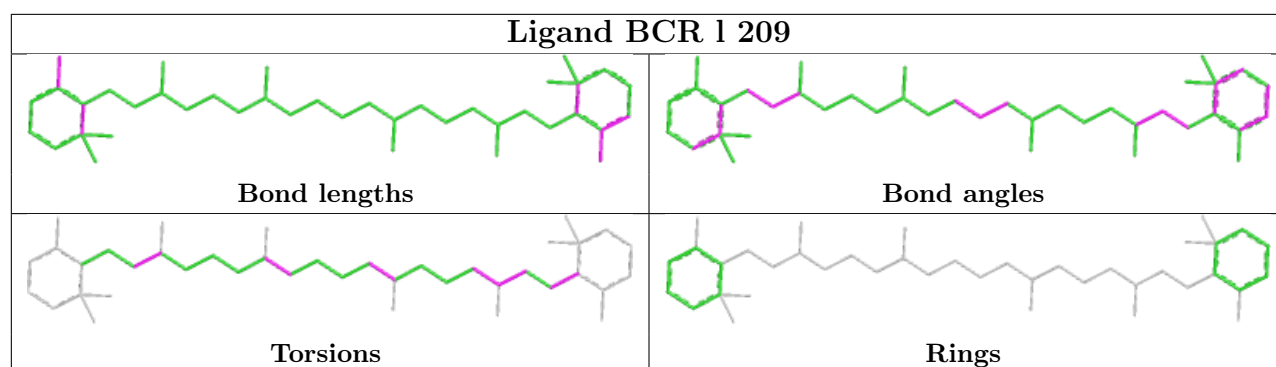


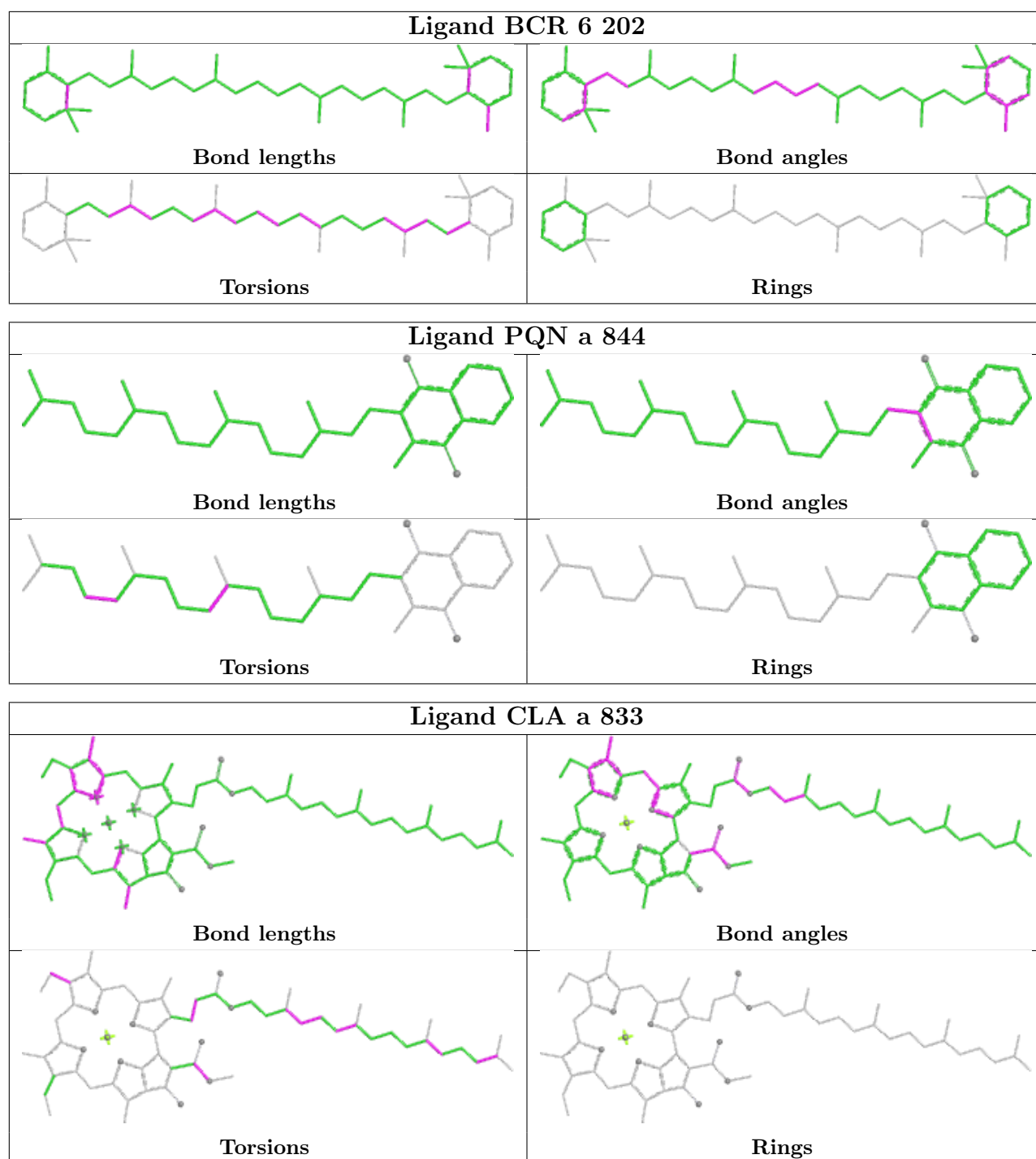
Ligand CLA F 204

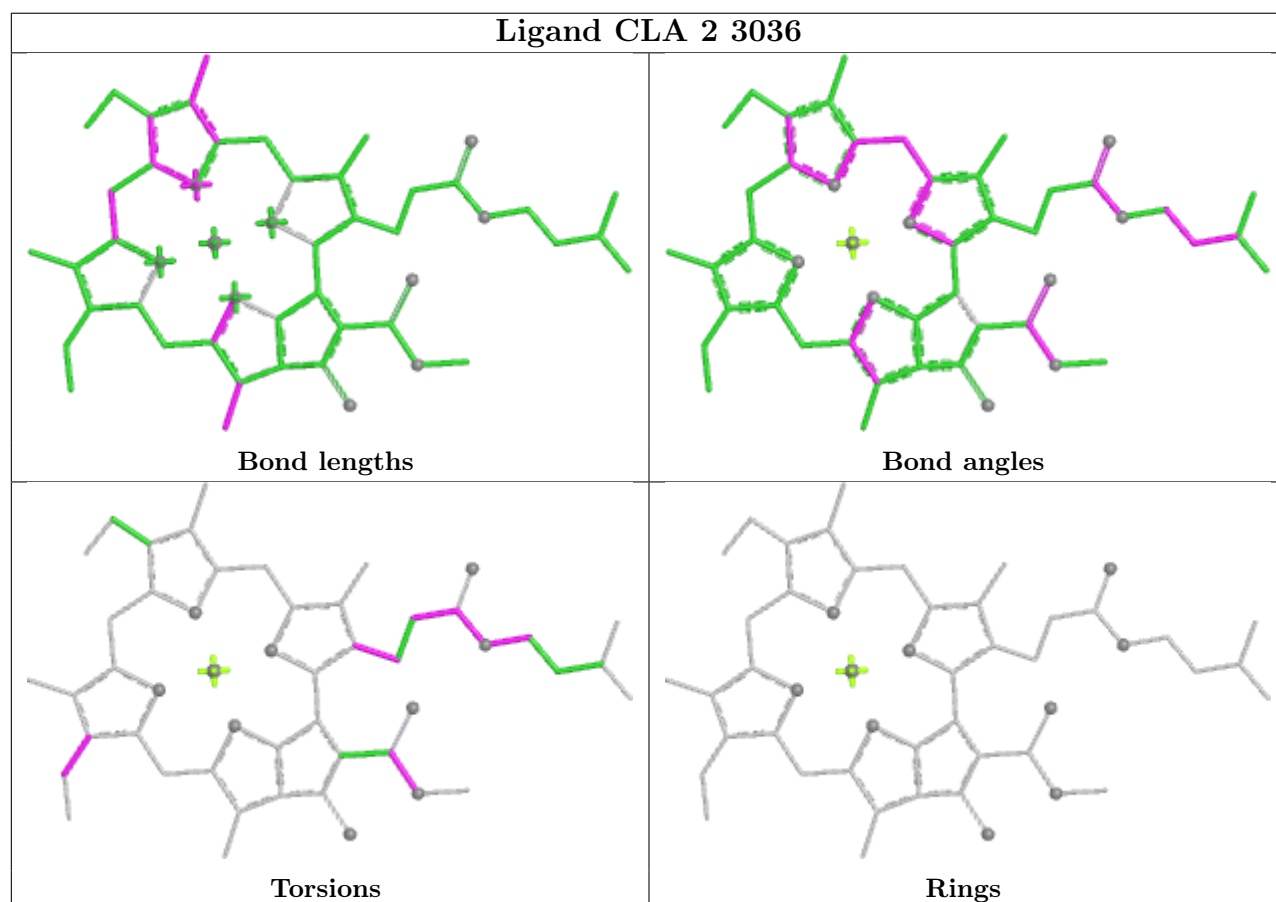
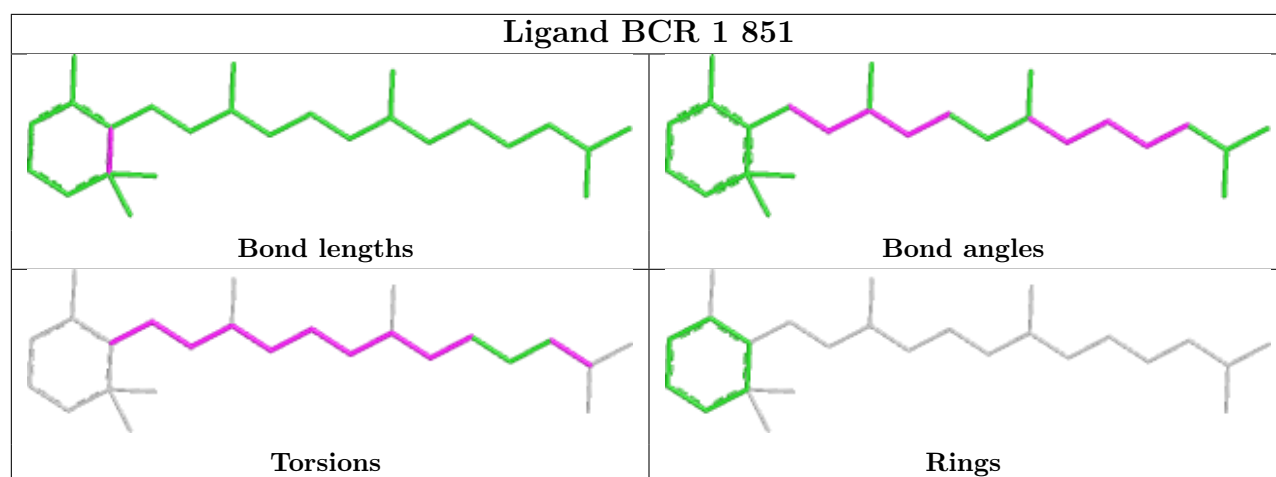


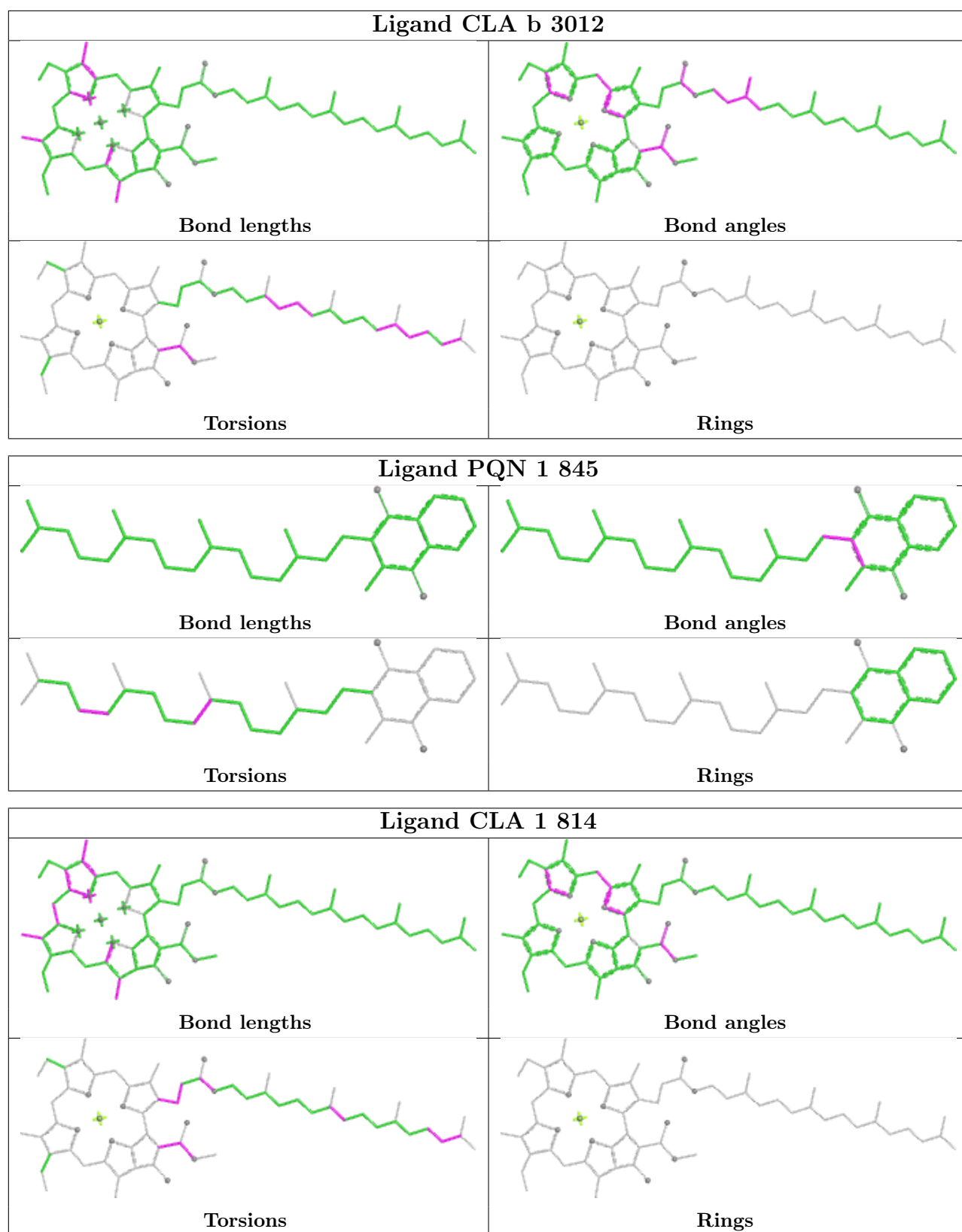




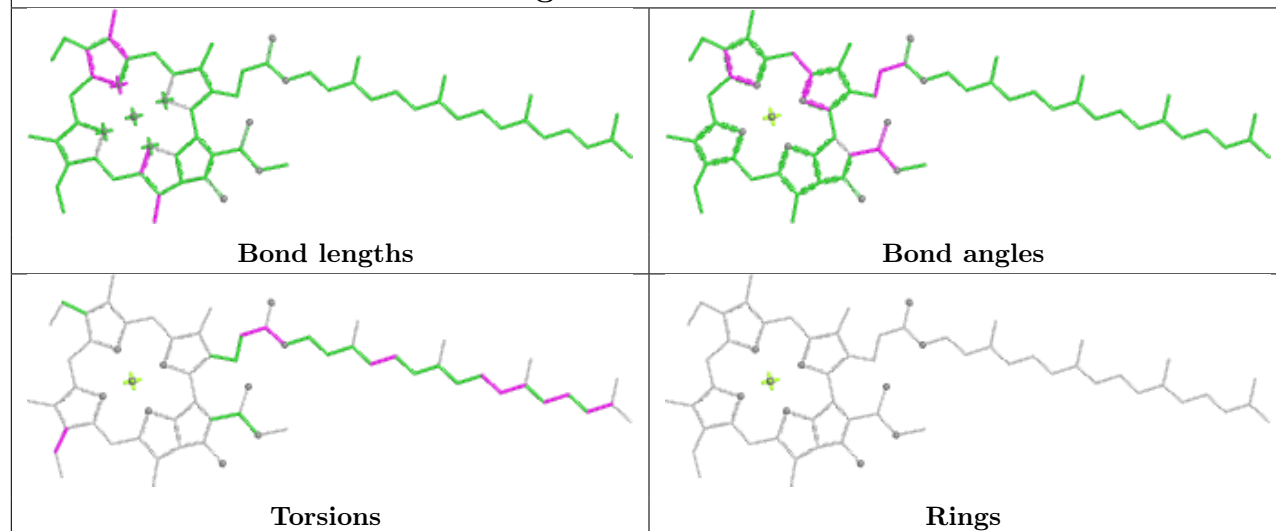




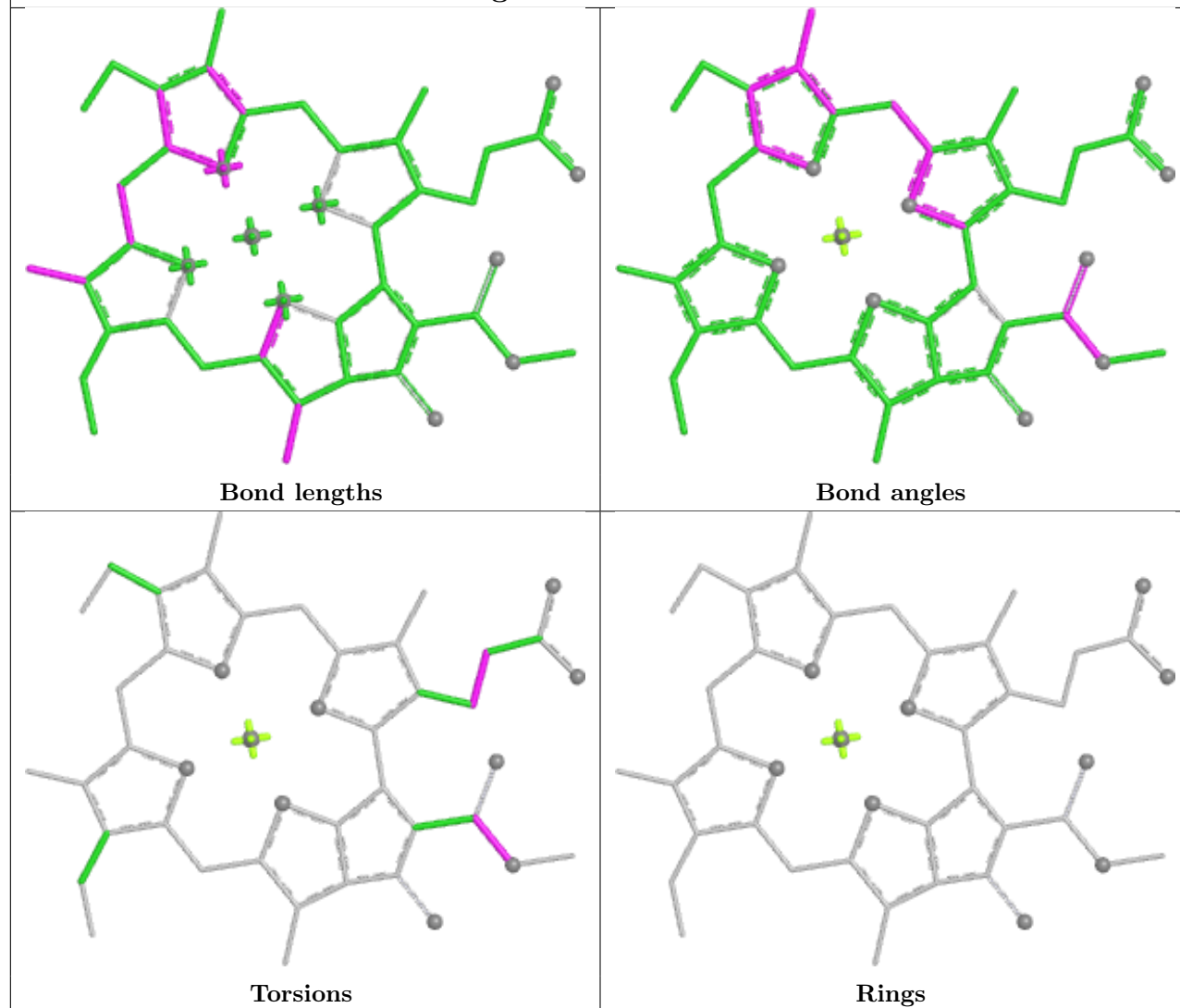


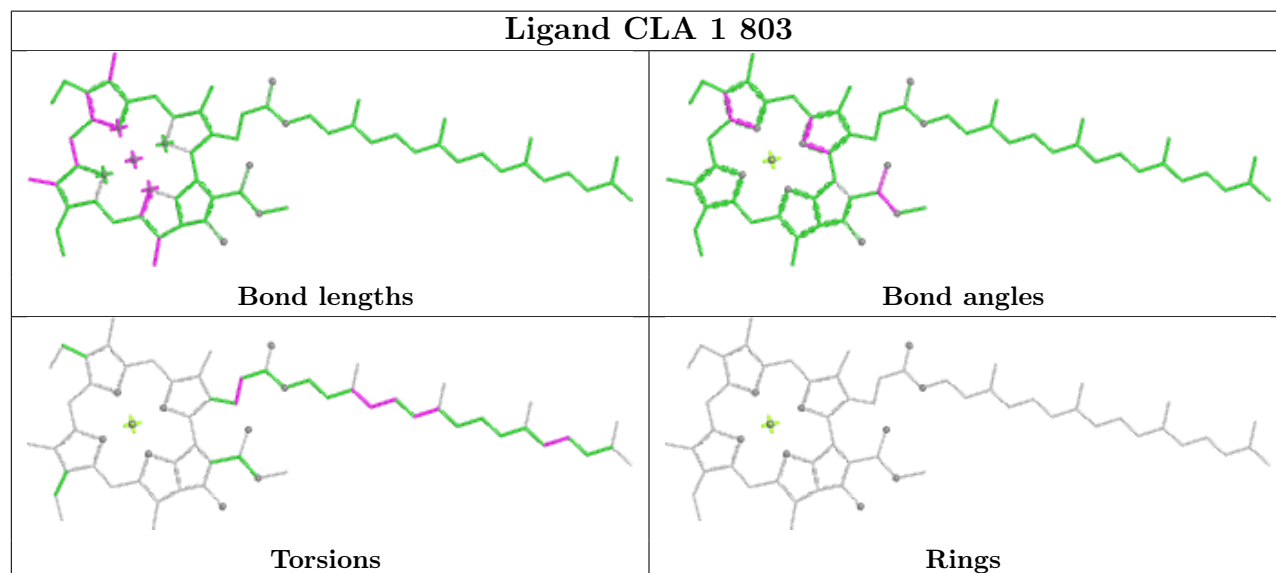
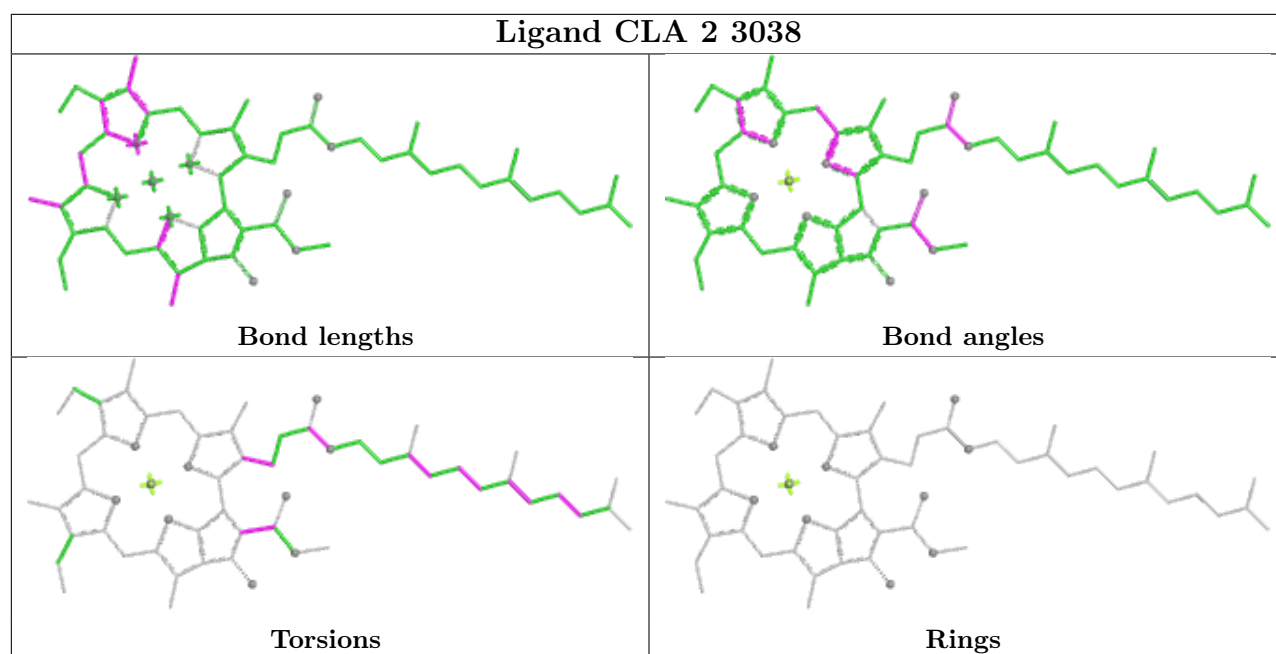


Ligand CLA 1 840

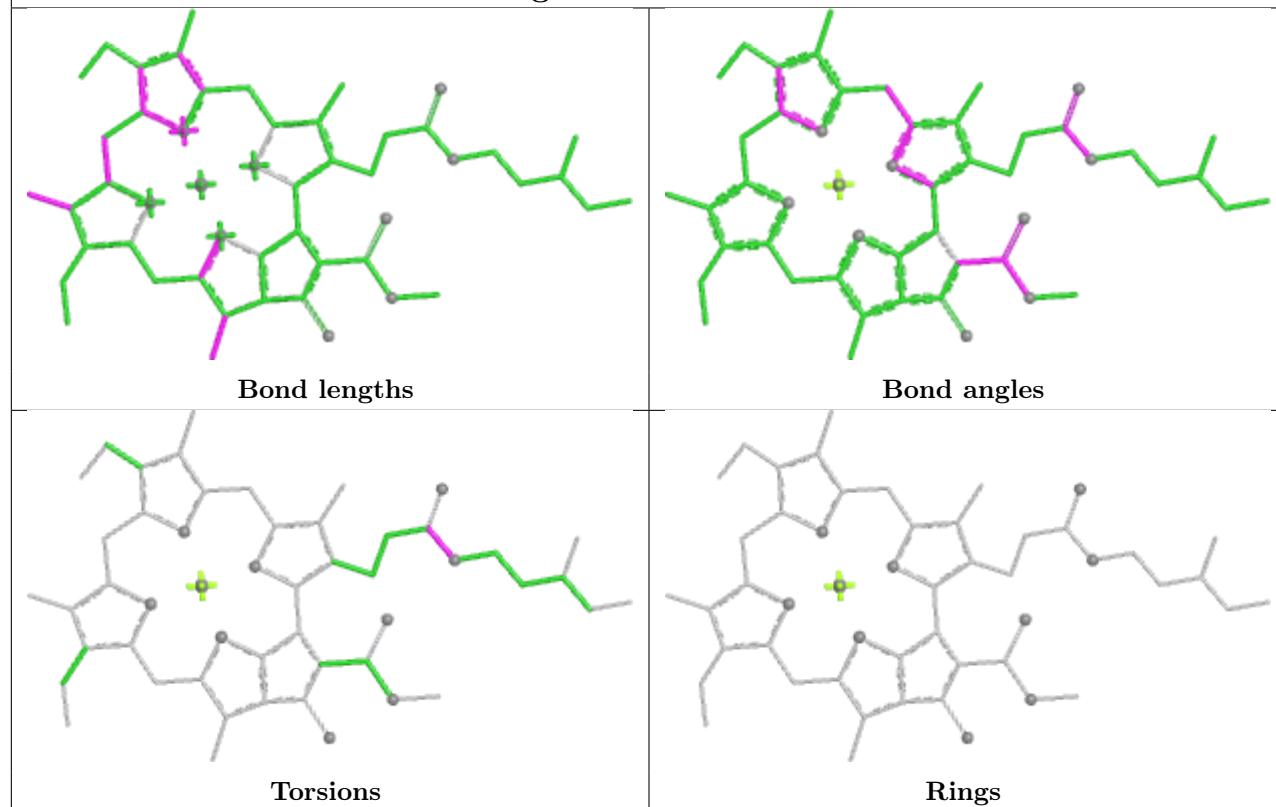


Ligand CLA A 823

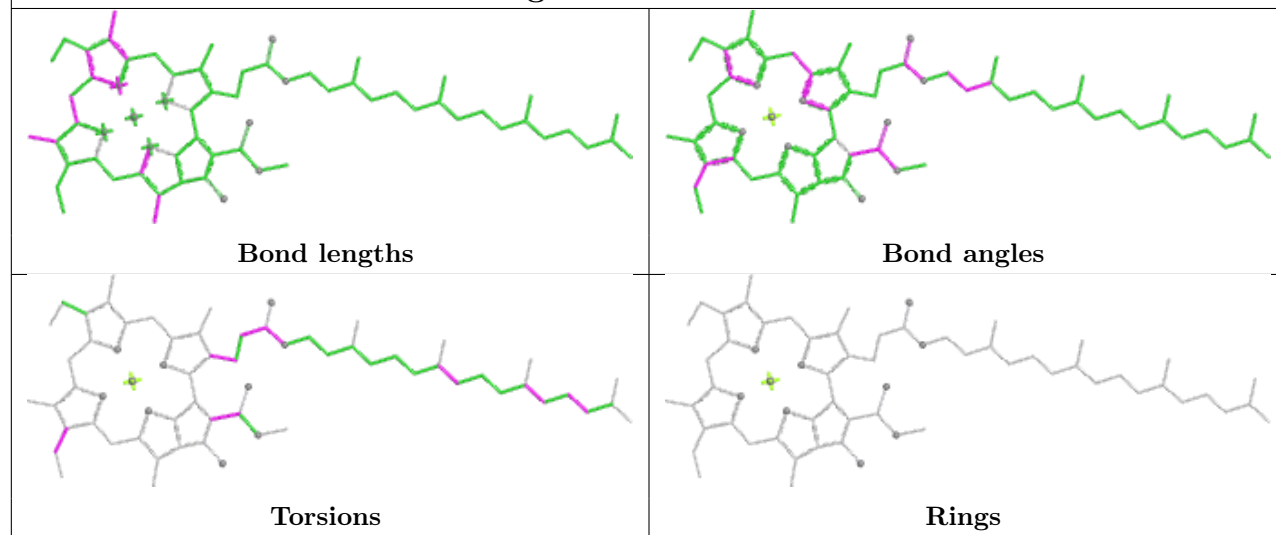


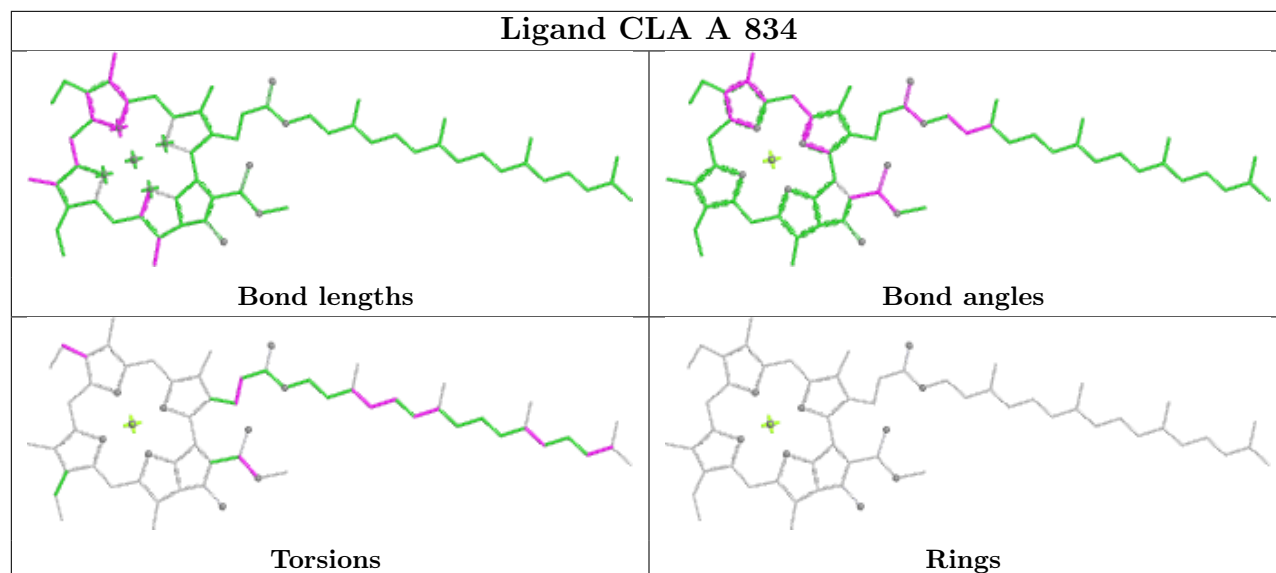
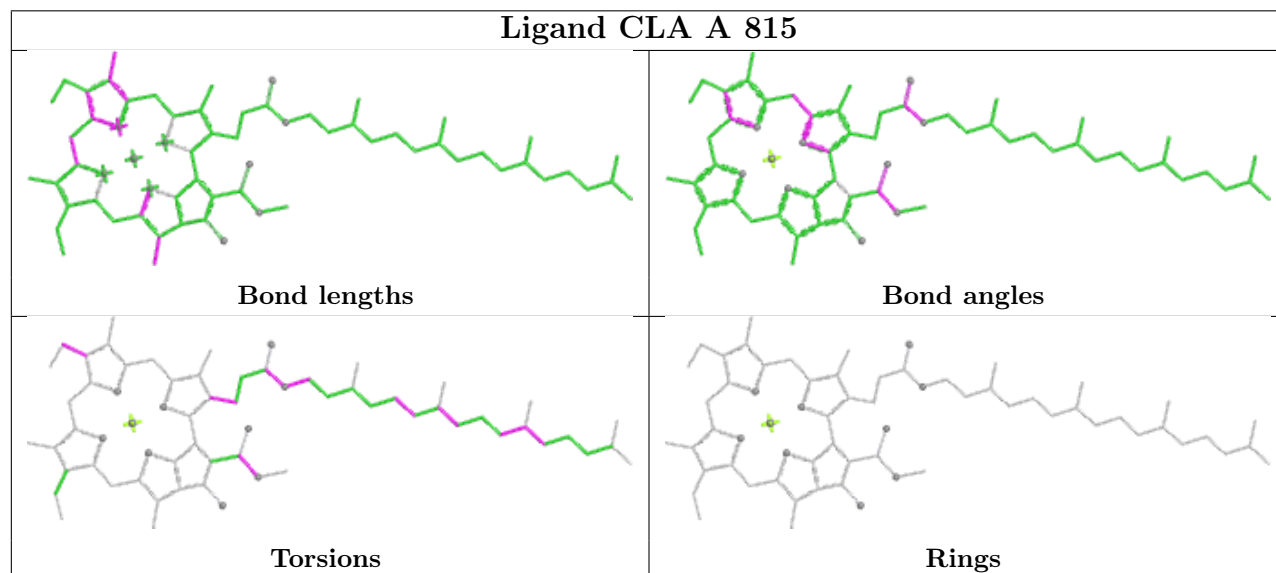
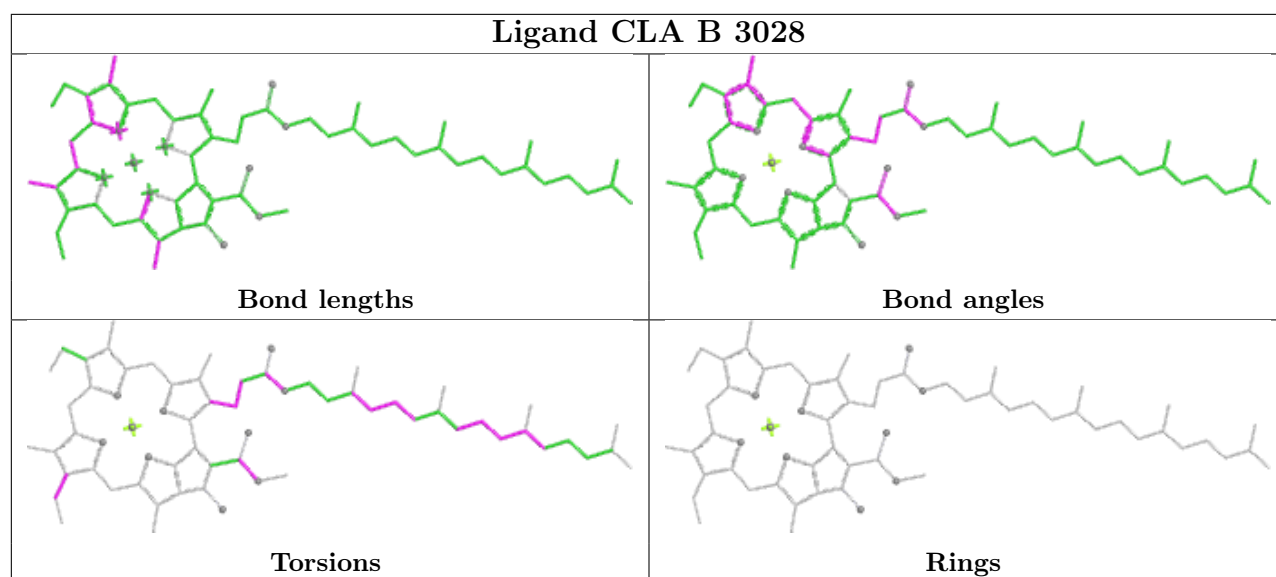


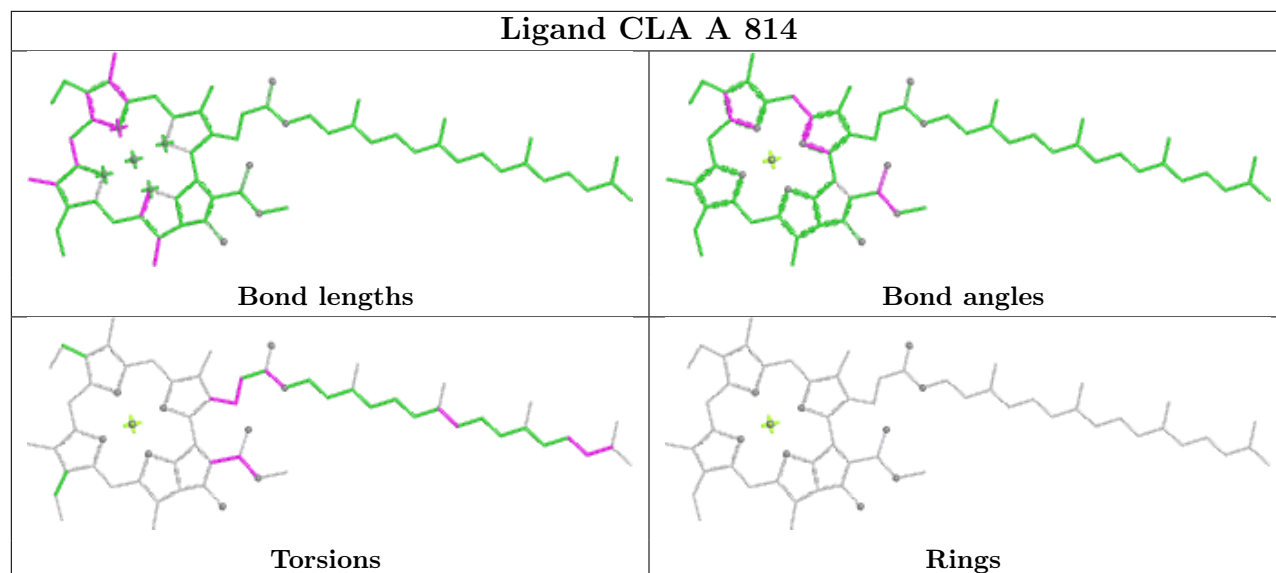
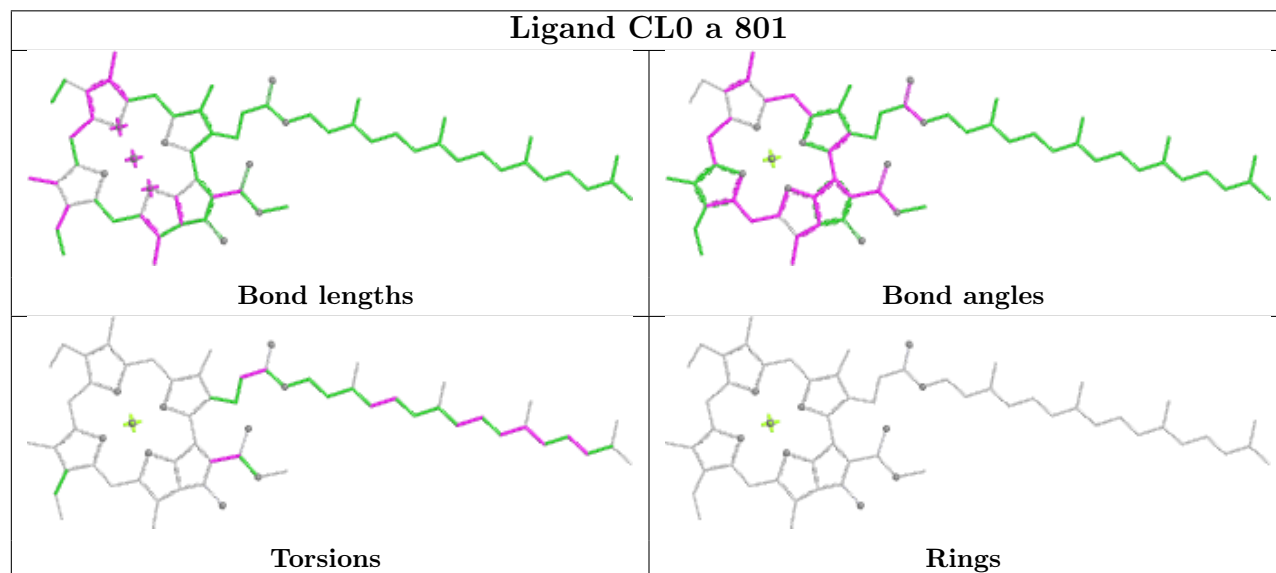
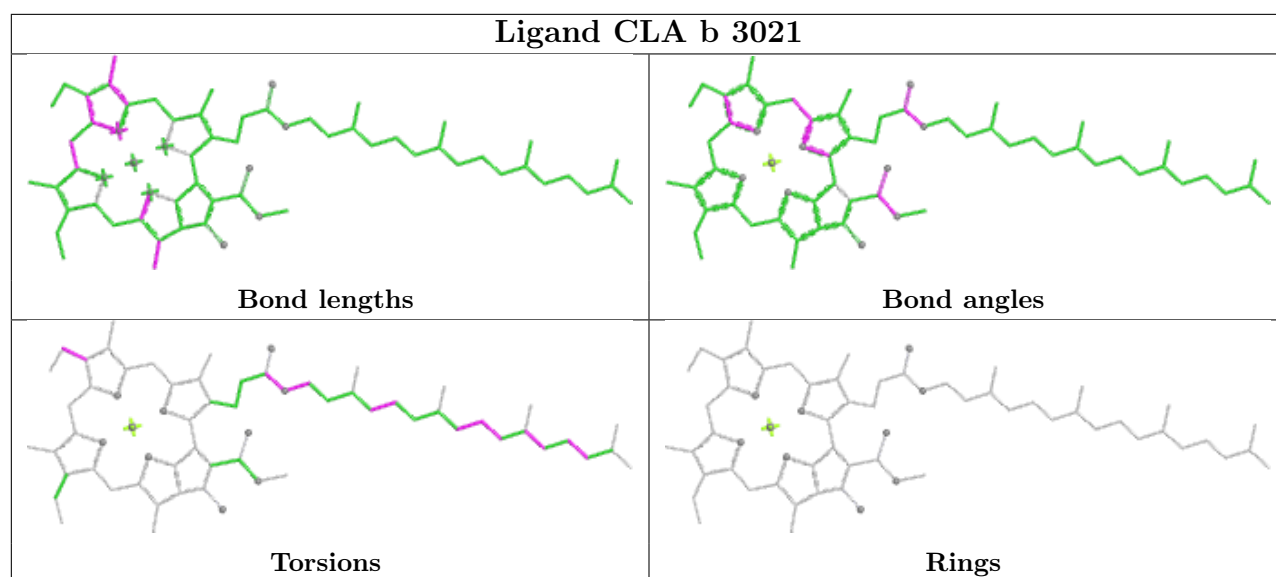
Ligand CLA A 808

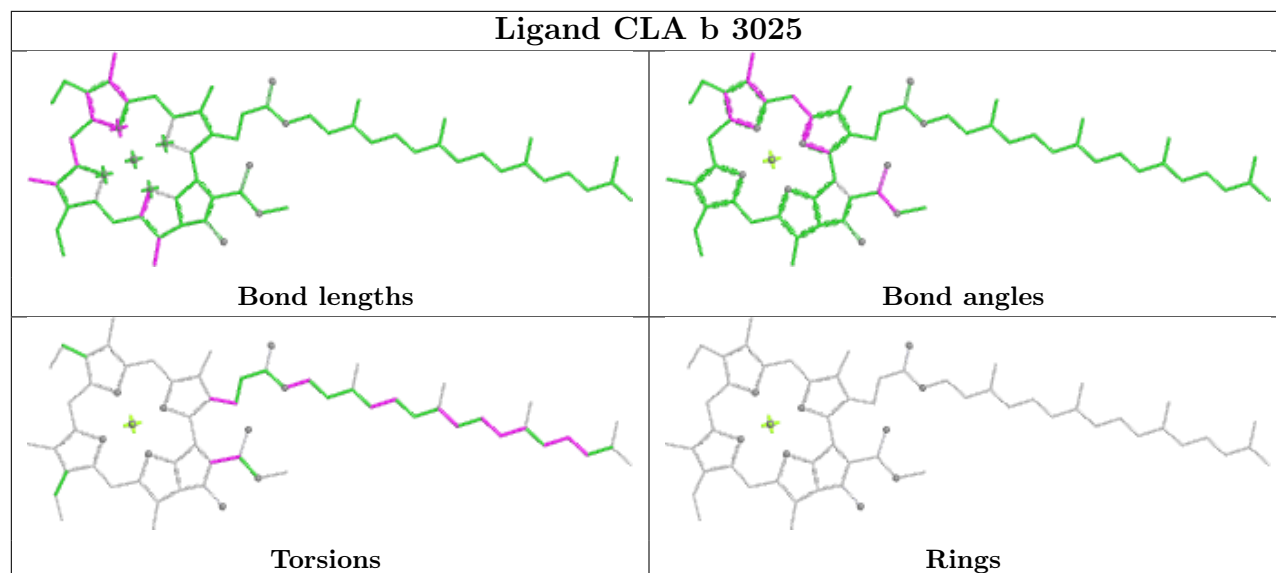
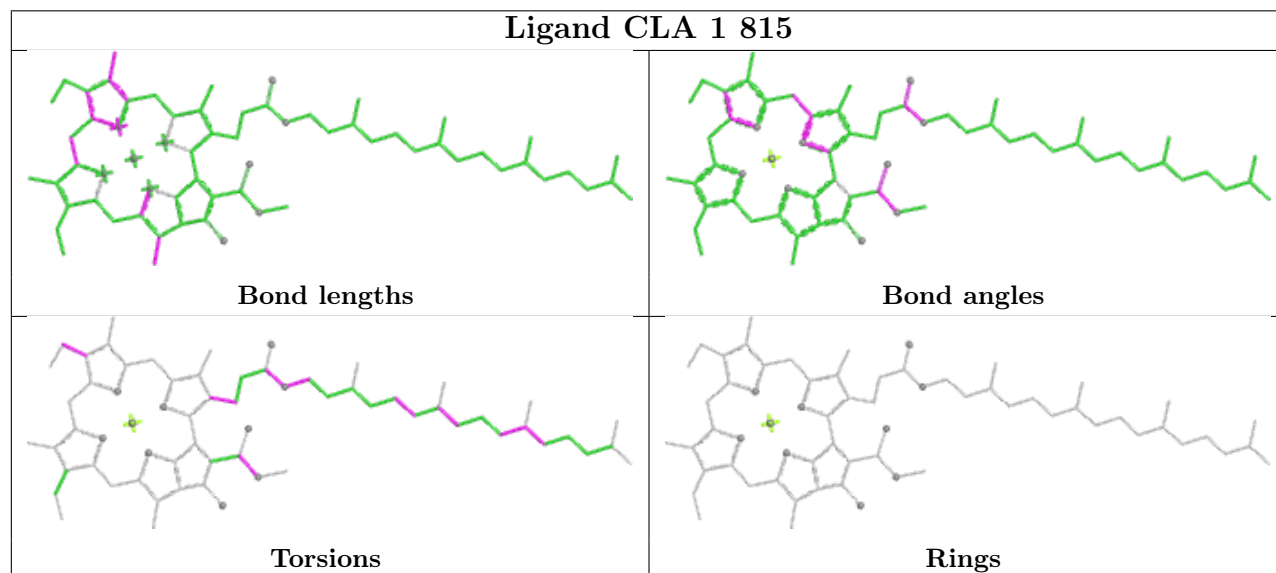
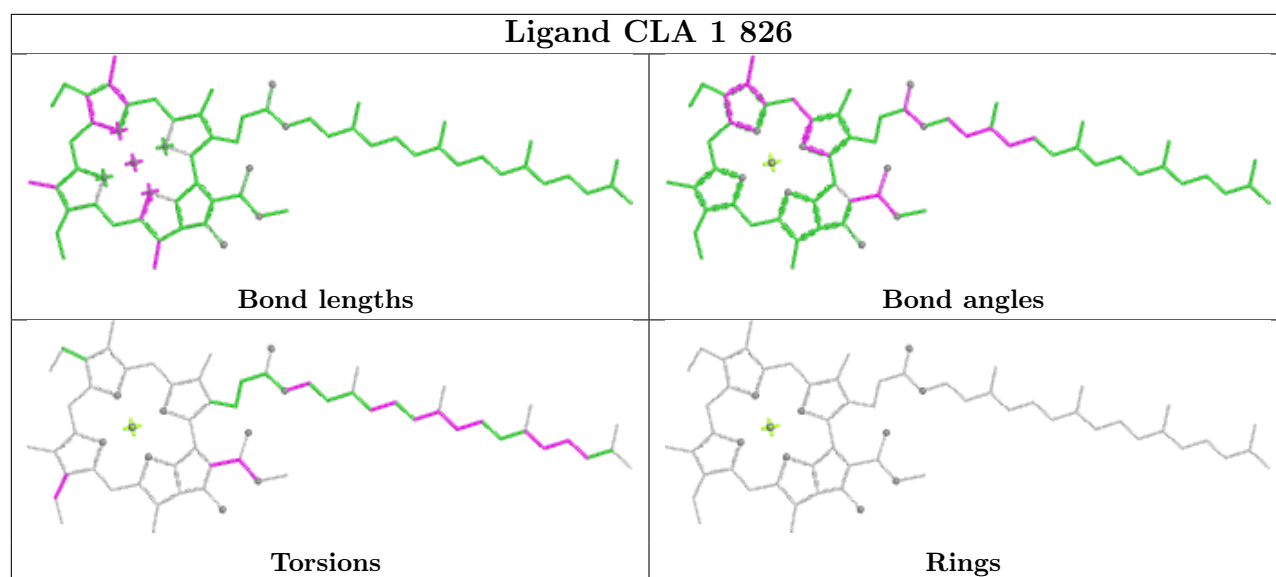


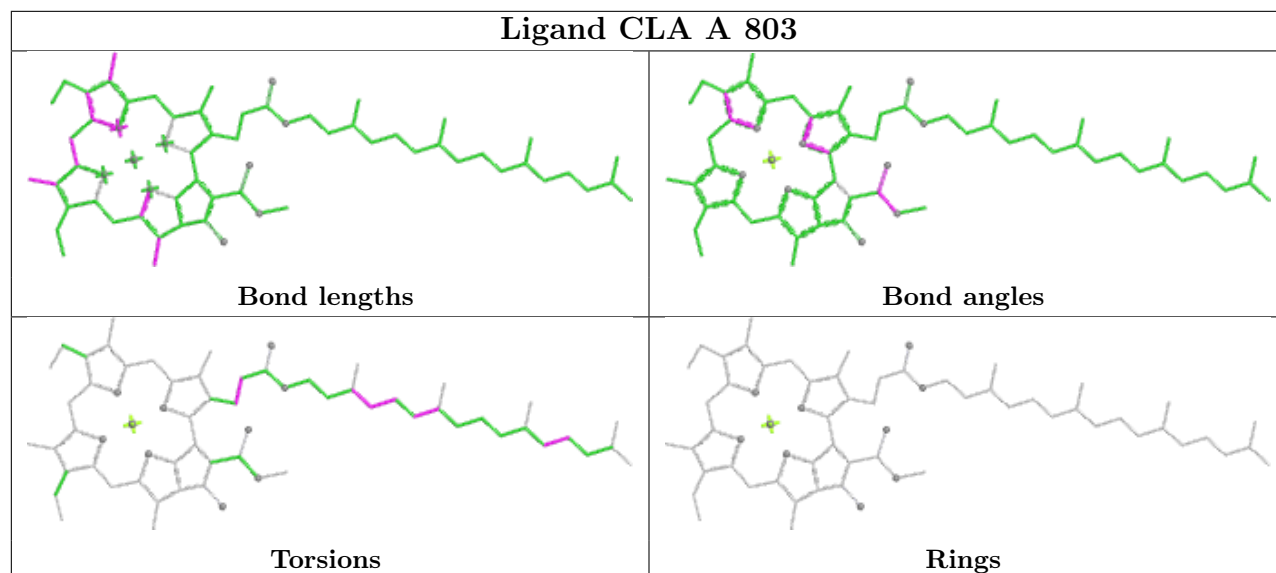
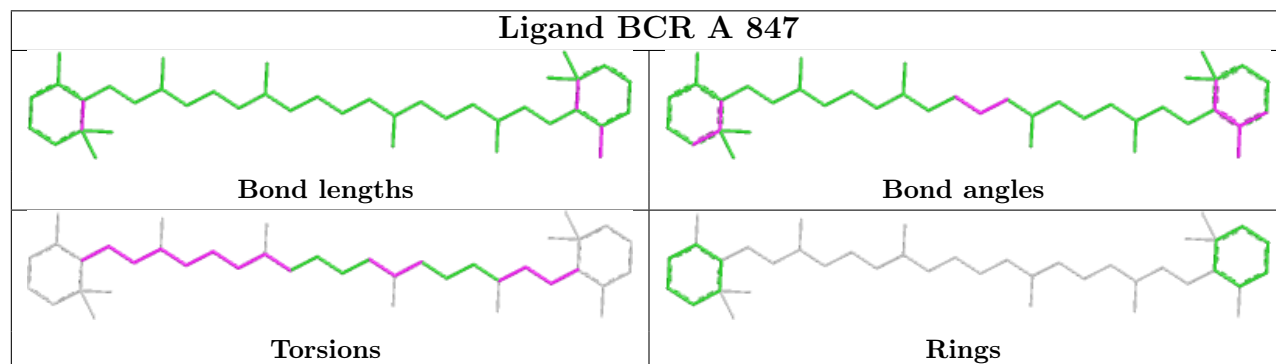
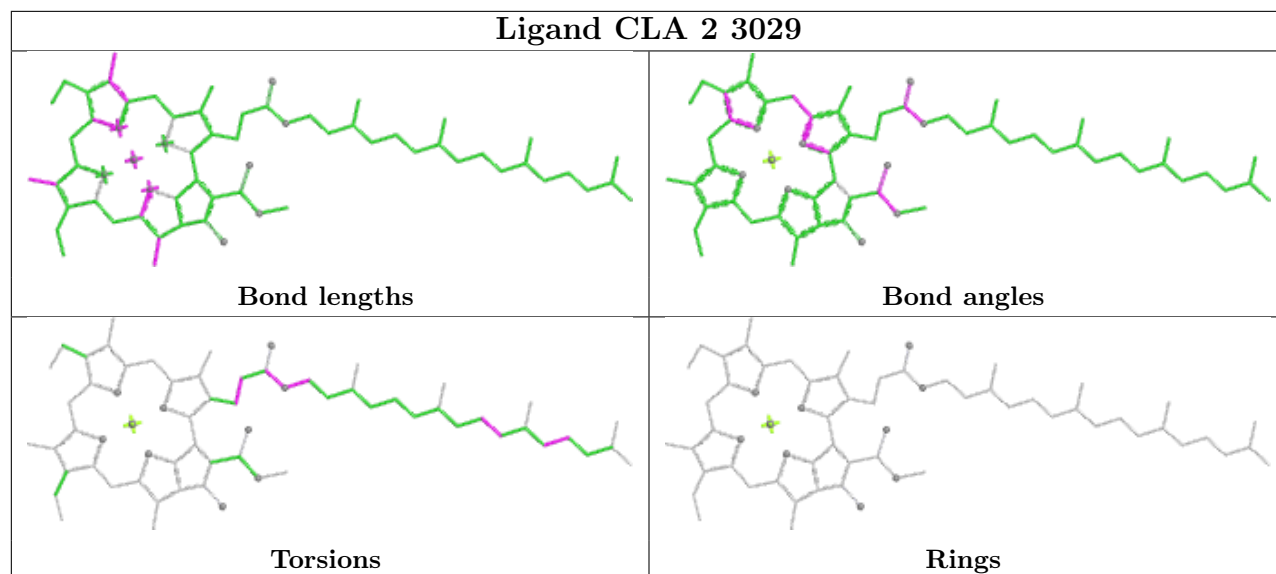
Ligand CLA 2 3033

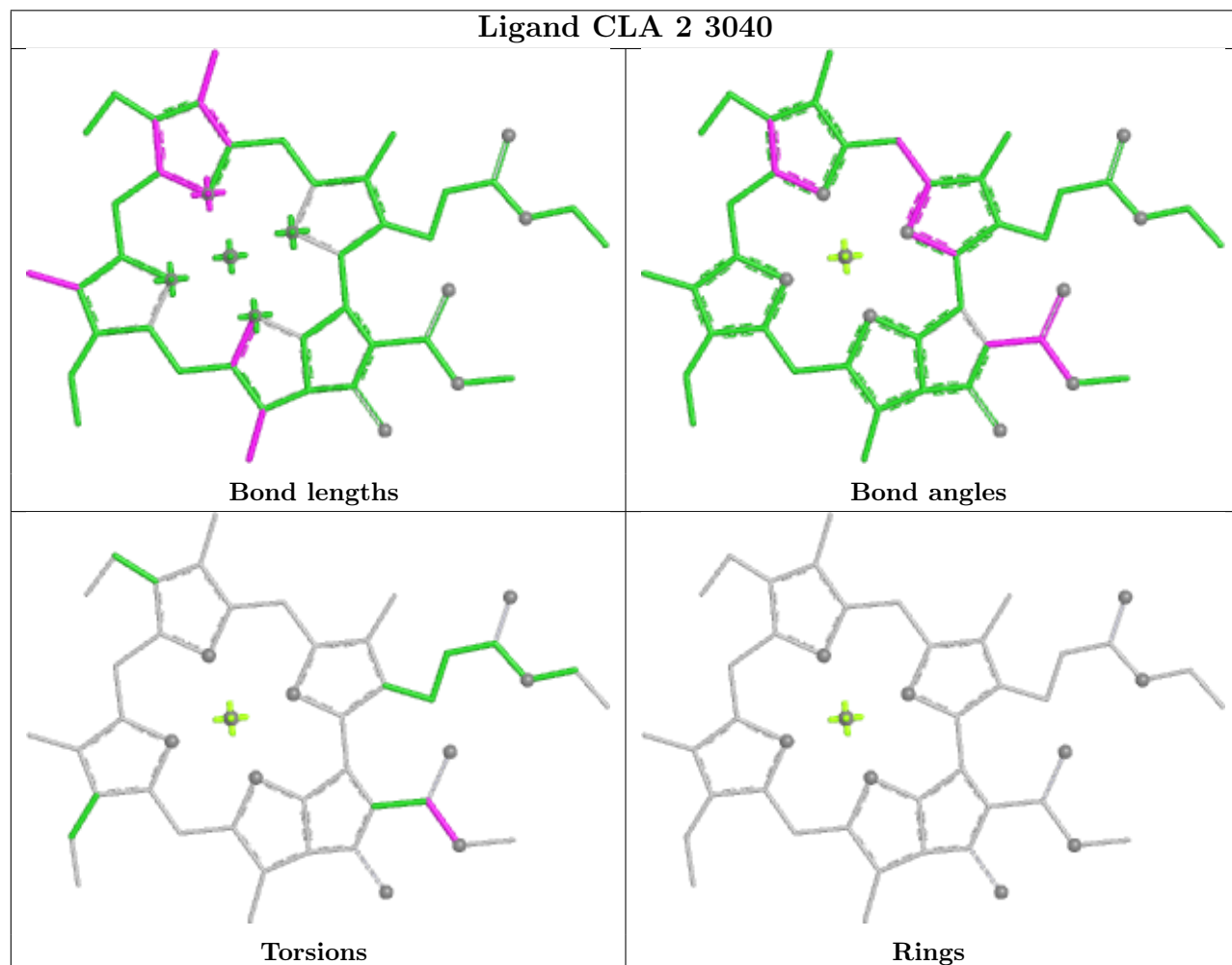
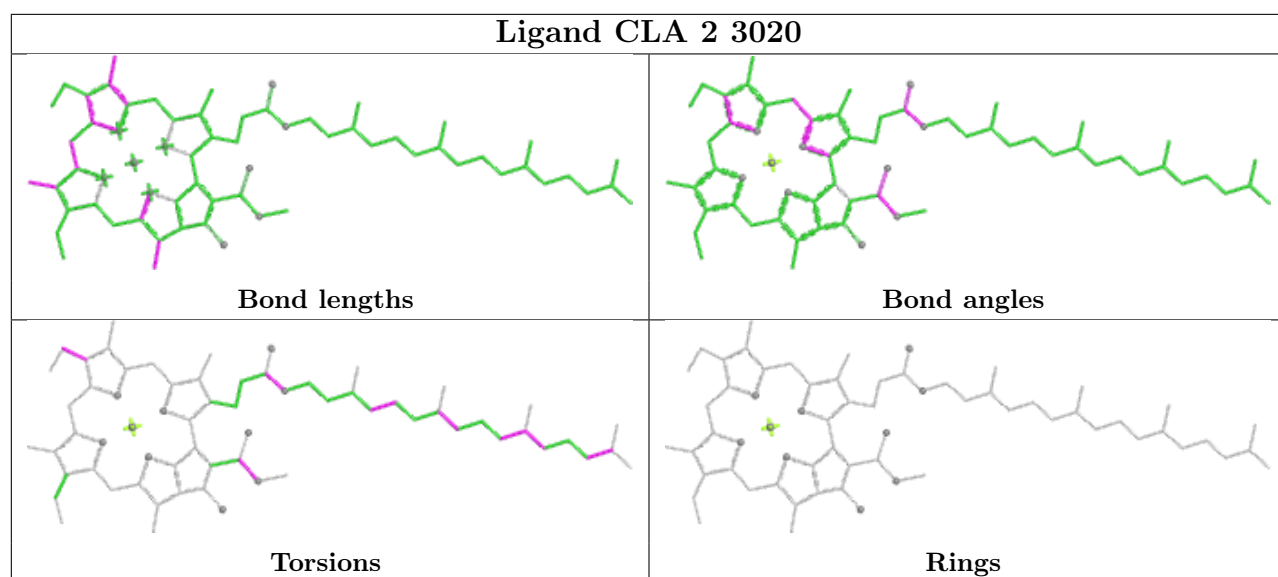




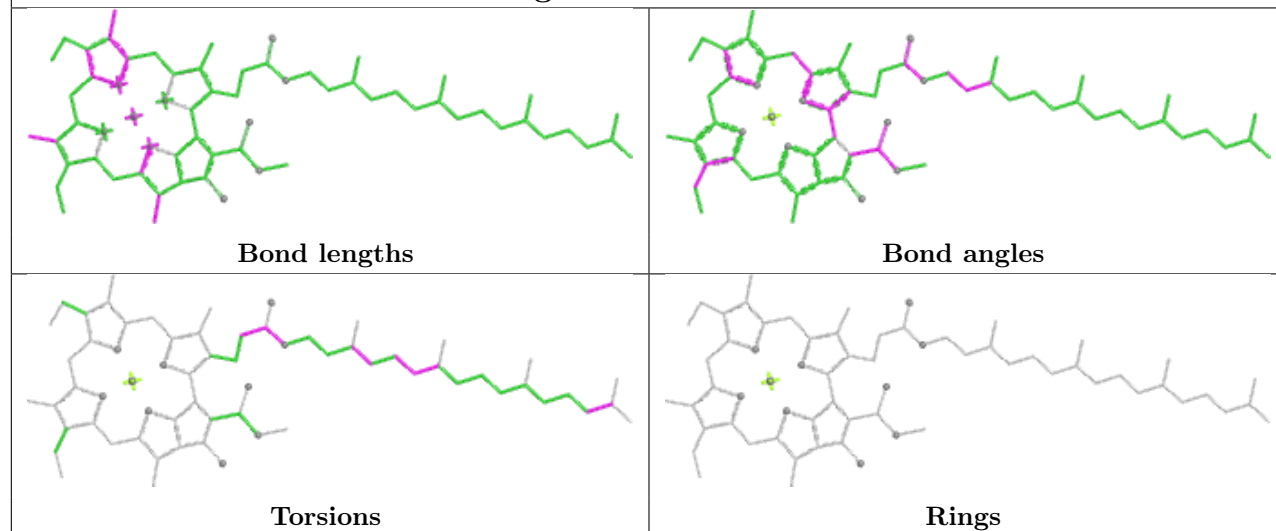




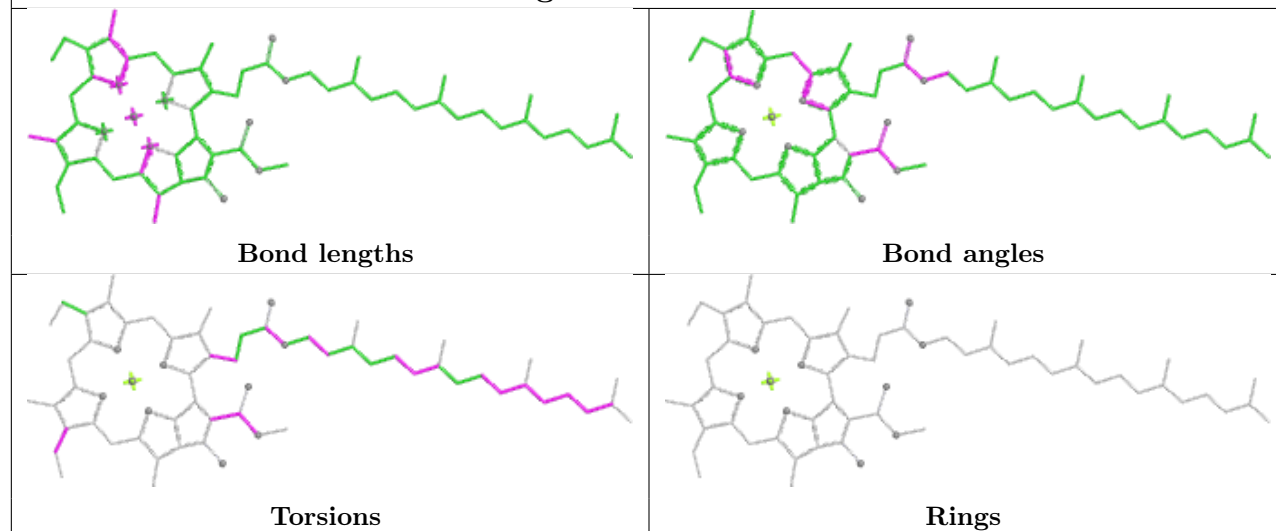




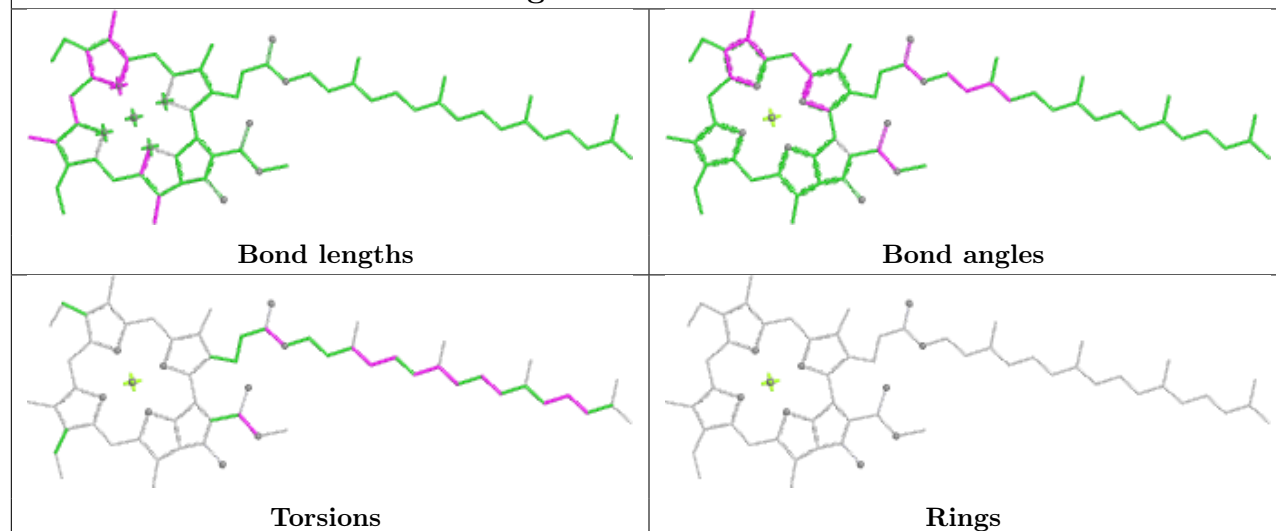
Ligand CLA L 201

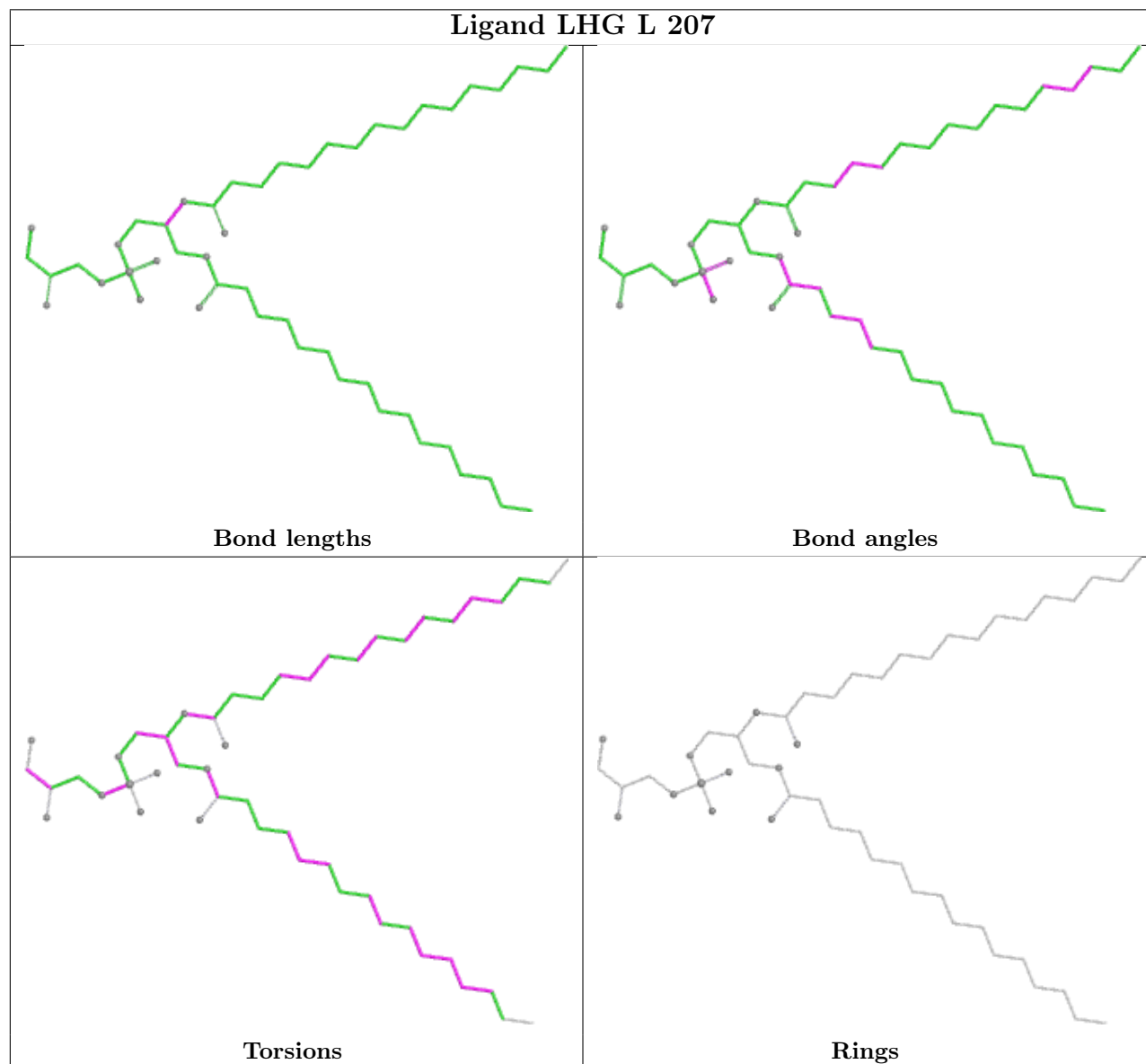
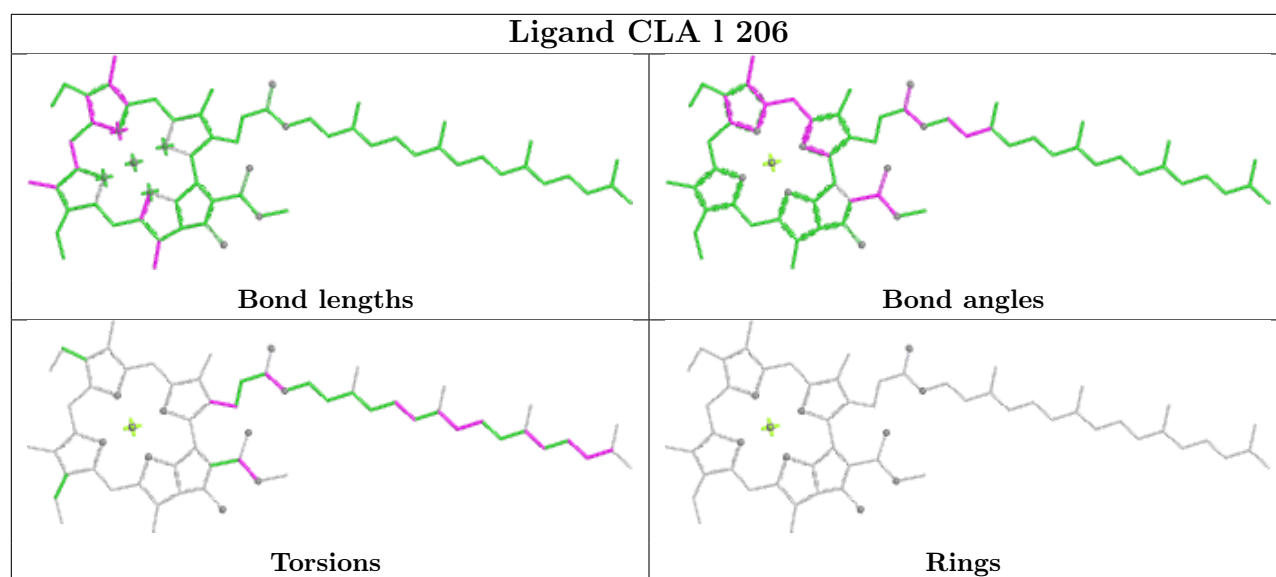


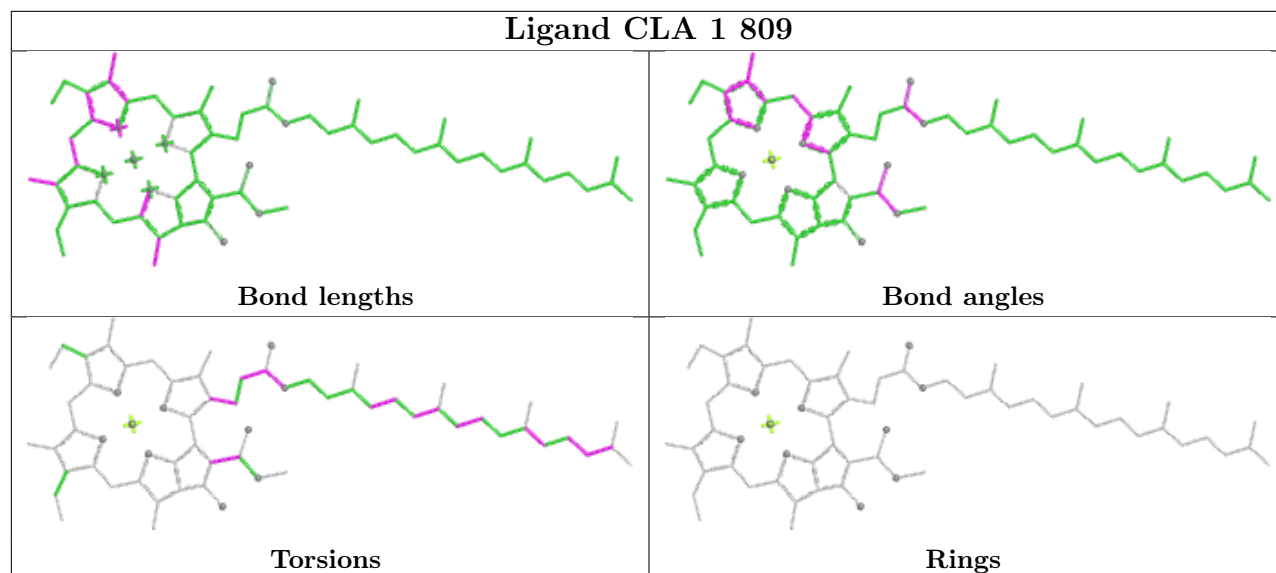
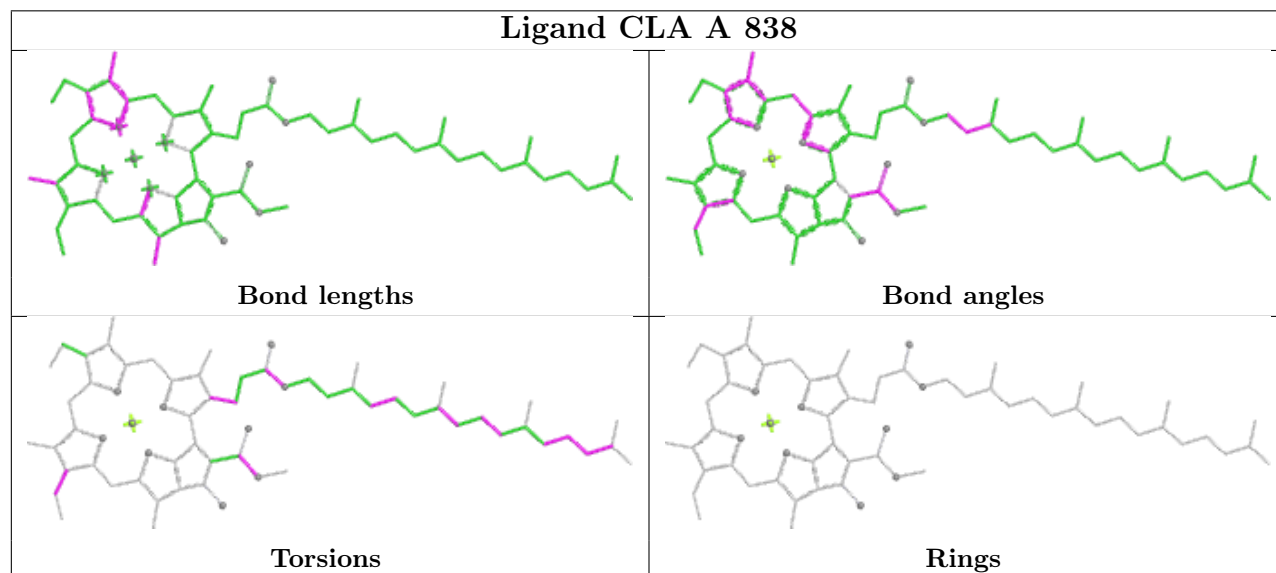
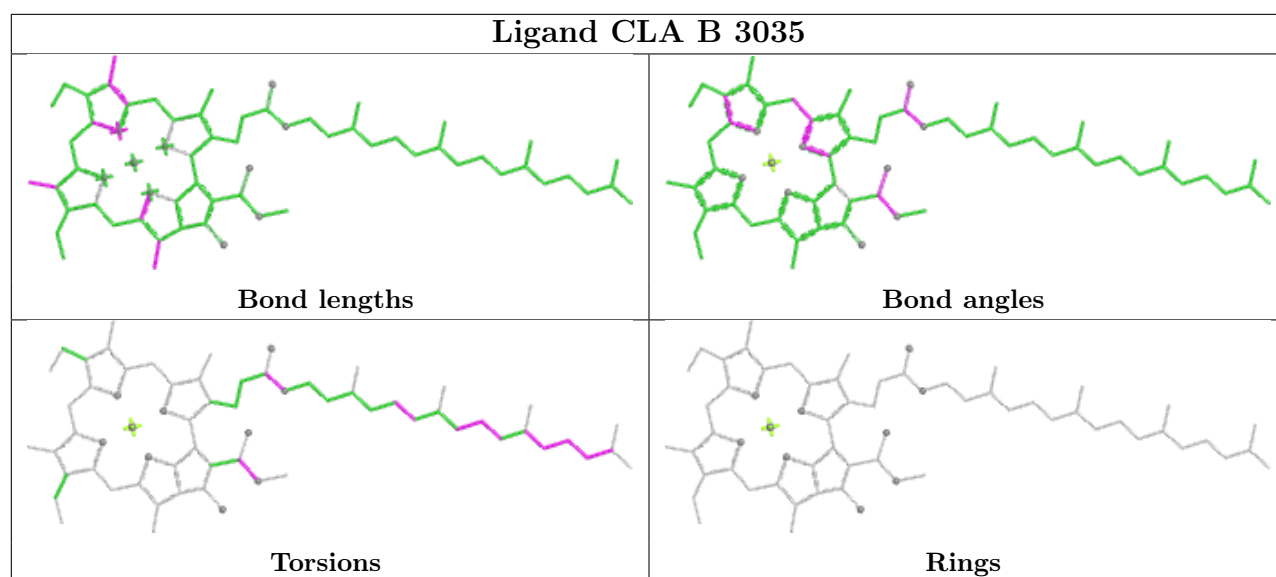
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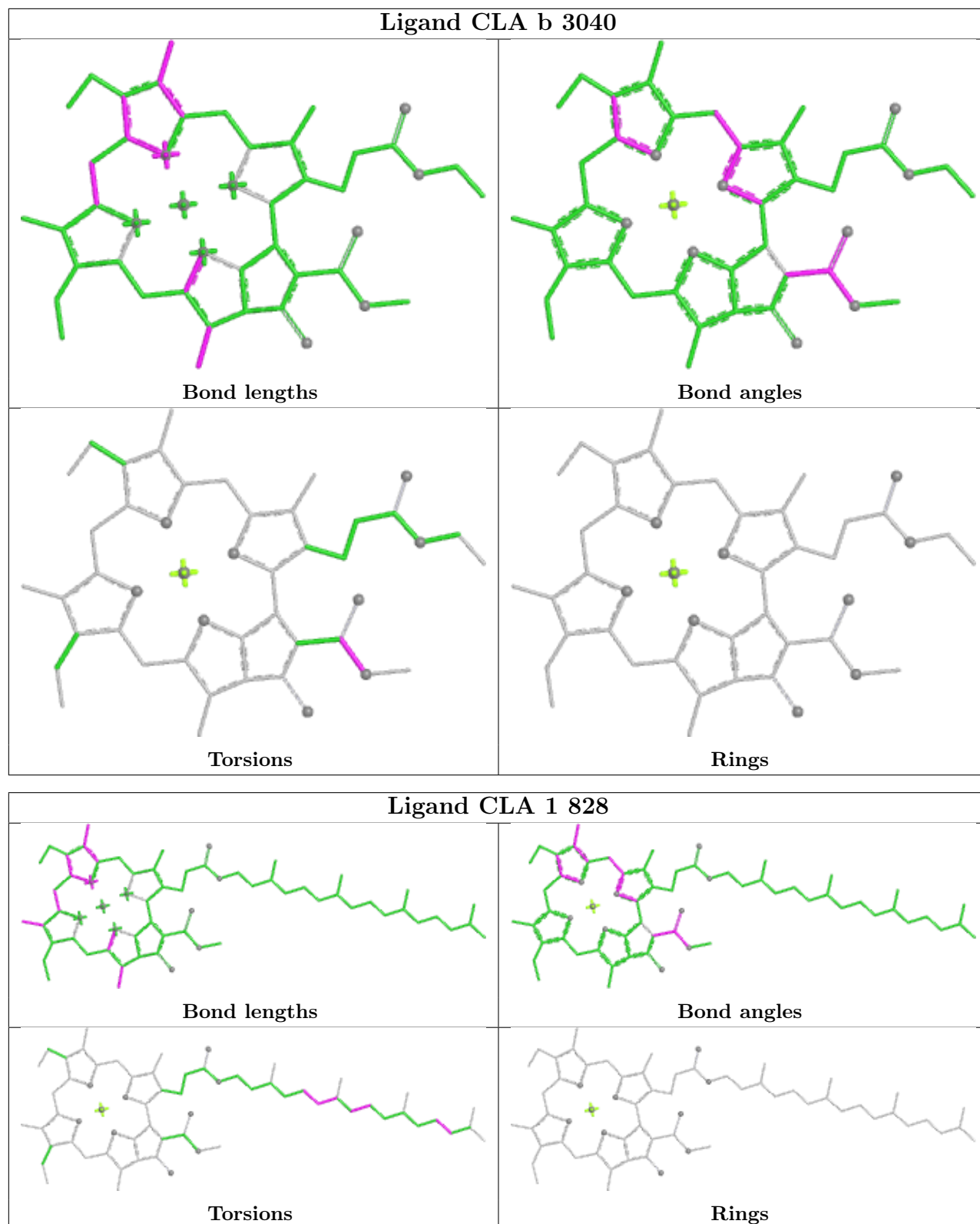


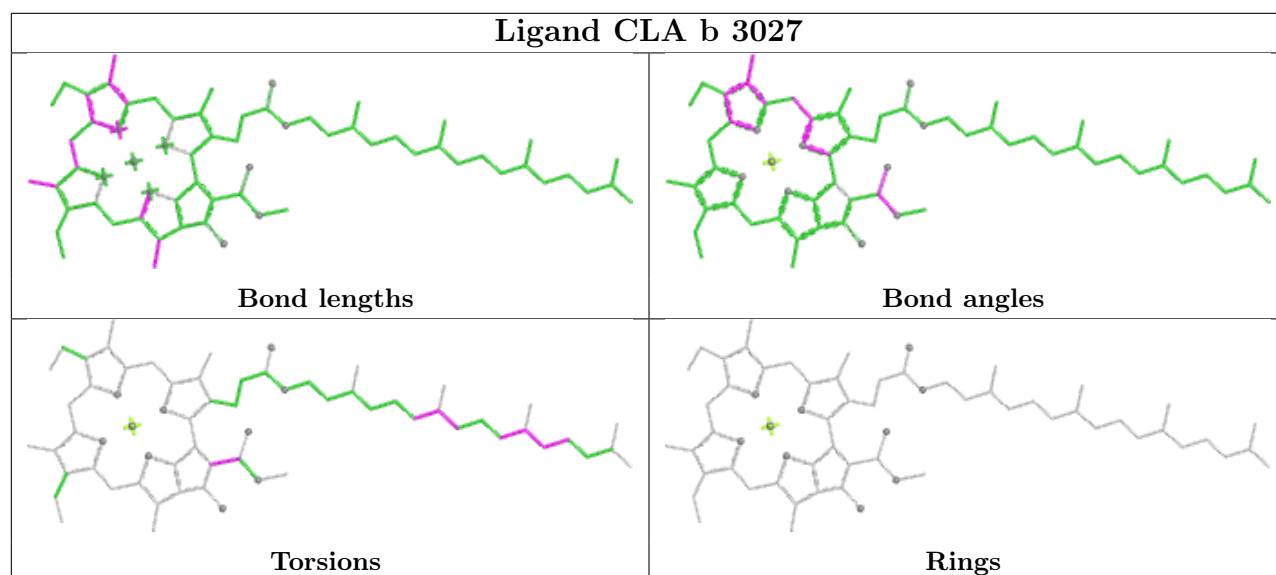
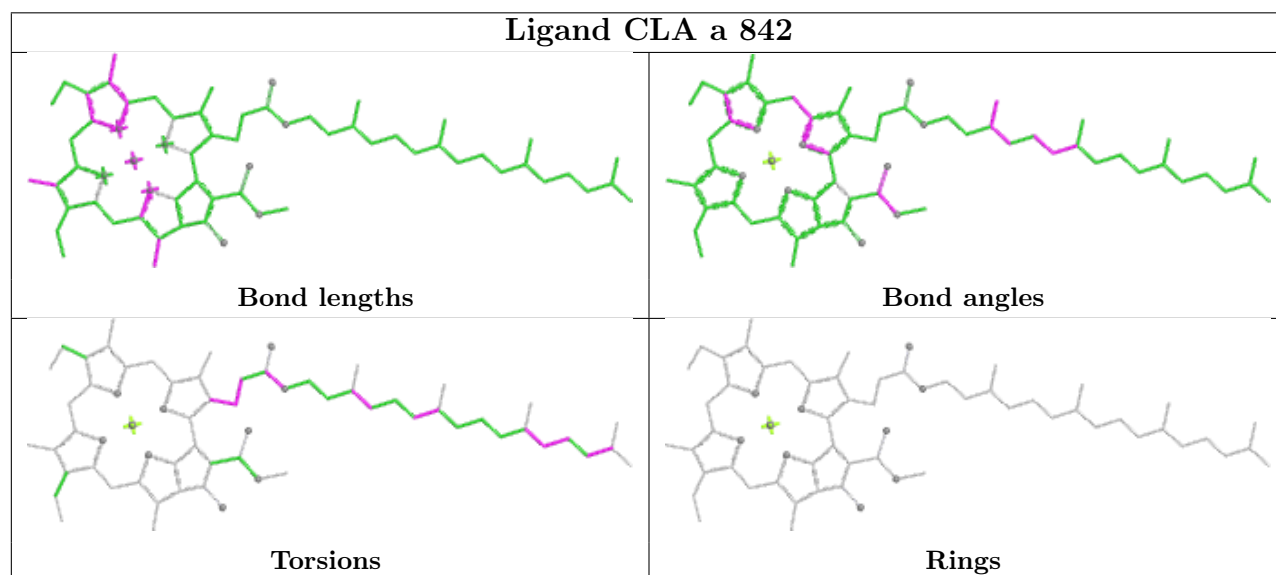
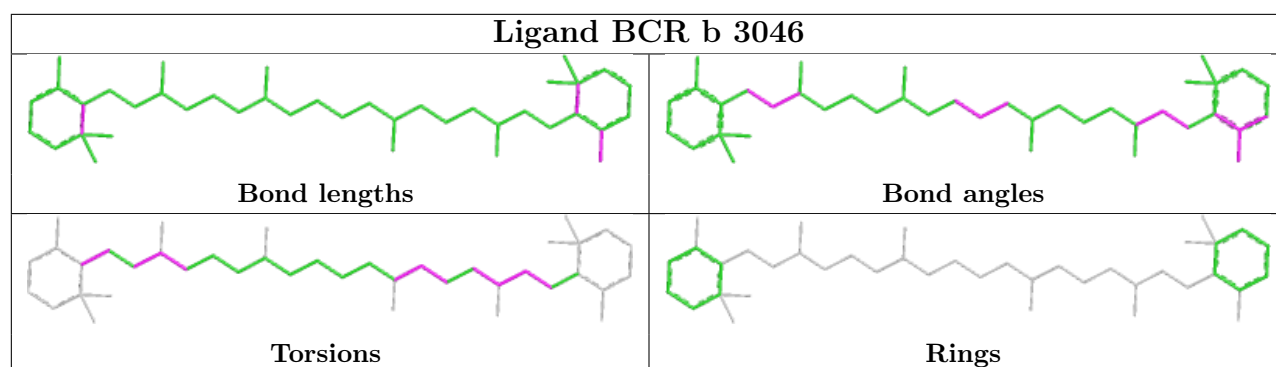
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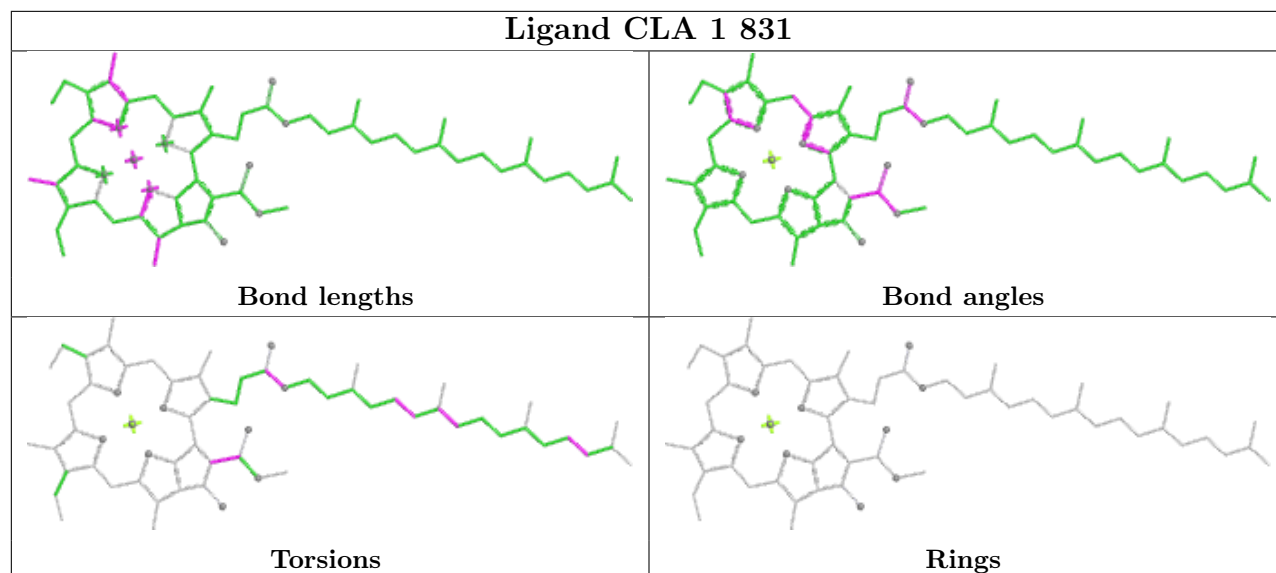
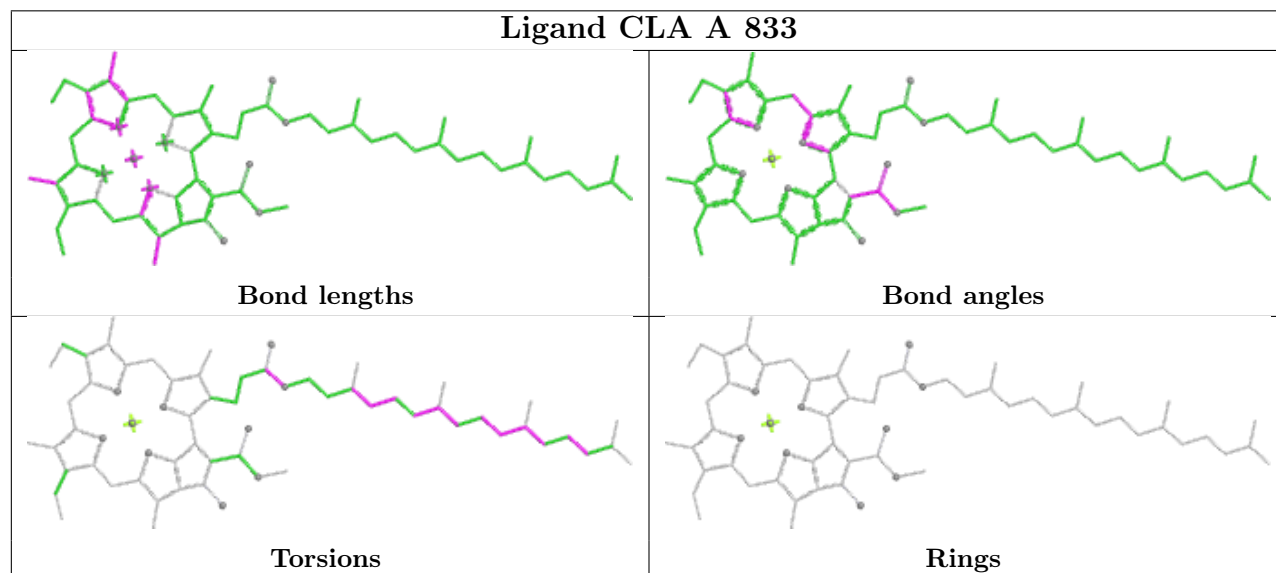
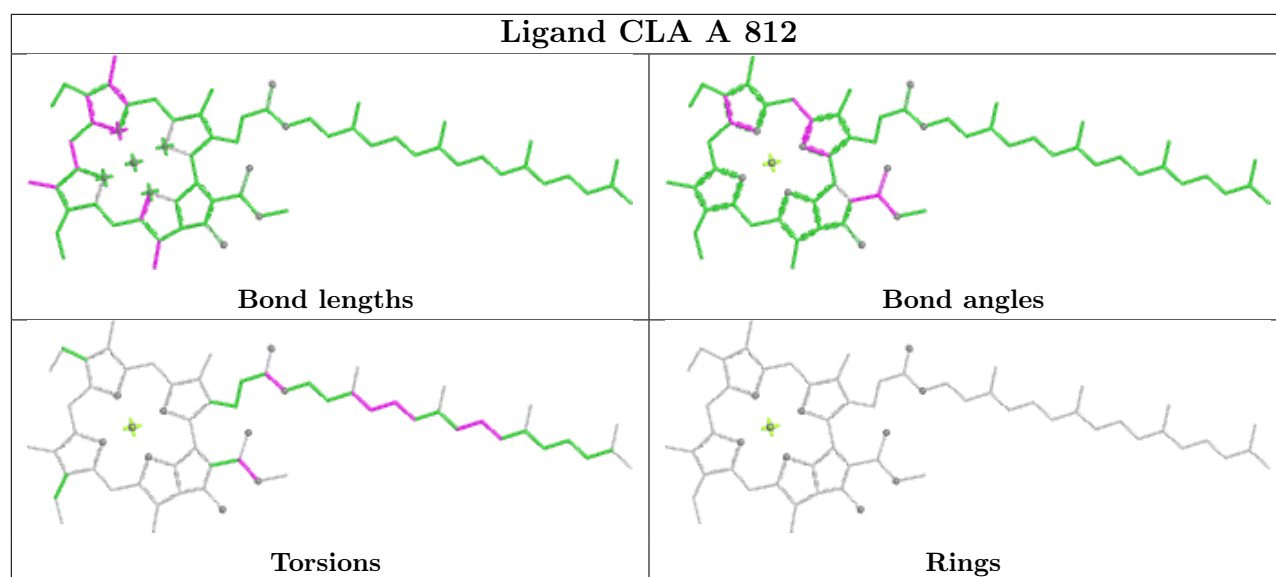




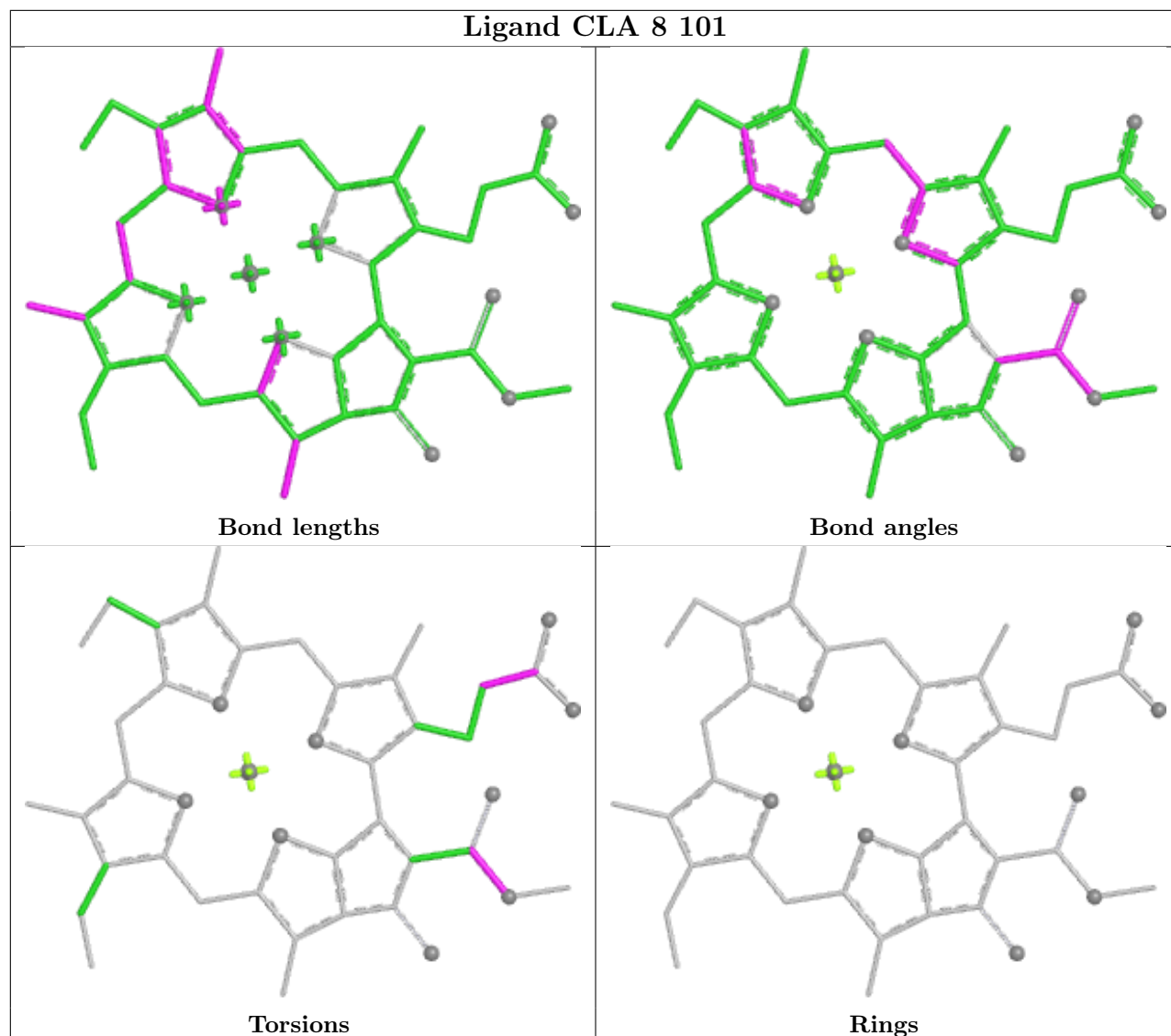




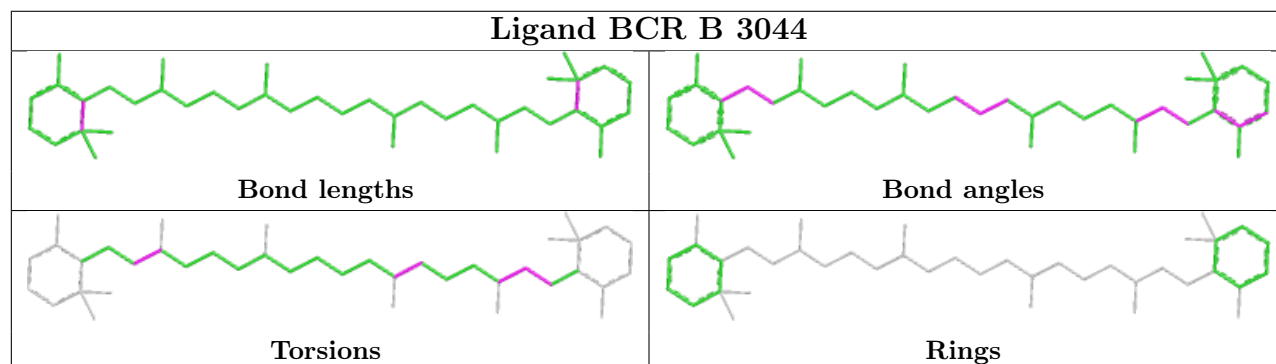




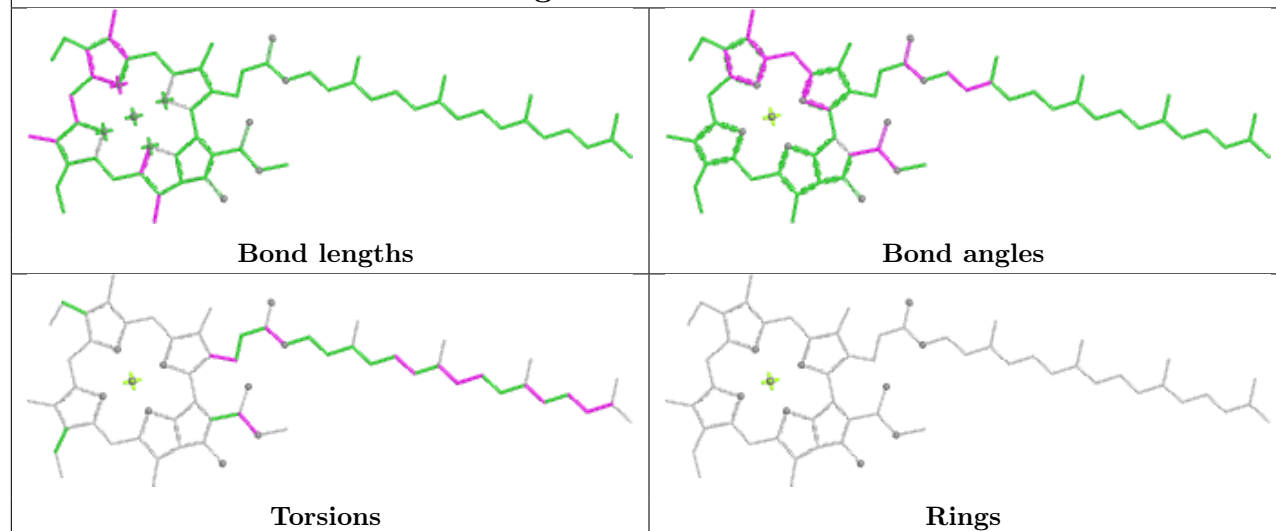
Ligand CLA 8 101



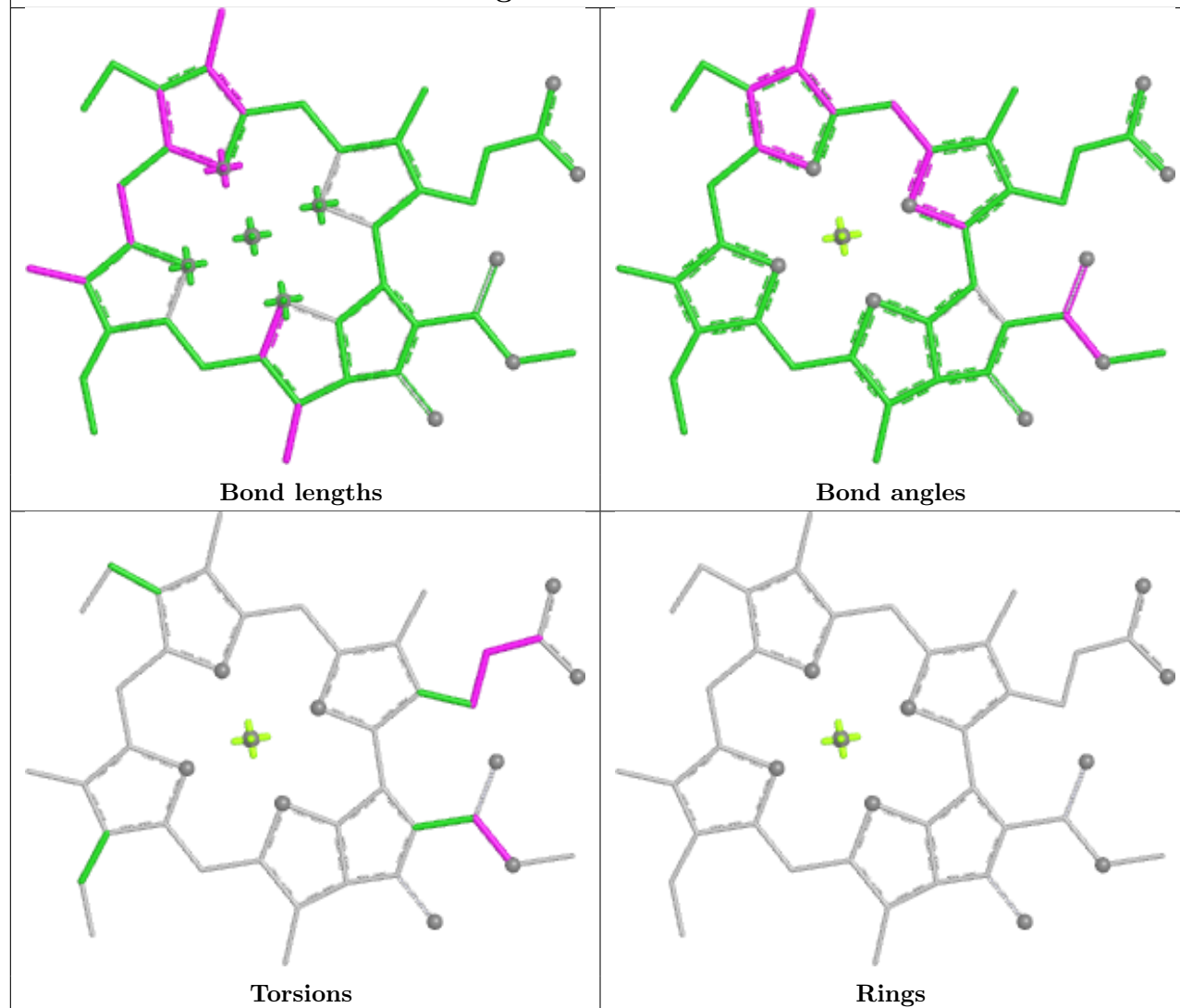
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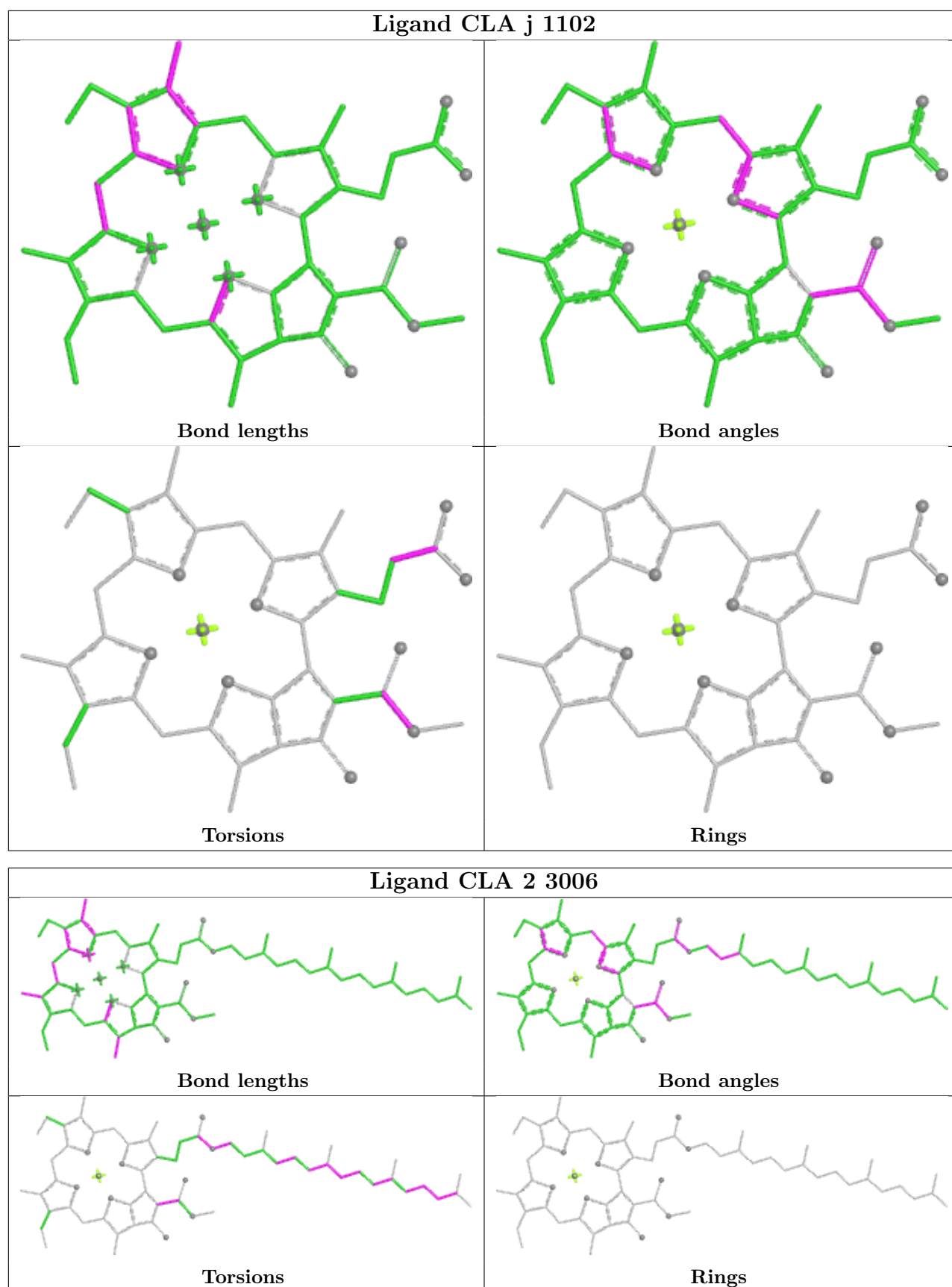


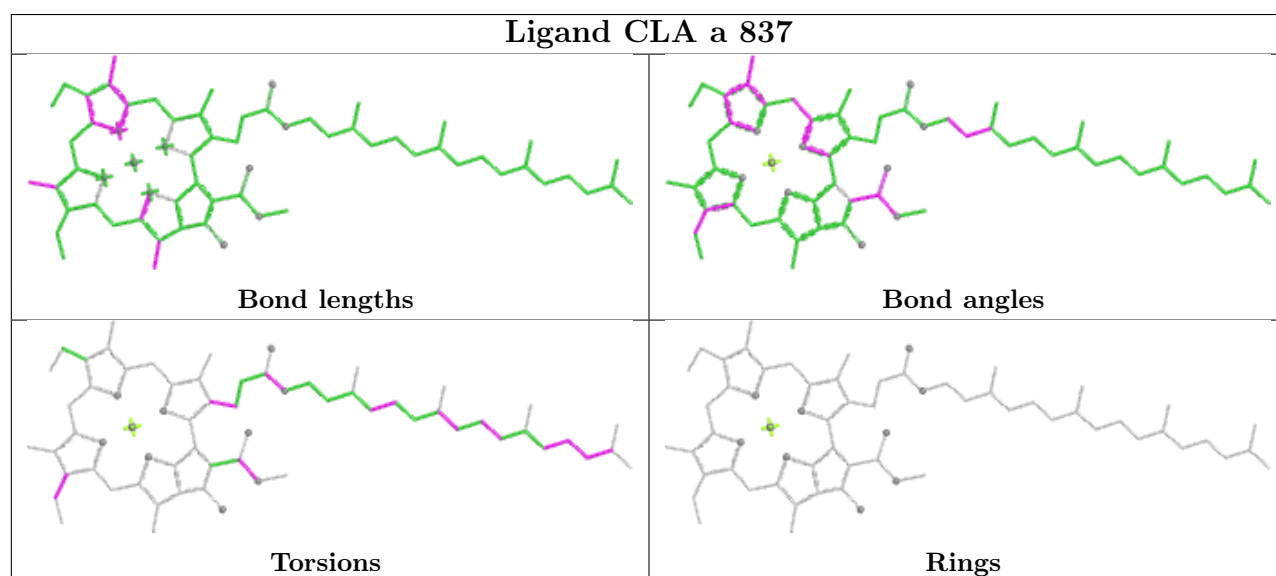
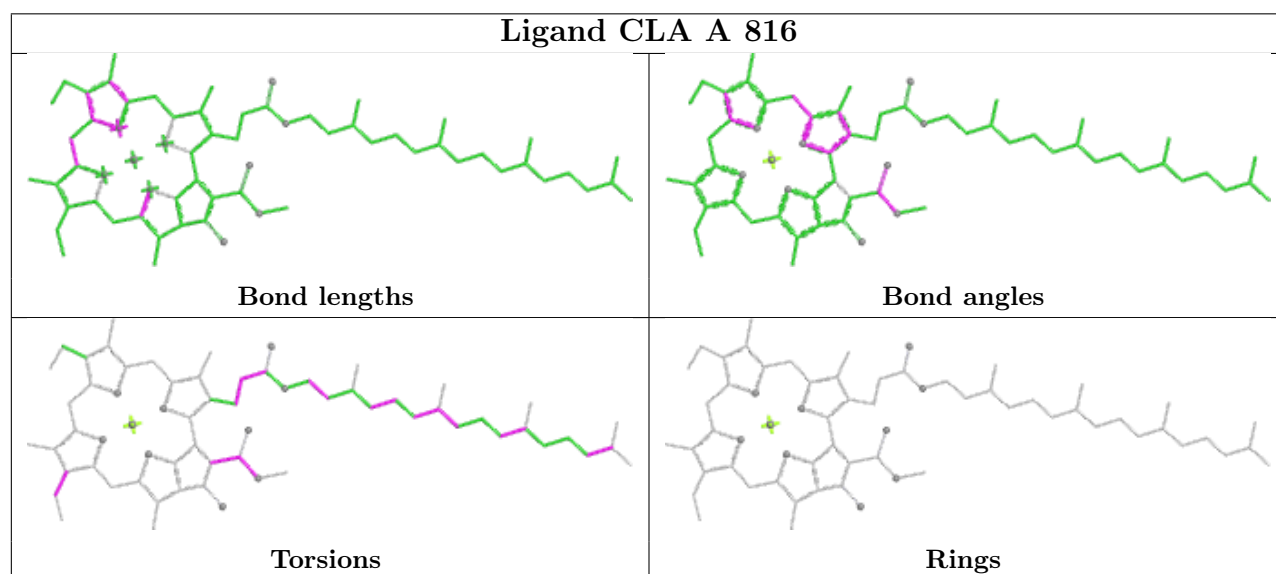
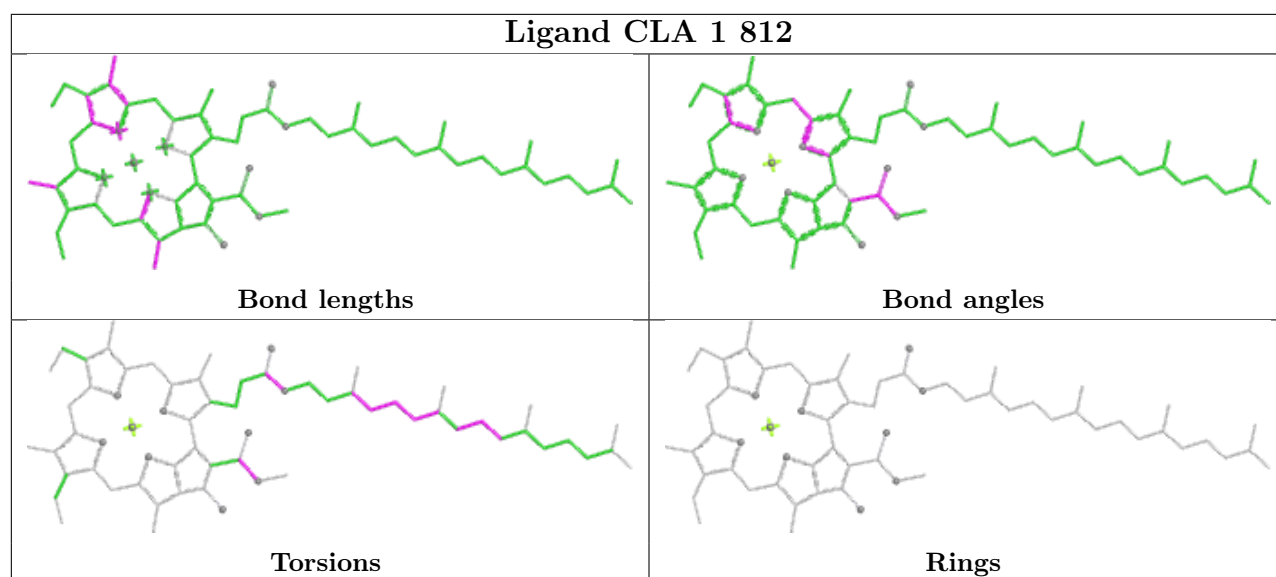
Ligand CLA L 203

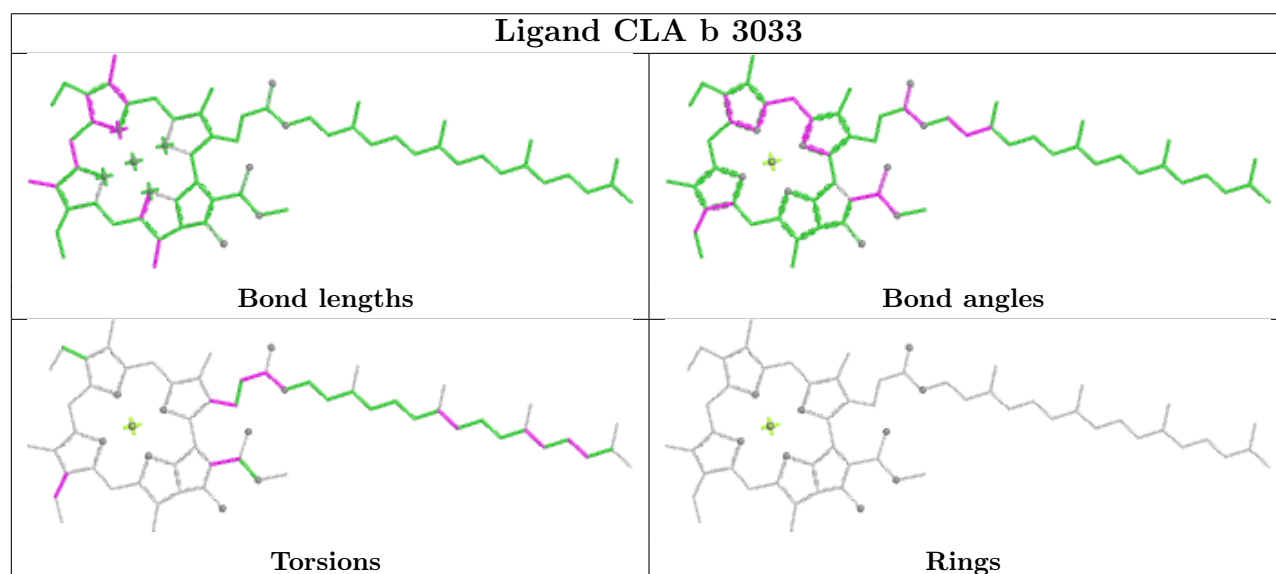
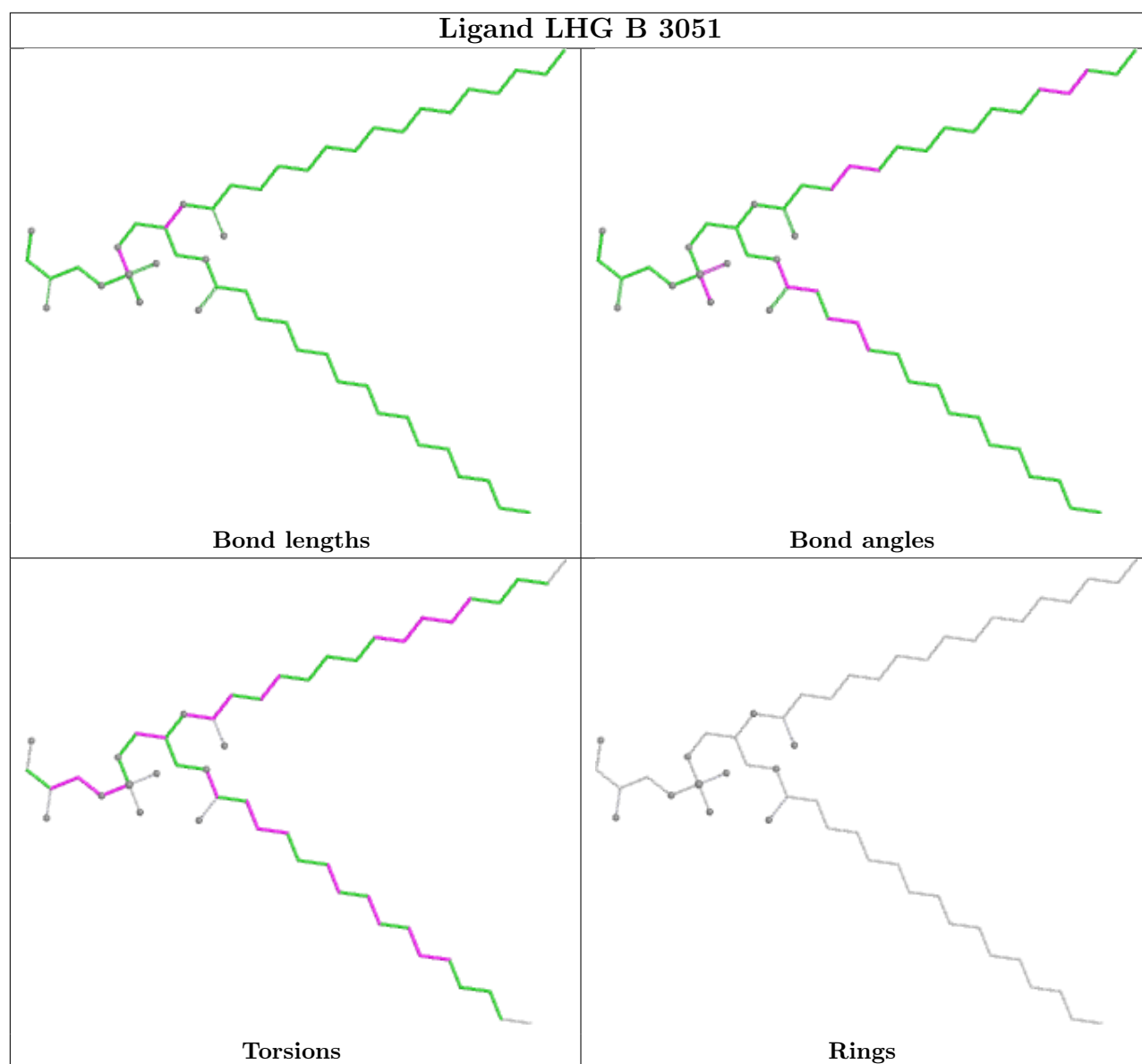


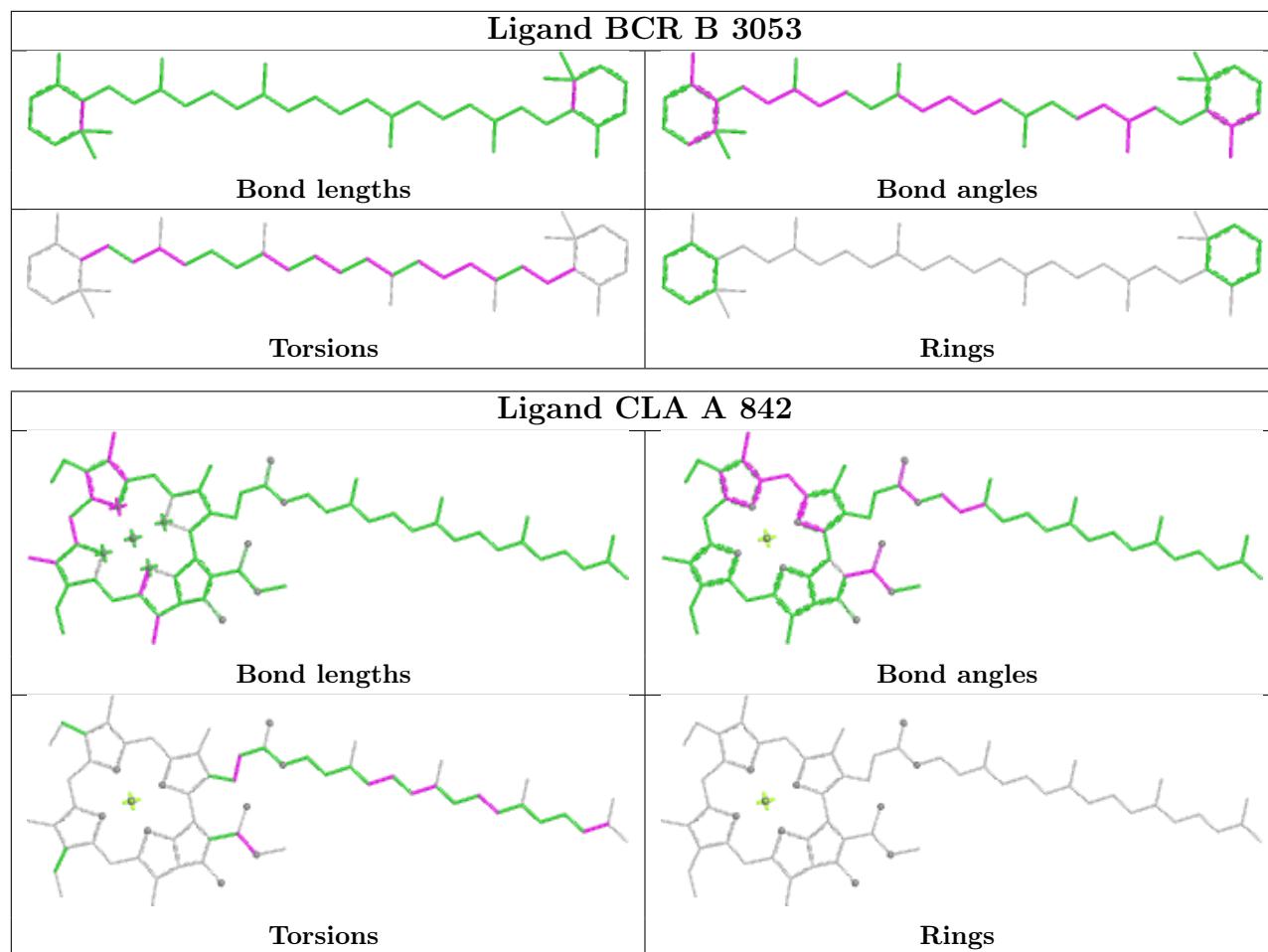
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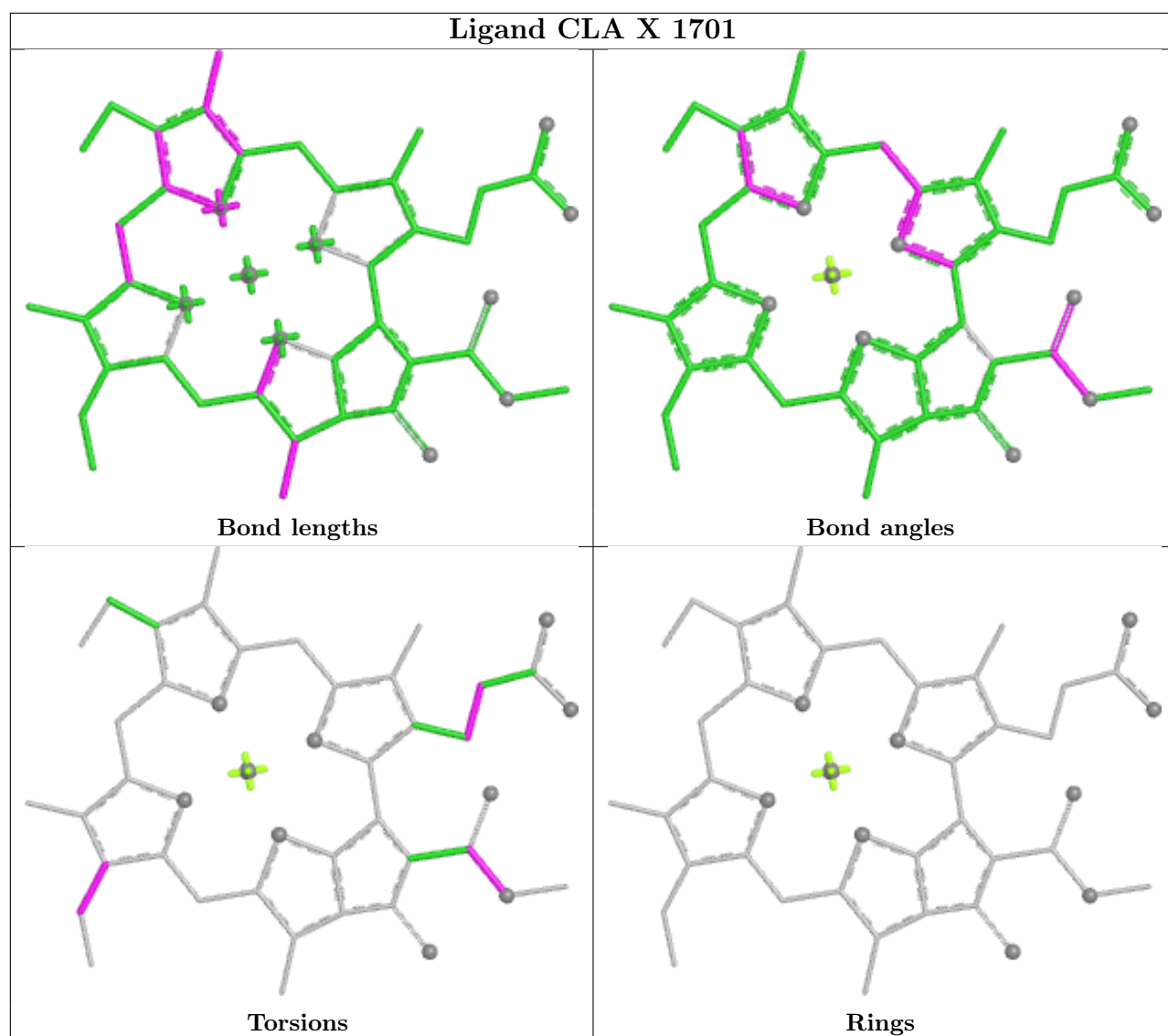


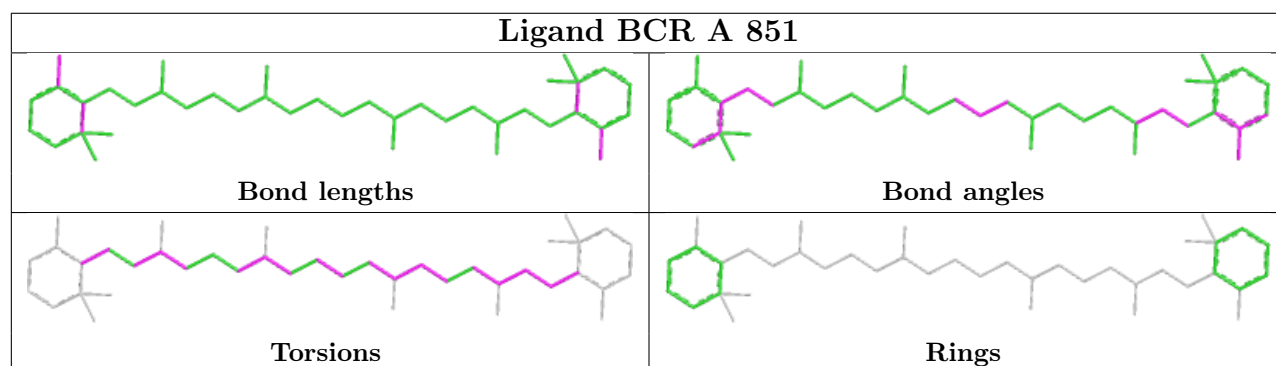
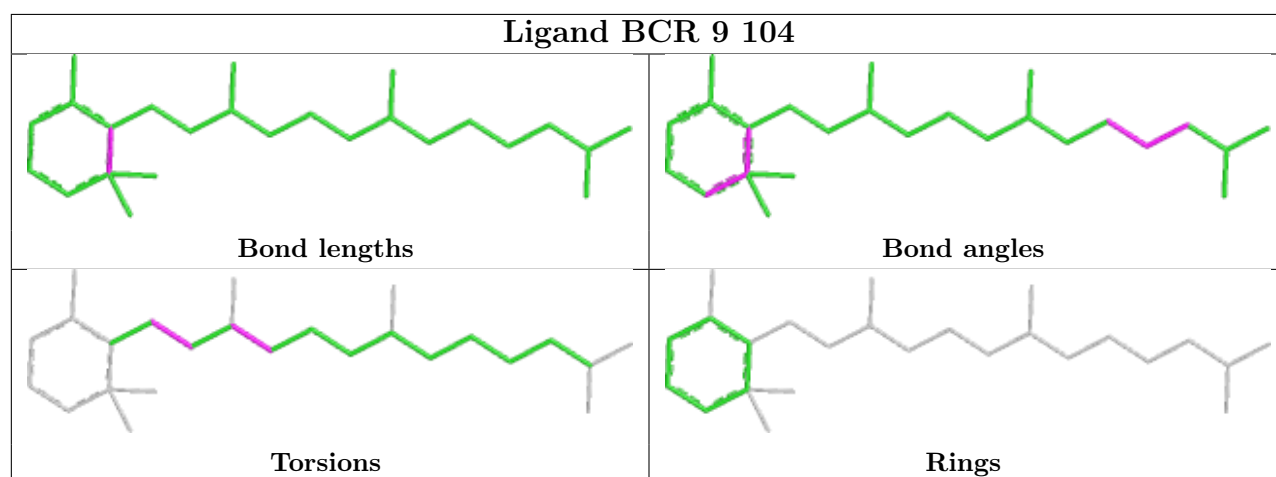
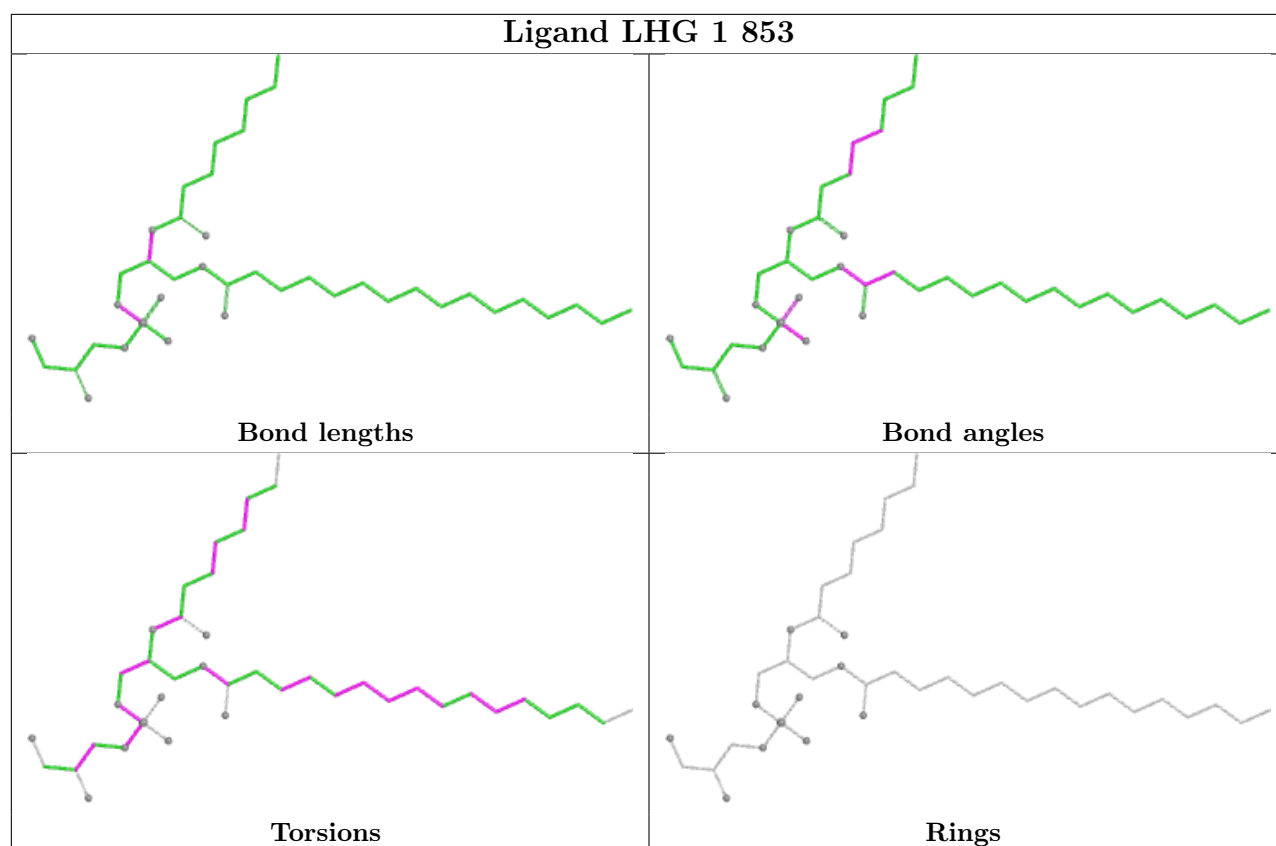


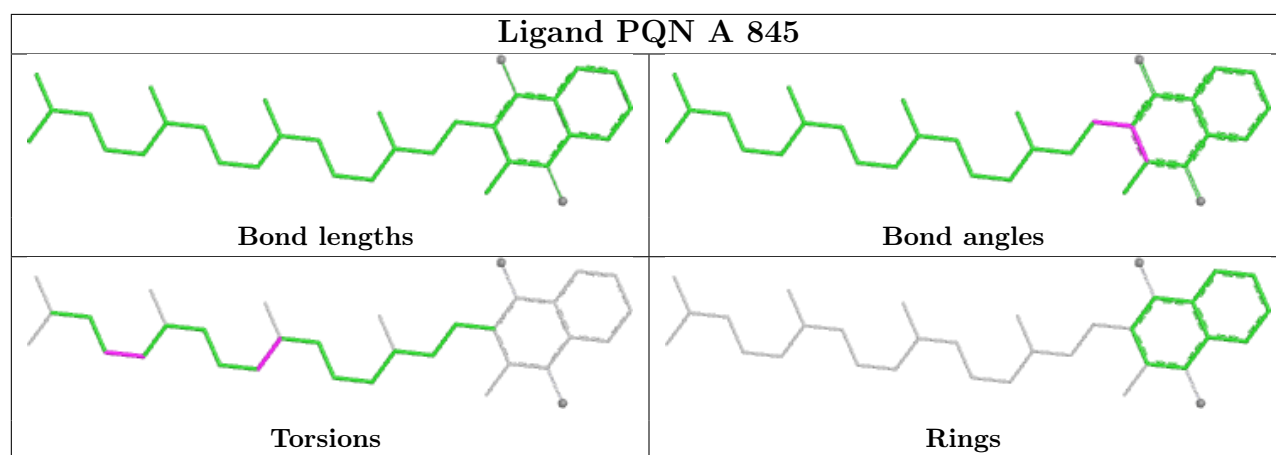
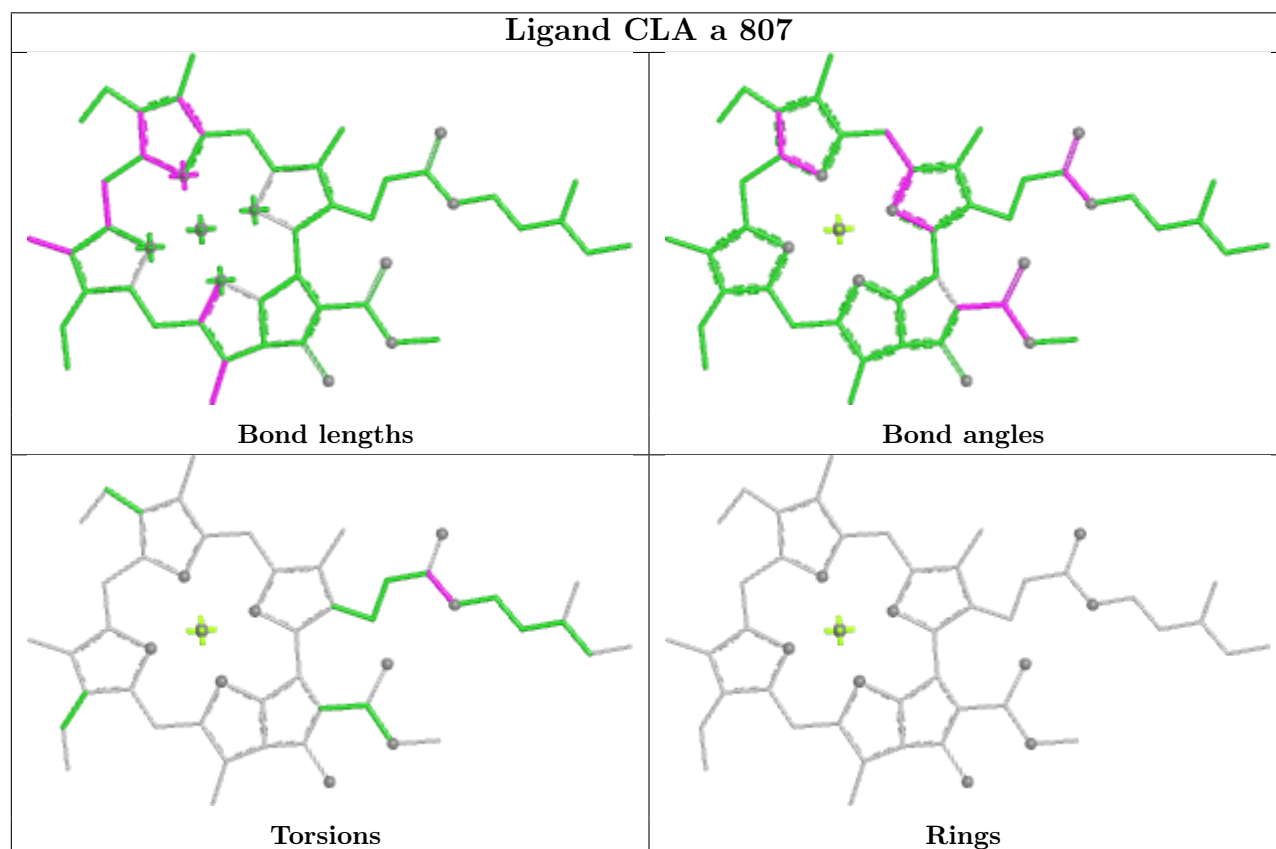
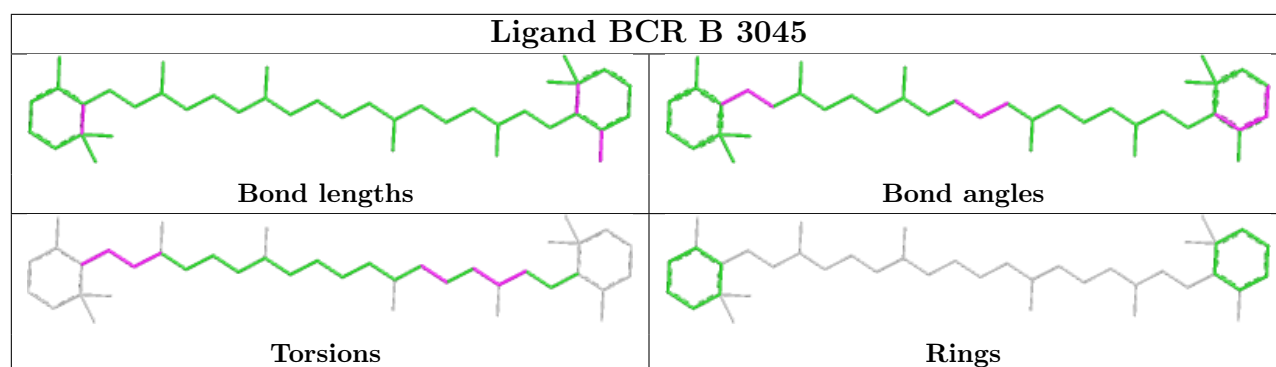


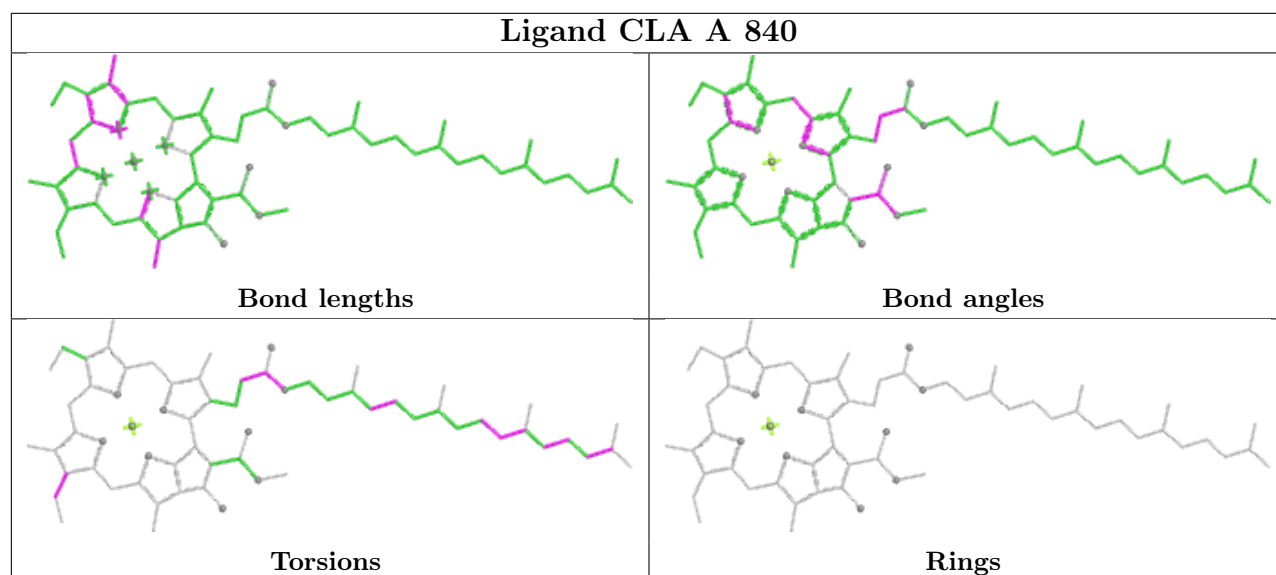
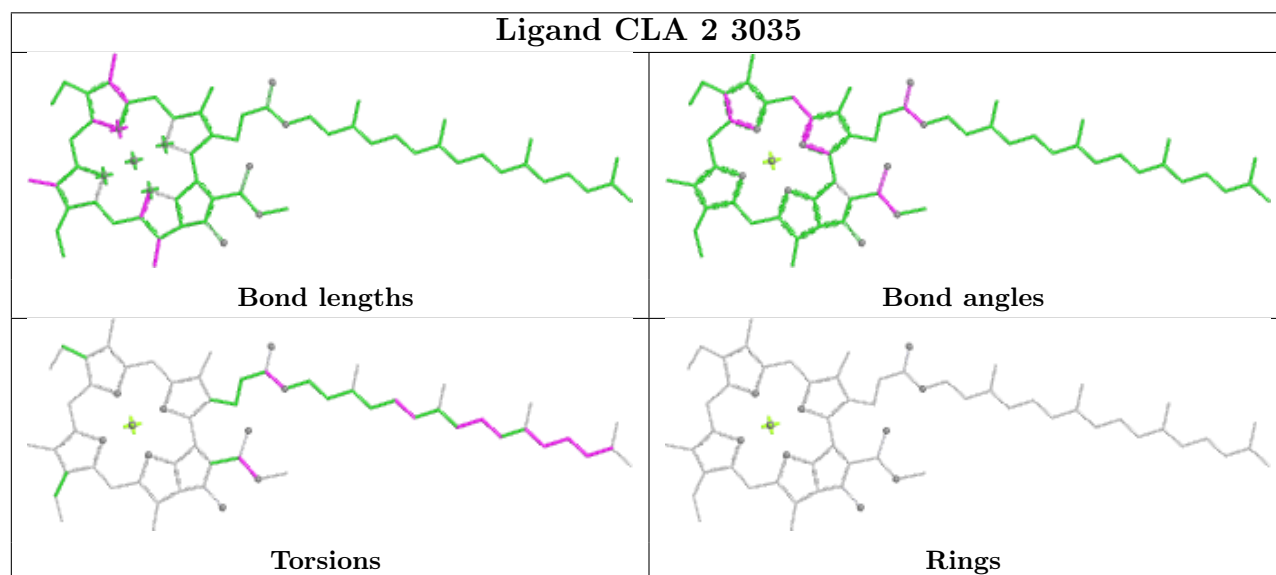
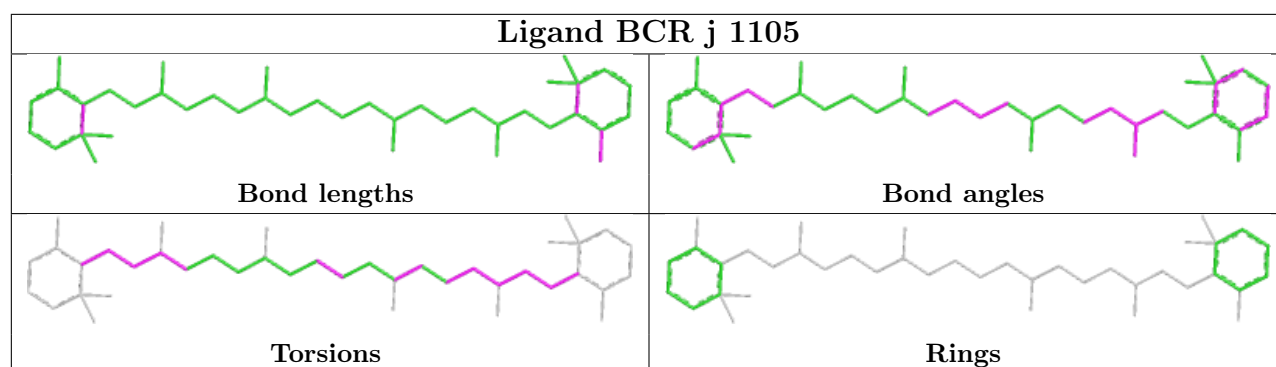


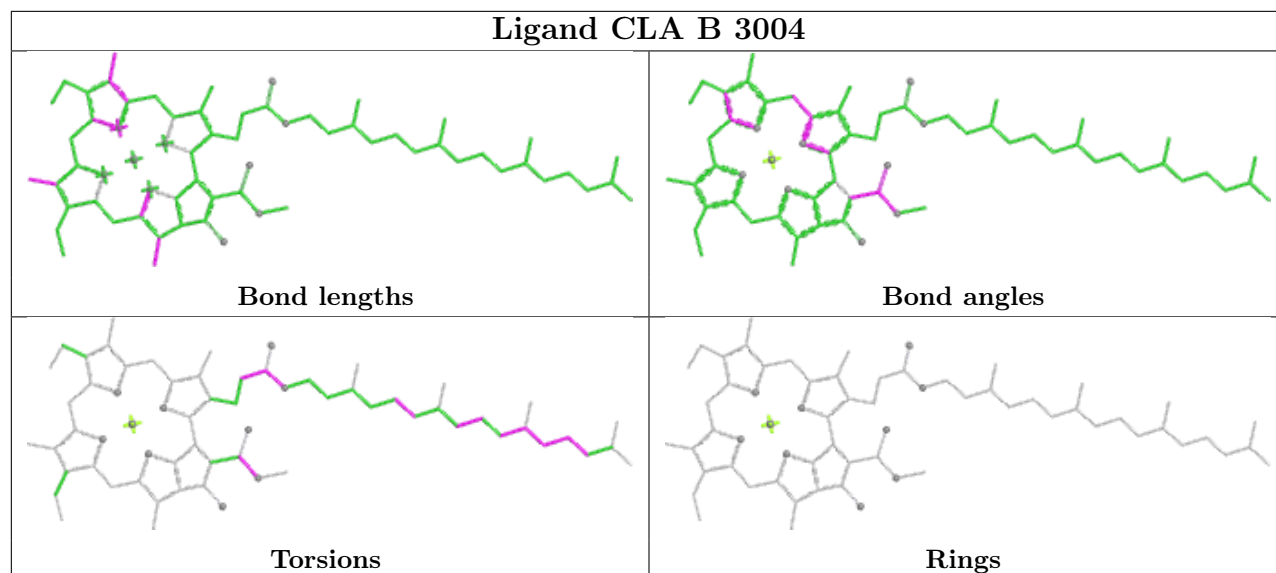
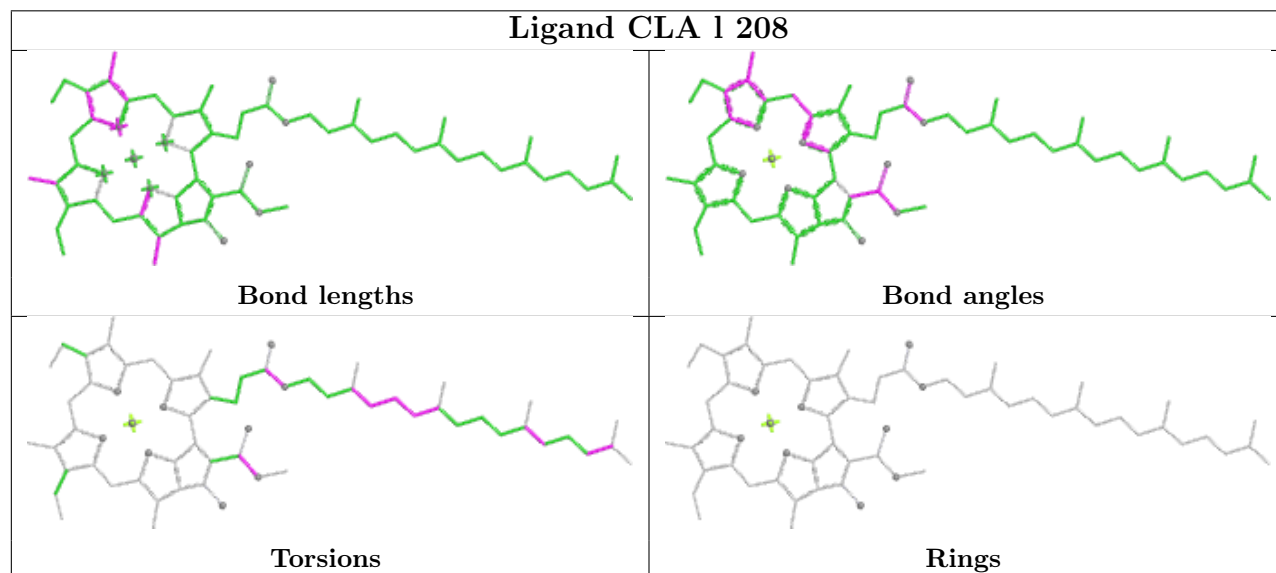
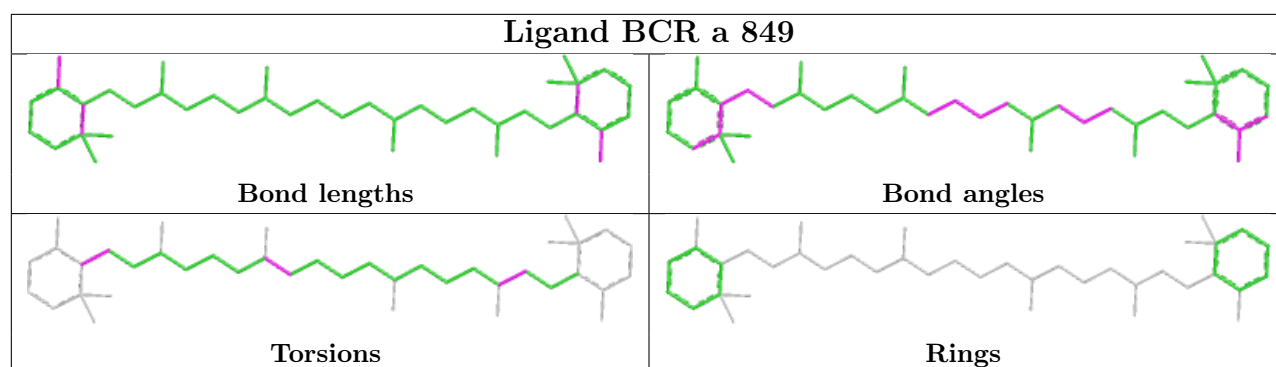


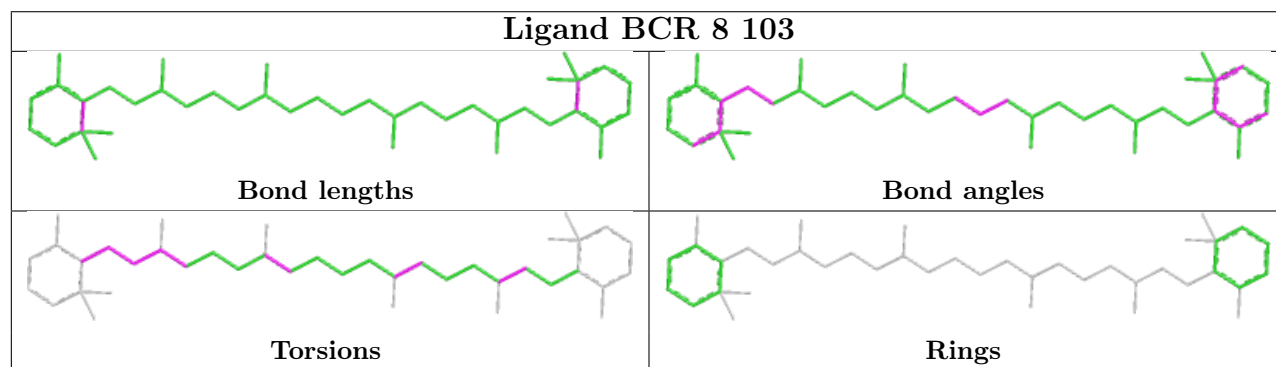
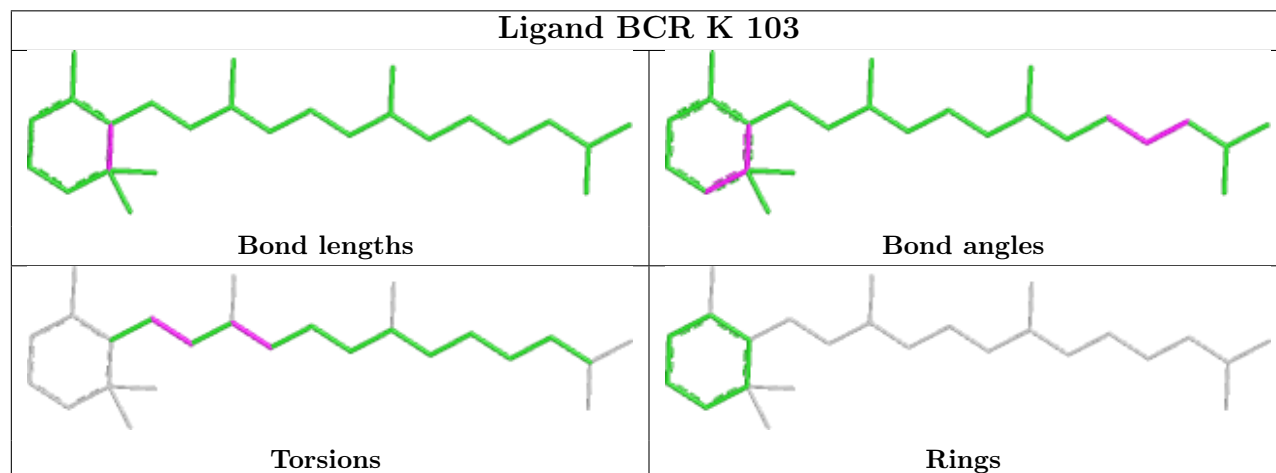
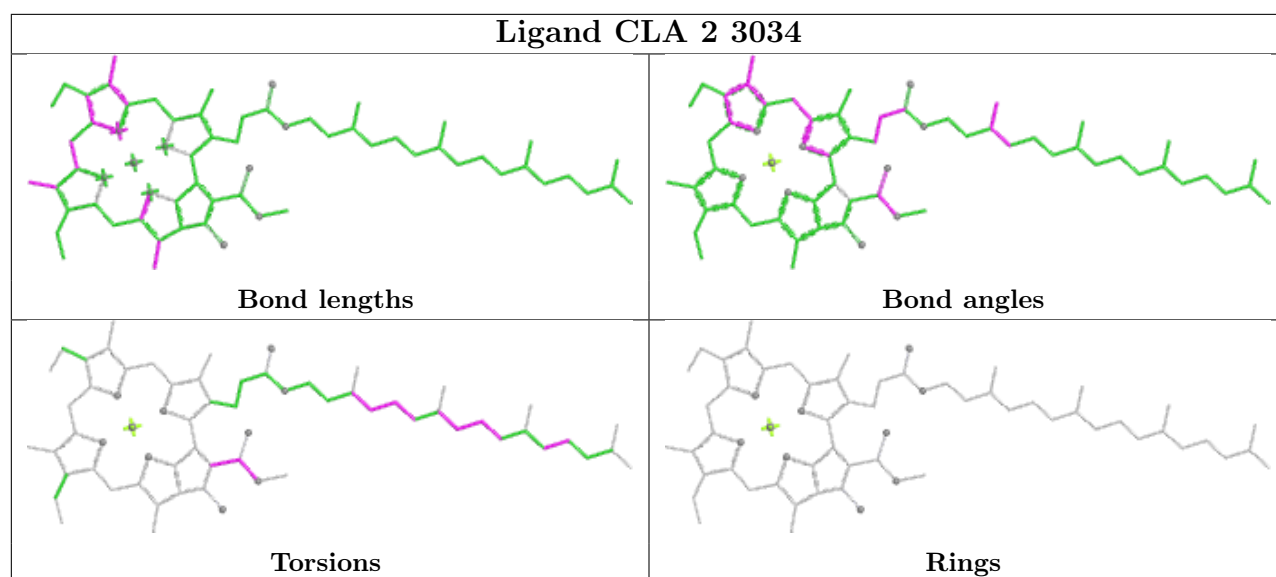


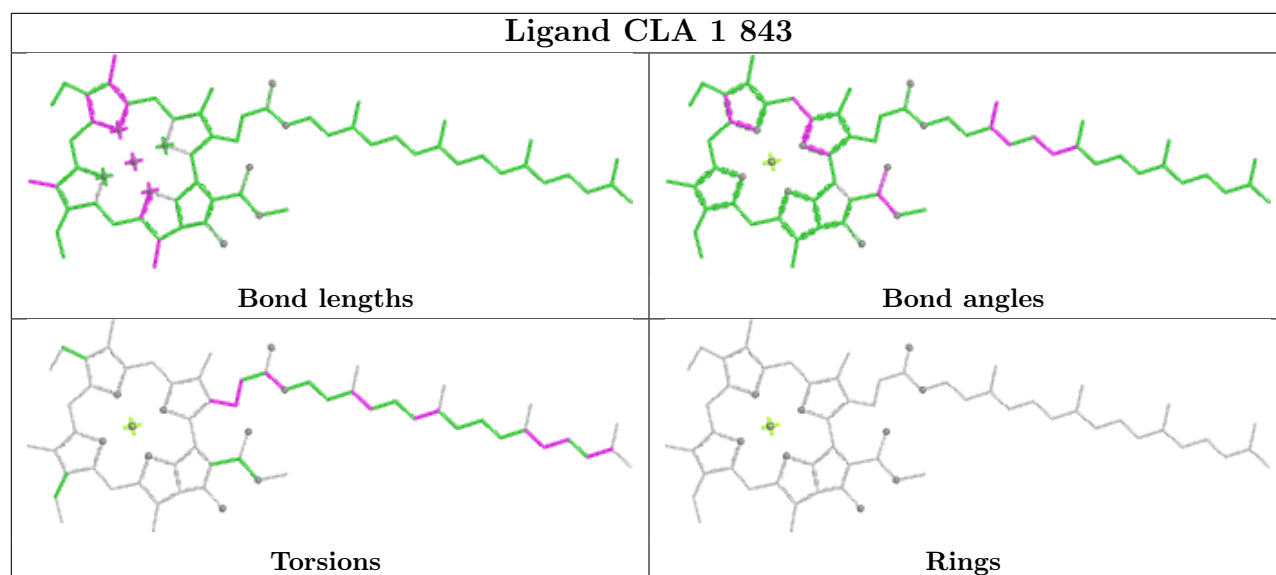
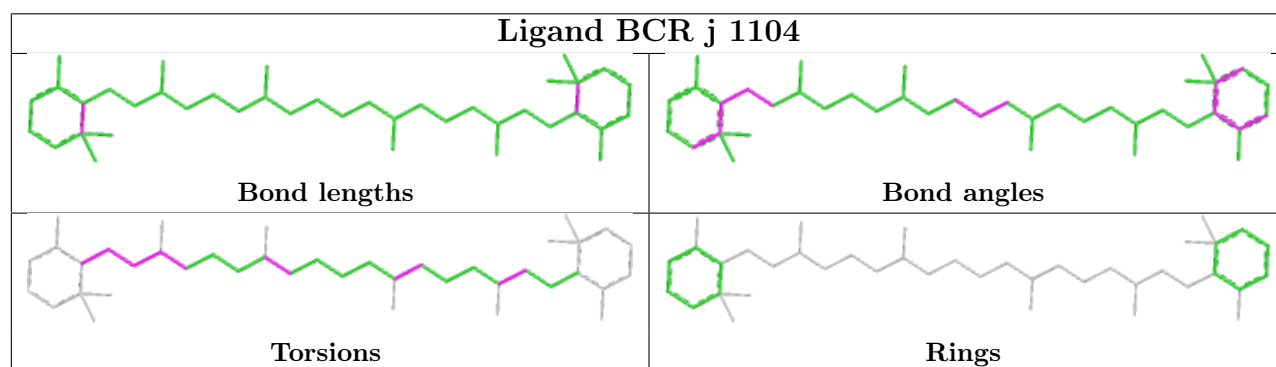
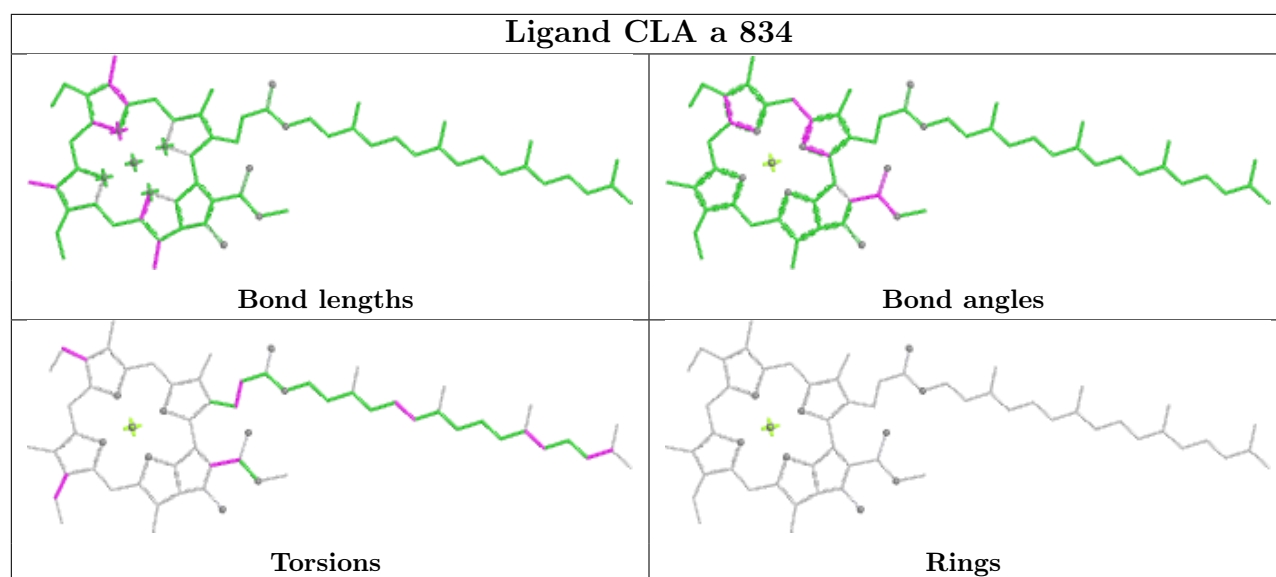


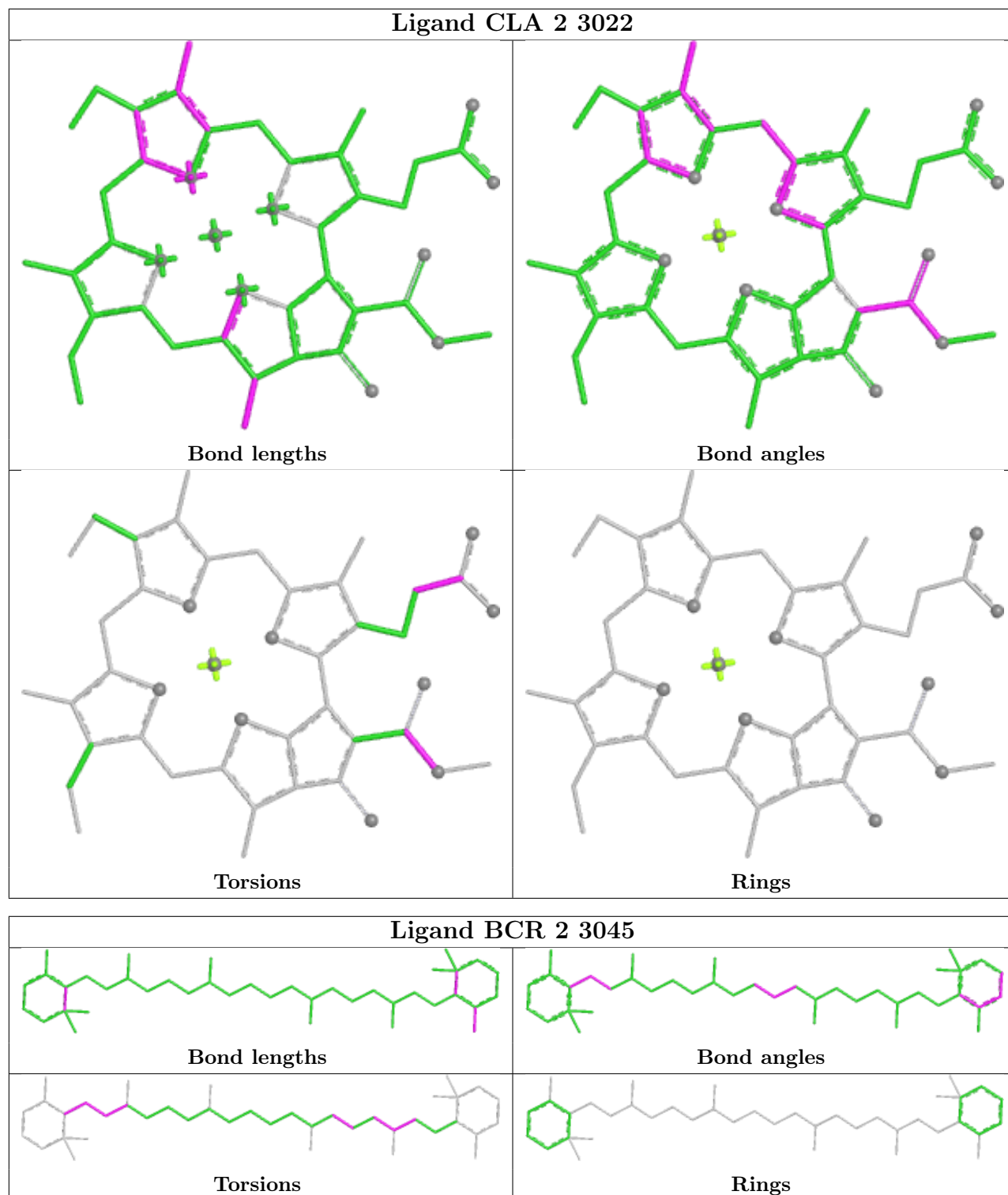


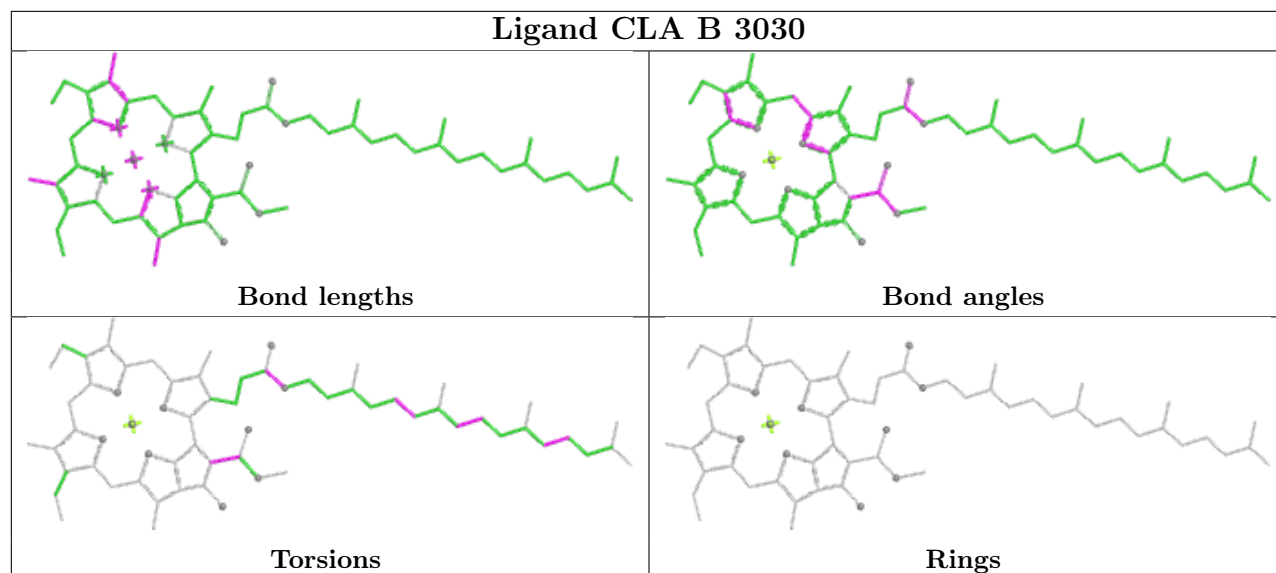
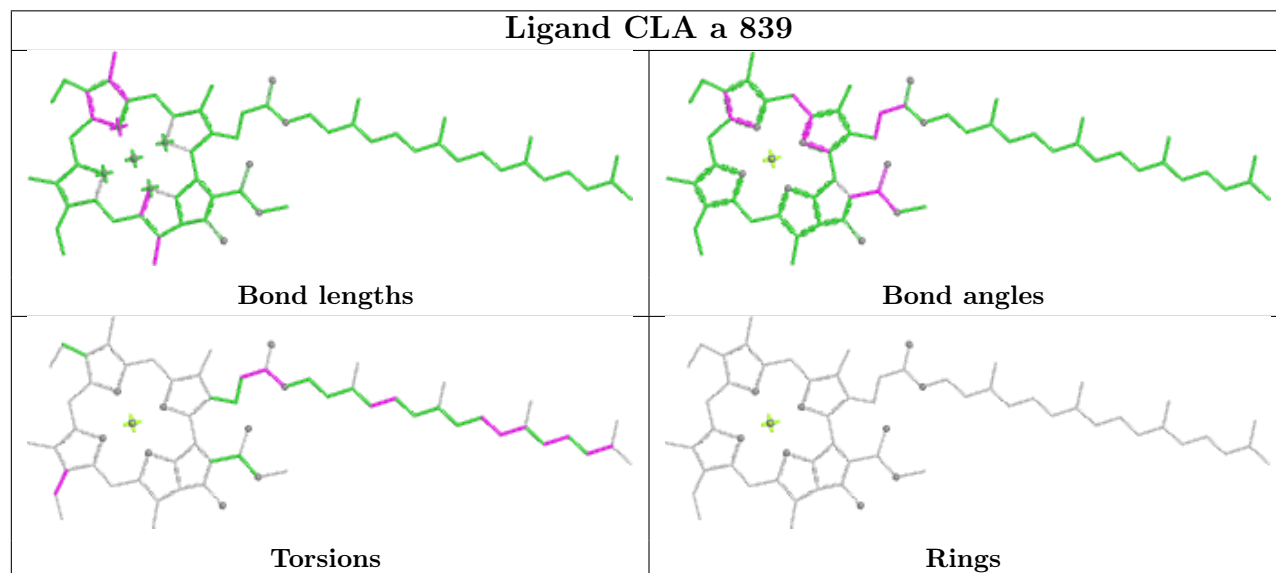
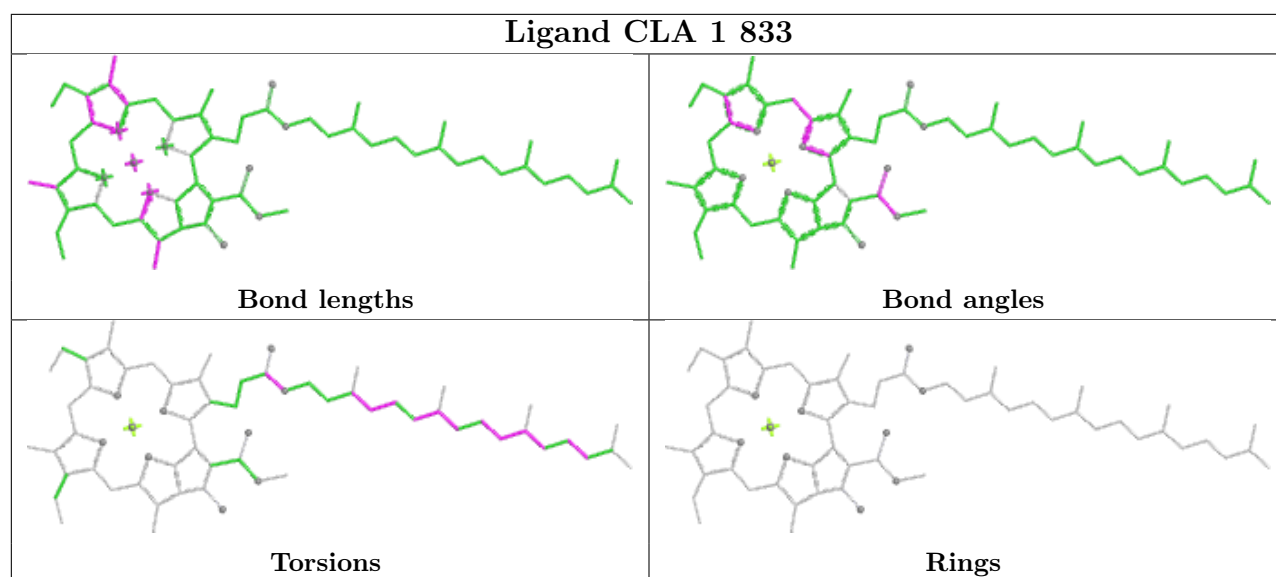


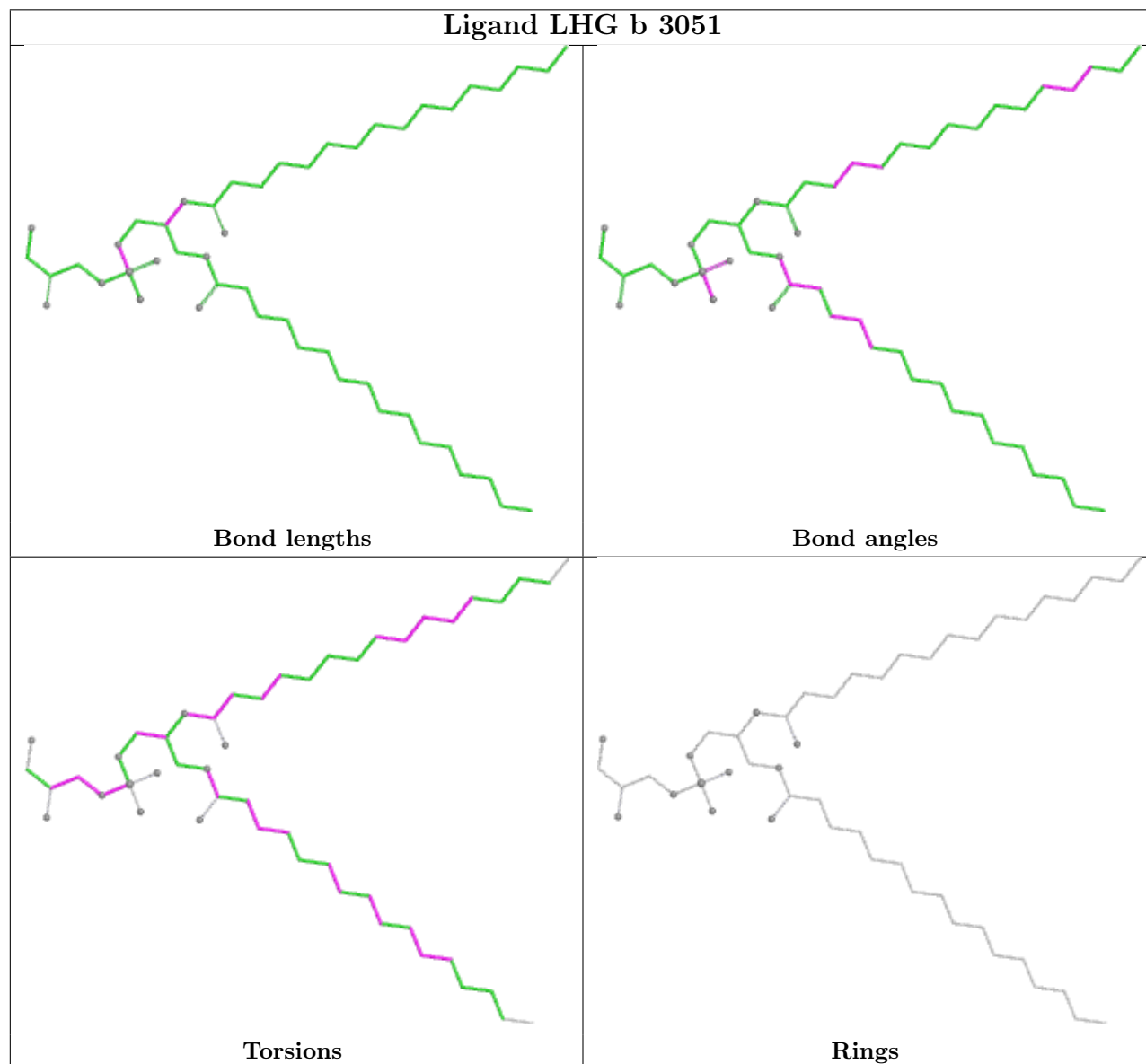
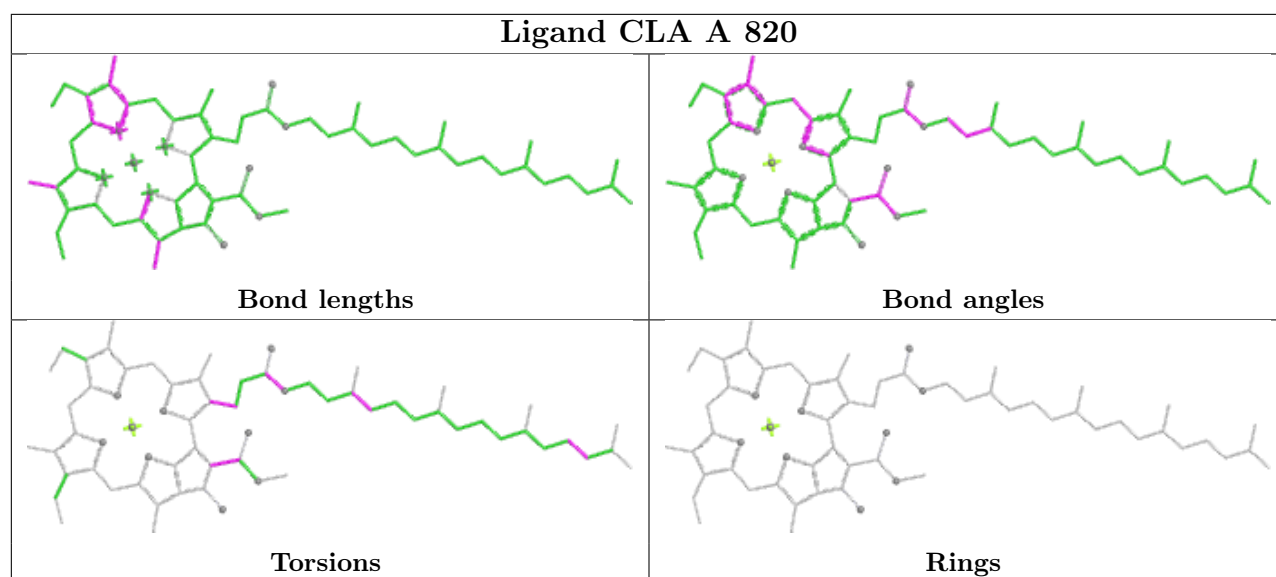


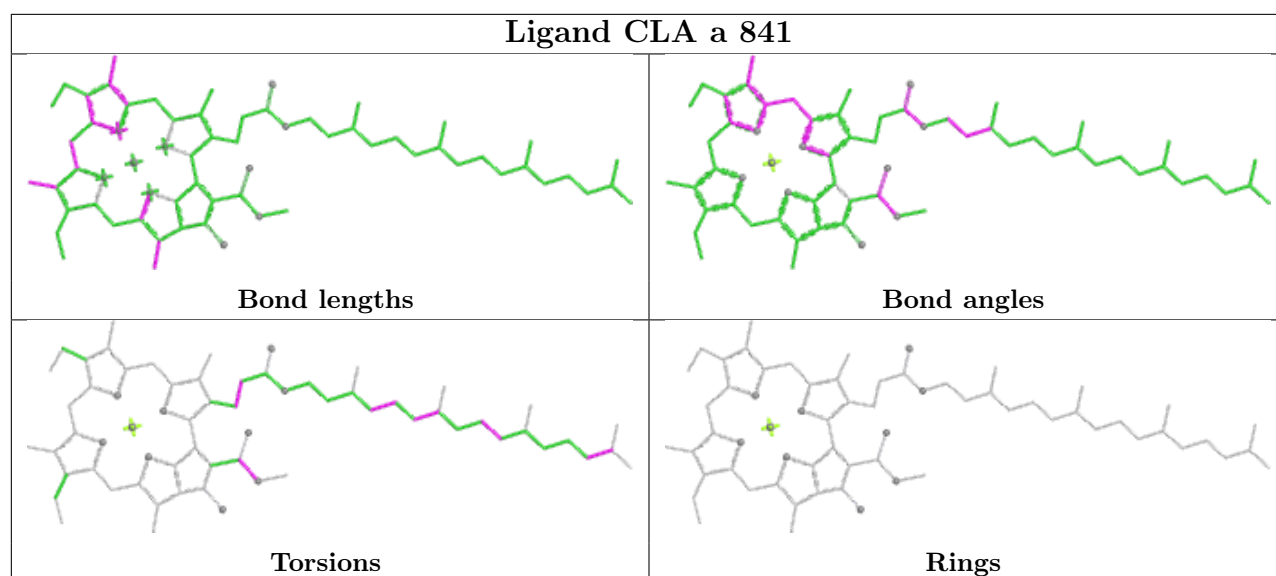
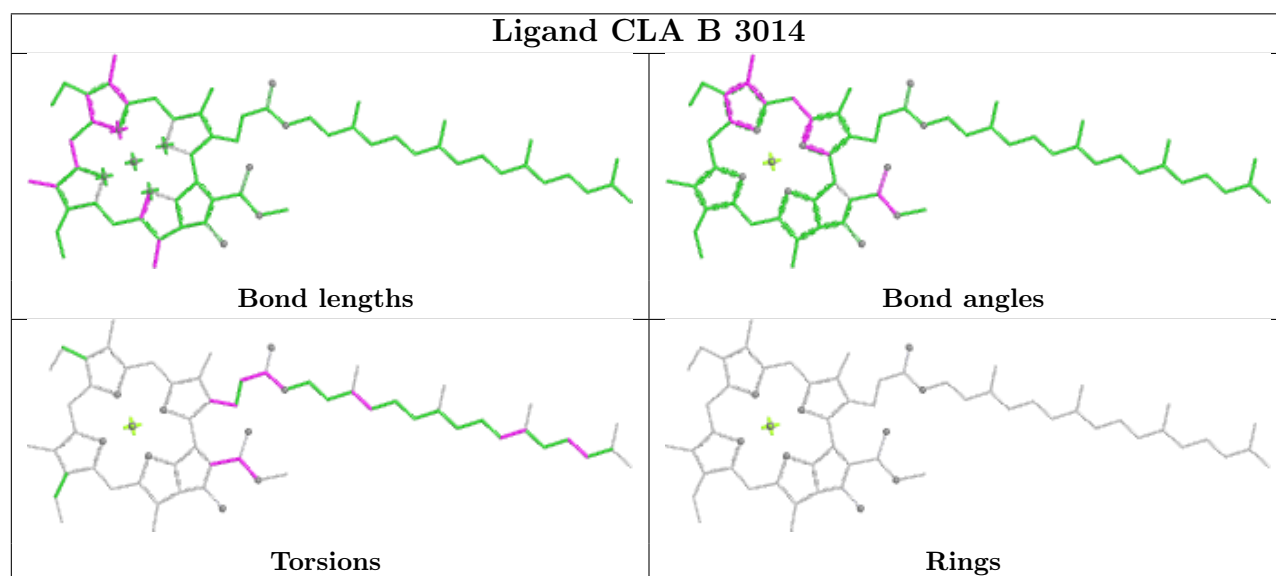
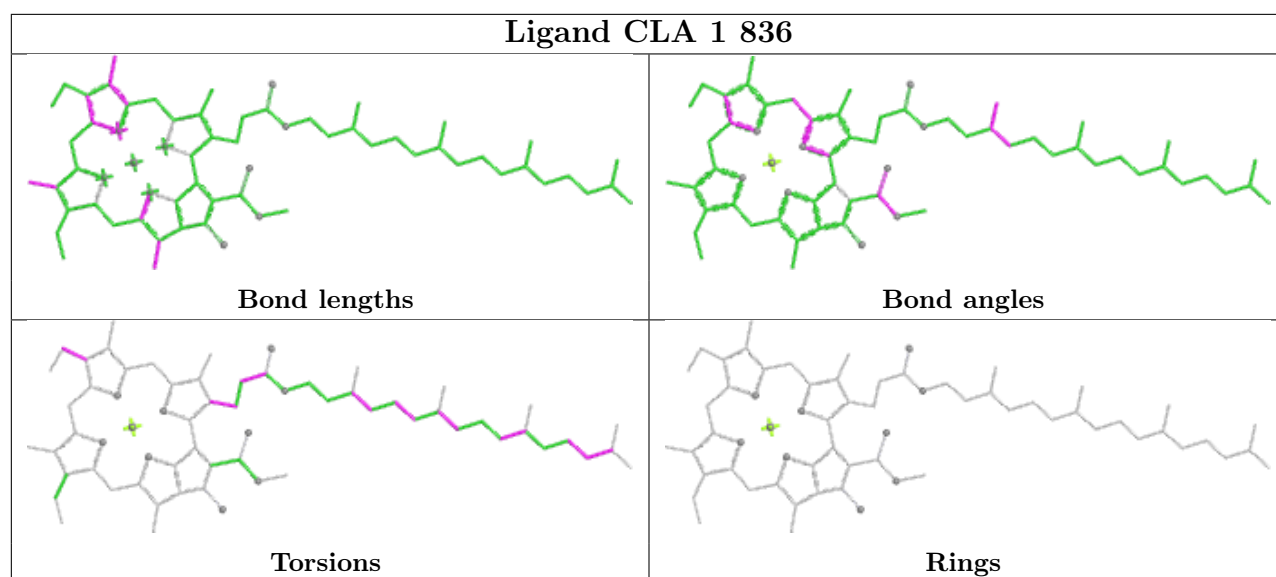


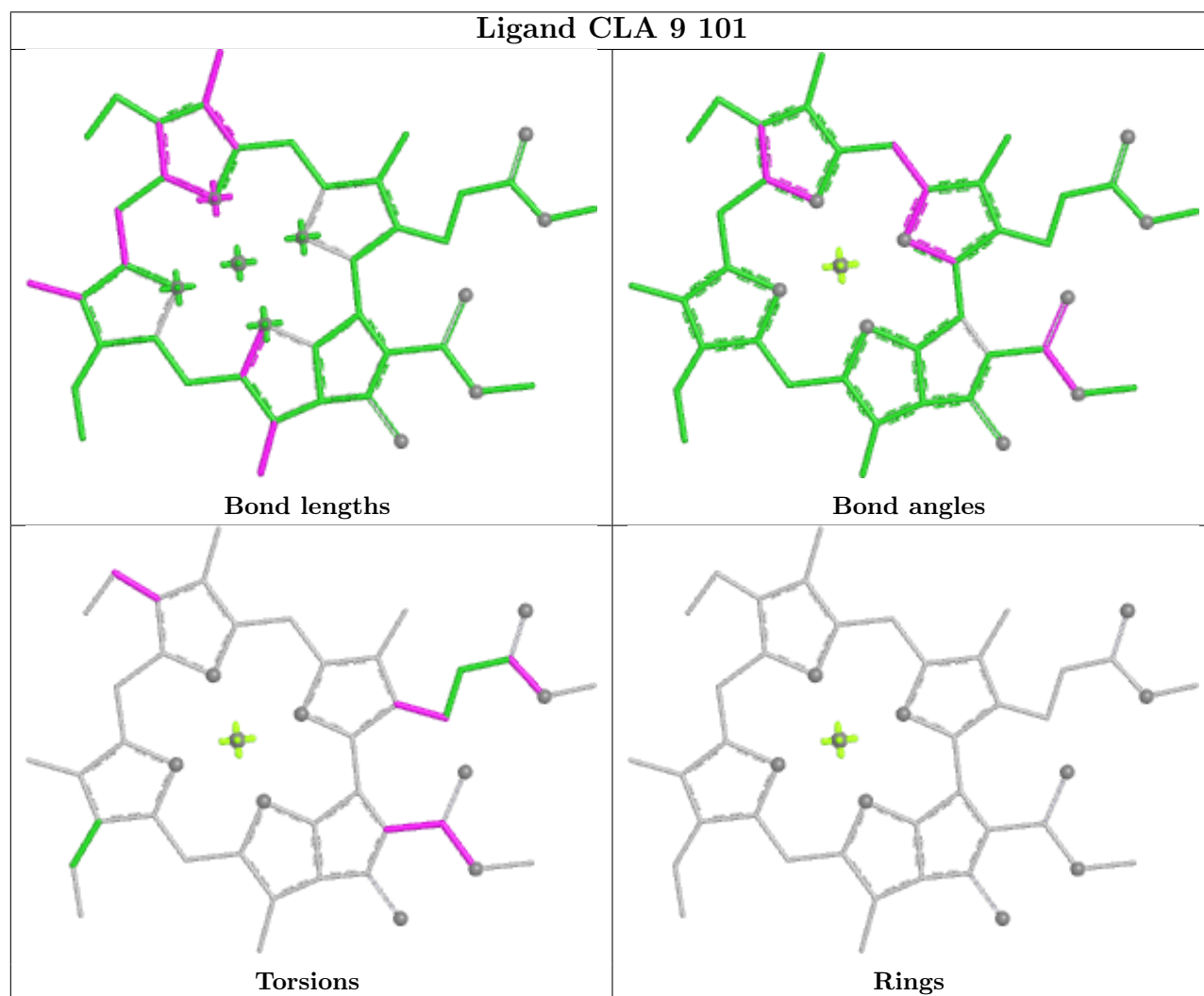
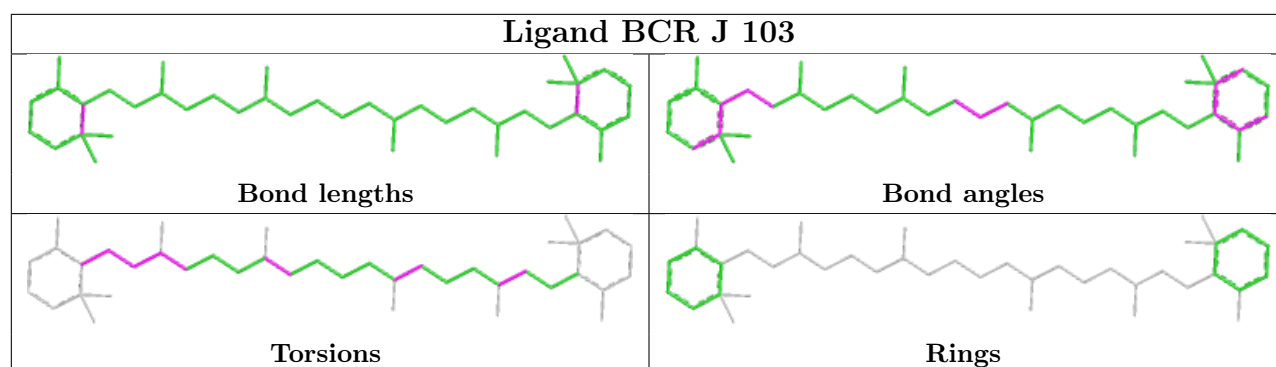


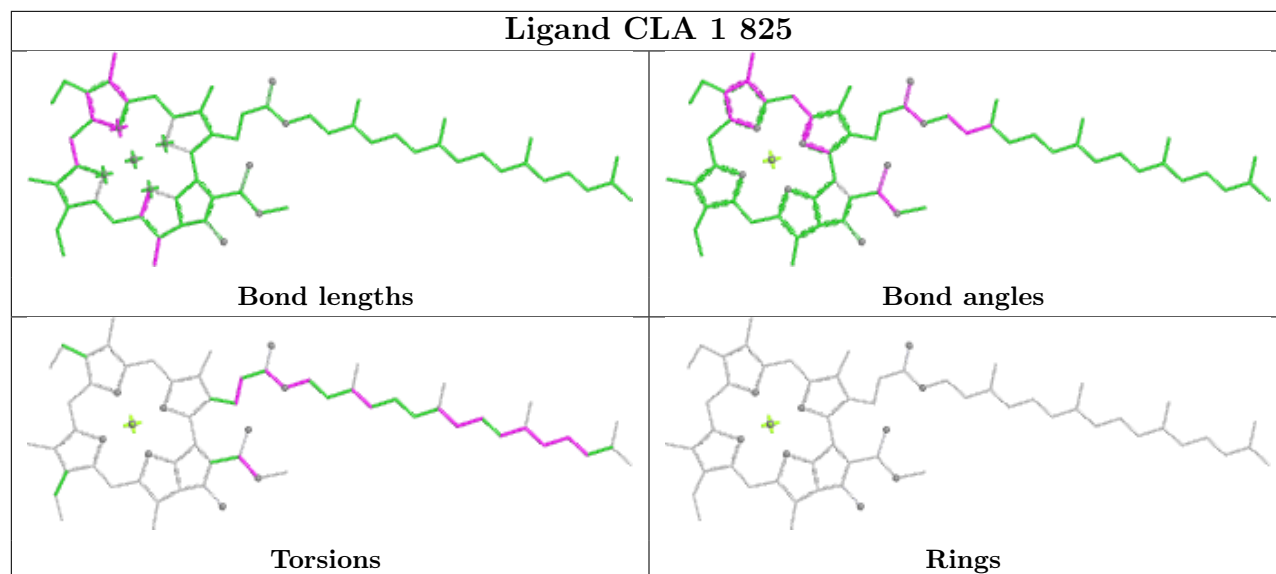
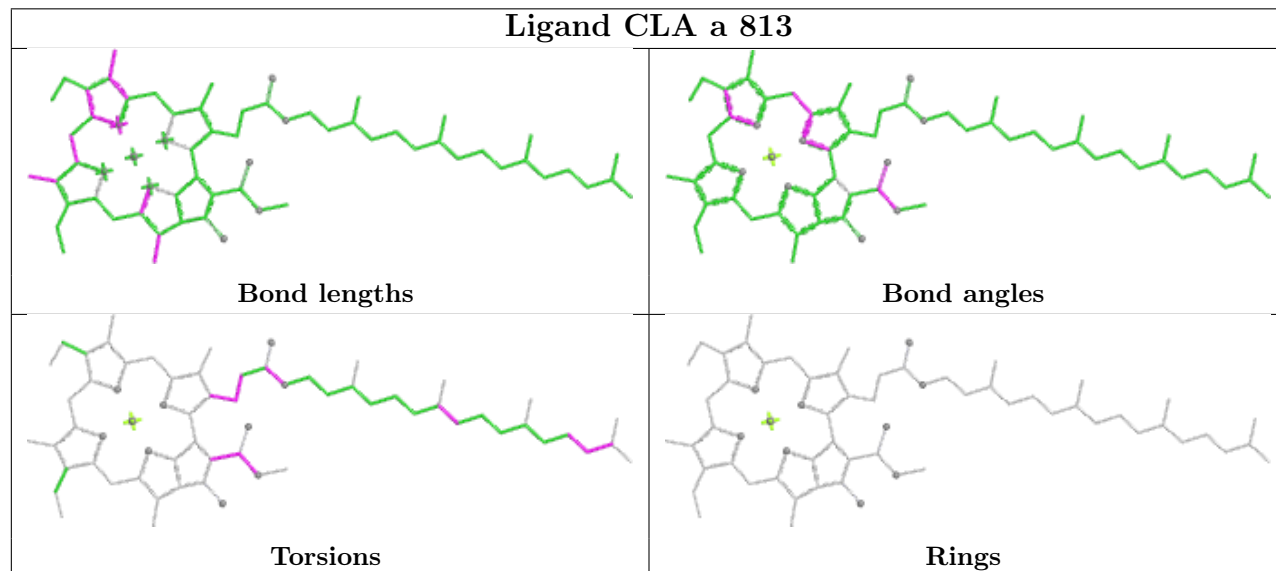




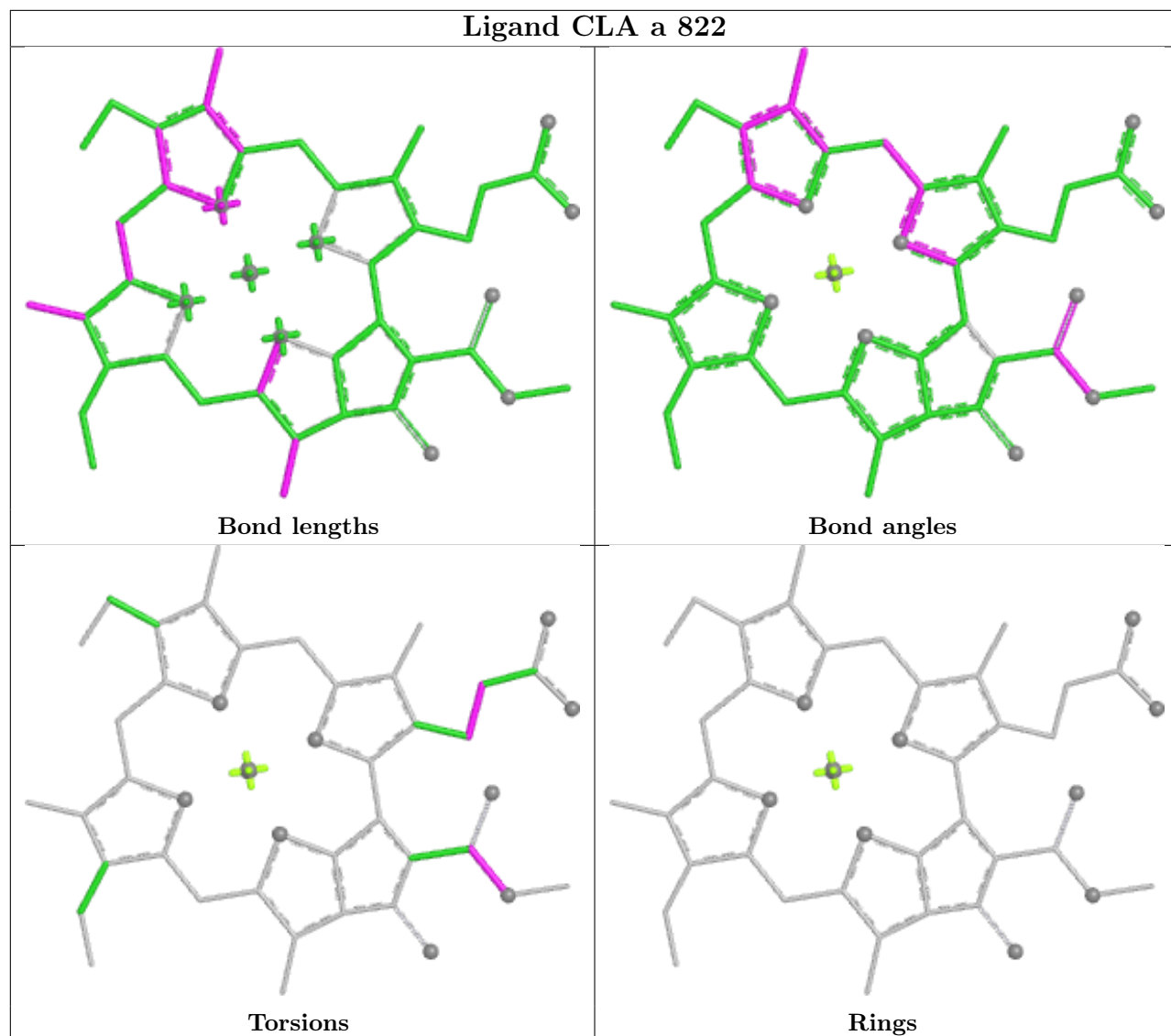


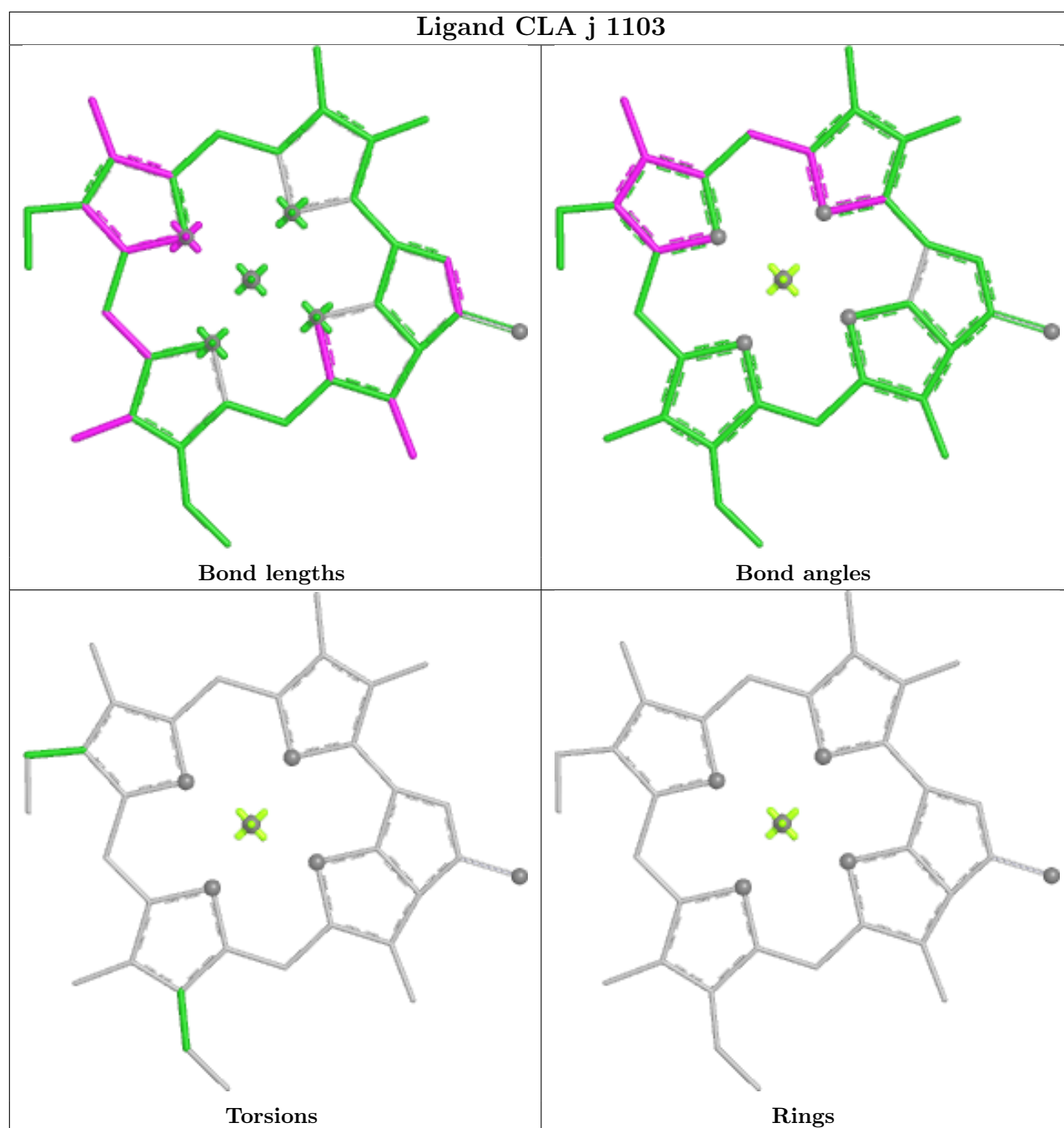


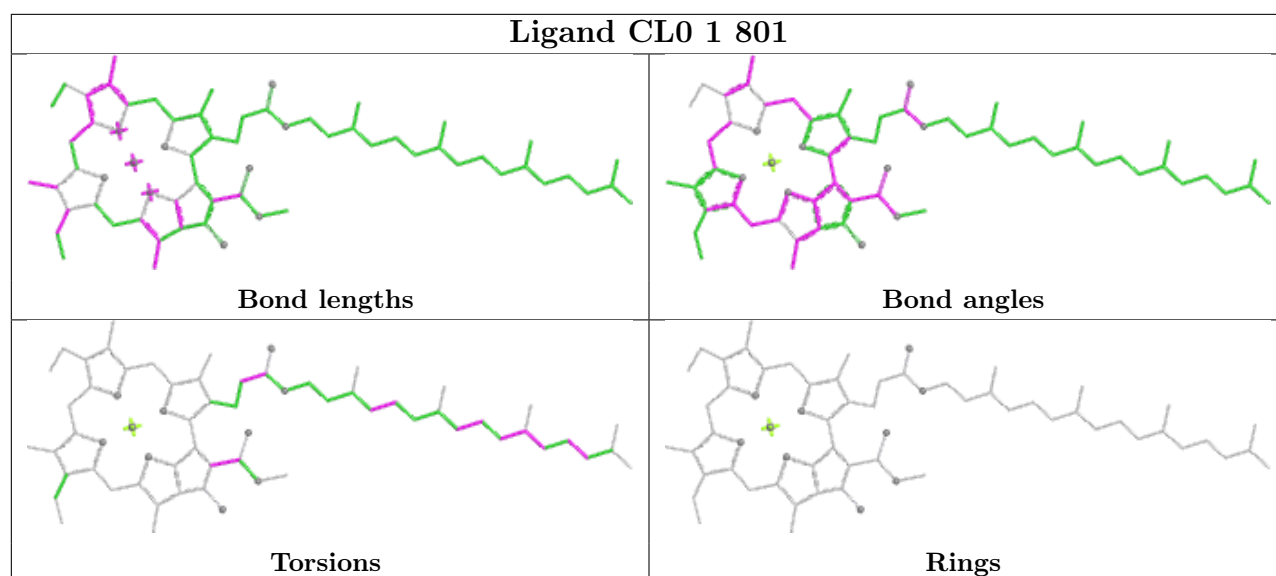
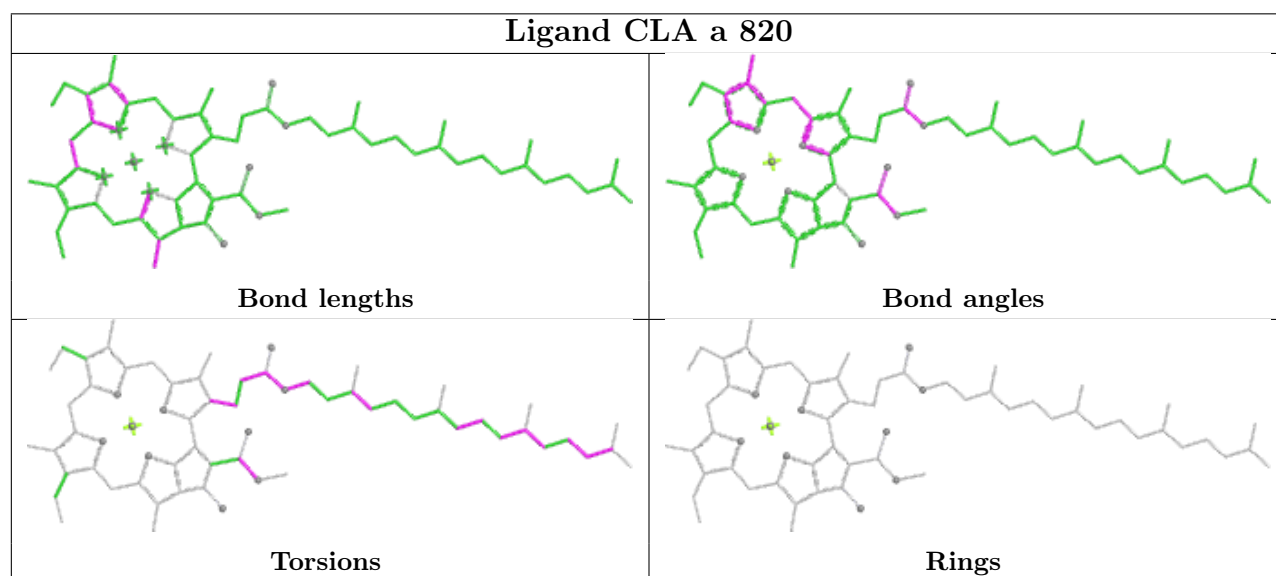
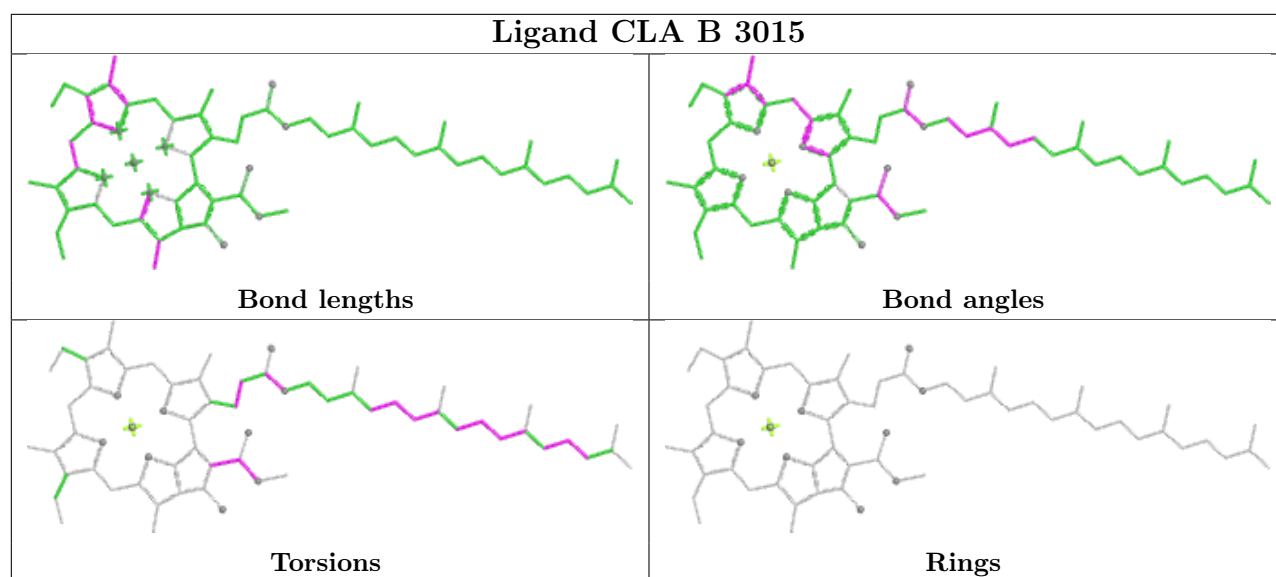


Ligand CLA 1 825**Ligand CLA a 813**

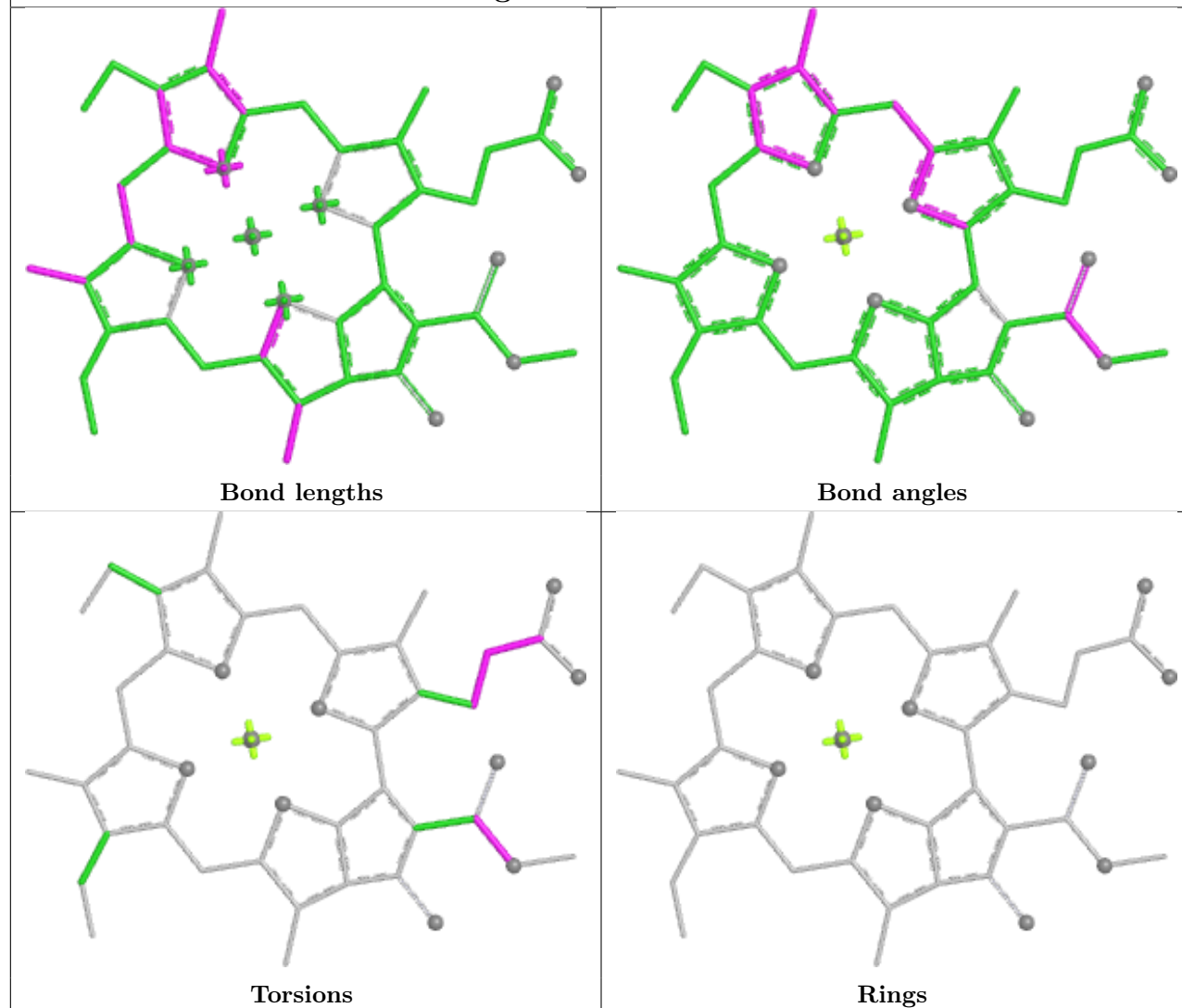
Ligand CLA a 822



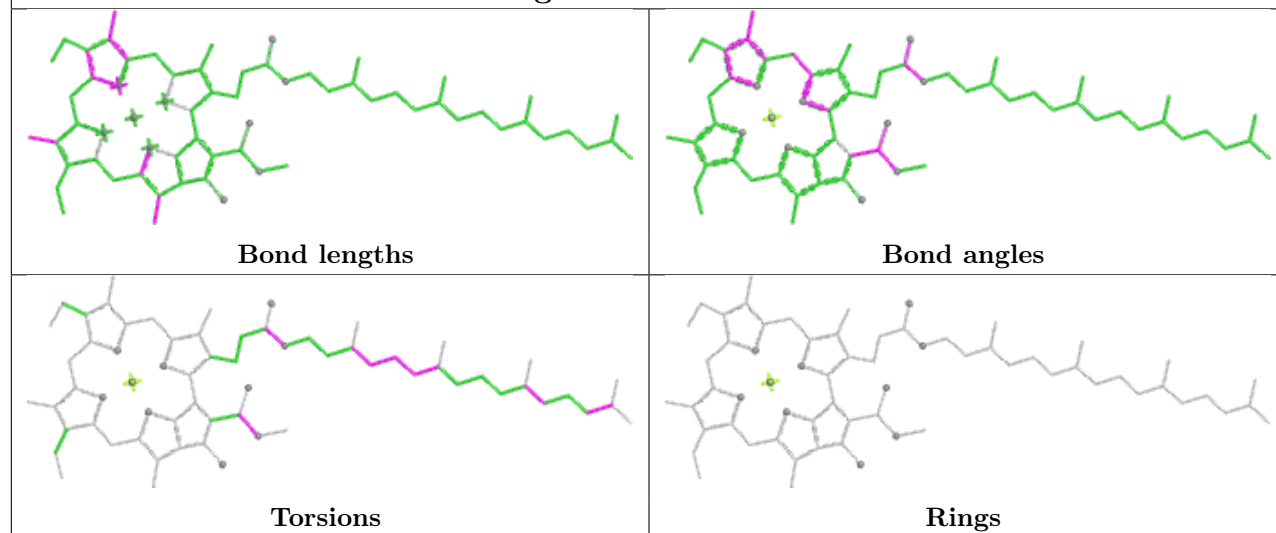


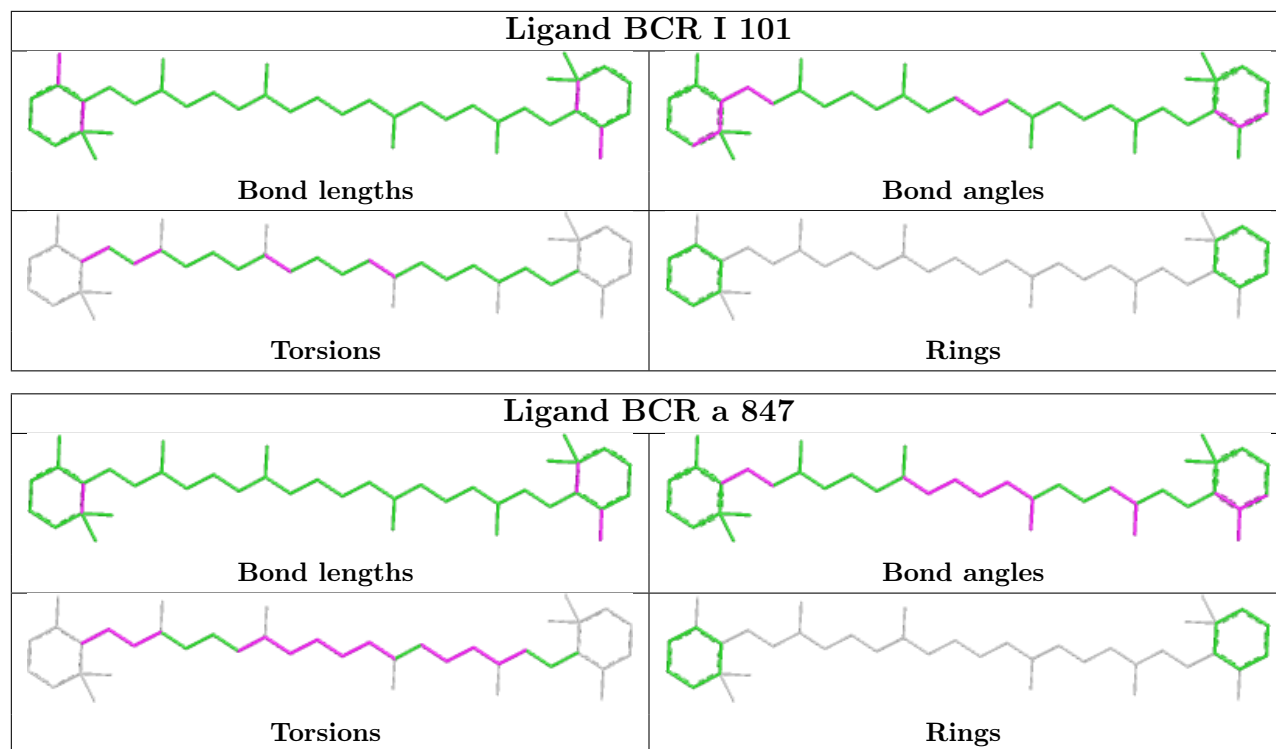


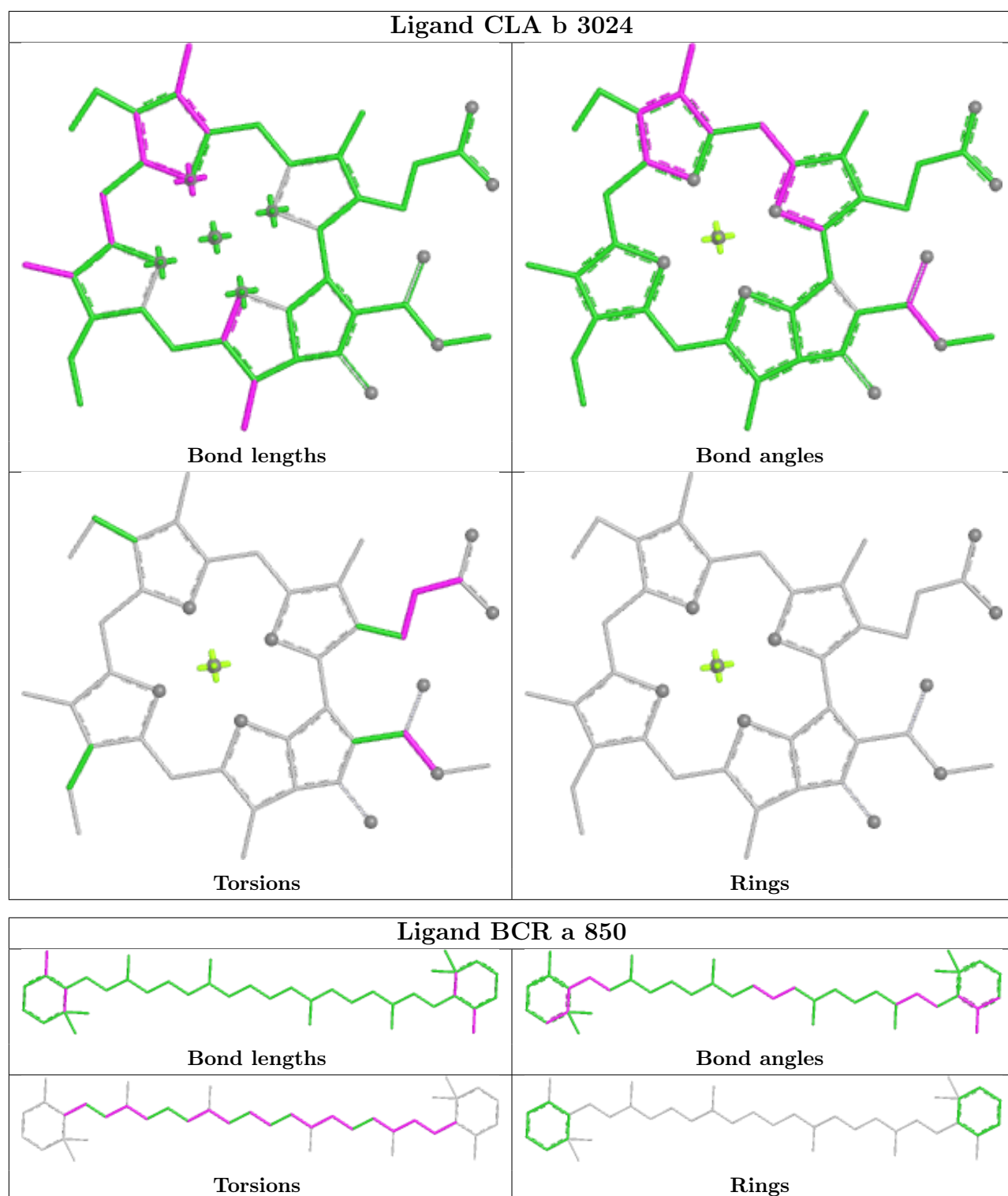
Ligand CLA F 203

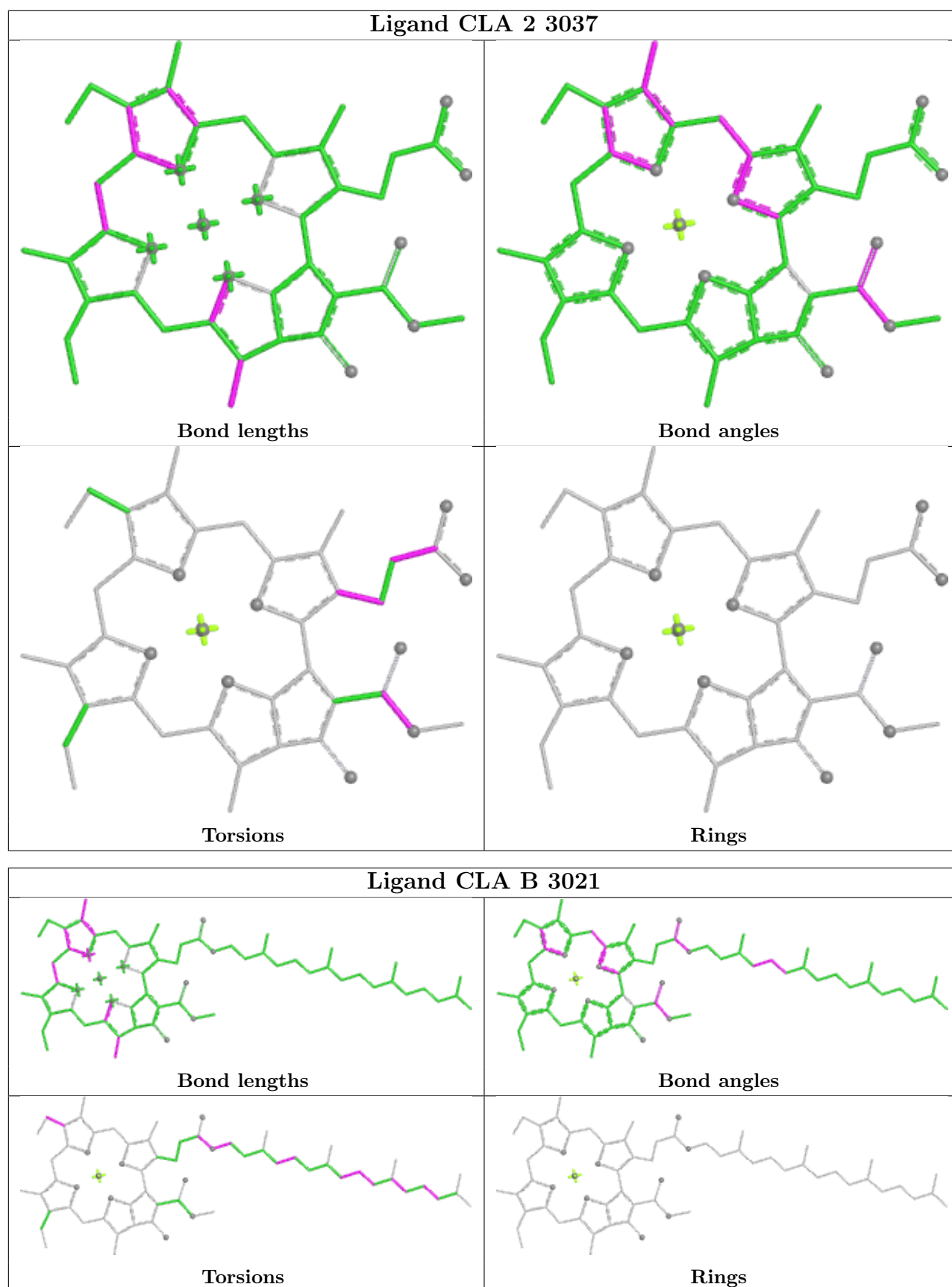


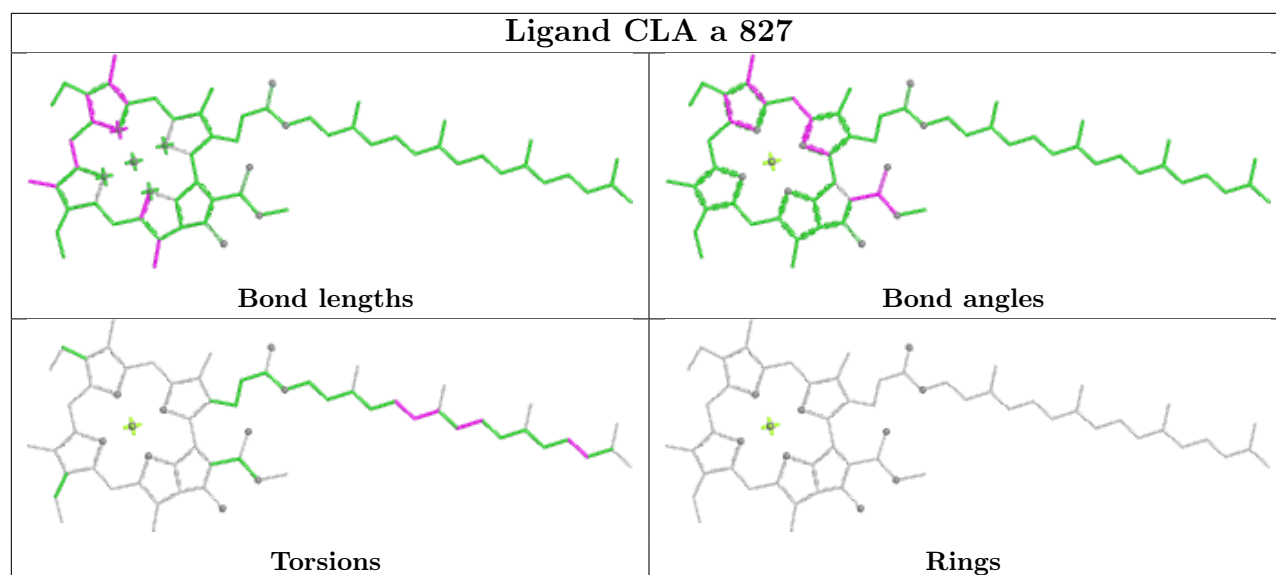
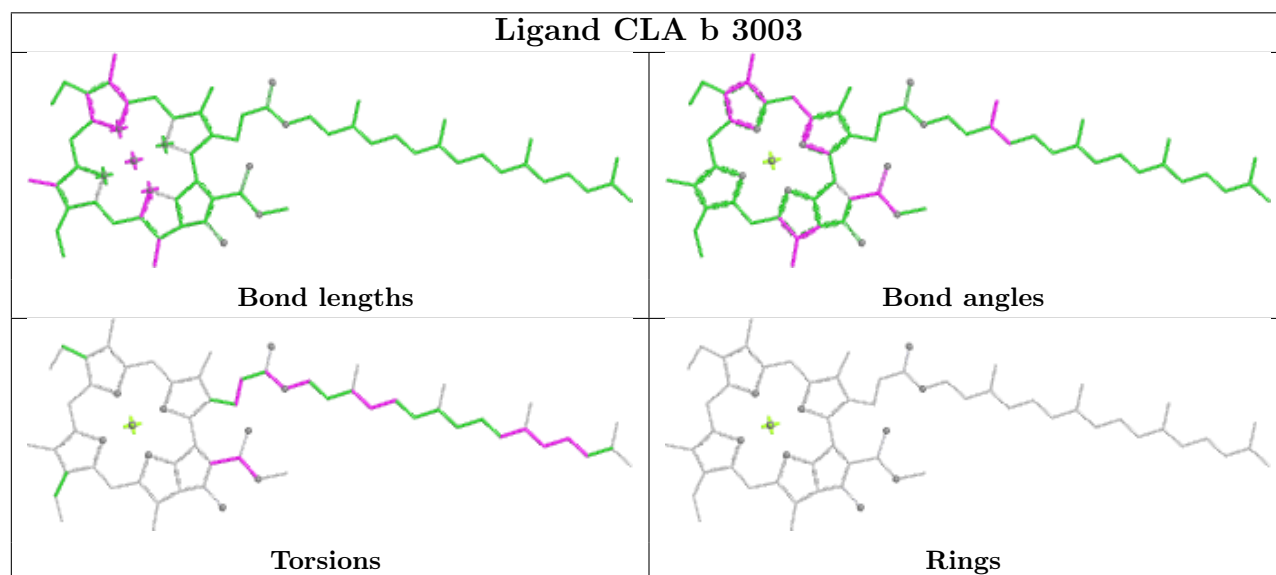
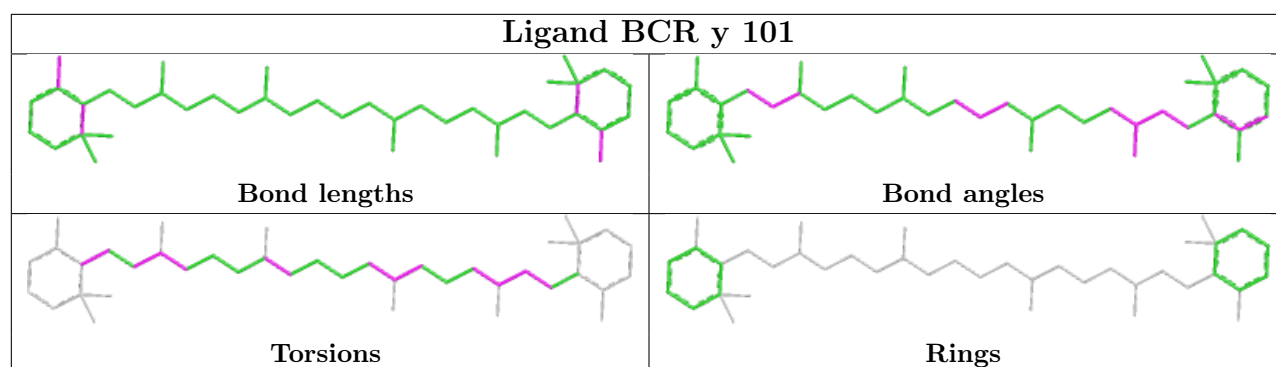
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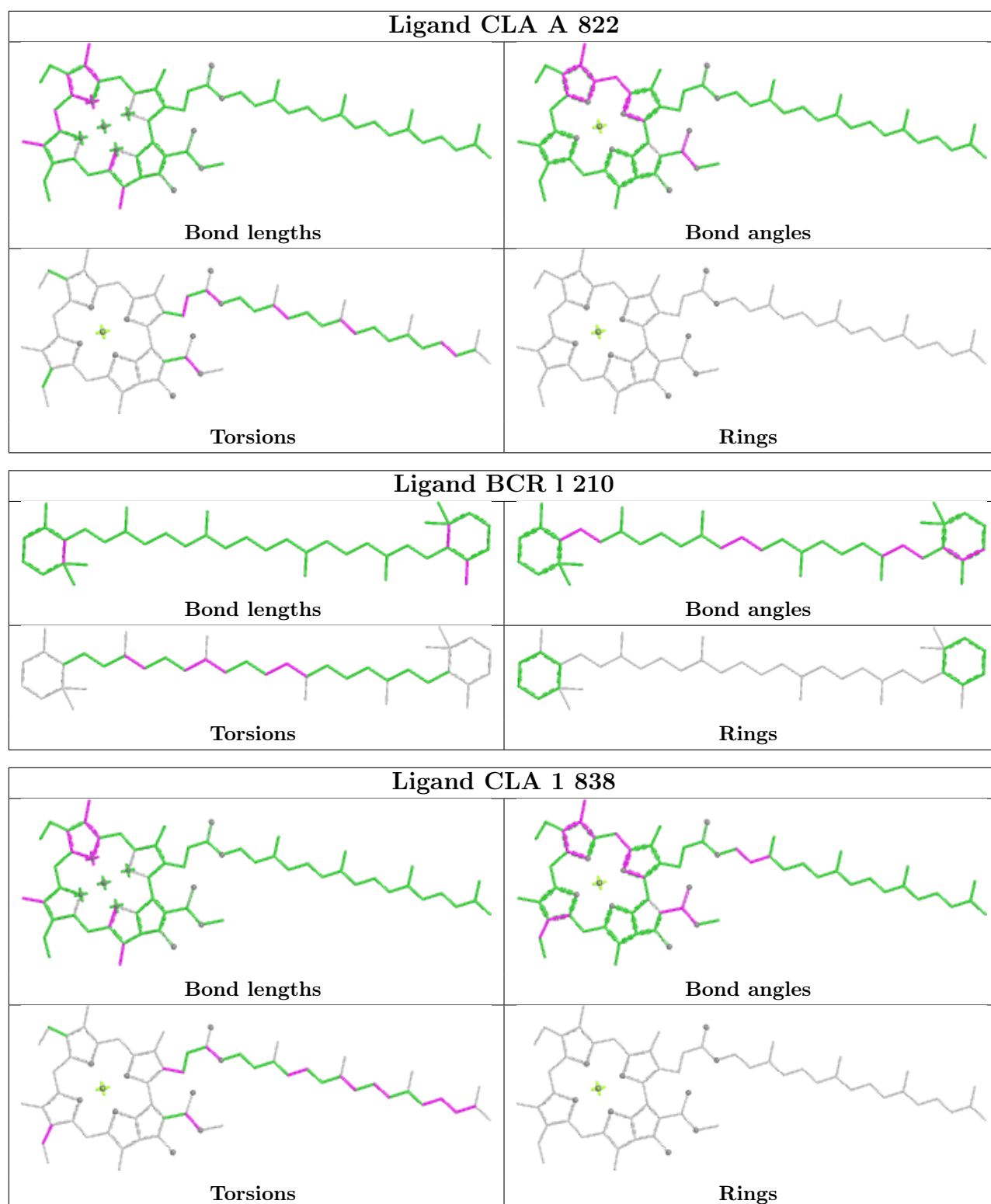


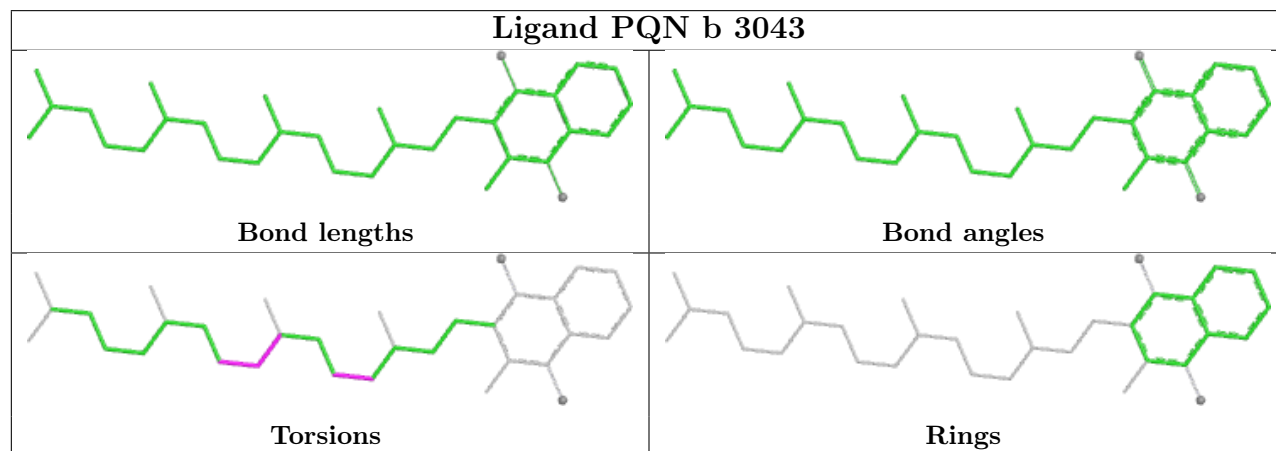
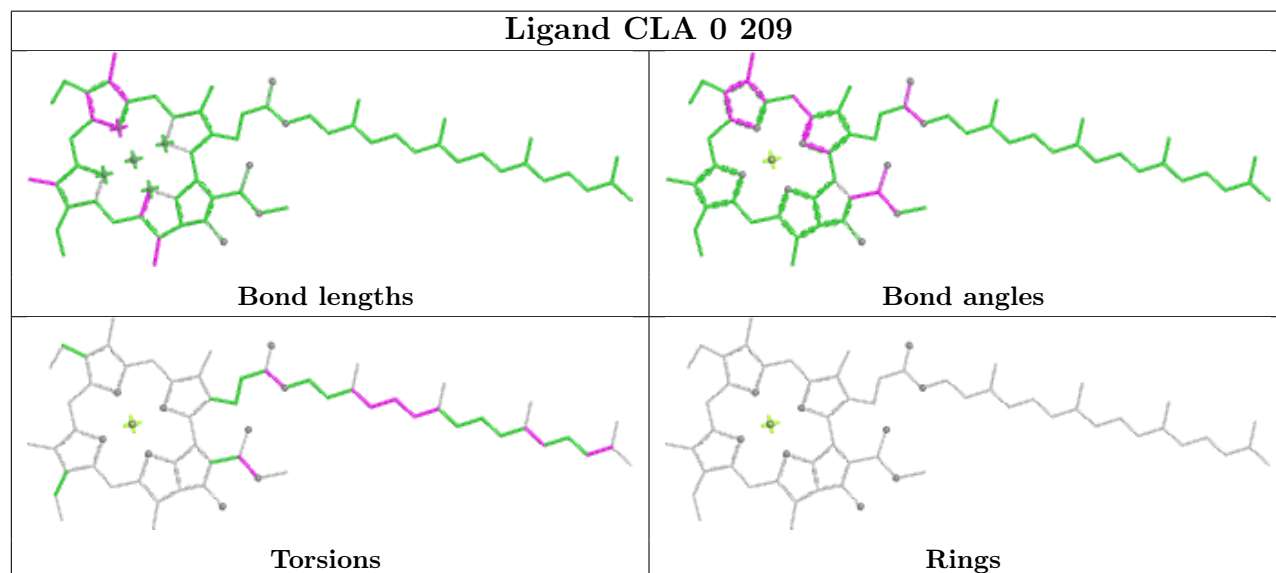
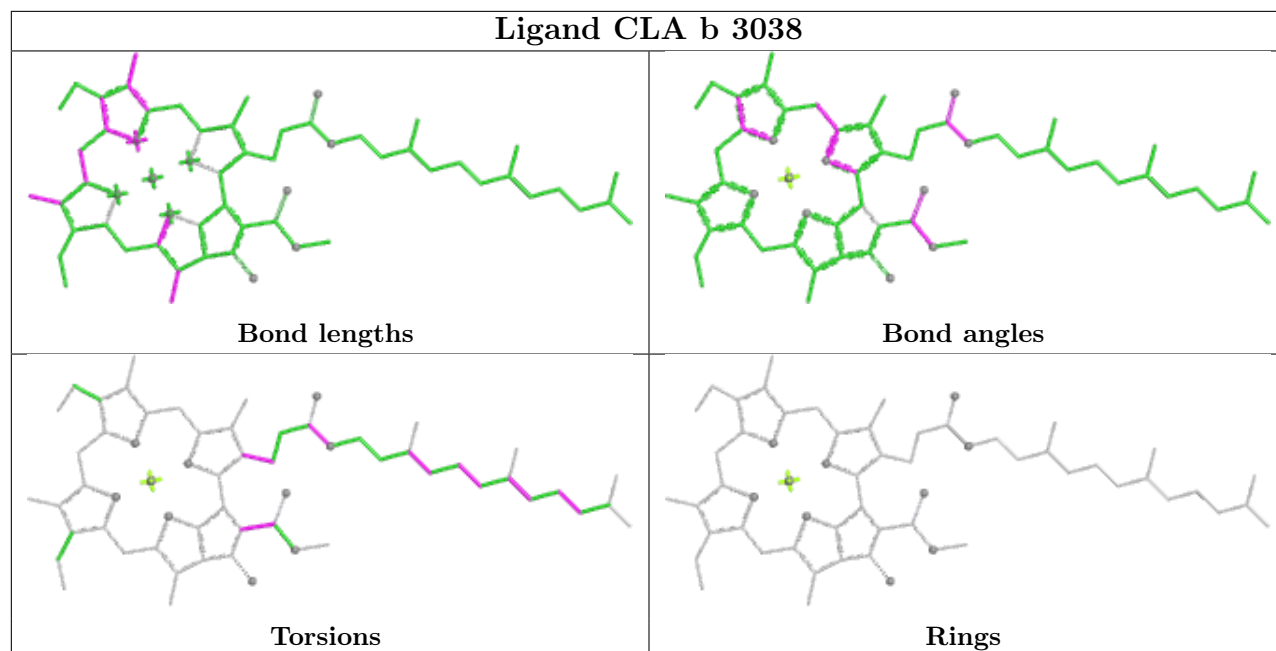


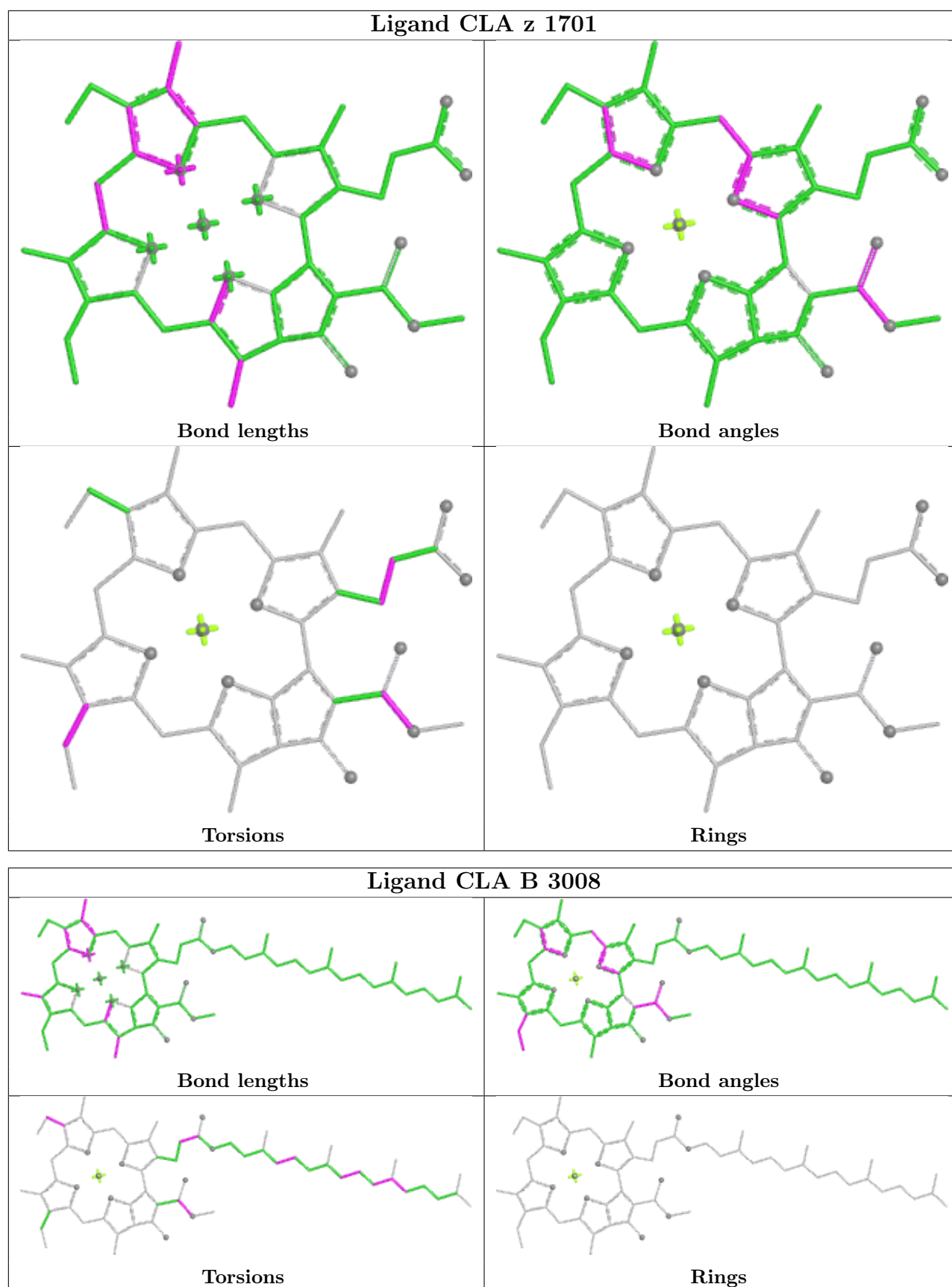


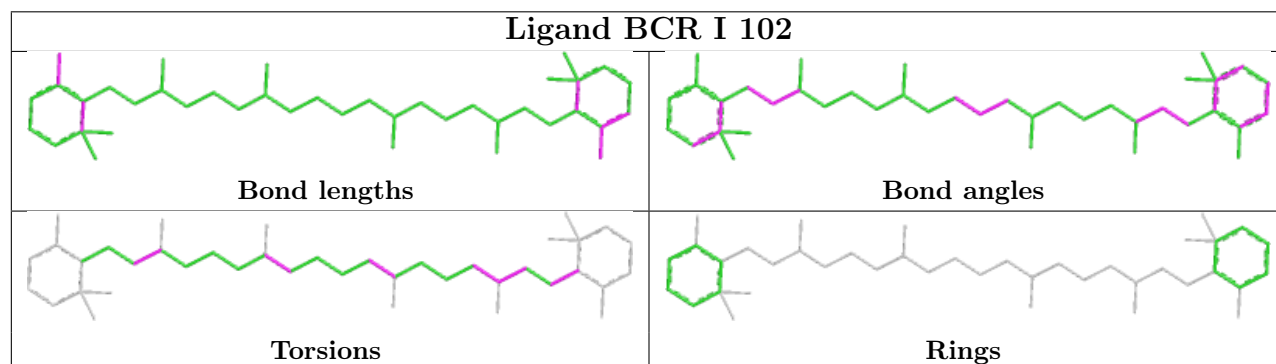
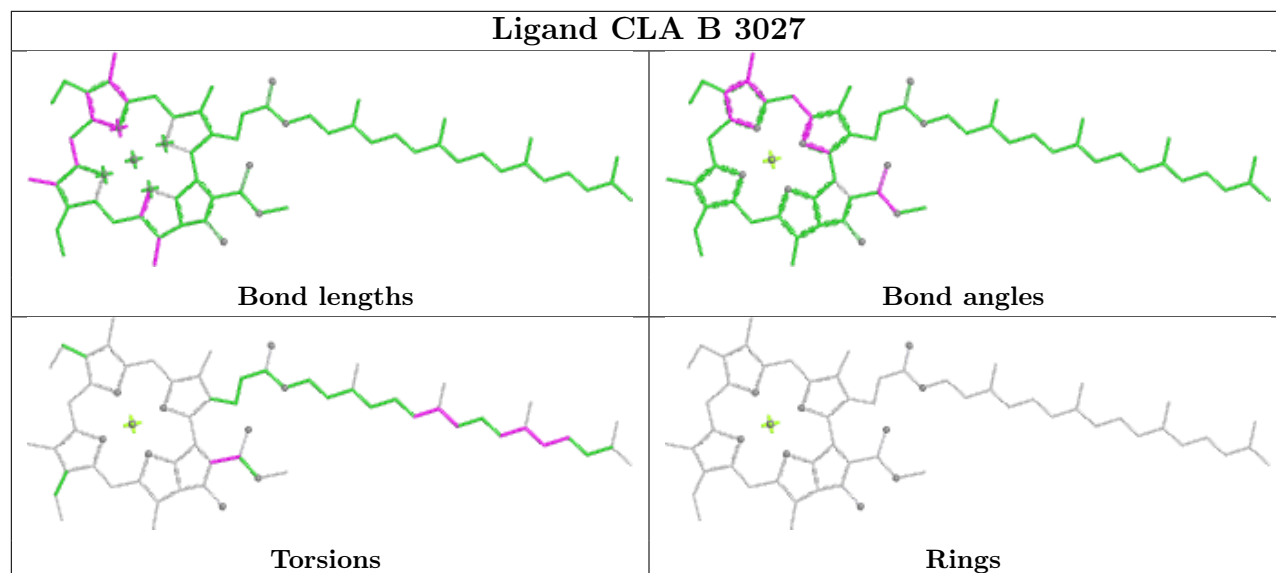
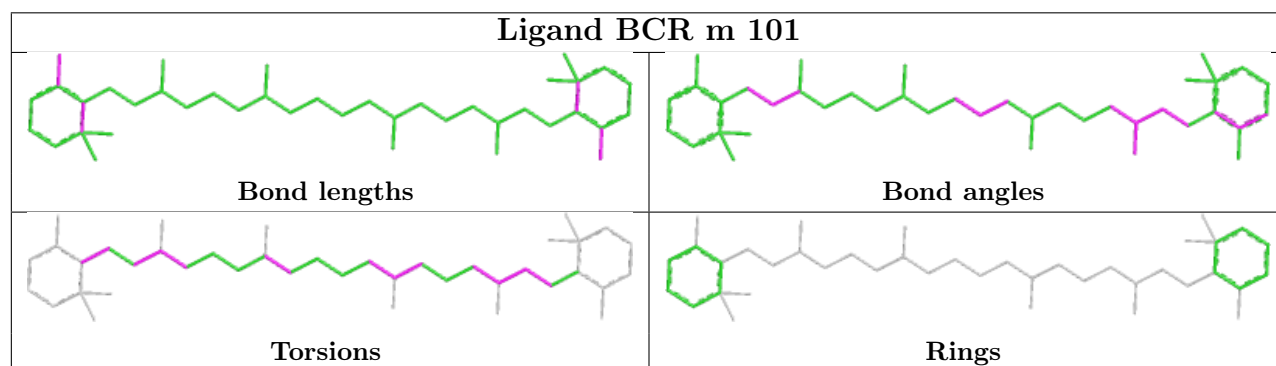
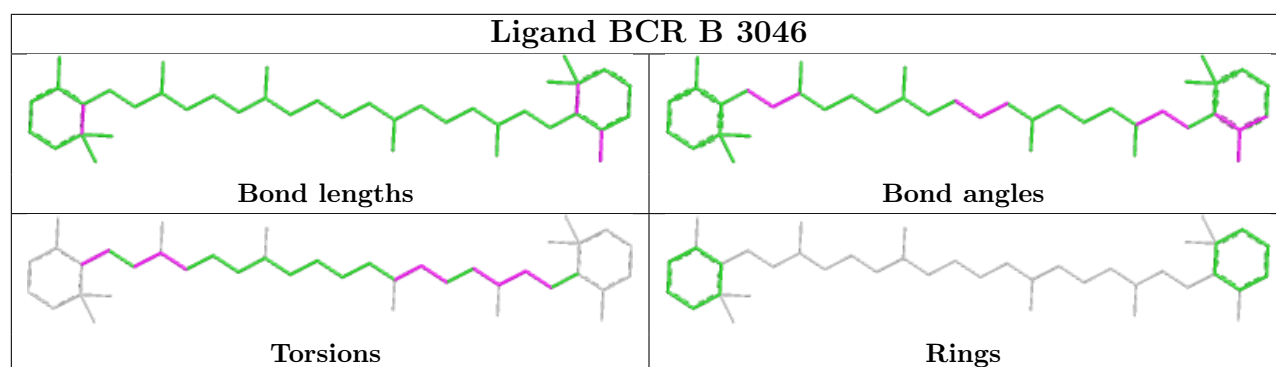


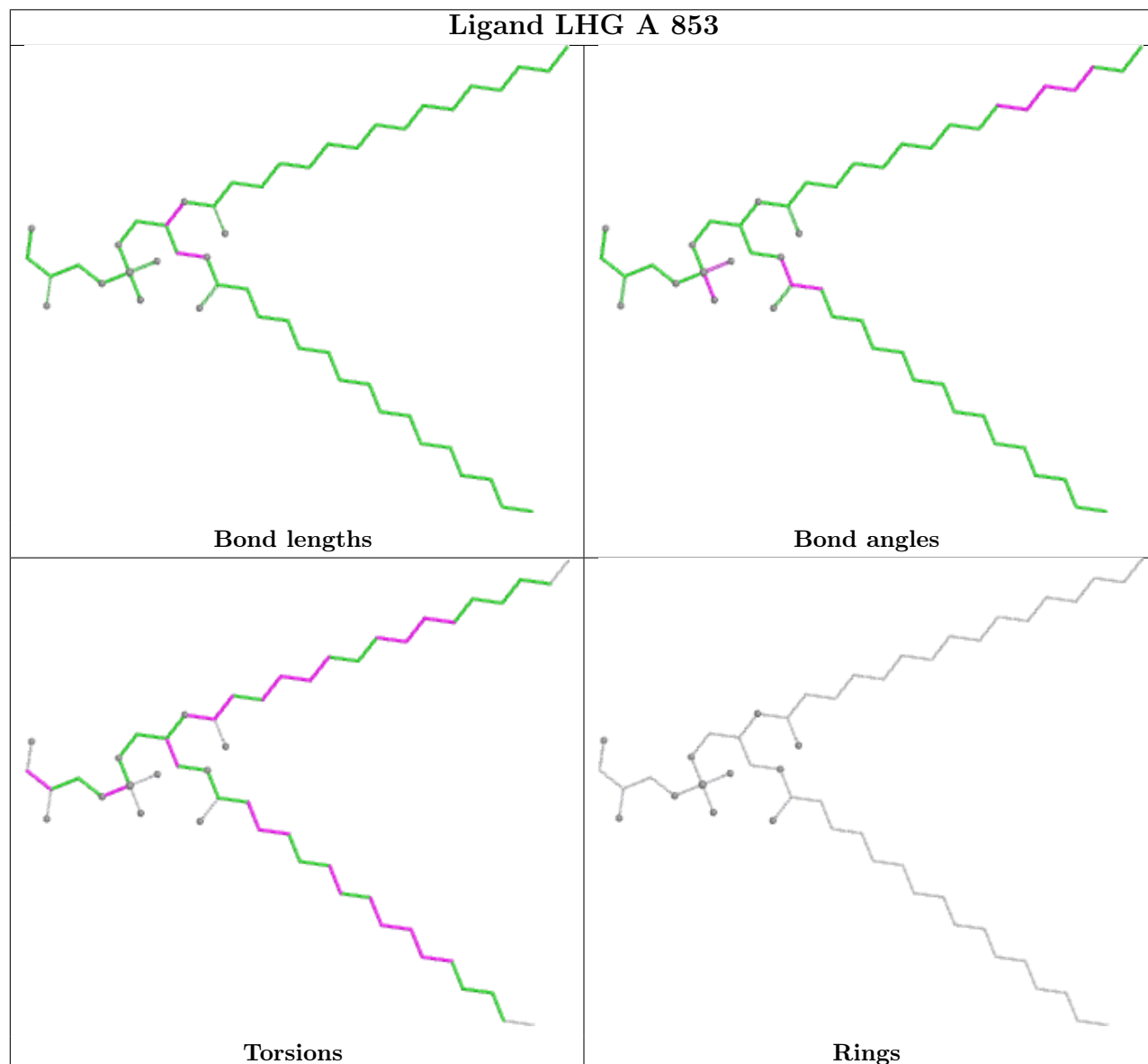
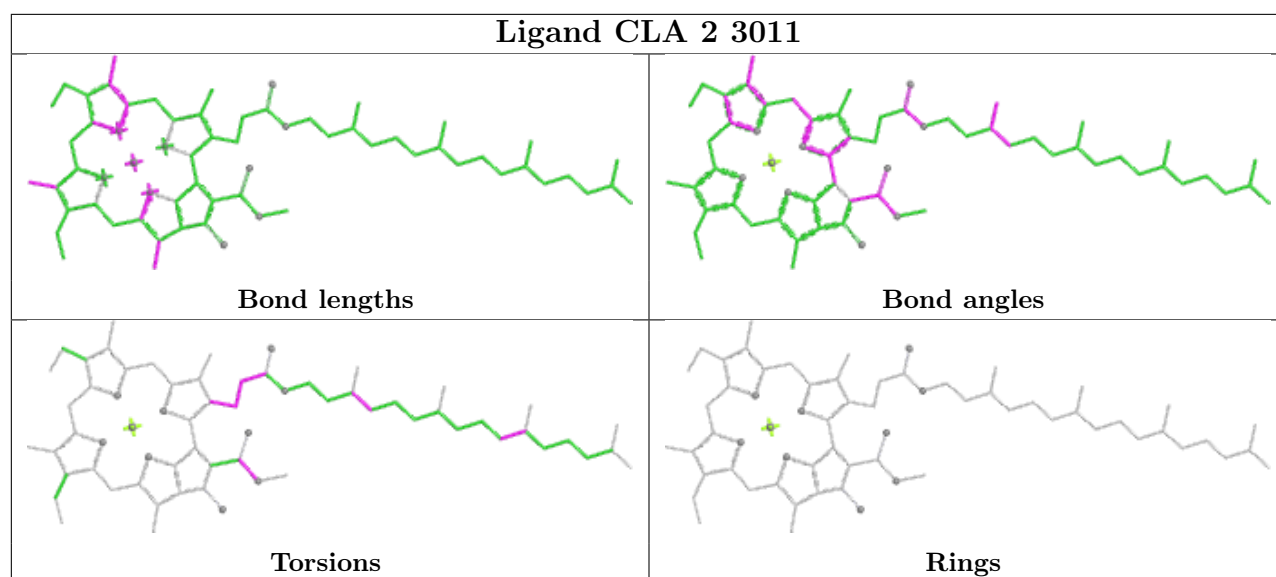


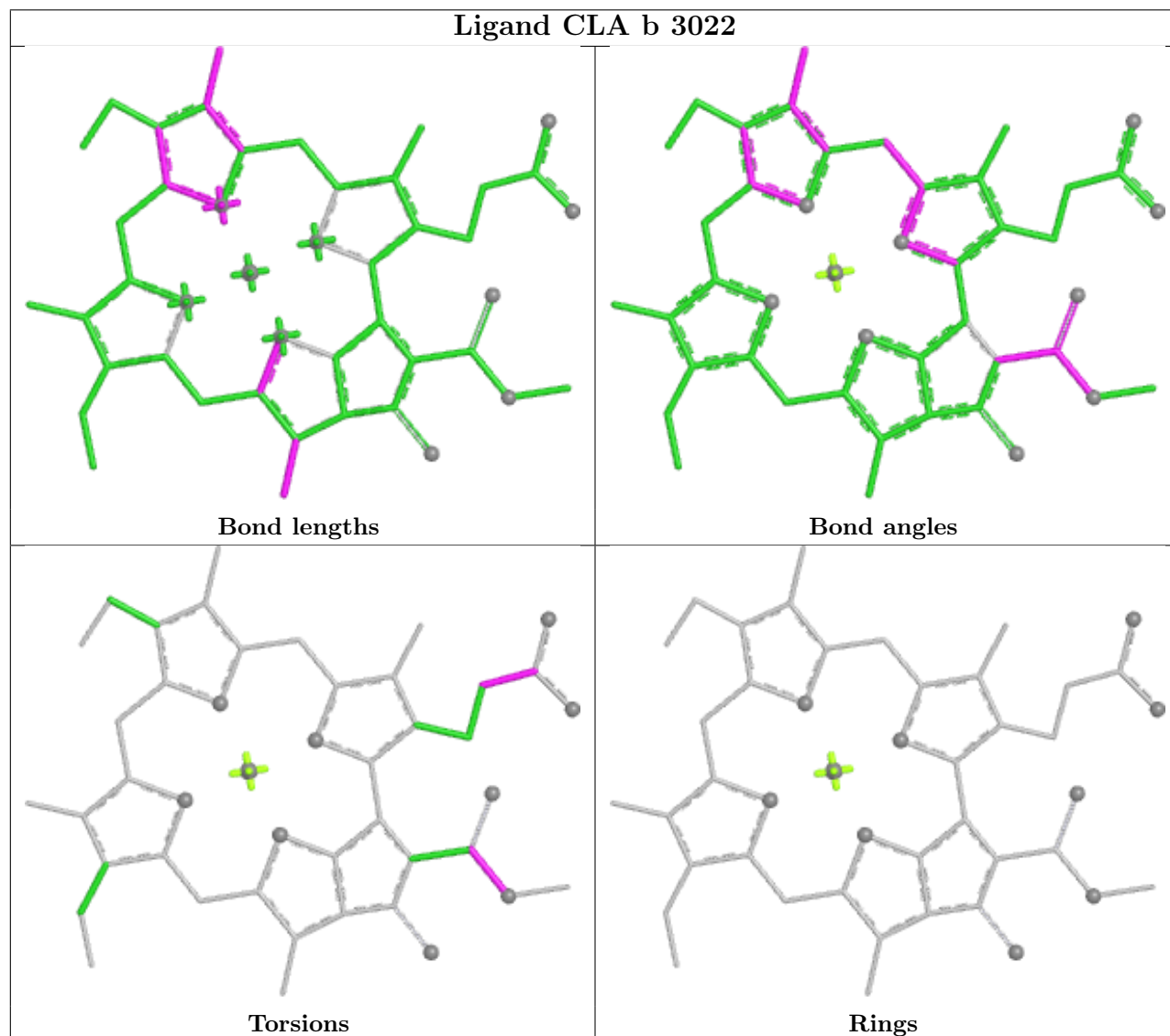
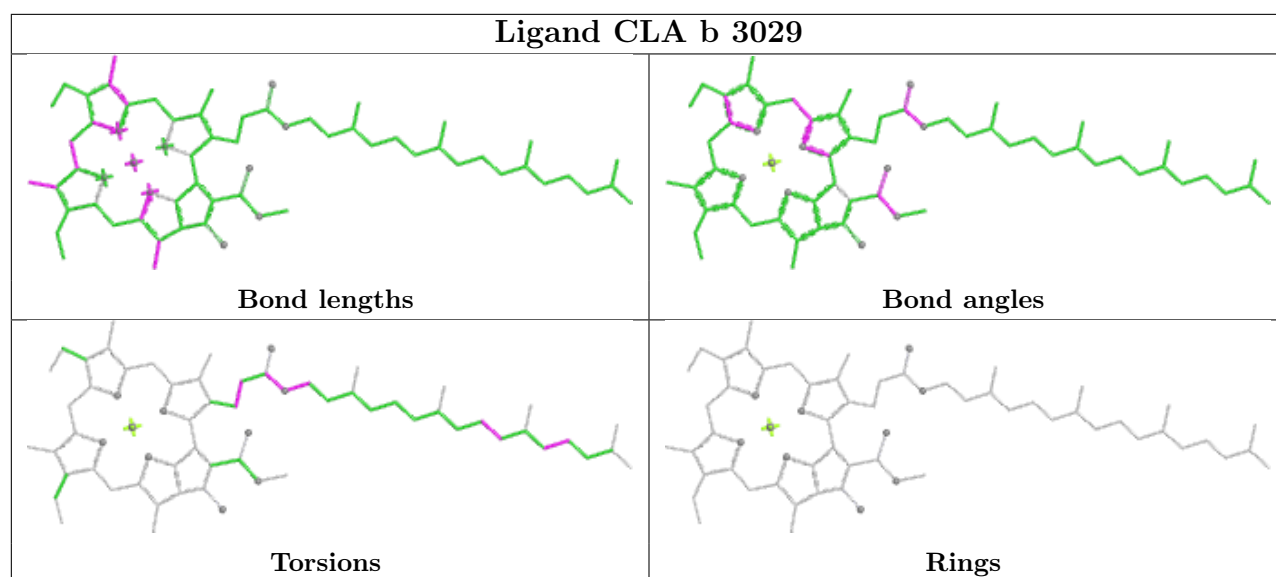


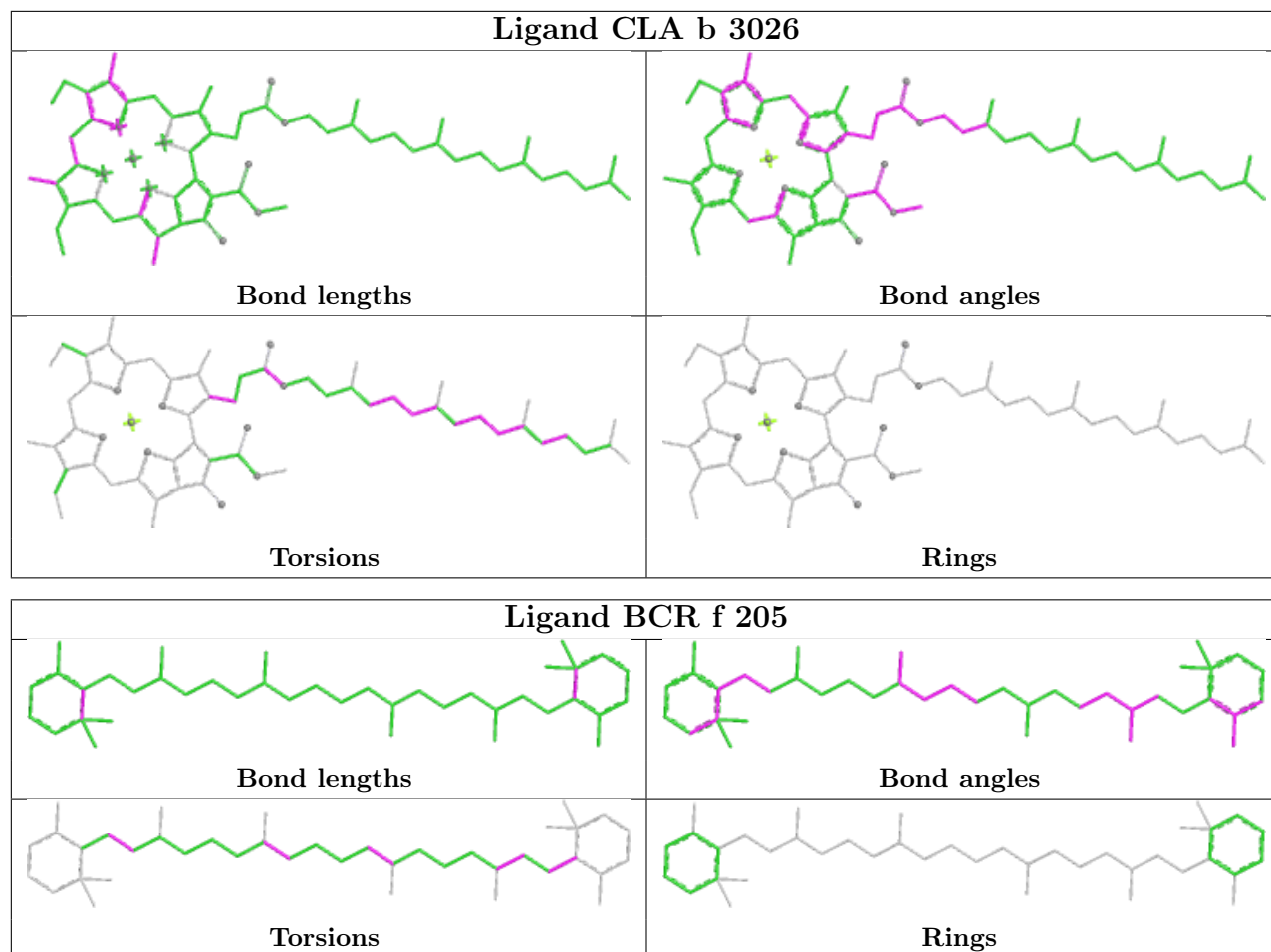


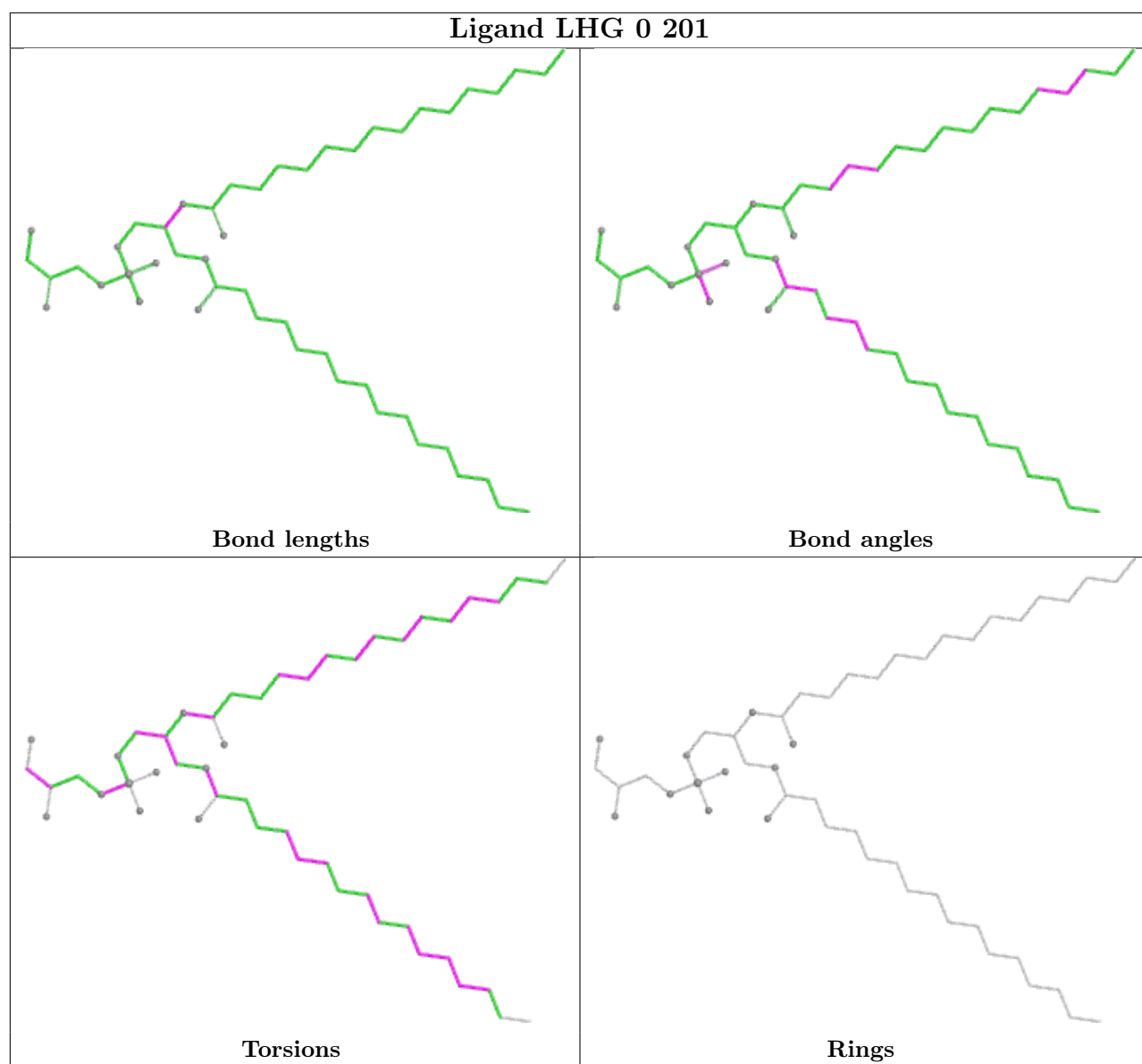


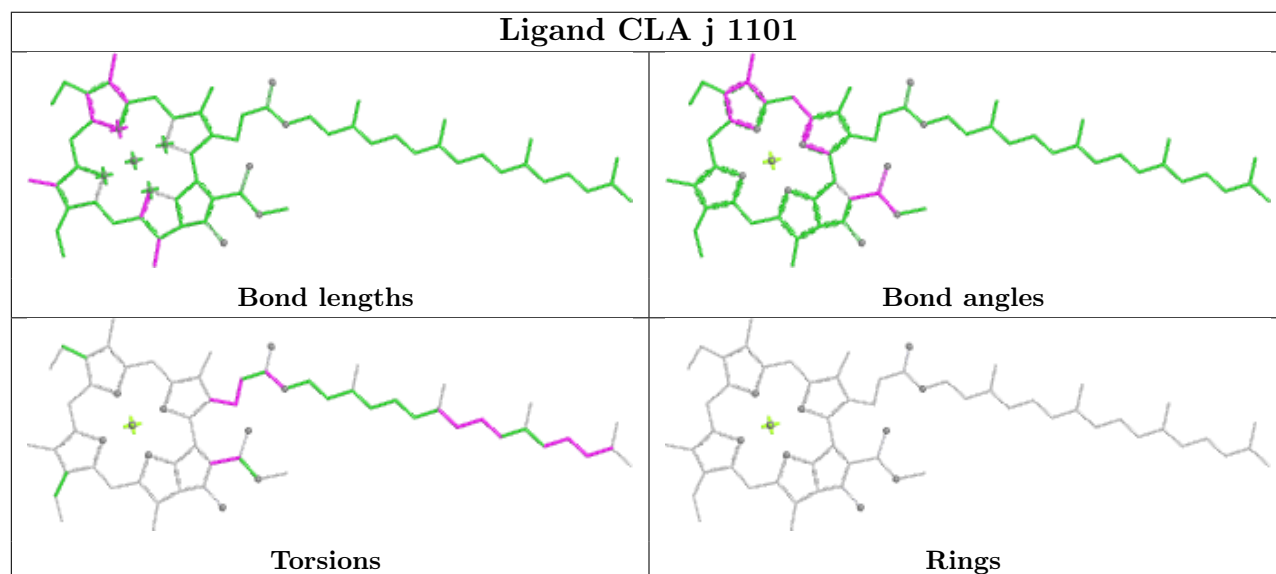
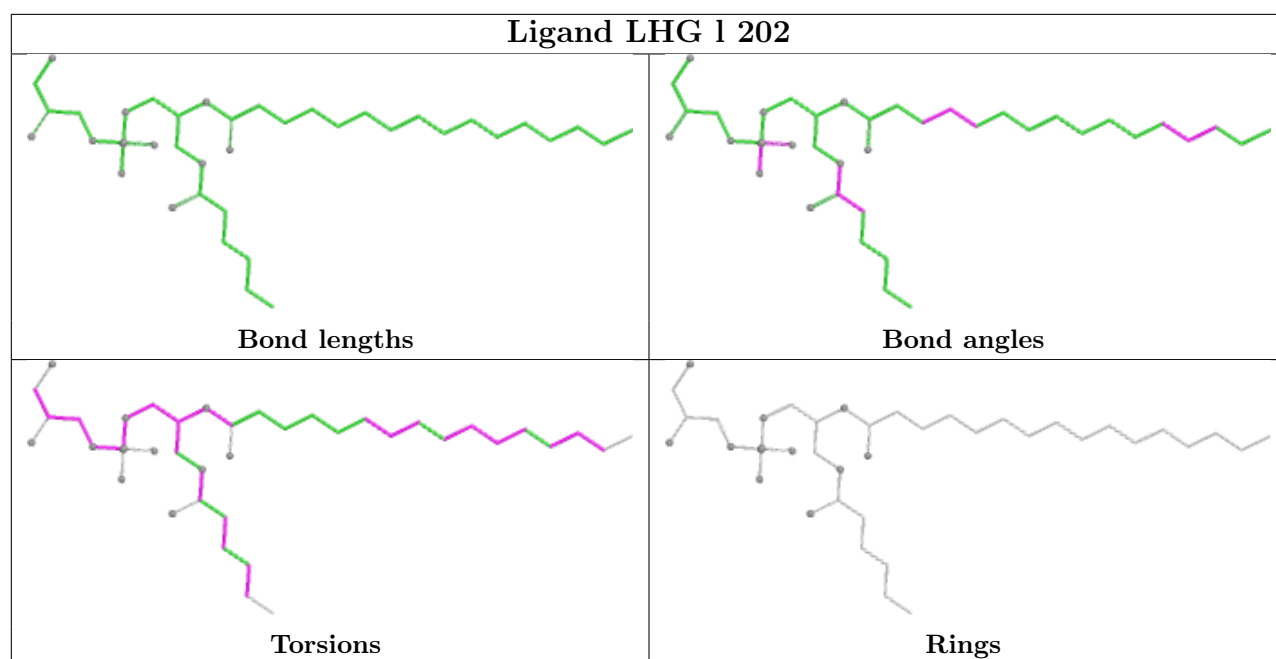


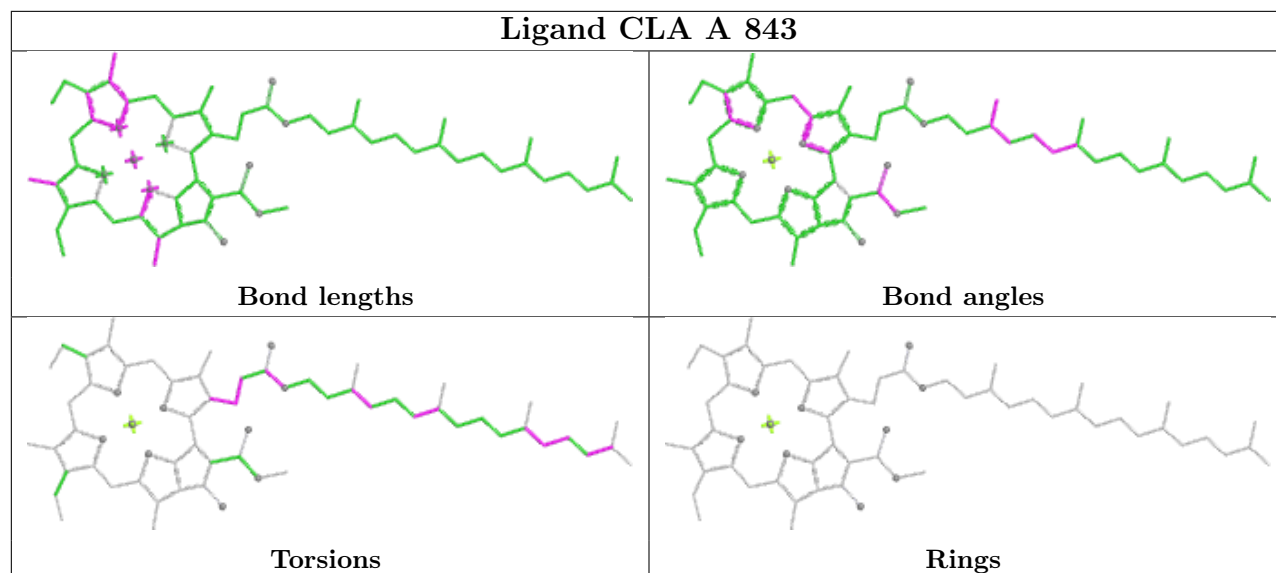
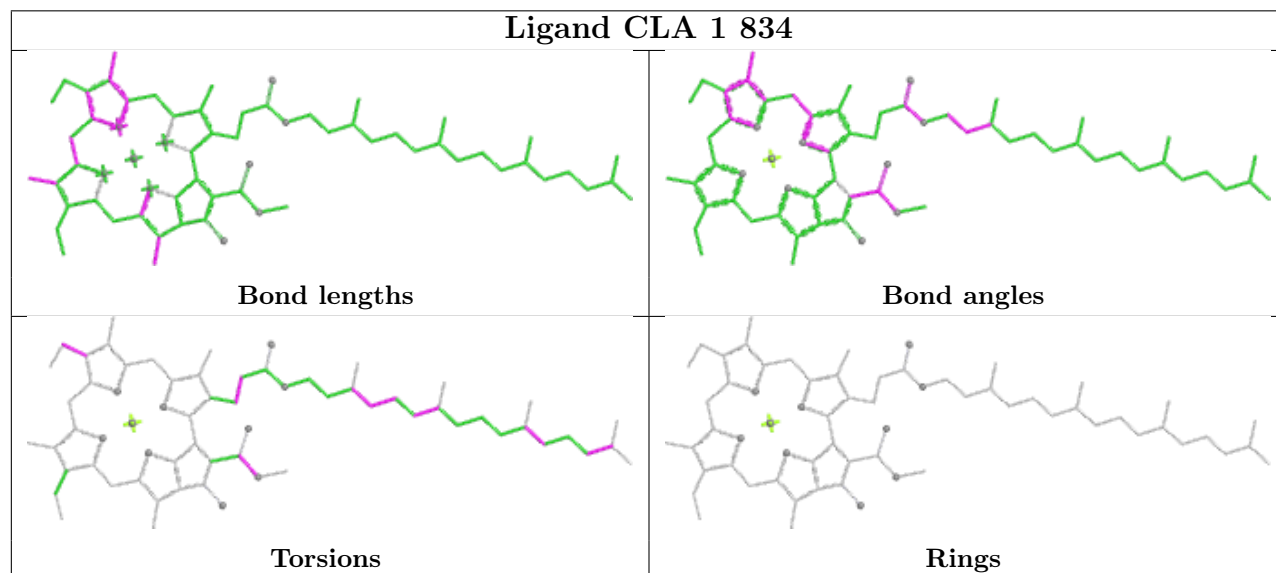
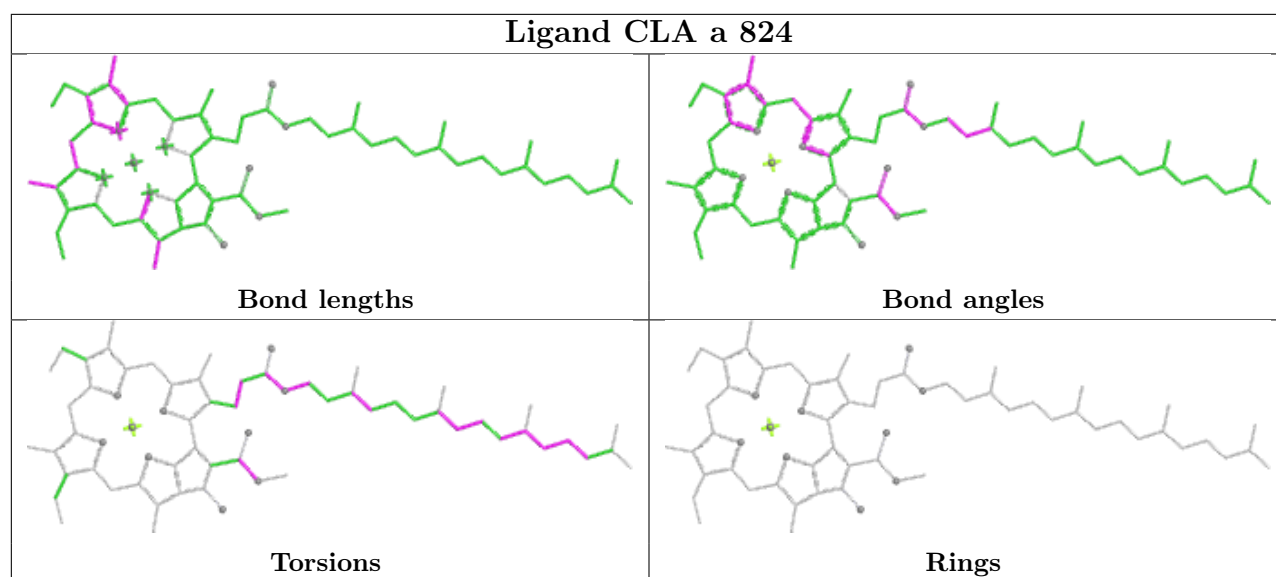


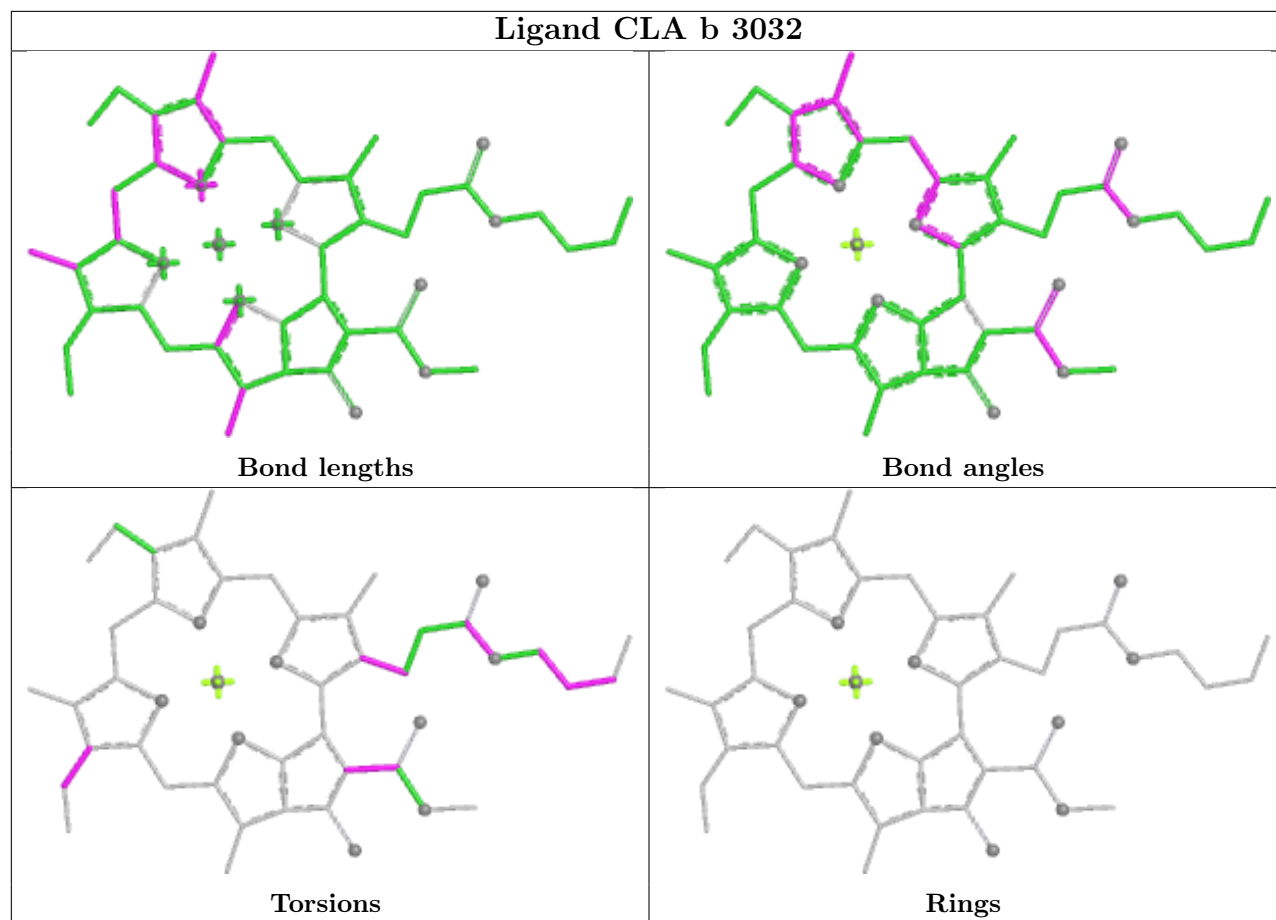




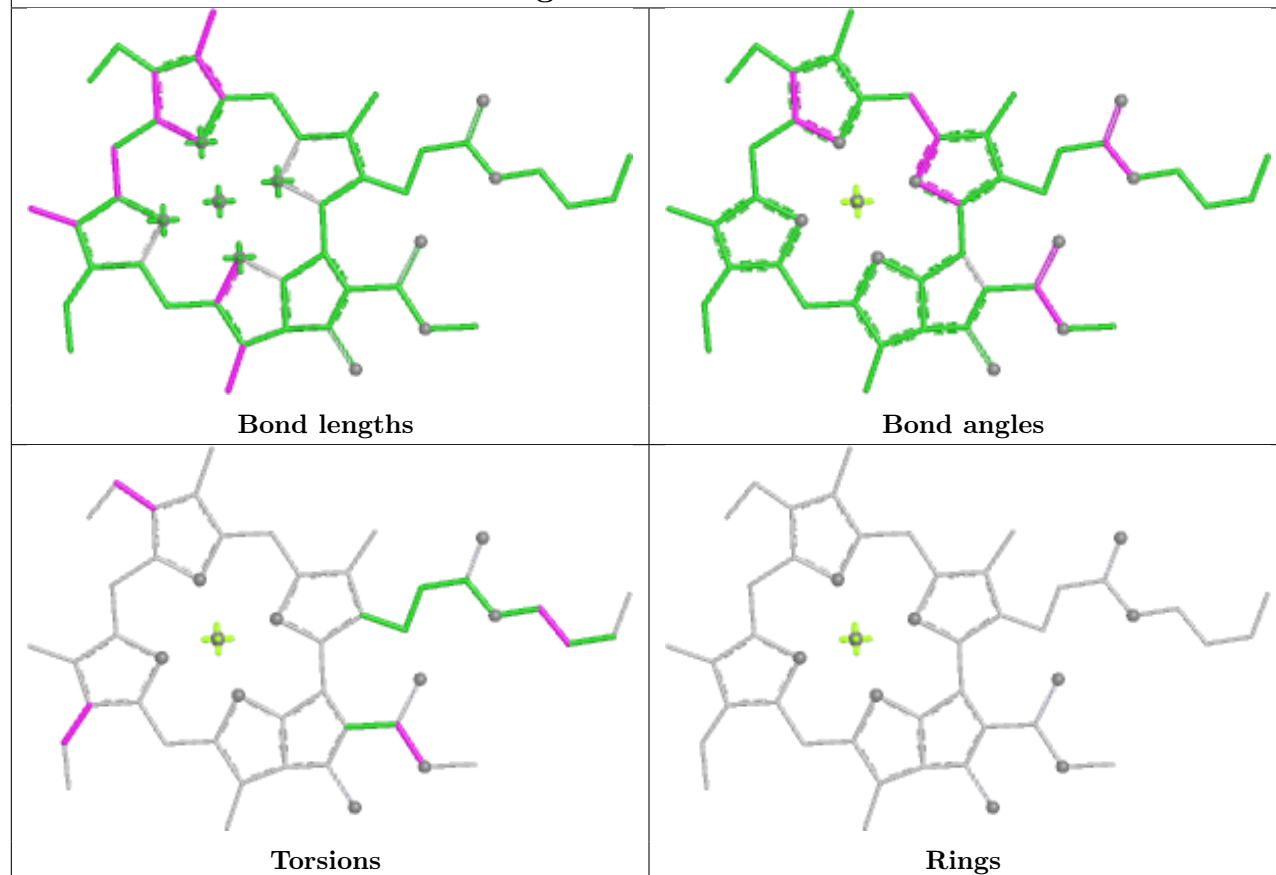




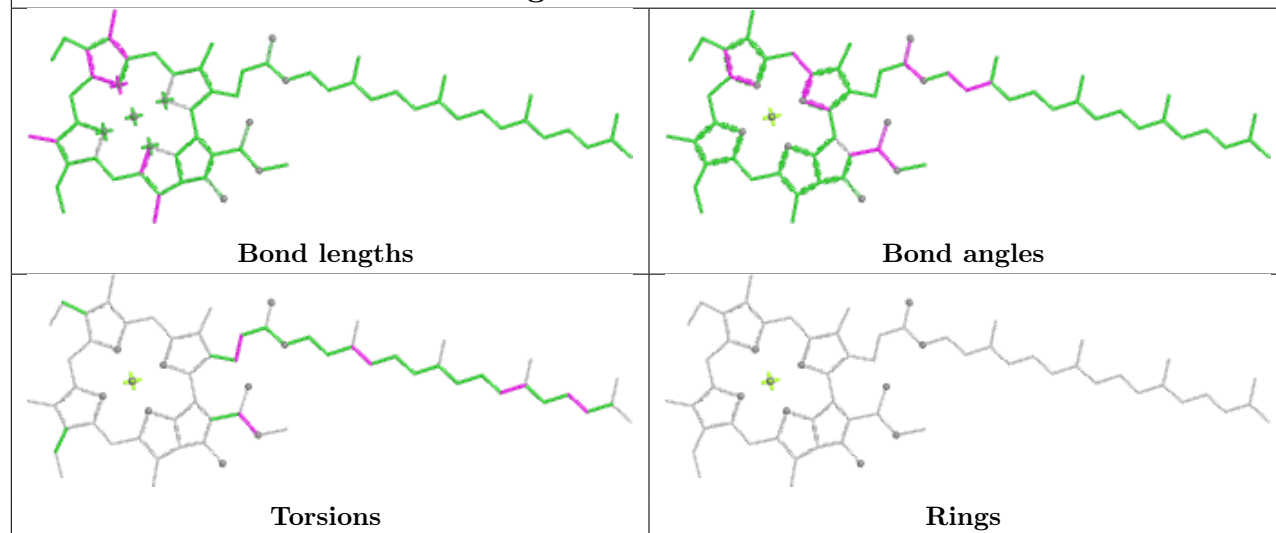


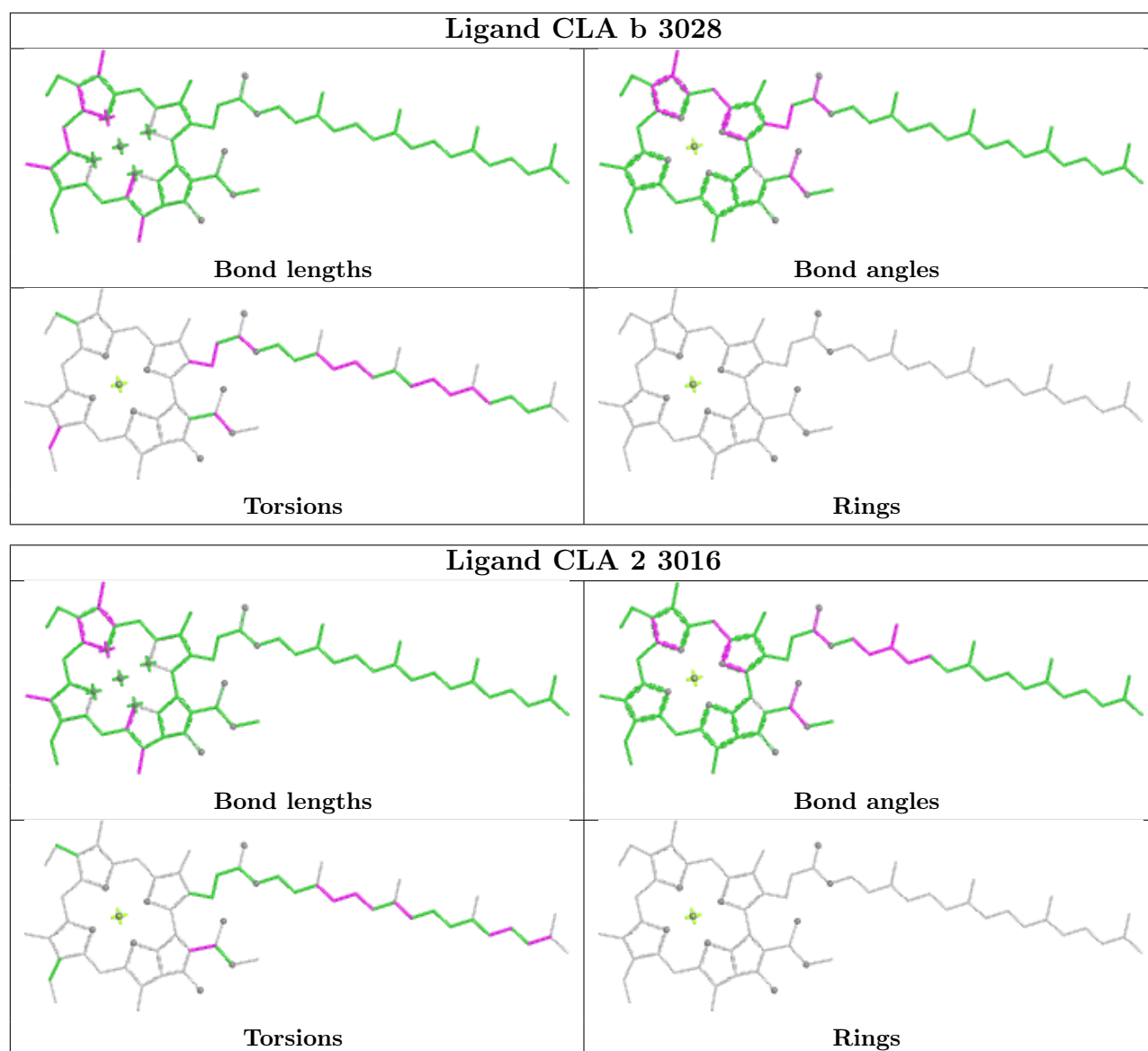


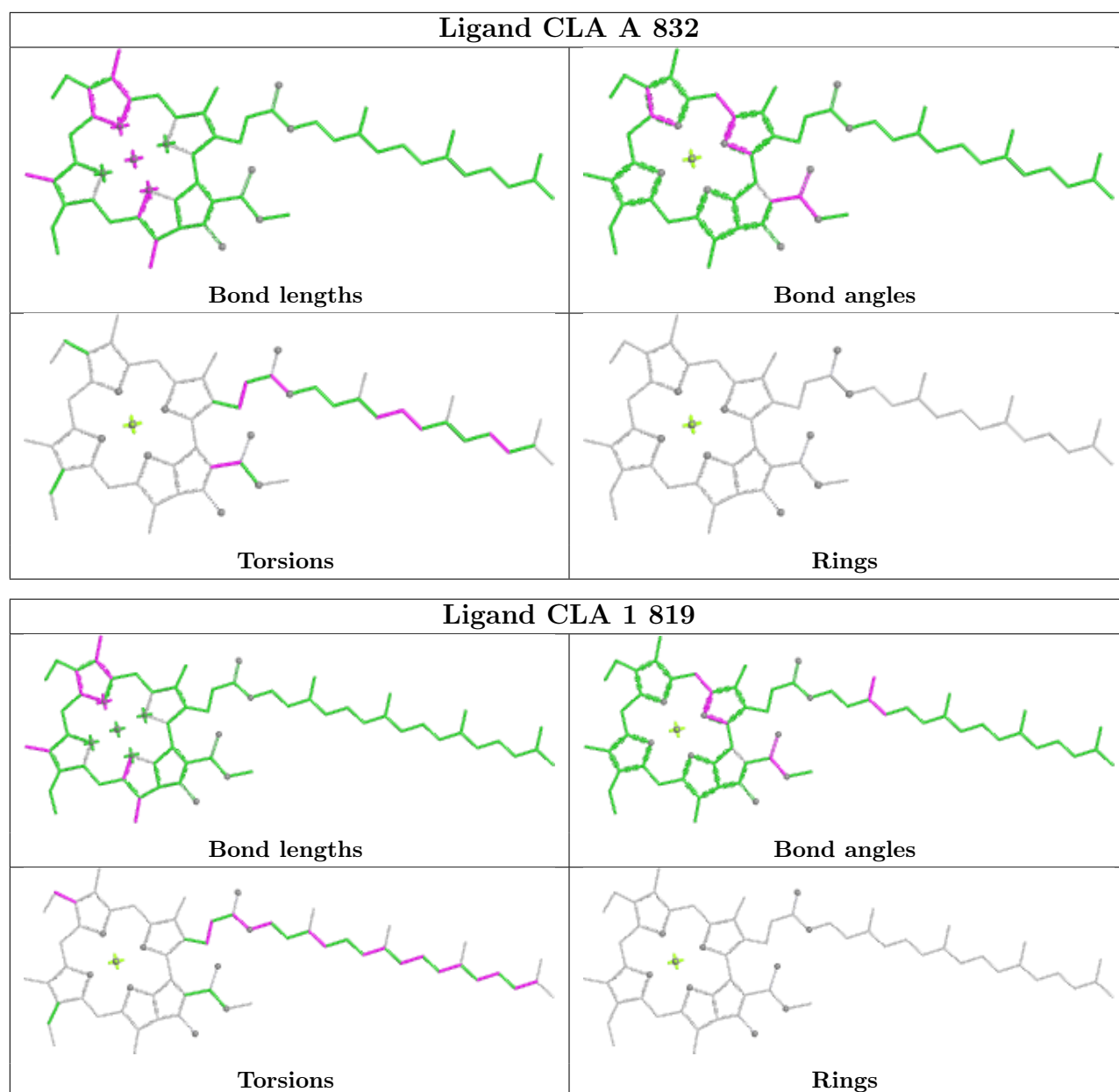
Ligand CLA a 810



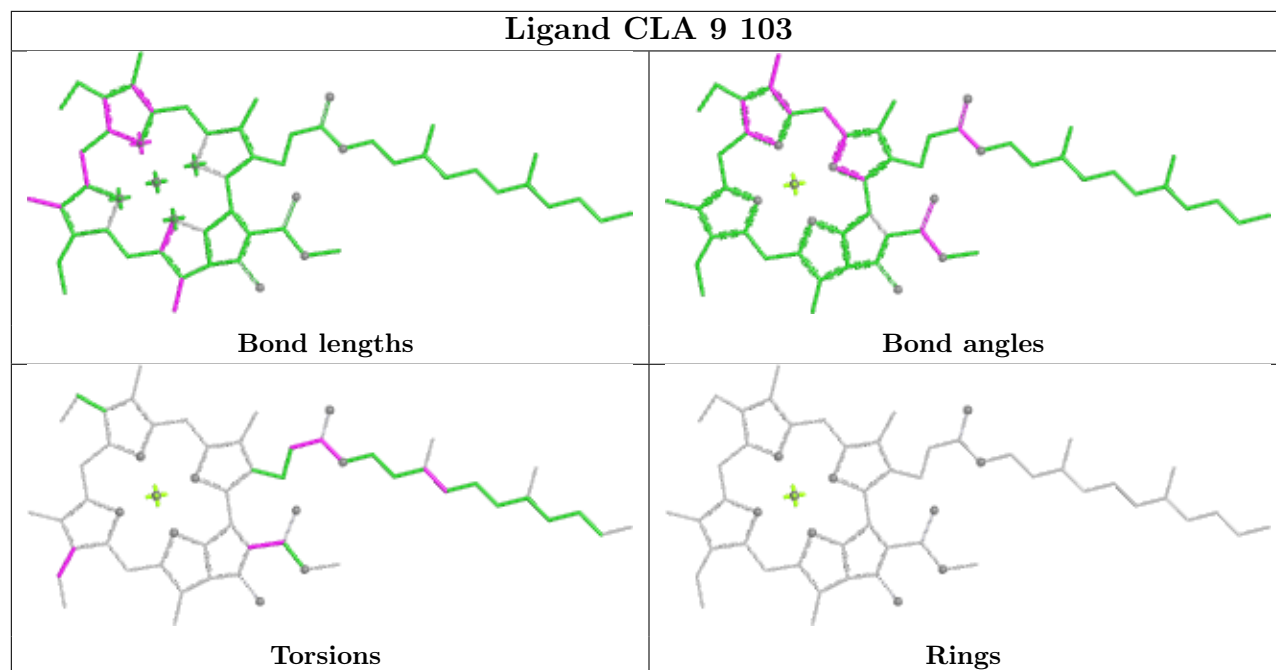
Ligand CLA 2 3009



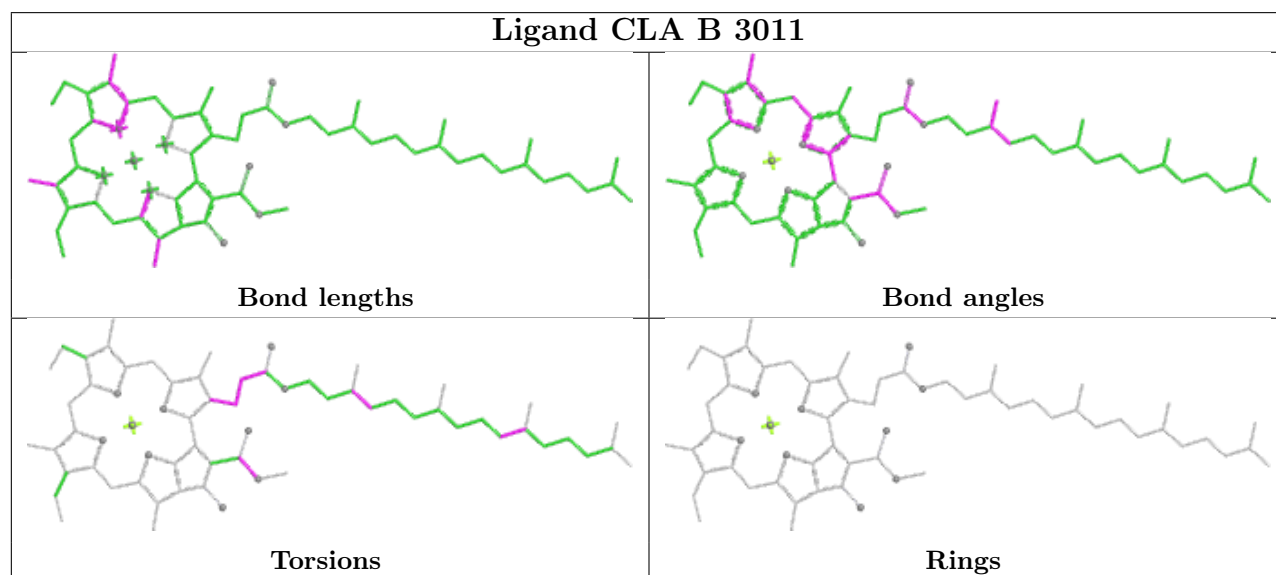


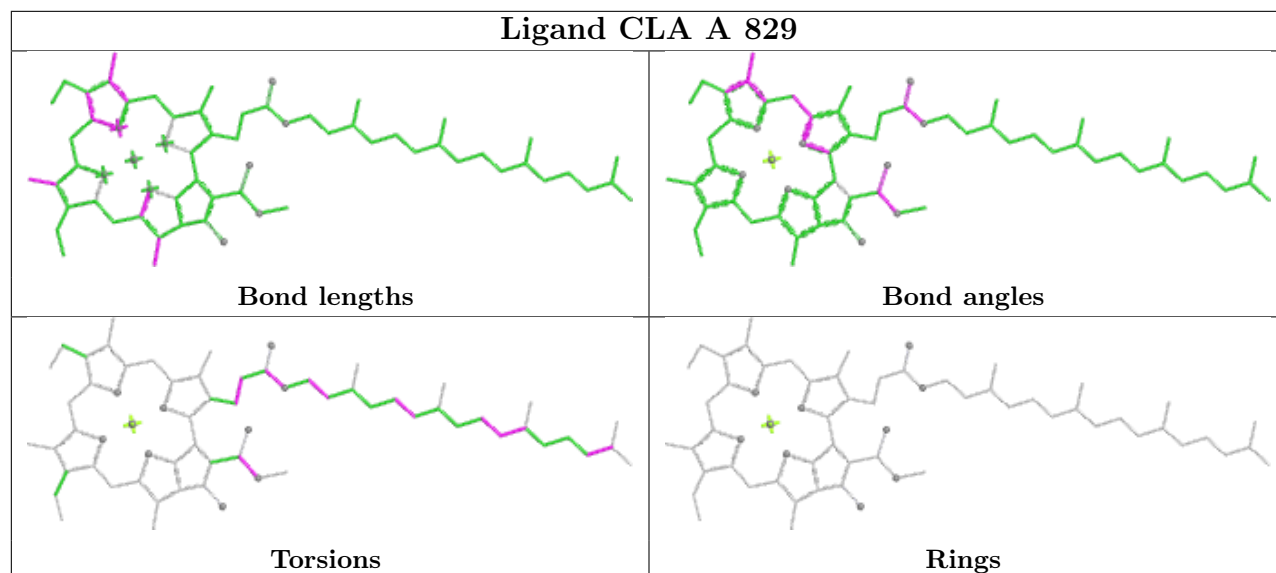
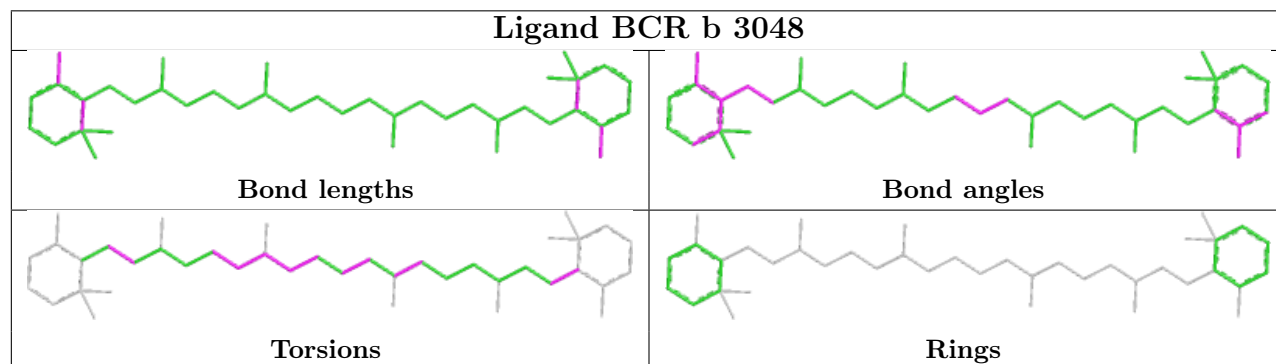
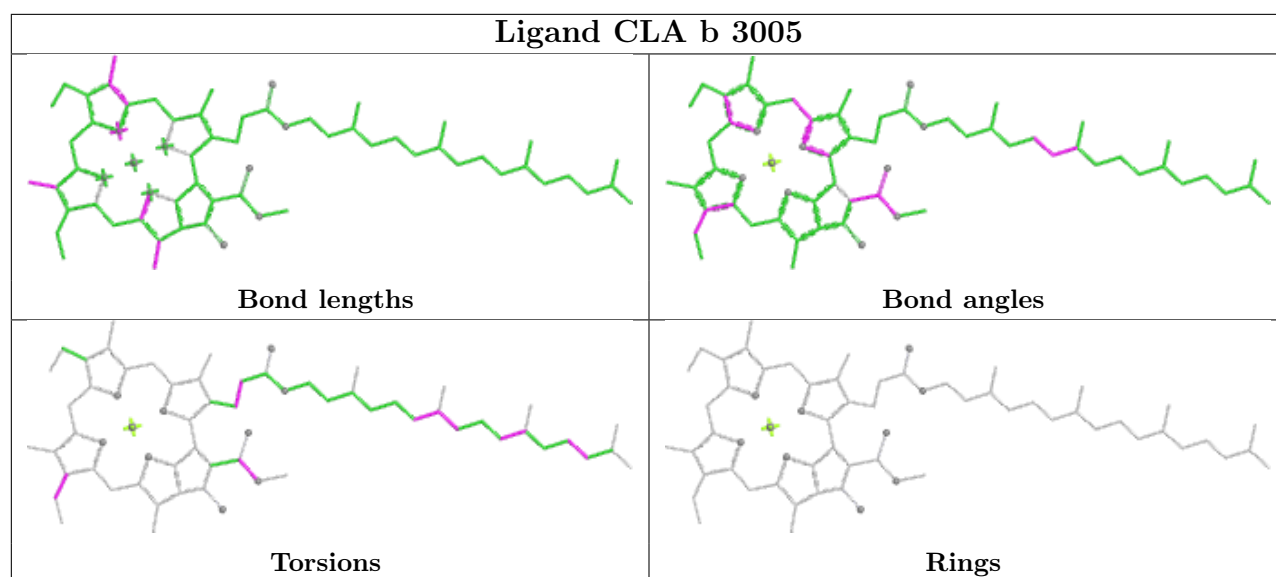


Ligand CLA 9 103

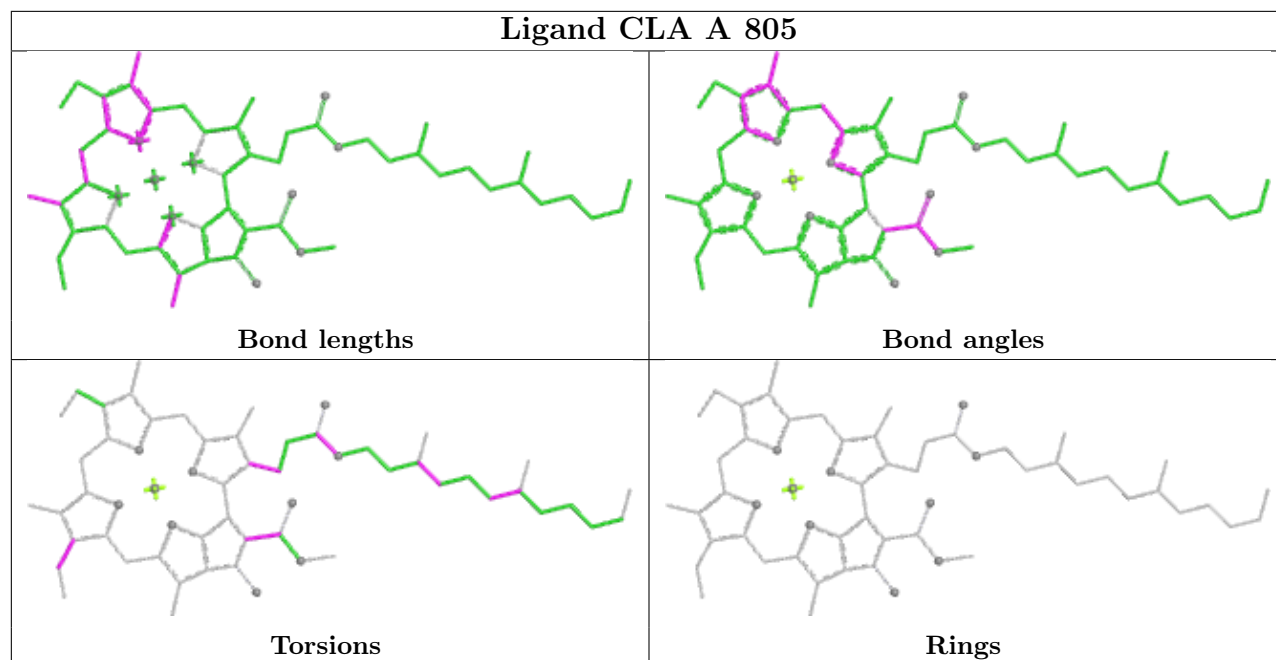


Ligand CLA B 3011

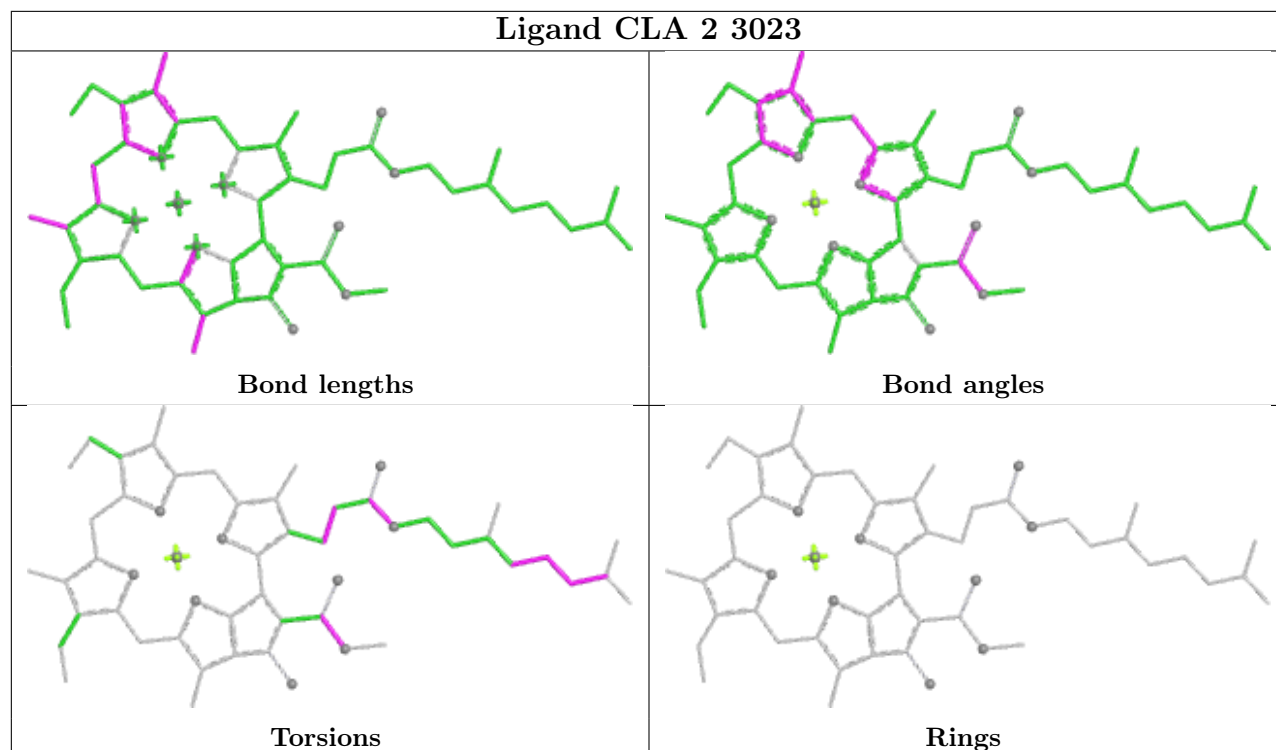




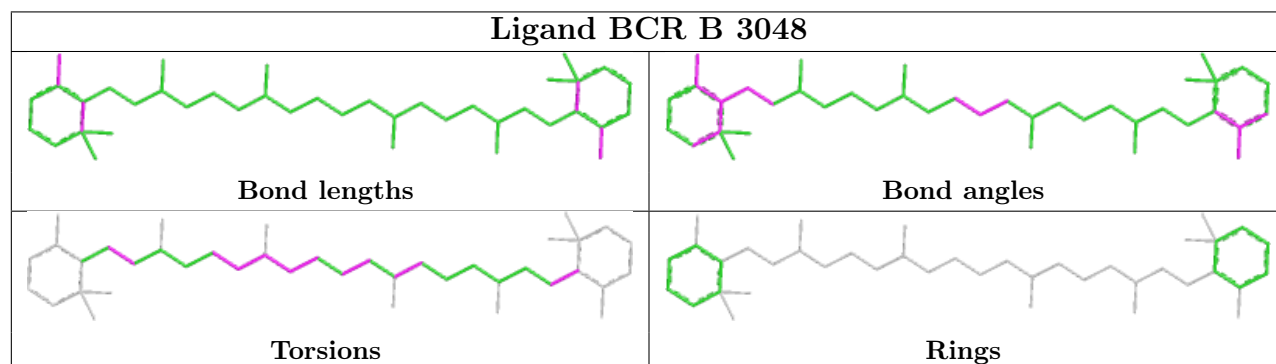
Ligand CLA A 805

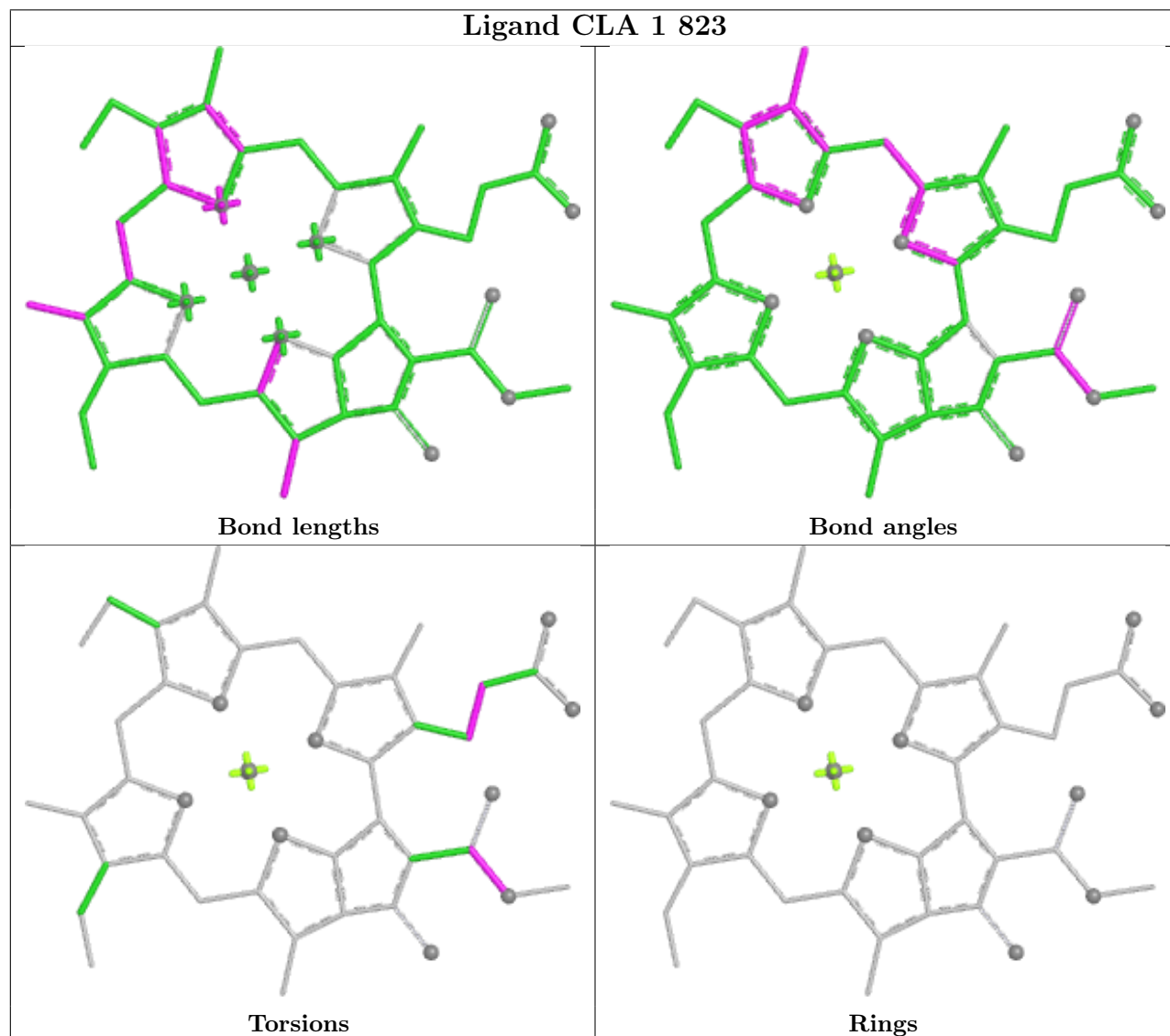
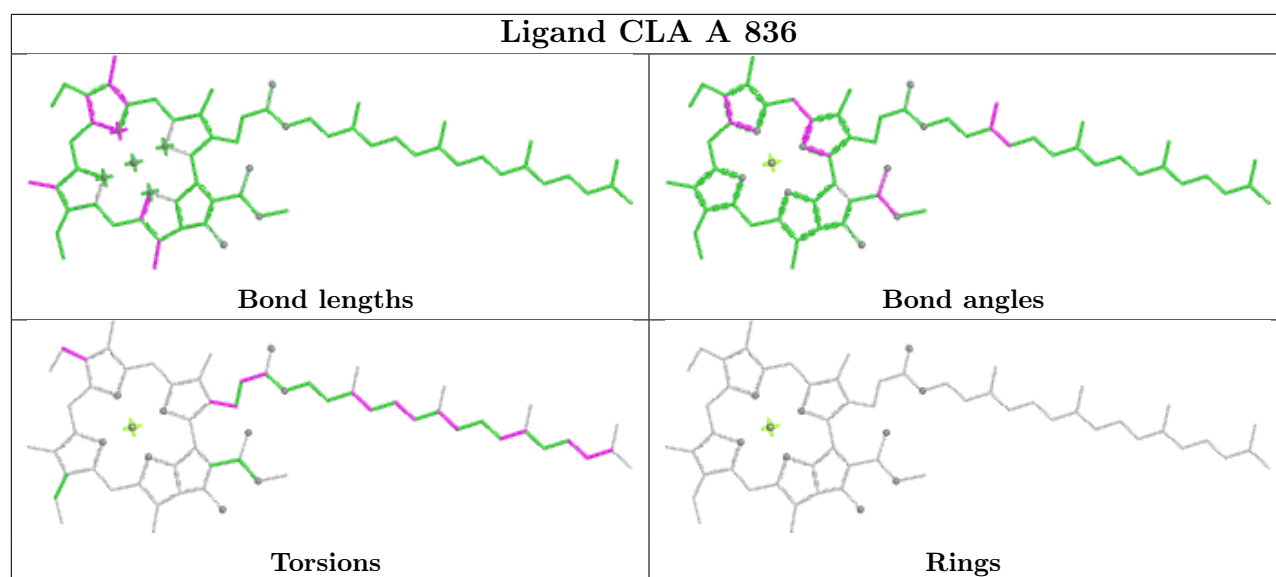


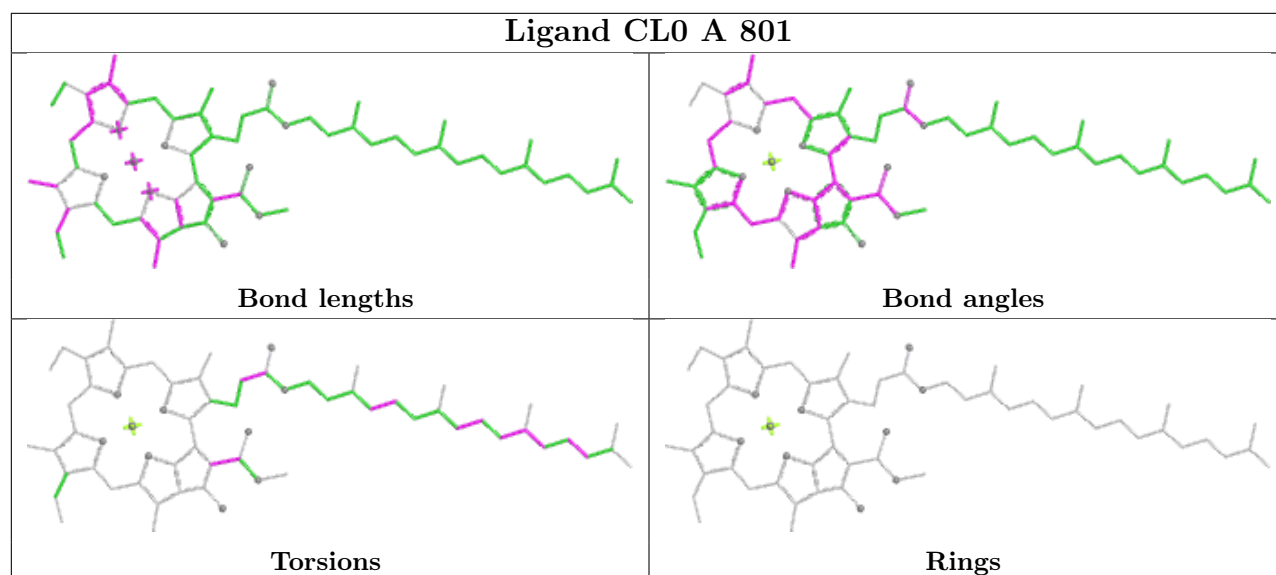
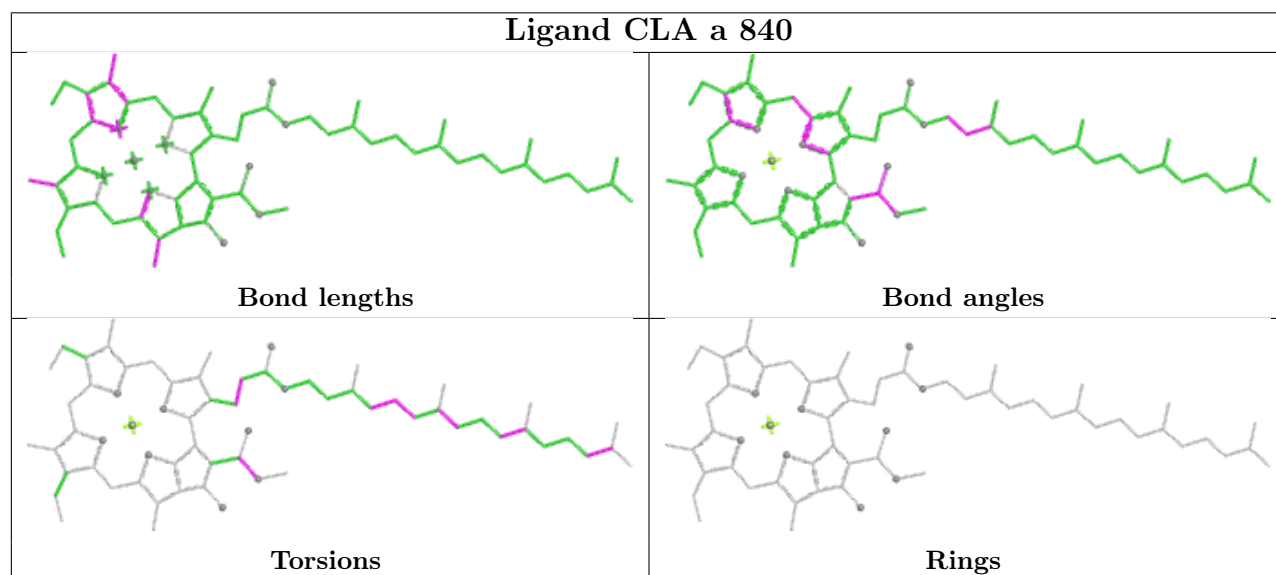
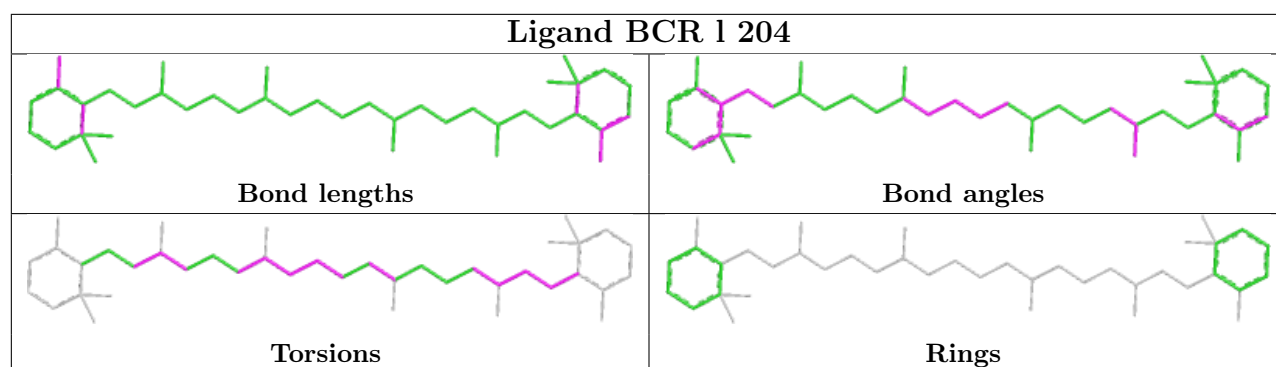
Ligand CLA 2 3023

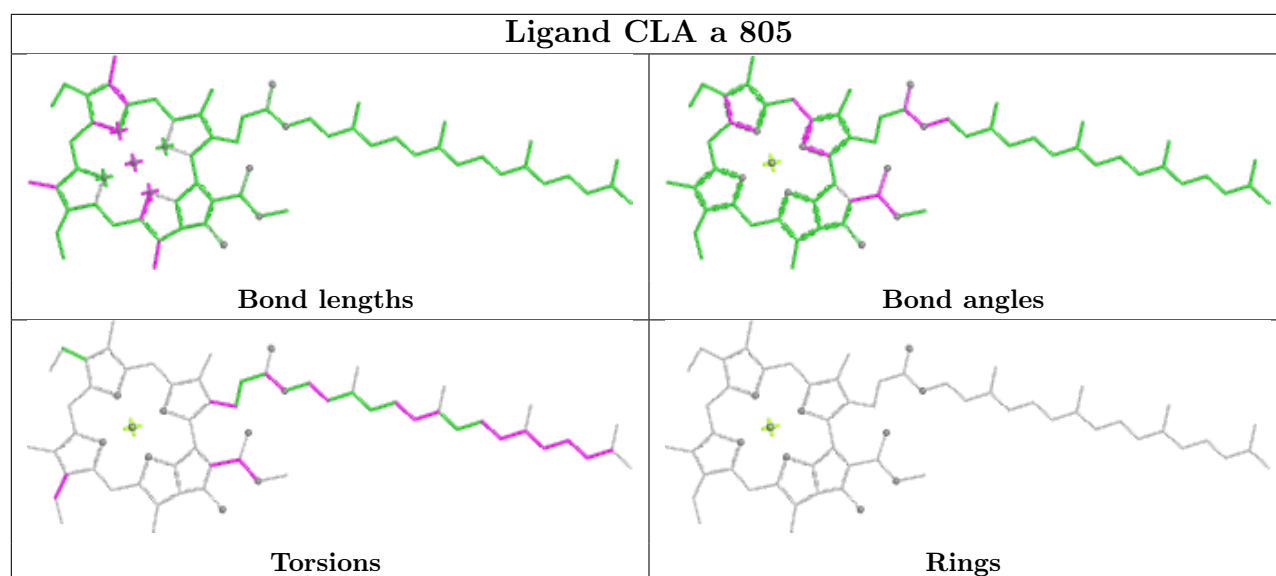
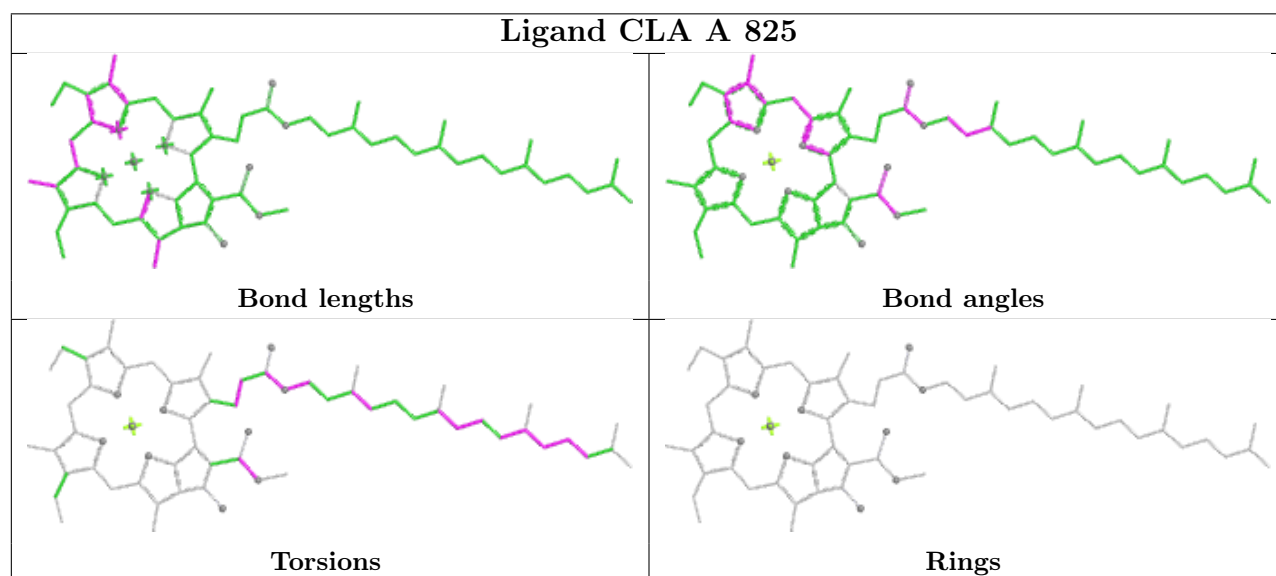
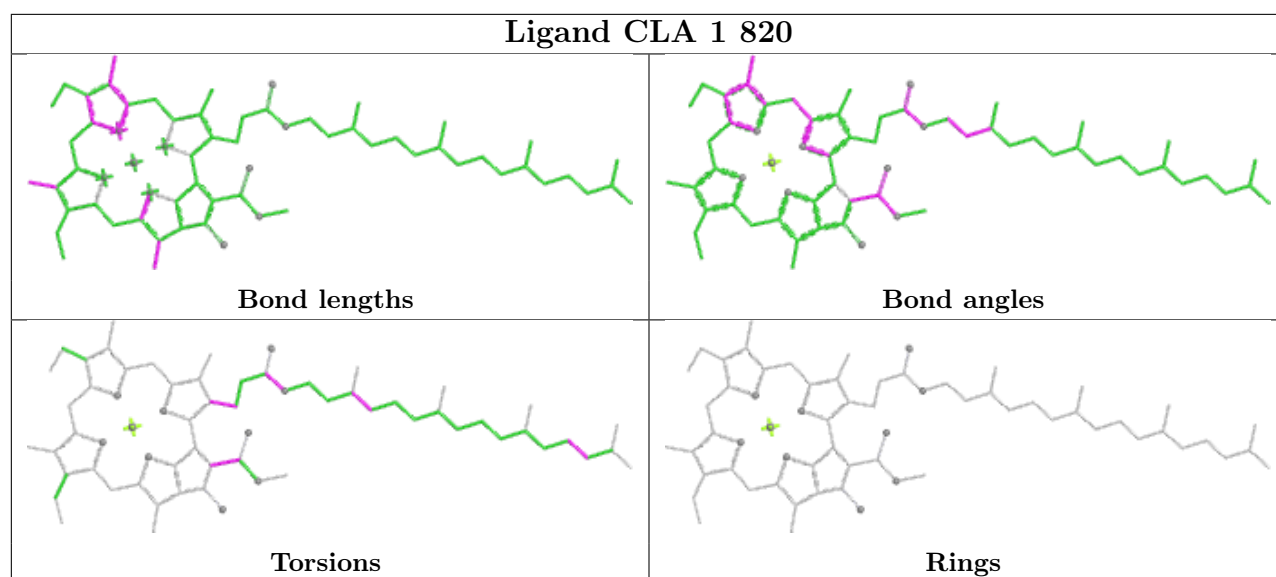


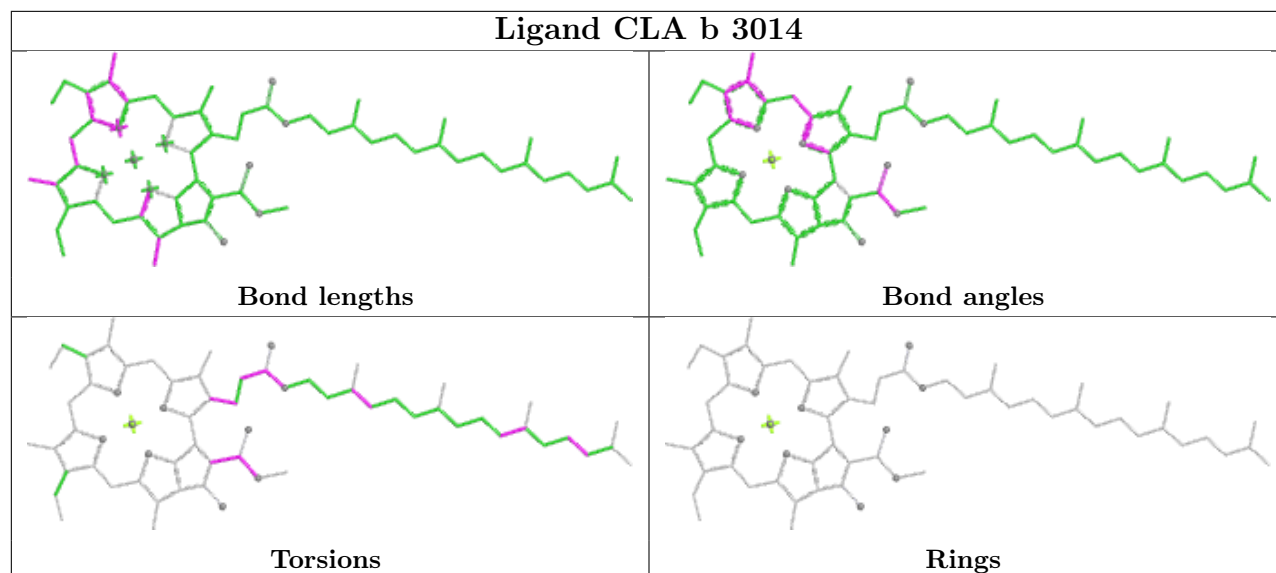
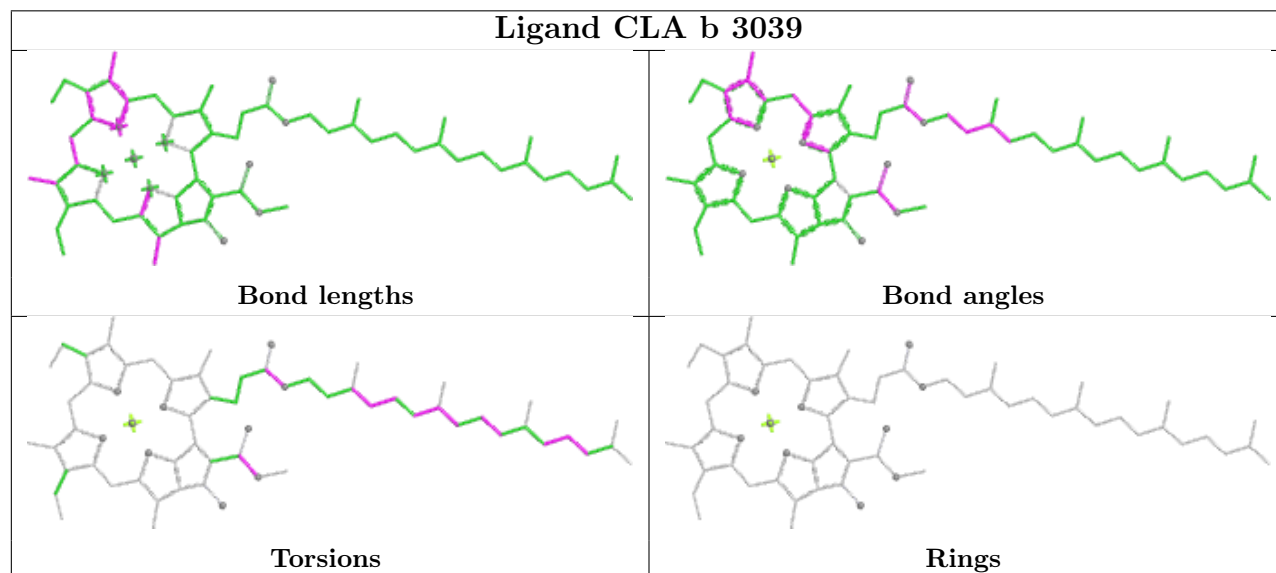
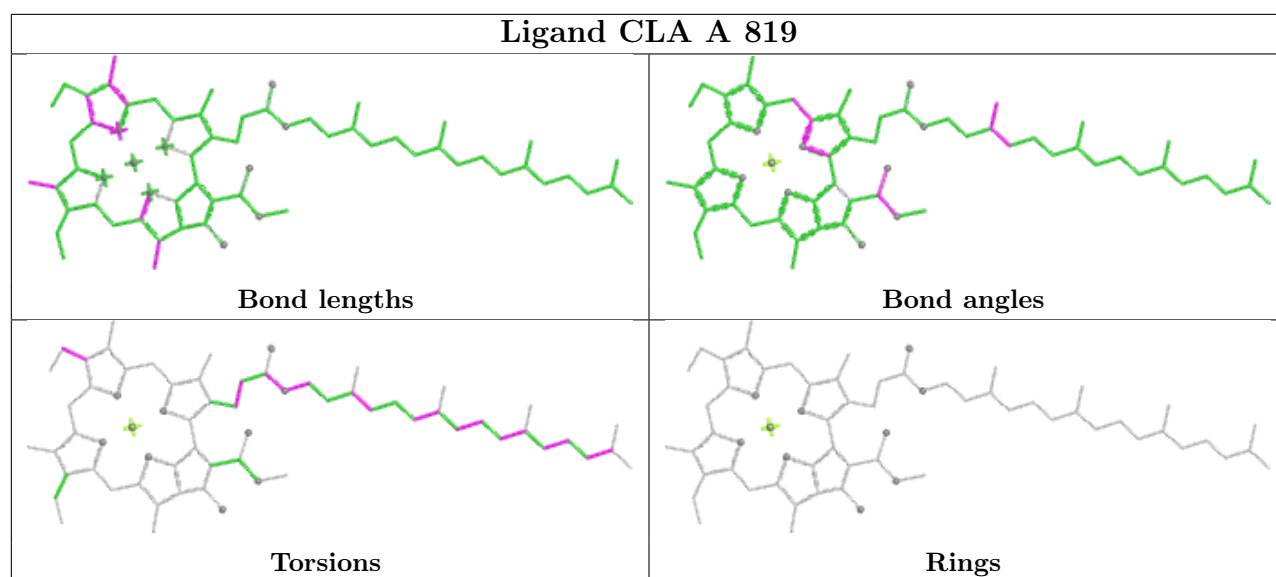
Ligand BCR B 3048

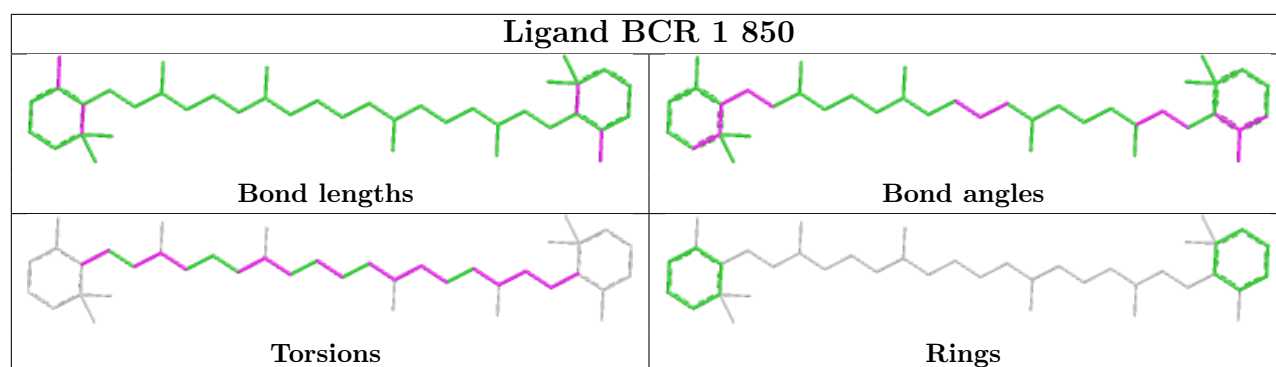
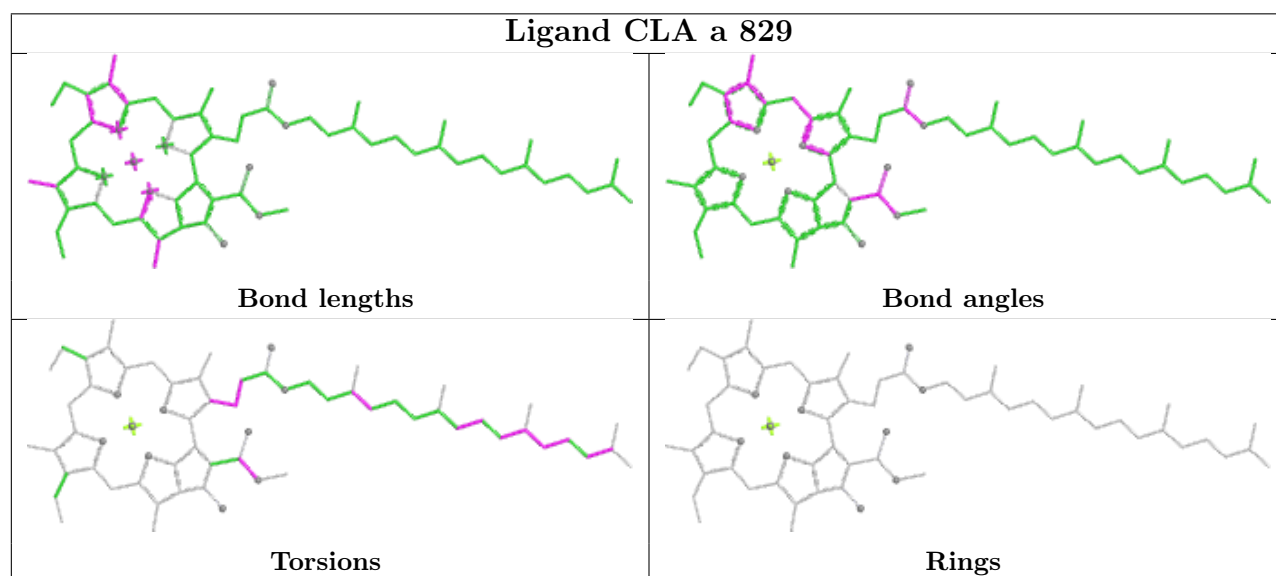
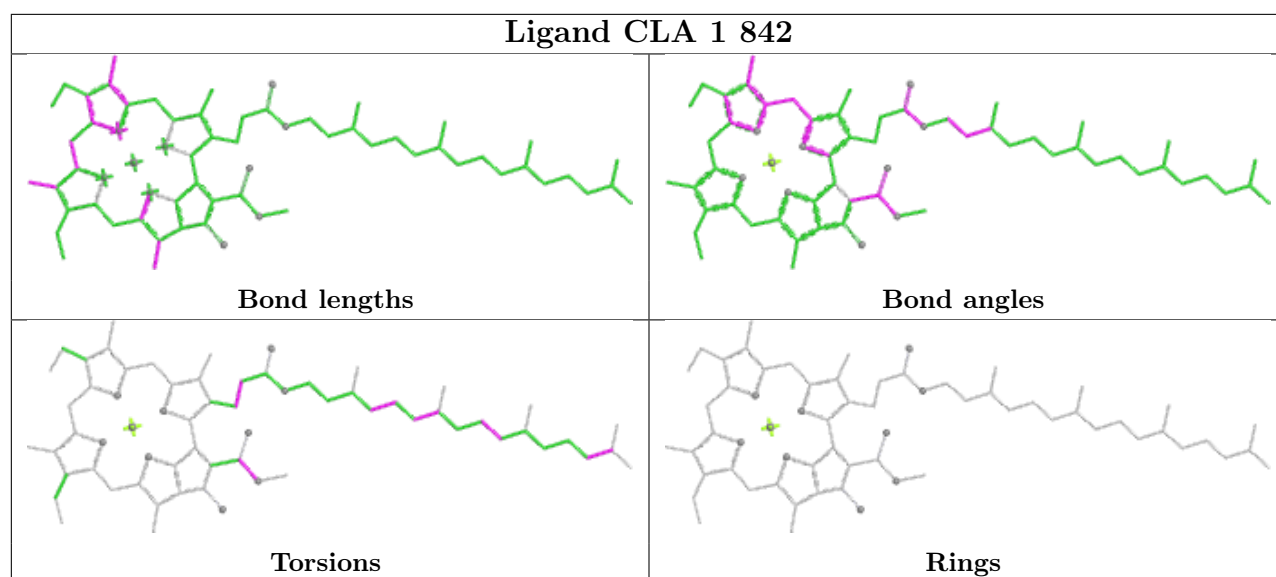


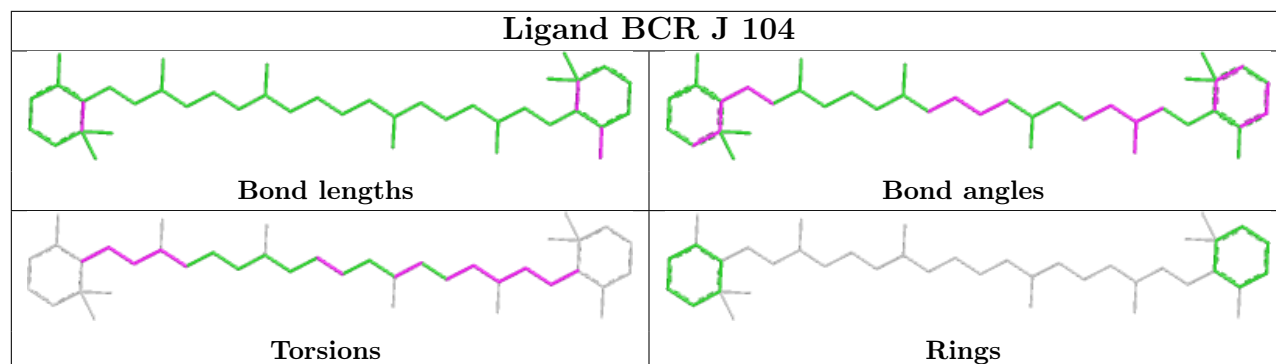
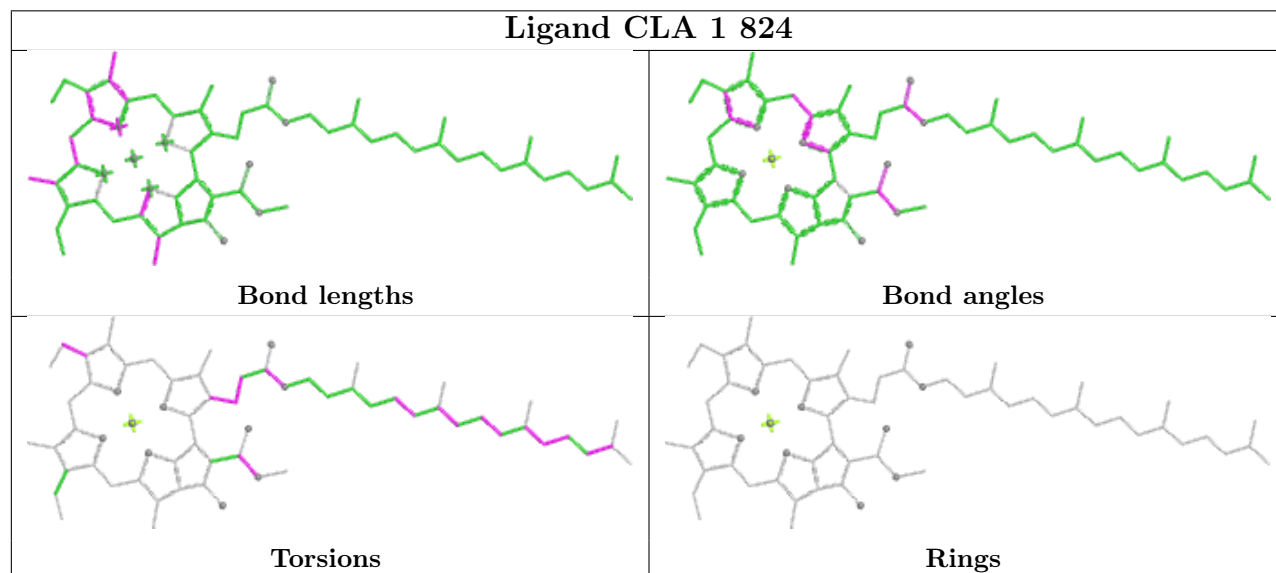
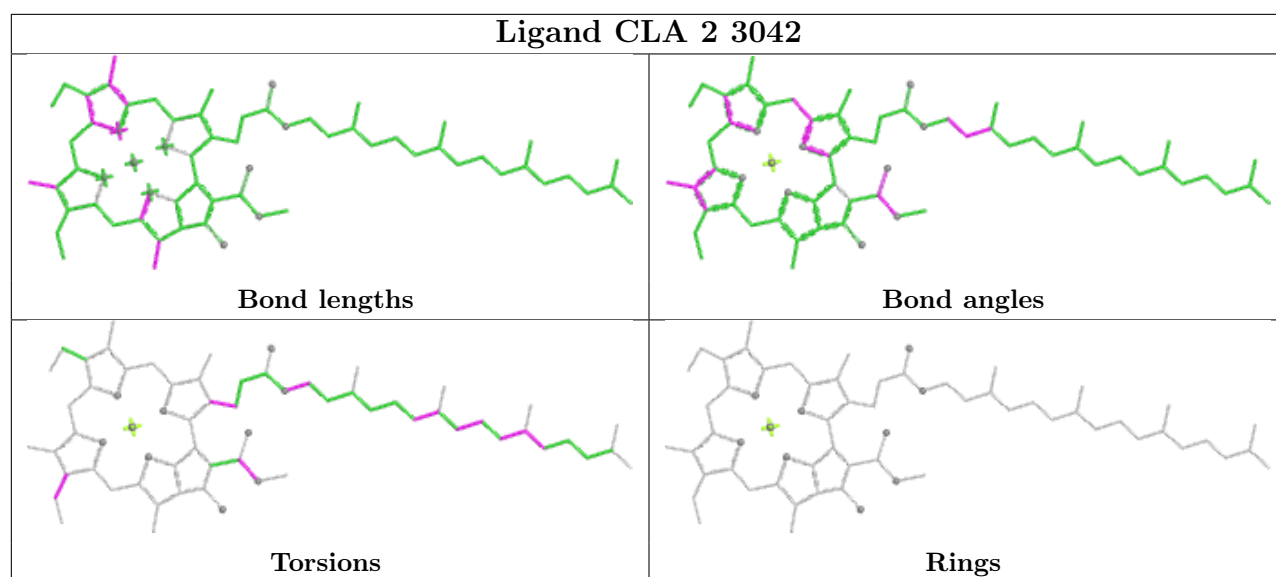


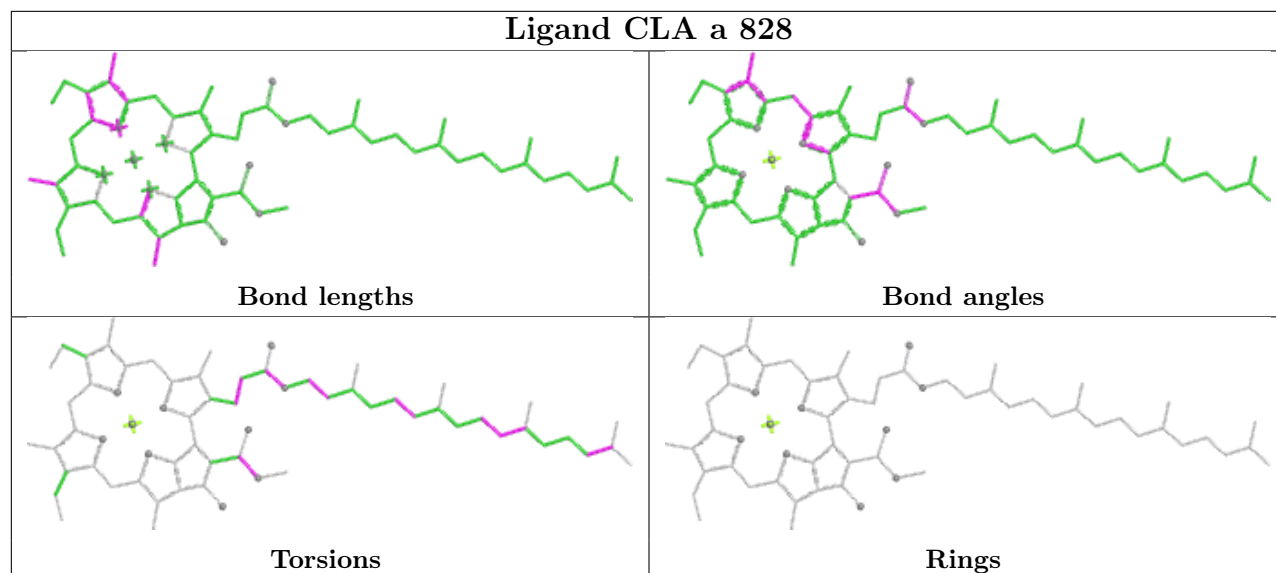
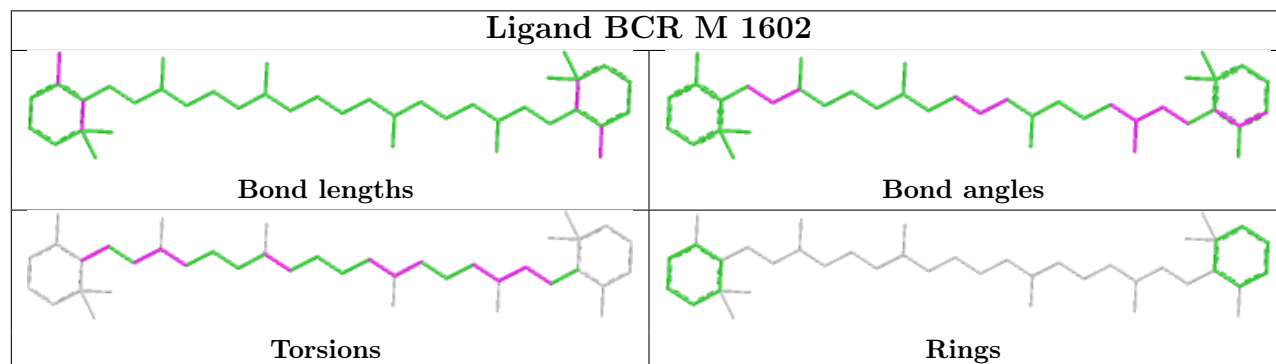
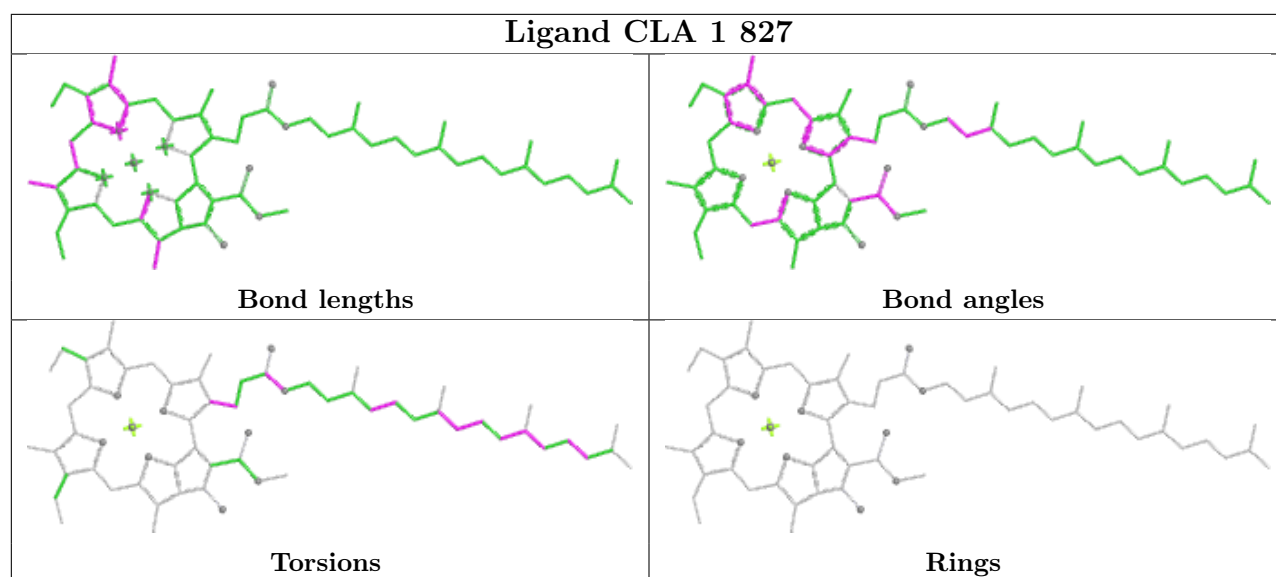


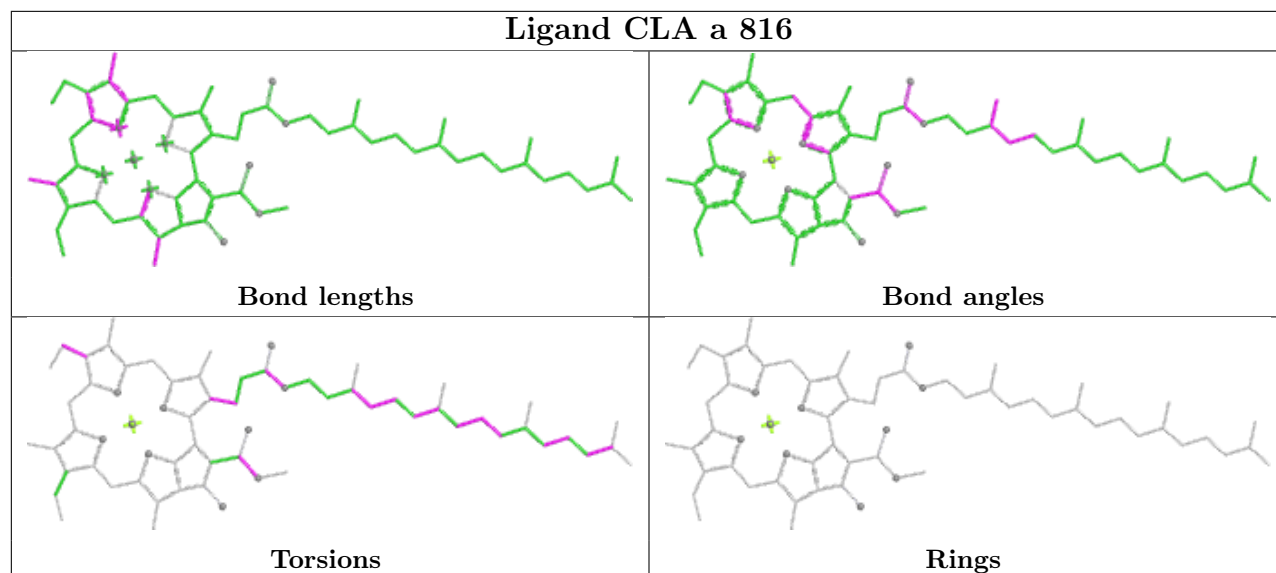
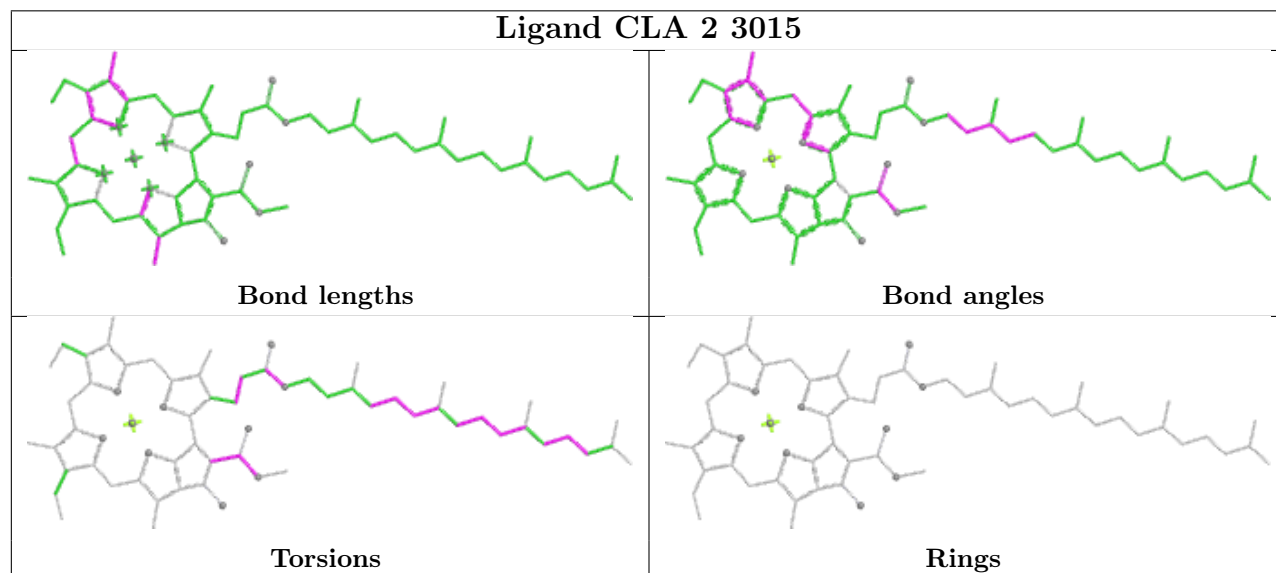
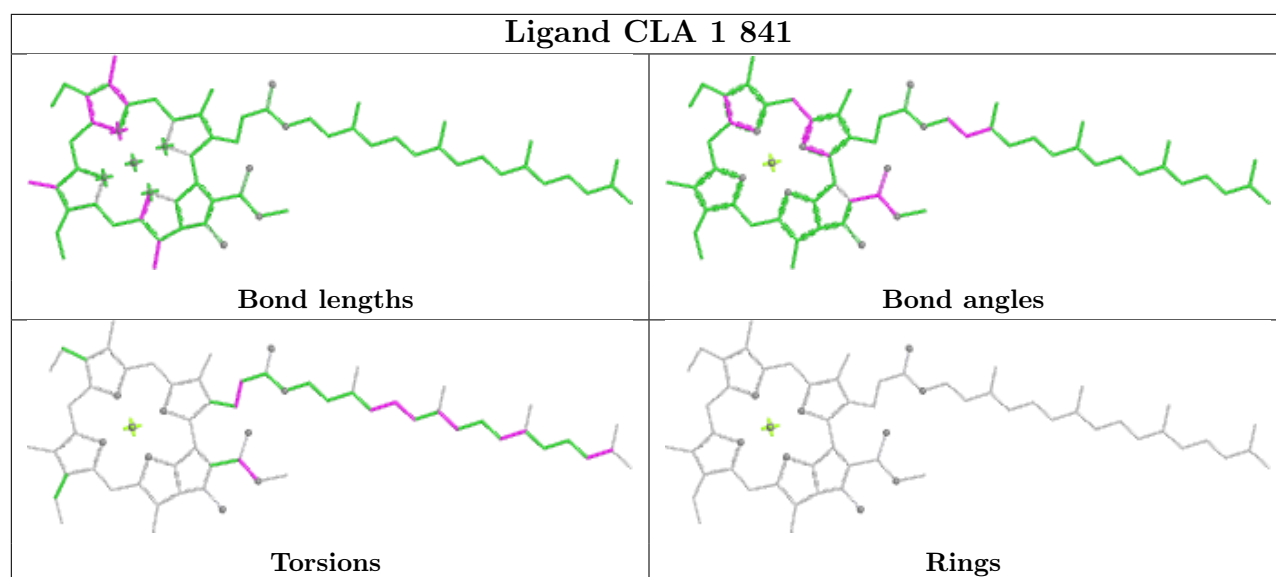


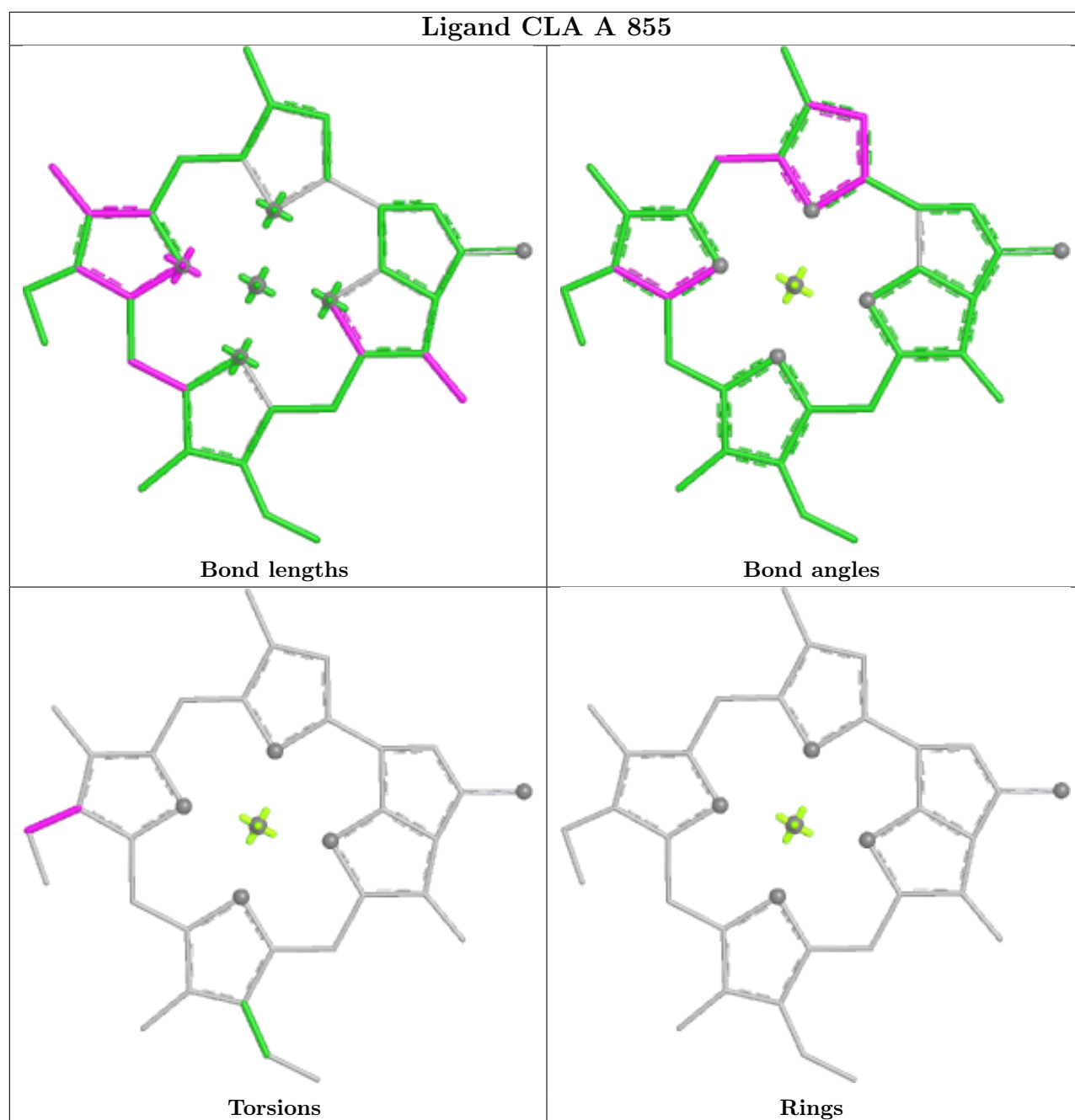


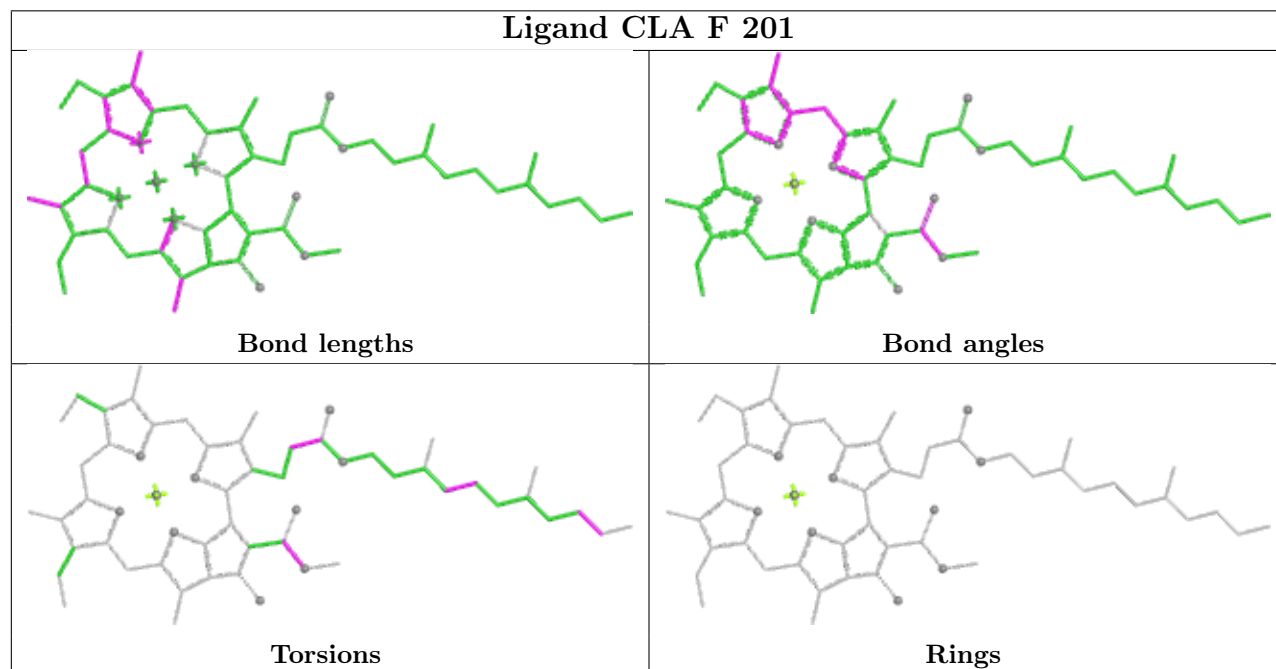
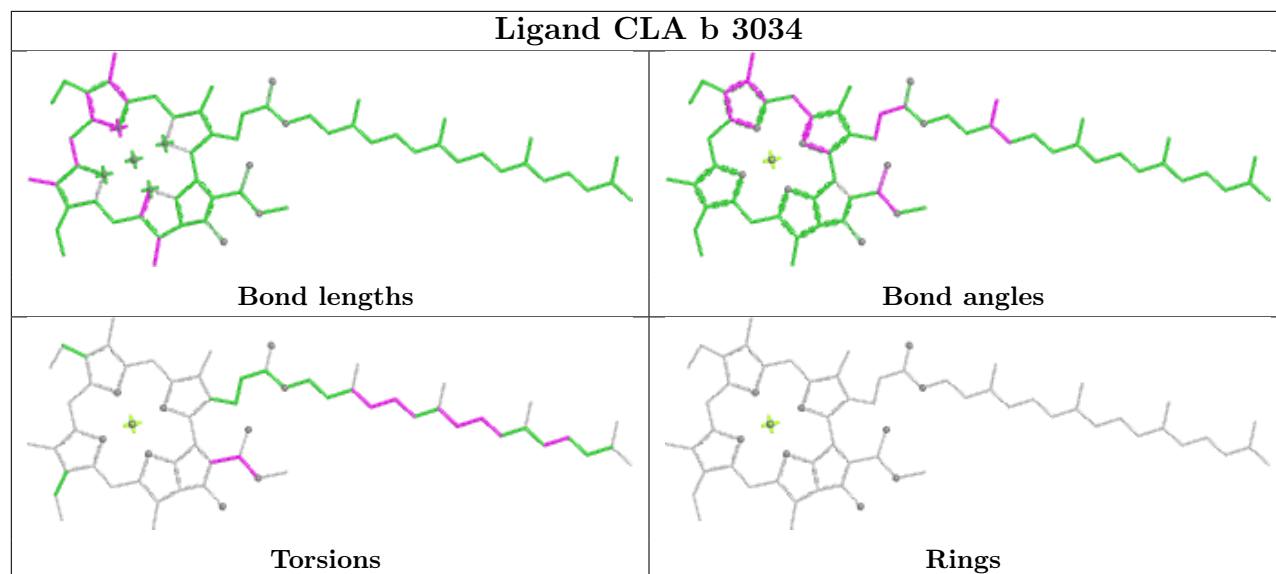




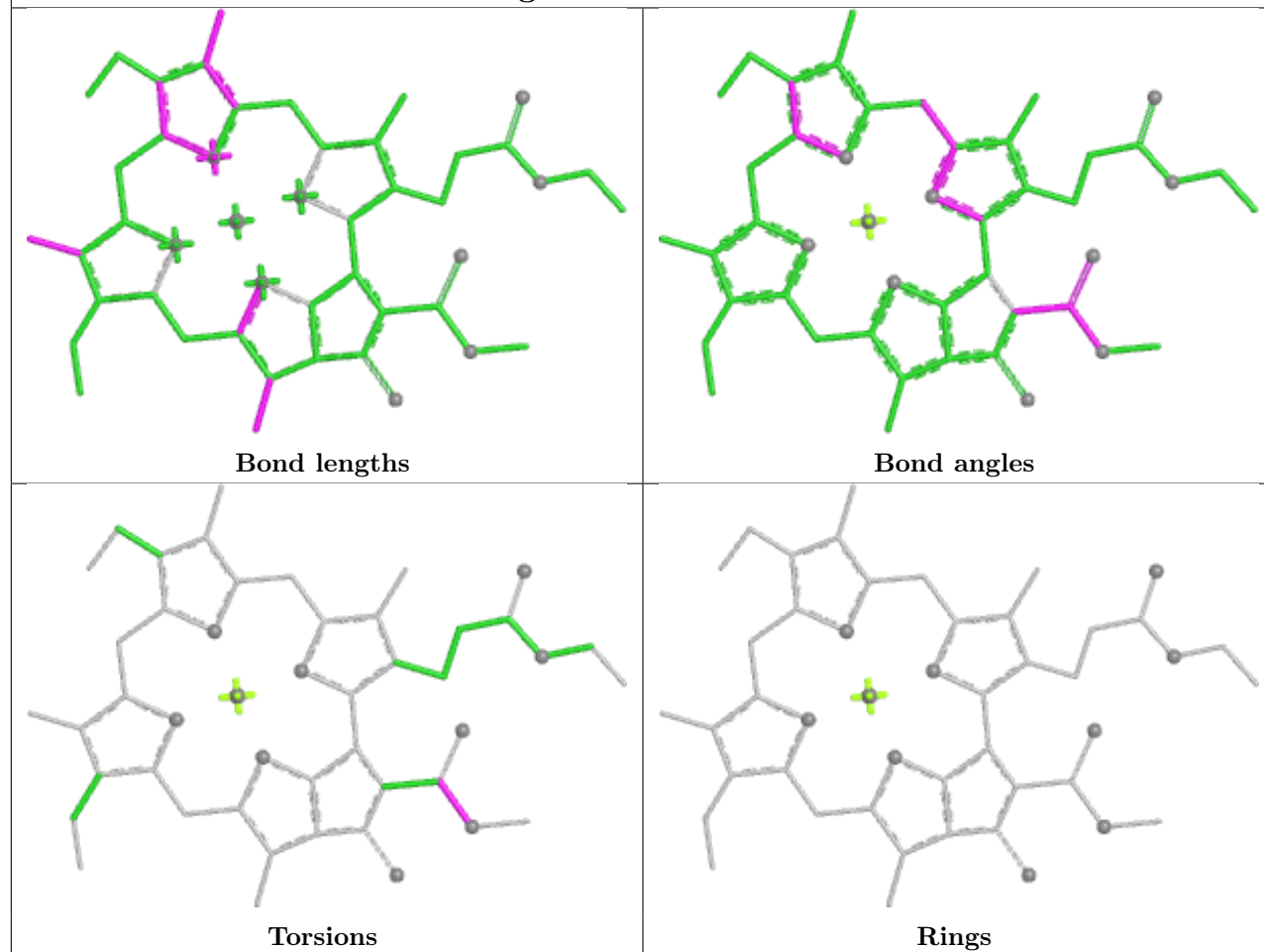




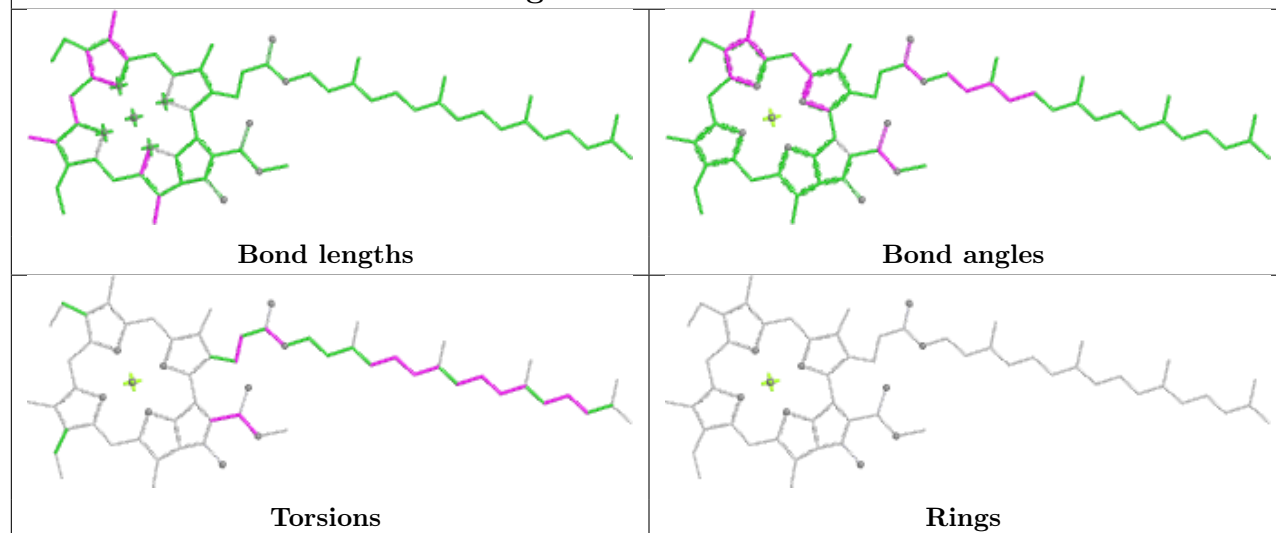


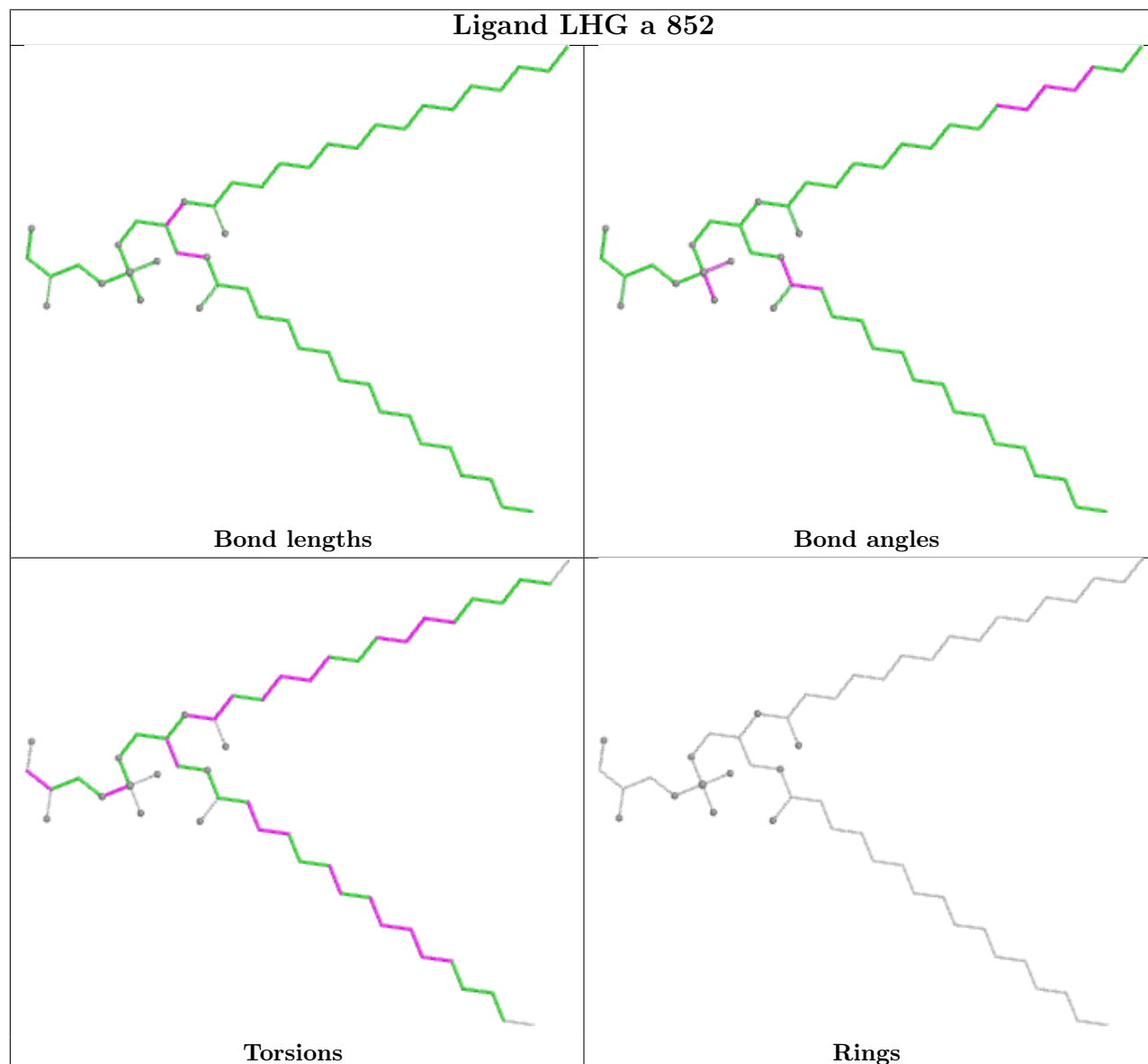
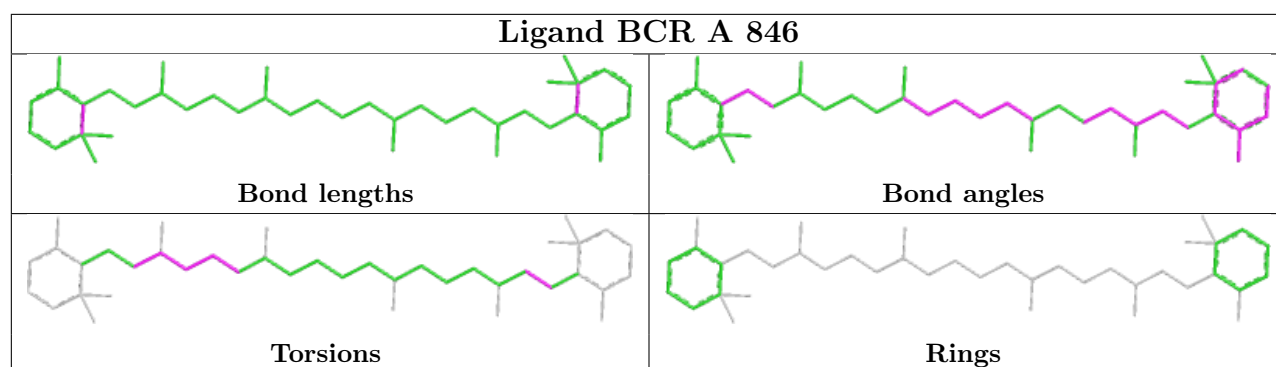


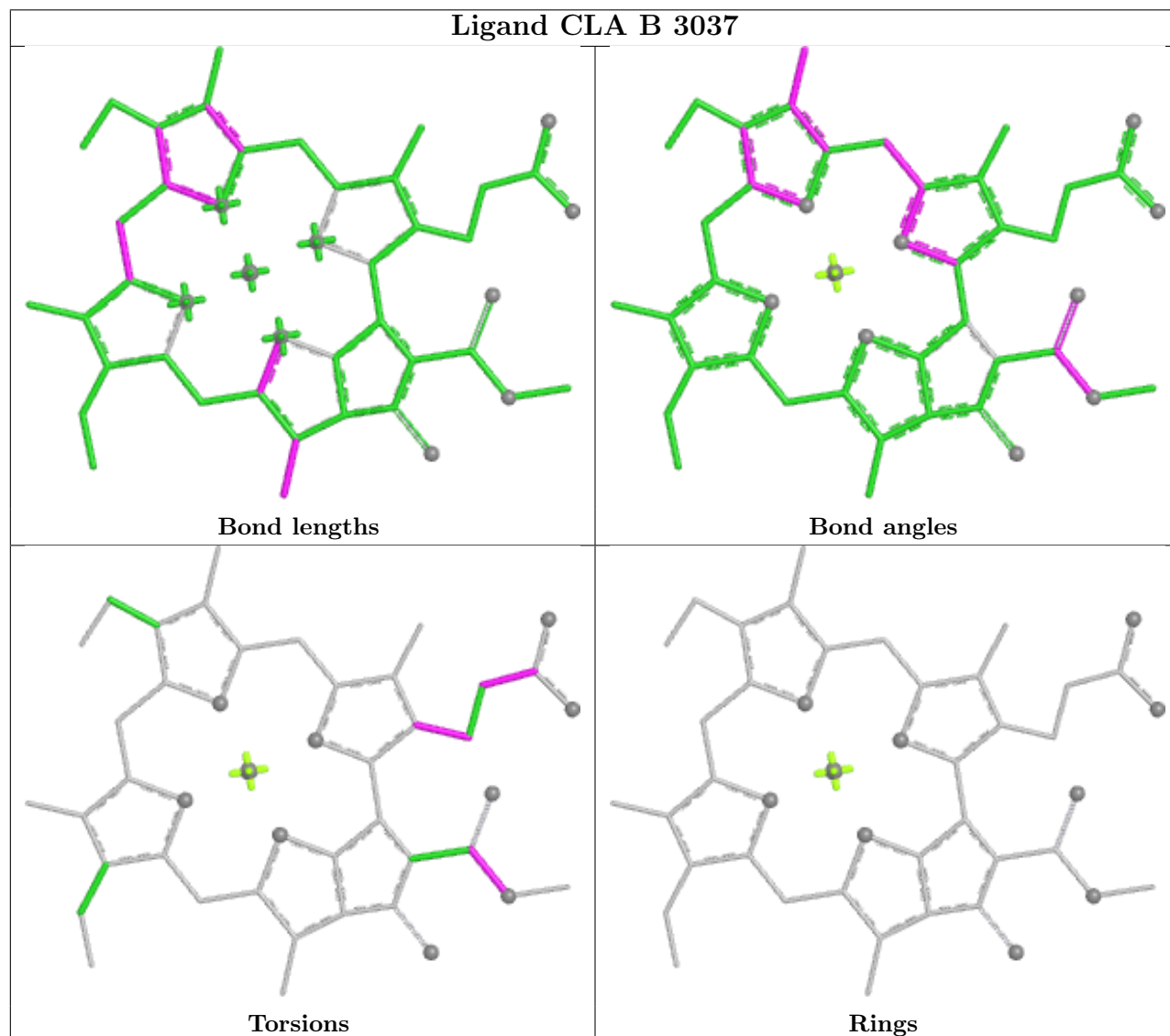
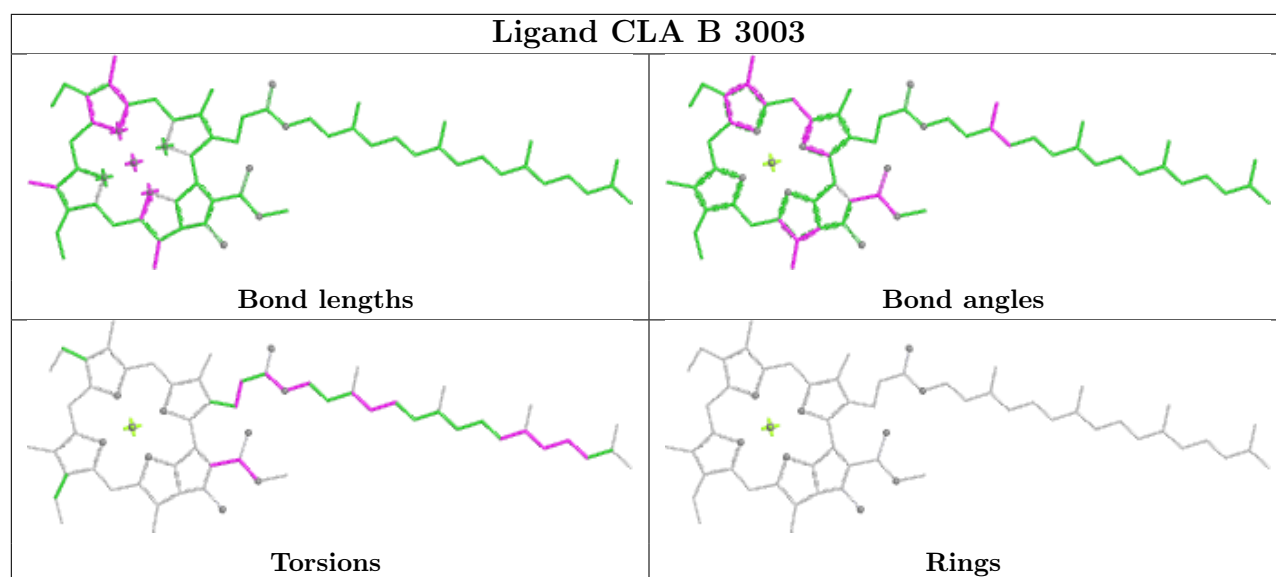
Ligand CLA B 3040

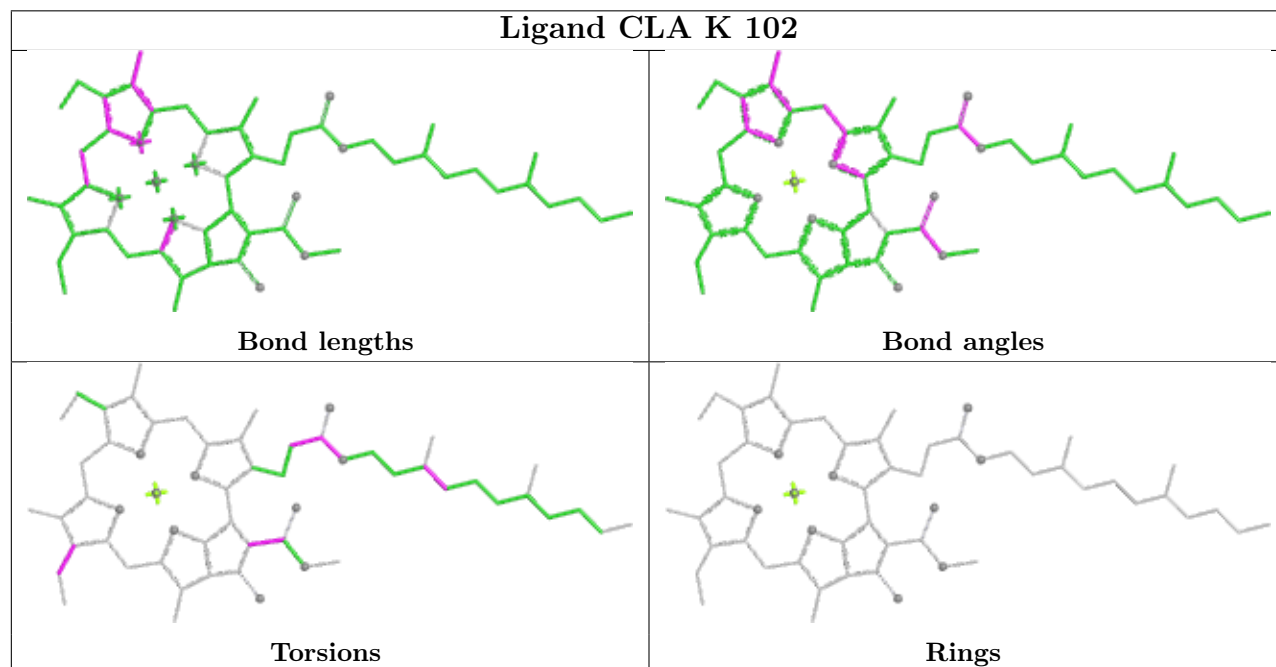
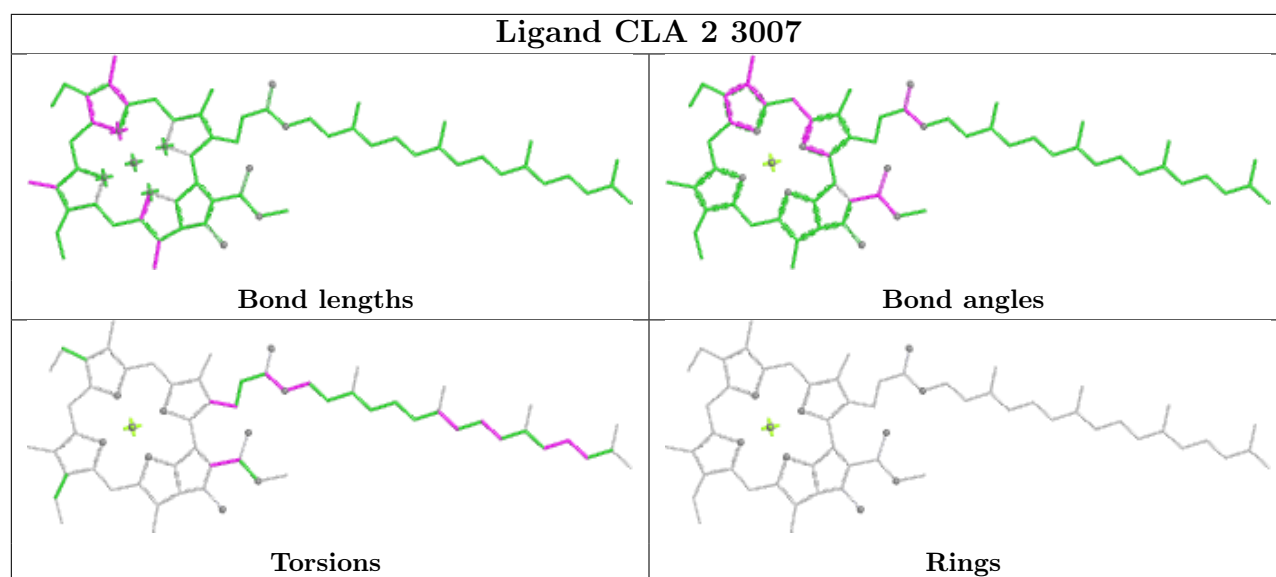


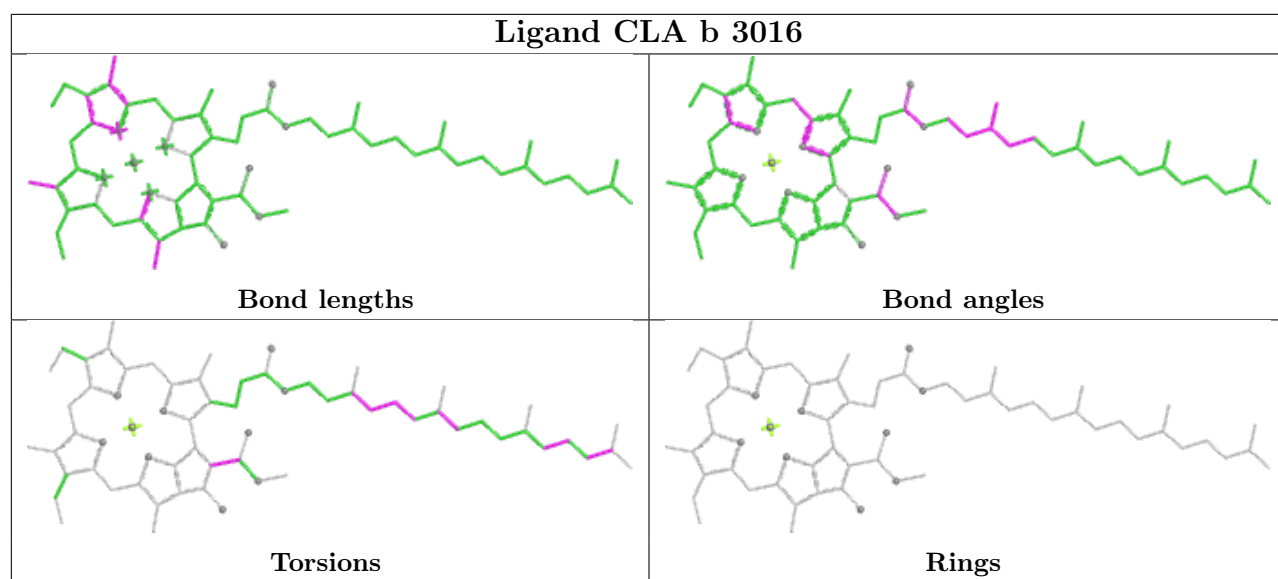
Ligand CLA b 3015



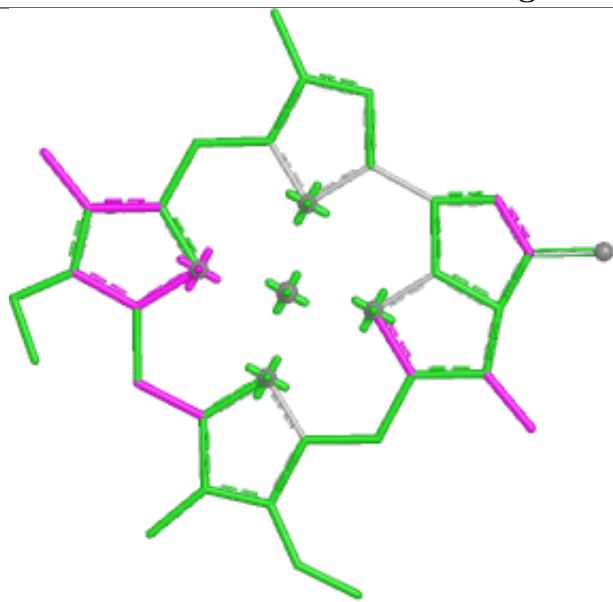




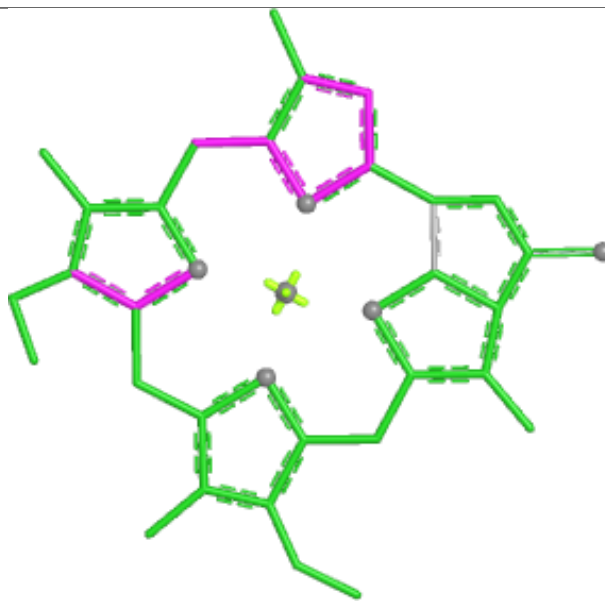




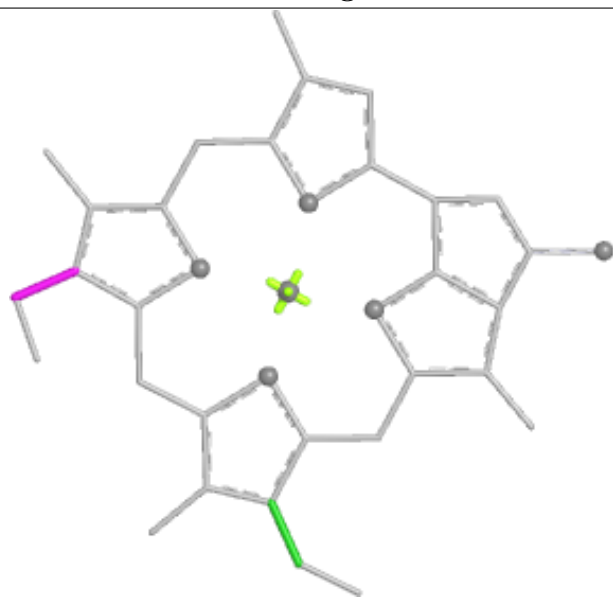
Ligand CLA 0 203



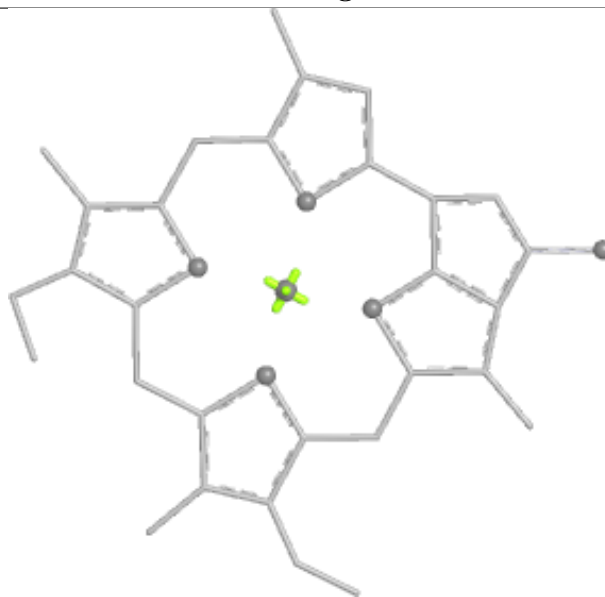
Bond lengths



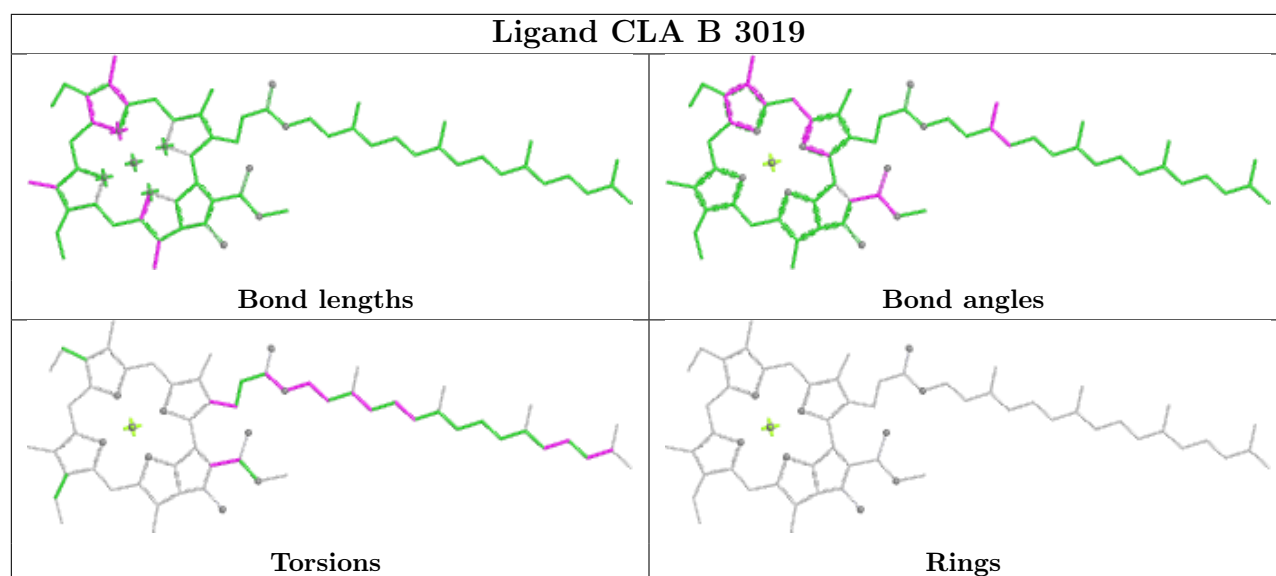
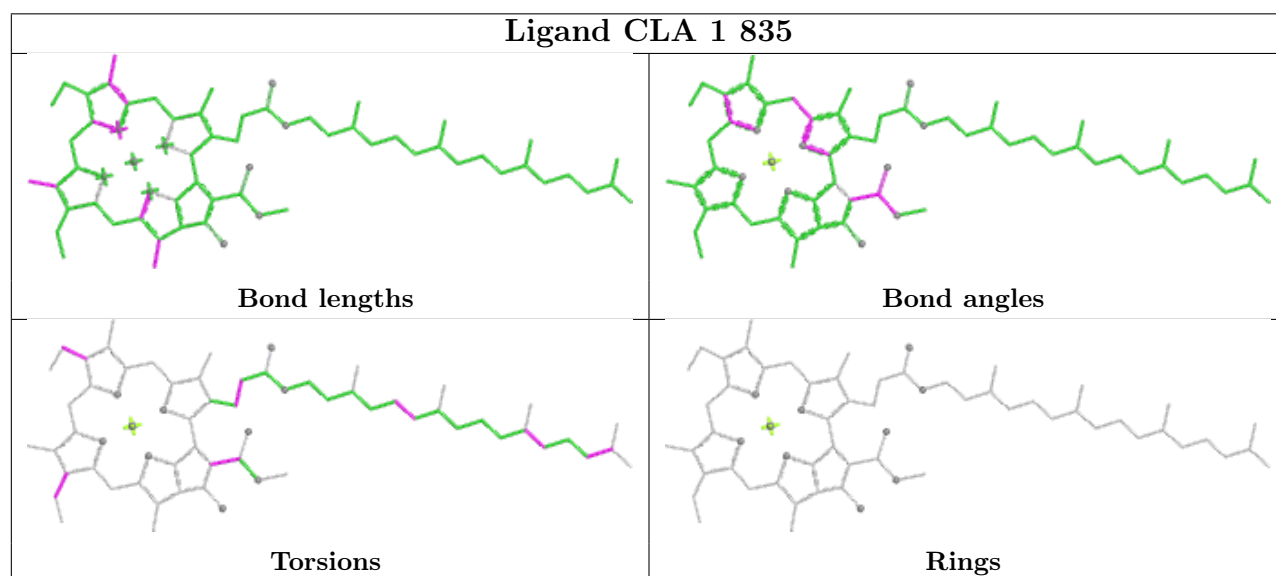
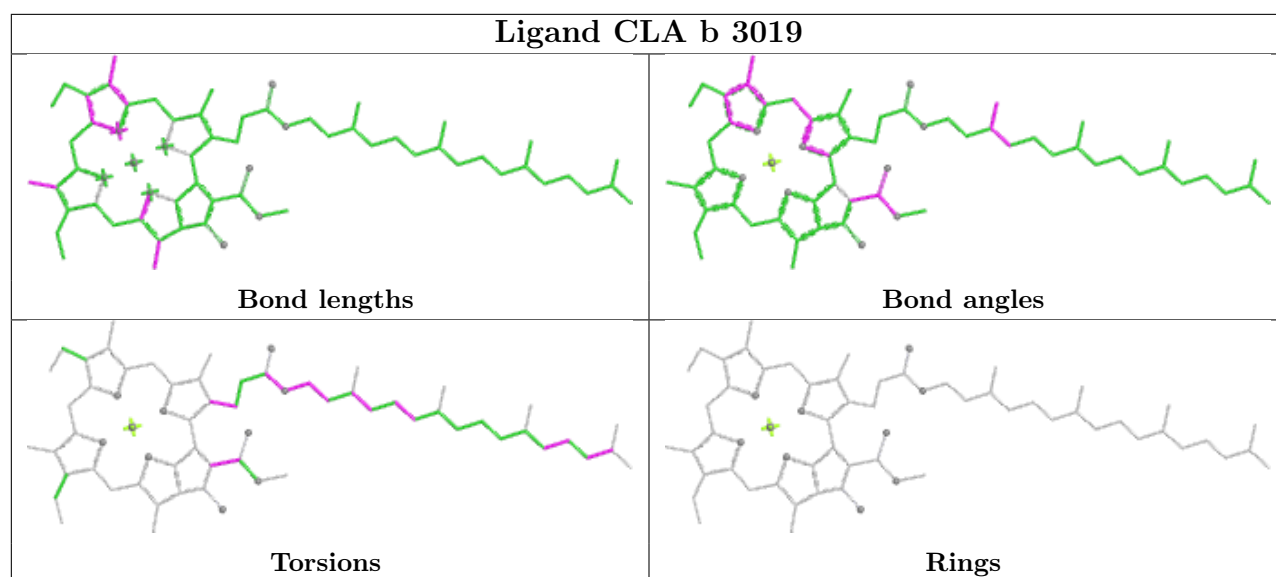
Bond angles



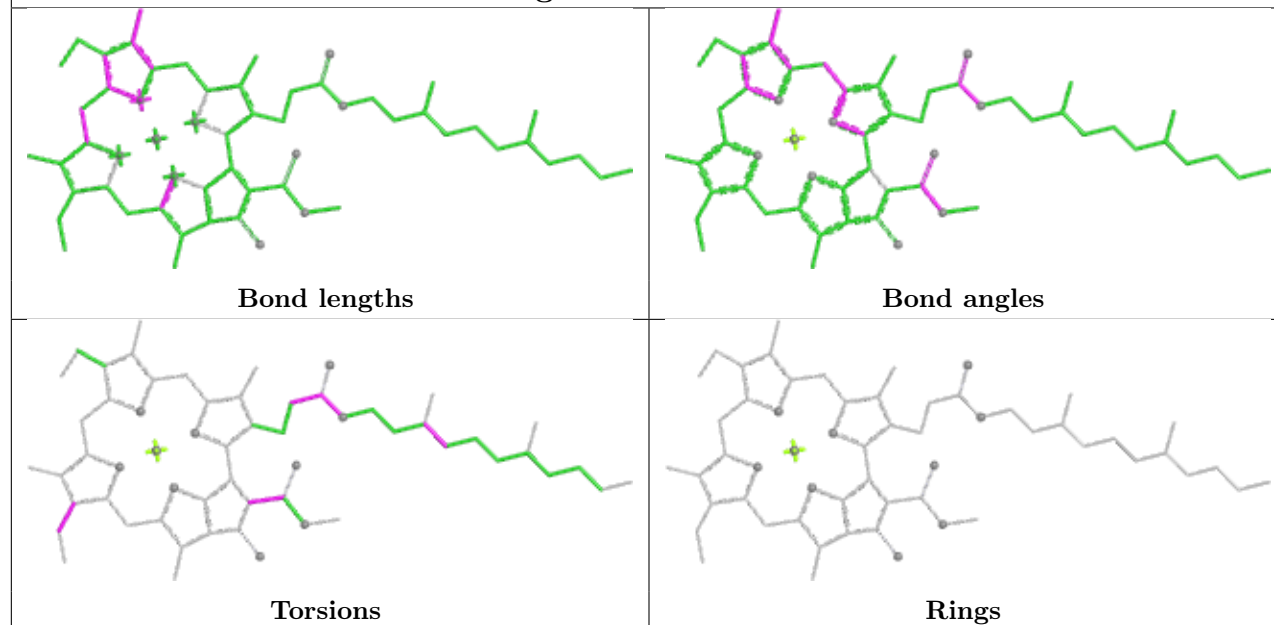
Torsions



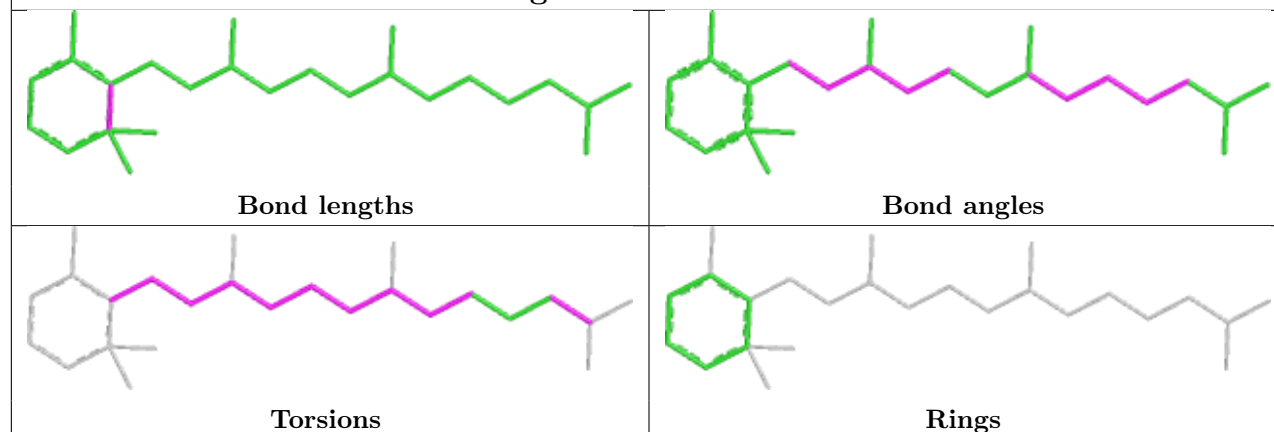
Rings



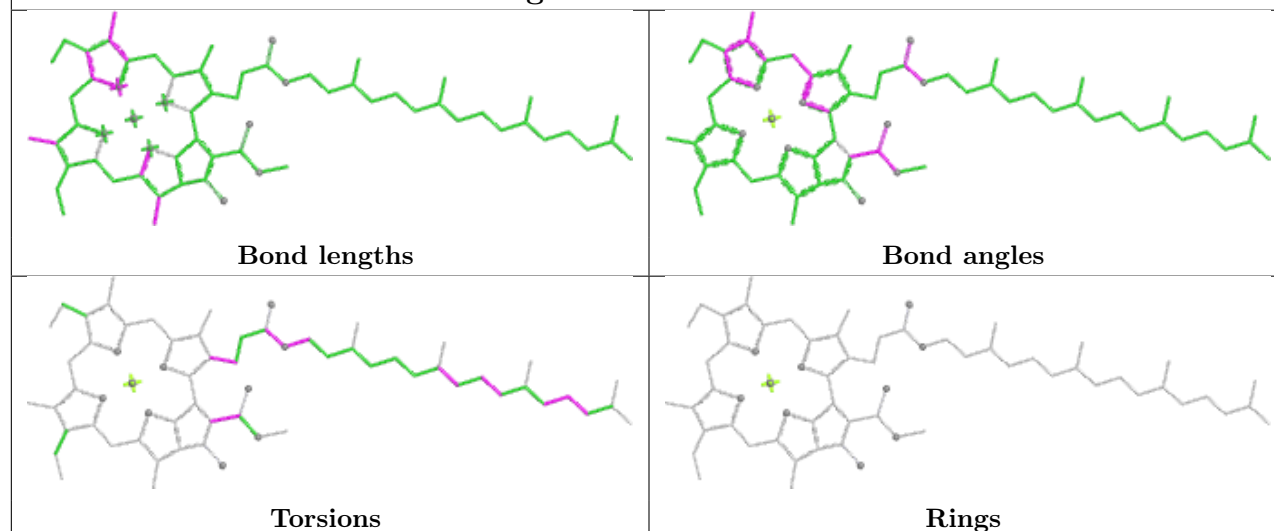
Ligand CLA k 102

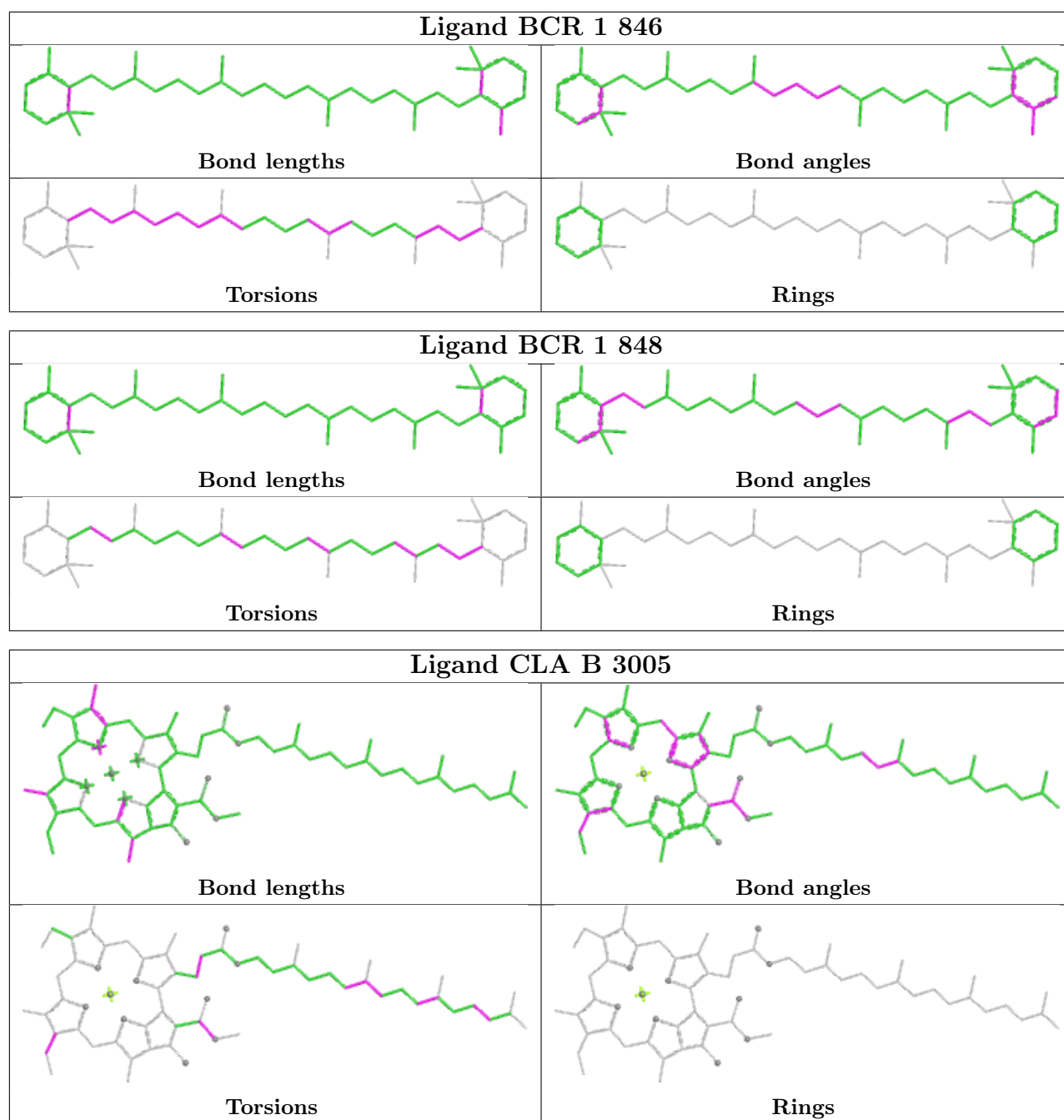


Ligand BCR A 852

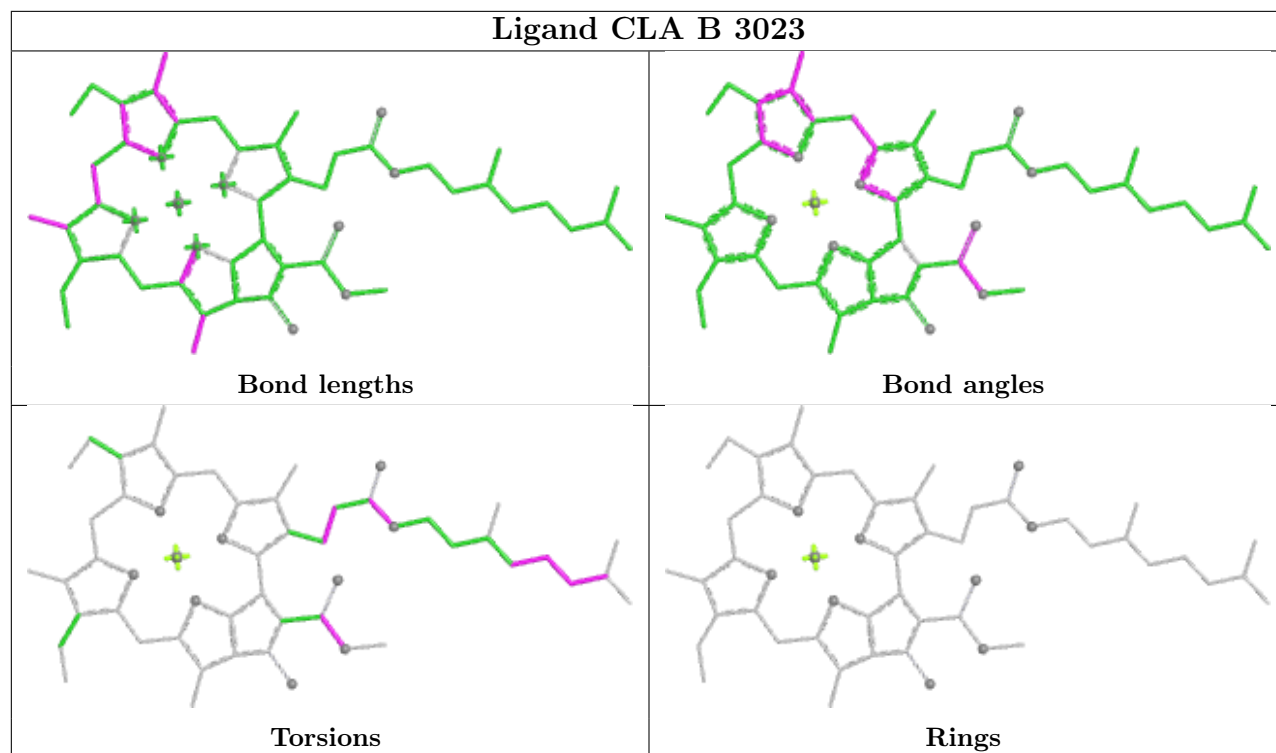


Ligand CLA b 3007

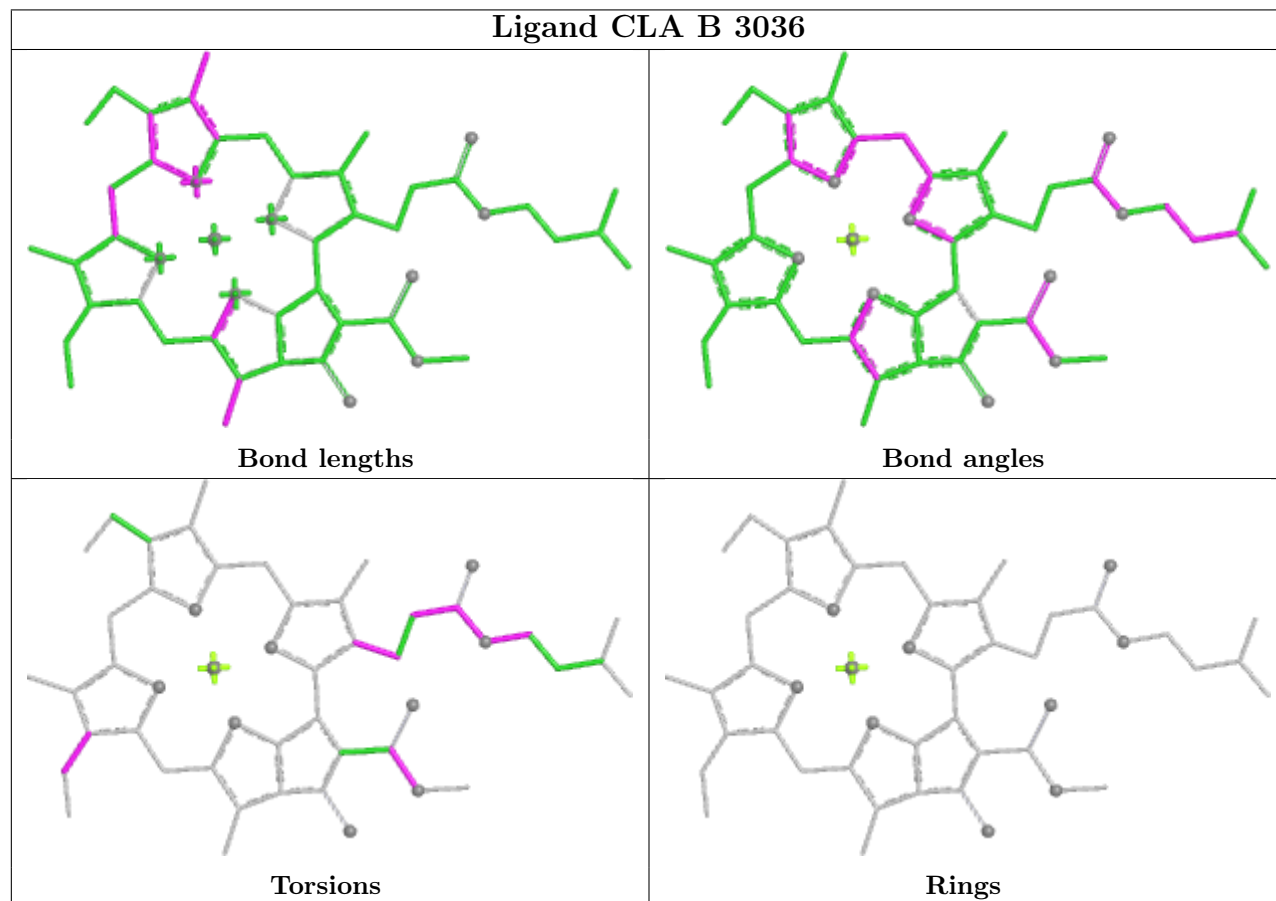


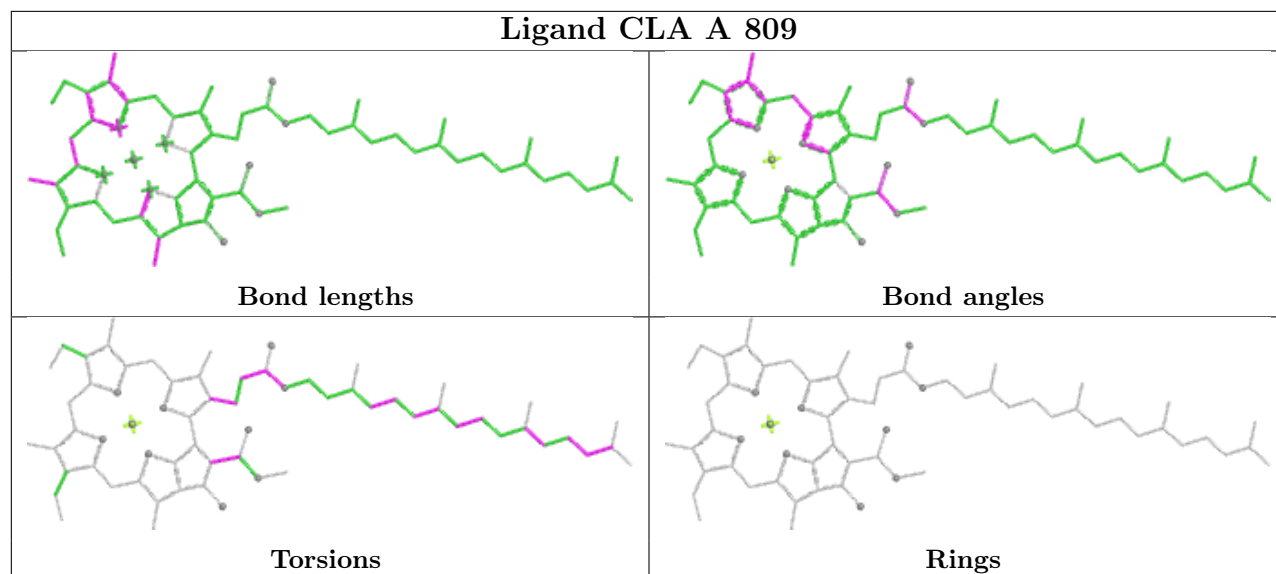
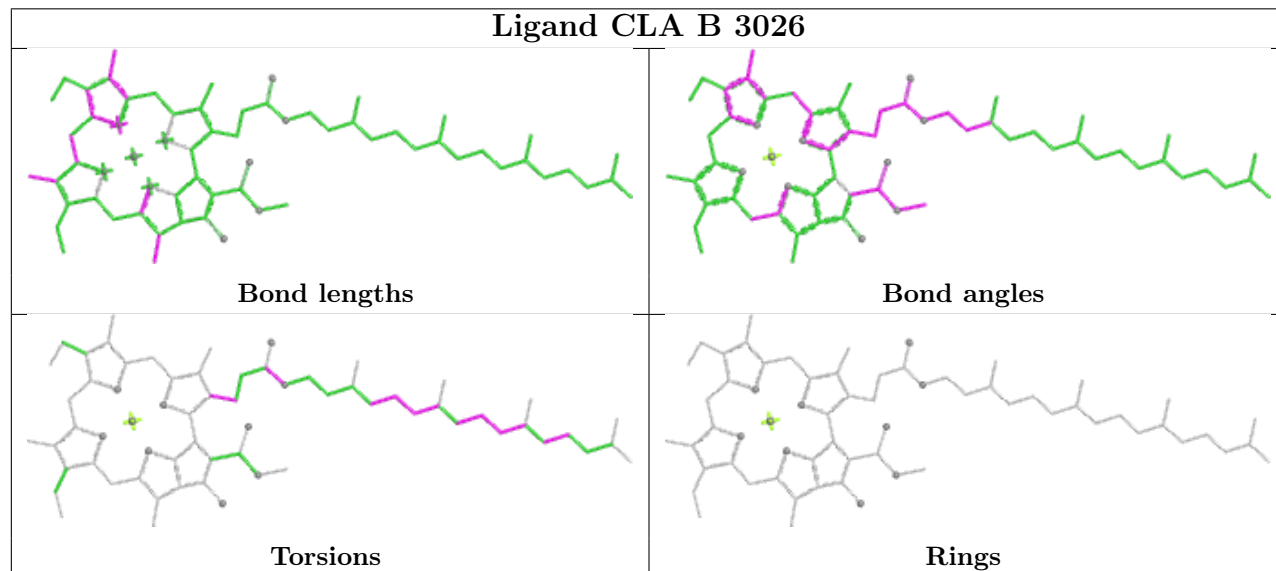


Ligand CLA B 3023

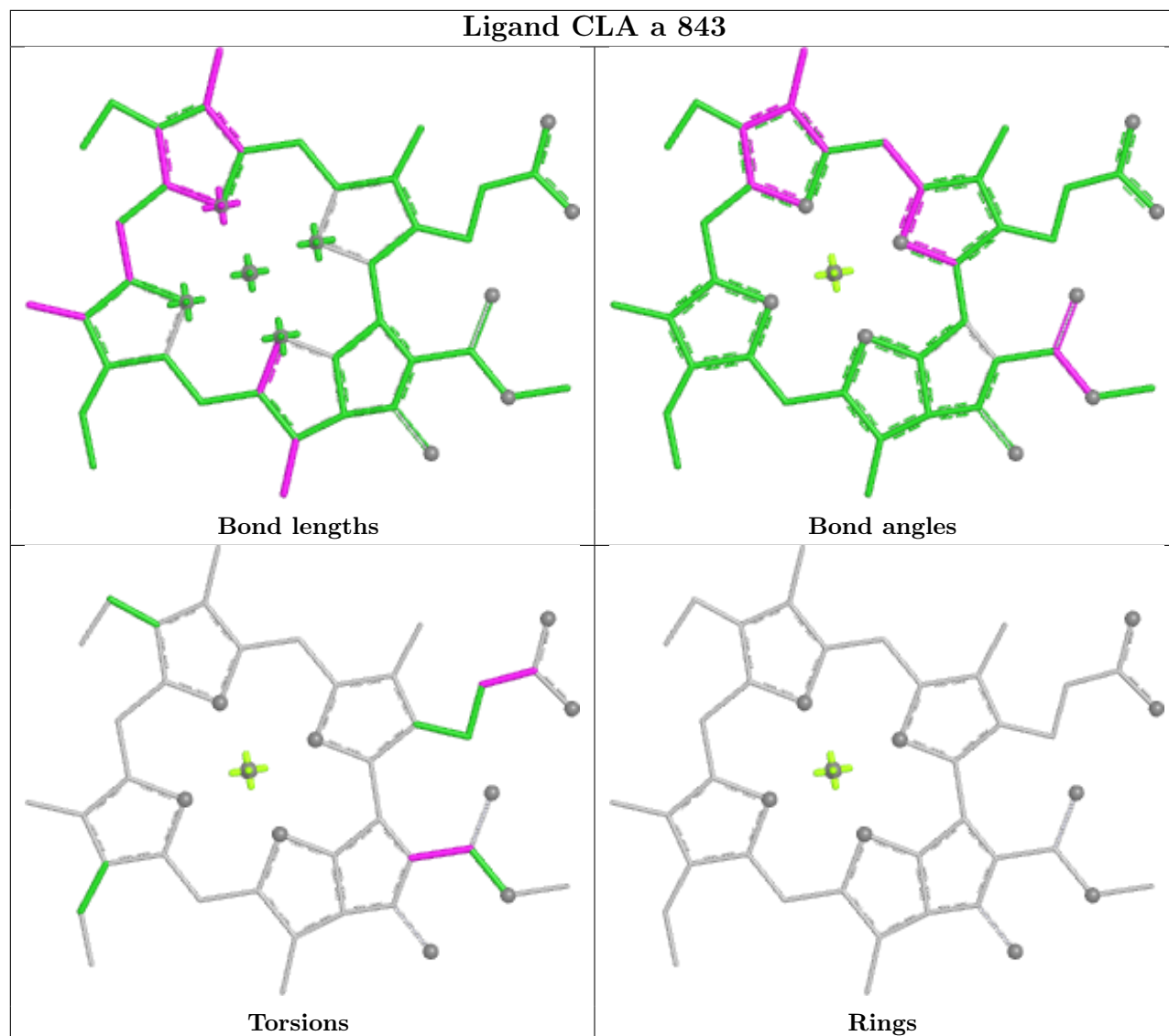


Ligand CLA B 3036

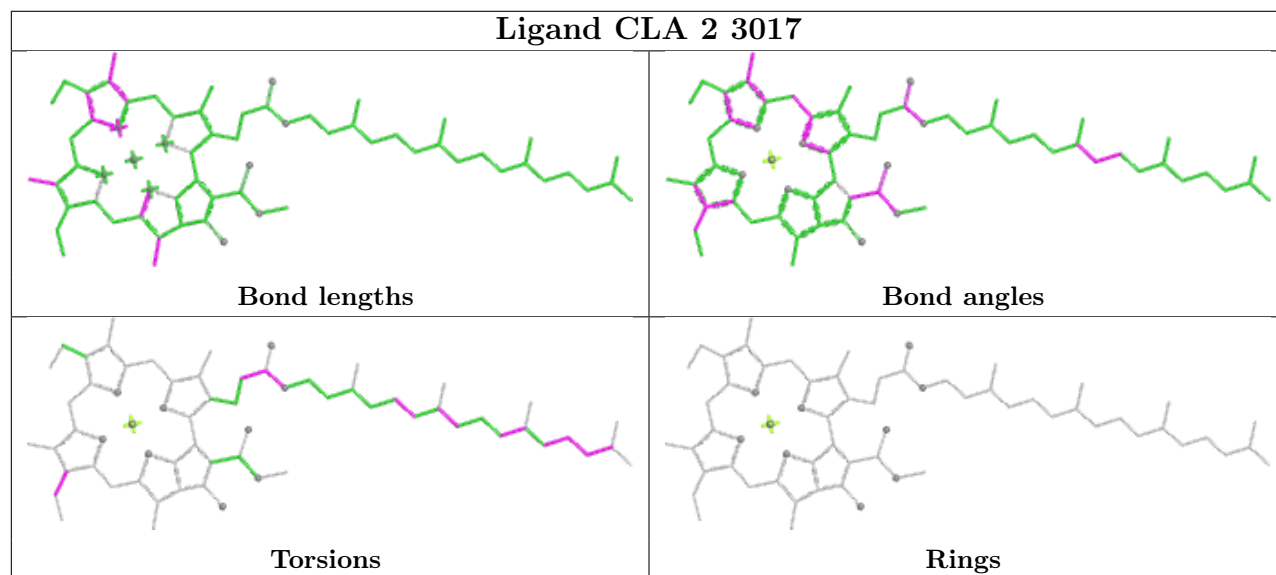


Ligand CLA A 809**Ligand CLA B 3026**

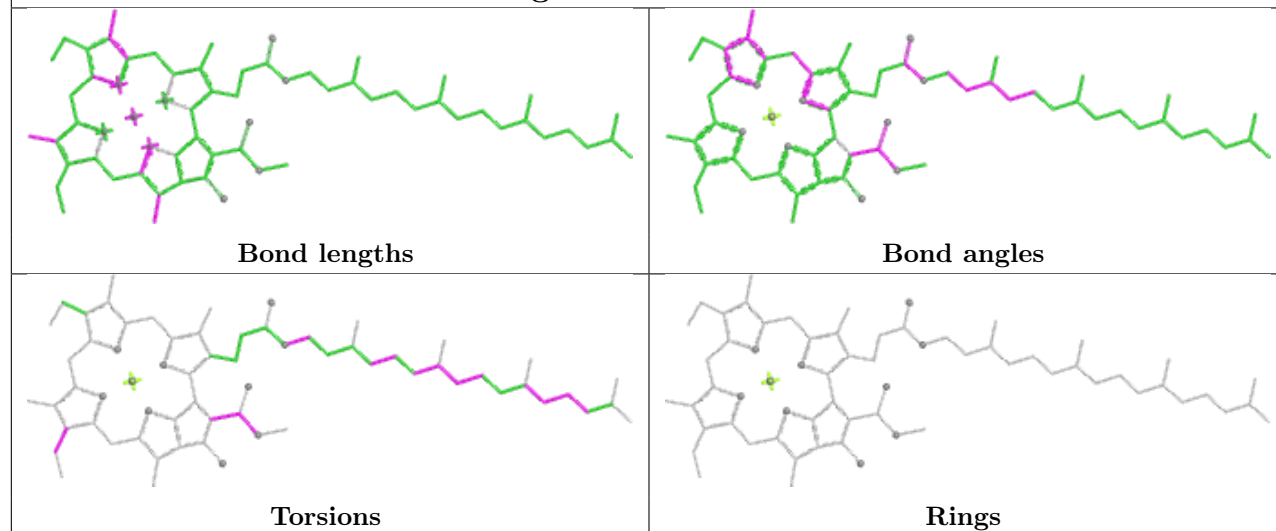
Ligand CLA a 843



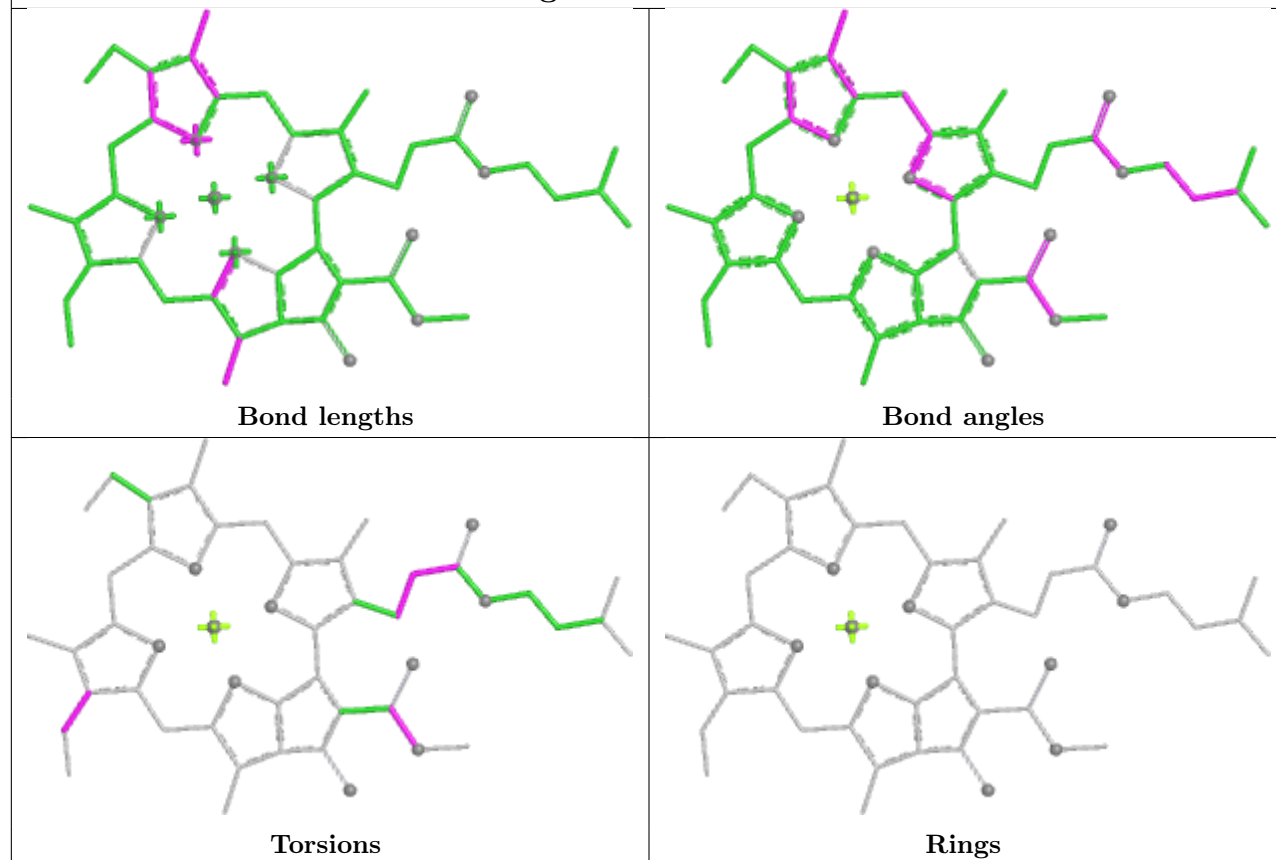
Ligand CLA 2 3017



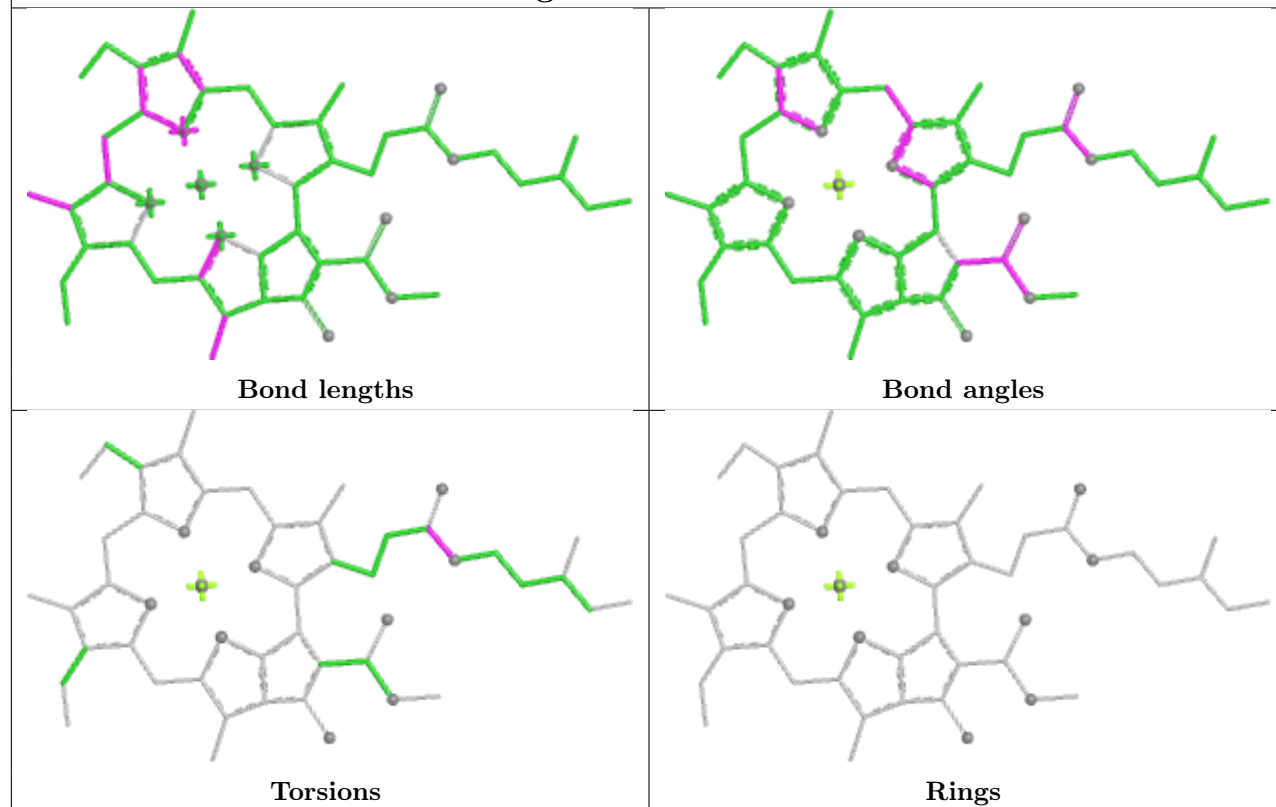
Ligand CLA A 826



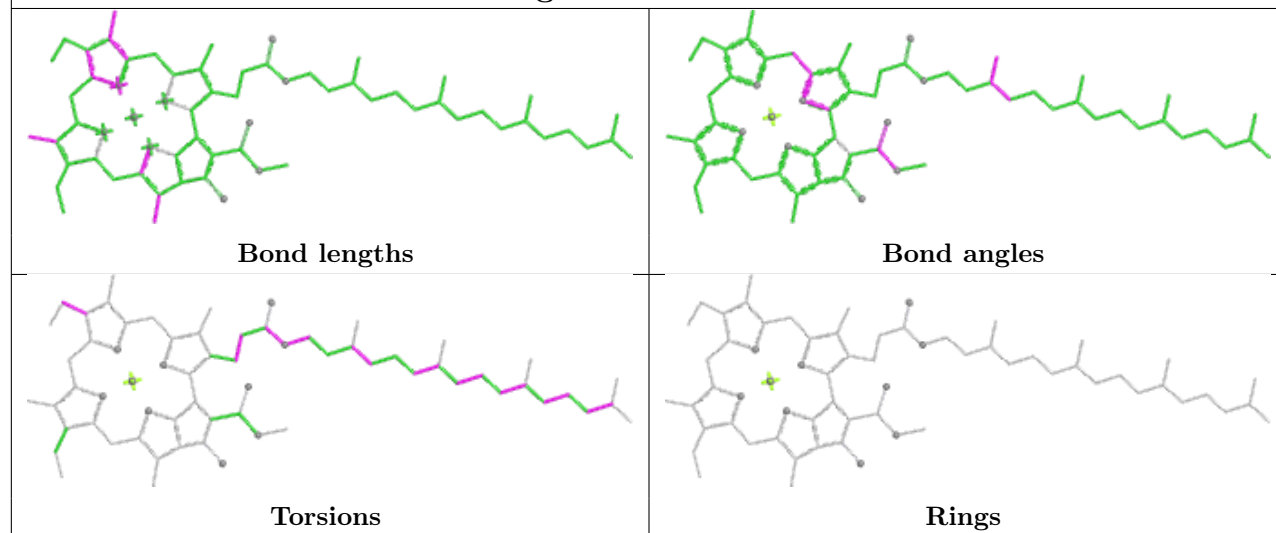
Ligand CLA f 204

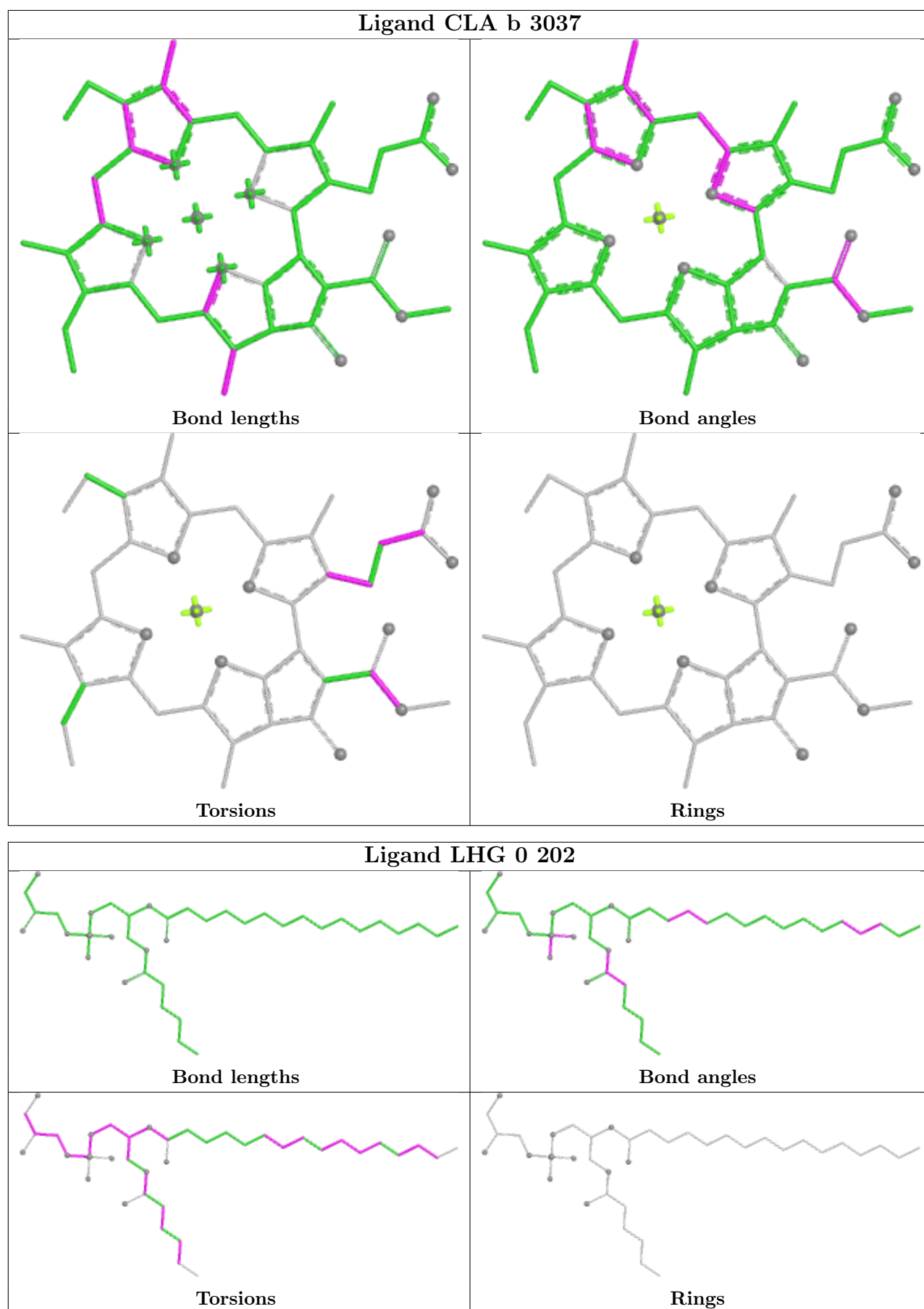


Ligand CLA 1 808

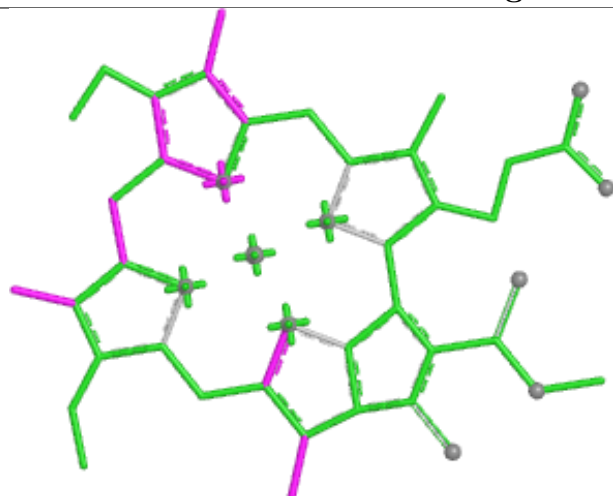


Ligand CLA a 818

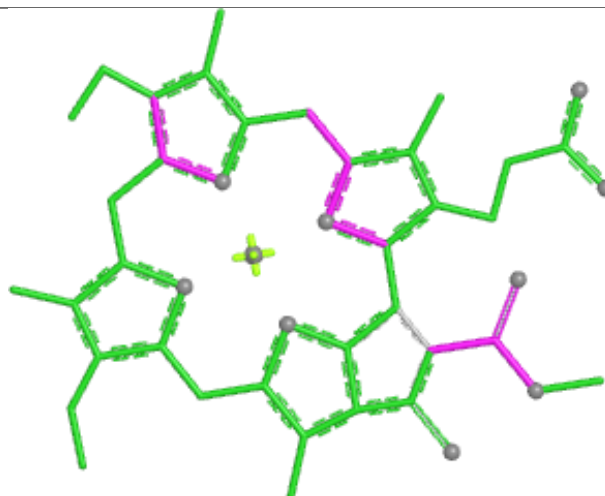




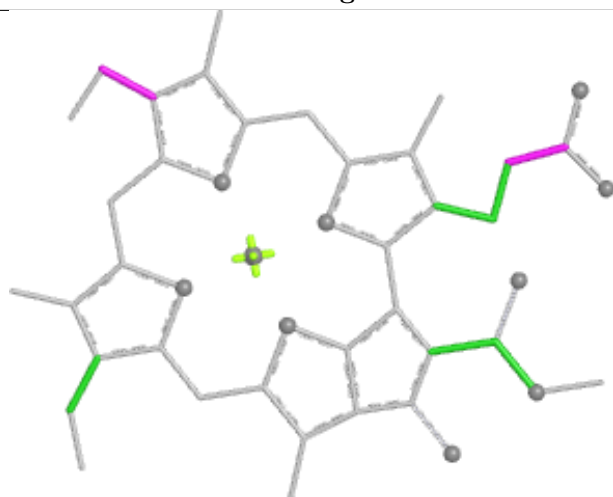
Ligand CLA B 3013



Bond lengths



Bond angles

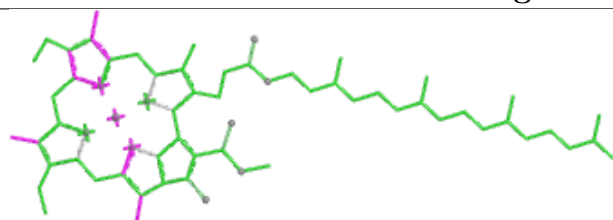


Torsions

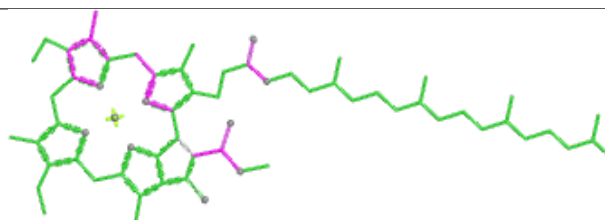


Rings

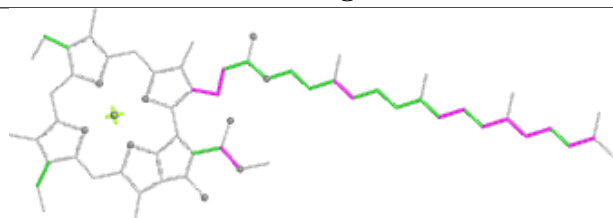
Ligand CLA A 830



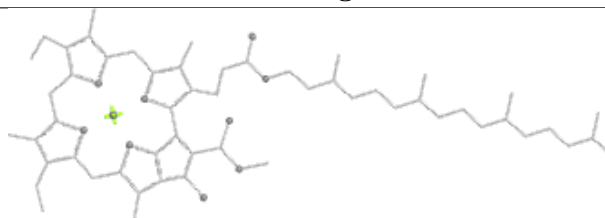
Bond lengths



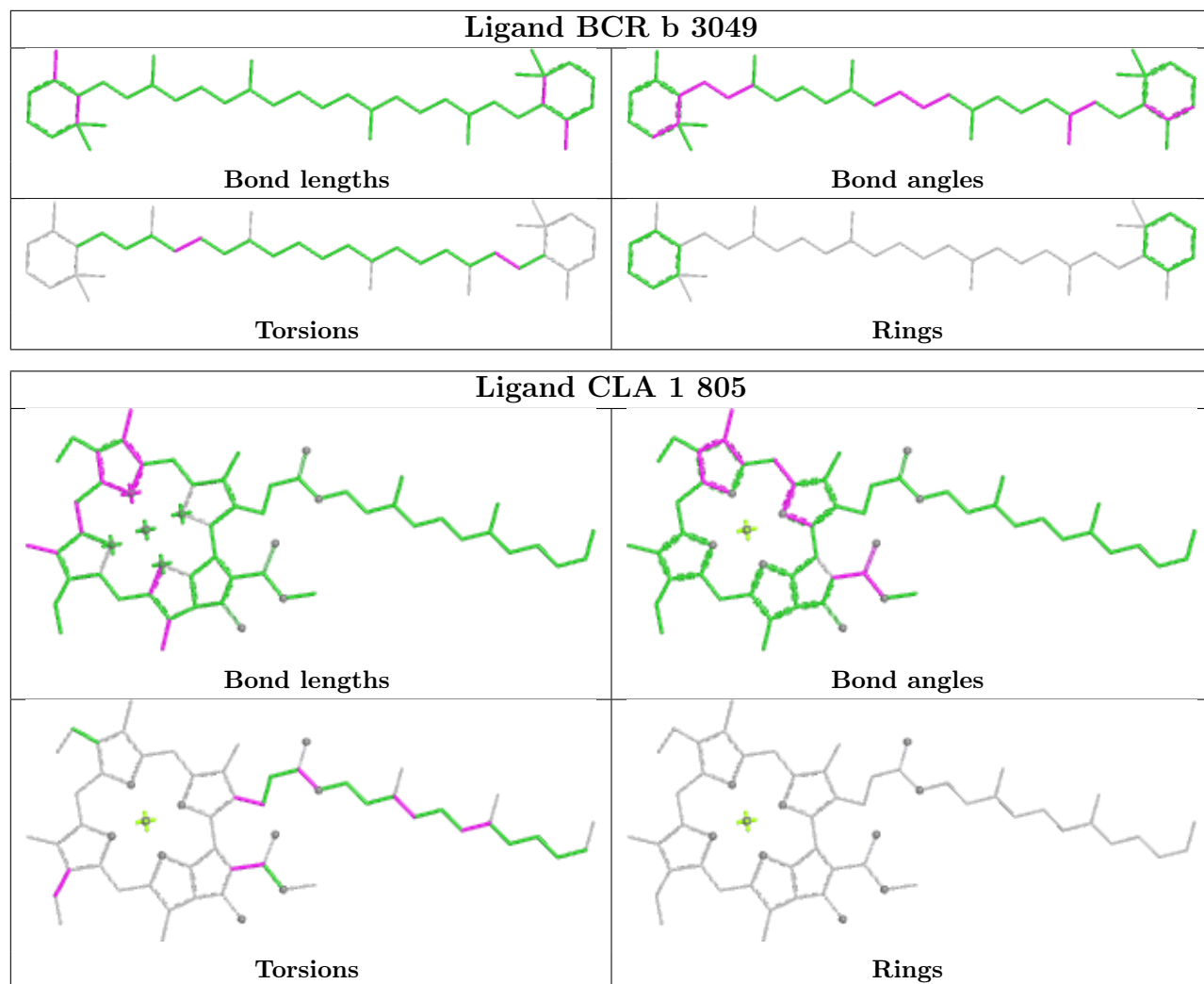
Bond angles

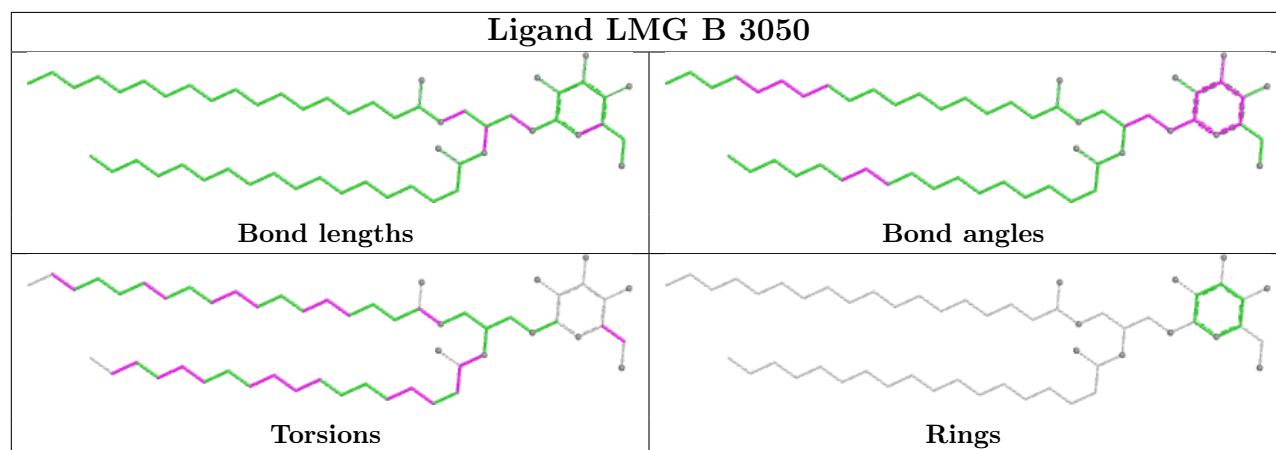
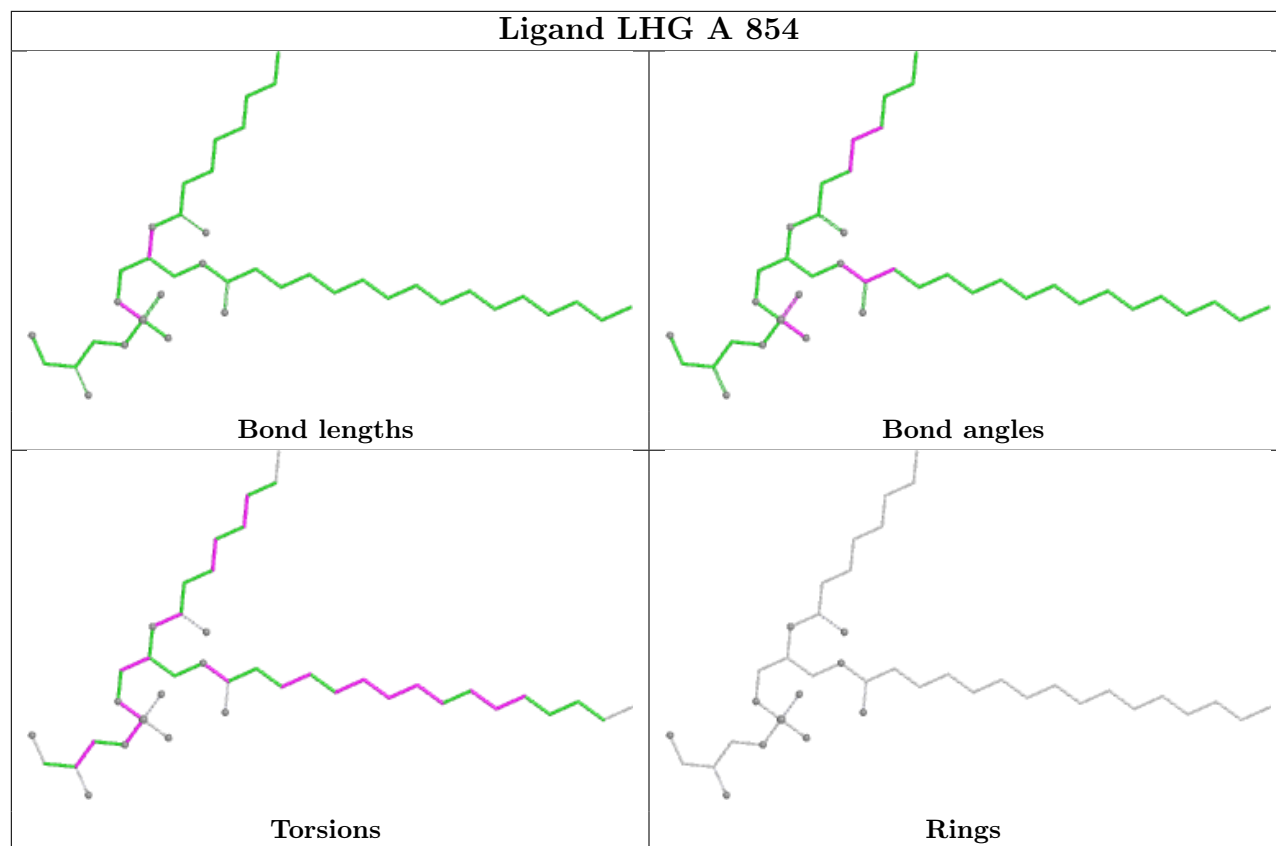


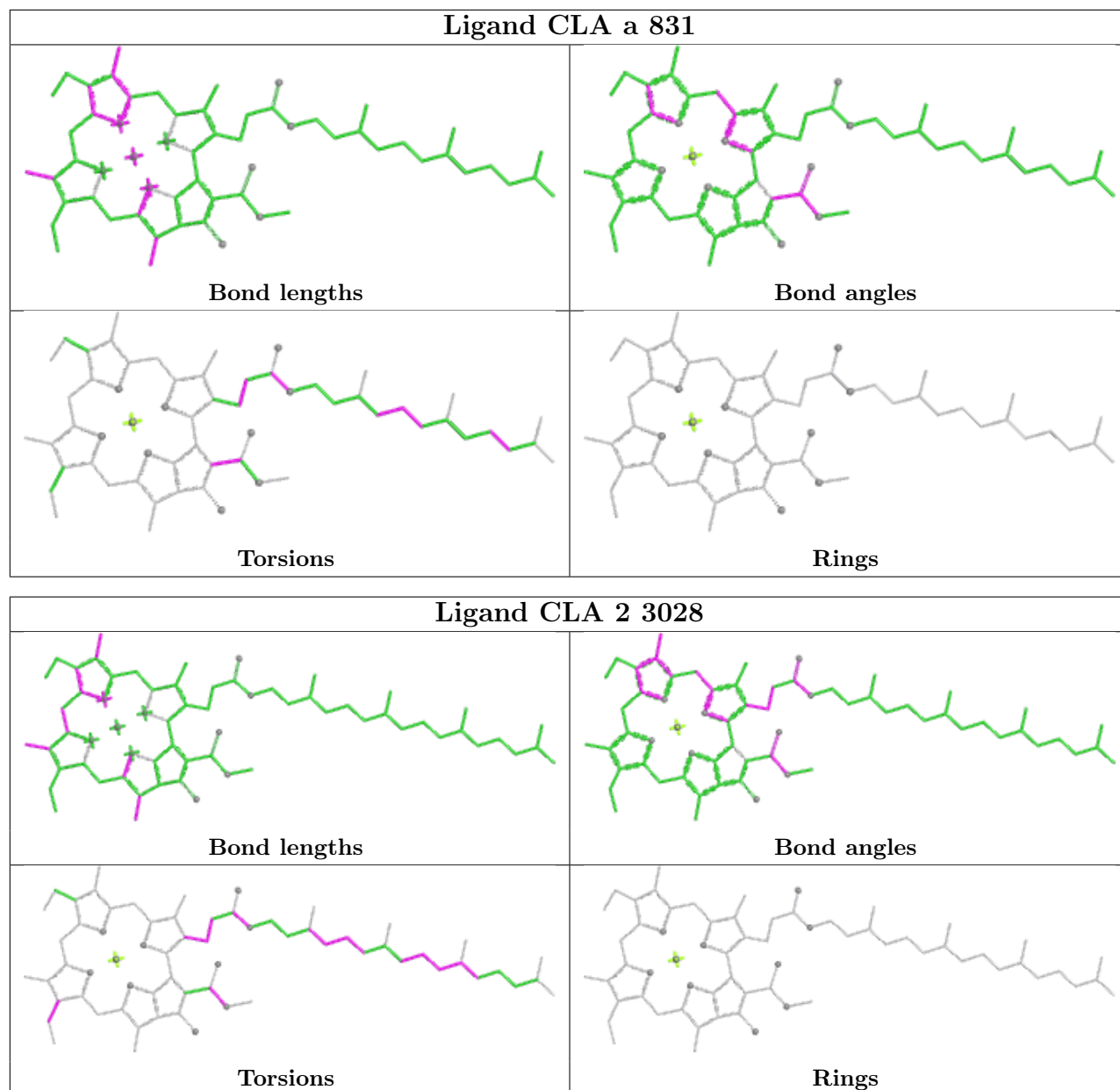
Torsions

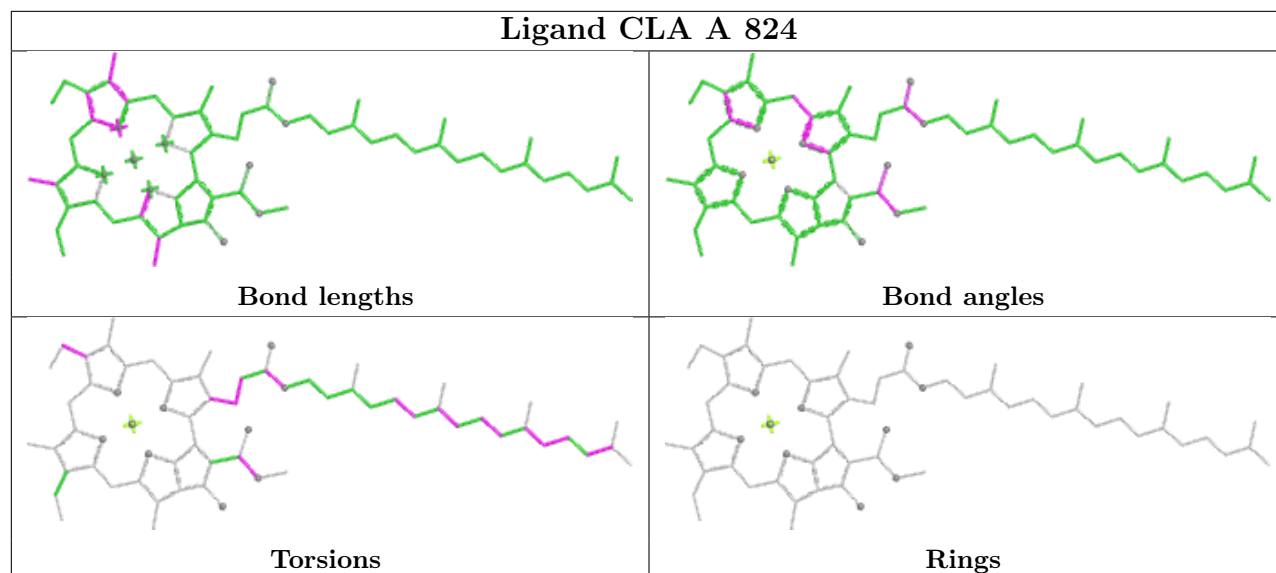
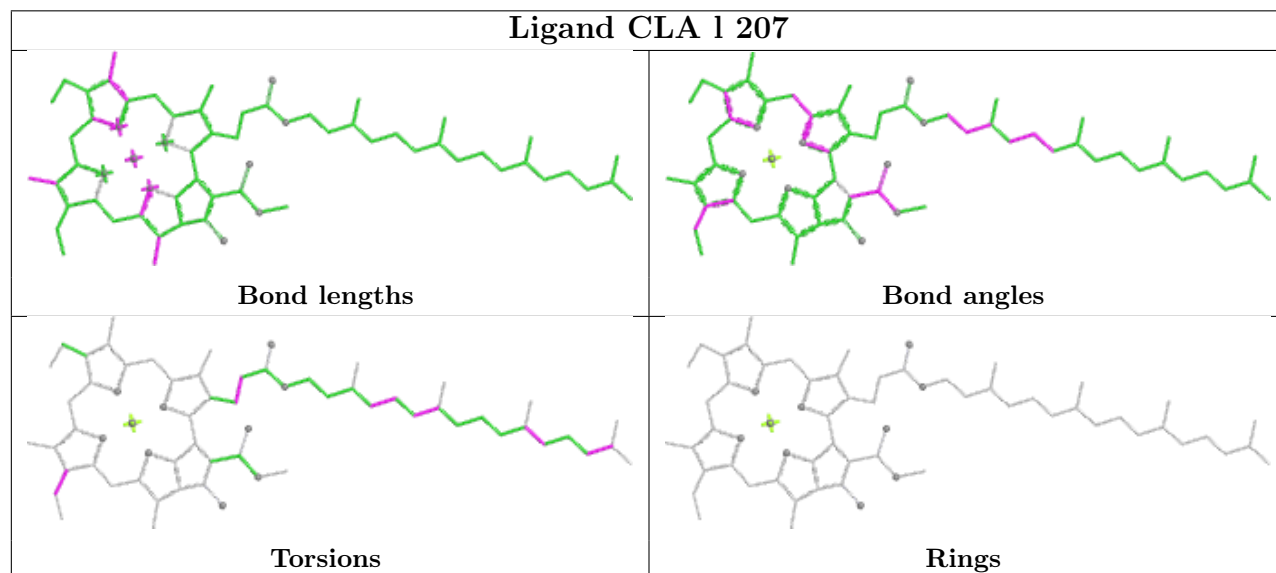
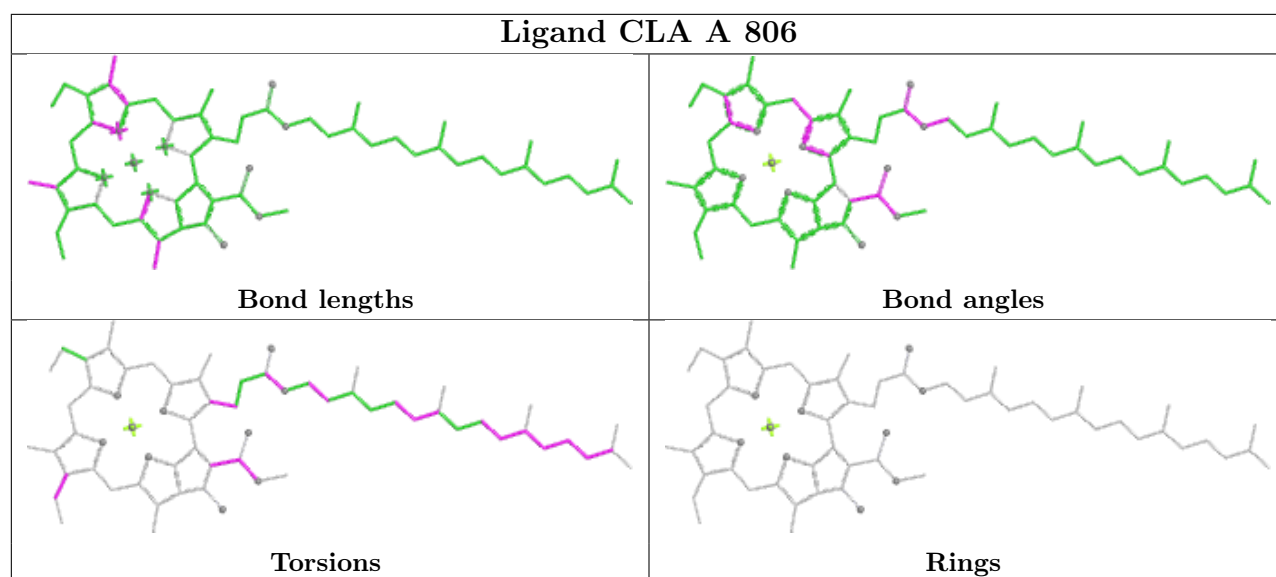


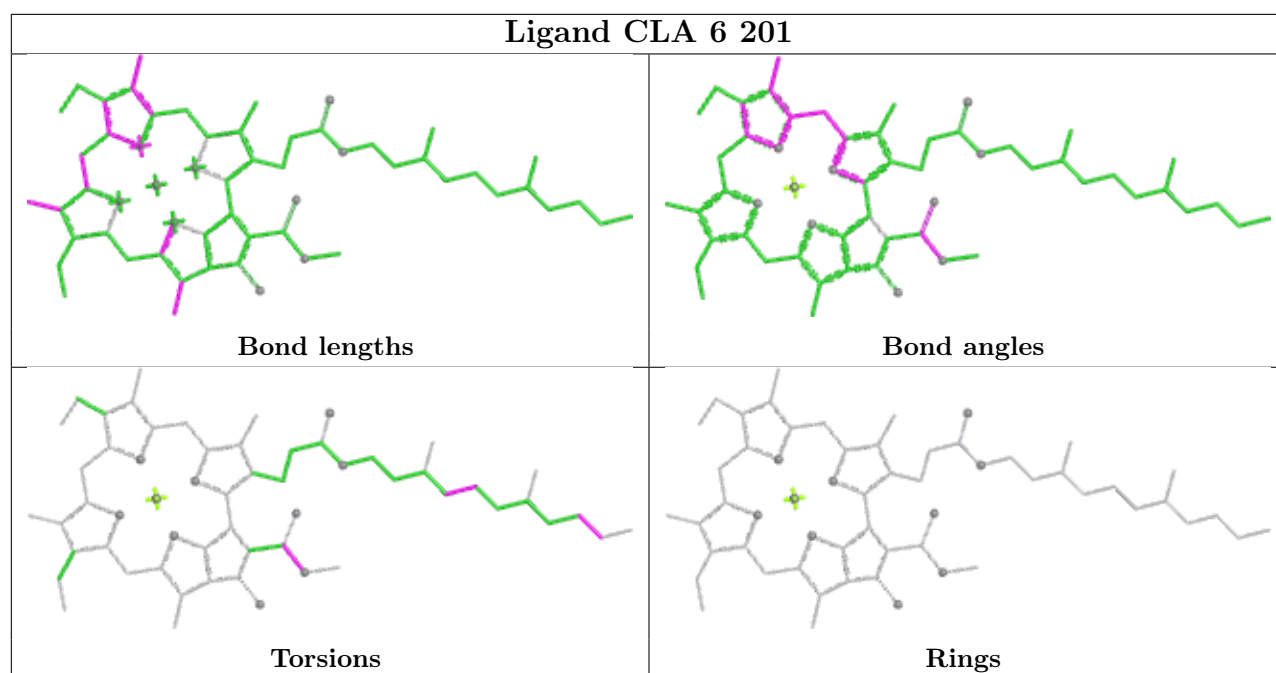
Rings

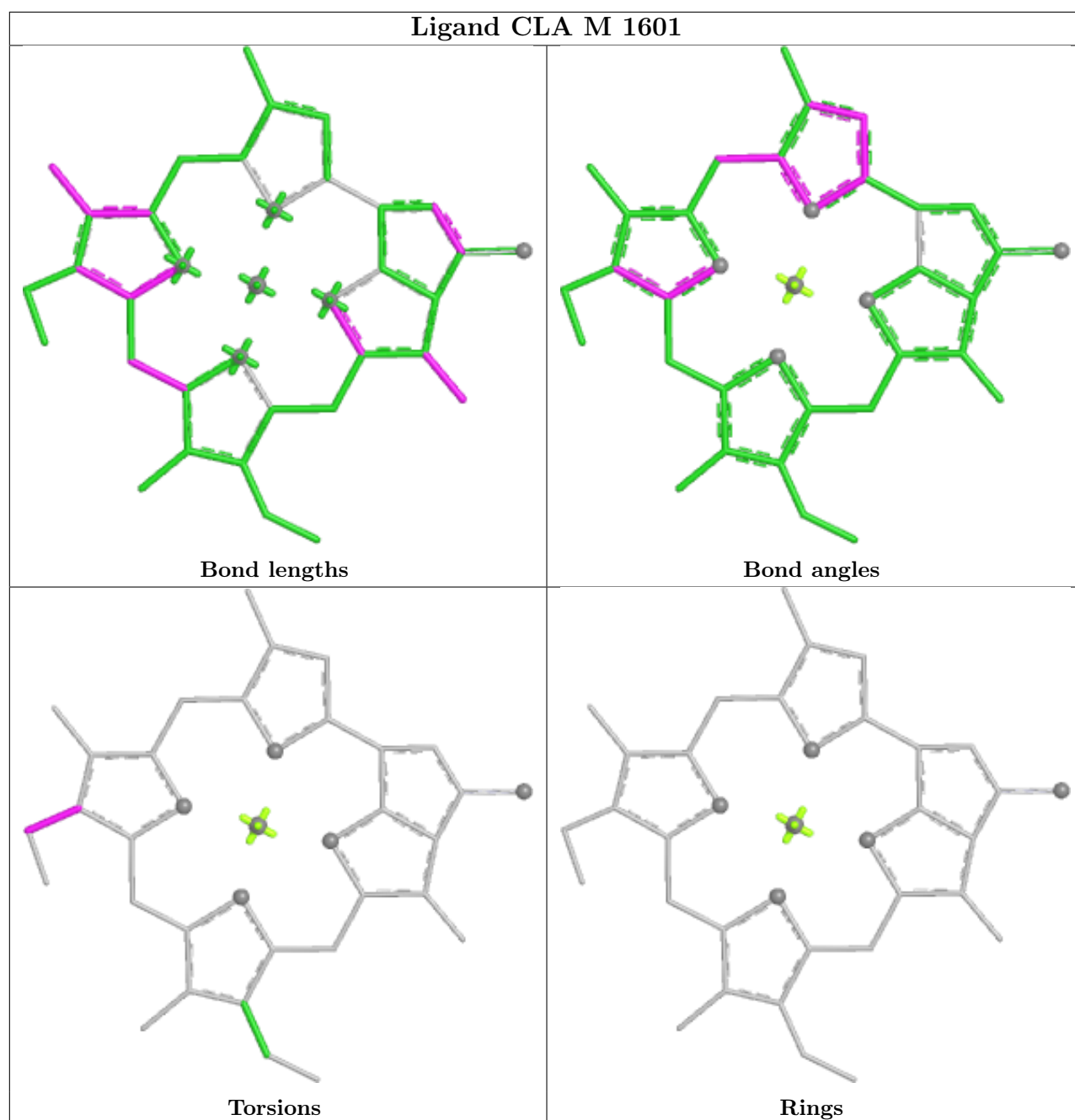




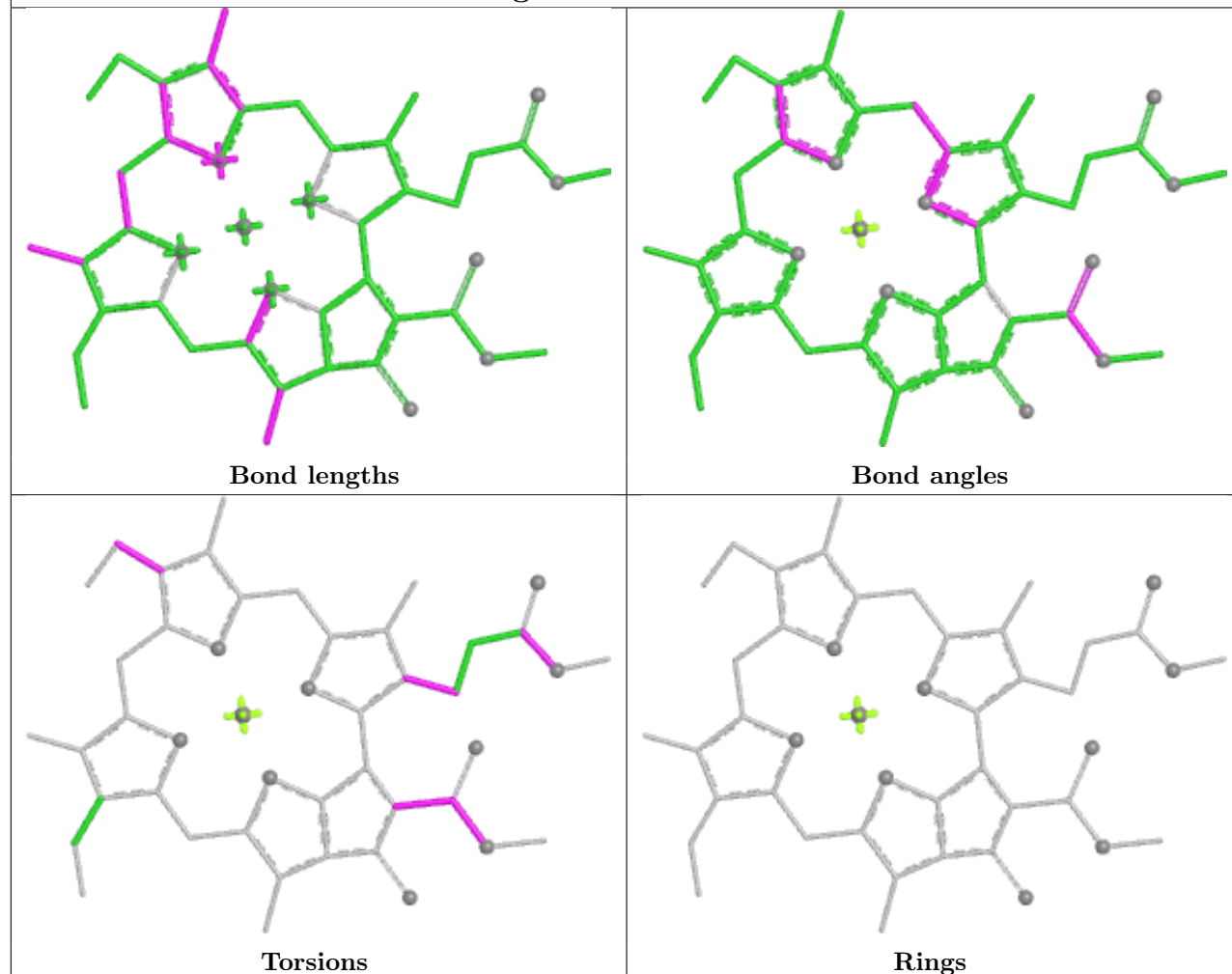




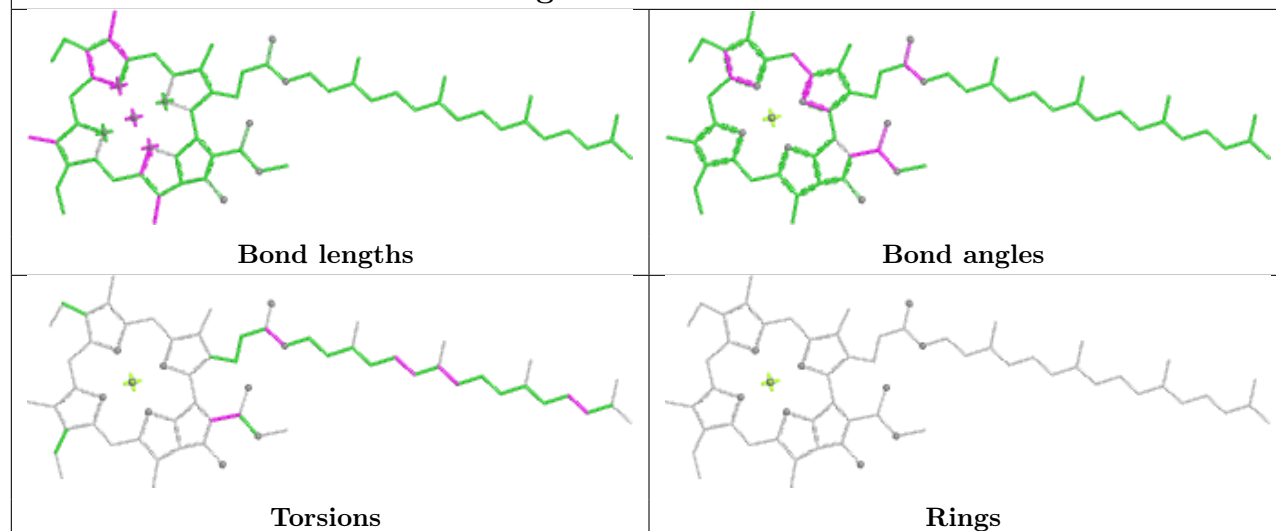


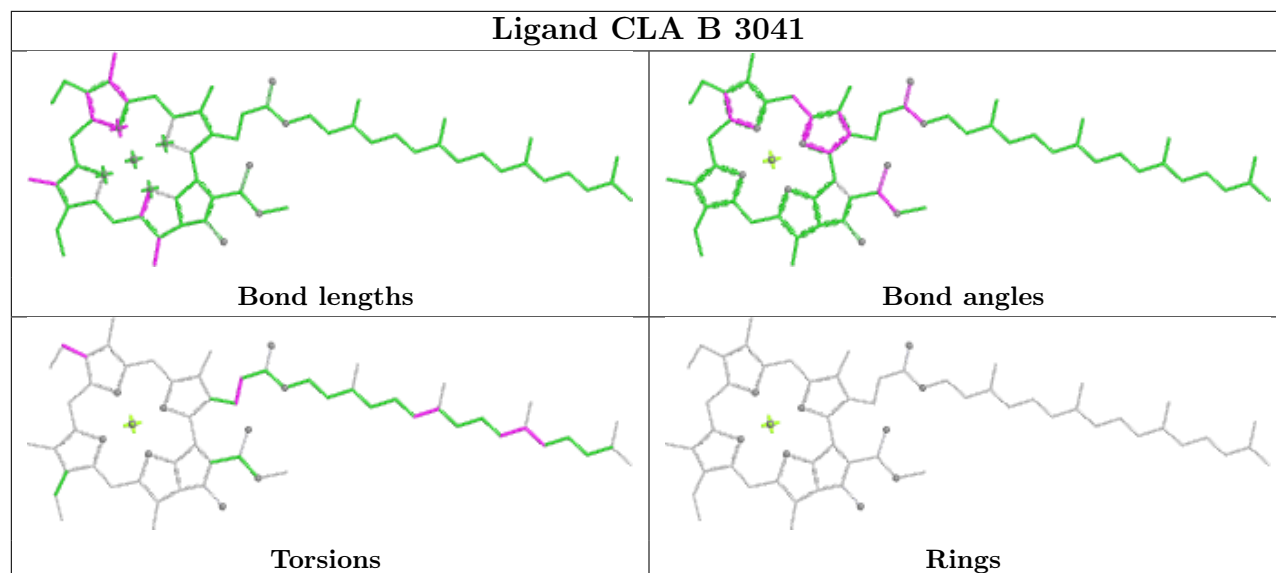
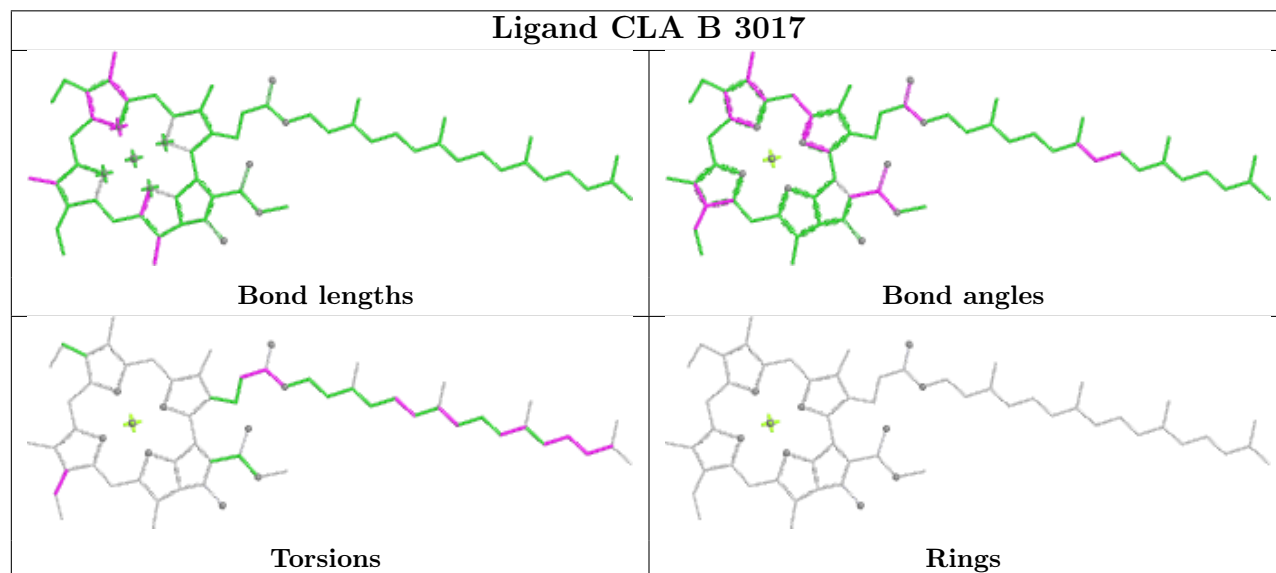
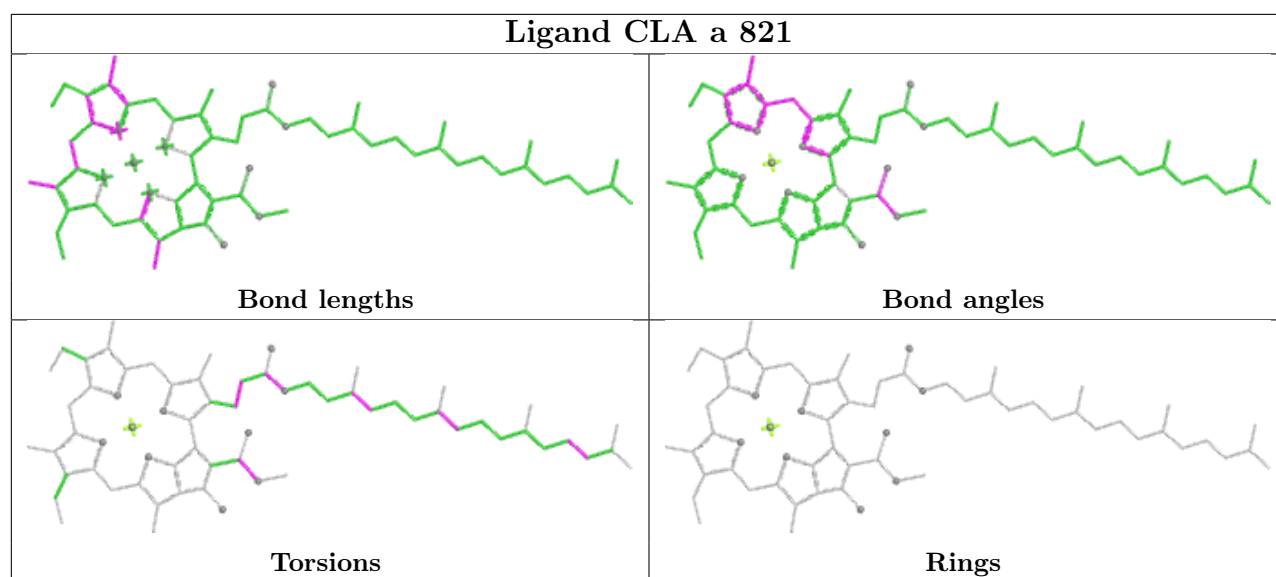


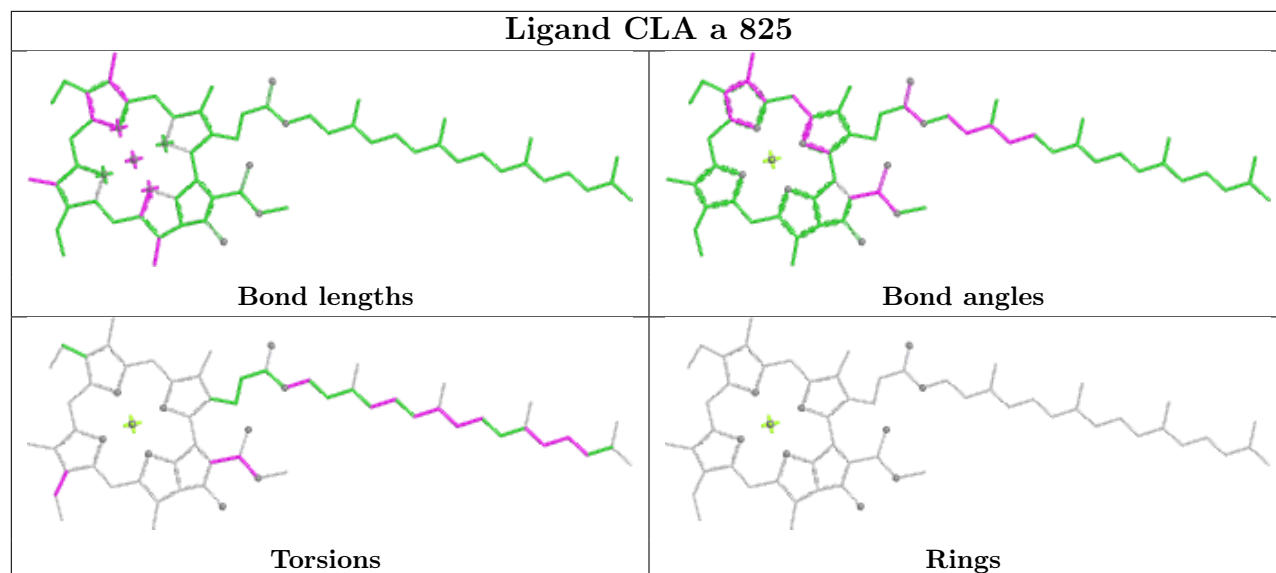
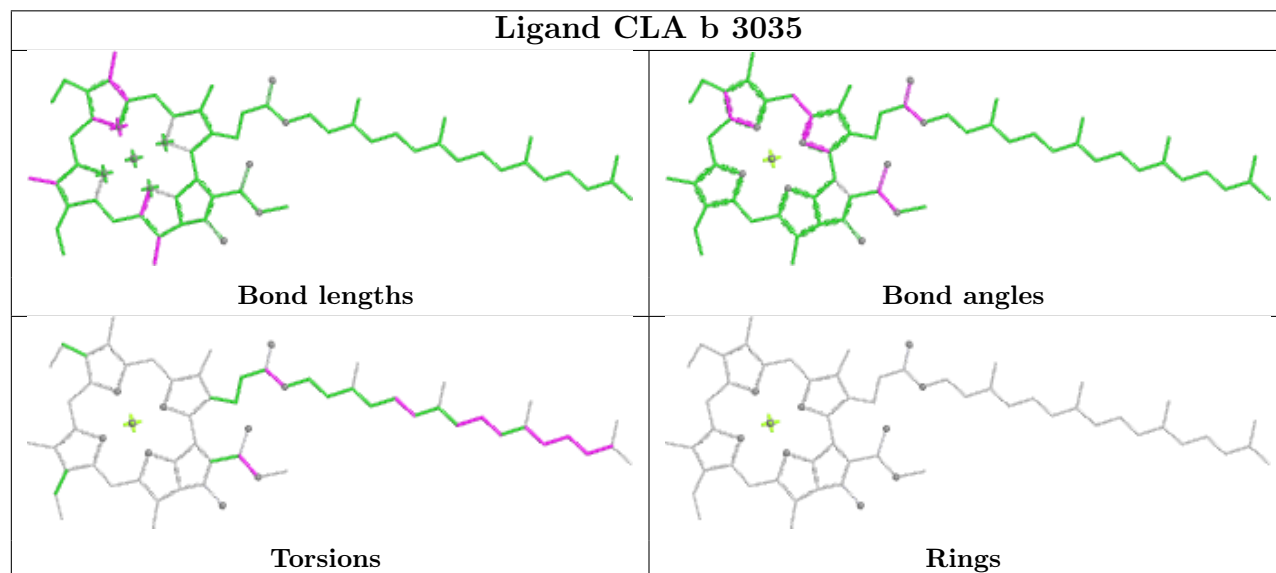
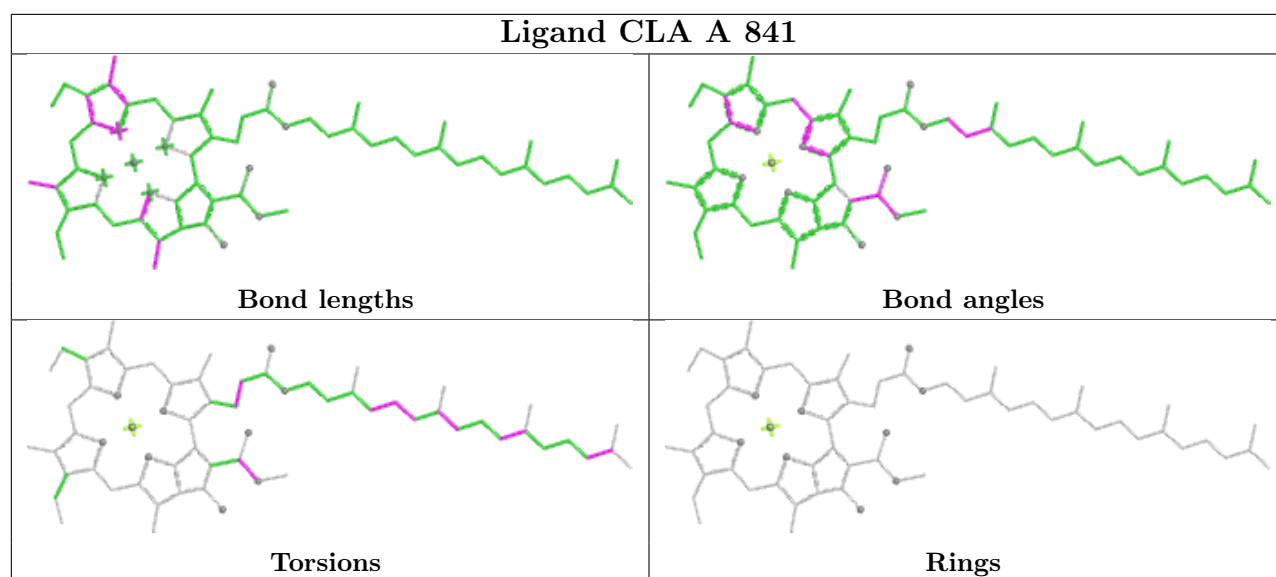
Ligand CLA K 101

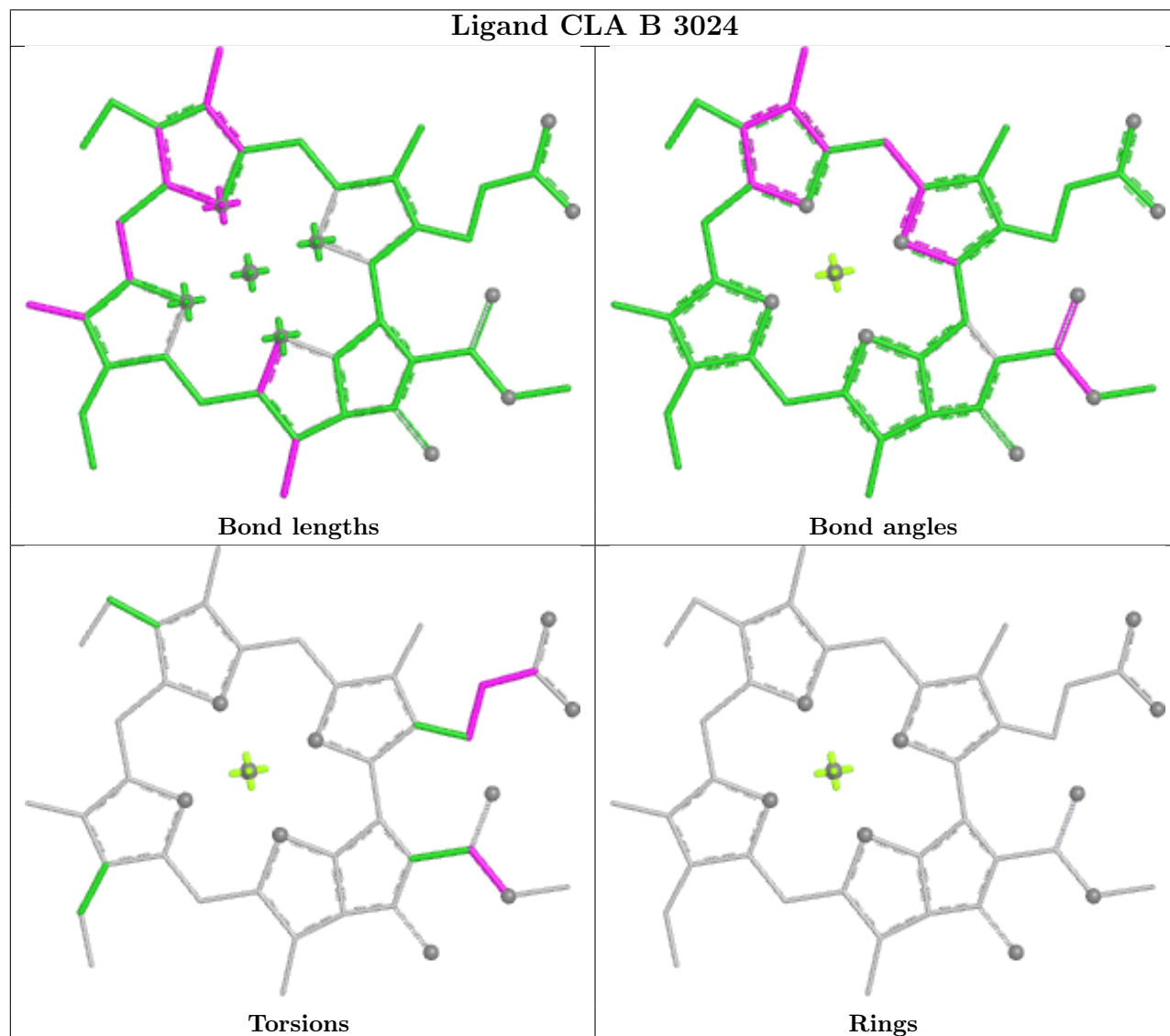
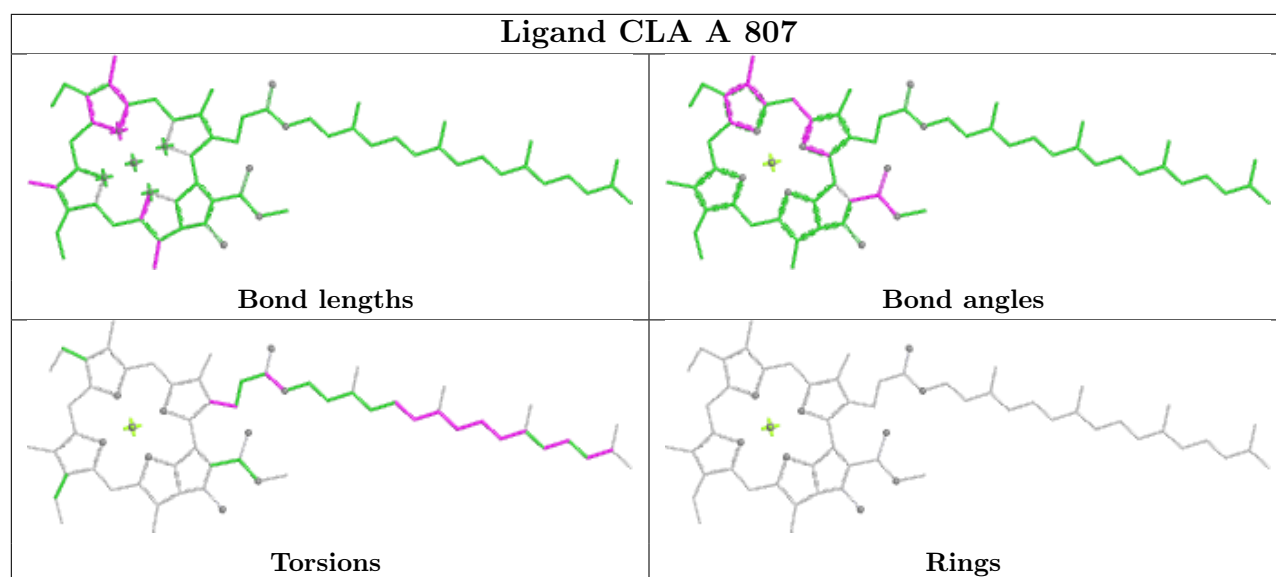


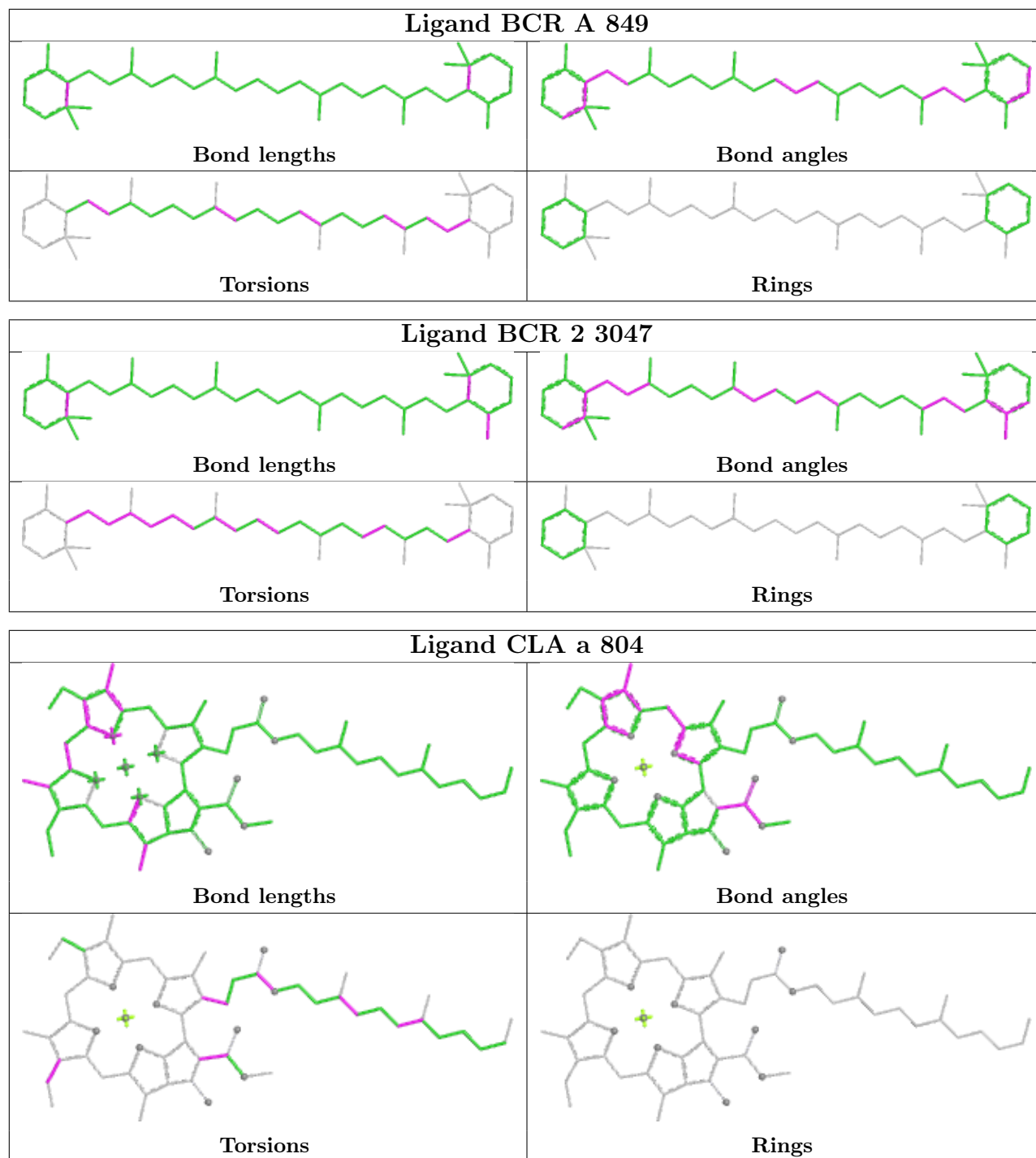
Ligand CLA a 830

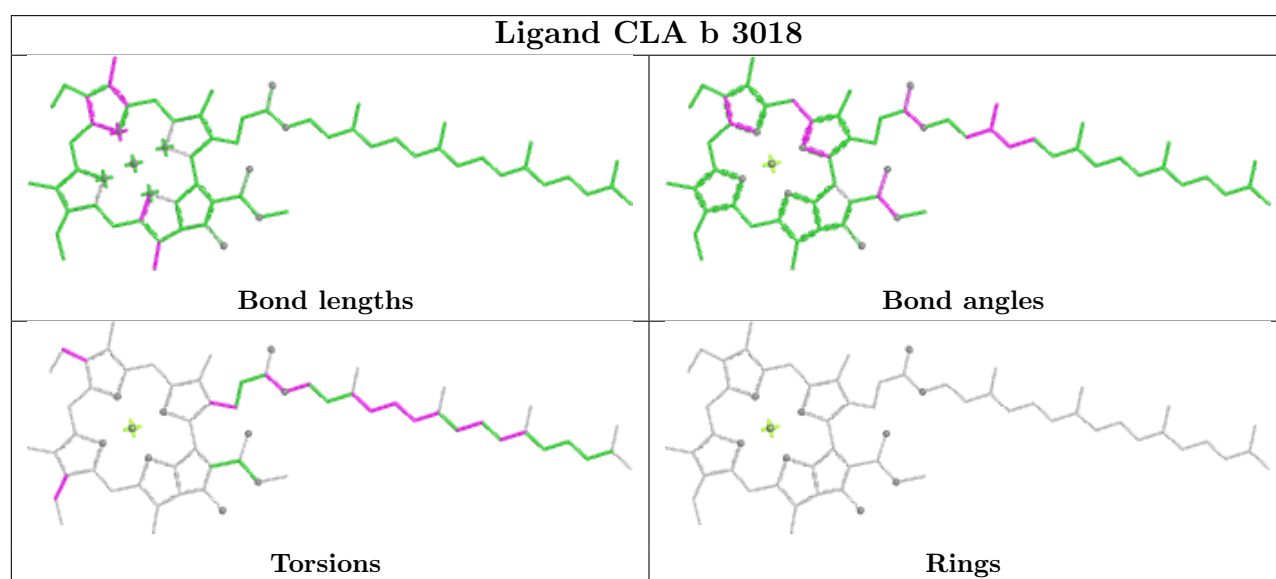
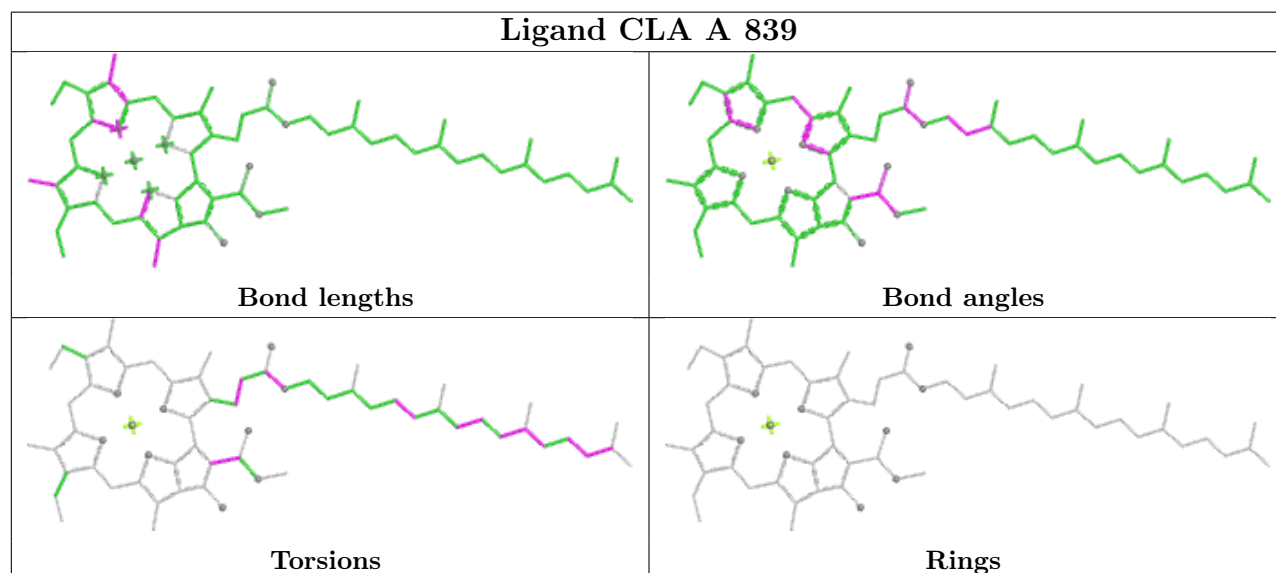
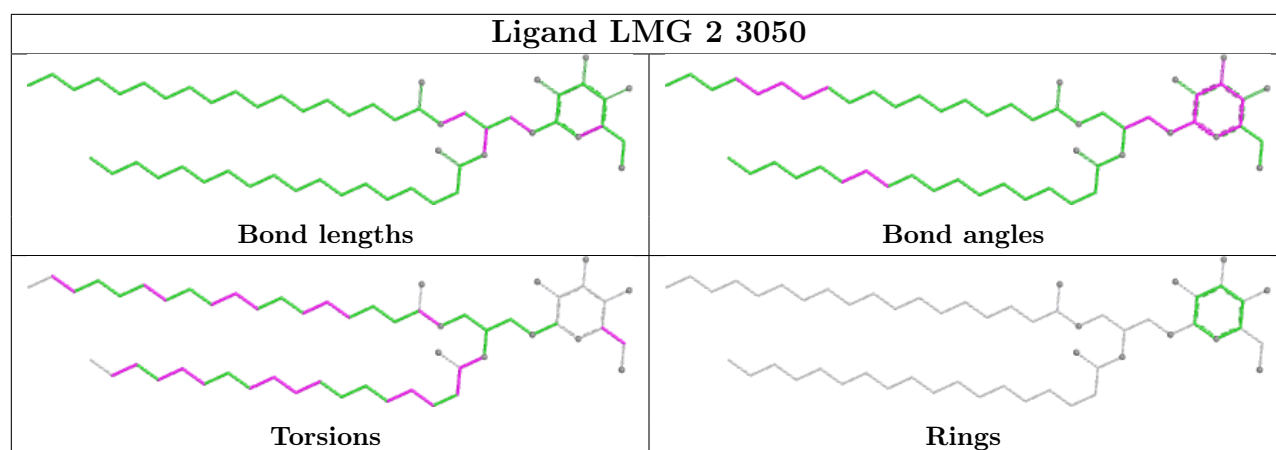




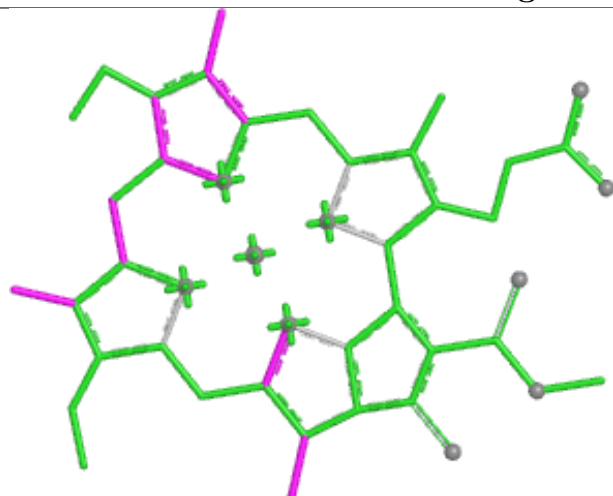




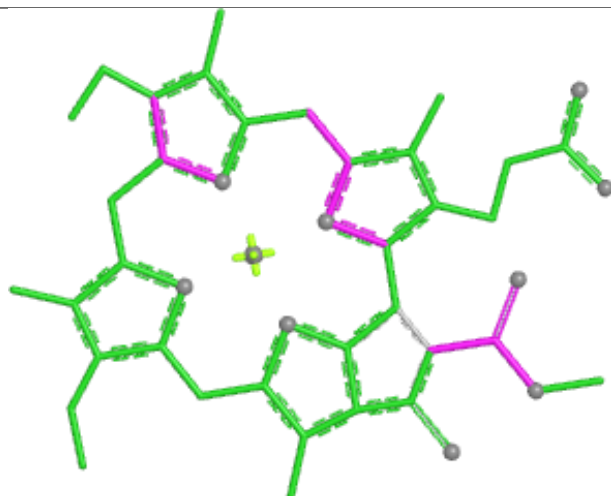




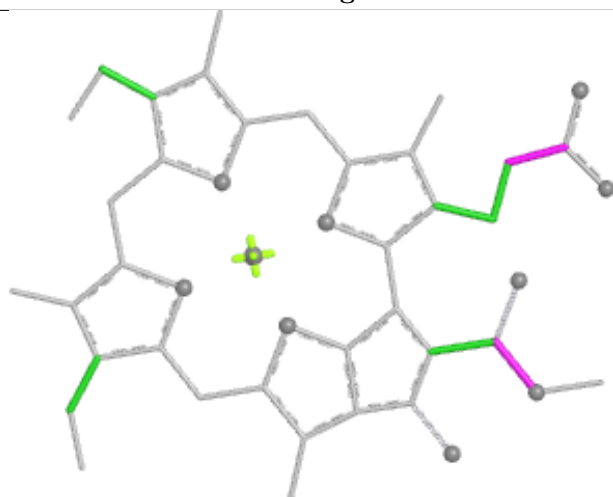
Ligand CLA J 101



Bond lengths



Bond angles

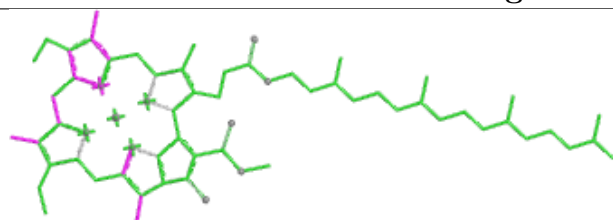


Torsions

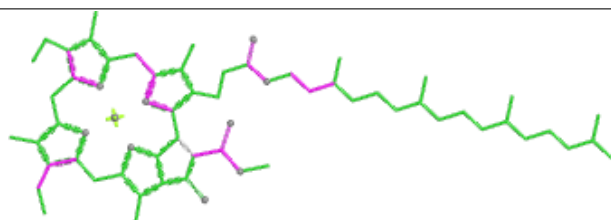


Rings

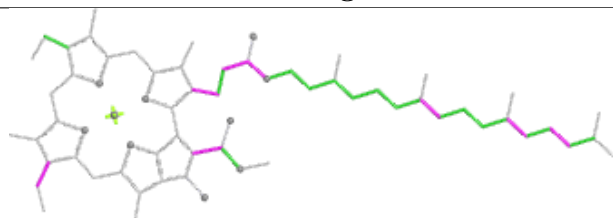
Ligand CLA B 3033



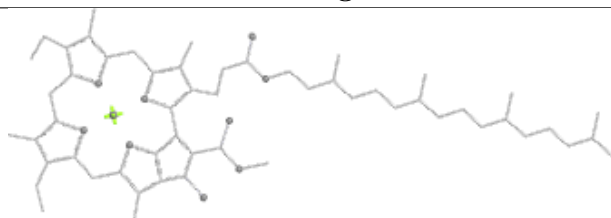
Bond lengths



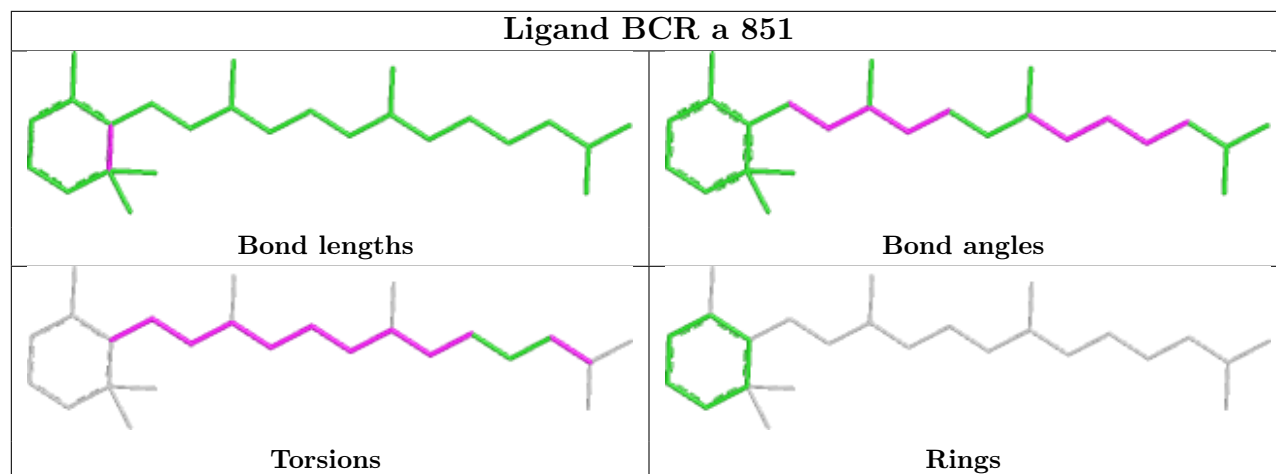
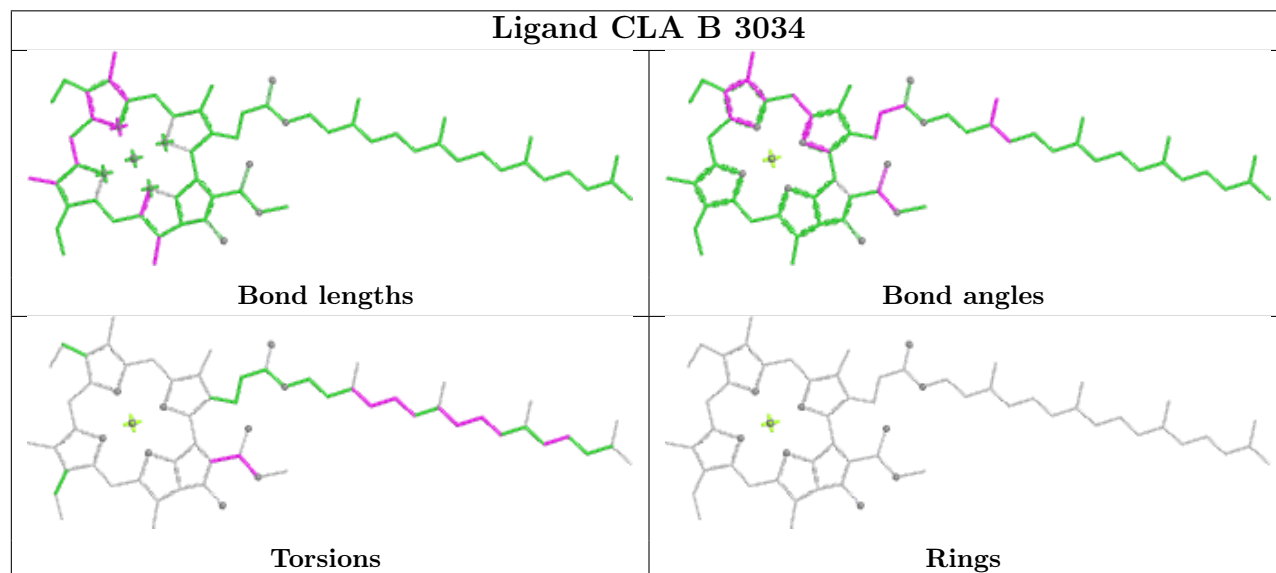
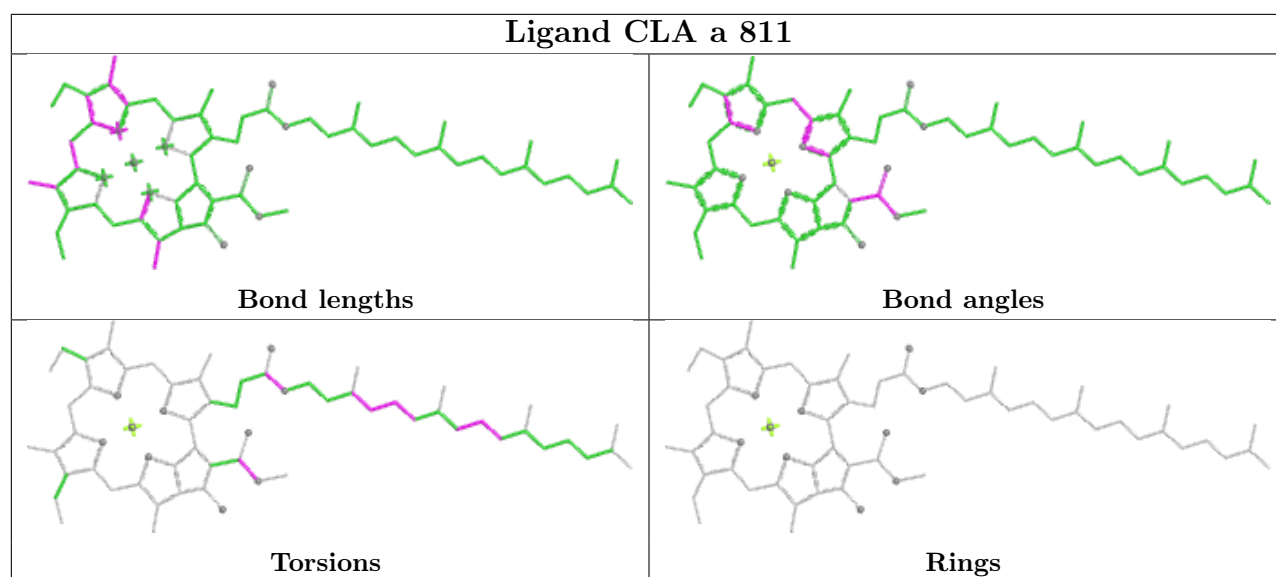
Bond angles

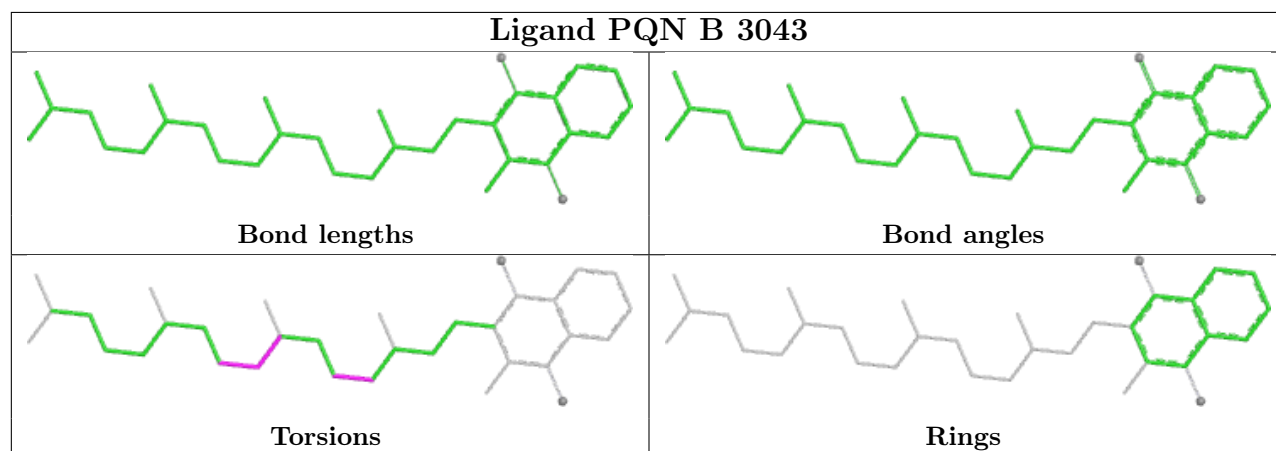
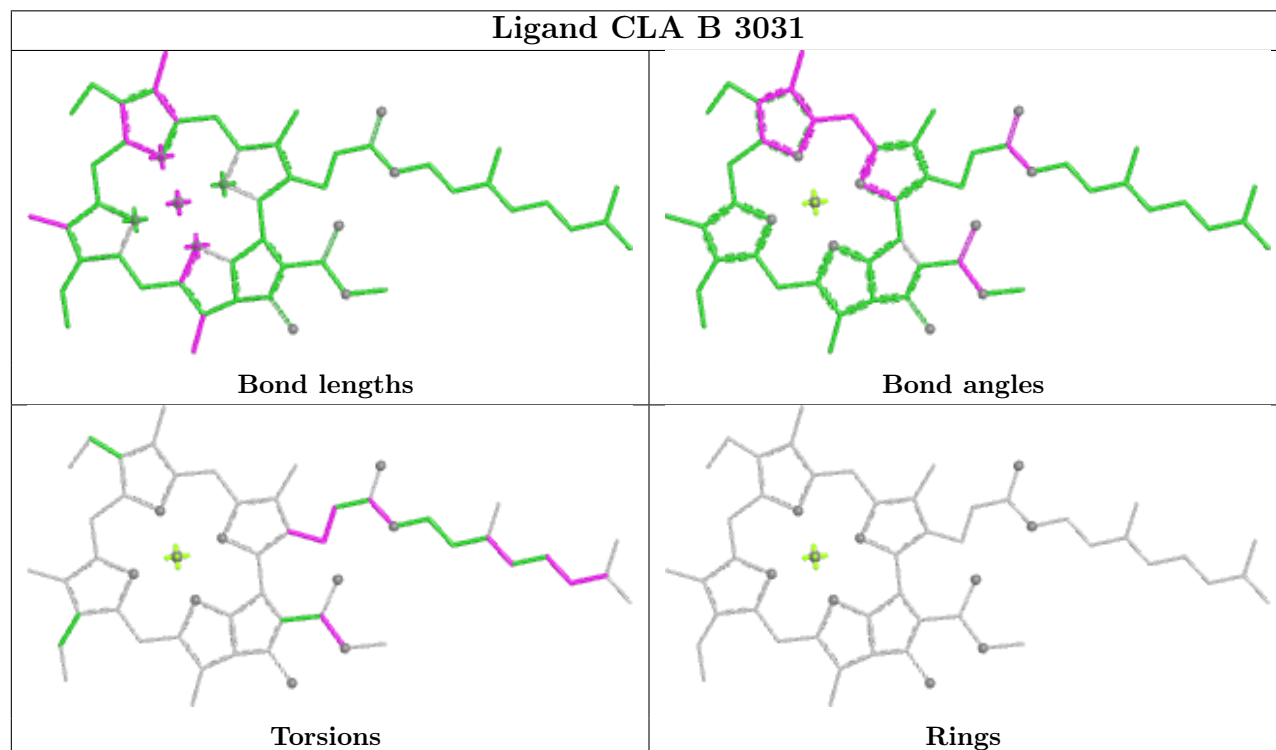
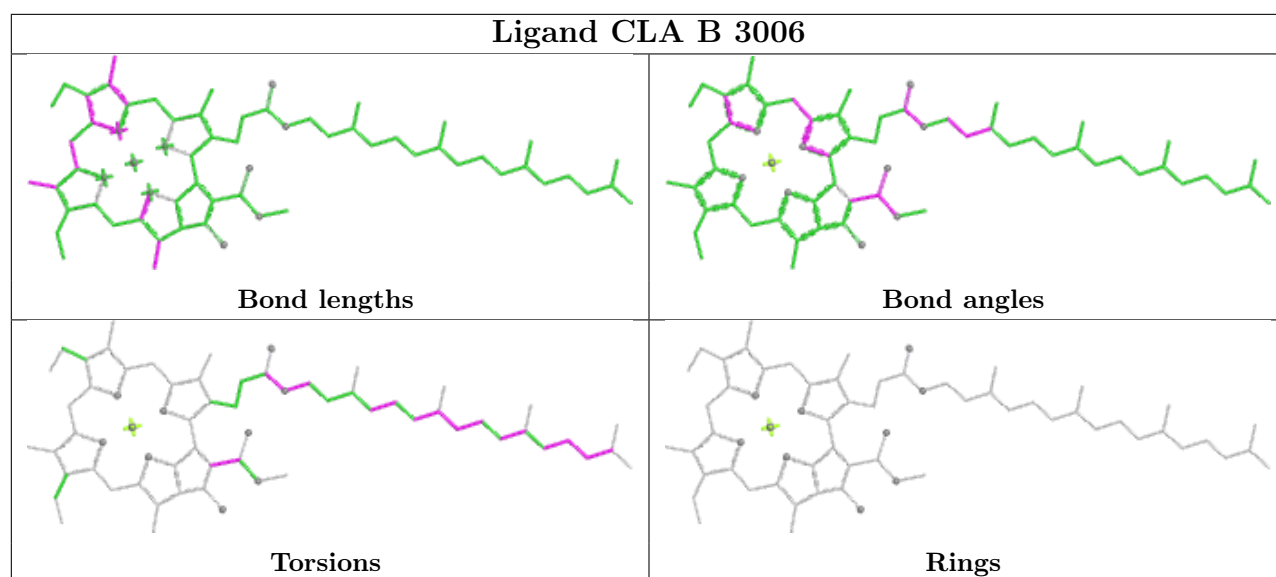


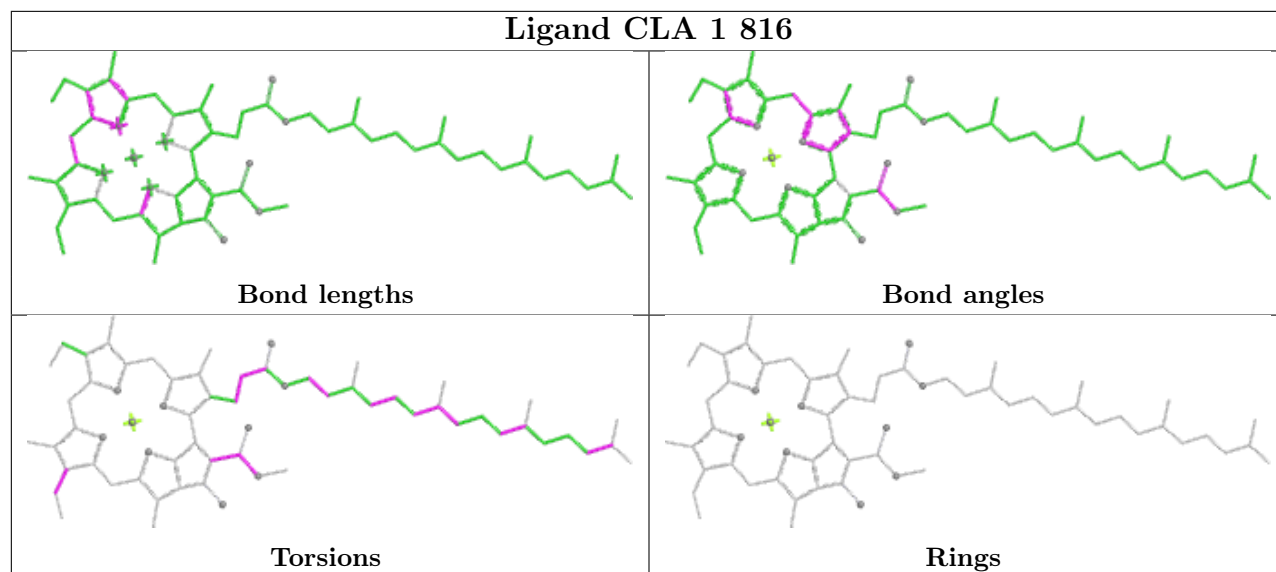
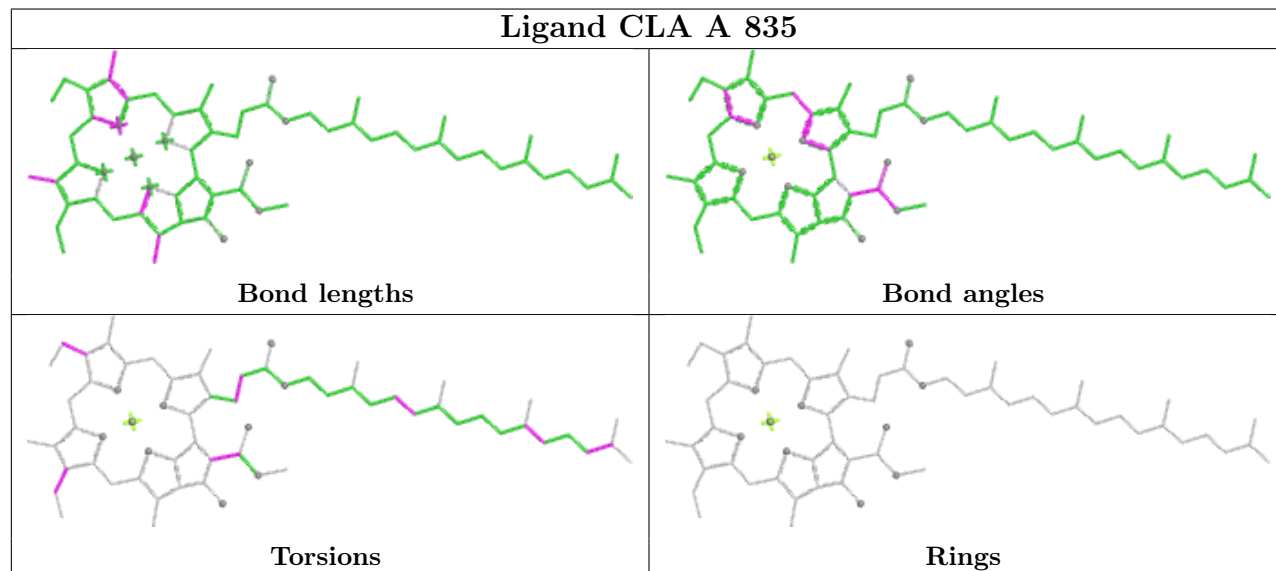
Torsions



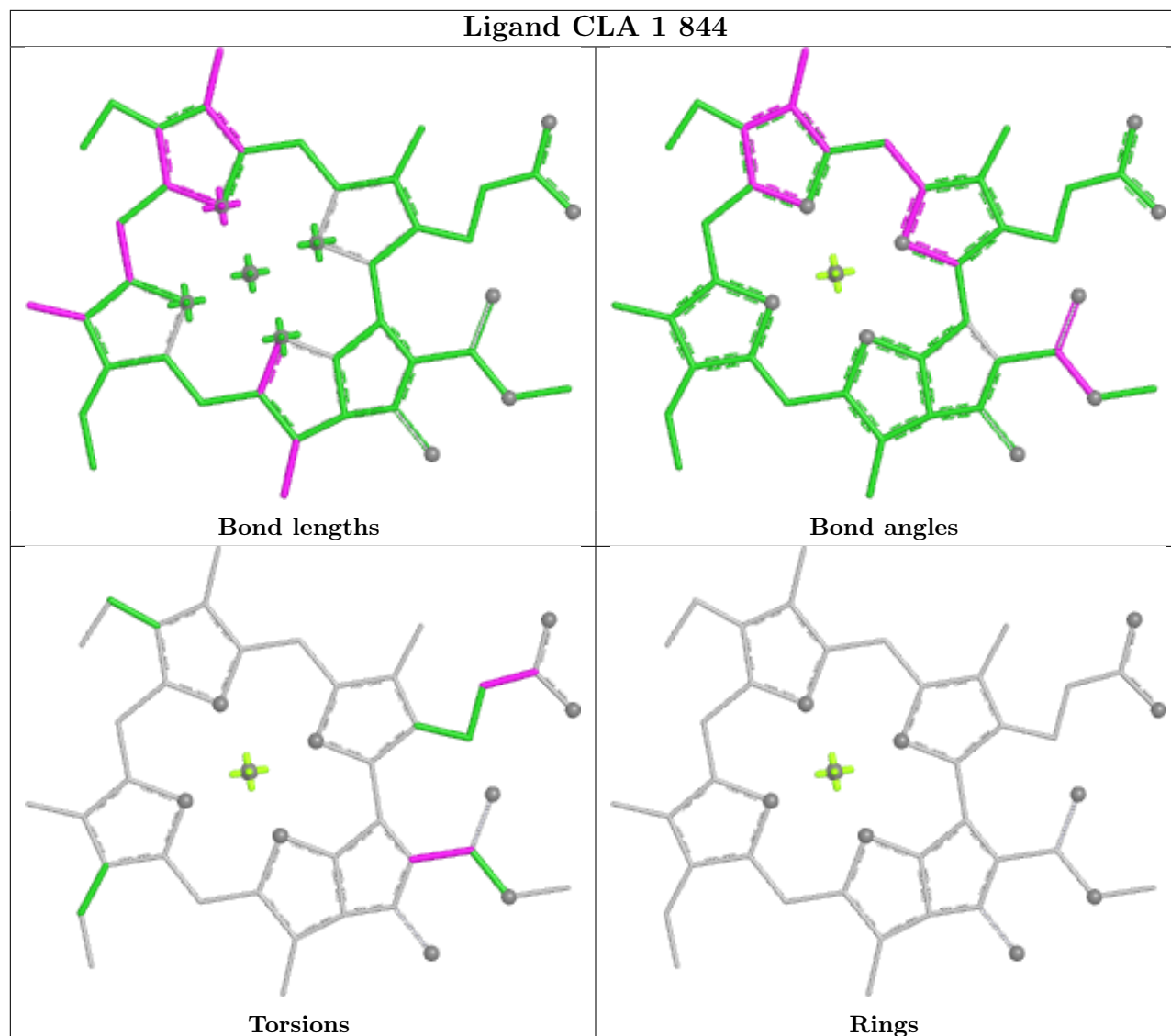
Rings



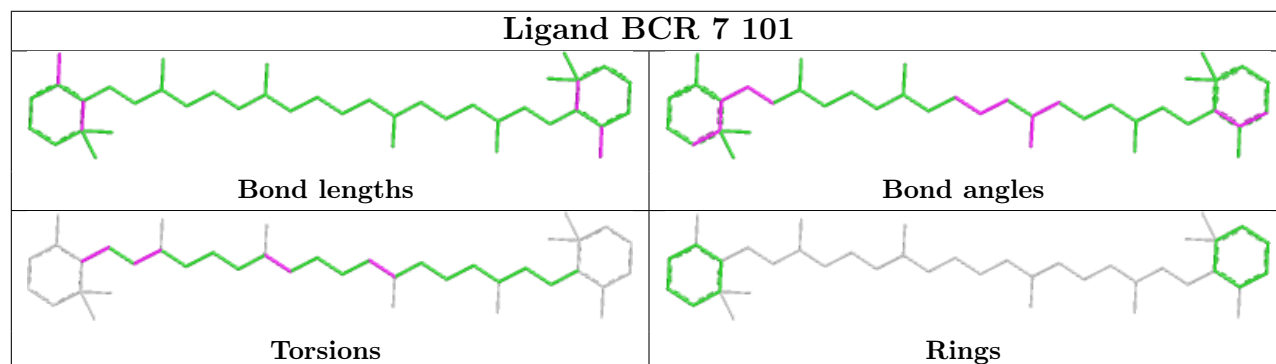


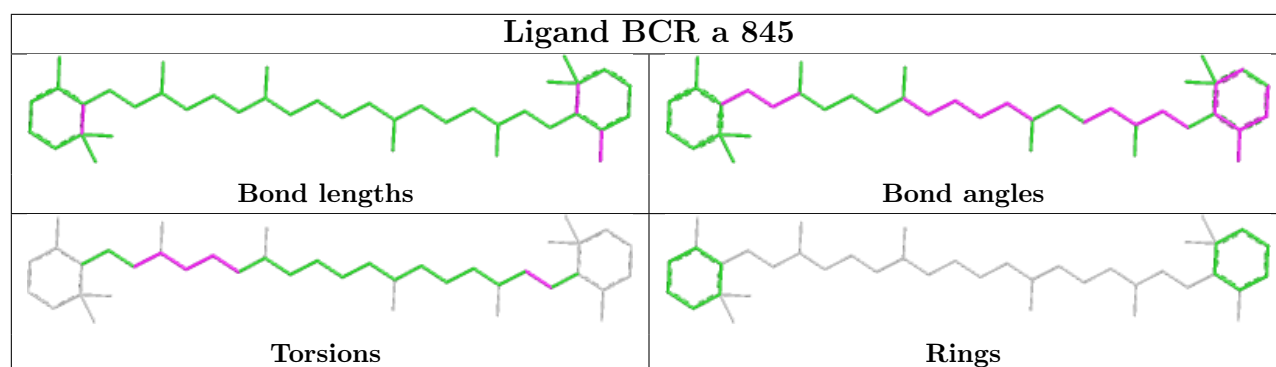
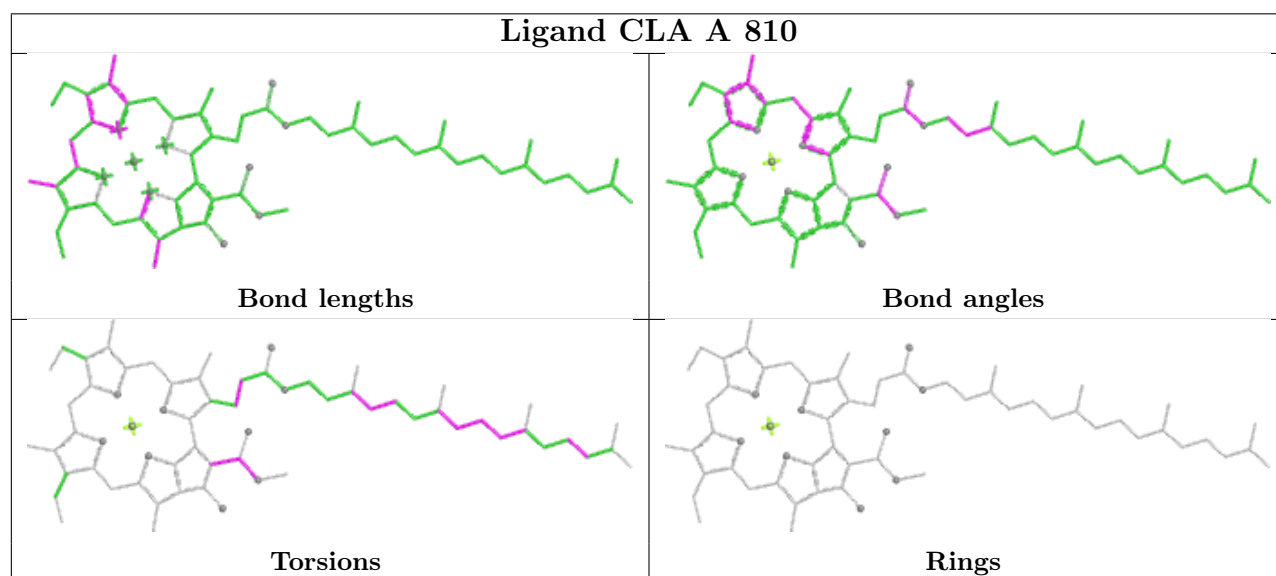
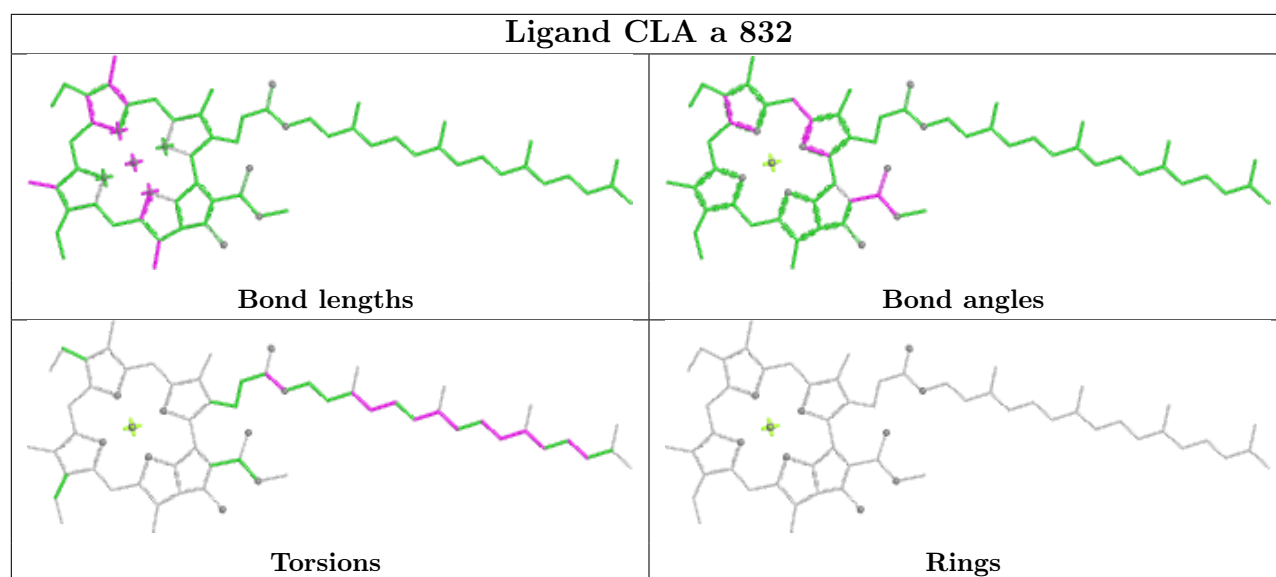
Ligand CLA 1 816**Ligand CLA A 835**

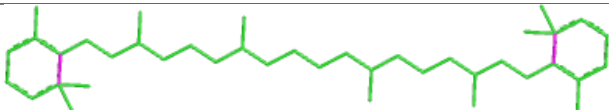
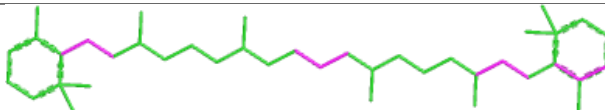
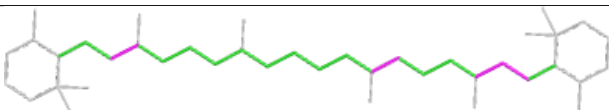
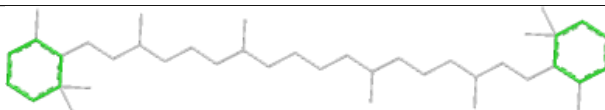
Ligand CLA 1 844

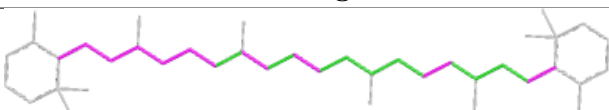
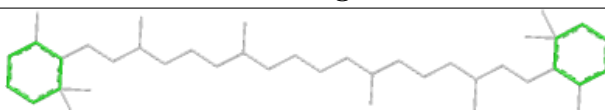


Ligand BCR 7 101

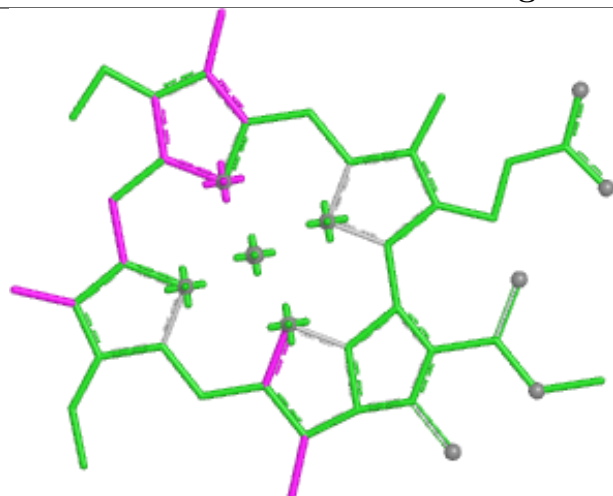




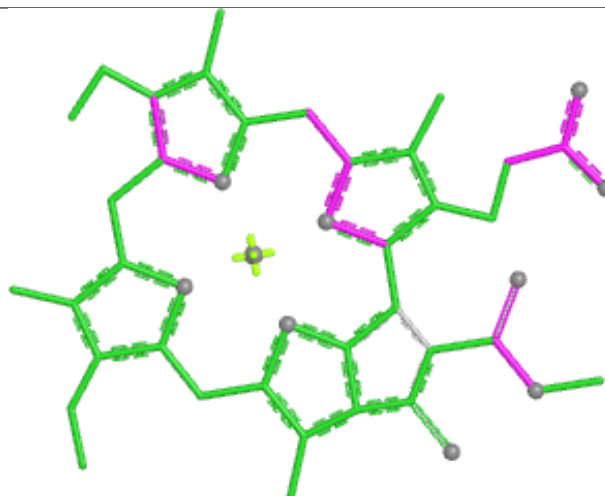
Ligand BCR 2 3044	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 3047	
	
Bond lengths	Bond angles
	
Torsions	Rings

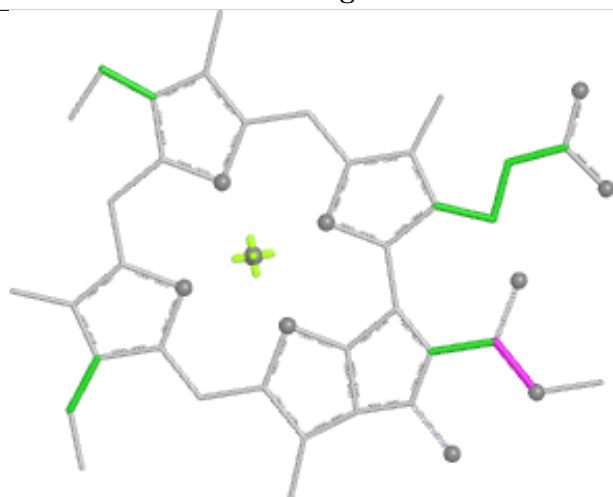
Ligand CLA a 836



Bond lengths



Bond angles

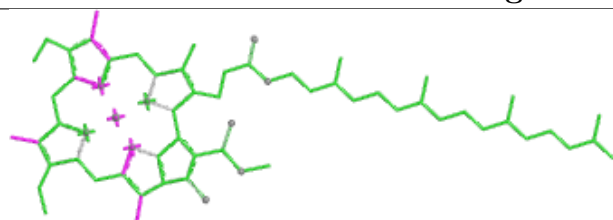


Torsions

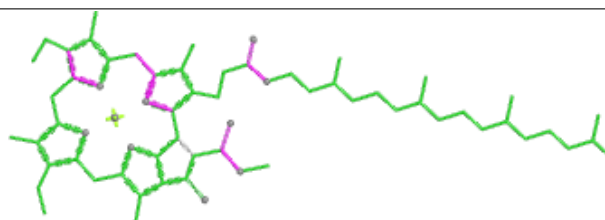


Rings

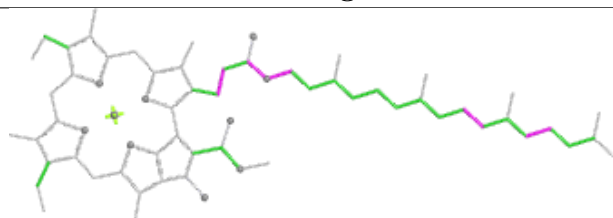
Ligand CLA B 3029



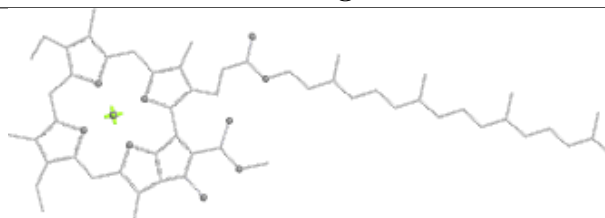
Bond lengths



Bond angles

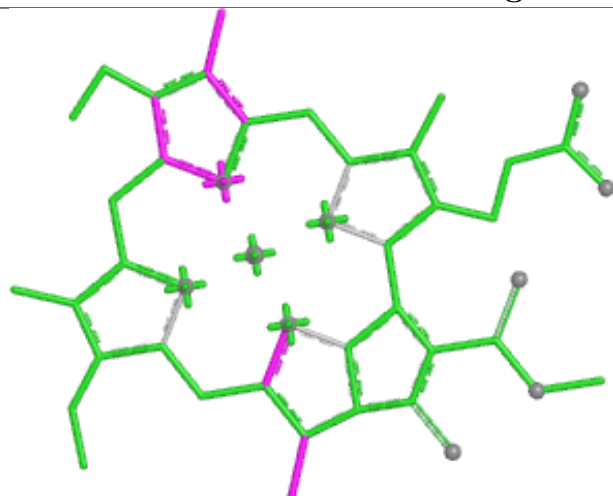


Torsions

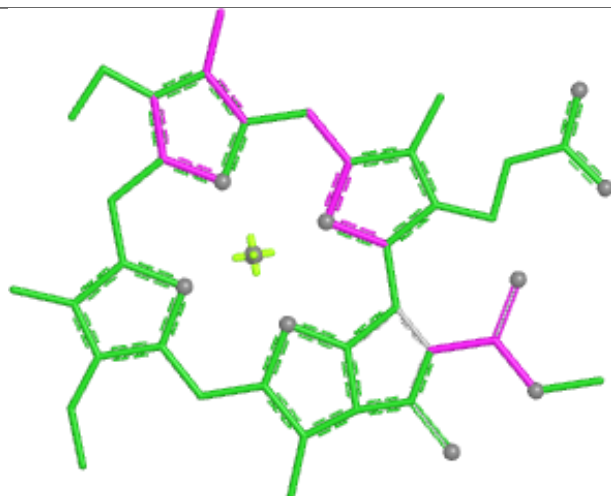


Rings

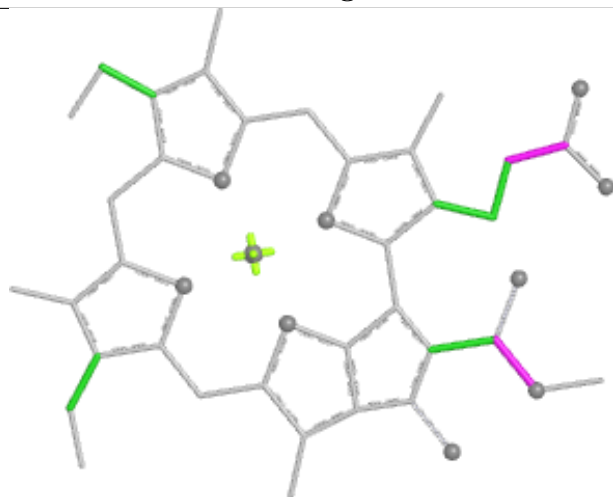
Ligand CLA B 3022



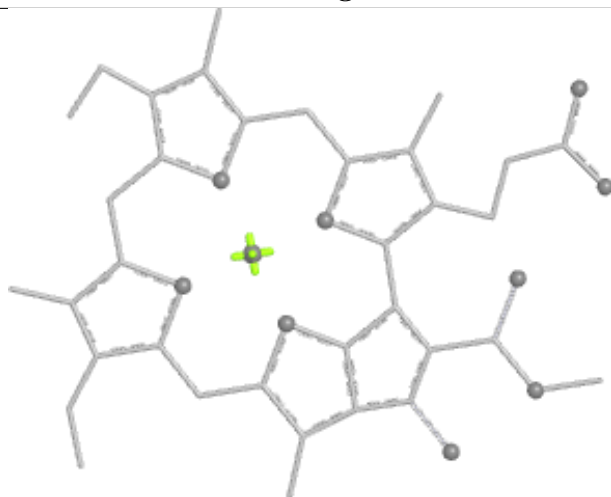
Bond lengths



Bond angles

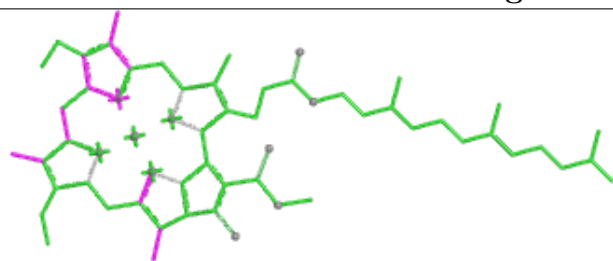


Torsions

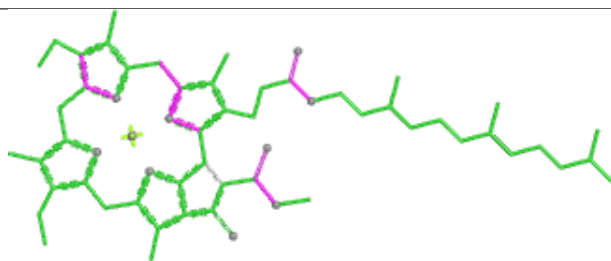


Rings

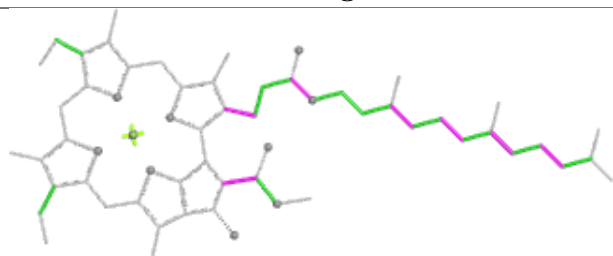
Ligand CLA B 3038



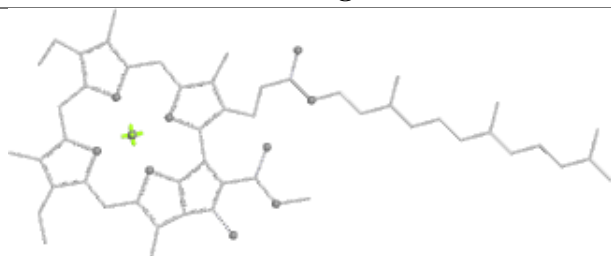
Bond lengths



Bond angles

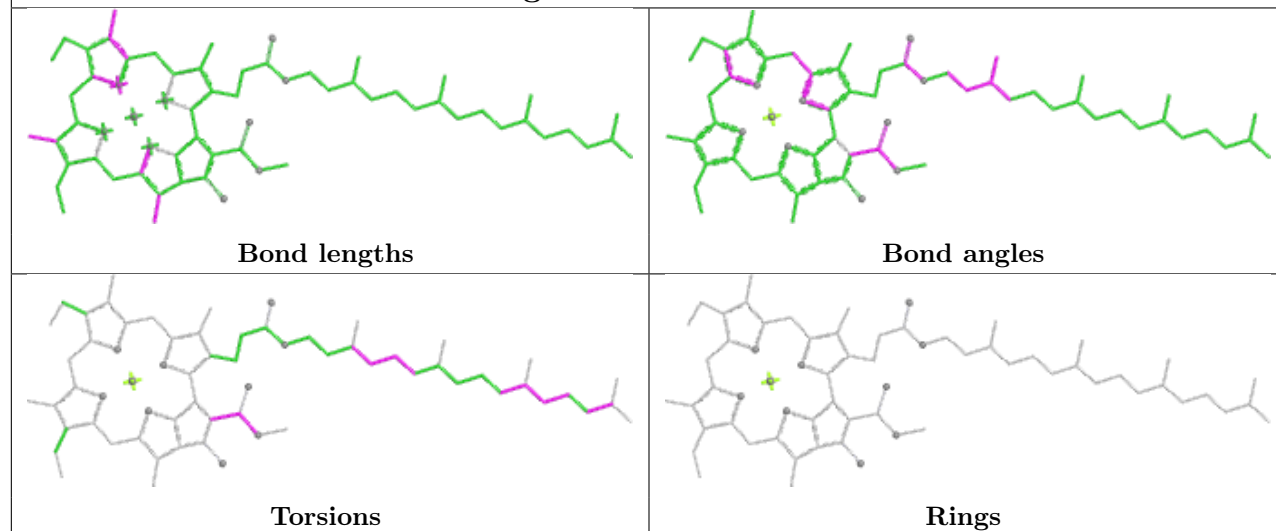


Torsions

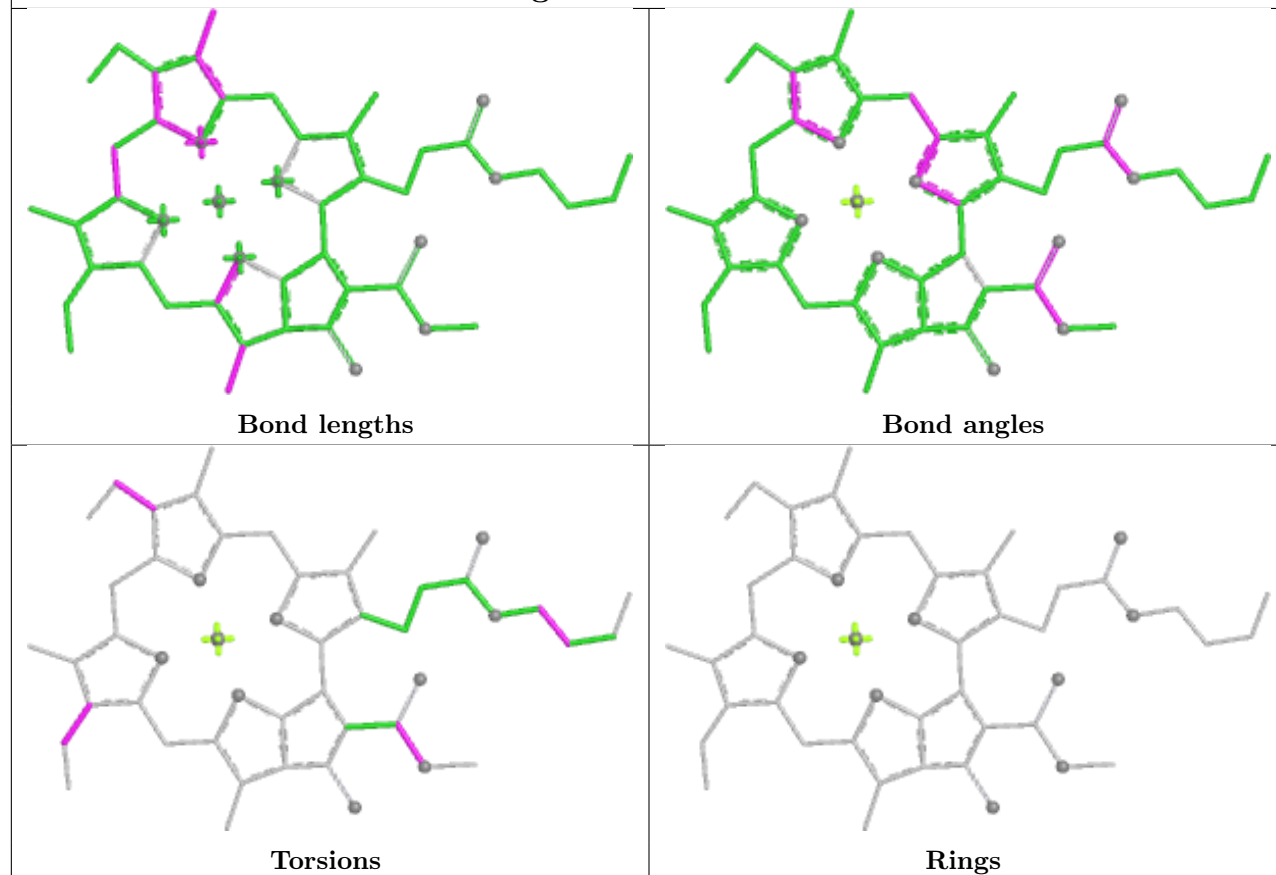


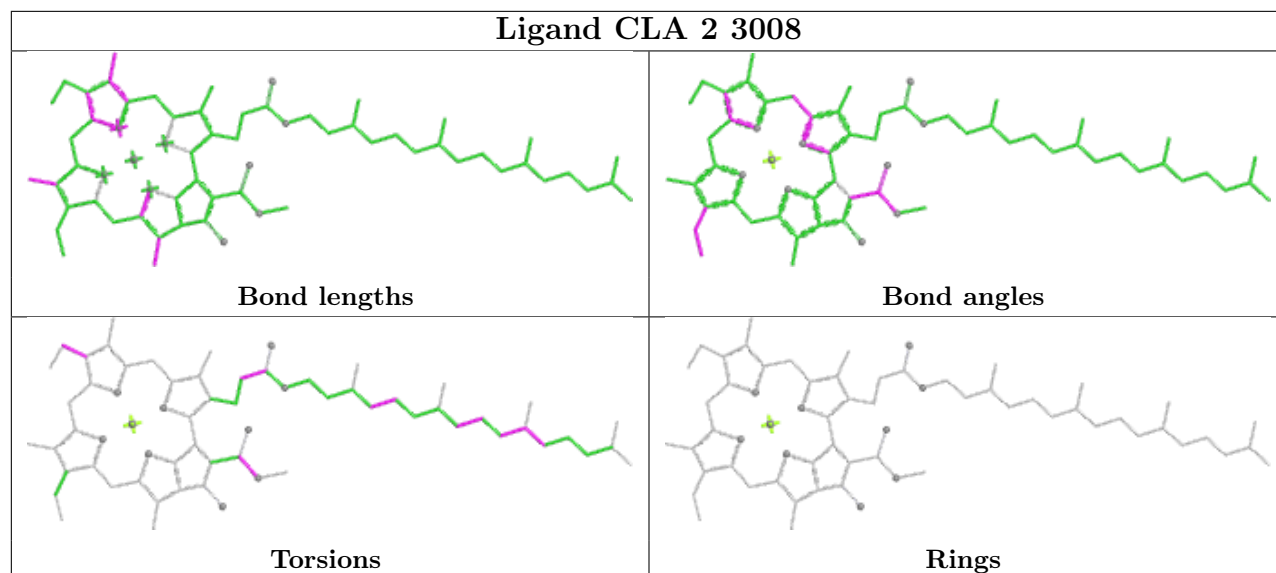
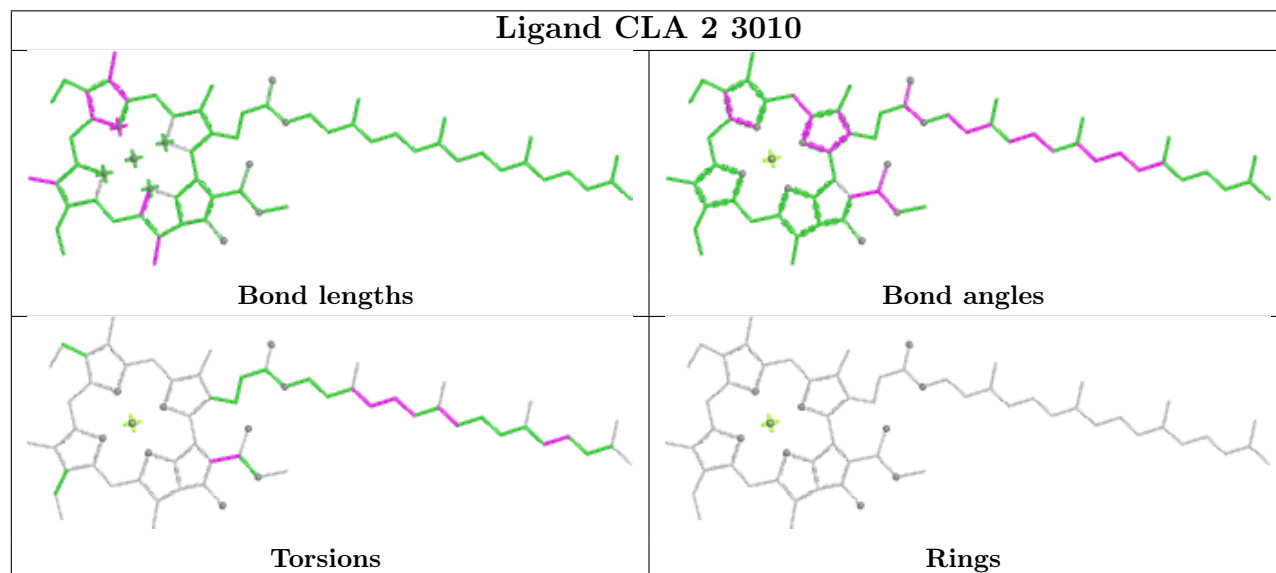
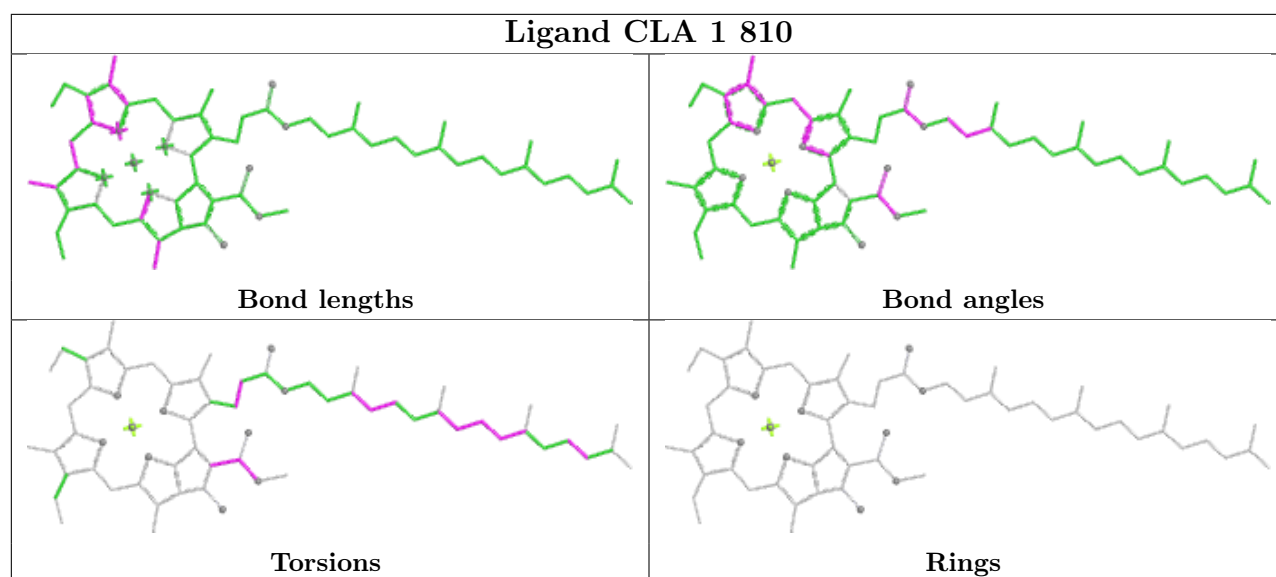
Rings

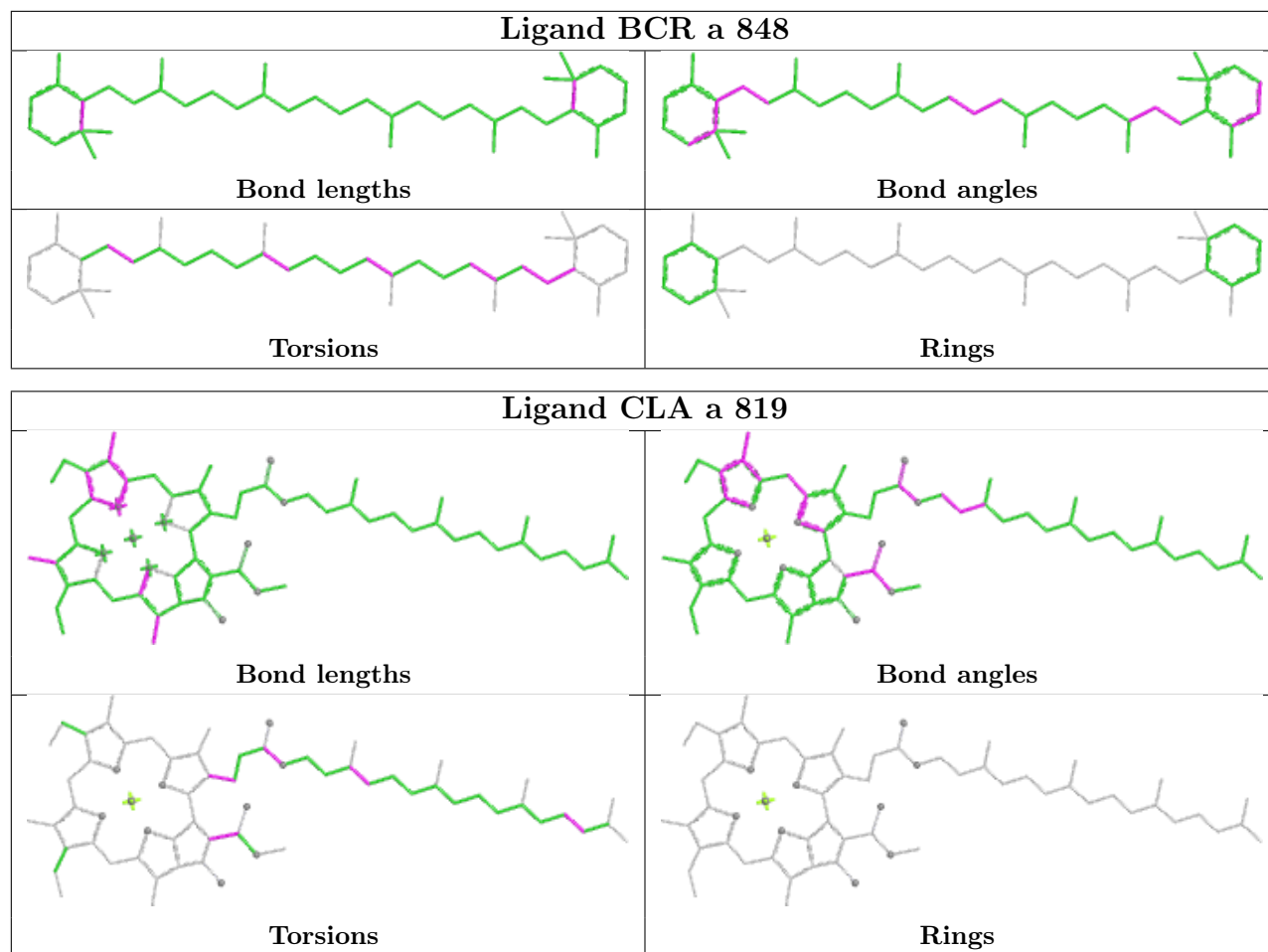
Ligand CLA B 3012

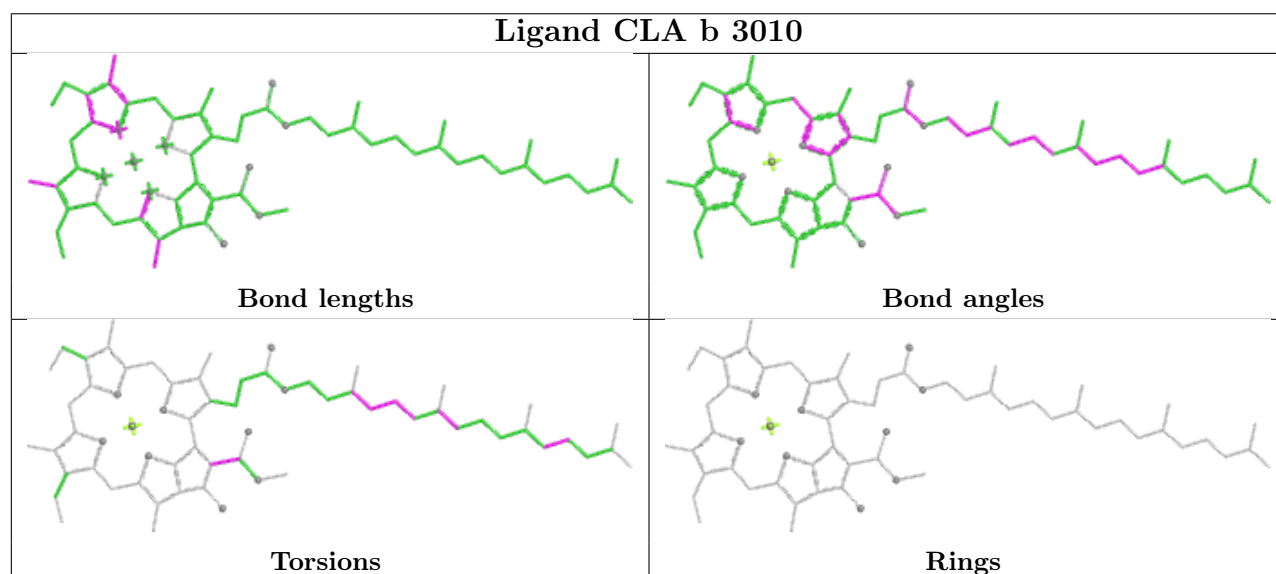
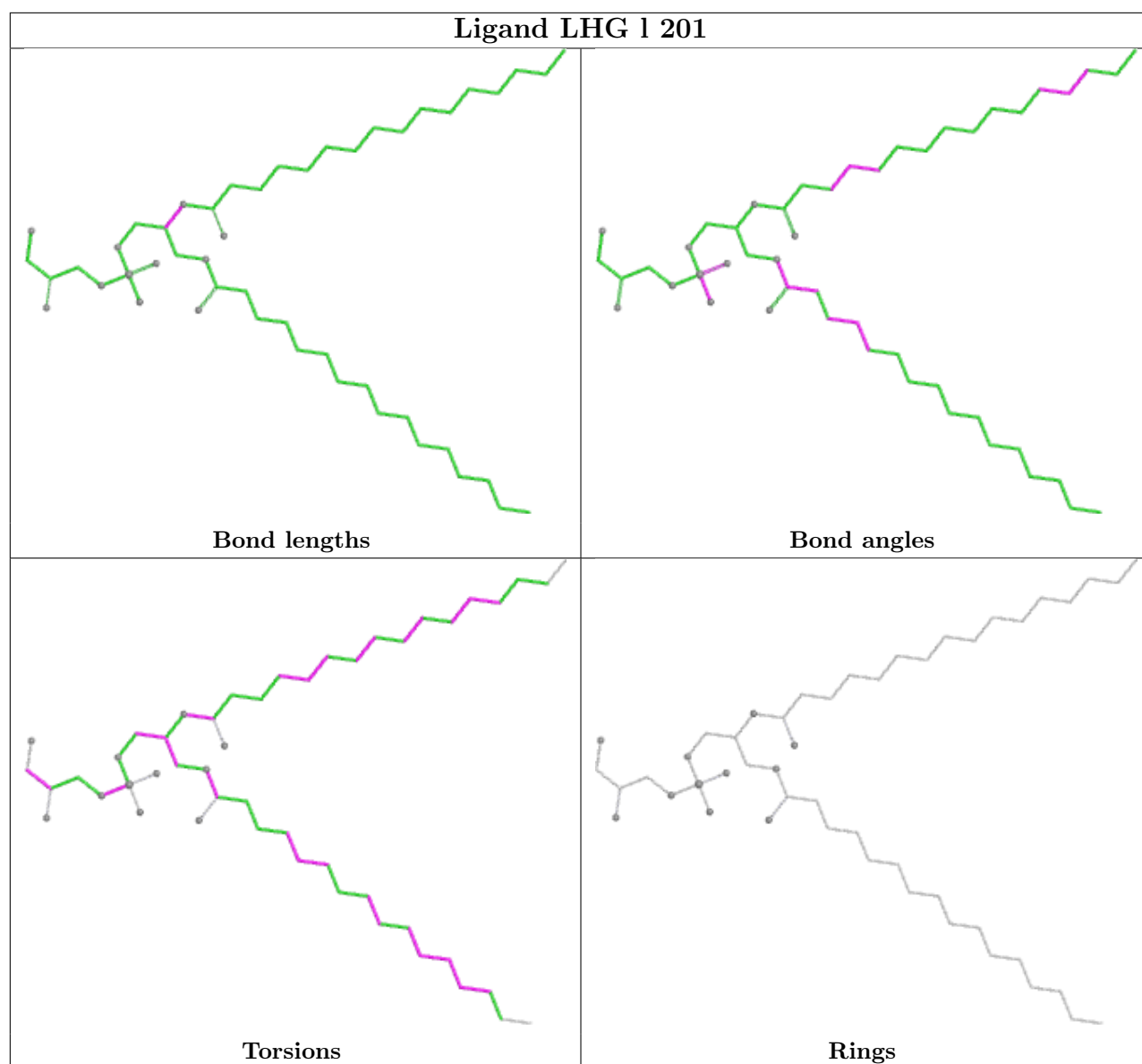


Ligand CLA A 811

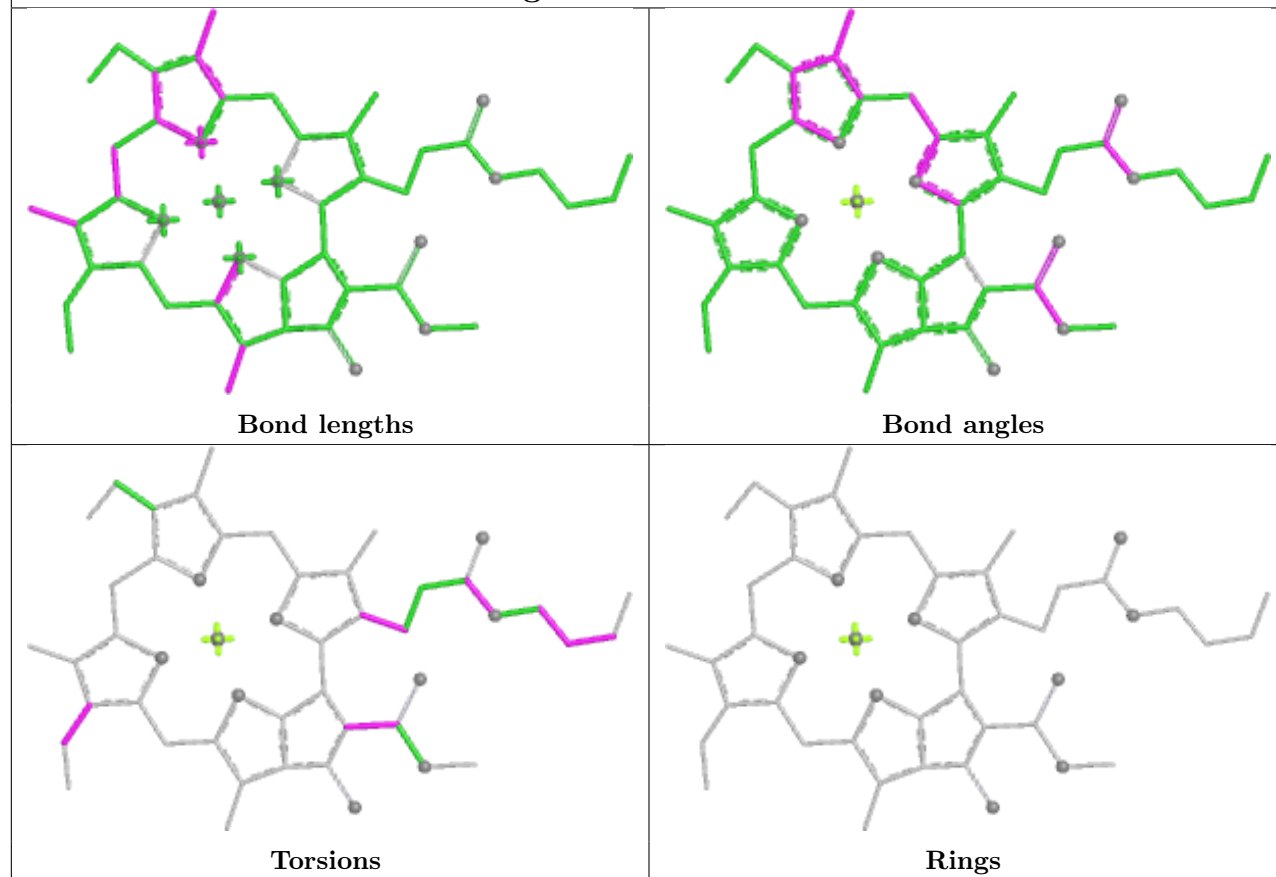




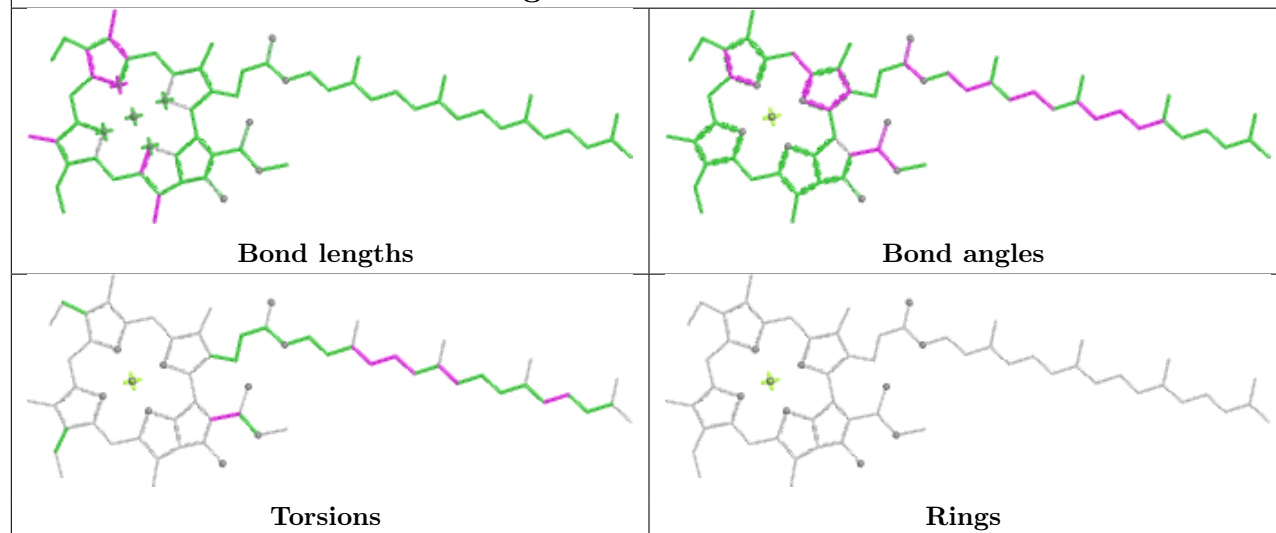


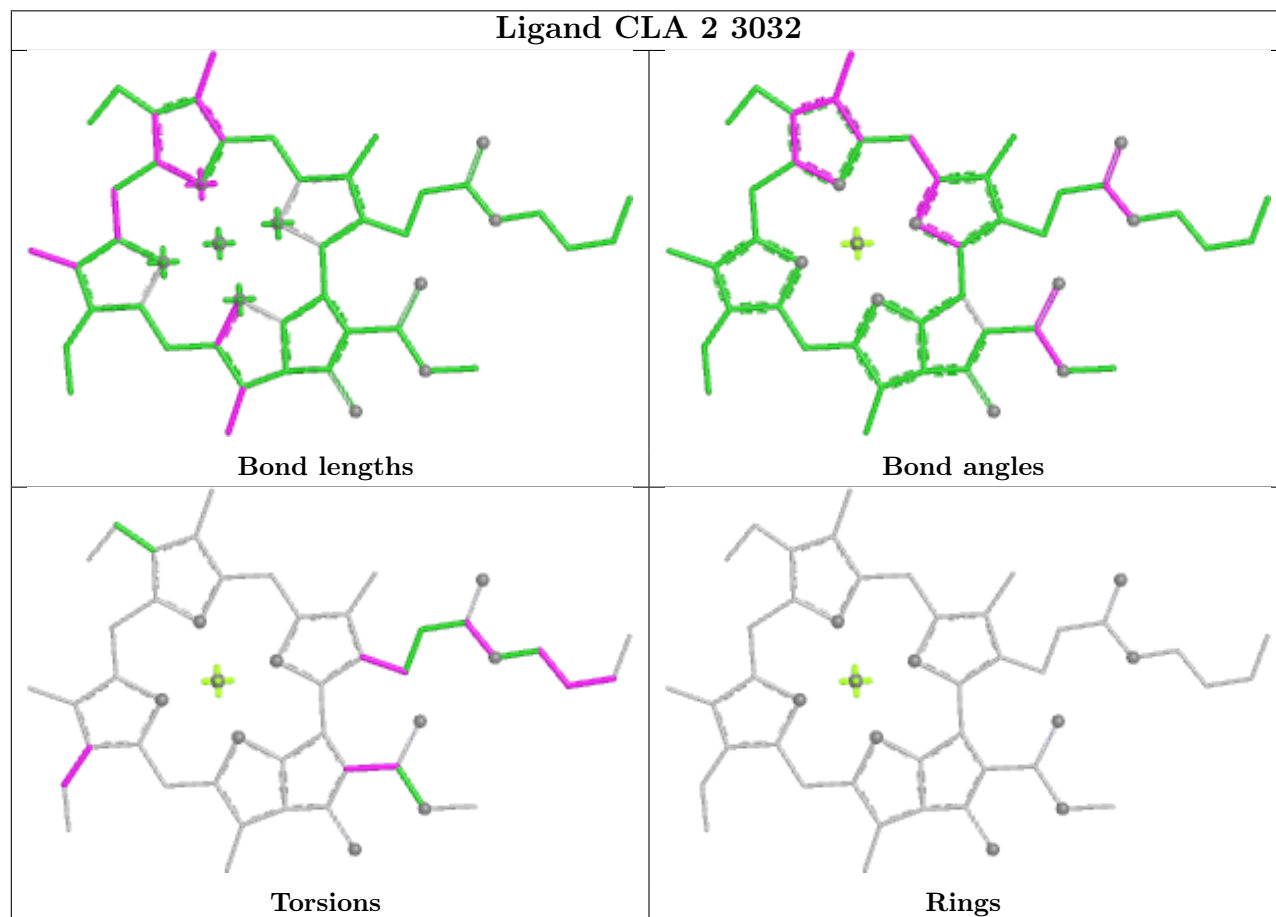
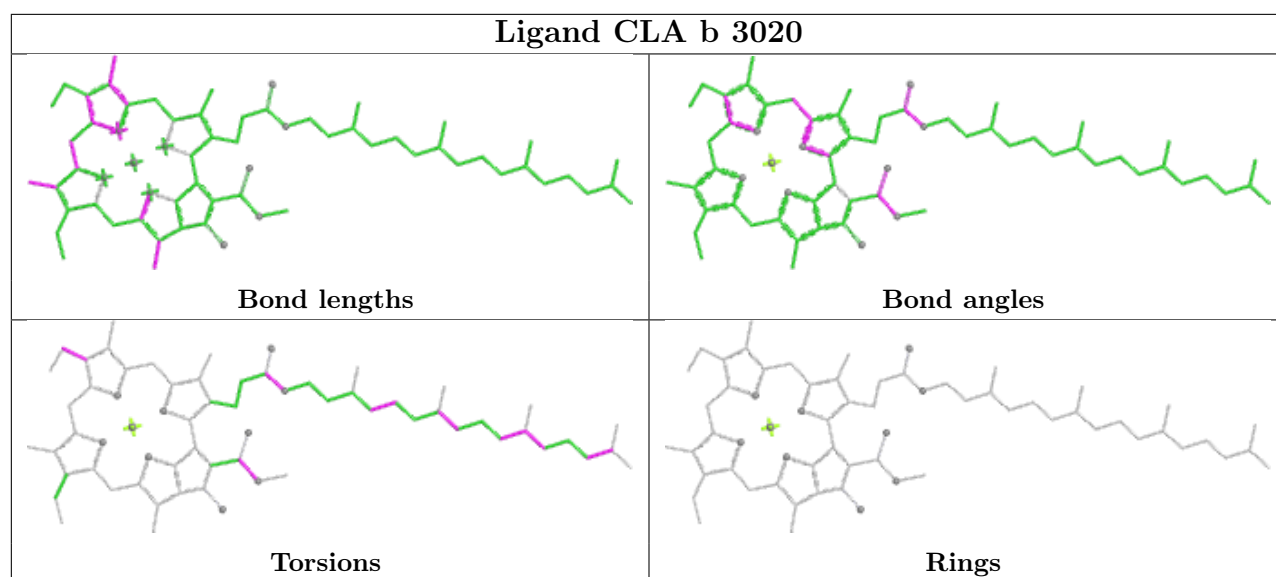


Ligand CLA B 3032

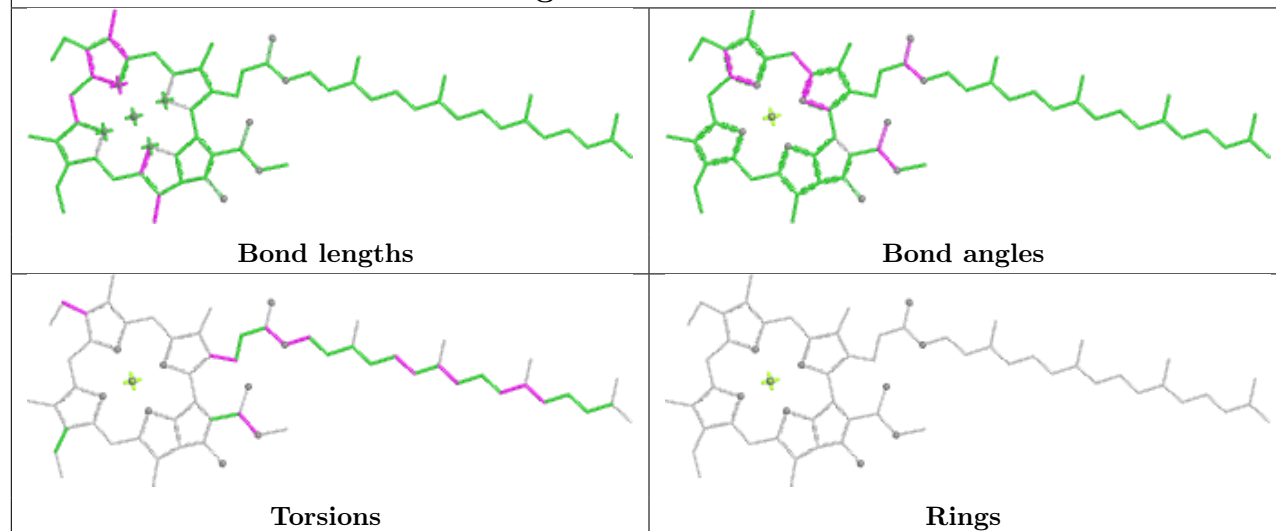


Ligand CLA B 3010

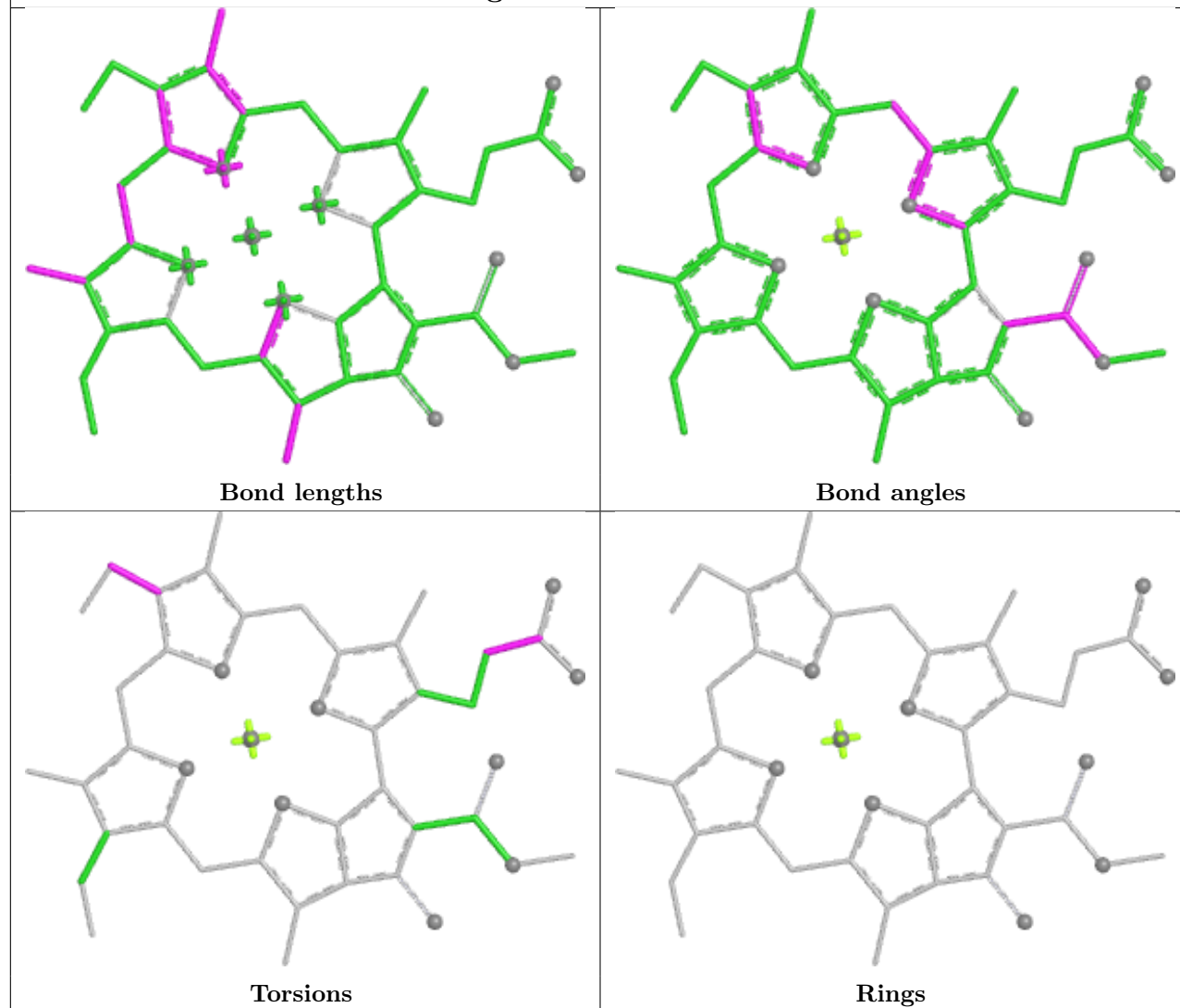




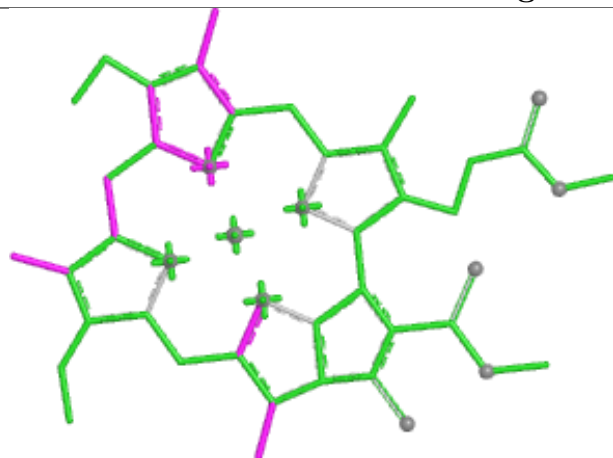
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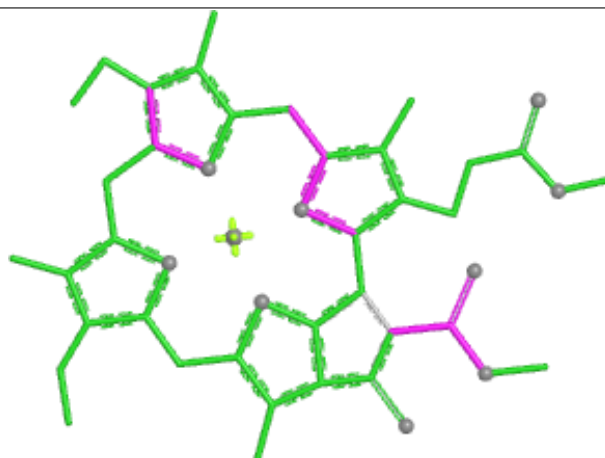
Ligand CLA b 3013



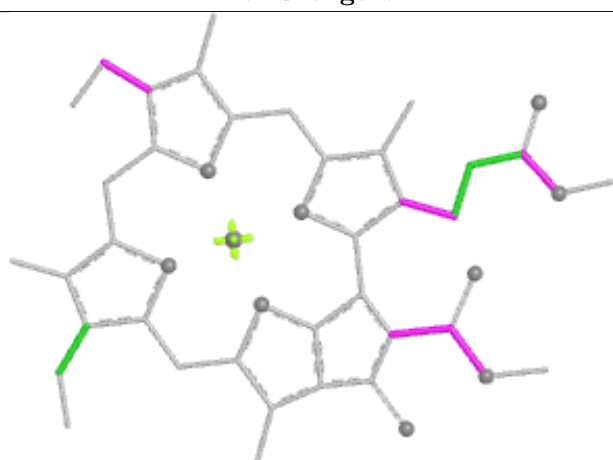
Ligand CLA k 101



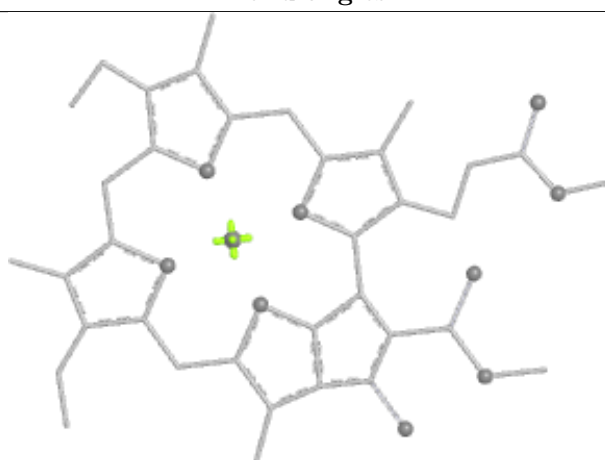
Bond lengths



Bond angles

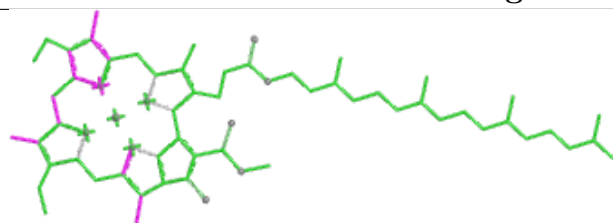


Torsions

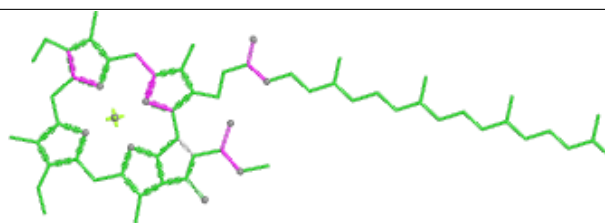


Rings

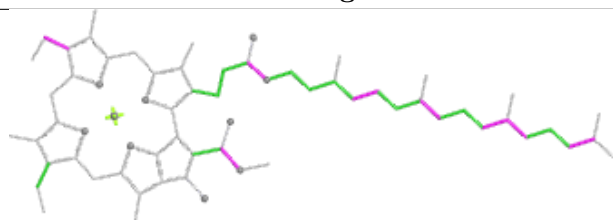
Ligand CLA B 3020



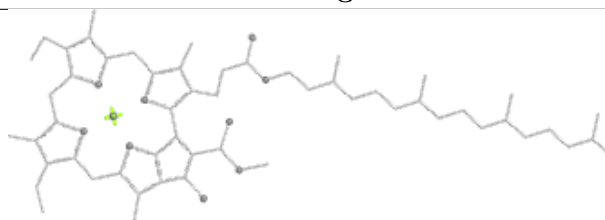
Bond lengths



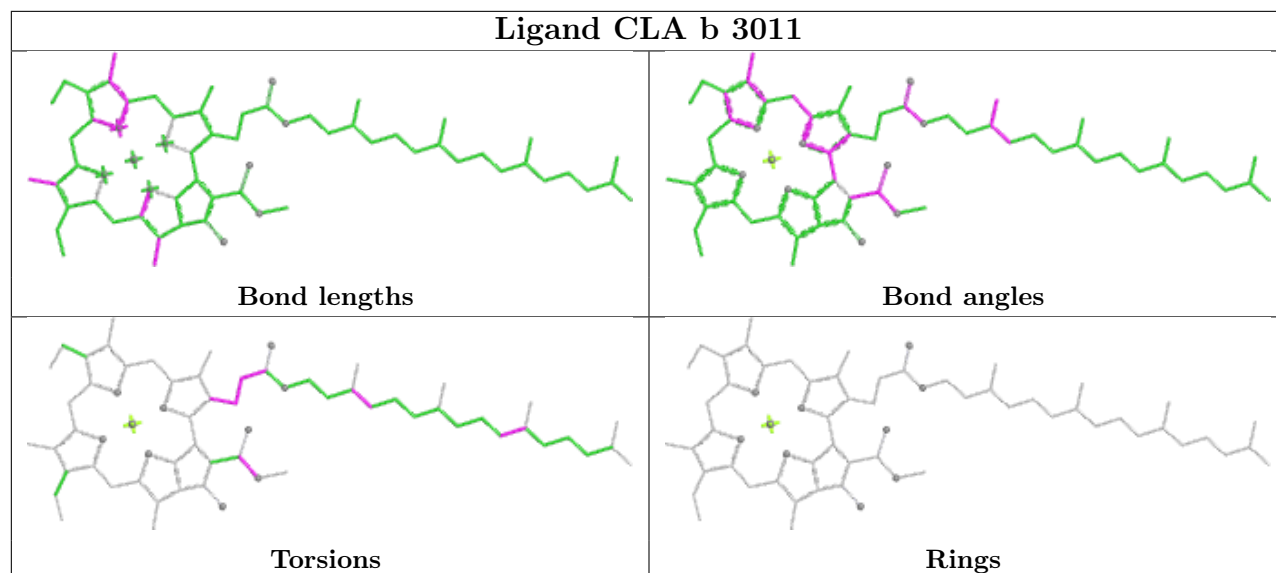
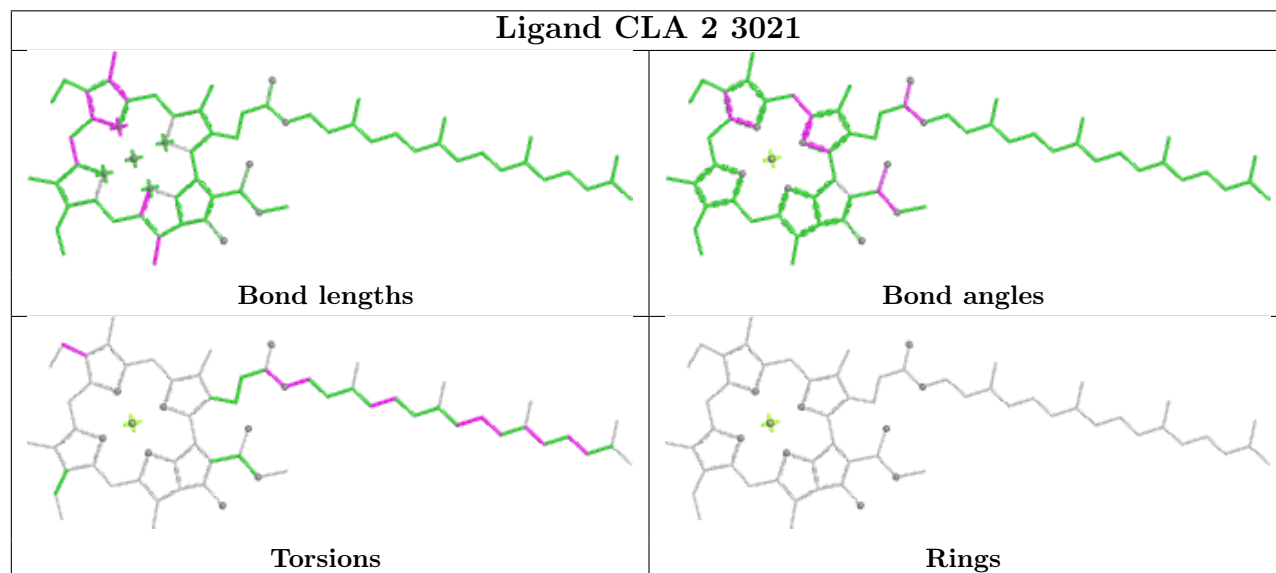
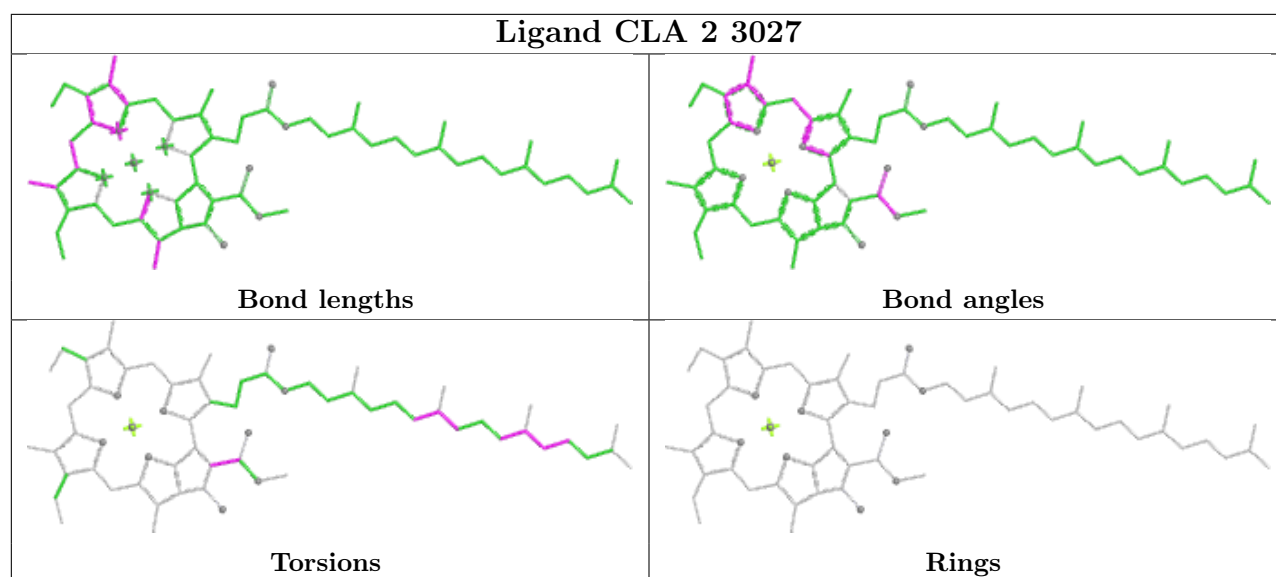
Bond angles

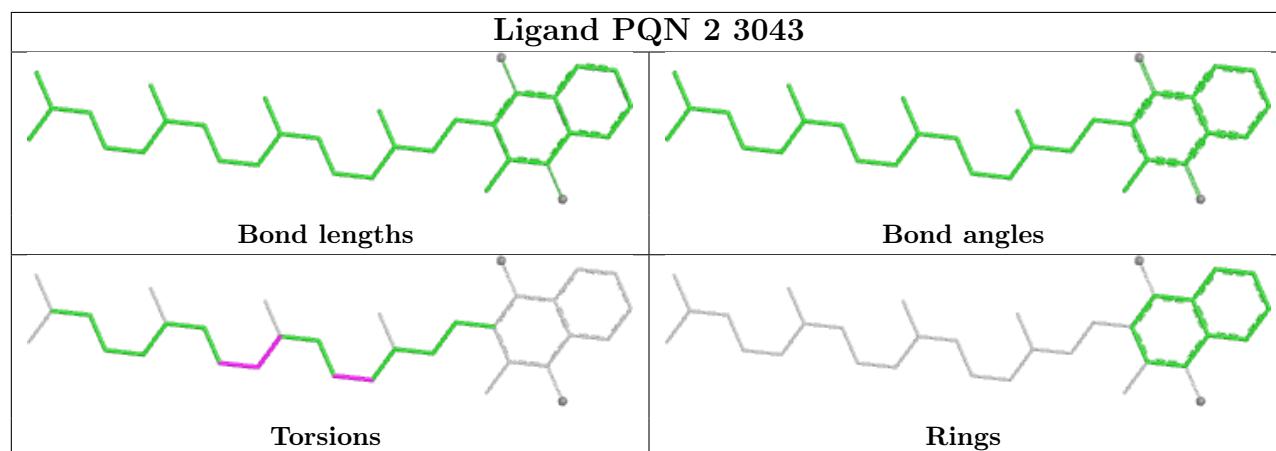
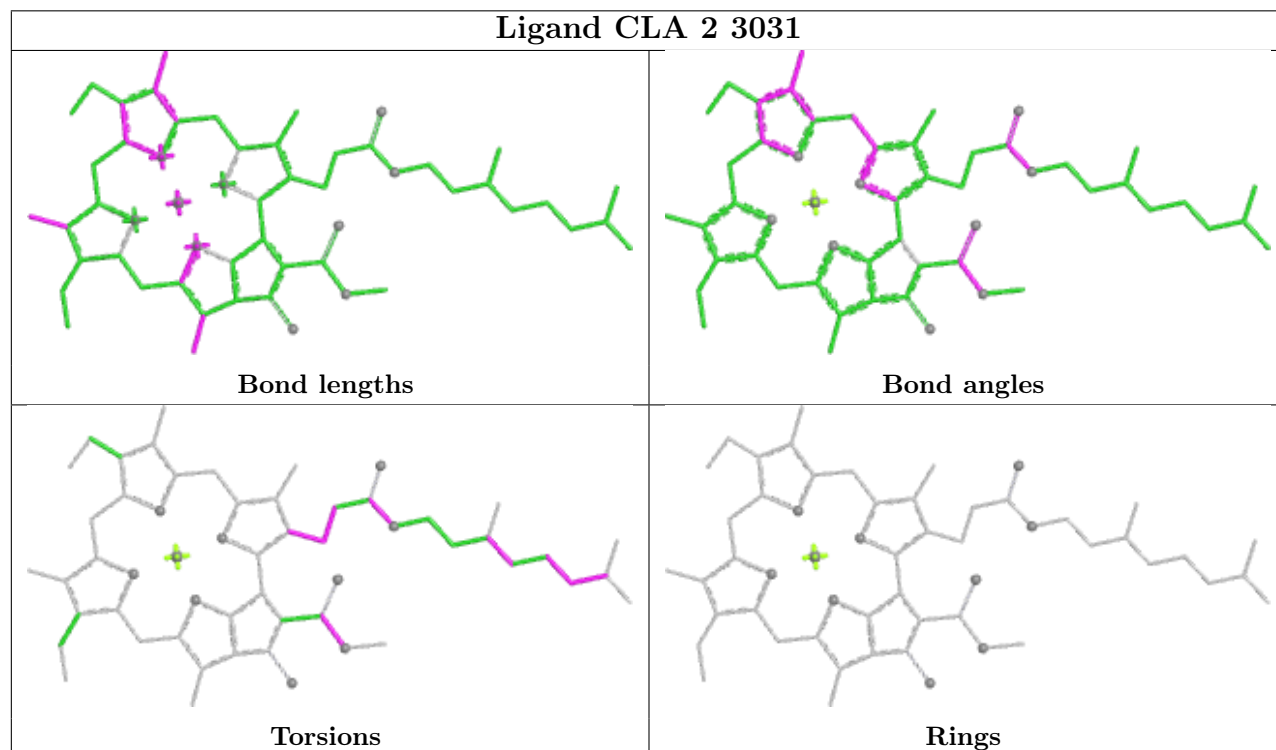
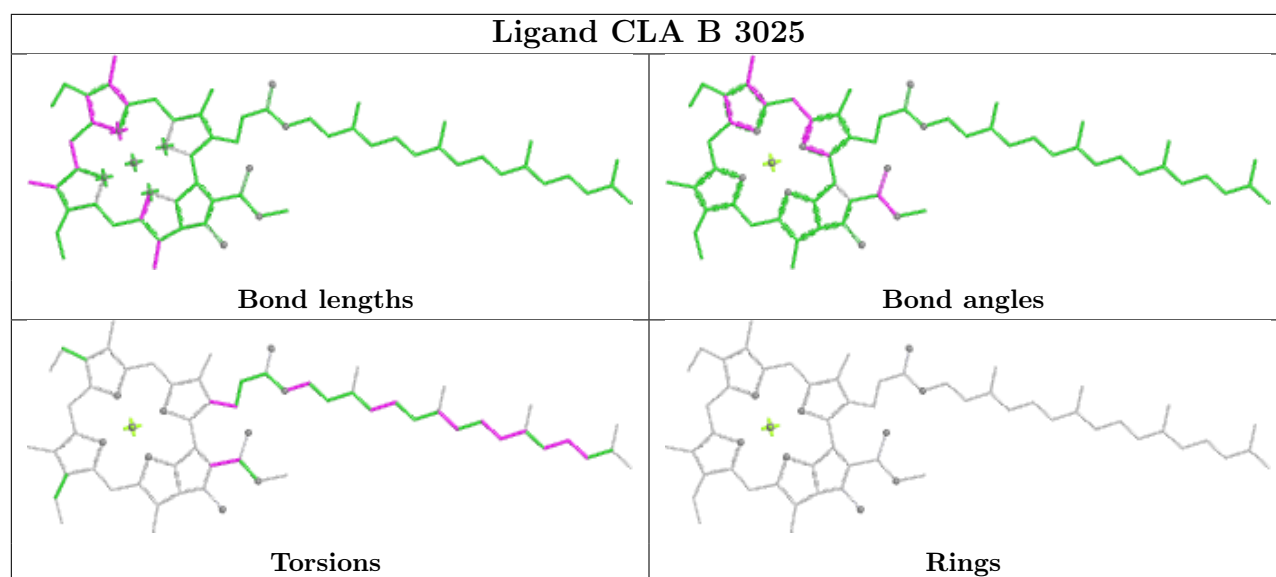


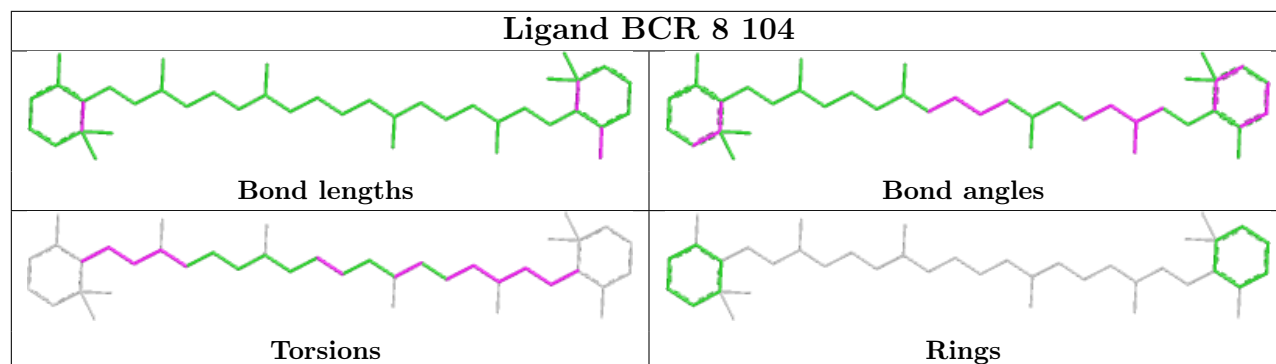
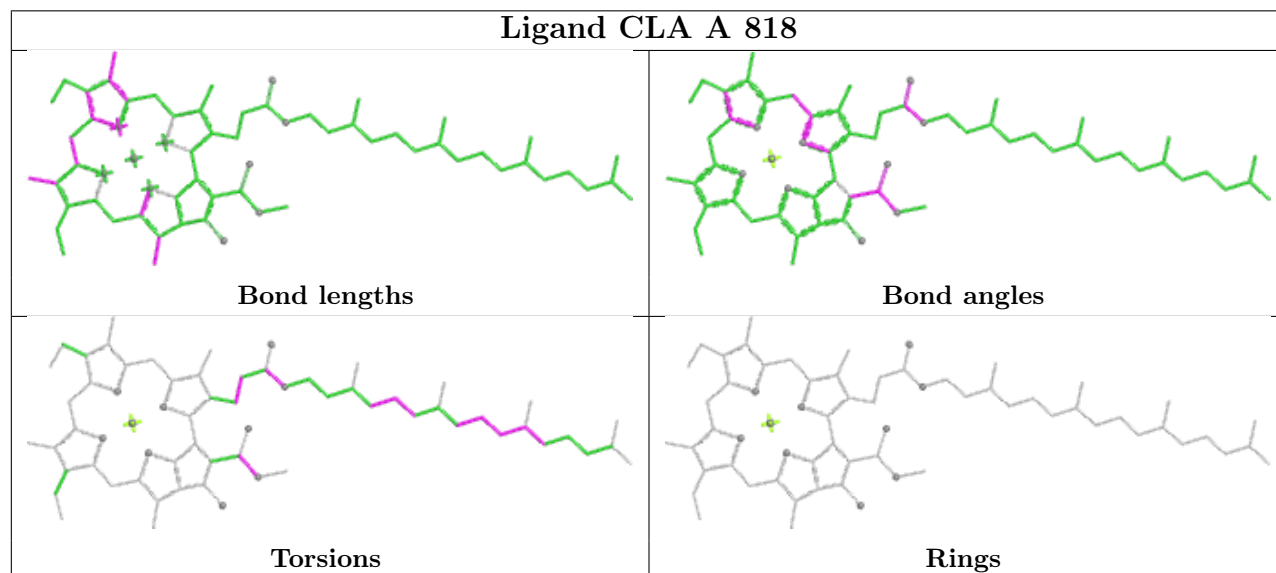
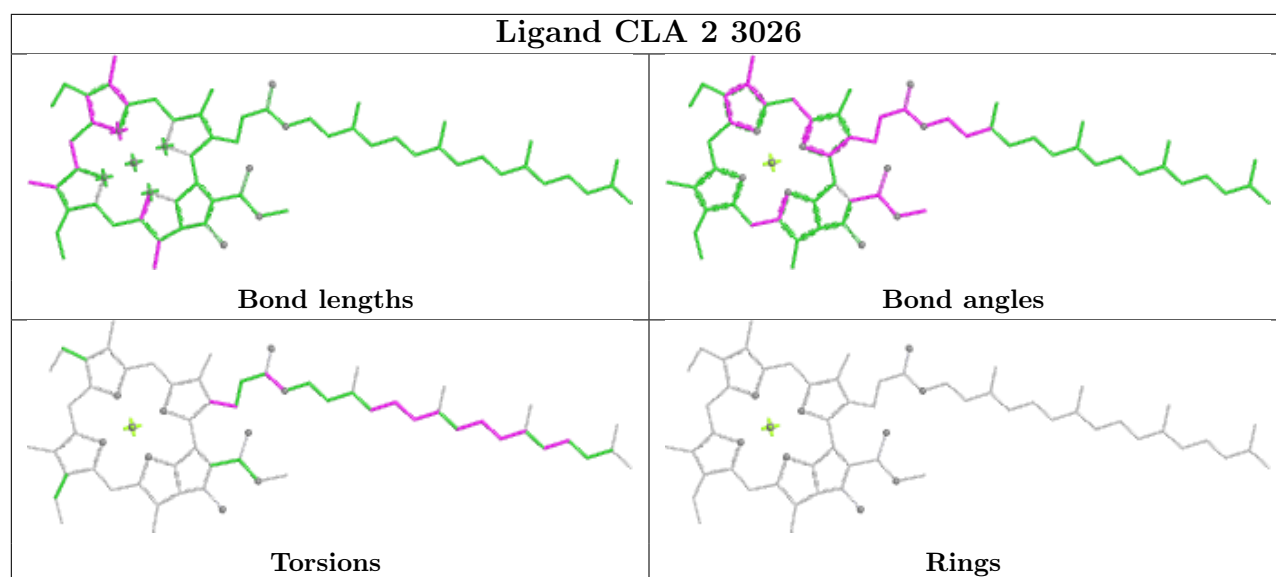
Torsions



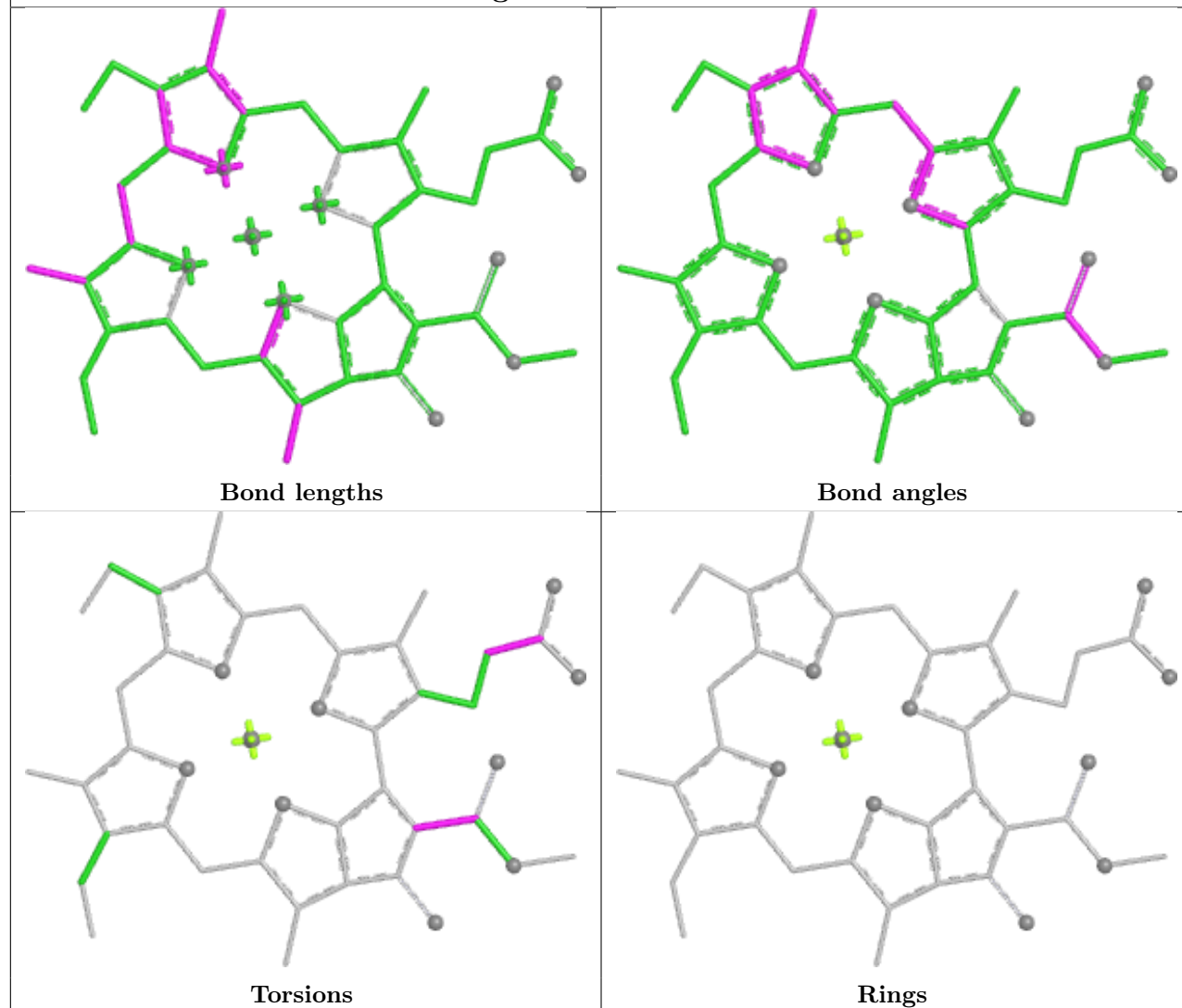
Rings



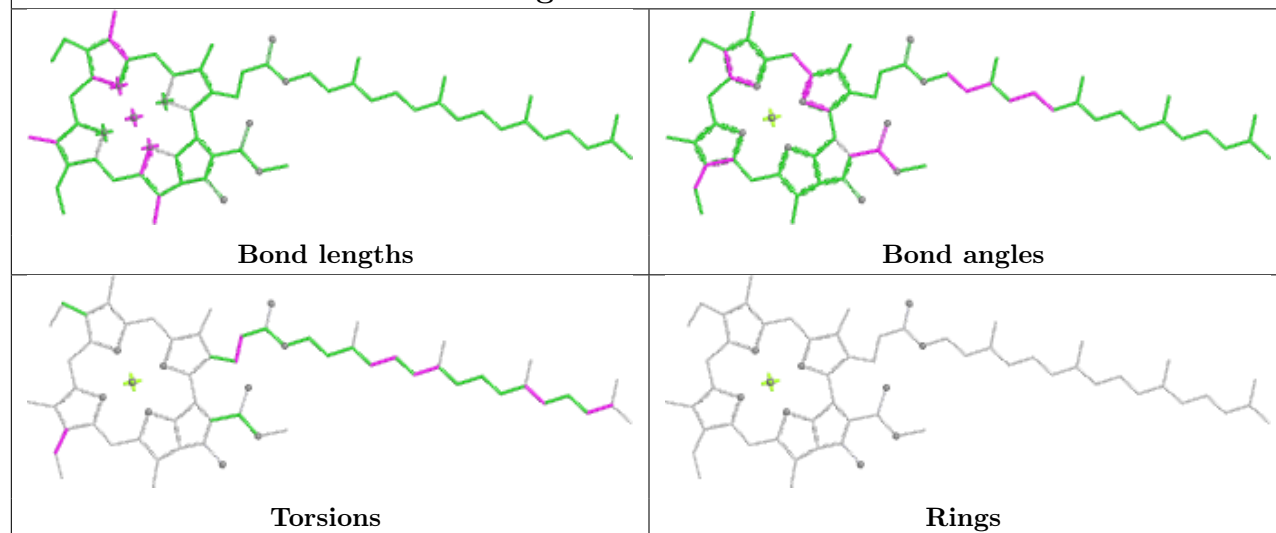


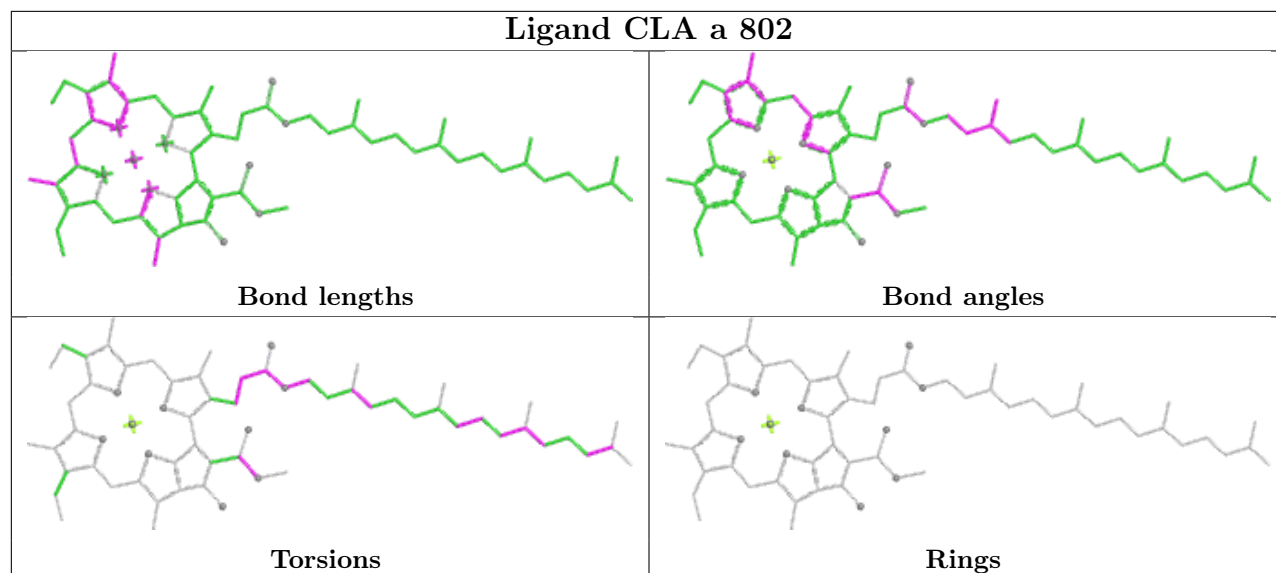
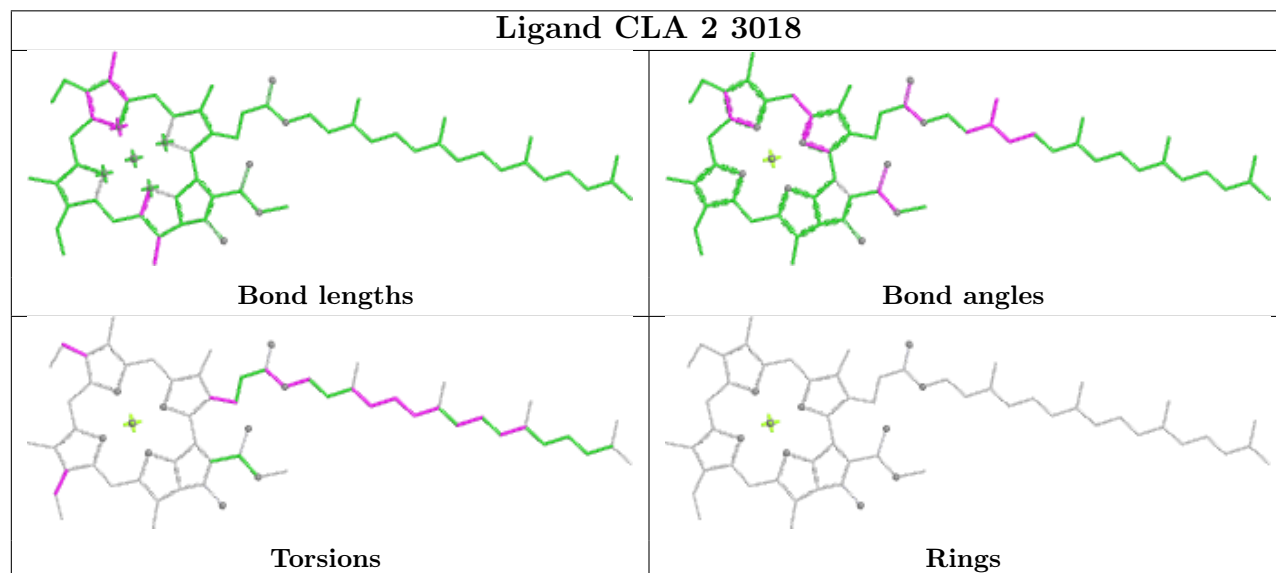
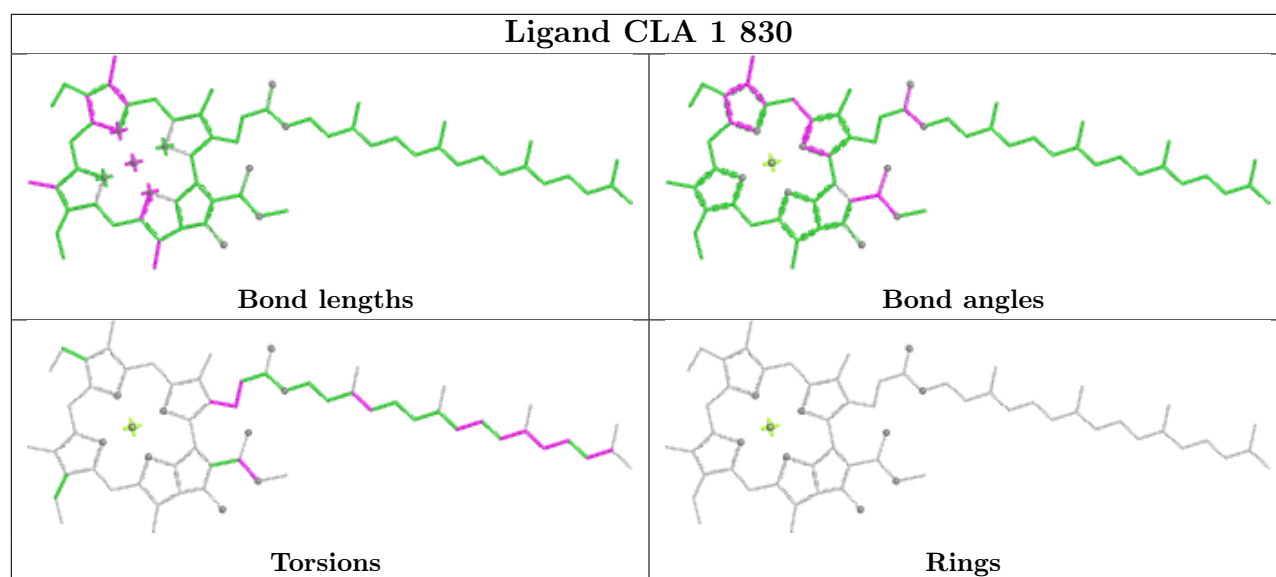


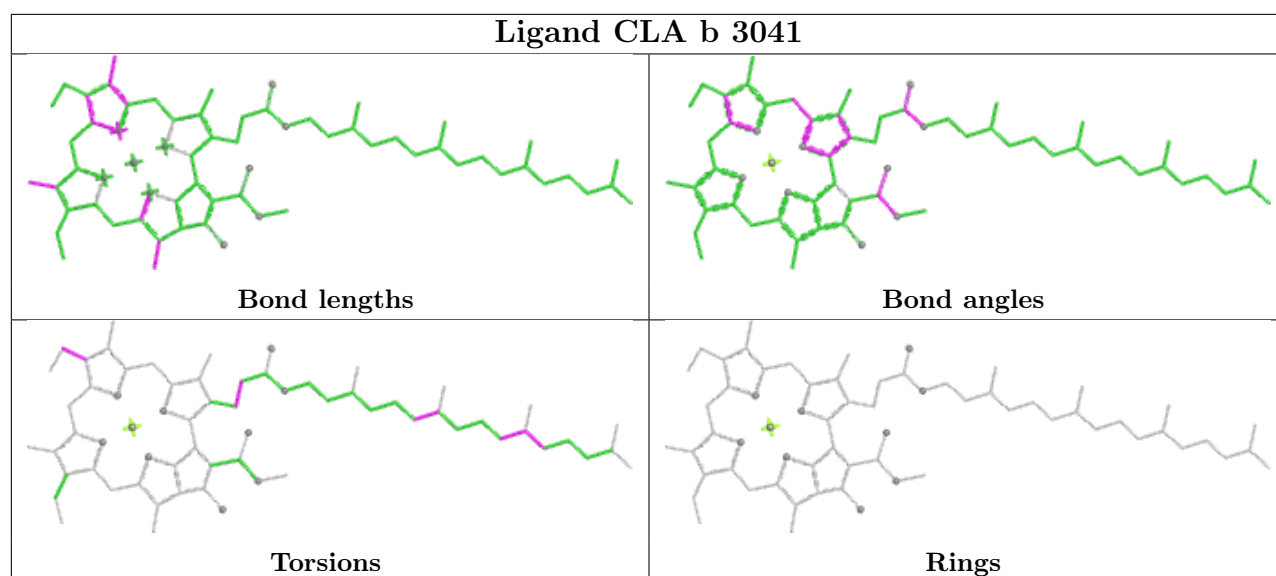
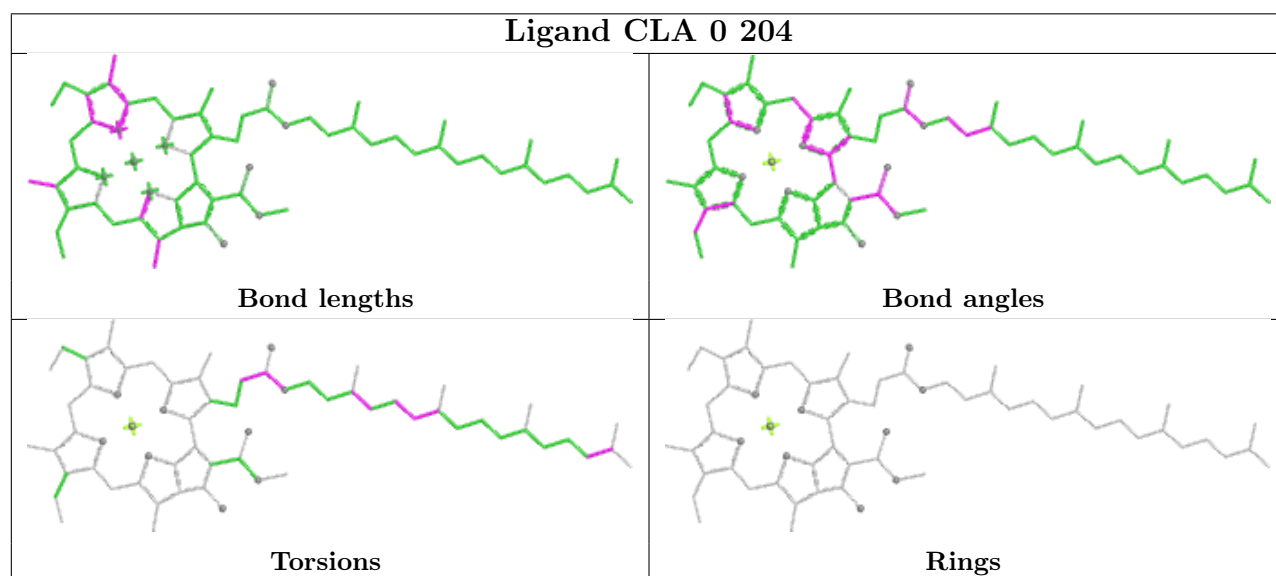
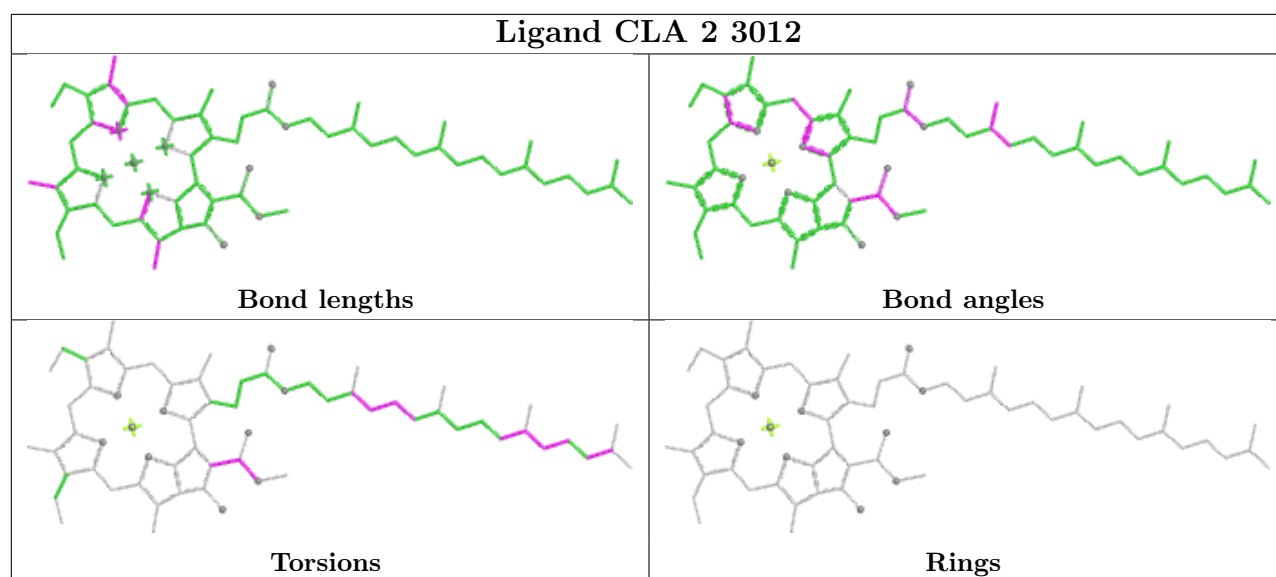
Ligand CLA A 844

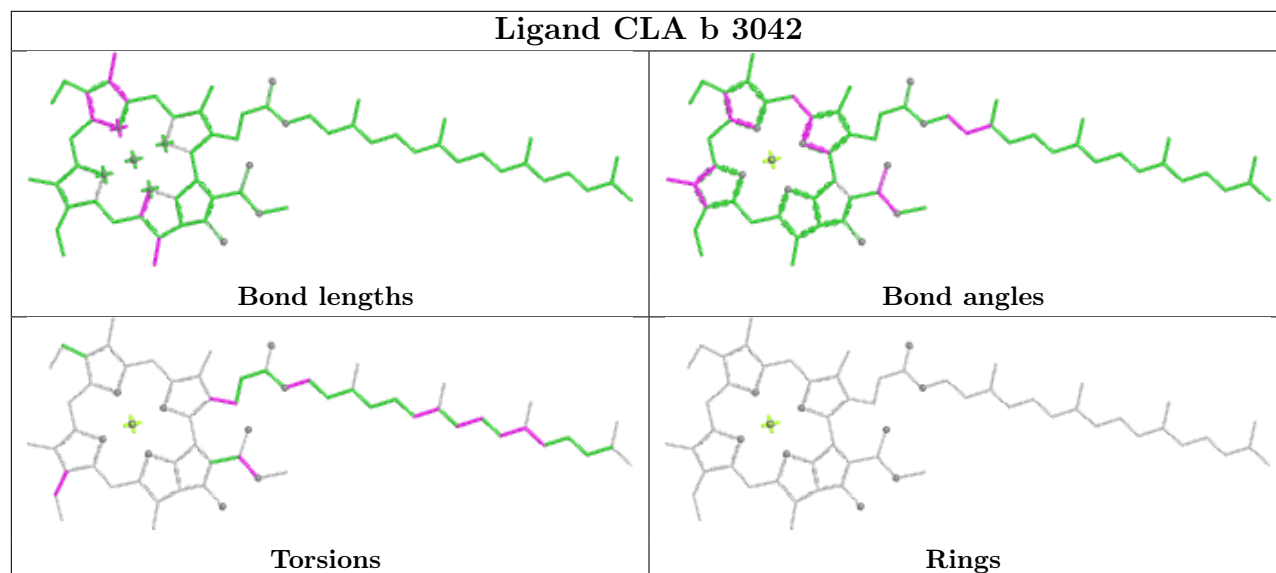
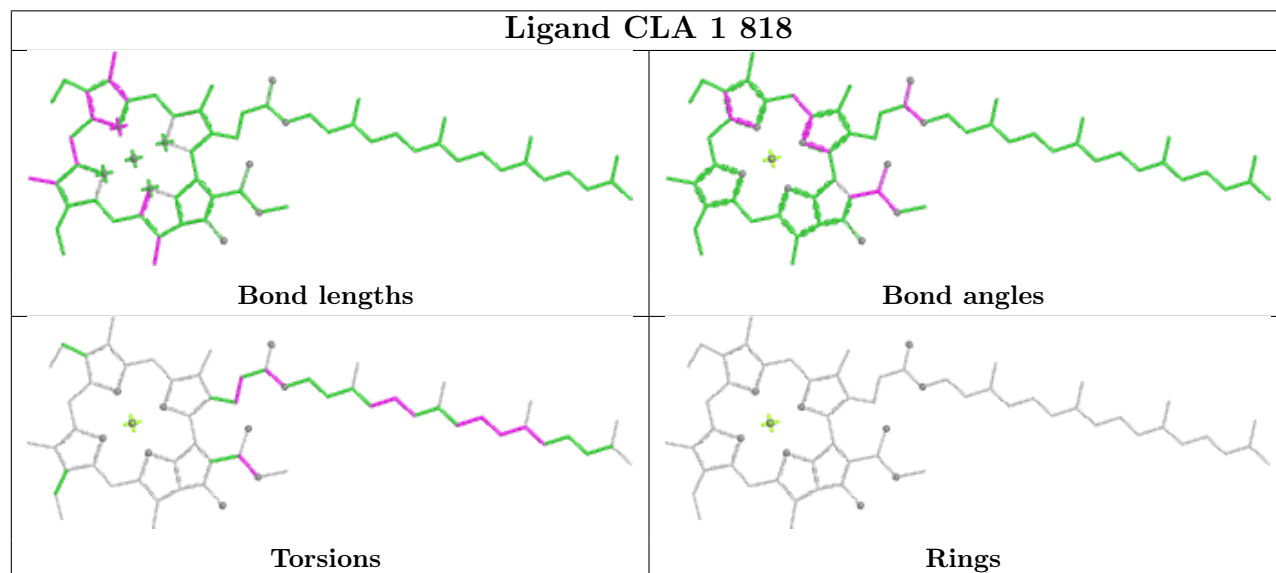
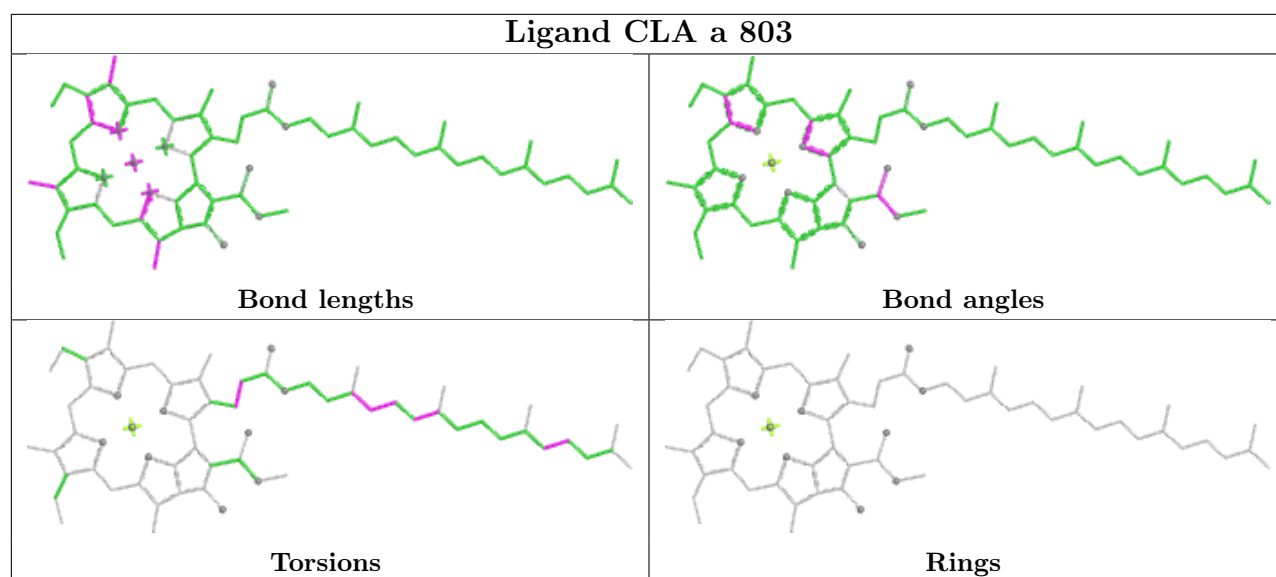


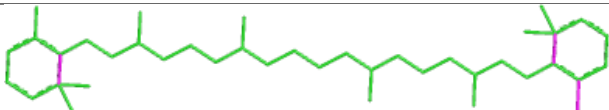
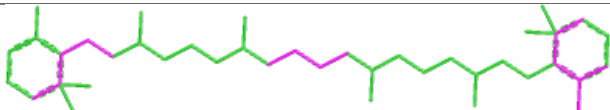
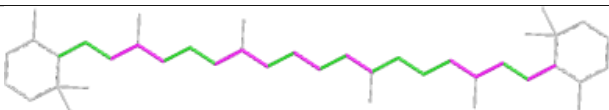
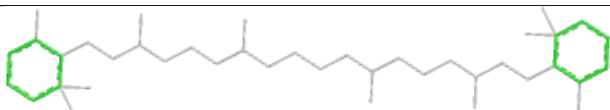
Ligand CLA 0 208

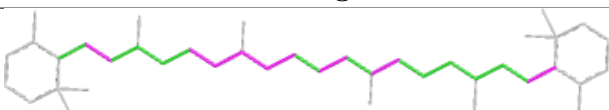
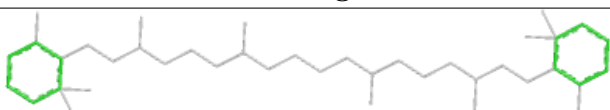


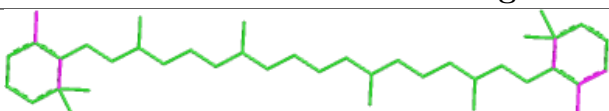
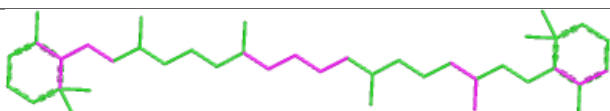
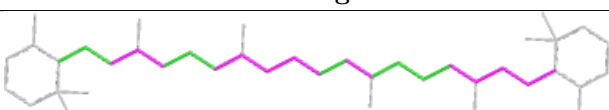
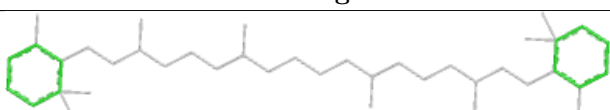




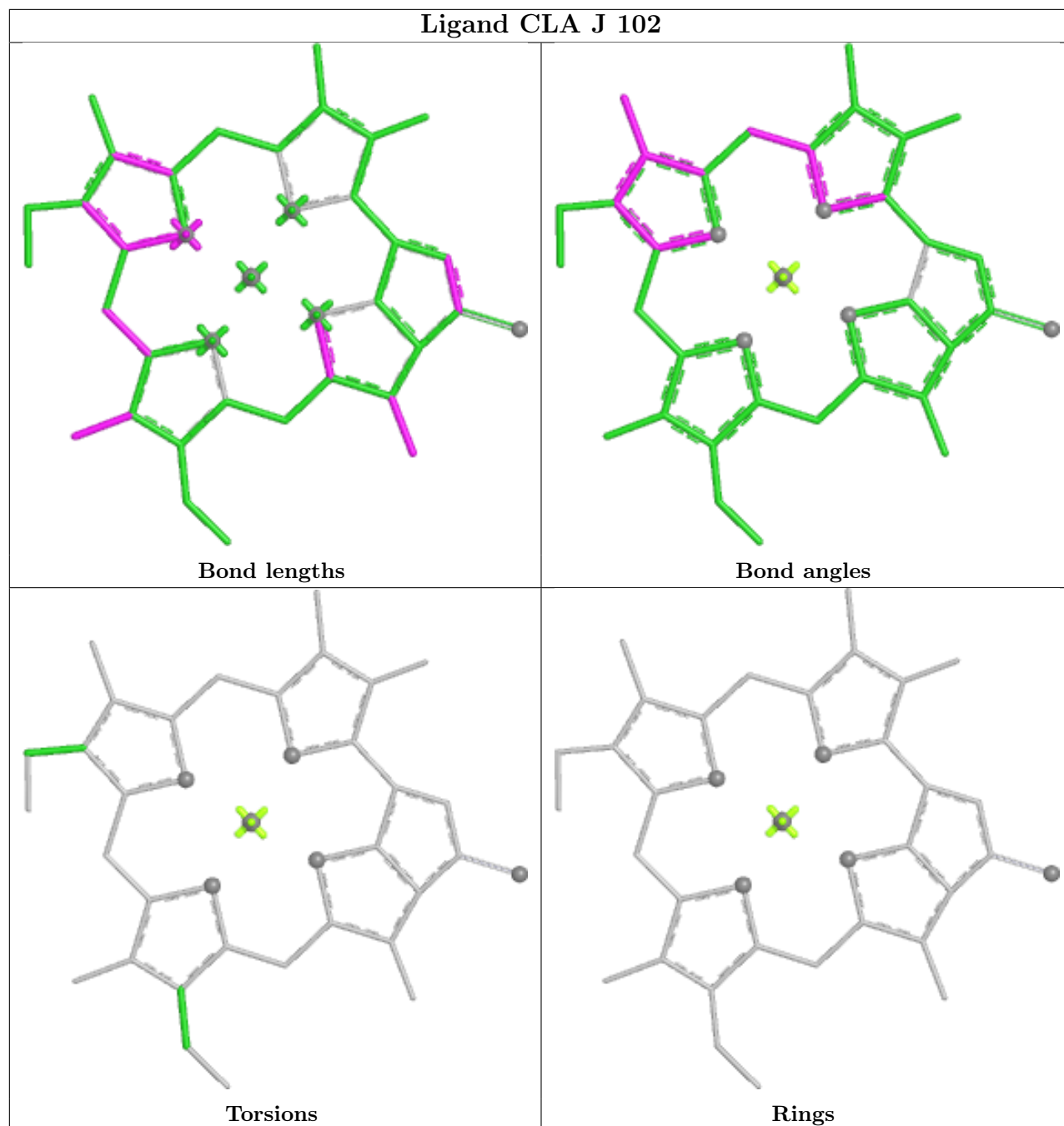


Ligand BCR f 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

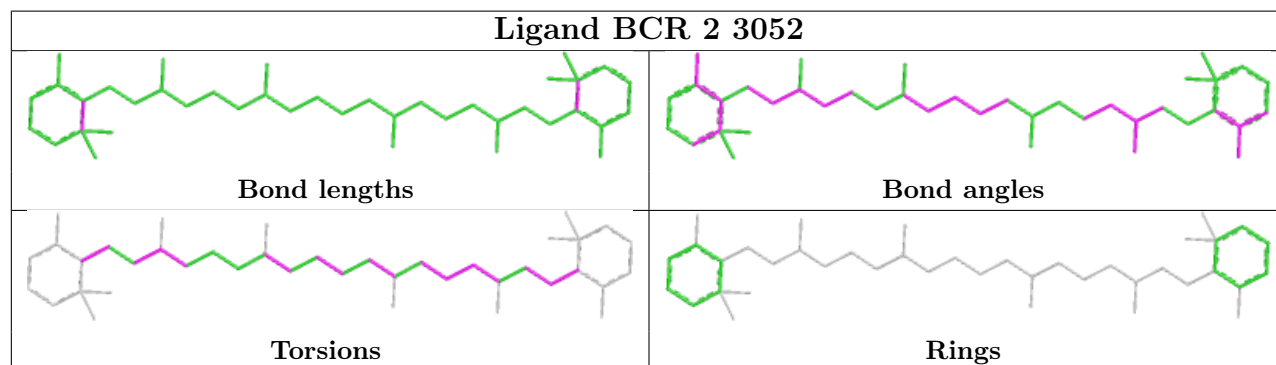
Ligand BCR 2 3048	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 3052	
	
Bond lengths	Bond angles
	
Torsions	Rings

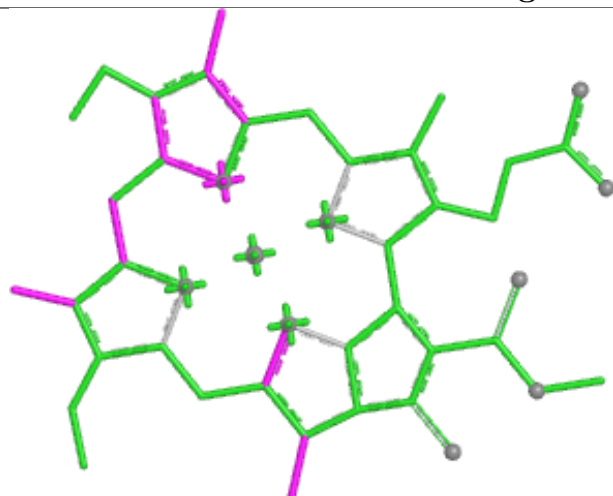
Ligand CLA J 102



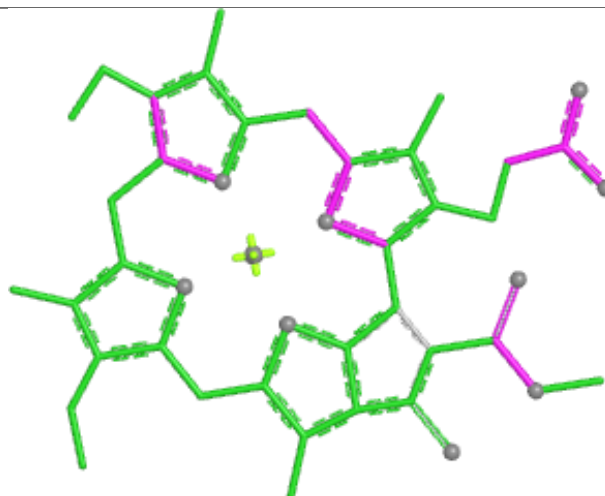
Ligand BCR 2 3052



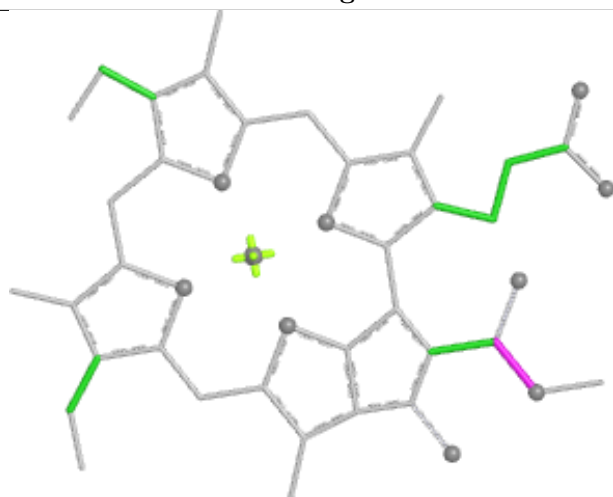
Ligand CLA 1 837



Bond lengths



Bond angles

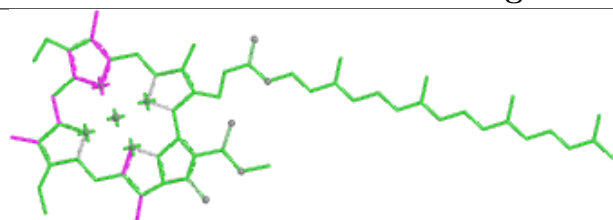


Torsions

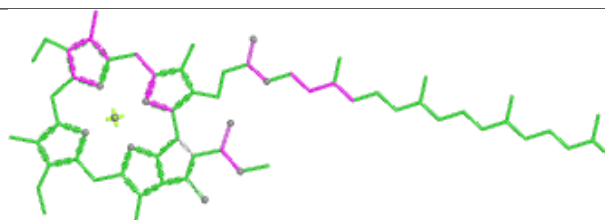


Rings

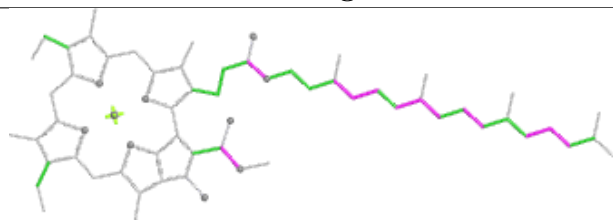
Ligand CLA B 3039



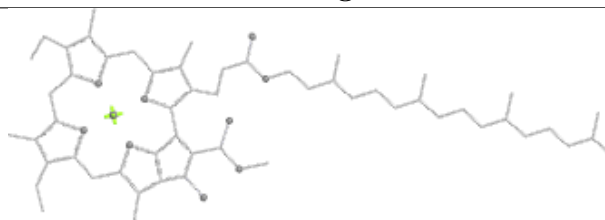
Bond lengths



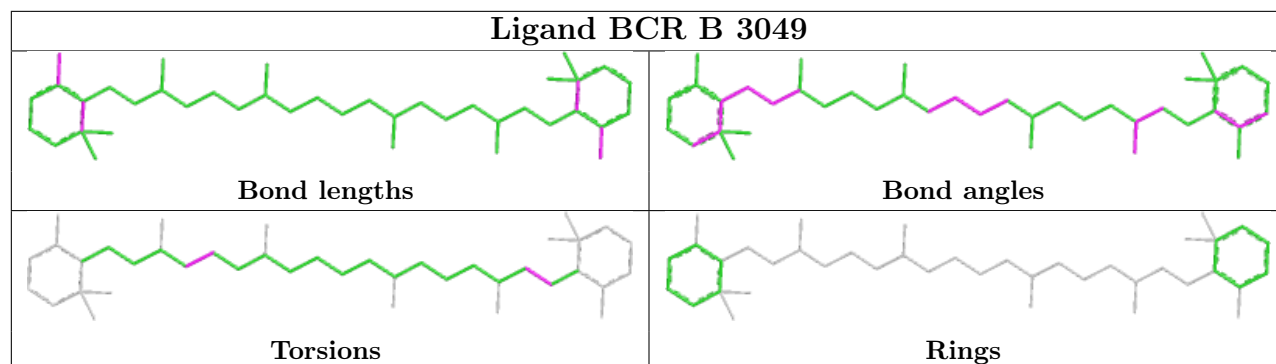
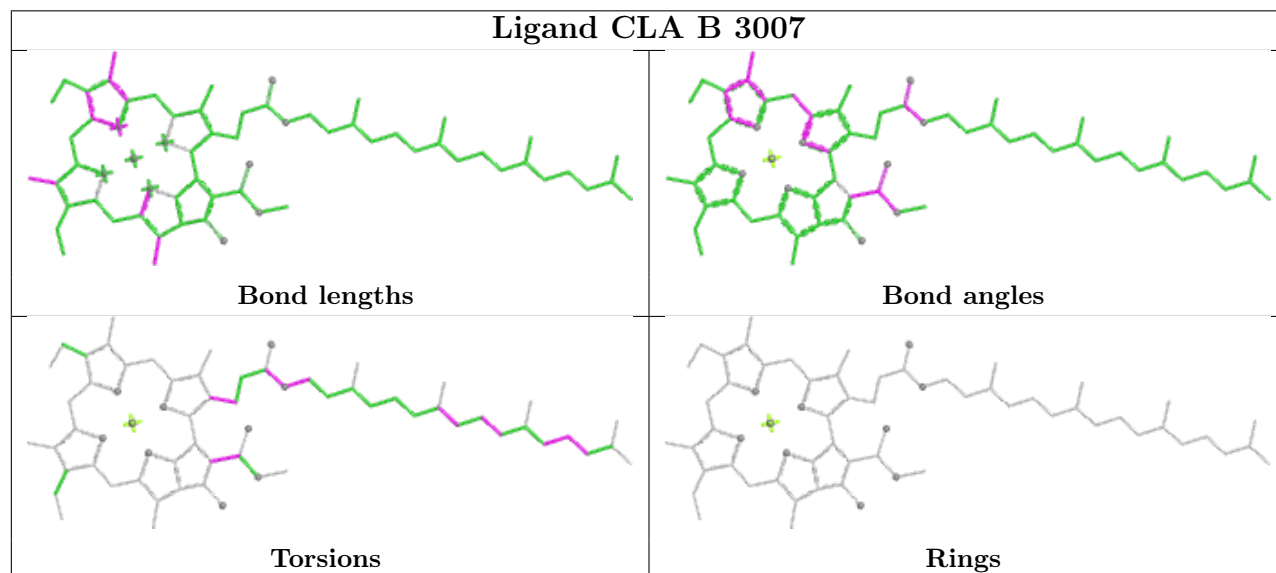
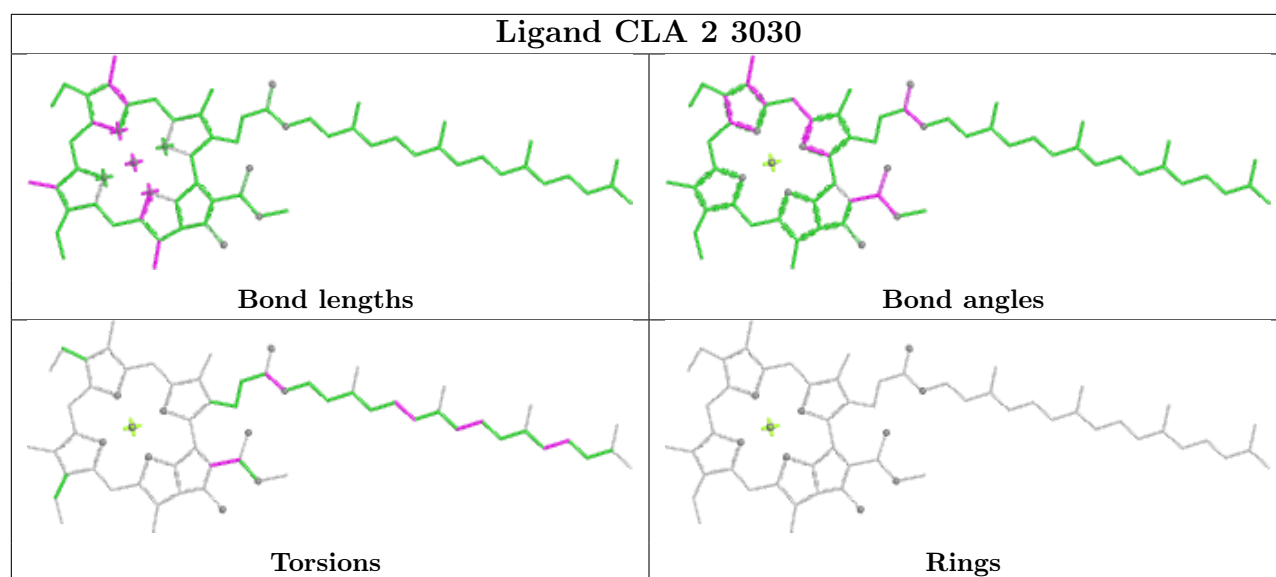
Bond angles

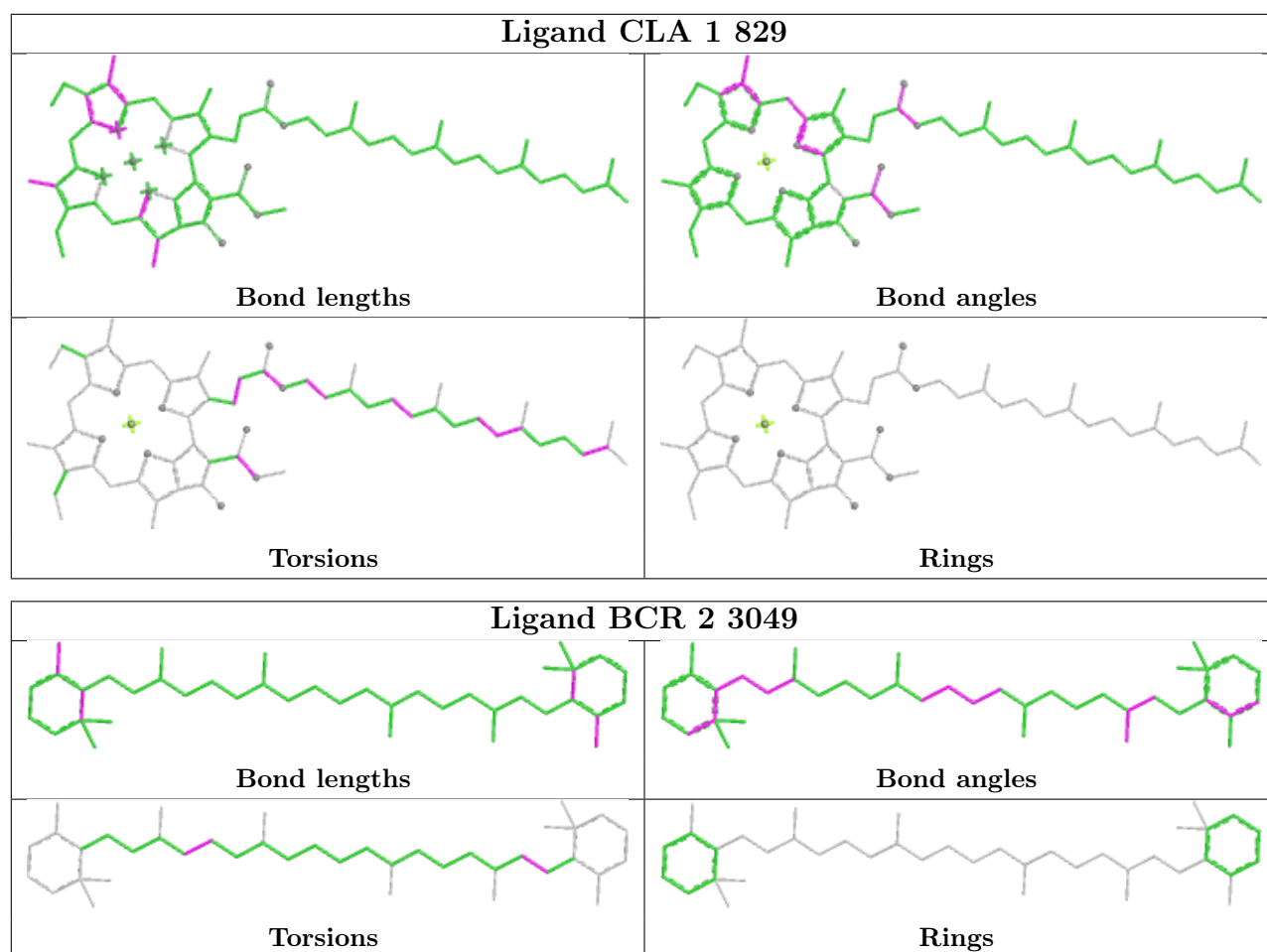


Torsions

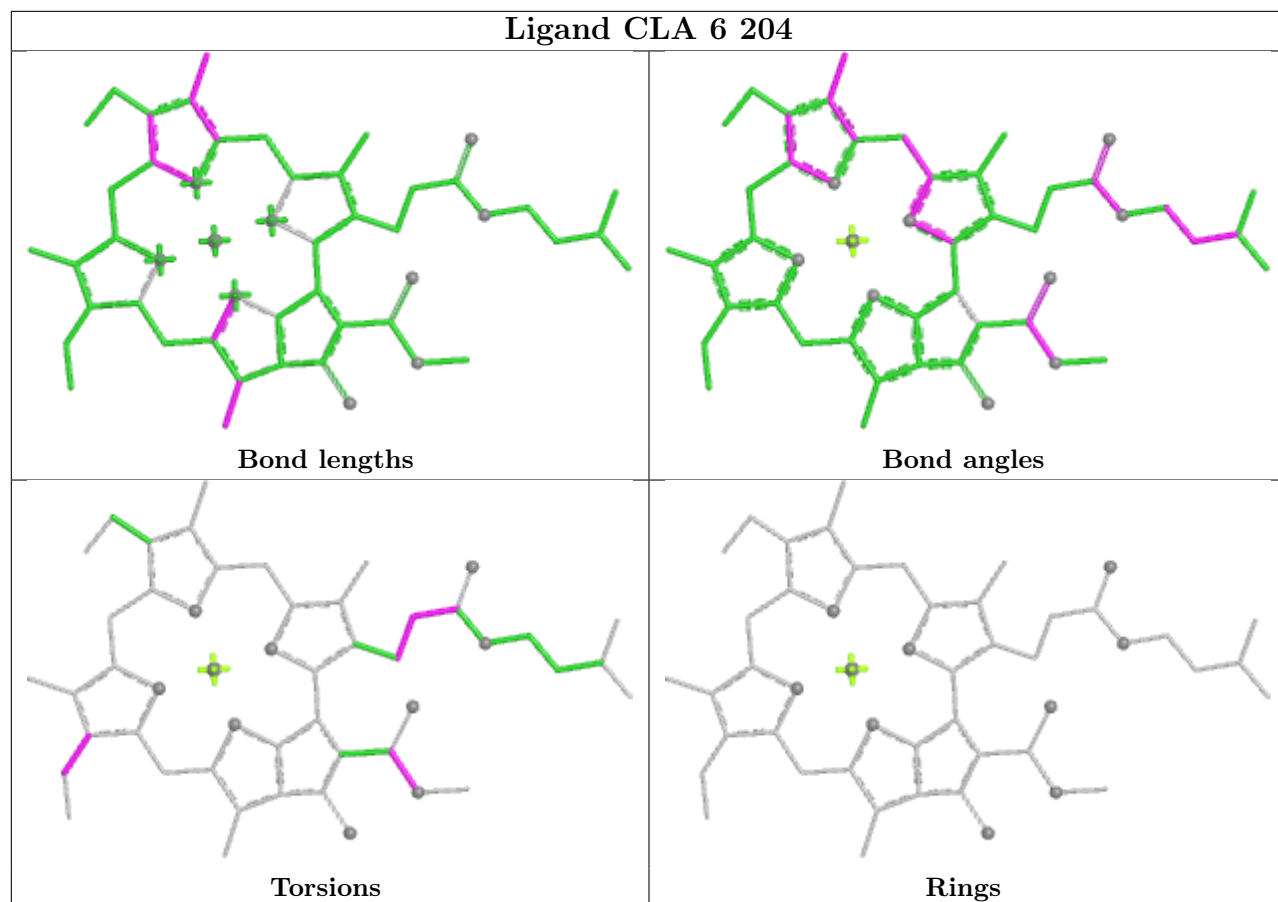


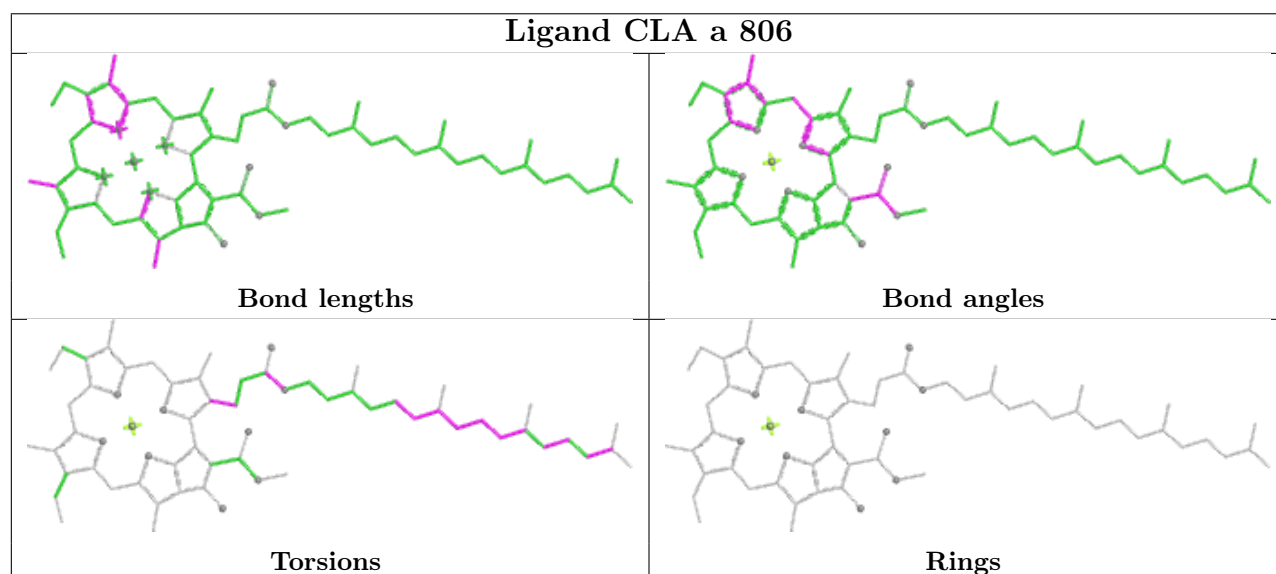
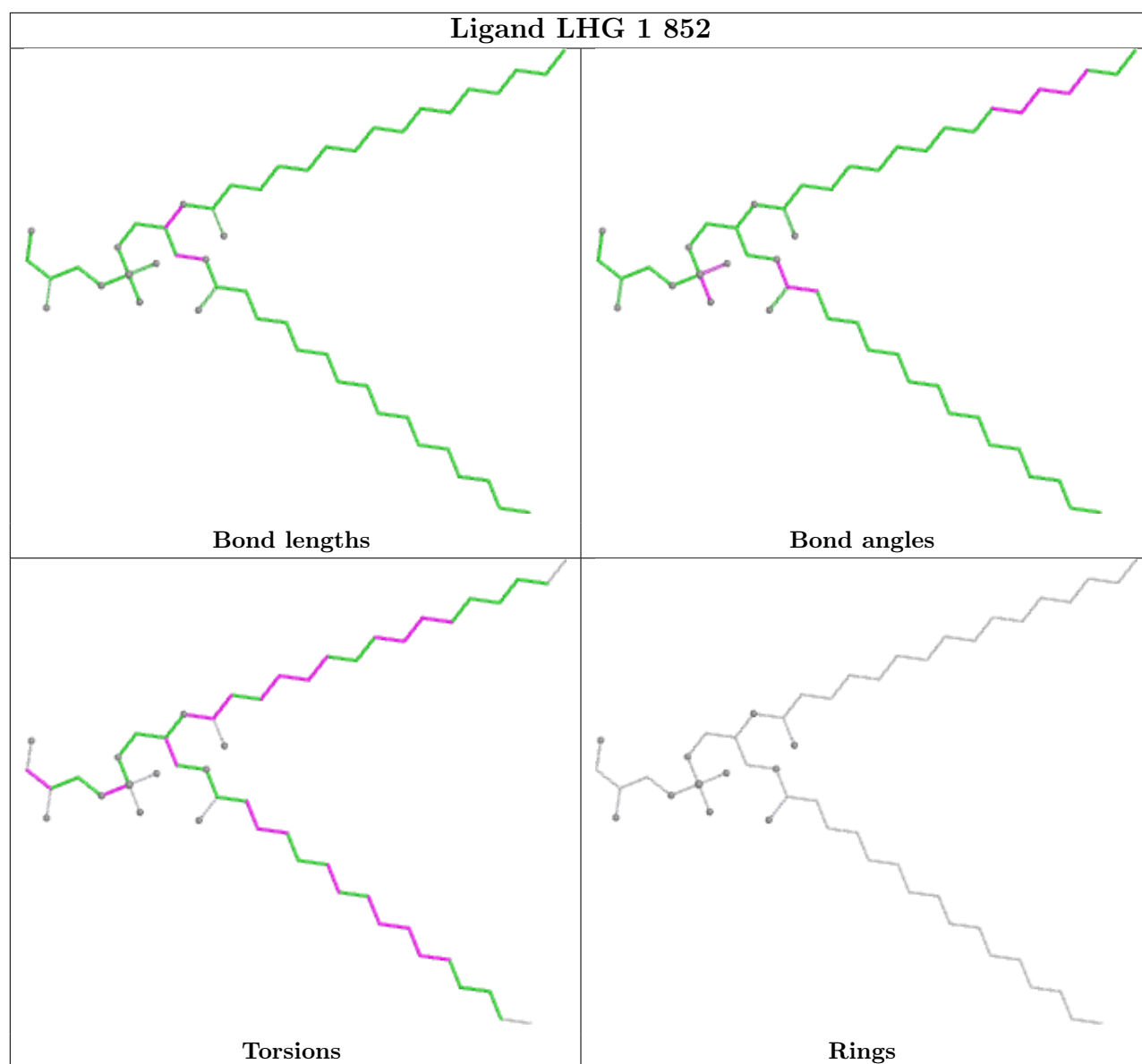
Rings



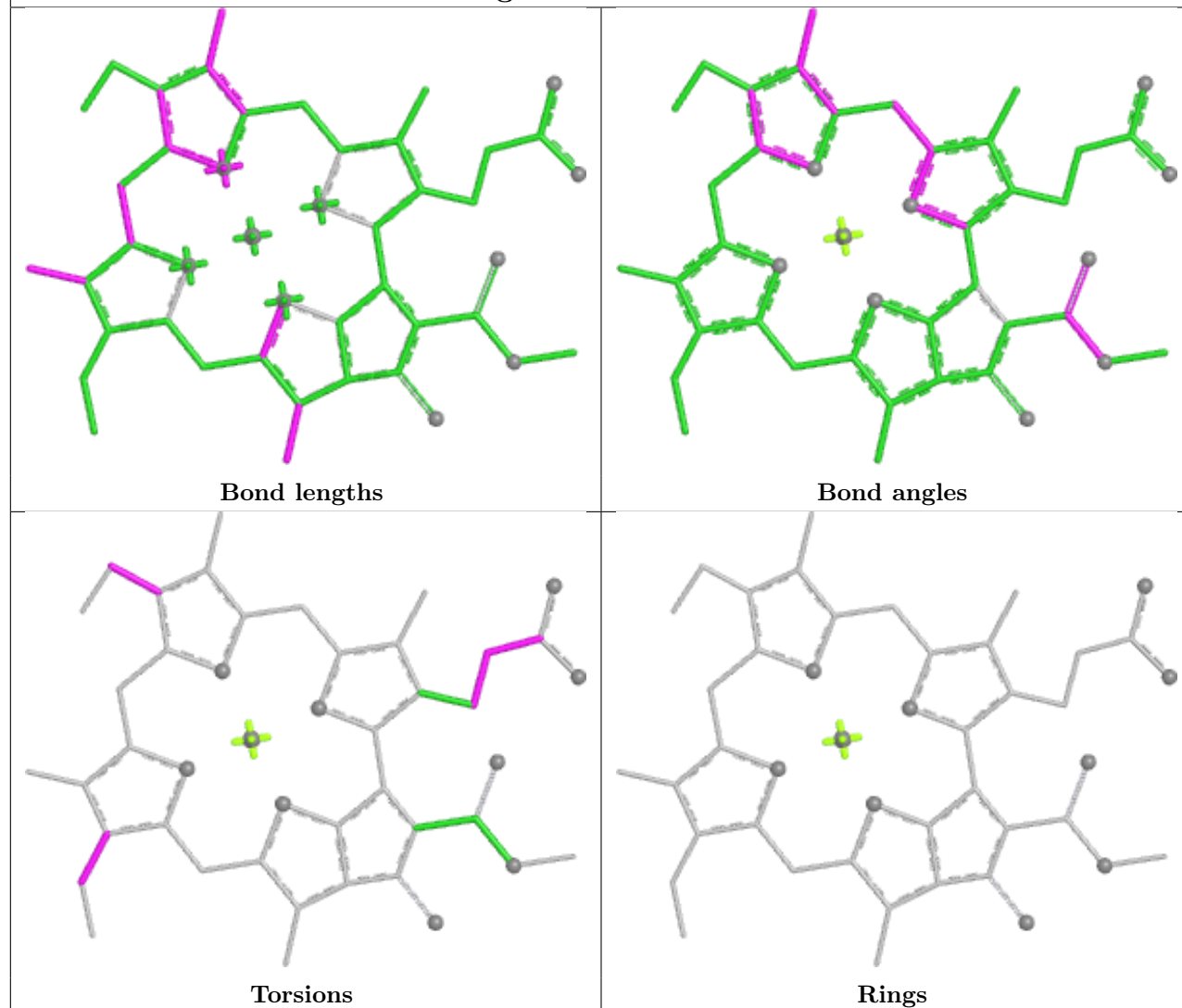


Ligand CLA 6 204

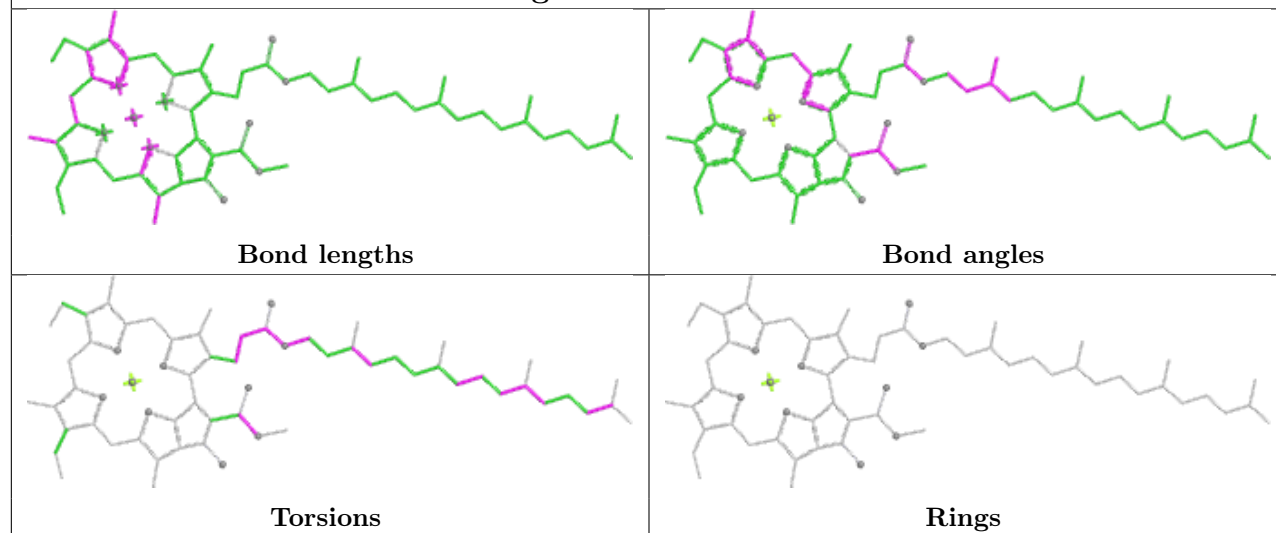


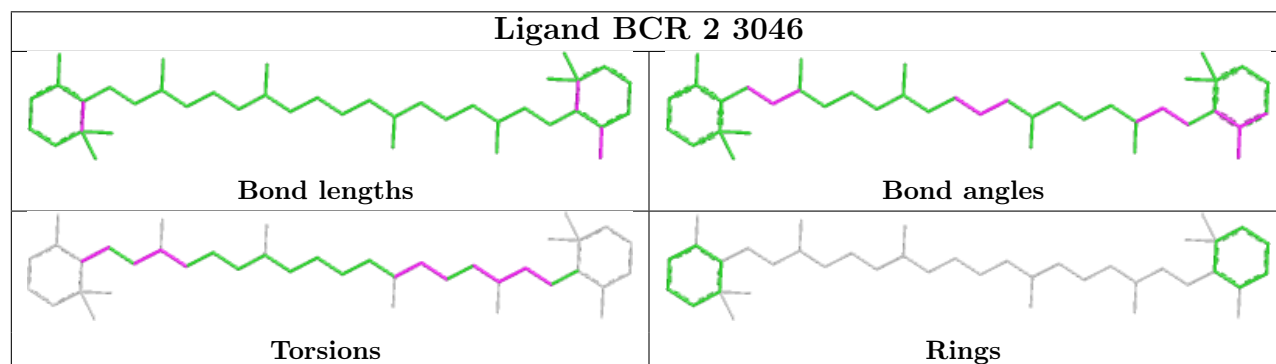
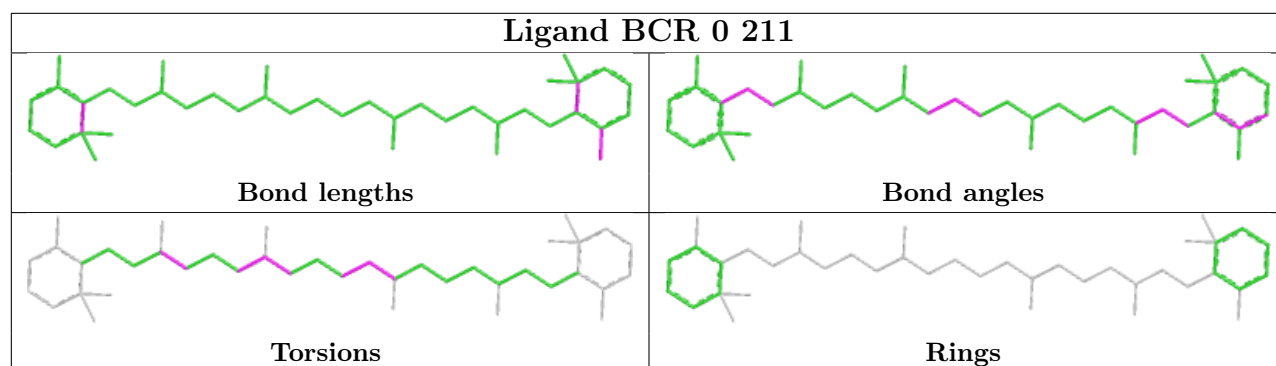
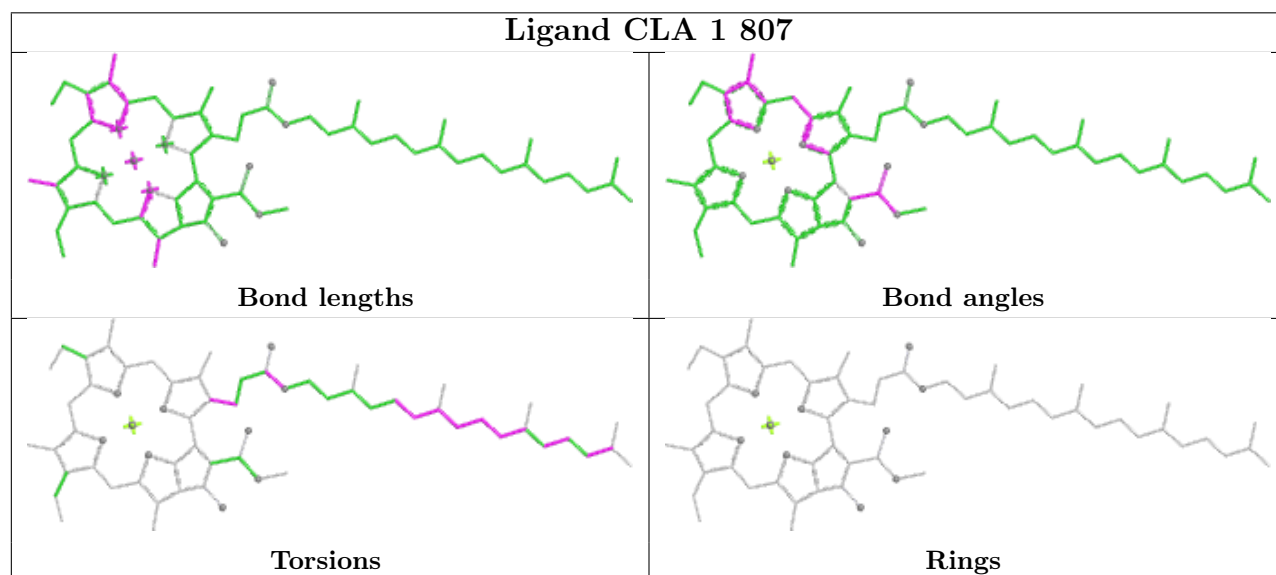
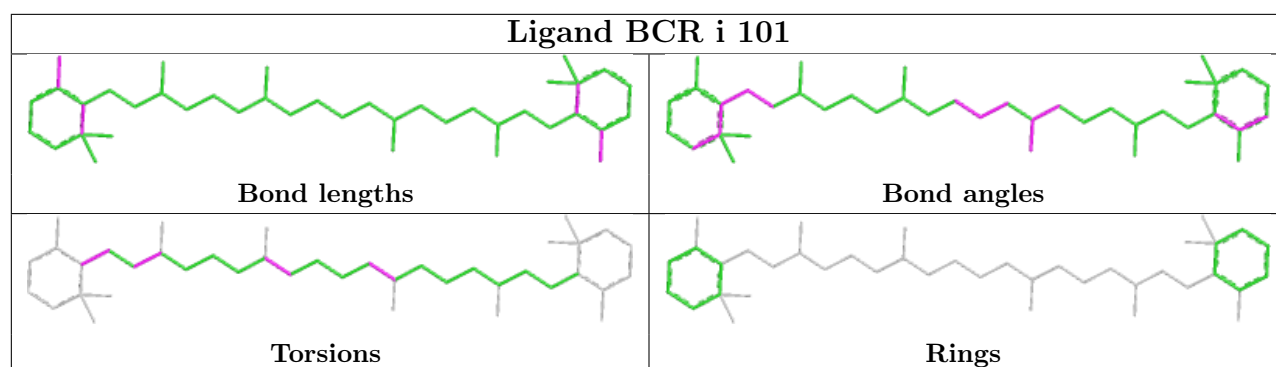


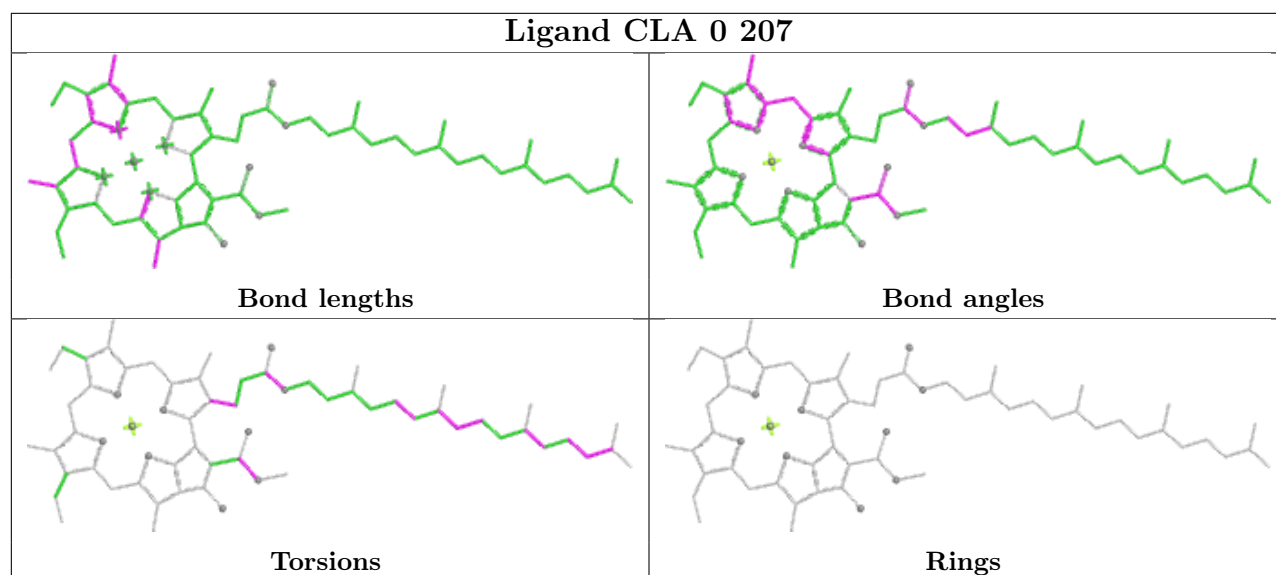
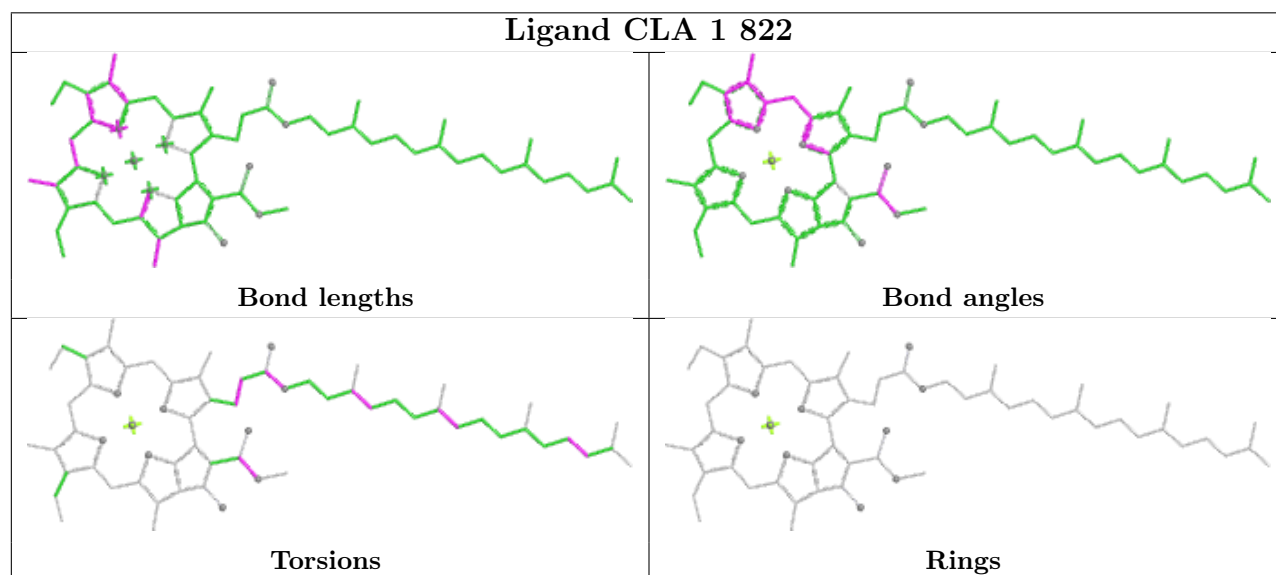
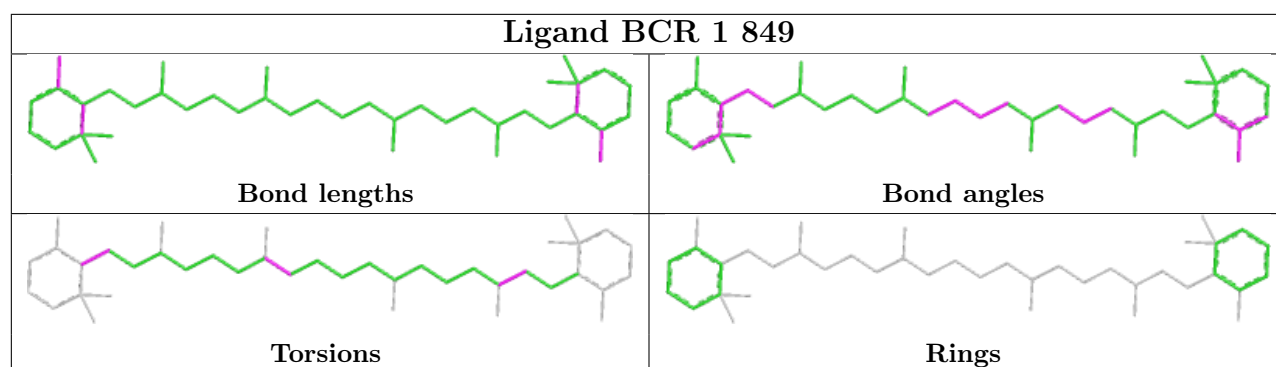
Ligand CLA a 812

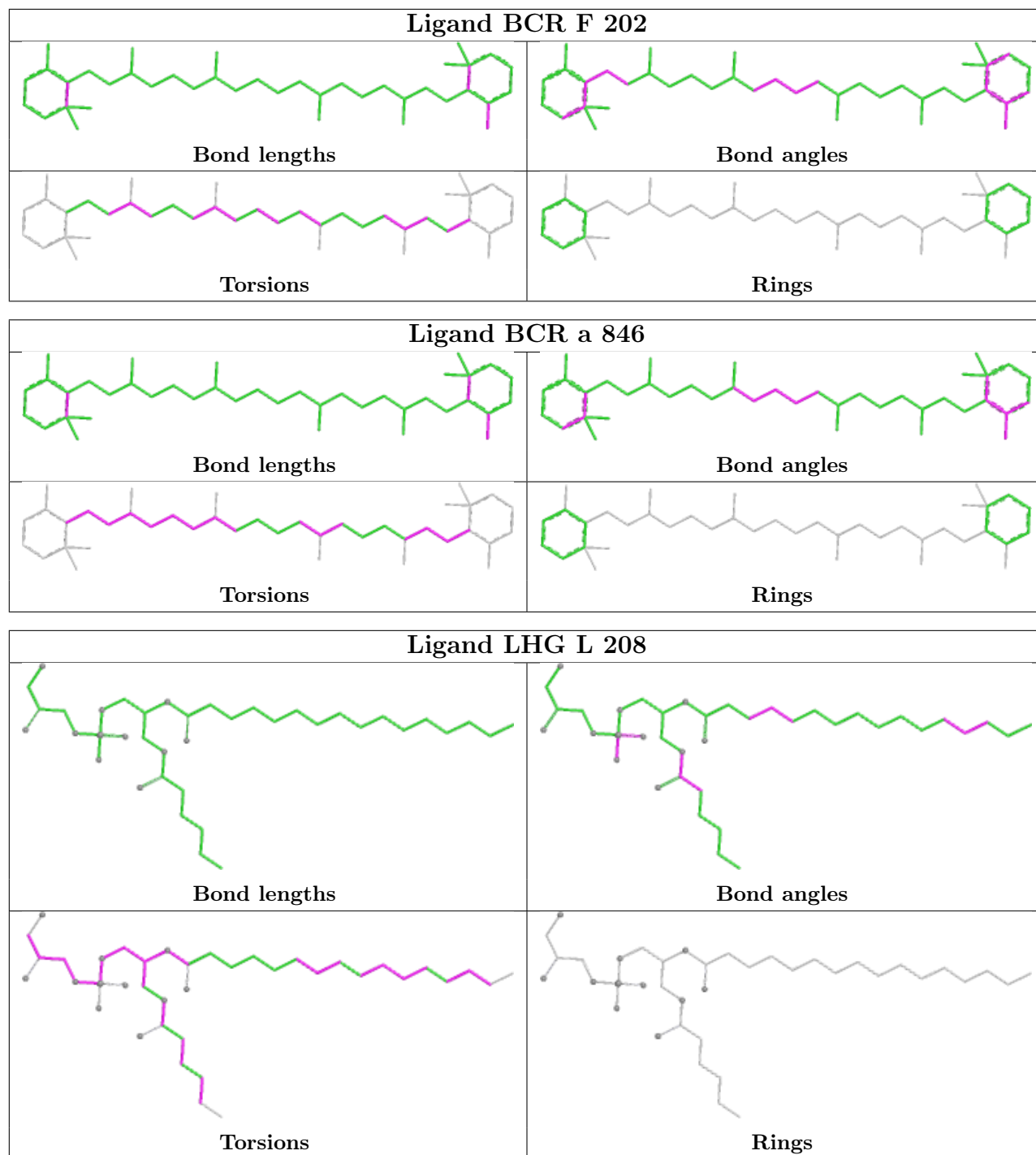


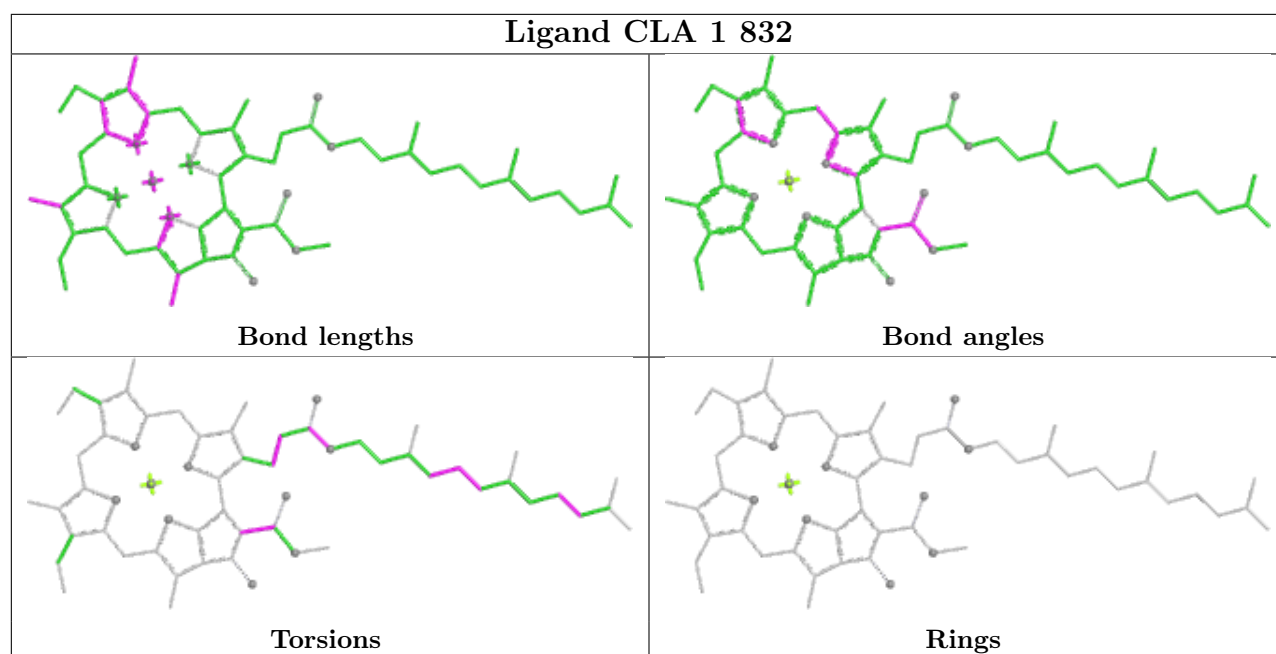
Ligand CLA A 802











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.

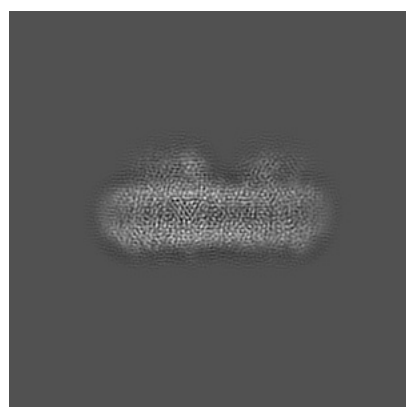
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10558. These allow visual inspection of the internal detail of the map and identification of artifacts.

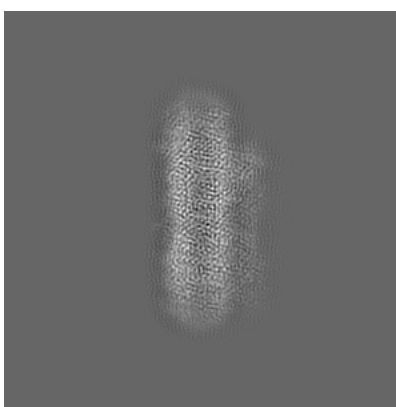
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

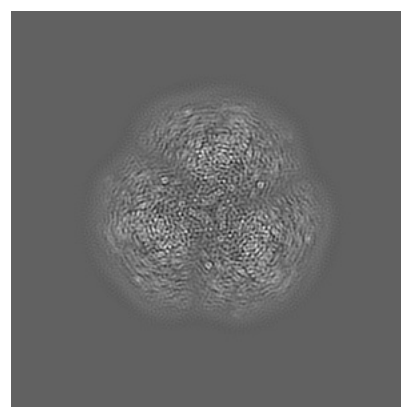
6.1.1 Primary map



X



Y

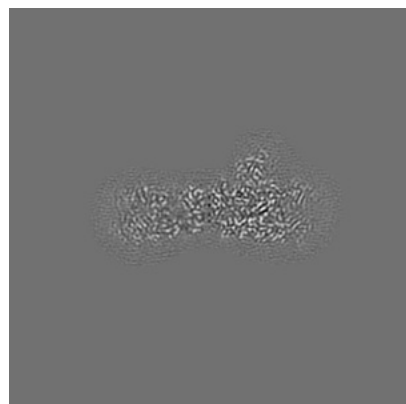


Z

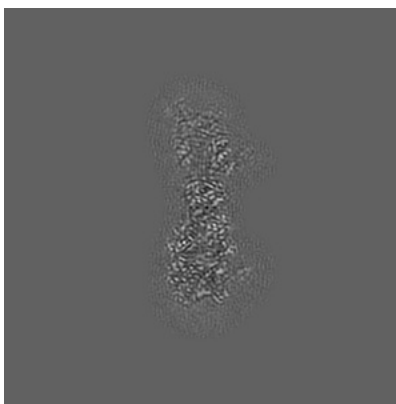
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

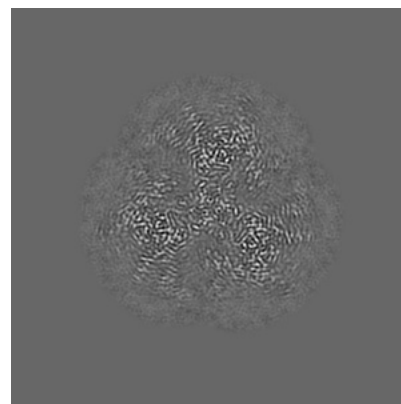
6.2.1 Primary map



X Index: 280



Y Index: 280

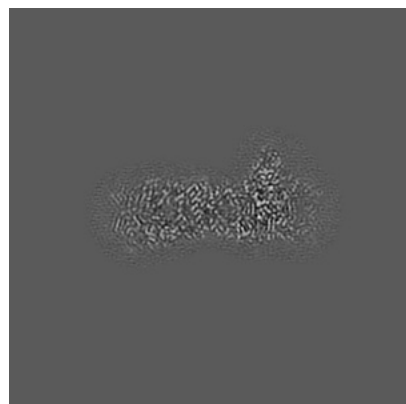


Z Index: 280

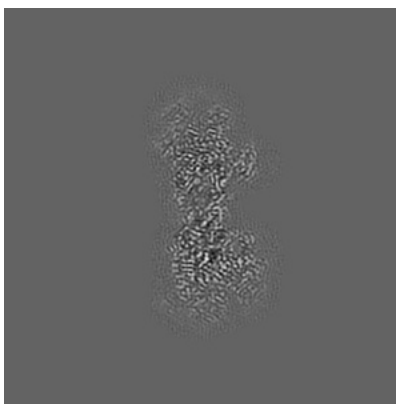
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

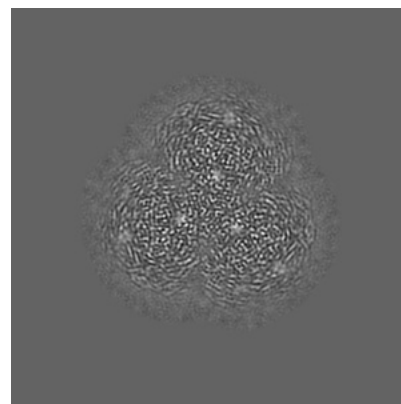
6.3.1 Primary map



X Index: 297



Y Index: 253

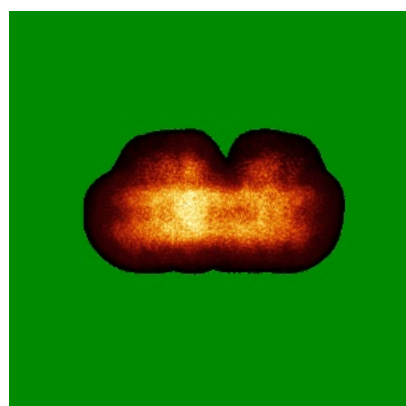


Z Index: 298

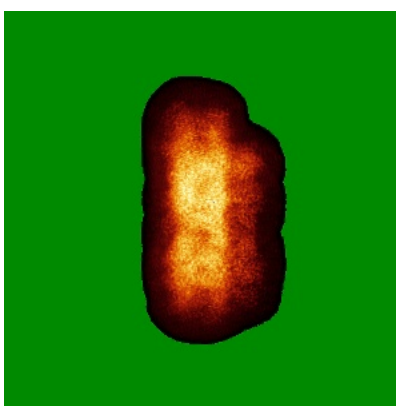
The images above show the largest variance slices of the map in three orthogonal directions.

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

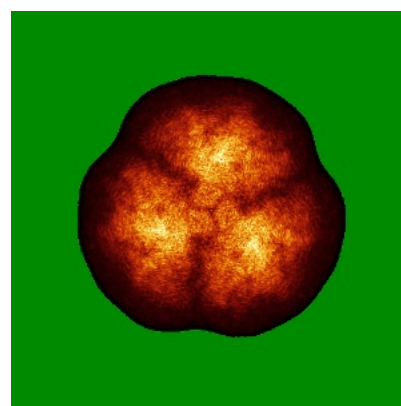
6.4.1 Primary map



X



Y

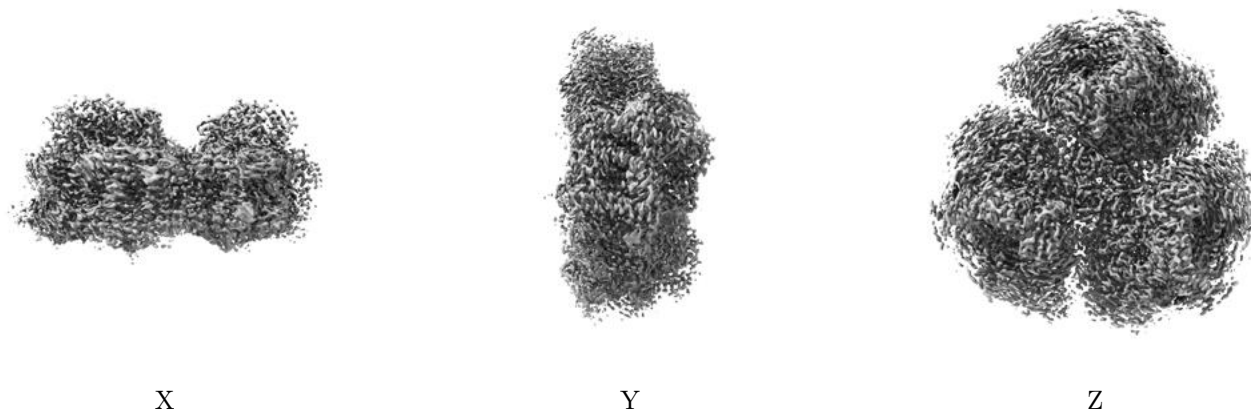


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

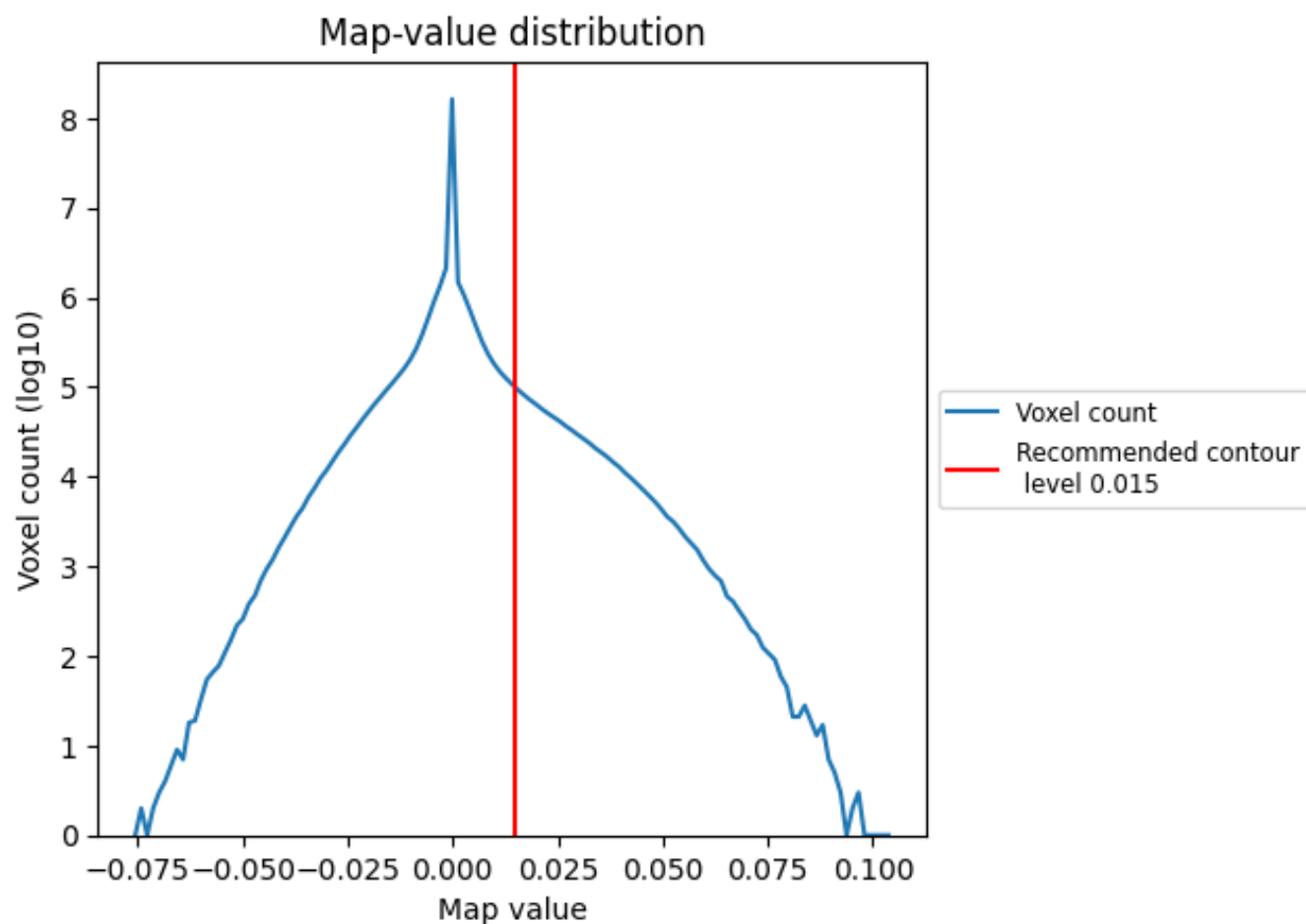
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

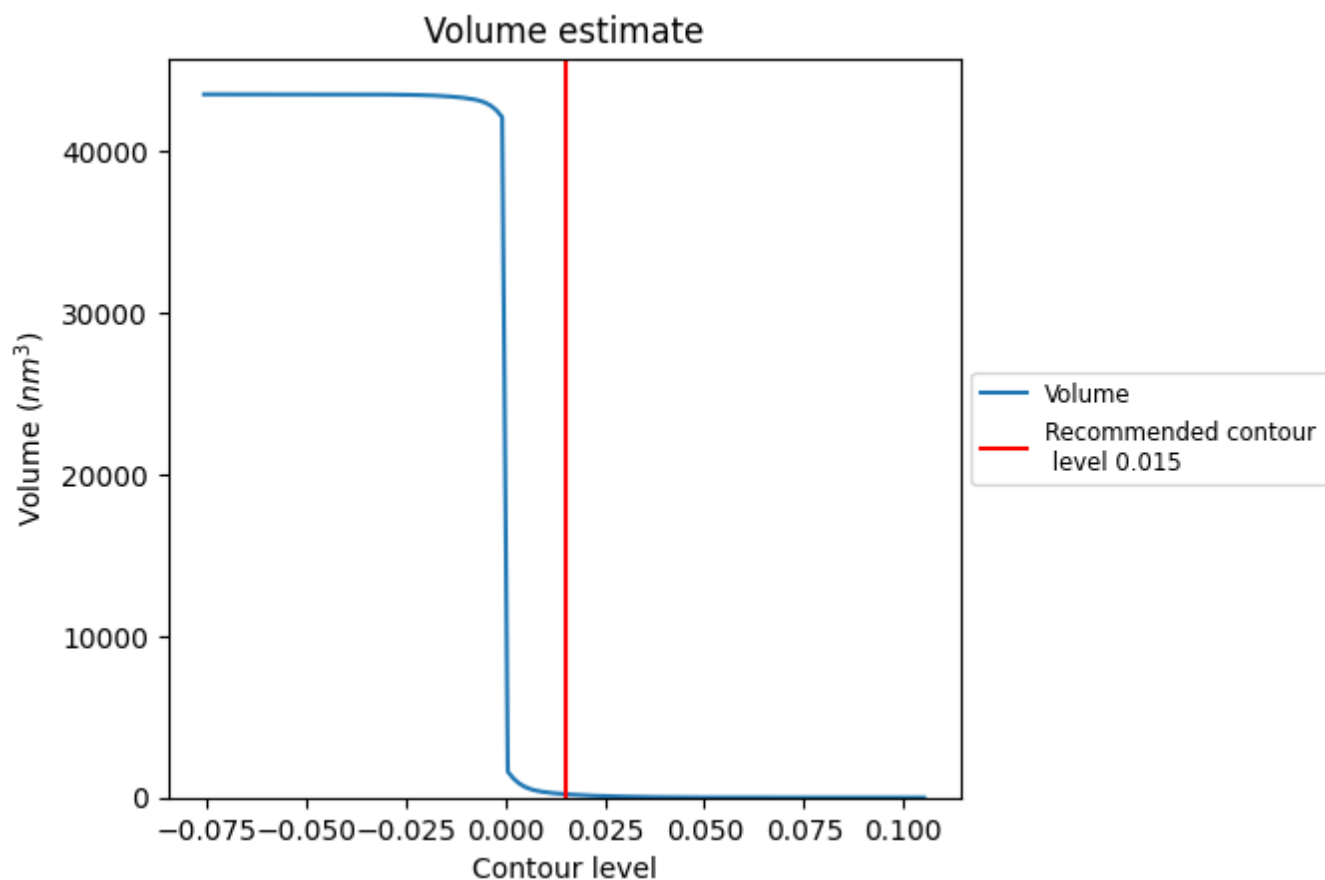
This section contains the results of statistical analysis of the map.

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.

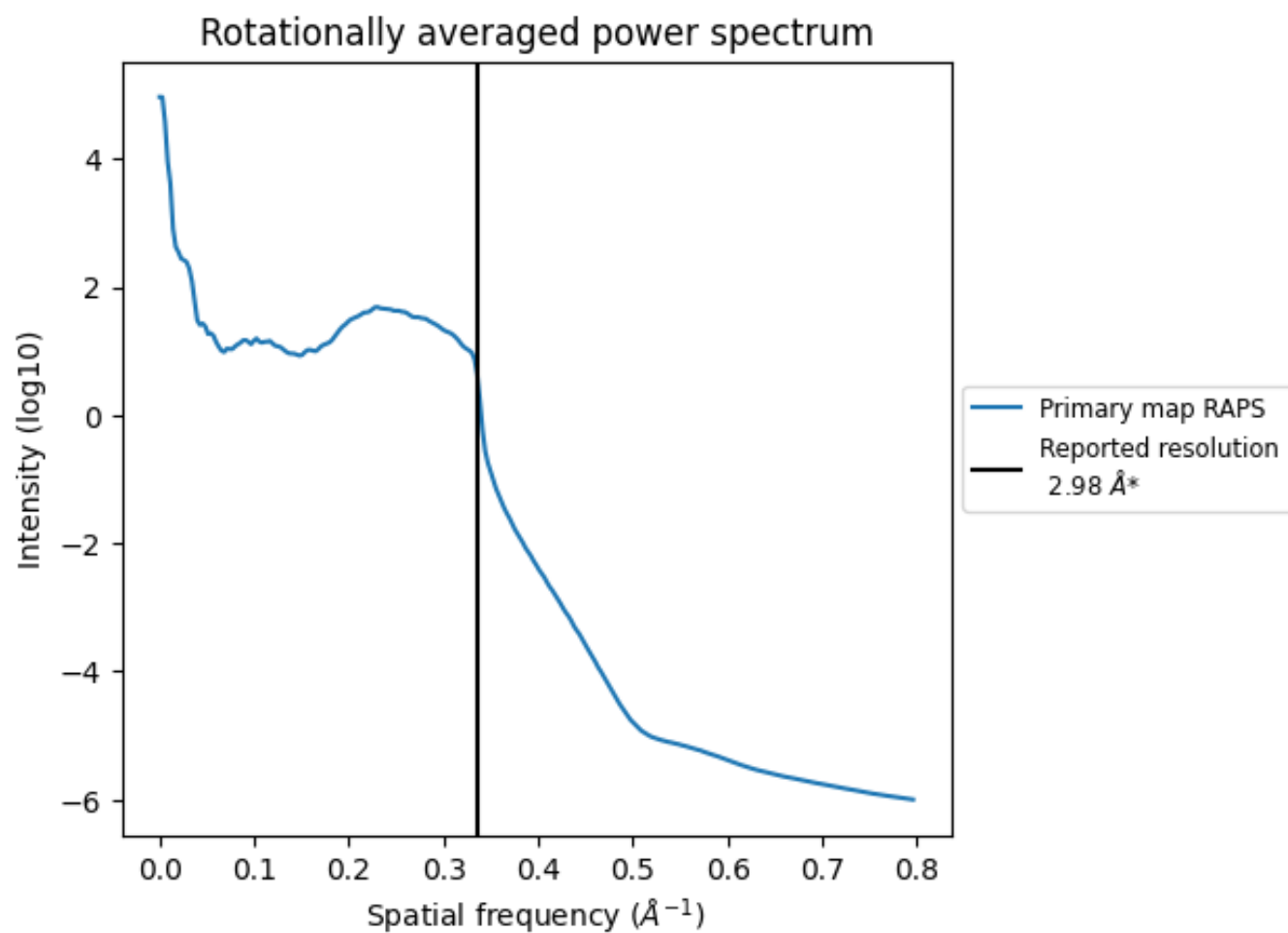
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 ⓘ

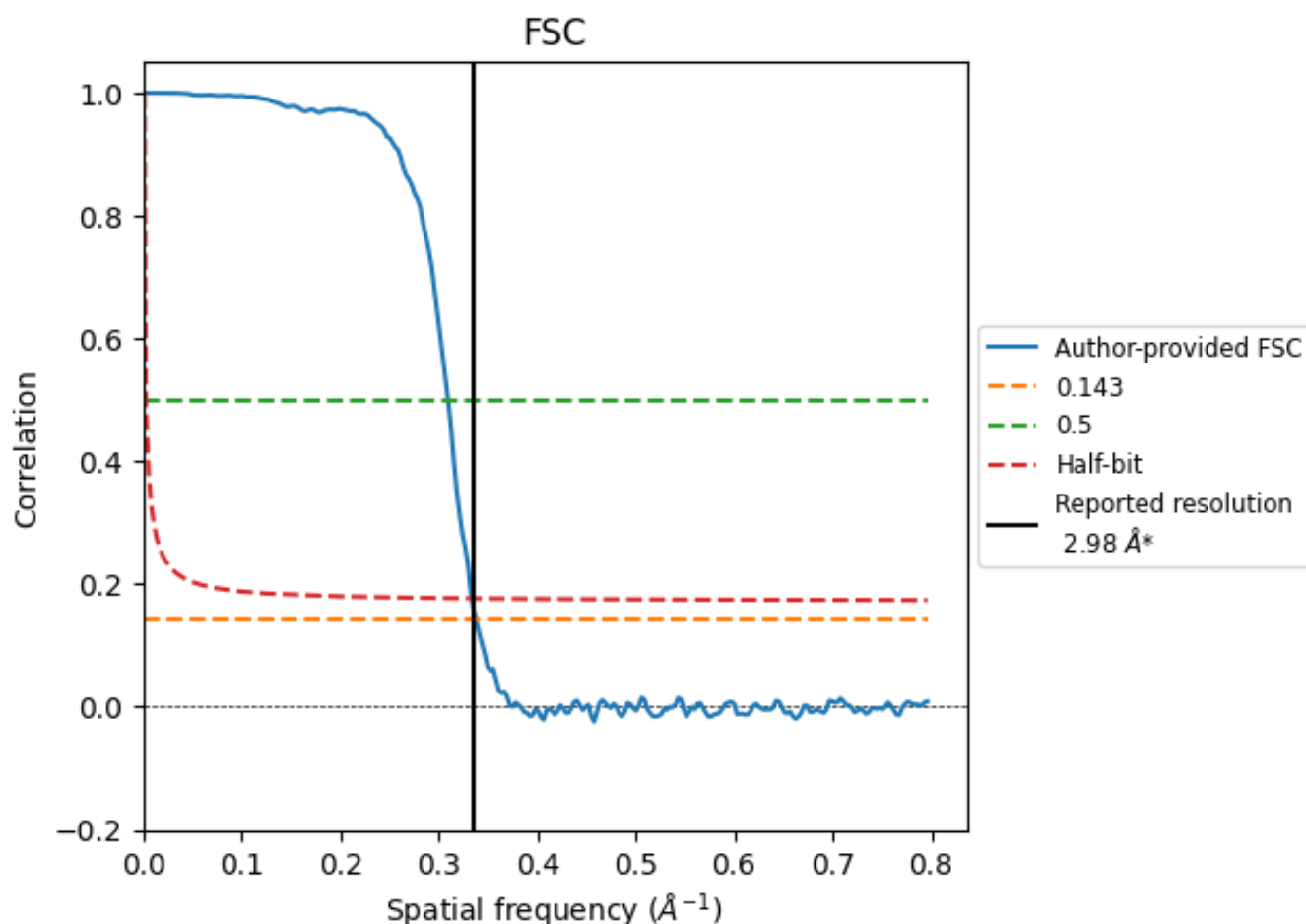


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

8.2 Resolution estimates [i](#)

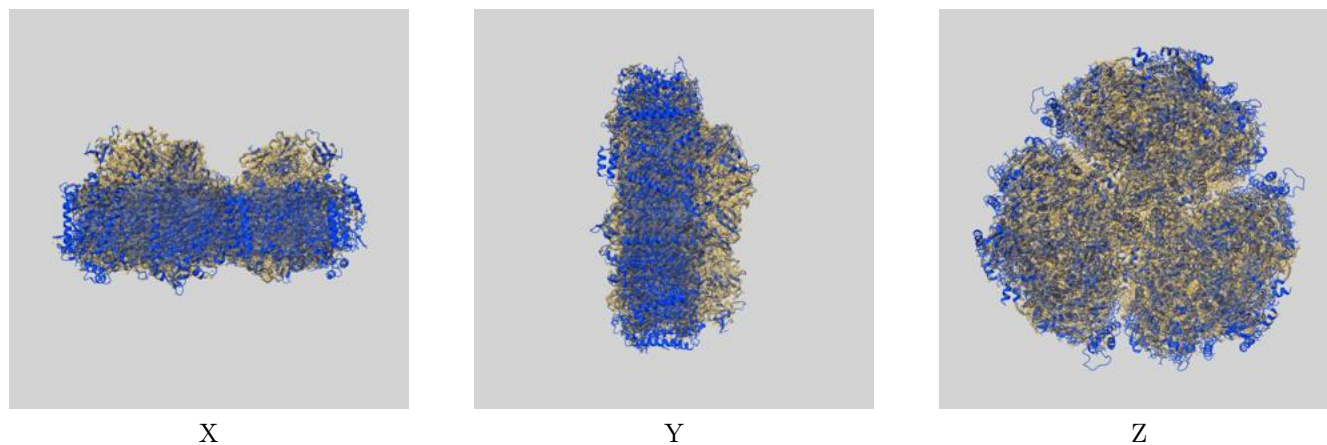
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.96	3.23	3.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

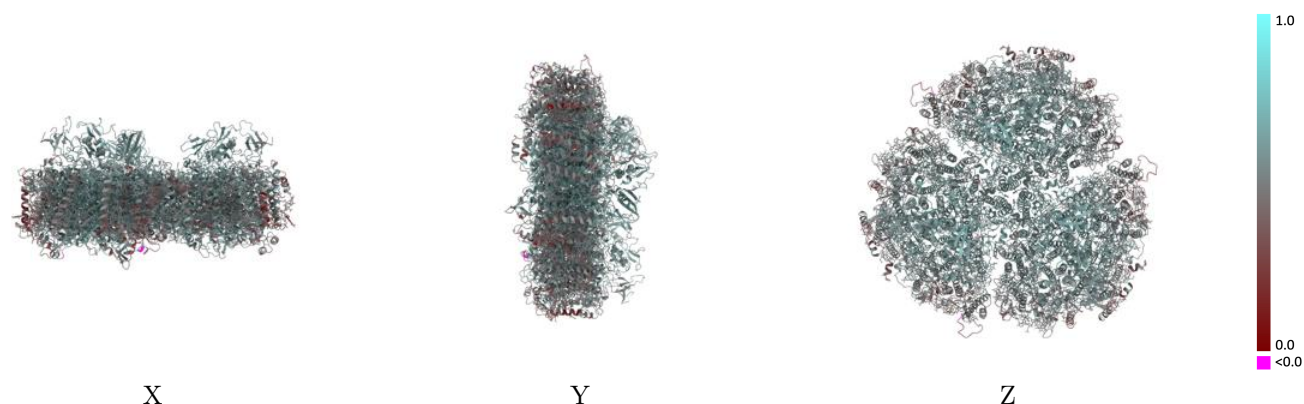
This section contains information regarding the fit between EMDB map EMD-10558 and PDB model 6TRC. Per-residue inclusion information can be found in section 3 on page 40.

9.1 Map-model overlay [i](#)



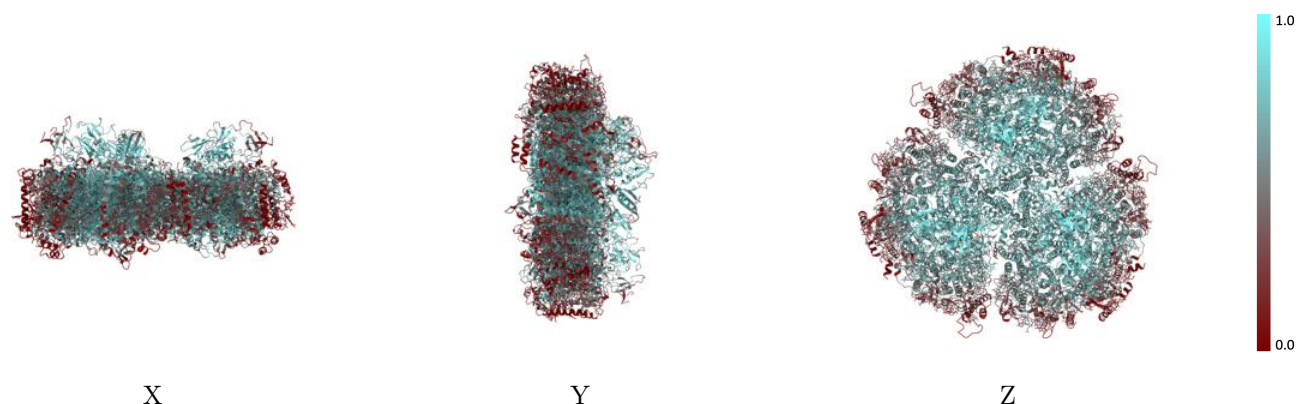
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



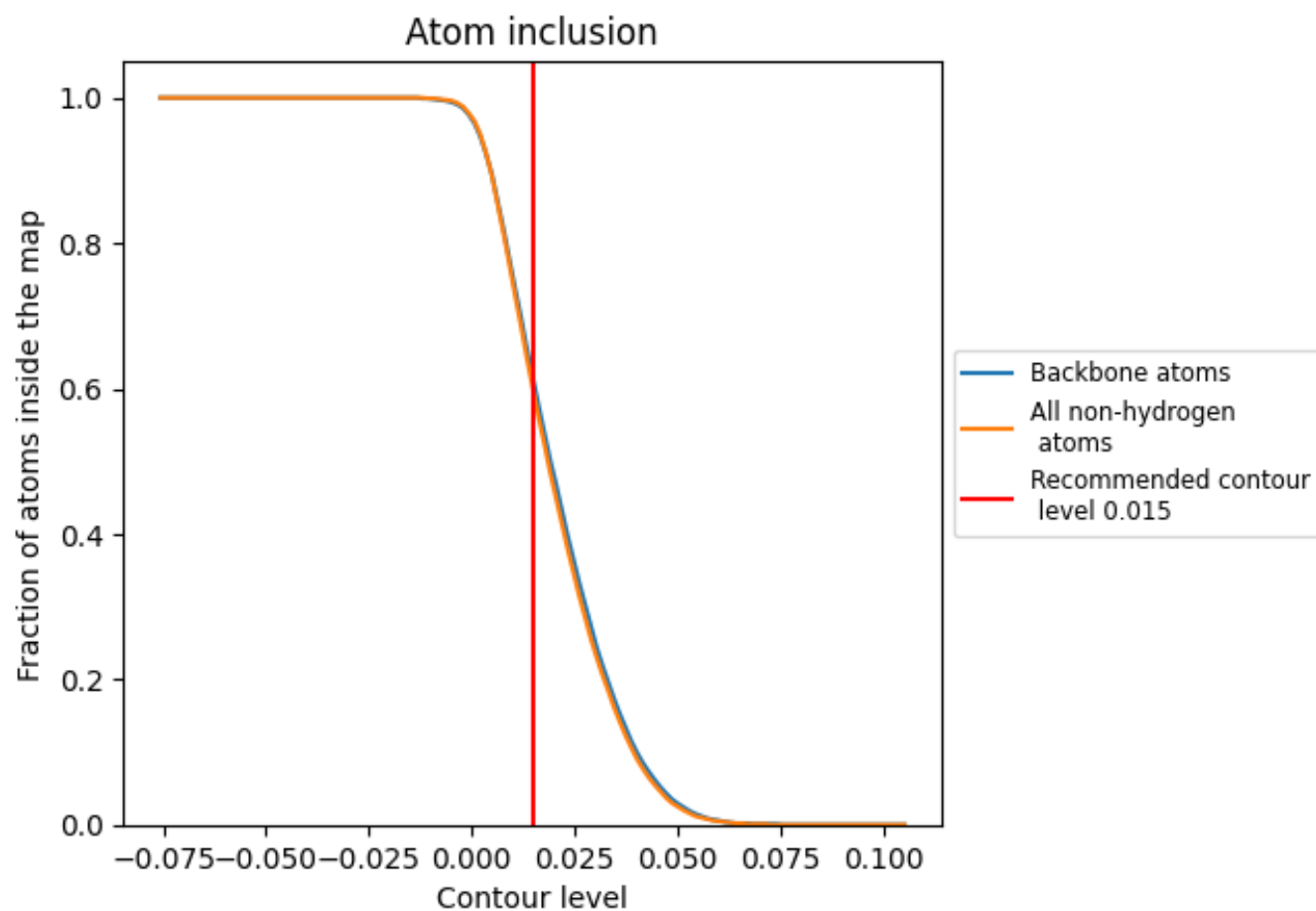
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 60% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5950	 0.5490
0	 0.7680	 0.6070
1	 0.6210	 0.5490
2	 0.6490	 0.5630
3	 0.7950	 0.6000
4	 0.6730	 0.5830
5	 0.4570	 0.5410
6	 0.2080	 0.4670
7	 0.7960	 0.6020
8	 0.1840	 0.4360
9	 0.1320	 0.4570
A	 0.6180	 0.5480
B	 0.6500	 0.5630
C	 0.7900	 0.6000
D	 0.6720	 0.5830
E	 0.4530	 0.5430
F	 0.2040	 0.4630
I	 0.8180	 0.6090
J	 0.1740	 0.4340
K	 0.1140	 0.4490
L	 0.7650	 0.6070
M	 0.6310	 0.5810
X	 0.0000	 0.3130
a	 0.6200	 0.5470
b	 0.6520	 0.5650
c	 0.7930	 0.6000
d	 0.6750	 0.5830
e	 0.4610	 0.5420
f	 0.2050	 0.4670
i	 0.7930	 0.6050
j	 0.2120	 0.4530
k	 0.1110	 0.4450
l	 0.7780	 0.6080
m	 0.6610	 0.5880
x	 0.0110	 0.3160



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
y	 0.6530	 0.5740
z	 0.0040	 0.3140